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NL MIND-BEST: a web server for ligands & proteins discovery; theoretic-experimental study of proteins of *Giardia lamblia* and new compounds active against *Plasmodium falciparum*

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Abstract.

There are many protein ligands and/or drugs described with very different affinity to a large number of target proteins or receptors. In this work, we selected Ligands or Drug-Target pairs (DTPs/nDTPs) of drugs with high affinity/non-affinity for different targets. Quantitative Structure-Activity Relationships (QSAR) models become a very useful tool in this context to substantially reduce time and resources consuming experiments. Unfortunately, most QSAR models predict activity against only one protein target and/or have not been implemented in the form of public web-server freely accessible online to the scientific community. To solve this problem, we developed here a multi-target QSAR (mt-QSAR) classifier using the MARCH-INSIDE technique to calculate structural parameters of drug and target plus one Artificial Neuronal Network (ANN) to seek the model. The best ANN model found is a Multi-Layer Perceptron (MLP) with profile MLP 20:20-15-1:1. This MLP classifies correctly 611 out of 678 DTPs (Sensitivity = 90.12%) and 3083 out of 3408 nDTPs (Specificity = 90.46%), corresponding to training Accuracy = 90.41%. The validation of the model was carried out by means of external predicting series. The model classifies correctly 310 out of 338 DTPs (Sensitivity = 91.72%) and 1527 out of 1674 nDTP (Specificity = 91.22%) in validation series, corresponding to total Accuracy = 91.30% for validation series (Predictability). This model favorably compares with other ANN models developed in this work and Machine Learning classifiers published before to address the same problem in different aspects. We implemented the present model at web portal Bio-AIMS in the form of an online server called: **Non-Linear MARCH-INSIDE Nested Drug-Bank Exploration & Screening Tool (NL MIND-BEST)**; which is located at URL: <http://miaja.tic.udc.es/Bio-AIMS/NL-MIND-BEST.php>. This online tool is based on PHP/HTML/Python and MARCH-INSIDE routines. Finally, we illustrated two practical uses of this server with two different experiments. In experiment 1, we report by first time Quantum QSAR study, synthesis, characterization, and experimental assay of antiplasmodial and cytotoxic activities of oxoisoaporphine alkaloids derivatives as well as NL MIND-BEST prediction of potential target proteins. In experiment 2, we report sampling, parasite culture, sample preparation, 2-DE, MALDI-TOF and -TOF/TOF MS, MASCOT search, MM/MD 3D structure modeling, and **NL MIND-BEST** prediction for different peptides a new protein of the found in the proteome of the human parasite *Giardia lamblia*; which is promising for anti-parasite drug targets discovery.

Keywords: Ligands-Protein interaction; Drugs-Targets prediction, Protein Structure Networks; *Giardia lamblia* proteome; Anti-Malarial drugs; *Plasmodium falciparum*; multi-target QSAR; Markov Model.

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1. Introduction

The fast and accurate prediction of interactions between protein ligands and/or drugs and target proteins is a keystone piece on the application of theoretical biology and chemistry towards drug discovery. Therefore, there is a strong incentive to develop new methods capable of detecting these potential drug-target interactions efficiently (Yamanishi et al., 2008). In this sense, graphs and complex network theory may play an important role at different stages of modeling process with different degrees of organization of matter (Barabasi and Oltvai, 2004; Bornholdt and Schuster, 2003; Estrada, 2006a; Estrada, 2006b; Giuliani, 2010; Réka and Barabasi, 2002; Wu et al., 2010; Xiao et al., 2006; Xiao et al., 2008b; Xiao et al., 2005a; Xiao et al., 2005b). In a first stage, we can use molecular graphs to represent and calculate structural parameters for drugs sometimes called Topological Indices (TIs) but also estimate physicochemical parameters based on a graph method, see our recent review (González-Díaz et al., 2007a). At a higher level we can use graphs to represent structure of the drug-target proteins, proteins structure, protein interactions networks, metabolic systems, and more complex systems see for instance the works after Barabasi *et al.* (Barabasi, 2005; Barabasi, 2007; Goh et al., 2007; Loscalzo et al., 2007; Onnela et al., 2007; Park and Barabasi, 2007), Bonchev *et al.* (Apte et al., 2008; Bonchev, 2003; Bonchev, 2004; Bonchev and Buck, 2007; Bonchev et al., 2010; Kier et al., 2005; Managbanag et al., 2008; Mazurie et al., 2008; Mazurie et al., 2010; Thomas and Bonchev, 2010), or recent reviews/journal issues co-authored and/or guest-edited by González-Díaz *et al.* (Concu et al., 2010; Gonzalez-Diaz, 2010; González-Díaz, 2010; González-Díaz et al., 2008). We can also develop a kind of computer program with network topology called Artificial Neural Networks (ANNs) that after adequate training learns to predict target proteins for a given drug. It means, ANNs are network-like software that may use as inputs TIs and/or physicochemical parameters calculated in the previous steps to predict which molecular structures, which are also network-like structures, present or not a desire property (Gonzalez-Diaz et al., 2007b; Vilar et al., 2006).

In particular, using the parameters of the drug and the target ANNs may select Drug-Target pairs of drugs with high affinity (DTPs) out of those pairs for drugs with none affinity for different targets (nDTPs). In general, this technique (using or not ANNs) lie within the kind of studies called Quantitative Structure-Activity Relationships (QSAR) models and may become a very useful tool in this context to substantially reduce time and resources consuming experiments. In a previous work, our group have reported a QSAR model base on the MARCH-INSIDE method to predict a large network of DTPs (Vina et al., 2009). However, even when this model is useful to predict targets for many proteins it presents some weak points. The database used to fit and validate the model was not the official FDA benchmark data. The model does not consider the 3D structure of the protein target, which is a determinant aspect in drug-protein docking. Last, the previous classifier lacks of availability for public research due to it was not implemented as an online web server. The problem with many QSAR models is more serious because many of them work only for one target protein or for a limited family of organic compounds. We then should develop new models to predict unknown DTPs from chemical structure considering 3D structure of different target proteins, using official databases with well-curated annotation and making this method online-available to public research if possible.

In principle, we can select between more than 1,600 different drug molecular descriptors to solve the former problem (Todeschini and Consonni, 2002). However, not many methods offer one unique software platform to calculate parameters for both drugs and protein structures based on unified theoretic background more easily to rationalize. Our group has introduced elsewhere a Markov Chain Model (MCM) method named **MARKov CHains Invariants for Network SIMulation and Design (MARCH-INSIDE)**. The **MARCH-INSIDE** approach makes use of the same MCM theoretic formulation to calculate the average values of different molecular TIs and physicochemical properties from 2D, 3D, and/or sequence chemical

structures including drugs, DNA, RNA, and proteins, see a recent review (Gonzalez-Diaz et al., 2008). **MARCH-INSIDE** parameters not only offers these advantages but also may be used as inputs to train ANNs with the software STATISTICA (*e.g.*) easily generate C+ codes of ANNs. The codes generated show high compatibility and/or may be integrated into BioPython routines to implement public servers for proteome research and drug discovery (Aguero-Chapin et al., 2009; Concu et al., 2009b; Concu et al., 2009c; Gonzalez-Diaz et al., 2007a; Lin et al., 2009; Munteanu et al., 2009; Rodriguez-Soca et al., 2009a; Xiao and Lin, 2009; Xiao et al., 2008a; Xiao et al., 2009; Xiao et al., 2010).

In this work, we developed a multi-target QSAR (mt-QSAR) classifier using the **MARCH-INSIDE** technique to calculate structural parameters of drugs and targets plus one ANN algorithm to seek the model. The validation of the model was carried out by means of external predicting series. We also compare this model with other ANN models developed in this work and Machine Learning (ML) classifiers published before to address the same problem. We implemented the present model at web portal Bio-AIMS in the form of an online server called: **Non-Linear MARCH-INSIDE Nested Drug-Bank Exploration & Screening Tool (NL MIND-BEST)**; which is located at URL: <http://miaja.tic.udc.es/Bio-AIMS/NL-MIND-BEST.php>. This online-free public tool is based on PHP/HTML/Python and MARCH-INSIDE routines. Finally, we illustrated two practical uses of this server with two different experiments. In experiment 1, we report by first time **NL MIND-BEST** prediction, synthesis, characterization, and experimental assay of antiplasmodial and cytotoxic activities of oxo-isoaporphine alkaloids derivatives. In experiment 2, we report sampling, parasite culture, sample preparation, 2-DE, MALDI-TOF and -TOF/TOF MS, MASCOT search, MM/MD 3D structure modeling, and **NL MIND-BEST** prediction for different peptides a new protein of the found in the proteome of the human parasite *Giardia lamblia* (*G. lamblia*). In **Figure 1** we depict a flowchart with the main steps given in this work to train and validate the ANN classifier as well as implement the **NL MIND-BEST** server.

Figure 1 comes about here

2. Materials and Methods

2.1. Computational methods

2.1.1. MARCH-INSIDE technique

2.1.1.1. Parameters for drugs

The **MARCH-INSIDE** approach (Gonzalez-Diaz et al., 2008; González-Díaz et al., 2007a; González-Díaz et al., 2008) is based on the calculation of the different physicochemical molecular properties as an average of atomic properties (ap). For instance, it is possible to derive average estimations of molecular descriptors or group indices such as electro-negativities ${}^k\chi(G)$ (Santana et al., 2006b; Santana et al., 2008) values.

$${}^k\chi(G) = \sum_{j \in G} p_k(\chi_j) \cdot \chi_j \quad (1)$$

It is possible to consider isolated atoms ($k = 0$) in the estimation of the molecular properties ${}^0\chi(G)$. In this case the probabilities ${}^0p(\chi_j)$ are determined without considering the formation of chemical bonds (simple additive scheme). However, it is possible to consider the gradual effects of the neighboring atoms at different distances in the molecular backbone. In order to reach this goal the method uses a MM, which determines the absolute probabilities $p_k(\chi_j)$ with which the atoms placed at different distances k affect the contribution of the atom j to the molecular property in question. For example, in the case of electro-negativities ${}^k\chi(G)$ values:

$${}^k\chi(G) = [p(\chi_1) p_0(\chi_2) \dots p_0(\chi_n)] \cdot \begin{bmatrix} {}^1p_{1,2} & {}^1p_{1,2} & {}^1p_{1,3} & \cdot & {}^1p_{1,n} \\ {}^1p_{2,1} & {}^1p_{2,2} & {}^1p_{2,3} & \cdot & {}^1p_{2,n} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ {}^1p_{n,1} & \cdot & \cdot & \cdot & {}^1p_{n,n} \end{bmatrix}^k \cdot \begin{bmatrix} \chi_1 \\ \chi_2 \\ \cdot \\ \cdot \\ \chi_n \end{bmatrix} = \sum_{j=1 \in G}^n p_k(\chi_j) \cdot \chi_j \quad (2)$$

Where, from left to right, the first term is ${}^k\alpha$, which is the average molecular polarizability of the molecule considering the effects of all the atoms placed at distance k over every atomic polarizability α_j . The vector on the left-hand side of the equation contains the probabilities ${}^0p(\chi_j)$ for every atom in the molecule, without considering chemical bonds. The matrix in the center of the equation is the so-called stochastic matrix. The values of this matrix (${}^1p_{ij}$) are the probabilities with which every atom affects the electronegativity of the atom bonded to it. Both kinds of probabilities ${}^0p(\chi_j)$ and ${}^1p_{ij}$ are easily calculated from atomic electronegativities (χ_j) and the chemical bonding information:

$${}^0p_{ij} = \frac{\chi_j}{\sum_{k=1}^n \chi_k} \quad (3) \quad {}^1p_{ij} = \frac{\delta_{ij} \cdot \chi_j}{\sum_{k=1}^n \delta_{ik} \cdot \chi_k} \quad (4)$$

The only difference is that in the probabilities ${}^0p(\chi_j)$ we consider isolated atoms by carrying out the sum in the denominator over all n atoms in the molecule. On the other hand, for ${}^1p_{ij}$ chemical bonding is taken into consideration by means of the factor δ_{ij} . This factor has a value of 1 if atoms i and j are chemically bonded and is 0 otherwise. Finally, it is interesting to note that one can sum only the atoms included in a specific group (G) rather than all atoms. In this way we can approach specific classes of average properties such as average electronegativity for sp_3 carbon atoms (C_{sp3}) or average electronegativity for heteroatoms (Het). All calculations were performed using the program **MARCH-INSIDE** (Gonzalez-Diaz et al., 2008; González-Díaz et al., 2007a; González-Díaz et al., 2008), which was developed in-house, see recent reviews for details.

2.1.1.2. Parameters for proteins

In previous works, we have predicted protein function based on 3D-Potentials for different types of interactions. The main types of potentials used are: averaged values of Electrostatic, vdW, and HINT potentials (Concu et al., 2009a; Humberto González-Díaz, 2008). In this paper, we used only the Electrostatic ξ_k and HINT Potentials μ_k ; we omitted vDW since the HINT potential includes a vDW component. The values were used as inputs to construct the QSAR model. The detailed explanation of the procedure has been published before (see also method supplementary material with details) and therefore we only provide the more general formula for these potentials and some general explanations (González-Díaz et al., 2008):

$$\xi_k(R) = \sum_{j=1 \in R}^n p_k(j) \cdot \xi(j) \quad (5)$$

The average general potentials depend on the absolute probabilities $p_k(j)$ and the total potential with which the aminoacid j -th interact with the rest of aminoacids. These are the probabilities with which the amino acids interact with other amino acids placed at a distance equals to k -times the cut-off distance ($r_{ij} = k \cdot r_{\text{cut-off}}$). The method uses an MCM to calculate these probabilities; which also depend on the 3D interactions between all pairs of aminoacids placed at distance r_{ij} in \mathbf{r}_3 in the protein structure. However, for the sake of simplicity, a truncation or cut-off function α_{ij} is applied in such a way that a short-term interaction takes place in a first approximation only between neighboring aa ($\alpha_{ij} = 1$ if $r_{ij} < r_{\text{cut-off}}$). Otherwise, the interaction is banished ($\alpha_{ij} = 0$). The relationship α_{ij} may be visualized in the form of a protein structure complex network. In this network the nodes are the C_α atoms of the aminoacids and the edges connect pairs of aminoacids with $\alpha_{ij} = 1$. This network can be understood in terms of aminoacid - aminoacid protein contact maps (Vassura et al., 2008) in Euclidean 3D space $\mathbf{r}_3 = (x, y, z)$ coordinates of the C_α atoms of aminoacids listed on protein PDB files. In recent works we published different examples of these networks (Rodriguez-Soca et al., 2009a; Rodriguez-Soca et al., 2009b). For the purposes of the calculation, all water molecules and metal ions were removed (González-Díaz et al., 2008). All calculations were carried out with our in-house software **MARCH-INSIDE** (González-Díaz et al., 2008). For calculation the **MARCH-INSIDE** software always uses the full matrix, never a sub-matrix, but may run the last

summation term either for all amino acids or only for some specific groups called regions (R). These regions are often defined in geometric terms and are referred to as core, inner, middle and surface regions. The protein regions (c correspond to core, i to inner, m to middle, and s to surface regions, respectively) are shown in different figures published in previous works (González-Díaz et al., 2007b). The diameters of the regions, as a percentage of the longest distance r_{\max} with respect to the centre of charge, are 0 to 25 for region c, 26 to 50 for region i, 51 to 75 for region m, and 76 to 100 for region s. Additionally, we consider the total region (t) that contains all the amino acids in the protein (region diameter 0 to 100% of r_{\max}). Consequently, we can calculate different ${}^o\xi_k$ and ${}^o\mu_k$ values for the amino acids contained in different Regions (c, i, m, s, or t) and placed at topological distance k within this region (k is the named the order). In this work, we calculated in total 2(type of potentials) x 5regions x 6(higher order considered) = 30 (${}^o\xi_k$ values) = 30 indices for each protein.

2.1.2. ANN analysis

Let be ${}^k\chi(G)$ drugs molecular descriptors and ${}^k\xi(R)$ receptor or drug target descriptors for different drugs (d) with different receptor; we can attempt to develop a simple linear classifier of mt-QSAR type with the general formula:

$$S(\text{DTP})_{\text{pred}} = \sum_{k=0}^5 b(G_k) \cdot {}^k\chi(G) + \sum_{k=0}^5 b(R_k) \cdot {}^k\xi(R) + b \quad (6)$$

We can use a very simple type of ANN called Linear Neural Network (LNN) to fit this discriminant function. The model deals with the classification of a compound set with or without affinity on different receptors. A dummy variable Affinity Class (AC) was used as input to codify the affinity. This variable indicates either high (AC = 1) or low (AC = 0) affinity of the drug by the receptor. $S(\text{DTP})_{\text{pred}}$ or DTP affinity predicted score is the output of the model and it is a continuous dimensionless score that sorts compounds from low to high affinity to the target coinciding DTPs with higher values of $S(\text{DTP})_{\text{pred}}$ and nDTPs with lowest values. In equation (6), b represents the coefficients of the LNN classification function, determined by the ANN module of the STATISTICA 6.0 software package (StatSoft.Inc., 2002). We used Forward Stepwise algorithm for a variable selection.

In addition, we can explore more complicated non-linear ANNs in order to improve the accuracy of the classifier. We processed our data with different ANNs looking for a better model. Four types of ANNs were used, namely, Probabilistic Neural Network (PNN), Radial Basic Function (RBF), Three Layers Perceptron (MLP-3), and Four Layer Perceptron (MLP-4) (Prado-Prado et al., 2010; Rodriguez-Soca et al., 2010).

The quality of all the ANNs (linear or non-linear) was determined calculating values of Specificity, Sensitivity, and total Accuracy to determine the quality-of-fit to data in training. The validation of the model was corroborated with external prediction series. We also reported ROC-curve analysis (ROC curve can be used to select an optimum decision) for both training and validation series (Prado-Prado et al., 2010; Prado-Prado et al., 2007).

2.1.3. Data set

The data set was formed by a set of marketed and/or reported drugs/receptors (proteins) pairs where affinity of drugs with the receptors was established taking into consideration the Drug Bank. The data set was formed to more than 500 drugs with respectively 323 protein receptors, so we were able to collect already 6098 cases (drug/protein receptors) instead of 500 x 323 cases. The data set were used to perform the ANN analysis. The names or codes for all compounds are depicted in **Table 1SM** of the supplementary material, due to space constraints, as well as the references consulted to compile the data in this table.

2.1.4. Theoretical study of antiplasmodial compounds (experiment 1)

Density-functional theory (DFT) is a new tool for describing the ground states of molecular systems. Chemical concepts like electronic potential (μ), absolute hardness (η), electron affinity (EA), and electrophilicity (ω) are well defined quantities that conveniently rationalize

molecular reactivity and chemical bonding (Parr et al., 1978). The electronic chemical potential μ is the natural descriptor of the direction of charge transfer during a chemical interaction (Parr and Pearson, 1983). The descriptor η is related to the resistance of the system to charge transfer. A good approximation based on Koopman's theorem allows μ and η to be calculated in terms of the electron energies of the frontier molecular orbitals HOMO and LUMO according to Eqs. 1 and 2 (Parr and Pearson, 1983):

$$\mu \approx (\varepsilon_L + \varepsilon_H) / 2 \quad (7)$$

$$\eta \approx \varepsilon_L - \varepsilon_H \quad (8)$$

In where ε_L and ε_H are the energies of the LUMO and HOMO levels, respectively. The link with classical structural chemistry is achieved by making $\mu = -\chi$, where χ is the well-known electronegativity. The EA is defined as an approximation of the energy of the frontier molecular orbital LUMO, being the following approximate versions of χ and EA widely used according to Eqs. 3 and 4:

$$\chi = -\mu \approx (\varepsilon_L + \varepsilon_H) \quad (9)$$

$$EA \approx -\varepsilon_L \quad (10)$$

Recently the global ω of an atom or molecule has been introduced by Parr *et al.* (Parr et al., 1999) through the simple expression:

$$\omega = \mu^2 / 2\eta \quad (11)$$

The global ω measures the energy stabilization when the system acquires an amount of electronic charge from the environment. It is necessary taking into account that the Koopman's theorem is not exactly correct and will fail when strong electronic relaxation and correlation effects occur. Thus, in the studied systems that are structurally related, the relaxation and correlation effects are expected to be about the same for all systems allowing the comparison of electronic properties obtained from the Koopman's theorem to give insights on the relative behavior of the systems. Since these oxoisoaporphines are good electron acceptors, we will study a possible relationship between the EA, χ , and global ω of the structurally related oxoisoaporphines **1-8** with both their cytotoxic and antiplasmodial activities. For it, Hartree-Fock/6-31G(d) (HF) and B3LYP/6-31++G(d,p) calculations have been performed using the Gaussian 03 package of programs (Frisch, 2003). The structures included in this study were fully optimized at the HF/6-31G(d) level of theory and single point calculation at the B3LYP/6-311++G(d,p) level of theory was carried out to afford the molecular electronic properties such as molecular orbital energies and local reactivity indices. The calculation of the electronic chemical potential and the chemical hardness were obtained from the expressions $\mu \approx (\varepsilon_L + \varepsilon_H) / 2$ and $\eta \approx \varepsilon_L - \varepsilon_H$, in terms of the one electron energies of the HOMO and LUMO frontier molecular orbitals, ε_H and ε_L , respectively (Parr et al., 1989). With these quantities at hand, χ and ω values were obtained using Eq. 3 and 4, respectively. The electron affinity, absolute electronegativity, and electrophilicity index of neutral as well as ionic species of the oxoisoaporphines were calculated using HF and DFT methods. Table 3 shows the calculated values of electron affinity, absolute electronegativity, and electrophilicity index for neutral species using B3LYP/6-311++G(d,p) method.

2.1.5. Theoretical study of protein fingerprints on *G. lamblia* proteome (experiment 2)

2.1.5.1. BLAST Search

The most relevant peptide fragments of the new protein were submitted to BLASTp to determine the similarity of the sequence compared to other protein (Altschul et al., 1997). The BLASTp procedure was carried out with the non-redundant NCI database as the query database and allowing BLASTp to search for conserved domains through the CD search tool (Marchler-Bauer and Bryant, 2004).

2.1.5.2. MM/MD study

Molecular Mechanics (MC) and Molecular Dynamics (MD) study. For MM study we first introduced the sequence of the 29 peptides in the HyperChem (Hypercube.Inc., 2002); the optimization of their geometries was carried out by the Molecular Mechanics Force Field BIO+(CHARMM). In setup we keep the options implemented by default, but allowing a cut-off switching truncation $r_{in} = 15\text{\AA}$ and $r_{out} = 17\text{\AA}$. We refer here to MD in the sense of MD stochastic simulation by the Monte Carlo (MC) method, although some authors understand MD as only the MD deterministic search. The Molecular Dynamics Trajectories (MDTs) or energetic profiles of all the starting structure of peptides were obtained by means of MC method, with the Hyper-Chem package (Froimowitz, 1993; Hypercube, 2002). In this sense, the force field AMBER (Liu and Beveridge, 2002) of molecular mechanics was used with distant-dependent dielectric constant (scale factor 1), electrostatic and Van der Waals values by default and a cut-off switched function with $r_{in} = 15$ and $r_{out} = 17\text{\AA}$ (see **Figure 2**). All the components in the force field were included and the atom type was recalculated by maintaining the current charges. Finally, MD simulation was carried out by use of the Monte Carlo algorithm in the *vacuo* at 300 K and 1000 optimization steps, thus obtaining MDTs with 100 potential energy dE_j ($j = 1, 2, 3, \dots, 100$) values for each. We obtained 22 MDTs for 19 peptides. In order to obtain realistic MDTs we monitored an additional parameter in MD algorithms; this is known as the acceptance ratio (ACCR). It appears as ACCR on the list of possible selections in the MC Averages dialog box of HyperChem (see **Figure 2**). The ACCR is a running average of the ratio of the number of accepted moves to attempted moves. Varying the step size can have a large effect on the ACCR value. The step size, Δr , is the maximum allowed atomic displacement used in the generation of trial configurations. The default value of r in HyperChem is 0.05\AA (Froimowitz, 1993). For most organic molecules, this will result in an ACCR of about 0.5\AA , which means that about 50% of all moves are accepted. Increasing the size of the trial displacements may lead to a more complete search of configuration space, but the acceptance ratio will, in general, decrease. Smaller displacements generally lead to higher acceptance ratios but result in more limited sampling. There has been little research to date as regards the optimum value of the acceptance ratio.

Figure 2 comes about here

2.2. Experimental methods

2.2.1. Experimental study of antiplasmodial compounds (experiment 1)

2.2.1.1. Synthesis of compounds

Synthesis of compounds **1-8** has been previously reported¹¹⁻¹⁴. However in order to obtain sufficient amounts for pharmacological tests we carried out the preparative synthesis of all these compounds again, see **Figure 3**.

2.2.1.2. Cytotoxicity

The samples of lines J-774 (murine macrophages) and HL-60 cell (Human acute promyelocytic leukaemia cell) were cultured with Flow RPMI 1640 medium supplemented with heat-inactivated foetal bovine serum; 0.33% L-glutamine, 1% non essential amino acids, 1% sodium pyruvate and penicillin-streptomycin (100 UI/ml - 100 $\mu\text{g/ml}$). The cell lines HeLa (human cervix carcinoma cells), Mel-43 and WI-38 (human lung fibroblasts) were grown in Gibco MEM supplemented with 10% heat-inactivated fetal bovine serum and penicillin (100 UI/ml). Cells were incubated in a humidified atmosphere with 5% CO_2 , at 37 °C. Stock solutions of pure compounds were prepared at 10 mg/ml in DMSO. The effects of synthetic compounds on all cell lines were evaluated using MTT (Sigma) colorimetric assay based on cleavage of the reagent by dehydrogenases in viable cells.⁴⁴ The cell lines 5000 HeLa, Gal-43, WI-38 and J-774 (adherent cells) in 200 μl medium were seeded in each well of 96-well plates. Cells were first incubated 24h, then, the medium was removed and replaced by 200 μl /well fresh medium containing various concentrations of compounds or DMSO at the same final concentration. After 72h treatment, the medium was removed and replaced by 100 μl of DMEM

(without serum) containing 10 μ l of MTT (3mg/ml in PBS). After 5 min in the incubator, the medium containing MTT was removed, and 100 μ l of DMSO were added to each well.

The samples for line HL-60 at 50000 cells (non-adherent cells) in 100 μ l medium were seeded in each well of 96-well plates. A volume of 100 μ l of fresh medium containing various drug concentrations or analogous DMSO concentrations was added to HL-60 wells. After 72h treatment, the medium was supplemented by 10 μ l MTT (5mg/ml in PBS) added to each well. After 2h in the incubator, the reaction was stopped by adding 100 μ l of 0.04M HCl in 2-propanol.⁴ For all cell lines, plates were shaken and absorbance values (Spectra Max 190, Molecular Devices) recorded at two wavelengths (570-620nm) against a background control as blank. The relative absorbance was expressed as a percentage of corresponding control considered as 100%. Camptothecin (Sigma) was used as positive cytotoxic reference compound. Each substance was tested in a concentration range from 3.1 μ g/ml to 100 μ g/ml; each concentration was tested in at least 8 wells. IC₅₀ determinations were achieved via regression analysis of the results of at least six different concentrations of each substance. Results are expressed as percentages of the control cultures, considered as 100% and are given as mean \pm SEM of three independent experiments.

2.2.1.3. Plasmodium *in vitro* culture and antiplasmodial activity

Parasites were cultured according to the method described by Trager and Jensen⁴⁵ with modifications described by Benoit *et al.* (1995).⁴⁶ The cultures were synchronized every 48 h by 5% D-sorbitol lysis⁴⁷ (Merck, Darmstadt, Germany). The FcB1-Columbia strain was considered as chloroquino-resistant strain (chloroquine IC₅₀: 145 nM). *In vitro* antimalarial activity testing was performed by [³H]-hypoxanthine (Amersham-France) incorporation as described by Desjardins *et al.* (1979)⁴⁸ with modifications.⁴⁹

2.2.2. Experimental study of protein fingerprints on *G. lamblia* proteome (experiment 2)

2.2.2.1. Parasite culture

Trophozoites of *Giardia* (ATCC® 203333) were grown for 48 h in a modified YI-S-33 medium: 3% yeast extract, 1% glucose, 0.1% NaCl, 0.2% L-cysteine, 0.02% ascorbic acid, 0.1% K₂HPO₄, 0.06% KH₂PO₄, 10% calf serum, 0.05% dehydrated bovine bile, 22.8 mg/l ferric ammonium citrate and 2% vitamin mixture (Sigma), pH 7.

2.2.2.2. Sample preparation

Trophozoites were recovered on day 2 post-inoculum (*p.i.*) and the parasites were centrifuged at 3000 rpm for 10 minutes at 4°C. The resulting pellet was washed five times with 0.5 mM Tris-HCl pH 7.8, and resuspended in this same buffer. Glycoproteins isolation was carried with the Qproteome Total Glycoprotein Kit (Qiagen). In order to achieve a well focused first-dimension separation, sample proteins must be completely disaggregated and fully solubilized, in a sample buffer containing 7M urea, 2M Thiourea, 4% Chaps, Destreak buffer (Amersham Biosciences), 5mM CO₃K₂, 2% IPG buffer (Amersham Biosciences) and incubated at room temperature for 30 minutes. Following clarification by centrifugation at room temperature (12,000 rpm, 10 min) the supernatants were stored frozen.

2.2.2.3. 2D-Electrophoresis (2-DE)

An amount of 340 μ l of rehydration buffer was added to solubilized glycoproteins (7 M urea, 2 M thiourea, 2% Chaps, 0,75% IPG buffer 4-7, bromophenol blue) and immediately were adsorbed onto 11 cm immobilized pH 3-10 gradient (IPG) strips (Amersham Biosciences). Optimal IEF was carried out at 20 °C, with an active rehydration step of 12 h (50 V), and then focused on an IPGphor IEF unit (Amersham Biosciences) by using the following program: 150 V for 2 h, 500 V for 1 h, 1000 V for 1 h, 1000-2000 V for 1 h and 8000 V for 12 h. After focusing, IPG strips were equilibrated for 15 min in 10 ml of 50 mM Tris-HCl, pH 8.8, 6 M urea, 30% v/v glycerol, 2% w/v SDS, traces of bromophenol blue containing 100 mg of DTT; and further incubated for 25 min in the same buffer replacing DTT by 300 mg of iodoacetamide. After equilibration, the IPG strips were placed onto 12, 5% SDS-polyacrilamide gels and sealed with 0,5% (w/v) agarose. SDS-PAGE was run at 15 mA/gel for

20 min as initial migration and increased to 30 mA/gel for separation until front dye reached the bottom of the gel. 2D gels were stained with Colloidal Coomassie stain.

2.2.2.4. MALDI-TOF and -TOF/TOF MS

The spot of interest was manually excised from silver stained 2-DE gels after being destained as described by Gharahdaghi *et al.* (1999). Briefly, gel spots were incubated in 100 mM sodium thiosulfate and 30 mM potassium ferricyanide, rinsed twice in 25 mM ammonium bicarbonate (AmBic) and once in water, shrunk with 100% acetonitrile (ACN) for 15 min, and dried in a Savant SpeedVac for 20–30 min. Then, the spots were reduced with 10 mM dithioerythritol in 25 mM AmBic for 30 min at 56 °C and subsequently alkylated with 55 mM iodoacetamide in 25 mM AmBic for 20 min in the dark. Gel pieces were alternately washed with 25 mM AmBic and ACN, and dried under vacuum. Gel pieces were incubated with 12.5 ng/μl sequencing grade trypsin (Roche Molecular Biochemicals) in 25 mM AmBic overnight at 37 °C. After digestion, the supernatants (crude extracts) were separated. Peptides were extracted from the gel pieces first into 50% ACN, 1% trifluoroacetic acid and then into 100% ACN. Then, one microliter of each sample and 0,4 μl of 3mg/ml α-cyano-4-hydroxycinnamic acid matrix (Sigma) in 50% ACN, 0,01% trifluoroacetic acid were spotted onto a MALDI target. MALDI-TOF MS analyses were performed on a Voyager-DE STR mass spectrometer (PerSeptive Biosystems, Framingham, MA, USA). The following parameters were used: cysteine as S-carbamidomethyl derivative and methionine in oxidized form. Spectra were acquired over the m/z range of 700-4500 Da. Tryptic, monoisotopic peptide mass lists were generated and exploited for database searching. MS/MS sequencing analysis were carried out using the MALDI-tandem time-of-flight mass spectrometer 4700 Proteomics Analyzer (Applied Biosystems, Framingham, MA). Mass spectrometry was performed at the University Complutense de Madrid Proteome Facility.

2.2.2.5. Database Search

The PMF and peptide fragment-ion data obtained from MALDI-TOF and MS/MS analyses, respectively, were used to search for protein candidates in two sequence databases: SWISS-PROT/TrEMBL non-redundant protein database (www.expasy.ch/sprot) using MASCOT search engine (www.matrixscience.com) (Fink, 1965; Hirosawa *et al.*, 1993; Koenig *et al.*, 2008; Leung *et al.*, 2005; Rudnick *et al.*, 2005; Tamura and Takano, 1965). Initial search parameters were as follows: Cys as S-carbamidomethyl derivative and Met in oxidized form, one missed cleavage site, peptide mass tolerance of 50 ppm, and MS/MS tolerance of ± 0.5 Da. When this approach failed, amino acid sequences were deduced manually from the charge-state de-encrypted spectra and used as queries for searches using BLAST.

3. Results

3.1. Drug-Target QSAR models

3.1.1. ANN models

The present model shows good results with a relatively small number of parameters (15 parameters) and a linear equation. To show how important is this result, we compared the present model with other models used to address the same problem. We processed our data with different Artificial Neural Networks (ANNs) looking for a better model. Four types of ANNs were used, namely, Probabilistic Neural Network (PNN), Radial Basic Function (RBF), Three Layers Perceptron (MLP-3), and Four Layer Perceptron (MLP-4). The **Figure 4** depicts the networks maps for some of the ANN models tested. In general, at least one ANN of every type tested was statically significant. However, one must note that the profiles of each network indicate that these are highly nonlinear and complicated models.

Figure 4 comes about here

One network found was MLP and it showed training performance higher than 91%. We compare different types of networks to obtain a better model; **Table 1** shows the classification matrix of the different networks. Was taken as the main network (MLP 20:20-15-1:1) because it presents a wider range of variables, presents 20 inputs in the first layer and 20 neurons in

second layer, two sets of cases (Training and Validation). Another tested networks found were MLP 28:28-22-1:1, RBF 1:1-1-1:1 presents the same type of variables; Linear 65:65-1:1 present many variables and PNN 65:65-4086-2-2:1 has a very low percentage of DTPs leading to possible errors in the model although your accuracy is very well, see **Table 1**. We depict the ROC-curve for MLP 20:20-15-1:1 to show how reliable was the network model developed, see **Figure 4**. Notably, almost the model presented was under curve higher than 0.5. The model presented an area greater than 0.93. The vitality of this type of procedures developing ANN-QSAR models has been demonstrated before; see, for instance, the works of Fernandez and Caballero (Caballero and Fernandez, 2006; Fernandez et al., 2006). The same is true about the other kinds of ANNs tested.

Table 1 comes about here

3.1.2. Comparison to previous ML models

The MLP model shows excellent results with a relatively small number of parameters (only 20) with respect to some previously published Machine-Learning (ML) models. To assess the importance of this result, we compared these ML models with other models used to address the same problem. For a example, have been reported a notably more complicated ML model, which included a non-linear SVM model, a large number of parameters as well as many class-to-class trials rather than the single QSAR equation used in this work (Chen et al., 2007; Li et al., 2008). All the other models included less than (20) input parameters or unknown parameters and some with 1000 or more (5000+) cases, and non-linear techniques such as Support vector Machine (SVM) and others (Bas et al., 2008; Bleakley and Yamanishi, 2009; Li and Lai, 2007; Vina et al., 2009; Yang et al., 2009). Our model is notably simpler. However, some of these other models has low accuracy, or use ROC curve or Correlation coefficient as good classification at which makes the task more difficult (Mascarenhas and Ghoshal, 2008; Vijayan et al., 2009). Other studies do not show the number of variables (NV) involved in the model, see **Table 2** for details (Michel et al., 2006; Naumann and Matter, 2002; Pham and Jain, 2006; Raha et al., 2007; Zhang et al., 2006).

Table 2 comes about here

3.2. NL MIND-BEST web server

In addition, internet era training and validation of a QSAR and/or computational model in general should be considered the first step towards the development of a valuable tool towards bioinformatics application in proteome research. At the present time, is not enough to seek a fast and accurate predictive model we should also to implement it a public servers, preferably of open access, online available to the scientific community. The server packages developed by Chou and Shen to predict the function of proteins from structural parameters or explore protein structures (Chou and Shen, 2007; Chou and Shen, 2008; Shen and Chou, 2007; Shen and Chou, 2008) are good examples in this sense. These may be used by proteome research scientists by interacting with user-friendly interfaces. It means that the user do not need to be expert on the theoretical details behind this kind of models including the vast literature published by Chou *et al.* on the development of models with pseudo-aminoacid composition parameters or the use of ML classification techniques and other algorithms (Chou, 2005; Chou and Elrod, 2002; Chou and Elrod, 2003; Chou and Shen, 2006a; Chou and Shen, 2006b). However, there are not many reports of DTPs prediction QSAR-based servers based on fully curated databases like FDA approved drugs and targets as well as with automatic upload of new proteins by means of online connection to PDB. In this sense, we implemented the best ANN model found here (MLP 28:28-22-1:1) at web portal Bio-AIMS in the form of an online server called **NL MIND-BEST**. We can spell out this acronym as **NL MIND-BEST: Non-Linear MARCH-INSIDE Nested Drug-Bank Exploration & Screening Tool**. The web server **NL MIND-BEST** is located at URL: <http://miaja.tic.udc.es/Bio-AIMS/MIND-BEST.php>. This online tool is based on PHP/HTML and Python routines coupled to nested MARCH-INSIDE classic algorithm to calculate input molecular structure parameters (Gonzalez-Diaz et al., 2008).

3.2.1. MIND-BEST mode 1

In this user friendly interface the user only has to paste the names (identification codes) and the SMILE code for drugs. We this SMILE code MIND-BEST construct the Markov matrix of electronic delocalization and calculates the total and atom groups (G) average electronegativity values ${}^k\chi(G)_{\text{query}}$ for each query drug candidate. In **Figure 5 (A)** we depict the user interface for MIND-BEST including **mode 1** (at web page top). The user has to paste also the PDB ID of the potential drug target proteins or query proteins. With these PDB ID codes **NL MIND-BEST** automatically connects to PDB, upload the .pdb, .ent, or .txt files with the 3D structure of the protein, construct the Markov matrix of electrostatic interactions and calculates the total and region (R) average electrostatic potential values ${}^k\xi(R)_{\text{query}}$ for each query protein. MIND-BEST have also an internal database with all information related to names, DB codes, PDB code, ${}^k\chi(G)_{\text{fdai}}$, ${}^k\xi(R)_{\text{fdaj}}$ for all DTPs formed by any i^{th} -drug and j^{th} -protein approved by FDA of USA until January-2010. We give all this information free as only supplementary material to this manuscript. Using these values MIND-BEST compares all query drugs and proteins introduced by the user with FDA approved drugs and proteins. For a DTPs and nDTPs previously present at FDA data the server **NL MIND-BEST** do not evaluate the pair (run the ANN model) but give directly the unknown answer. Otherwise, **NL MIND-BEST** evaluate the query drugs vs. all query proteins. Taking into consideration that the name of a drug may present many other synonym names and the SMILE code is not unique for a drug **NL MIND-BEST** use a drug-drug similarity (DDS) score to decide if a drug is already present on FDA data or a very close analogue. There are different similarity values for drugs and proteins in the literature (Campillos et al., 2008; Geppert et al., 2009; Good et al., 1992; Lam and Welch, 2004; Thimm et al., 2004; Wang and Bajorath, 2009; Xie et al., 2009). Some important databases like ChEMBL with more than 2,000,000 activity outcomes (<http://www.ebi.ac.uk/chembl/db/index.php/compound/search>) implement search algorithms based on similarity scores; which evidence the importance of incorporating this feature to new servers. One of the salient features of **NL MIND-BEST** is the use of only one theoretic background for structure characterization in terms of drug structure, protein structure, drug-drug similarity, protein-protein similarity, and DTP-DTP similarity. In this sense, **NL MIND-BEST** use the MARCH-INSIDE parameters for all these purposes. In so doing, we introduce here by first time a DDS score for **NL MIND-BEST** using the ${}^k\chi(G)$ values of the r^{th} query drugs ${}^k\chi(G)_{\text{rquery}}$ and s^{th} FDA approved drugs ${}^k\chi(G)_{\text{sFDA}}$. The server use a similar procedure to calculate protein-protein similarity $\text{PPS}_{\text{F-Q}}$ scores for u^{th} query and v^{th} FDA approved drug protein targets. By analogy to drug-drug case **NL MIND-BEST** decide when a protein is already in the FDA list using first the PDB ID and for negative case adding a search with $\text{PPS}_{\text{F-Q}}$ scores. Last, and based on the same idea this server determines similarity between $r^{\text{th}} + u^{\text{th}}$ DTPs in query list vs. s^{th} and v^{th} DTPs in FDA list using a DTP-DTP similarity score DPS. For pairs already present in FDA list $\text{DPS}(\%) = 100\%$ the server **NL MIND-BEST** omit evaluation with ANN and give the experimental answer. Otherwise the server carry out evaluation and give predicted answer but also give the result for the DTP formed by the more similar drug and the more similar protein in the FDA list. At follows we give the mathematical formula for these scores were the subscripts F = FDA and Q = query.

$$\text{DDS}_{\text{F-Q}}(\%) = 100 \cdot \left[1 - \frac{\left(\sum_{G,k} |{}^k\chi(G)_F - {}^k\chi(G)_Q| \right)}{\left(\sum_{G,k} {}^k\chi(G)_Q \right)} \right] \quad (12)$$

$$\text{PPS}_{\text{F-Q}}(\%) = 100 \cdot \left[1 - \frac{\left(\sum_{R,k} |{}^k\xi(R)_F - {}^k\xi(R)_Q| \right)}{\left(\sum_{R,k} {}^k\xi(R)_Q \right)} \right] \quad (13)$$

$$DPS (\%) = 100 \cdot \left[1 - \frac{\left(\sum_{G,k} |{}^k\chi(G)_F - {}^k\chi(G)_Q| \right)}{\left(\sum_{G,k} {}^k\chi(G)_Q \right)} \right] \cdot \left[1 - \frac{\left(\sum_{R,k} |{}^k\xi(R)_F - {}^k\xi(R)_Q| \right)}{\left(\sum_{R,k} {}^k\xi(R)_Q \right)} \right] \quad (14)$$

Figure 5 comes about here

3.2.2. NL MIND-BEST mode 2

The present server was trained and validated to use the SMILE codes of new organic compounds to predict target proteins for these compounds from the list of previously approved FDA proteins (mode 1). In **mode 1** this server may be also used to select potential targets for new compounds between proteins currently unknown as drug targets but with known 3D structures that have been released to PDB. However, there are other potentials uses of this server. How should one predict DTPs for 3D structures of proteins not represented on the FDA list given before and not released to PDB? Certainly, the server was created to calculate S_{pred} values only for these proteins so for other proteins the answer is simply in general: you should use another server based on a classifier trained and validated with a database that contained other proteins. However, we should not forget that the model was trained using protein parameters for many different protein structures. Consequently, it is technically possible to estimate DPPs for other proteins if we introduce as inputs for the classifier protein or peptide 3D structural models created by us using MM/MD techniques. The reader should remember at this point that the classifier was trained with proteins of many different DTPs. For these situations, we incorporated to the server the input mode 2. This input mode is essentially the same than mode 1 but the server prompts you to upload .ent files with 3D structures of proteins of peptides generated by you using MM/MD algorithms. In **Figure 5 (B)** we depict the user interface for **NL MIND-BEST** including **mode 2** (at web page bottom). We have to be aware that by using this input mode 2 we predict S_{pred} scores for DTPs using structural models generated only by modeling. Consequently, predictions derived with input mode 2 have to be used with higher caution than predictions with input mode 1.

3.3. NL MIND-BEST illustrative experiments

3.3.1. Theoretic-experimental study of antiplasmodial compounds (experiment 1)

3.3.1.1. Cytotoxicity and biological activity assay

In **Figure 6** and **Table 3** we show that oxoisoaporphines exhibited cytotoxic activities at the same dose range than their isomers, oxoaporphines or some aporphine derivatives lacking a methylenedioxy substituent (IC_{50} from 15 to 60 μM) (Stevigny et al., 2005; Stévigny et al., 2002). This work also showed the selective cytotoxic effect of some oxoisoaporphine alkaloids towards different cell lines and indicated that position and nature of substituents are more important for the cytotoxic activity than the isomerisation. Compound **7**, which exhibited a low cytotoxic activity against WI-38 cells, may be considered as not cytotoxic against HL-60, HeLa and Mel-43 lines. This compound displayed a selective cytotoxic activity on J-774 cells while this line seems to be more resistant to alkaloids **4**, **5**, **6** and **8**, see **Figure 7**. Such a selective activity has already been observed in the case of oxoisoaporphines previously isolated from *Menispermum dauricum* (Yu et al., 2001). Alkaloid **7** is the only compound of the series bearing a hydroxyl group on C-5, which may be an important feature for this selective toxicity.

Figure 6 comes about here

Table 3 comes about here

Furthermore, the isomerisation and/or the absence of methoxy groups at certain position seems to be important for the cytotoxic activity since lysicamine (**9**), an oxoaporphine similar to **5** with an additional methoxy group at C-1 was shown to be inactive.¹ Nevertheless, isomerisation does not seem to have any influence on the Cytotoxicity of this type of compounds since the tested oxoisoaporphines have a similar Cytotoxicity than related

oxoaporphines derivatives. Previous results have shown the importance of the presence of a methylenedioxy group for a high Cytotoxicity of aporphines and oxoaporphines alkaloids (Boustie et al., 1998; Likhitwitayawuid et al., 1993; Montanha et al., 1995; Stevigny et al., 2005; Stévigny et al., 2002). These results are in good agreement with this present work since the tested synthetic compounds lack this chemical moiety and are less active than the aporphines bearing the methylenedioxy substituent. Since oxoaporphine alkaloids have been shown to exhibit antiparasitic properties, we decided to submit compounds **1–8** to antiplasmodial tests. The corresponding IC_{50} values of the eight compounds and chloroquine are listed in **Table 4**.

Table 4 comes about here

Compound **8** exhibited the strongest antiplasmodial activity ($IC_{50} = 1.45 \mu\text{M}$), whereas **5** exhibited a lower activity ($IC_{50} \sim 10 \mu\text{M}$), **2**, **4** and **6** had a moderate effect ($IC_{50} \sim 50 \mu\text{M}$) and **1**, **3** and **7** possessed a very low activity ($IC_{50} > 80 \mu\text{M}$). Since **5** and **8**, two isomers bearing a methoxy group on C-5 and carbonyl group at C-7 or C-6, are the most active compounds, it suggests the important role of these two substituents in the antiplasmodial activity. Moreover, the higher antiplasmodial activity shown by the compound **8** regarding its isomer **5** is influenced by the migration of the carbonyl group from C-7 to C-6. Thus, an important redistribution of electronic density would exist in the isoquinolone framework that apparently determines its higher pharmacological reactivity. Indeed, when a hydroxyl group is added to compound **5** at C-6, the antimalarial activity diminishes notably. This is confirmed by the very low antiplasmodial activity of **6**, which possesses both hydroxy and methoxy moieties. In addition, the most active compound **8** possesses three conjugated rings, inducing a more planar configuration, which may be an important feature for antiplasmodial activity. This is also in agreement with the results for compounds **4**, **5**, and **6**, all possessing a double bond in the N-containing ring, thus being more planar. Thus, comparison between compounds **1/4**, **2/5** and **3/6**, which possess similar structures only differing by the double bond between C-2 and C-3, indicates the importance of the planarity in the oxoisoaporphine framework for the antiplasmodial activity since **4**, **5** and **6** are respectively 2-fold, 5-fold and 2-fold more active than **1**, **2** and **3**. There is no information available dealing with the antiplasmodial properties of oxoisoaporphines and relatively little information about those of oxoaporphine and aporphine alkaloids. Among the studied compounds, the most active one against *P. falciparum* is (–)-roemrefidine (**10**), an aporphine alkaloids bearing a 1,2-methylenedioxy substituent, isolated from *Sparattanthelium amazonum* ($IC_{50} = 0.58 \mu\text{M}$, INDO, chloroquine resistant strain of *P. falciparum*) (Munoz et al., 1999). In addition, liriiodenine (**11**), an oxoaporphine alkaloid was found to be active against *P. falciparum* ($IC_{50} = 25.1 \mu\text{M}$, K1, chloroquine resistant strain) (Camacho et al., 2000). The importance of the presence of the methylenedioxy substituent has been shown for the Cytotoxicity of aporphine alkaloids but since dicentrinone, an oxoaporphine bearing a 1,2-methylenedioxy substituent and two methoxy groups at C-9 and C-10 isolated from *Stephania dinklagei*, have been shown to be devoid of activity towards *P. falciparum* ($IC_{50} = 189.2 \mu\text{M}$, K1, chloroquine resistant strain) (Boustie et al., 1998; Likhitwitayawuid et al., 1993; Montanha et al., 1995; Stevigny et al., 2005; Stévigny et al., 2002). We can suppose that the involvement of this group for the antiplasmodial activity is weaker than for the Cytotoxicity. Nevertheless, the weak numbers of studies realized on the antiplasmodial activities of aporphines as well as the major structural differences between the tested compounds do not allow us to deduct structure-activity relationships for these aporphine alkaloids. Further studies have to be carried out to draw further conclusions concerning the involvement of the different moieties.

3.3.1.2. Quantum Chemistry QSAR prediction

Taking into consideration that there is not apparent single-variable relationship between activity and/or Cytotoxicity with electronic properties, we carried out a QSAR study to unravel multivariable effects. In this sense, we perform a Linear Discriminant Analysis (LDA) to

discriminate between active/toxic compound and non-effective compounds(Gonzalez-Diaz et al., 2008). The best model found was:

$$S_j(L,c) = 0.071 \cdot I(L) - 2.866 \cdot EA + 0.027 \cdot I(L) \cdot \left(\frac{\chi}{c}\right) + 2.771 \quad (15)$$

$$N = 204 \quad Chi - sqr = 39.3 \quad p < 0.001$$

In this QSAR model, $S_j(L,c)$ is a real-value variable that scores both the Cytotoxicity or activity of compound j th against line L at concentration c . For it, we have to substitute in the QSAR the line susceptibility value $I(L) = (\text{active compounds})/(\text{total compounds})$ for *P. falciparum* in the case we pretend to predict antiparasitic activity. By the contrary, we substitute the value of $I(L)$ for one of the cellular lines if we pretend to predict Cytotoxicity against one specific line. According to Chi-square test the model is significant in statistical terms with low error-level ($p < 0.05$). In addition, in **Table 5** we give the values of Accuracy, Sensitivity, and Specificity for both training and external validation series. These results have been considered as characteristic of a model with good fit to data for this type of models(Gia et al., 2005; Santana et al., 2006a).

Table 5 comes about here

In **Figure 8**, we map the multivariate relationships between drug cellular inhibition and the electronic properties. We can note that the both active as cytotoxic compounds are predicted to lie within regions with low EA and high χ . Consequently, optimized compounds in terms of Activity/Cytotoxicity ratio are expected to be found in the middle region. In this sense, further synthetic efforts should be directed towards new compounds predicted within this area. In a similar manner, if we substitute in the equation the EA and χ values for specific groups of atoms we can approach to the contribution of these atomic groups to the biological activity or toxicity. These values can be used to map backwards the biological activity on the chemical structure.

These kinds of maps have been known as back-projection maps(Gia et al., 2005; Prado-Prado et al., 2008; Prado-Prado et al., 2009). For instance, in **Figure 8** we illustrate the construction of back-projection maps for two molecules at $c = 1.6 \mu\text{g/mL}$ with respect to activity against *P. falciparum* and Cytotoxicity against HeLa cell line. We can note that the Cytotoxicity values for **6** and **8** are clearly nearby in the activity with a 43-44 of score regarding the chemical structure of the quinoline in the molecule, however, the presence of the keto-enol system in **6** increases significantly its contribution to the Cytotoxicity. The polarity and the possibility to afford hydrogen bond of both, carbonyl and hydroxyl groups, jointly with the methoxy group at C-5, they would be the driving force for the above mentioned reactivity. In case of the antiparasitic activity, the contribution of the quinoline system in **8** is slightly superior to the quinolone framework in **6**, being able to be an important part in the reactivity of this molecule on the parasite. The design of molecules from of this small group of oxoisoaporphine alkaloids should consider this quinoline core to be a part of possibly drugs to study.

Figure 8 comes about here

The global index mentioned previously could give us an explanation about the reactivity of certain molecular moieties on the Cytotoxicity and antiparasitic behavior. Thus, compound **8** presents an ω and EA lower than its isomer **5**, which could be due to the electron-donating effect of the OMe group at C-5, diminishing the electron acceptor capacity of the quinoline moiety which seems to be linked with the antiplasmodial activity. The Cytotoxicity of some derivatives can be easily related to the polarity and/or electro negativity of certain moieties of the molecule. Thus, the compound **4** represents to the central core of the oxoisoaporphine derivatives which, when adding a methoxy group as in **5**, diminishes its electron-withdrawing capacity and, consequently, its Cytotoxicity. This is reflected in a small decrease of the EA, χ

and ω values, being very important this feature of the quinoline system for the pharmacological activity.

3.3.1.3. NL MIND-BEST prediction of targets for anti-malarial aporphine alkaloids

We used the best ANN model found to predict the possible interaction of 2,3-dihydrooxoisoaporphine, oxoisoaporphine and oxoaporphine alkaloids with proteins targets present in *P. falciparum*. For this study we selected 54 proteins out of all proteins of *P. falciparum* proteome reported in PDB. The criteria used to download structures from PDB were: 1) source organism is *P. falciparum* 3D7 and 2) Identity Cutoff = 50% in Homologue Removal tool. We predicted the interaction of the 8 compounds with all these proteins using the **NL MIND-BEST**. The **Table 6** shows some results obtained using the model MLP 20:20-15-1:1; which is a classifier implemented in the server. For it, firstly we generated the SMILE codes for these compounds and using the model predicted their propensity to form DTPs with 54 Plasmodium proteins obtained from Protein Data Bank (PDB).

Table 6 comes about here

Despite a positive or negative prediction we report all values to illustrate the results in **Table 6** and confront the results obtained using this server and the outcomes of the pharmacological assay. We also carried out a Two-Way-joining Analysis (TWJ) of these results. Using these predictions as inputs we carried out the TWJ. In **Figure 9** we show a TWJ analysis of the DTPs scores predicted with **NL MIND-BEST** for 54 proteins with respect to the list of 8 anti-malarial drugs presented in this work. It makes a total of $54 \times 8 = 432$ score values used as inputs for the TWJ analysis, the values are in **Table 2SM**. After TWJ analysis re-ordering the 432 score values were grouped into 63 blocks or clusters. In the figure we can see values and variability of the none-interaction/interaction score with total sample mean = 0.75 and standard deviation SD = 0.23. These results indicate a low average tendency of these drugs to bind the selected proteins. This is useful because our results presented will simultaneously contribute to the uncovering of meaningful patterns of drug-target interaction clusters (StatSoft.Inc., 2002). Interesting, the figure shows that **NL MIND-BEST** predicts that compounds 4, 5, and 8 have more propensity to interact with the proteins of *P. falciparum*. This result is significant because the compound 8 has shown activity against *P. falciparum* in the experimental assay carry out in this work, see **Table 4**. In particular, **NL MIND-BEST** predicts a high interaction for compound 8 with the protein with PDB ID 2ANL. This protein is an enzyme with action as aspartic protease also known as Plasmepsin IV. The prediction of 2ANL as potential target for compound 8 is interesting because there are other compounds that inhibit the same protein. In fact, the PDB file 2ANL is the X-ray structure of the complex between Plasmepsin IV with the compound JE2 (Clemente et al., 2006). JEA is a peptide inhibitor of plasmepsin IV with name: (R)-N-(2-Methylbenzyl)-3-[(2s,3s)-2-Hydroxy-3-(3-Hydroxy-2-Methylbenzoyl)Amino-4-Phenylbutanoyl]-5,5-Dimethyl-1,3-Thiazolidine-4-Carboxamide, see also **Figure 6**. So, compound 8 may open a new door to the design of new non-peptidic inhibitors of Plasmepsin IV.

Figure 9 comes about here

3.3.1.4. NL MIND-BEST search of targets for cytotoxicity of aporphine alkaloids

Compounds 2e, 3e, 6e presented the highest cytotoxicity in cellular lines MeL-43 and WI-38 (Boustie et al., 1998; Likhitwitayawuid et al., 1993; Montanha et al., 1995; Stevigny et al., 2005; Stévigny et al., 2002) (Table 3). Compound 8e is the most active against Plasmodium but not presented high cytotoxic effect. We used the NL MIND-BEST to predict targets for cytotoxic effect of compounds 2e, 3e, 6e and 8e. For it, firstly we predicted the target of these compounds in the parasite (see previous section). Next, we obtained the sequence of these proteins in PDB in FASTA format. Later, we carried out BLAST analysis of these sequences against human proteome. The outcomes of BLAST alignment allowed us to detect the more similar proteins in human for potential targets in parasite. These proteins are also reasonably

expected to interact with the new compounds as well. In the case that predicted targets in humans are important for cell viability they may offer an explanation for cytotoxicity effect.

The server predicted that compounds 2e and 3e present interaction with protein 2Z8W (Henderson et al., 2007), compound 6e interacts with protein 2PSS (Dufe et al., 2007; Pokkuluri et al., 1999). However, these compounds do not exhibit any activity against Plasmodium, which is why we only focus to the compound 8e, because it presented the more interesting anti-plasmodium activity. In **Table 7**, we show the PDB ID, and the protein type, and NL MIND-BEST (NL-MB) score for these proteins. More important for us is the prediction by our server of an interaction of compound 8e with protein 2ANL, a Plasmepsin IV protein (Clemente et al., 2006). Consequently, we decide to focus only on explaining the relative cytotoxicity of our most active compound 8e. Firstly, we performed a protein BLAST analysis of 2ANL. In this alignment study we obtained a similarity with respect to the human protein 3D91, see **Figure 10**. The 3D91 is a Renin protein, an enzyme which biological role is the blood pressure control at organ level and not totally demonstrated to present direct or indirect effect at intracellular level that may explain the mechanism by which the compound 8e produce cytotoxicity. In any case, recently has been published certain evidence on the relationships of the complex Renin-Angiotensin-Aldosterone (RAS) with immune system function and drug cytotoxicity. RAS with its respective receptors, the angiotensin AT1 and AT2 receptor (AT1R and AT2R), has been implicated in ethanol-induced cytotoxicity (Menk et al., 2010), to cite an example. In fact, while angiotensin II, which is produced by RAS system, is considered to be the major regulator molecule that controls both the blood pressure and fluid system, there is an increasing body of evidence that this bioactive peptide and its receptor might also contribute to the immune system. However, there are few details known about the direct effect that angiotensin type I receptors (AT1R) have on the cytotoxic T cell (CTL). The antigen-specific CTL induction by immunization with the CTL antigenic peptide was reduced by angiotensin II type I receptor blocker (ARB) in vivo. These findings suggested that ARBs might have the ability to suppress excessive antigen-specific activation and induction of CTLs promoted by angiotensin II (Maeda et al., 2009). However, a recent experimental work discarded a relationship between this system and the cytotoxicity of the drug Amiodarone (AM) or an AM metabolite called N-desethylamiodarone (DEA) (Mulder et al.). In conclusion, the present result, even interesting, do not allow us to propose a plausible mechanism for the relative level of cytotoxicity of compound 8e but we can speculate with an effect over Renin and consequently over all the RAS system.

Figure 10 comes about here

Table 7 comes about here

3.3.2. Theoretic-experimental study of peptides from *G. lamblia* proteome (experiment 2)

3.3.2.1. 2DE & MS study of peptides found on new protein PMF

In this section we present an example of the practical use of the QSAR model to predict enzyme scores for peptides found in the PMF of a new query protein. We illustrate an overall view of the 2DE map obtained from *G. lamblia*, see **Figure 11**. In this figure, we zoomed in to highlight a spot that corresponds to a protein of MW > 21 000 Da and pI < 7, which has not been investigated before. Our interest in this area derived from the fact that these spots remained unchanged from gel to gel repetitions and may correspond to a relevant but unknown protein of this parasite.

Figure 11 comes about here

The protein sample corresponding to this spot was submitted to in-gel trypsin digestion and the mass of the resulting peptides was measured by MALDI-TOF MS analysis. Once we obtained the data from MALDI-TOF MS analysis of the query spot, the most relevant MS signals were introduced into the MASCOT search engine (Giddings et al., 2003; Lei et al., 2005). In the MASCOT collection of annotated we used the database with MS recorded for *G. lamblia* (Arakaki et al., 2006) proteins. We obtained 13 hits (template proteins) for this protein

with MASCOT scores (M_s) higher than 59 ($p < 0.05$), the threshold value for significant match, see **Table 8**. The maximum score obtained was 421, which corresponded to protein gi159116163 of *G. lamblia* with mass 99 431 Da and annotated, as well as other relevant hits, gi121999104 of DNA topoisomerase III with score 82 or other with hypothetical protein or unknown function.

Table 8 comes about here

Moreover, almost all relative interesting matches found have also been recorded for predicted protein or hypothetical proteins. These aspects make it difficult to assign the sequence and function for the new protein, but at the same time, increase our interest in the PMF of this new query protein that does not match to known templates. As mentioned in the Introduction, the PMF of this type of protein may be of great interest. We provide detailed information on the results of the MS analysis of the PMF of the new protein by the MALDI TOF technique and MASCOT search engine, in **Table 8**. Similar combinations have been successfully used in the past to study *Trichinella* antigens (Dea-Ayuela and Bolás-Fernández, 2005) and possible *Leshmania* dynein proteins (Dea-Ayuela et al., 2008). The table includes only the 13 most interesting peptides matched with the MS of other proteins in the MASCOT search. We found an excellent match between the mass of the peptide detected and the mass of the template peptide recorded in MASCOT database with known sequence for all these peptides. Interestingly, we found an excellent match between MS signals not only for template protein 1 (higher M_s) but also for the second one template protein. Consequently, we decided to investigate the structure-function relationships for all sequences of peptides found on the PMF of the new protein.

3.3.2.2. MM/MC study of peptides found on new protein PMF

Our main interest on the study of the peptides in the PMF of the new unknown proteins is to find which of them make a positive contribution to the ligand interaction. This may allow us to select peptides for drug design and/or obtain information for drug-target discovery. We therefore have to calculate the ξ_k and μ_k for all peptides and substitute these values in the QSAR model to predict ligand interaction score for one ligand (levulinic acid). For this, we first need the 3D structures of the peptides in order to calculate the ξ_k and μ_k values. For this study we used the same 13 peptides found by PMF of the new protein. Unfortunately, we only have the sequences of the peptides but not the 3D structures. We therefore first obtained the optimal 3D folded structures by use of a MM geometry optimization for the 13 peptides (see **Figure 2**). We complemented the MM by MC search in order to explore alternative geometrical structures for the peptides. We summarized the results of MC simulation of these peptides in **Table 9**. In this table we reported the initial energy (E_0) based on the starting structure constructed with standard parameters for α -helixes (bond distances, angles, and dihedral angles) set as default on the sequence editor of Hyperchem (Froimowitz, 1993; Hypercube, 2002). We also reported the (E_1) obtained after optimization of the structure with AMBER force field obtained by MC method using 1000 steps for 13 peptides. Lastly, we report the ACCR values for the MDT of the 13 peptides in **Table 9**. In the MD study most researchers tend to try for an average ACCR value around 0.5; smaller values may be appropriate when longer runs are acceptable and more extensive sampling is necessary. In the present study all the ACCR values were between 0.66 and 0.71 because MC simulation has been realized by 1000 steps; in consequence, we can accept the MD results as valid (Froimowitz, 1993; Hypercube, 2002).

Table 9 comes about here

3.3.2.3. NL MIND-BEST prediction for peptides of new protein (mode 2)

We illustrated this mode of use of the server NL MIND-BEST with the study of the interaction of peptides against different ligands. In mode 2, first we have to carry out the calculation of plausible 3D structure of the 13 peptides using the software Hyperchem. This program generates files of type .ent with possible structures of peptides. Next, we used the files

with extension .ent as inputs for the server **NL MIND-BEST**. With these files the server calculated the ξ_k and μ_k values for the 13 peptides. Next, the web server substituted these values in the model as well as the average parameters for the different ligands and predicted the probability with which the 13 peptides interact with the different ligands. For the present study we selected as potential ligands 9 known drugs with different mechanisms of action, see list at follows:

1. Levamisole, target Ion-channel Nicotinic acetylcholine receptor (nematodes) (Evans and Martin, 1996; Martin, 1993; Robertson and Martin, 1993).
2. Piperazine, target Ion-channel GABA receptors (in large intestinal nematodes) (Martin, 1985).
3. Ivermectin, target Ion-channel GluCl⁻ receptor (in nematodes and insect parasites) (Cully et al., 1996; Martin, 1996).
4. Praziquantel, target Membrane Ion-channel calcium permeability (in cestodes and trematodes) (Redman et al., 1996).
5. Mebendazole, target β -Tubulin (in nematodes, cestodes and trematodes) (Roos et al., 1995).
6. Closantel, Proton ionophore against blood feeders: Flukes, *Haemonchus contortus*, *Oestrus ovis* (McKellar et al., 1991).
7. Diamfenetide, target Malate metabolism (in immature *Fasciola hepatica*) (Edwards et al., 1981a; Edwards et al., 1981b).
8. Clorsulon, target Phosphoglycerate kinase and mutase (Schulman et al., 1982).
9. Diethylcarbamazina, target Arachidonic acid metabolism and host immunity, effective against *Filaria* (Maizels and Denham, 1992).

We used the best ANN model implemented in the web server **NL MIND-BEST** to predict the possible interaction of these drugs with the 13 peptides. In **Figure 12 (A)** we show a TWJ analysis of the DTPs scores predicted with this sever for all the peptides with respect to the list of nine representative drugs. In this figure we can see a very low values and variability of the scores indicating low tendency of peptides studied to bind these drugs. As a result, we can see that MIND-BEST do not predict significant contribution to DTP formation between the peptides of relevant protein and the nine drugs representative of nine different mechanisms of action. These results coincide for all peptide investigated (100%) with the results found by MASCOT and BLAST analysis, see **Table 8**. In **Figure 12 (B)** we show a typical BLAST alignment result found for one of these peptides showing very low similarity scores with known parasite proteins (algorithm adjusted for short peptides). In conclusion, all **NL MIND-BEST**, MASCOT, and BLAST predict very low propensity of these peptides to be involved on DTPs formation with some of the nine anti-parasite drugs with known mechanism of action. It could indicate that this protein may be interesting to be investigated as a new target for drugs with a mechanism different from those mechanisms more representative of anti-parasite drugs. These results are relevant because they show that we can use both QSAR (alignment-free) and BLAST (relies upon alignment) as complementary methods (Aguero-Chapin et al., 2008; Agüero-Chapin et al., 2006; González-Díaz et al., 2005; Han et al., 2006; Sternberg et al., 1994). In **Table 10**, as an example for test our system using well established drug-protein interaction, such as interaction between imatinib (Gleevec) with protein OPL1 (Proto-oncogene tyrosine-protein kinase ABL1). The all drug-protein interaction were able on **Table 1SM**.

Figure 12 comes about here

Table 10 comes about here

4. Conclusions

Combining **MARCH-INSIDE** approach and ANNs is possible to seek one mt-QSAR classifier to predict with Accuracy > 90% the probability of drugs to bind more than 500 different drug target proteins approved by FDA of USA. This ANN classifier was implemented in the form a web server called **NL MIND-BEST** that may be used online and free by the research community to carry out public research. The server is useful to carry out Data Mining of PDB automatically in order to discovery new targets for any drug giving as inputs the SMILE code of the drug and the PDB ID of the protein only. We can also predict the interactions with specific drugs of peptides or protein 3D structures generated by MM/MD modeling.

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References

- Aguero-Chapin, G., Antunes, A., Ubeira, F.M., Chou, K.C., and Gonzalez-Diaz, H., 2008. Comparative Study of Topological Indices of Macro/Supramolecular RNA Complex Networks. *J Chem Inf Model* 48, 2265–2277.
- Aguero-Chapin, G., Varona-Santos, J., de la Riva, G.A., Antunes, A., Gonzalez-Villa, T., Uriarte, E., and Gonzalez-Diaz, H., 2009. Alignment-Free Prediction of Polygalacturonases with Pseudofolding Topological Indices: Experimental Isolation from *Coffea arabica* and Prediction of a New Sequence. *J Proteome Res* 8, 2122-2128.
- Agüero-Chapin, G., Gonzalez-Diaz, H., Molina, R., Varona-Santos, J., Uriarte, E., and Gonzalez-Diaz, Y., 2006. Novel 2D maps and coupling numbers for protein sequences. The first QSAR study of polygalacturonases; isolation and prediction of a novel sequence from *Psidium guajava* L. *FEBS Lett* 580 723-730.
- Altschul, S.F., Madden, T.L., Schaffer, A.A., Zhang, J., Zhang, Z., Miller, W., and J., L.D., 1997. Gapped BLAST and PSI-BLAST: a new generation of protein database search programs. *Nucleic Acids Res.* 25, 389-402.
- Apte, A.A., Cain, J.W., Bonchev, D.G., and Fong, S.S., 2008. Cellular automata simulation of topological effects on the dynamics of feed-forward motifs. *J Biol Eng* 2, 2.
- Arakaki, T., Le Trong, I., Phizicky, E., Quartley, E., DeTitta, G., Luft, J., Lauricella, A., Anderson, L., Kalyuzhniy, O., Worthey, E., Myler, P.J., Kim, D., Baker, D., Hol, W.G., and Merritt, E.A., 2006. Structure of Lmaj006129AAA, a hypothetical protein from *Leishmania major*. *Acta Crystallograph Sect F Struct Biol Cryst Commun* 62, 175-9.
- Barabasi, A.L., 2005. Sociology. Network theory--the emergence of the creative enterprise. *Science* 308, 639-41.
- Barabasi, A.L., 2007. Network medicine--from obesity to the "diseasome". *N Engl J Med* 357, 404-7.
- Barabasi, A.L., and Oltvai, Z.N., 2004. Network biology: understanding the cell's functional organization. *Nat Rev Genet* 5, 101-13.
- Bas, D.C., Rogers, D.M., and Jensen, J.H., 2008. Very fast prediction and rationalization of pKa values for protein-ligand complexes. *Proteins* 73, 765-83.
- Bleakley, K., and Yamanishi, Y., 2009. Supervised prediction of drug-target interactions using bipartite local models. *Bioinformatics* 25, 2397-403.
- Bonchev, D., 2003. On the complexity of directed biological networks. *SAR QSAR Environ Res* 14, 199-214.
- Bonchev, D., 2004. Complexity analysis of yeast proteome network. *Chem Biodivers* 1, 312-26.
- Bonchev, D., and Buck, G.A., 2007. From molecular to biological structure and back. *J Chem Inf Model* 47, 909-17.
- Bonchev, D., Thomas, S., Apte, A., and Kier, L.B., 2010. Cellular automata modelling of biomolecular networks dynamics. *SAR QSAR Environ Res* 21, 77-102.
- Bornholdt, S., and Schuster, H.G., 2003. *Handbook of Graphs and Complex Networks: From the Genome to the Internet*. WILEY-VCH GmbH & CO. KGa., Weinheim.
- Boustie, J., Stigliani, J.L., Montanha, J., Amoros, M., Payard, M., and Girre, L., 1998. Antipoliiovirus structure-activity relationships of some aporphine alkaloids. *J Nat Prod* 61, 480-4.
- Caballero, J., and Fernandez, M., 2006. Linear and nonlinear modeling of antifungal activity of some heterocyclic ring derivatives using multiple linear regression and Bayesian-regularized neural networks. *J Mol Model* 12, 168-81.
- Camacho, M.R., Kirby, G.C., Warhurst, D.C., Croft, S.L., and Phillipson, J.D., 2000. Oxoaporphine alkaloids and quinones from *Stephania dinklagei* and evaluation of their antiprotozoal activities. *Planta Med* 66, 478-80.
- Campillos, M., Kuhn, M., Gavin, A.C., Jensen, L.J., and Bork, P., 2008. Drug target identification using side-effect similarity. *Science* 321, 263-6.
- Chen, X., Fang, Y., Yao, L., Chen, Y., and Xu, H., 2007. Does drug-target have a likeness? *Methods Inf Med* 46, 360-6.
- Chou, K.C., 2005. Prediction of G-protein-coupled receptor classes. *J Proteome Res* 4, 1413-8.

- Chou, K.C., and Elrod, D.W., 2002. Bioinformatical analysis of G-protein-coupled receptors. *J Proteome Res* 1, 429-33.
- Chou, K.C., and Elrod, D.W., 2003. Prediction of enzyme family classes. *J Proteome Res* 2, 183-90.
- Chou, K.C., and Shen, H.B., 2006a. Predicting eukaryotic protein subcellular location by fusing optimized evidence-theoretic K-nearest neighbor classifiers *J Proteome Res* 5, 1888-1897.
- Chou, K.C., and Shen, H.B., 2006b. Large-scale predictions of Gram-negative bacterial protein subcellular locations. *J Proteome Res* 5, 3420-3428.
- Chou, K.C., and Shen, H.B., 2007. MemType-2L: A Web server for predicting membrane proteins and their types by incorporating evolution information through Pse-PSSM. *Biochem Biophys Res Commun* doi:10.1016/j.bbrc.2007.1006.1027.
- Chou, K.C., and Shen, H.B., 2008. Cell-PLoc: a package of Web servers for predicting subcellular localization of proteins in various organisms. *Nat Protoc* 3, 153-62.
- Clemente, J.C., Govindasamy, L., Madabushi, A., Fisher, S.Z., Moose, R.E., Yowell, C.A., Hidaka, K., Kimura, T., Hayashi, Y., Kiso, Y., Agbandje-McKenna, M., Dame, J.B., Dunn, B.M., and McKenna, R., 2006. Structure of the aspartic protease plasmepsin 4 from the malarial parasite *Plasmodium malariae* bound to an allophenylnorstatine-based inhibitor. *Acta Crystallogr D Biol Crystallogr* 62, 246-52.
- Concu, R., Podda, G., Uriarte, E., and Gonzalez-Diaz, H., 2009a. Computational chemistry study of 3D-structure-function relationships for enzymes based on Markov models for protein electrostatic, HINT, and van der Waals potentials. *J Comput Chem* 30, 1510-20.
- Concu, R., Podda, G., Ubeira, F.M., and Gonzalez-Diaz, H., 2010. Review of QSAR Models for Enzyme Classes of Drug Targets: Theoretical Background and Applications in Parasites, Hosts, and other Organisms. *Curr Pharm Des* 16, 2710-23.
- Concu, R., Dea-Ayuela, M.A., Perez-Montoto, L.G., Bolas-Fernandez, F., Prado-Prado, F.J., Podda, G., Uriarte, E., Ubeira, F.M., and Gonzalez-Diaz, H., 2009b. Prediction of enzyme classes from 3D structure: a general model and examples of experimental-theoretic scoring of peptide mass fingerprints of *Leishmania* proteins. *J Proteome Res* 8, 4372-82.
- Concu, R., Dea-Ayuela, M.A., Perez-Montoto, L.G., Prado-Prado, F.J., Uriarte, E., Bolas-Fernandez, F., Podda, G., Pazos, A., Munteanu, C.R., Ubeira, F.M., and Gonzalez-Diaz, H., 2009c. 3D entropy and moments prediction of enzyme classes and experimental-theoretic study of peptide fingerprints in *Leishmania* parasites. *Biochim Biophys Acta* 1794, 1784-94.
- Cully, D.F., Wilkinson, H., Vassilatis, D.K., Etter, A., and Arena, J.P., 1996. Molecular biology and electrophysiology of glutamate-gated chloride channels of invertebrates. *Parasitology* 113 Suppl, S191-200.
- Dea-Ayuela, M.A., and Bolás-Fernández, F., 2005. Two-dimensional electrophoresis and mass spectrometry for the identification of species-specific *Trichinella* antigens. *Vet Parasitol* 132, 43-49.
- Dea-Ayuela, M.A., Perez-Castillo, Y., Meneses-Marcel, A., Ubeira, F.M., Bolas-Fernandez, F., Chou, K.C., and Gonzalez-Diaz, H., 2008. HP-Lattice QSAR for dynein proteins: experimental proteomics (2D-electrophoresis, mass spectrometry) and theoretic study of a *Leishmania infantum* sequence. *Bioorg Med Chem* 16, 7770-6.
- Edwards, S.R., Campbell, A.J., Sheers, M., Moore, R.J., and Montague, P.E., 1981a. Protection of *Fasciola hepatica* against flukicidal action of the amine of diamphenethide in vitro. *Mol Biochem Parasitol* 2, 339-48.
- Edwards, S.R., Campbell, A.J., Sheers, M., Moore, R.J., and Montague, P.E., 1981b. Studies of the effect of diamphenethide and oxyclozanide on the metabolism of *Fasciola hepatica*. *Mol Biochem Parasitol* 2, 323-38.
- Estrada, E., 2006a. Protein bipartivity and essentiality in the yeast protein-protein interaction network. *J Proteome Res* 5, 2177-84.
- Estrada, E., 2006b. Virtual identification of essential proteins within the protein interaction network of yeast. *1615-9853* 6, 35-40.

- Evans, A.M., and Martin, R.J., 1996. Activation and cooperative multi-ion block of single nicotinic-acetylcholine channel currents of *Ascaris* muscle by the tetrahydropyrimidine anthelmintic, morantel. *Br J Pharmacol* 118, 1127-40.
- Fernandez, M., Caballero, J., and Tundidor-Camba, A., 2006. Linear and nonlinear QSAR study of N-hydroxy-2-[(phenylsulfonyl)amino]acetamide derivatives as matrix metalloproteinase inhibitors. *Bioorg Med Chem* 14, 4137-50.
- Fink, H., 1965. On the problem of the minimal inhibitory concentration (MIC) of oxacillin against staphylococci. *Arzneim-Forsch* 15, 630-2.
- Frisch, M.J.T., G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A., 2003. Gaussian 03, Revision B.03, Gaussian, Inc., Pittsburgh, PA.
- Froimowitz, M., 1993. HyperChem: a software package for computational chemistry and molecular modeling. *BioTechniques* 14, 1010-3.
- Geppert, H., Humrich, J., Stumpfe, D., Gartner, T., and Bajorath, J., 2009. Ligand prediction from protein sequence and small molecule information using support vector machines and fingerprint descriptors. *J Chem Inf Model* 49, 767-79.
- Gia, O., Marciani Magno, S., González-Díaz, H., Quezada, E., Santana, L., Uriarte, E., and Dalla Via, L., 2005. Design, synthesis and photobiological properties of 3,4-cyclopentenepsoralens. *Bioorg Med Chem* 13, 809-17.
- Giddings, M.C., Shah, A.A., Gesteland, R., and Moore, B., 2003. Genome-based peptide fingerprint scanning. *Proc Natl Acad Sci U S A* 100, 20-5.
- Giuliani, A., 2010. Collective motions and specific effectors: a statistical mechanics perspective on biological regulation. *1471-2164* 11 Suppl 1, S2.
- Goh, K.I., Cusick, M.E., Valle, D., Childs, B., Vidal, M., and Barabasi, A.L., 2007. The human disease network. *Proc Natl Acad Sci U S A* 104, 8685-90.
- Gonzalez-Diaz, H., 2010. Network topological indices, drug metabolism, and distribution. *Curr Drug Metab* 11, 283-4.
- Gonzalez-Diaz, H., Prado-Prado, F., and Ubeira, F.M., 2008. Predicting antimicrobial drugs and targets with the MARCH-INSIDE approach. *Curr Top Med Chem* 8, 1676-90.
- Gonzalez-Diaz, H., Saiz-Urra, L., Molina, R., Santana, L., and Uriarte, E., 2007a. A model for the recognition of protein kinases based on the entropy of 3D van der Waals interactions. *J Proteome Res* 6, 904-8.
- Gonzalez-Diaz, H., Bonet, I., Teran, C., De Clercq, E., Bello, R., Garcia, M.M., Santana, L., and Uriarte, E., 2007b. ANN-QSAR model for selection of anticancer leads from structurally heterogeneous series of compounds. *Eur J Med Chem* 42, 580-5.
- González-Díaz, H., 2010. QSAR and Complex Networks in Pharmaceutical Design, Microbiology, Parasitology, Toxicology, Cancer and Neurosciences *Curr Pharm Des* 16, 2598-2600.
- González-Díaz, H., Vilar, S., Santana, L., and Uriarte, E., 2007a. Medicinal Chemistry and Bioinformatics – Current Trends in Drugs Discovery with Networks Topological Indices. *Curr Top Med Chem* 7, 1025-39.
- González-Díaz, H., Pérez-Castillo, Y., Podda, G., and Uriarte, E., 2007b. Computational Chemistry Comparison of Stable/Nonstable Protein Mutants Classification Models Based on 3D and Topological Indices. *J Comput Chem* 28, 1990-1995.

- González-Díaz, H., González-Díaz, Y., Santana, L., Ubeira, F.M., and Uriarte, E., 2008. Proteomics, networks and connectivity indices. *1615-9853* 8, 750-778.
- González-Díaz, H., Agüero-Chapin, G., Varona-Santos, J., Molina, R., de la Riva, G., and Uriarte, E., 2005. 2D RNA-QSAR: assigning ACC oxidase family membership with stochastic molecular descriptors; isolation and prediction of a sequence from *Psidium guajava* L. *Bioorg Med Chem Lett* 15, 2932-7.
- Good, A.C., Hodgkin, E.E., and Richards, W.G., 1992. Similarity screening of molecular data sets. *J Comput Aided Mol Des* 6, 513-20.
- Han, L., Cui, J., Lin, H., Ji, Z., Cao, Z., Li, Y., and Chen, Y., 2006. Recent progresses in the application of machine learning approach for predicting protein functional class independent of sequence similarity. *1615-9853* 6, 4023-4037.
- Hirosawa, M., Hoshida, M., Ishikawa, M., and Toya, T., 1993. MASCOT: multiple alignment system for protein sequences based on three-way dynamic programming. *Comput Appl Biosci* 9, 161-7.
- Humberto González-Díaz, F.P.-P.a.F.M.U., 2008. Predicting Antimicrobial Drugs and Targets with the MARCH INSIDE Approach. *Current Topics in Medicinal Chemistry* 8, 1676-1690.
- Hypercube, I., 2002. Hyperchem 7.0, Gainesville, FL, USA
- Hypercube.Inc., 2002. Hyperchem software. Release 7.5 for windows, Molecular Modeling System., Hypercube Inc. , Gainesville, FL, USA
- Kier, L.B., Bonchev, D., and Buck, G.A., 2005. Modeling biochemical networks: a cellular-automata approach. *Chem Biodivers* 2, 233-43.
- Koenig, T., Menze, B.H., Kirchner, M., Monigatti, F., Parker, K.C., Patterson, T., Steen, J.J., Hamprecht, F.A., and Steen, H., 2008. Robust prediction of the MASCOT score for an improved quality assessment in mass spectrometric proteomics. *J Proteome Res* 7, 3708-17.
- Lam, R.L., and Welch, W.J., 2004. Comparison of methods based on diversity and similarity for molecule selection and the analysis of drug discovery data. *Methods Mol Biol* 275, 301-16.
- Lei, Z., Elmer, A.M., Watson, B.S., Dixon, R.A., Mendes, P.J., and Sumner, L.W., 2005. A two-dimensional electrophoresis proteomic reference map and systematic identification of 1367 proteins from a cell suspension culture of the model legume *Medicago truncatula*. *Mol Cell Proteomics* 4, 1812-25.
- Leung, K.Y., Lescuyer, P., Campbell, J., Byers, H.L., Allard, L., Sanchez, J.C., and Ward, M.A., 2005. A novel strategy using MASCOT Distiller for analysis of cleavable isotope-coded affinity tag data to quantify protein changes in plasma. *1615-9853* 5, 3040-4.
- Li, J., Lei, B., Liu, H., Li, S., Yao, X., Liu, M., and Gramatica, P., 2008. QSAR study of malonyl-CoA decarboxylase inhibitors using GA-MLR and a new strategy of consensus modeling. *J Comput Chem* 29, 2636-47.
- Li, Q., and Lai, L., 2007. Prediction of potential drug targets based on simple sequence properties. *BMC Bioinformatics* 8, 353.
- Likhitwitayawuid, K., Angerhofer, C.K., Chai, H., Pezzuto, J.M., Cordell, G.A., and Ruangrunsi, N., 1993. Cytotoxic and antimalarial alkaloids from the tubers of *Stephania pierrei*. *J Nat Prod* 56, 1468-78.
- Lin, W.Z., Xiao, X., and Chou, K.C., 2009. GPCR-GIA: a web-server for identifying G-protein coupled receptors and their families with grey incidence analysis. *Protein Eng Des Sel* 22, 699-705.
- Liu, Y., and Beveridge, D.L., 2002. Exploratory studies of ab initio protein structure prediction: multiple copy simulated annealing, AMBER energy functions, and a generalized born/solvent accessibility solvation model. *Proteins* 46, 128-46.
- Loscalzo, J., Kohane, I., and Barabasi, A.L., 2007. Human disease classification in the postgenomic era: a complex systems approach to human pathobiology. *Mol Syst Biol* 3, 124.
- Maeda, A., Okazaki, T., Inoue, M., Kitazono, T., Yamasaki, M., Lemonnier, F.A., and Ozaki, S., 2009. Immunosuppressive effect of angiotensin receptor blocker on stimulation of mice CTLs by angiotensin II. *Int Immunopharmacol* 9, 1183-8.
- Maizels, R.M., and Denham, D.A., 1992. Diethylcarbamazine (DEC): immunopharmacological interactions of an anti-filarial drug. *Parasitology* 105 Suppl, S49-60.

- Managbanag, J.R., Witten, T.M., Bonchev, D., Fox, L.A., Tsuchiya, M., Kennedy, B.K., and Kaeberlein, M., 2008. Shortest-path network analysis is a useful approach toward identifying genetic determinants of longevity. *PLoS ONE* 3, e3802.
- Marchler-Bauer, A., and Bryant, S.H., 2004. CD-Search: protein domain annotations on the fly. *Nucleic Acids Res.* 32, W327-31.
- Martin, R.J., 1985. gamma-Aminobutyric acid- and piperazine-activated single-channel currents from *Ascaris suum* body muscle. *Br J Pharmacol* 84, 445-61.
- Martin, R.J., 1993. Neuromuscular transmission in nematode parasites and antinematodal drug action. *Pharmacol Ther* 58, 13-50.
- Martin, R.J., 1996. An electrophysiological preparation of *Ascaris suum* pharyngeal muscle reveals a glutamate-gated chloride channel sensitive to the avermectin analogue, milbemycin D. *Parasitology* 112 (Pt 2), 247-52.
- Mascarenhas, N.M., and Ghoshal, N., 2008. Combined ligand and structure based approaches for narrowing on the essential physicochemical characteristics for CDK4 inhibition. *J Chem Inf Model* 48, 1325-36.
- Mazurie, A., Bonchev, D., Schwikowski, B., and Buck, G.A., 2008. Phylogenetic distances are encoded in networks of interacting pathways. *Bioinformatics* 24, 2579-85.
- Mazurie, A., Bonchev, D., Schwikowski, B., and Buck, G.A., 2010. Evolution of metabolic network organization. *BMC Syst Biol* 4, 59.
- McKellar, Q.A., Bogan, J.A., von Fellenberg, R.L., Ludwig, B., and Cawley, G.D., 1991. Pharmacokinetic, biochemical and tolerance studies on carprofen in the horse. *Equine Vet J* 23, 280-4.
- Menk, M., von Haefen, C., Funke-Kaiser, H., Sifringer, M., Scheffe, J.H., Kirsch, S., Seidel, K., Reinemund, J., Steckelings, U.M., Unger, T., and Spies, C.D., 2010. Ethanol-induced downregulation of the angiotensin AT2 receptor in murine fibroblasts is mediated by PARP-1. *Alcohol* 44, 495-506.
- Michel, J., Verdonk, M.L., and Essex, J.W., 2006. Protein-ligand binding affinity predictions by implicit solvent simulations: a tool for lead optimization? *J Med Chem* 49, 7427-39.
- Montanha, J.A., Amoros, M., Boustie, J., and Girre, L., 1995. Anti-herpes virus activity of aporphine alkaloids. *Planta Med* 61, 419-24.
- Mulder, J.E., Brien, J.F., Racz, W.J., Takahashi, T., and Massey, T.E., Mechanisms of Amiodarone and Desethylamiodarone Cytotoxicity in Non-transformed Human Peripheral Lung Epithelial Cells. *J Pharmacol Exp Ther*.
- Munoz, V., Sauvain, M., Mollinedo, P., Callapa, J., Rojas, I., Gimenez, A., Valentin, A., and Mallie, M., 1999. Antimalarial activity and cytotoxicity of (-)-roemrefidine isolated from the stem bark of *Sparattanthelium amazonum*. *Planta Med* 65, 448-9.
- Munteanu, C.R., Vazquez, J.M., Dorado, J., Sierra, A.P., Sanchez-Gonzalez, A., Prado-Prado, F.J., and Gonzalez-Diaz, H., 2009. Complex network spectral moments for ATCUN motif DNA cleavage: first predictive study on proteins of human pathogen parasites. *J Proteome Res* 8, 5219-28.
- Naumann, T., and Matter, H., 2002. Structural classification of protein kinases using 3D molecular interaction field analysis of their ligand binding sites: target family landscapes. *J Med Chem* 45, 2366-78.
- Onnela, J.P., Saramaki, J., Hyvonen, J., Szabo, G., Lazer, D., Kaski, K., Kertesz, J., and Barabasi, A.L., 2007. Structure and tie strengths in mobile communication networks. *Proc Natl Acad Sci U S A* 104, 7332-6.
- Park, J., and Barabasi, A.L., 2007. Distribution of node characteristics in complex networks. *Proc Natl Acad Sci U S A* 104, 17916-20.
- Parr, R.G., and Pearson, R.G., 1983. Absolute hardness: companion parameter to absolute electronegativity. *Journal of the American Chemical Society* 105, 7512-7516.
- Parr, R.G., Szentpály, L.v., and Liu, S., 1989. Density functional theory of atoms and molecules. Oxford University Press, New York.
- Parr, R.G., Szentpály, L.v., and Liu, S., 1999. Electrophilicity Index. *Journal of the American Chemical Society* 121, 1922-1924.
- Parr, R.G., Donnelly, R.A., Levy, M., and Palke, W.E., 1978. Electronegativity: The density functional viewpoint. *Journal of Chemical Physics* 68, 3801.

- Pham, T.A., and Jain, A.N., 2006. Parameter estimation for scoring protein-ligand interactions using negative training data. *J Med Chem* 49, 5856-68.
- Prado-Prado, F.J., Garcia-Mera, X., and Gonzalez-Diaz, H., 2010. Multi-target spectral moment QSAR versus ANN for antiparasitic drugs against different parasite species. *Bioorg Med Chem* 18, 2225-31.
- Prado-Prado, F.J., Gonzalez-Diaz, H., Santana, L., and Uriarte, E., 2007. Unified QSAR approach to antimicrobials. Part 2: predicting activity against more than 90 different species in order to halt antibacterial resistance. *Bioorg Med Chem* 15, 897-902.
- Prado-Prado, F.J., Gonzalez-Diaz, H., de la Vega, O.M., Ubeira, F.M., and Chou, K.C., 2008. Unified QSAR approach to antimicrobials. Part 3: first multi-tasking QSAR model for input-coded prediction, structural back-projection, and complex networks clustering of antiprotozoal compounds. *Bioorg Med Chem* 16, 5871-80.
- Prado-Prado, F.J., Martinez de la Vega, O., Uriarte, E., Ubeira, F.M., Chou, K.C., and Gonzalez-Diaz, H., 2009. Unified QSAR approach to antimicrobials. 4. Multi-target QSAR modeling and comparative multi-distance study of the giant components of antiviral drug-drug complex networks. *Bioorg Med Chem* 17, 569-75.
- Raha, K., Peters, M.B., Wang, B., Yu, N., Wollacott, A.M., Westerhoff, L.M., and Merz, K.M., Jr., 2007. The role of quantum mechanics in structure-based drug design. *Drug Discov Today* 12, 725-31.
- Redman, C.A., Robertson, A., Fallon, P.G., Modha, J., Kusel, J.R., Doenhoff, M.J., and Martin, R.J., 1996. Praziquantel: an urgent and exciting challenge. *Parasitol Today* 12, 14-20.
- Réka, A., and Barabasi, A.-L., 2002. Statistical mechanics of complex networks. *Rev Mod Phys* 74, 47-97.
- Robertson, S.J., and Martin, R.J., 1993. Levamisole-activated single-channel currents from muscle of the nematode parasite *Ascaris suum*. *Br J Pharmacol* 108, 170-8.
- Rodriguez-Soca, Y., Munteanu, C.R., Prado-Prado, F.J., Dorado, J., Pazos Sierra, A., and Gonzalez-Diaz, H., 2009a. Trypano-PPI: A Web Server for Prediction of Unique Targets in Trypanosome Proteome by using Electrostatic Parameters of Protein-Protein Interactions. *J Proteome Res*, doi:10.1021/pr900827b.
- Rodriguez-Soca, Y., Munteanu, C.R., Dorado, J., Rabuñal, J., Pazos, A., and González-Díaz, 2009b. Plasmod-PPI: A web-server predicting complex biopolymer targets in plasmodium with entropy measures of protein-protein interactions. *Polymer* 50, doi:10.1016/j.polymer.2009.11.029.
- Rodriguez-Soca, Y., Munteanu, C.R., Dorado, J., Pazos, A., Prado-Prado, F.J., and Gonzalez-Diaz, H., 2010. Trypano-PPI: a web server for prediction of unique targets in trypanosome proteome by using electrostatic parameters of protein-protein interactions. *J Proteome Res* 9, 1182-90.
- Roos, M.H., G., K.M.S., and N., G.W., 1995. New genetic and practical implications of selection for anthelmintic resistance in parasitic nematodes. *Parasitology Today* 11, 148-150.
- Rudnick, P.A., Wang, Y., Evans, E., Lee, C.S., and Balgley, B.M., 2005. Large scale analysis of MASCOT results using a Mass Accuracy-based THreshold (MATH) effectively improves data interpretation. *J Proteome Res* 4, 1353-60.
- Santana, L., Uriarte, E., Gonzalez-Diaz, H., Zagotto, G., Soto-Otero, R., and Mendez-Alvarez, E., 2006a. A QSAR model for in silico screening of MAO-A inhibitors. Prediction, synthesis, and biological assay of novel coumarins. *J Med Chem* 49, 1149-56.
- Santana, L., Uriarte, E., Gonzalez-Diaz, H., Zagotto, G., Soto-Otero, R., and Mendez-Alvarez, E., 2006b. A QSAR model for in silico screening of MAO-A inhibitors. Prediction, synthesis, and biological assay of novel coumarins. *J Med Chem* 49, 1149-56.
- Santana, L., Gonzalez-Diaz, H., Quezada, E., Uriarte, E., Yanez, M., Vina, D., and Orallo, F., 2008. Quantitative structure-activity relationship and complex network approach to monoamine oxidase a and B inhibitors. *J Med Chem* 51, 6740-51.
- Schulman, M.D., Ostlind, D.A., and Valentino, D., 1982. Mechanism of action of MK-401 against *Fasciola hepatica*: inhibition of phosphoglycerate kinase. *Mol Biochem Parasitol* 5, 133-45.
- Shen, H.B., and Chou, K.C., 2007. Nuc-PLoc: a new web-server for predicting protein subnuclear localization by fusing PseAA composition and PsePSSM. *Protein Eng Des Sel* 20, 561-7.
- Shen, H.B., and Chou, K.C., 2008. PseAAC: A flexible web server for generating various kinds of protein pseudo amino acid composition. *Anal Biochem* 373, 386-8.

- StatSoft.Inc., 2002. STATISTICA (data analysis software system), version 6.0, www.statsoft.com. Statsoft, Inc., 6.0,
- Sternberg, M.J., King, R.D., Lewis, R.A., and Muggleton, S., 1994. Application of machine learning to structural molecular biology. *Philos Trans R Soc Lond B Biol Sci* 344, 365-71.
- Stevigny, C., Bailly, C., and Quetin-Leclercq, J., 2005. Cytotoxic and antitumor potentialities of aporphinoid alkaloids. *Curr Med Chem Anticancer Agents* 5, 173-82.
- Stévigny, C., Block, S., Pauw-Gillet, M.C.D., Hoffmann, E.d., Llabrès, G., Adjakidjé, V., and Quetin-Leclercq, J., 2002. Cytotoxic Aporphine Alkaloids from *Cassytha filiformis*. *Planta Med* 68, 1042-1044.
- Tamura, M., and Takano, S., 1965. [Influence of pH of media on the minimal inhibitory concentration of cycloserine to *Mycobacterium tuberculosis*]. *Kekkaku* 40, 213-8.
- Thimm, M., Goede, A., Hougardy, S., and Preissner, R., 2004. Comparison of 2D similarity and 3D superposition. Application to searching a conformational drug database. *J Chem Inf Comput Sci* 44, 1816-22.
- Thomas, S., and Bonchev, D., 2010. A survey of current software for network analysis in molecular biology. *Hum Genomics* 4, 353-60.
- Todeschini, R., and Consonni, V., 2002. *Handbook of Molecular Descriptors*. Wiley-VCH.
- Vassura, M., Margara, L., Di Lena, P., Medri, F., Fariselli, P., and Casadio, R., 2008. Reconstruction of 3D structures from protein contact maps. *IEEE/ACM Trans Comput Biol Bioinform* 5, 357-67.
- Vijayan, R.S., Bera, I., Prabu, M., Saha, S., and Ghoshal, N., 2009. Combinatorial library enumeration and lead hopping using comparative interaction fingerprint analysis and classical 2D QSAR methods for seeking novel GABA(A) alpha(3) modulators. *J Chem Inf Model* 49, 2498-511.
- Vilar, S., Santana, L., and Uriarte, E., 2006. Probabilistic neural network model for the in silico evaluation of anti-HIV activity and mechanism of action. *J Med Chem* 49, 1118-1124.
- Vina, D., Uriarte, E., Orallo, F., and Gonzalez-Diaz, H., 2009. Alignment-free prediction of a drug-target complex network based on parameters of drug connectivity and protein sequence of receptors. *Mol Pharm* 6, 825-35.
- Wang, Y., and Bajorath, J., 2009. Development of a compound class-directed similarity coefficient that accounts for molecular complexity effects in fingerprint searching. *J Chem Inf Model* 49, 1369-76.
- Wu, Z.C., Xiao, X., and Chou, K.C., 2010. 2D-MH: A web-server for generating graphic representation of protein sequences based on the physicochemical properties of their constituent amino acids. *J Theor Biol* 267, 29-34.
- Xiao, X., and Lin, W.Z., 2009. Application of protein grey incidence degree measure to predict protein quaternary structural types. *Amino Acids* 37, 741-9.
- Xiao, X., Shao, S.H., and Chou, K.C., 2006. A probability cellular automaton model for hepatitis B viral infections. *Biochem Biophys Res Commun* 342, 605-10.
- Xiao, X., Lin, W.Z., and Chou, K.C., 2008a. Using grey dynamic modeling and pseudo amino acid composition to predict protein structural classes. *J Comput Chem* 29, 2018-24.
- Xiao, X., Wang, P., and Chou, K.C., 2008b. Predicting protein structural classes with pseudo amino acid composition: an approach using geometric moments of cellular automaton image. *J Theor Biol* 254, 691-6.
- Xiao, X., Wang, P., and Chou, K.C., 2009. GPCR-CA: A cellular automaton image approach for predicting G-protein-coupled receptor functional classes. *J Comput Chem* 30, 1414-23.
- Xiao, X., Wang, P., and Chou, K.C., 2010. Quat-2L: a web-server for predicting protein quaternary structural attributes. *Mol Divers*.
- Xiao, X., Shao, S., Ding, Y., Huang, Z., Chen, X., and Chou, K.C., 2005a. Using cellular automata to generate image representation for biological sequences. *Amino Acids* 28, 29-35.
- Xiao, X., Shao, S., Ding, Y., Huang, Z., Chen, X., and Chou, K.C., 2005b. An application of gene comparative image for predicting the effect on replication ratio by HBV virus gene missense mutation. *J Theor Biol* 235, 555-65.

- Xie, L., Xie, L., and Bourne, P.E., 2009. A unified statistical model to support local sequence order independent similarity searching for ligand-binding sites and its application to genome-based drug discovery. *Bioinformatics* 25, i305-12.
- Yamanishi, Y., Araki, M., Gutteridge, A., Honda, W., and Kanehisa, M., 2008. Prediction of drug-target interaction networks from the integration of chemical and genomic spaces. *Bioinformatics* 24, i232-40.
- Yang, C.Y., Sun, H., Chen, J., Nikolovska-Coleska, Z., and Wang, S., 2009. Importance of ligand reorganization free energy in protein-ligand binding-affinity prediction. *J Am Chem Soc* 131, 13709-21.
- Yu, B.W., Meng, L.H., Chen, J.Y., Zhou, T.X., Cheng, K.F., Ding, J., and Qin, G.W., 2001. Cytotoxic oxoisoaporphine alkaloids from *Menispermum dauricum*. *J Nat Prod* 64, 968-70.
- Zhang, S., Golbraikh, A., and Tropsha, A., 2006. Development of quantitative structure-binding affinity relationship models based on novel geometrical chemical descriptors of the protein-ligand interfaces. *J Med Chem* 49, 2713-24.

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Figure Legends:

Figure 1. Flowchart of all steps given in this work to develop MIND-BEST server

Figure 2. Snapshot of software Hyper-Chem with MM/MD study for one peptide

Figure 3. Synthesis of 2,3-dihydrooxoisoaporphine, oxoisoaporphine and oxoaporphine alkaloids.

Figure 4. (A) Topology of ANN models and **(B)** ROC Curve for MLP1 (20:20-15-1:1) classifier

Figure 5. Web interface for MIND-BEST server

Figure 6. Chemical structures of 2,3-dihydrooxoisoaporphine, oxoisoaporphine and oxoaporphine alkaloids.

Figure 7. Graphic of Cytotoxic activities IC_{50} (μ M) of oxoisoaporphine derivatives 1-8.

Figure 8. (A) Map of multivariate relationships between drug cellular inhibition and the electronic properties (EA) and χ . **(B)** Back-projection maps for **6** and **8** at $c = 1.6 \mu\text{g/mL}$ with respect to activity against *P. falciparum* and cytotoxicity against HeLa cell line.

Figure 9. BLAST score for similar PDB human protein.

Figure 10. TWJ analysis of 2,3-dihydrooxoisoaporphine, oxoisoaporphine and oxoaporphine alkaloids.

Figure 11. 2-DE map obtained for *G. lamblia* proteome

Figure 12. (A) MIND-BEST + TWJ analysis and **(B)** Typical BLAST for peptides from *G. lamblia* protein

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TABLES

Table 1. Comparison of LDA and different ANNs classification models.

Model profile	Class	Train			Statistical Parameters	Validation		
		DTPs	nDTPs	%		%	DTPs	nDTPs
LDA 15:15-1:1	DTPs	2931	477	86.00	Sensitivity	87.22	1460	214
	nDTPs	82	596	87.91	Specificity	88.76	38	300
	Total			86.32	Accuracy	87.48	1498	514
LNN 65:65-1:1	DTPs	598	80	88.20	Sensitivity	88.17	298	40
	nDTPs	418	2990	87.73	Specificity	88.35	195	1479
	Total			87.81	Accuracy	88.32		
PNN 65:65-4086 -2-2:1	DTPs	26	652	3.83	Sensitivity	3.85	13	325
	nDTPs	0	3408	100	Specificity	100	0	1674
	Total			84.04	Accuracy	83.85		
MLP 28:28-22-1:1	DTPs	568	110	83.78	Sensitivity	84.02	284	54
	nDTPs	525	2883	84.60	Specificity	83.75	272	1402
	Total			84.46	Accuracy	83.80		
RBF 1:1-1-1:1	DTPs	417	261	61.50	Sensitivity	60.36	204	134
	nDTPs	1343	2065	60.59	Specificity	61.41	646	1028
	Total			60.74	Accuracy	61.23		
MLP 20:20-15-1:1	DTPs	611	67	90.12	Sensitivity	91.72	310	28
	nDTPs	325	3083	90.46	Specificity	91.22	147	1527
	Total			90.41	Accuracy	91.30		

DTPs: Drug-Target Pairs for compounds with high affinity;
nDTPs: Drug-Target Pair for compounds with non-affinity.

Table 2. Input parameters for our model and output results compared with other models.

Drugs		Targets			MODEL						
I ^a	D ^b	Type ^c	I ^a	D ^b	Method ^d	N ^e	Nv ^f	Tech. ^g	Ac ^h	P ⁱ	Ref.
χ	2	Prot.	ξ	3	MI	6098	15	LDA	86.3	%	*
χ	2	Prot.	ξ	3	MI	6098	20	MLP	90.4	%	*
CTD	2	Prot.	σ	-	DTL	5367	2	SVM	94.4	%	(Chen et al., 2007)
PLB	2	Prot.	PLC	-	ReliefF	1300	-	LSVM	89.9	R	(Li et al., 2008)
S	2	MR	-	2	BLM	-	-	KRM	95.5	ROC	(Bleakley and Yamanishi, 2009)
ΔG	2	Prot.	ΔG	-	PROPKA	26	-	-	-	-	(Bas et al., 2008)
PP	2	Prot.	PP	3	-	372	-	RSVM	84.0	%	(Li and Lai, 2007)
ΔG	2	Prot.	ΔG	-	GBSA	2331	2	-	-	-	(Yang et al., 2009)
PP	2	MR	PP	1	MI	2559	10	LDA	72.3	%	(Vina et al., 2009)
PP	2	Prot.	PP	3	-	129	28	SMLR	73	R	(Mascarenhas and Ghoshal, 2008)
MOE	2	Prot.	MOE	3	CoIFA	133	17	GFA	81.2	%	(Vijayan et al., 2009)
SD	2	Prot.	SD	3	NTD	2274	-	ROC	99.3	ROC	(Pham and Jain, 2006)
ΔG	3	Prot.	ΔG	3	LBDD	-	-	QM	99.6	R	(Raha et al., 2007)
χ	2	Prot.	χ	3	nnsort	517	-	kNN	85	R	(Zhang et al., 2006)
ΔG	3	Enz.	ΔG	3	PBSA	48	-	PI	97	R	(Michel et al., 2006)
χ	3	Prot.	χ	3	CoMSIA	26	-	PCA	86	R	(Naumann and Matter, 2002)

^a Structural Indices: Drugs Total or Group Electronegativity (χ), Protein Total or Region Electrostatic Potential (ξ), Similarity (S), Gibbs Free energy (ΔG), Physicochemicals properties (PP), Composition (C), Transition (T), Distribution (D), Kernel parameter (σ), Protein sequence, Ligand-Structure And Binding-Pocket (PLB), Molecular Operating Environment (MOE), Surflex-Dock parameters (SD); ^b Dimension of the structures parameters: 1D-structure, 2D-Structure and 3D structure; ^c Types of drug targets: prot. (all types of proteins), MR (Membrane Receptor protein), Enz. (Enzymes). ^d Method: MARCH-INSIDE (MI), Bipartite Local Model (BLM), Drug-Target Likeness (DTL), pKa values for protein ligand complexes (PROPKA), comparative interaction fingerprint analysis (CoIFA), Negative Training Data (NTD), Ligand-Based drug design (LBDD), Quantum Mechanics (QM), Molecular Mechanics + Generalized Born Surface Area theory (GBSA). ^e N- Number of cases used to seek the model.

^f Nv- Number of variables in the model. ^g Statistical method used to seek the model: LDA-Linear Discriminant Analysis, SVM-Support Vector Machine, Kernel Regression-Based Method (KRM), Multi Layer Perceptron (MLP), Stepwise Multiple Linear Regression (SMLR), Genetic Function Approximation (GFA), k-Nearest Neighbors (kNN), Predictive Index (PI), Partial-Least-Square (PLS), Least-Square + Support-Vector Machine (LSVM), Radial-Basis Function + Support-Vector Machine (RSVM), Principal Component Analysis (PCA). ^h Accuracy (Ac). ⁱ Parameter used in the accuracy. * This work.

Table 3. Cytotoxic activities IC_{50} (μ M) of oxoisoaporphine derivatives **1-8** upon several cell lines

Compounds	J774	HL-60	HeLa	Mel-43	WI-38
1	15.3	14.2	12.2	8.1	21.4
2	24.4	19.4	18.5	2.7	20.7
3	14.7	12.5	9.3	4.7	19.6
4	37.7	17.4	21.0	26.7	13.4
5	64.3	31.6	33.7	35.3	10.1
6	46.6	9.9	16.7	26.3	4.5
7	45.0	158.1	196.5	120.6	71.1
8	38.8	15.0	16.0	16.4	16.0

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Table 4. Antiplasmodial activities of **1 – 8**.

Compounds	^a IC₅₀ (μM)
1	105.03 ± 9.34 ^b
2	51.78 ± 5.37
3	82.35 ± 12.66
4	59.38 ± 2.45
5	10.62 ± 2.77
6	44.96 ± 7.65
7	93.13 ± 11.69
8	1.45 ± 0.56
CQ ^c	0.097

^a *In vitro* activity on *Plasmodium falciparum* FcB1 (4).

^b Mean ± S.D.

^c CQ, chloroquine; positive control for *Plasmodium falciparum* inhibition.

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Table 5. Results of the QSPR model

Parameter	%	class	low	high
Training series				
Sensitivity	73.7	low	87	31
Specificity	76.7	high	20	66
Accuracy	75.0			
Validation series				
Sensitivity	75.0	low	24	8
Specificity	83.3	high	6	30
Accuracy	79.4			

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Table 6. Non-interaction c-level values for 8 compounds vs. selected proteins of *P. falciparum*

pdb	New compounds							
	1	2	3	4	5	6	7	8
1QNG	0.77	0.95	0.83	0.36	0.58	0.74	0.80	0.63
1LDG	0.89	1.00	1.00	0.97	0.99	0.99	0.99	0.98
3EWC	0.86	0.94	0.81	0.18	0.50	0.74	0.74	0.58
2AAW	0.89	0.96	0.84	0.27	0.51	0.69	0.73	1.00
1NHG	0.90	0.95	0.88	0.33	0.59	0.76	0.79	1.00
3LT2	0.87	1.00	0.88	1.00	1.00	1.00	0.79	0.47
2PSS	0.99	0.93	0.87	0.26	0.49	0.28	0.33	0.60
3F4B	0.83	0.95	0.88	0.35	1.00	0.72	0.76	0.55
3KR5	0.88	0.92	0.77	0.35	0.50	0.76	0.78	0.62
1CET	0.90	0.96	0.88	0.97	0.99	0.99	0.99	0.99
1YVB	1.00	1.00	0.84	0.29	0.44	0.58	0.72	0.62
3GGJ	0.87	0.94	0.88	0.36	0.51	0.69	0.73	0.56
3LSY	0.87	1.00	0.88	0.35	0.60	0.74	0.78	0.64
1ZXL	0.90	1.00	0.85	1.00	0.60	1.00	1.00	1.00
2ANL	0.90	0.91	0.99	0.26	0.57	0.68	0.71	0.21
1CJB	0.51	0.95	0.81	0.35	0.59	0.76	1.00	0.60
3KQX	0.88	0.93	0.86	0.22	0.39	0.76	0.72	0.65
1RSZ	0.89	0.95	0.89	0.36	0.58	0.99	0.99	0.99
1T2C	1.00	1.00	1.00	0.94	0.50	0.71	0.68	0.46

Table 7. Comparative cytotoxicity table for aporphines compounds.

Organism	Compound	2e	3e	6e	8e
Parasite	IC ₅₀	51.78	82.35	44.96	1.45
	PDB Parasite	2Z8W	2Z8W	2PSS	2ANL
	Protein	AMA1	AMA 1	Spermidine synth	Plasmepsin IV
	NL-MB Score	0.220574	0.270574	0.056099	0.205199
BLAST	Score	49.7	49.7	273	180
Human	Mel-43	2.7	4.7	26.3	16.4
	WI-38	20.7	19.6	4.5	16
	PDB Human	2CD0	2CD0	2O05	3D91
	Protein	λ -6 Ig	λ -6 Ig	Spermidine synth	Renin
	NL-MB Score	0.000024	0.000002	0.001336	0.000317

AMA1= Apical membrane antigen 1; λ -6 Ig = lambda-VI immunoglobuline; NL-MB = Non Linear Mind Best; Mel-43 and WI-38 are cancer cell lines.

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Table 8. Top-20 template proteins in *G. lamblia* found by MASCOT search

Protein	Accession	Mass	Score	Function
1	gi159116163	99431	421	Hypothetical protein GL50803_16507
2	gi121999104	89668	82	DNA topoisomerase III
3	gi83593171	46301	73	O-acetylserine sulfhydrylase
4	gi152970457	32953	72	putative transcriptional regulator (LysR family)
5	gi148256476	22222	67	hypothetical protein BBta
6	gi160878692	47367	65	GTP-binding proten HflX
7	gi19697420	11743	63	hypothetical protein Oryza sativa
8	gi66044158	46312	63	outer membrane porin syringae B728a]
9	gi168003694	13992	62	predicted protein
10	gi168017259	13848	62	predicted protein
11	gi116749322	109448	61	hypothetical protein Sfum_1889
12	gi1002271	11977	61	envelope glycoprotein, v3 region
13	gi116330615	19688	60	Transcriptional regulator
14	gi168048940	14081	60	predicted protein
15	gi116328728	19687	59	Transcriptional regulator
16	gi151221220	10082	59	hypothetical protein NWMN_1008
17	gi167931120	71384	59	hypothetical protein EcolS_26140
18	gi149200841	99260	59	DNA topoisomerase I
19	gi38569925	31855	59	TPR-repeat protein
20	gi78048009	44141	59	filamentous phage Cflc related protein

Table 9. MASCOT, MM/MD, and QSAR results for new peptides

Input		MS			
Pept.	sequence	Obs.	Mr(expt)	Mr(calc)	δ
P1	kataweyhealakt	965.5	964.5	964.5	0.0032
P2	kdahslyvkpsffghfrl	2309.2	2308.2	2308.2	-0.0094
P3	kkppapyehlatdteaslslire	2566.4	2565.4	2565.3	0.0073
P4	kkppapyehlatdteaslslireky	1389.7	1388.7	1388.7	-0.0004
P5	ksshgrlnsllsgdfyars	1908.0	1906.9	1906.9	-0.002
P6	ktgsvftldlptsvry	1480.8	1479.8	1479.8	0.0047
P7	kvfglpeqgdenlvftlvdgrs	1260.6	1259.6	1259.6	0.0033
P8	kwadkyvystks	1879.9	1878.9	1878.9	-0.0288
P9	ratypissarg	1355.7	1354.7	1354.7	0.0014
P10	rfafhqlfswdikthdwks	2533.4	2532.3	2532.3	0.0268
P11	rfsiysdtifnseddavra	2205.1	2204.1	2204.1	-0.005
P12	rlnsllsgdfyars	1978.9	1977.9	1977.9	0.0031
P13	rslkvfglpeqgdenlvftlvdgrs	2206.1	2205.1	2205.1	0.0297
Input		MM/MD			M/B ^a
Pept.	sequence	ACCR	E ₁	E ₀	Pred.
P1	kataweyhealakt	0.71	174.34	43.87	0
P2	kdahslyvkpsffghfrl	0.68	68.49	37.59	0
P3	kkppapyehlatdteaslslire	0.67	-19.13	42.33	0
P4	kkppapyehlatdteaslslireky	0.68	22.64	45.71	0
P5	ksshgrlnsllsgdfyars	0.66	109.75	31.45	0
P6	ktgsvftldlptsvry	0.66	185.31	23.77	0
P7	kvfglpeqgdenlvftlvdgrs	0.67	208.98	37.57	0
P8	kwadkyvystks	0.66	-0.14	20.73	0
P9	ratypissarg	0.66	137.30	20.74	0
P10	rfafhqlfswdikthdwks	0.66	111.81	38.79	0
P11	rfsiysdtifnseddavra	0.67	172.69	40.05	0
P12	rlnsllsgdfyars	0.66	217.09	27.09	0
P13	rslkvfglpeqgdenlvftlvdgrs	0.67	212.44	47.92	0

^aM/B is the MASCOT and BLAST prediction of peptides; M/B = 1 if MASCOT and/or BLAST find high similarity between the peptide and one protein that is known receptor for one of the nine ligands studied, M/B = 0 otherwise.

Table 10. Some examples of drug-protein interaction.

DB	Drug name	PDB	Protein	OC	PC	Score
DB00619	Imatinib	1OPL	ABL1	1	1	0
DB00132	Alpha-Linolenic Acid	1FE3	FABP	1	1	0.15
DB00162	Vitamin A	1BI9	Aldehyde hydrogenase	1	1	0.08
DB00162	Vitamin A	1CRB	Retinol binding protein	1	1	0.18
DB00178	Ramipril	1UZF	Metalloprotease	1	1	0.15
DB00178	Ramipril	1UZF	Metalloprotease	1	1	0.15
DB00210	Adapalene	1EXX	Gamma receptor	1	1	0.05
DB00227	Lovastatin	1HWL	Oxidoreductase	1	1	0.53
DB00270	Isradipine	1VYT	Transport protein	1	1	0.02
DB00273	Topiramate	1T9N	Lyase	1	1	0.13
DB00290	Bleomycin	1UW0	DNA ligase III	1	1	0
DB00294	Etonogestrel	1SQN	Progesterone receptor	1	1	0.29
DB00304	Desogestrel	1SQN	Progesterone receptor	1	1	0.38
DB00308	Ibutilide	1VYT	Transport protein	1	1	0.12
DB00342	Terfenadine	1BYW	Membrane protein	1	1	0.34
DB00351	Megestrol	1R5K	DNA binding protein	1	1	0.21
DB00367	Levonorgestrel	1SQN	Progesterone receptor	1	1	0.4
DB00370	Mirtazapine	1HOF	Membrane protein	1	1	0.02
DB00449	Dipivefrin	1HOF	Membrane protein	1	1	0.26
DB00506	Norgestrel	1SQN	Progesterone receptor	1	1	0.4
DB00519	Trandolapril	1UZF	Metalloprotease	1	1	0.3
DB00519	Trandolapril	1UZF	Metalloprotease	1	1	0.3
DB00548	Azelaic Acid	1KFD	Nucleotidyltransferase	1	1	0
DB00603	Medroxyprogesteron	1R5K	DNA binding protein	1	1	0.4
DB00616	Candoxatril	1DMT	Endopeptidase	1	1	0.59
DB00622	Nicardipine	1VYT	Transport protein	1	1	0.07
DB00711	Diethylcarbamazine	1OCZ	Oxidoreductase	1	1	0.1
DB00717	Norethindrone	1F5F	Binding globulin	1	1	0.32
DB00772	Malathion	1QON	Acetylcholinesterase	1	1	0.11
DB00790	Perindopril	1UZF	Metalloprotease	1	1	0.42
DB00799	Tazarotene	1EXX	Gamma receptor	1	1	0.05
DB00799	Tazarotene	1UHL	DNA binding protein	1	1	0.03
DB00806	Pentoxifylline	1T9R	Hydrolase	1	1	0.04
DB00822	Disulfiram	1OF7	Dehydrogenase	1	1	0.09
DB00823	Ethinodiol Diacetate	1R5K	DNA binding protein	1	1	0.06
DB00865	Benzphetamine	1AMO	Oxidoreductase	1	1	0
DB00926	Etretinate	1XDK	Retinol binding protein	1	1	0.05
DB00957	Norgestimate	1R5K	DNA binding protein	1	1	0.24
DB00989	Rivastigmine	1F8U	Acetylcholinesterase	1	1	0.06
DB01029	Irbesartan	1JNM	Proto-oncogene	1	1	0.03

Proto-oncogene tyrosine-protein kinase (ABL1); Fatty acid-binding protein (FABD).

TABLE SM1. Drug codes in Drug-Bank, names, PDB ID of proteins targets and ANN model results.

ANALYSIS					
DB	Drug name	PDB	OC	PC	PRO
DB01395	Drospirenone	1R5K	1	0	0.75
DB00001	Lepirudin	1HAG	1	0	0.97
DB00351	Megestrol	1SQN	1	0	0.68
DB01078	Deslanoside	1MO8	1	0	0.98
DB00137	Xanthophyll	1HA2	1	0	0.88
DB01396	Digitoxin	1HA2	1	0	0.97
DB00163	Vitamin E	1OLM	1	0	0.99
DB00163	Vitamin E	1NRL	1	0	0.97
DB00621	Oxandrolone	1E3G	1	0	0.80
DB01222	Budesonide	1NHZ	1	0	0.68
DB00396	Progesterone	1SQN	1	0	0.91
DB00169	Cholecalciferol	1KXP	1	0	0.80
DB00802	Alfentanil	1HA2	1	0	0.77
DB00492	Fosinopril	1UZF	1	0	0.97
DB00615	Rifabutin	1BDF	1	0	0.93
DB00926	Etretinate	2CBR	1	1	0.50
DB01089	Deserpidine	1UZF	1	0	0.87
DB00390	Digoxin	1MO8	1	0	0.98
DB00926	Etretinate	1EXX	1	1	0.48
DB00115	Cyanocobalamin	1UJW	1	0	0.79
DB00976	Telithromycin	1TQN	1	0	0.99
DB00511	Acetyldigitoxin	1MO8	1	0	0.99
DB00984	Nandrolone	1E3G	1	0	0.91
DB00188	Bortezomib	1IRU	1	0	0.98
DB00361	Vinorelbine	1SA1	1	0	0.98
DB00541	Vincristine	1SA1	1	0	0.97
DB00570	Vinblastine	1JNM	1	0	0.97
DB00661	Verapamil	1VYT	1	0	0.95
DB00661	Verapamil	1BYW	1	0	0.97
DB00188	Bortezomib	1IRU	1	0	0.98
DB00641	Simvastatin	1HWL	1	0	0.68
DB00862	Vardenafil	1T9R	1	1	0.63
DB00641	Simvastatin	1REW	1	0	0.90
DB06692	Aprotinin	1KI0	1	0	0.97
DB06692	Aprotinin	1TRN	1	0	0.96
DB00641	Simvastatin	1TQN	1	0	0.91
DB00603	Medroxyprogesterone	1SQN	1	0	0.82
DB00762	Irinotecan	1A36	1	1	0.64
DB00641	Simvastatin	1MQ8	1	0	0.68
DB06267	Udenafil	1T9R	1	0	0.69
DB00641	Simvastatin	2IL6	1	0	0.94

DB00641	Simvastatin	1ILQ	1	0	0.97
DB00641	Simvastatin	1K7L	1	1	0.65
DB01055	Mimosine	1DON	1	0	0.96
DB00378	Dydrogesterone	1SQN	1	0	0.75
DB01083	Orlistat	1XKT	1	0	0.99
DB00995	Auranofin	1OC3	1	0	0.94
DB00995	Auranofin	1HA2	1	0	0.95
DB00641	Simvastatin	1C5G	1	0	0.92
DB00769	Hydrocortamate	1NHZ	1	0	0.95
DB00834	Mifepristone	1NHZ	1	0	0.80
DB00626	Bacitracin	1BV8	1	0	0.97
DB00302	Tranexamic Acid	1BDA	1	0	0.81
DB00615	Rifabutin	1UYL	1	0	0.97
DB00641	Simvastatin	1I4L	1	0	0.91
DB00641	Simvastatin	1DON	1	0	0.98
DB00641	Simvastatin	1X86	1	0	0.93
DB00864	Tacrolimus	1Q6U	1	0	0.99
DB00641	Simvastatin	1A8M	1	0	0.94
DB00273	Topiramate	1BYY	1	1	0.66
DB00768	Olopatadine	1K2H	1	0	0.92
DB00954	Dirithromycin	1EMI	1	0	0.99
DB01244	Bepidil	1MO8	1	1	0.64
DB01564	Calusterone	1E3G	1	0	0.79
DB00091	Cyclosporine	1CWM	1	0	0.99
DB00858	Dromostanolone	1F5F	1	0	0.99
DB00775	Tirofiban	1TYE	1	0	0.79
DB00877	Sirolimus	1J4I	1	0	0.99
DB00858	Dromostanolone	1E3G	1	0	0.98
DB00115	Cyanocobalamin	1N2Z	1	0	0.92
DB00858	Dromostanolone	1R5K	1	0	0.93
DB01180	Rescinnamine	1UZF	1	0	0.93
DB01045	Rifampin	1NRL	1	1	0.65
DB00707	Porfimer	1N7D	1	0	0.69
DB01601	Lopinavir	1RV7	1	1	0.60
DB00503	Ritonavir	1ODW	1	1	0.61
DB00823	Ethinodiol Diacetate	1SQN	1	1	0.42
DB00624	Testosterone	1E3G	1	1	0.48
DB00926	Etretinate	1LBD	1	1	0.42
DB00843	Donepezil	1F8U	1	1	0.46
DB00162	Vitamin A	1EII	1	1	0.25
DB00624	Testosterone	1HA2	1	1	0.36
DB00772	Malathion	1QON	1	1	0.11
DB00822	Disulfiram	1OF7	1	1	0.09
DB01072	Atazanavir	1ODW	1	1	0.52

DB00616	Candoxatril	1DMT	1	1	0.59
DB00506	Norgestrel	1SQN	1	1	0.40
DB01406	Danazol	1F5F	1	1	0.38
DB00370	Mirtazapine	1HOF	1	1	0.02
DB00367	Levonorgestrel	1SQN	1	1	0.40
DB00162	Vitamin A	1BI9	1	1	0.08
DB00132	Alpha-Linolenic Acid	1FE3	1	1	0.15
DB00227	Lovastatin	1HWL	1	1	0.53
DB00162	Vitamin A	1CRB	1	1	0.18
DB00799	Tazarotene	1EXX	1	1	0.05
DB00711	Diethylcarbamazine	1OCZ	1	1	0.10
DB00799	Tazarotene	1UHL	1	1	0.03
DB00989	Rivastigmine	1F8U	1	1	0.06
DB00806	Pentoxifylline	1T9R	1	1	0.04
DB00823	Ethynodiol Diacetate	1R5K	1	1	0.06
DB01173	Orphenadrine	1PB7	1	1	0.02
DB00790	Perindopril	1UZF	1	1	0.42
DB00603	Medroxyprogesterone	1R5K	1	1	0.40
DB00717	Norethindrone	1F5F	1	1	0.32
DB00294	Etonogestrel	1SQN	1	1	0.29
DB01394	Colchicine	1SA1	1	1	0.03
DB00449	Dipivefrin	1HOF	1	1	0.26
DB00351	Megestrol	1R5K	1	1	0.21
DB00342	Terfenadine	1BYW	1	1	0.34
DB00210	Adapalene	1EXX	1	1	0.05
DB00290	Bleomycin	1UW0	1	1	0.00
DB00178	Ramipril	1UZF	1	1	0.15
DB00273	Topiramate	1T9N	1	1	0.13
DB00865	Benzphetamine	1AMO	1	1	0.00
DB00308	Ibutilide	1VYT	1	1	0.12
DB00622	Nicardipine	1VYT	1	1	0.07
DB00519	Trandolapril	1UZF	1	1	0.30
DB00519	Trandolapril	1UZF	1	1	0.30
DB00178	Ramipril	1UZF	1	1	0.15
DB00548	Azelaic Acid	1KFD	1	1	0.00
DB00926	Etretinate	1XDK	1	1	0.05
DB00957	Norgestimate	1R5K	1	1	0.24
DB00304	Desogestrel	1SQN	1	1	0.38
DB01029	Irbesartan	1JNM	1	1	0.03
DB00270	Isradipine	1VYT	1	1	0.02
DB01586	Ursodeoxycholic acid	1IHI	1	1	0.54
DB00691	Moexipril	1UZF	1	1	0.14
DB00410	Mupirocin	1QU2	1	1	0.39
DB00210	Adapalene	1EXX	1	1	0.05

DB00523	Alitretinoin	3CBS	1	1	0.05
DB00523	Alitretinoin	2CBR	1	1	0.05
DB00696	Ergotamine	1HOF	1	1	0.15
DB00830	Phenmetrazine	1O5W	1	1	0.01
DB00210	Adapalene	1UHL	1	1	0.02
DB01348	Spirapril	1UZF	1	1	0.10
DB00820	Tadalafil	1T9R	1	1	0.00
DB04967	Lucanthone	1HD7	1	1	0.01
DB01011	Metyrapone	1TQN	1	1	0.00
DB00675	Tamoxifen	1R5K	1	1	0.00
DB00799	Tazarotene	1XDK	1	1	0.00
DB00935	Oxymetazoline	1HOF	1	1	0.02
DB01109	Heparin	1G1S	1	1	0.01
DB00655	Estrone	1F5F	1	1	0.02
DB00906	Tiagabine	1OHY	1	1	0.01
DB00307	Bexarotene	1UHL	1	1	0.01
DB00159	Icosapent	1FE3	1	1	0.04
DB00159	Icosapent	1I7I	1	1	0.01
DB00908	Quinidine	1BYW	1	1	0.02
DB00506	Norgestrel	1R5K	1	1	0.06
DB00572	Atropine	1F8U	1	1	0.01
DB00655	Estrone	1HA2	1	1	0.01
DB01406	Danazol	1R5K	1	1	0.04
DB00755	Tretinoin	1BI9	1	1	0.02
DB00755	Tretinoin	1EXX	1	1	0.04
DB00294	Etonogestrel	1R5K	1	1	0.04
DB00313	Valproic Acid	1OHY	1	1	0.00
DB00459	Acitretin	1EXX	1	1	0.01
DB00459	Acitretin	1LBD	1	1	0.01
DB00459	Acitretin	1HA2	1	1	0.01
DB00162	Vitamin A	1BXS	1	1	0.01
DB00727	Nitroglycerin	1OF7	1	1	0.00
DB00367	Levonorgestrel	1R5K	1	1	0.06
DB00545	Pyridostigmine	1F8U	1	1	0.00
DB00523	Alitretinoin	1UHL	1	1	0.02
DB00523	Alitretinoin	1EXX	1	1	0.04
DB00523	Alitretinoin	1EXX	1	1	0.04
DB00848	Levamisole	1EW2	1	1	0.00
DB01392	Yohimbine	1HOF	1	1	0.06
DB00304	Desogestrel	1R5K	1	1	0.06
DB01392	Yohimbine	1HOF	1	1	0.06
DB00674	Galantamine	1ODC	1	1	0.01
DB00635	Prednisone	1NHZ	1	1	0.06
DB01032	Probenecid	1HA2	1	1	0.00

DB01182	Propafenone	1BYW	1	1	0.01
DB00691	Moexipril	1R4L	1	1	0.02
DB00881	Quinapril	1UZF	1	1	0.01
DB00881	Quinapril	1UZF	1	1	0.01
DB00212	Remikiren	1BBS	1	1	0.26
DB00286	Conjugated Estrogens	1R5K	1	1	0.00
DB00412	Rosiglitazone	1I7I	1	1	0.00
DB00959	Methylprednisolone	1NHZ	1	1	0.09
DB00936	Salicylic acid	1HA2	1	1	0.00
DB01037	Selegiline	2BK3	1	1	0.00
DB00692	Phentolamine	1HOF	1	1	0.00
DB00170	Menadione	1SG0	1	1	0.00
DB01241	Gemfibrozil	1K7L	1	1	0.00
DB00122	Choline	1F8U	1	1	0.00
DB04967	Lucanthone	1A36	1	1	0.00
DB00675	Tamoxifen	1VJ5	1	1	0.00
DB01109	Heparin	1JVQ	1	1	0.00
DB01109	Heparin	1RFN	1	1	0.00
DB01109	Heparin	1HAG	1	1	0.00
DB01092	Ouabain	1MO8	1	1	0.15
DB01606	Tazobactam	1Q2P	1	1	0.00
DB00741	Hydrocortisone	1NHZ	1	1	0.11
DB00201	Caffeine	1TB5	1	1	0.00
DB01194	Brinzolamide	1T9N	1	1	0.00
DB01194	Brinzolamide	1CZM	1	1	0.00
DB00290	Bleomycin	1X9N	1	1	0.00
DB04794	Bifonazole	1PO5	1	1	0.00
DB01041	Thalidomide	1SVC	1	1	0.00
DB00281	Lidocaine	1IVO	1	1	0.00
DB01050	Ibuprofen	1HA2	1	1	0.00
DB00277	Theophylline	1T9R	1	1	0.00
DB00775	Tirofiban	1M1X	1	1	0.04
DB00273	Topiramate	1ZNC	1	1	0.01
DB00542	Benazepril	1UZF	1	1	0.01
DB00374	Treprostinil	1Y0S	1	1	0.04
DB00755	Tretinoin	1BXS	1	1	0.00
DB00197	Troglitazone	1I7I	1	1	0.01
DB01010	Edrophonium	1F8U	1	1	0.00
DB00197	Troglitazone	1C5G	1	1	0.02
DB01169	Arsenic trioxide	1JNM	1	1	0.00
DB00584	Enalapril	1UZF	1	1	0.02
DB00459	Acitretin	1XDK	1	1	0.00
DB00488	Altretamine	1BNA	1	1	0.00
DB00184	Nicotine	1I9B	1	1	0.00

DB01225	Enoxaparin	1JVQ	1	1	0.00
DB01225	Enoxaparin	1P0S	1	1	0.00
DB00783	Estradiol	1F5F	1	1	0.01
DB01006	Letrozole	1S78	1	1	0.00
DB00530	Erlotinib	1IVO	1	1	0.00
DB00122	Choline	1P0Q	1	1	0.00
DB00783	Estradiol	1QKM	1	1	0.01
DB00783	Estradiol	1R5K	1	1	0.00
DB00751	Epinastine	1HOF	1	1	0.00
DB00824	Enprofylline	1TB5	1	1	0.00
DB04573	Estriol	1EA1	1	1	0.00
DB04573	Estriol	1R5K	1	1	0.00
DB00651	Dyphylline	1TB5	1	1	0.00
DB00204	Dofetilide	1BYW	1	1	0.00
DB01096	Oxamniquine	1BNA	1	1	0.00
DB00780	Phenelzine	1O5W	1	1	0.00
DB00946	Phenprocoumon	1HA2	1	1	0.00
DB00191	Phentermine	2BK3	1	1	0.00
DB00397	Phenylpropanolamine	1HOF	1	1	0.00
DB00255	Diethylstilbestrol	1KED	1	1	0.00
DB01031	Ethinamate	1CZM	1	1	0.00
DB00977	Ethinyl Estradiol	1R5K	1	1	0.00
DB00977	Ethinyl Estradiol	1NRL	1	1	0.00
DB00255	Diethylstilbestrol	1VJB	1	1	0.00
DB00252	Phenytoin	1BYY	1	1	0.00
DB01411	Pranlukast	1HUL	1	1	0.00
DB01411	Pranlukast	1SVC	1	1	0.00
DB00175	Pravastatin	1HWL	1	1	0.01
DB00175	Pravastatin	1I4L	1	1	0.08
DB00852	Pseudoephedrine	1HOF	1	1	0.00
DB00147	Pyridoxal	1RFV	1	1	0.00
DB00819	Acetazolamide	1T9N	1	1	0.00
DB00093	Felypressin	1YTV	1	1	0.00
DB00705	Delavirdine	1VRU	1	1	0.00
DB00819	Acetazolamide	1CZM	1	1	0.00
DB01183	Naloxone	1R5K	1	1	0.00
DB00779	Nalidixic Acid	1BNA	1	1	0.00
DB04840	Debrisoquin	1HOF	1	1	0.00
DB00157	NADH	1FYC	1	1	0.00
DB04840	Debrisoquin	1HOF	1	1	0.00
DB00819	Acetazolamide	1H6I	1	1	0.00
DB00119	Pyruvic acid	1NI4	1	1	0.00
DB01264	Darunavir	1ODW	1	1	0.05
DB01219	Dantrolene	1HA2	1	1	0.00

DB00481	Raloxifene	1R5K	1	1	0.00
DB00916	Metronidazole	1C4C	1	1	0.00
DB00817	Rosoxacin	1EI1	1	1	0.00
DB00992	Methyl aminolevulinate	1N7D	1	1	0.00
DB00553	Methoxsalen	1BNA	1	1	0.00
DB00760	Meropenem	1K6R	1	1	0.01
DB01213	Fomepizole	1HSO	1	1	0.00
DB01213	Fomepizole	1HT0	1	1	0.00
DB01213	Fomepizole	1F4J	1	1	0.00
DB00170	Menadione	1AUT	1	1	0.00
DB01319	Fosamprenavir	1ODW	1	1	0.01
DB00828	Fosfomycin	1UAE	1	1	0.00
DB01232	Saquinavir	1ODW	1	1	0.29
DB01232	Saquinavir	1A8M	1	1	0.24
DB00170	Menadione	1KBQ	1	1	0.00
DB00614	Furazolidone	1BNA	1	1	0.00
DB00170	Menadione	1P0S	1	1	0.00
DB00766	Clavulanate	3BLM	1	1	0.00
DB00170	Menadione	1RFN	1	1	0.00
DB01065	Melatonin	1J3S	1	1	0.00
DB00827	Cinoxacin	1BNA	1	1	0.00
DB01065	Melatonin	1CP3	1	1	0.00
DB00489	Sotalol	1BYW	1	1	0.00
DB01120	Gliclazide	1TZI	1	1	0.00
DB00649	Stavudine	1VRU	1	1	0.00
DB00870	Suprofen	1HA2	1	1	0.00
DB00382	Tacrine	1F8U	1	1	0.00
DB00643	Mebendazole	1SA1	1	1	0.00
DB00643	Mebendazole	1SA1	1	1	0.00
DB00786	Marimastat	1L6J	1	1	0.00
DB00786	Marimastat	1GXD	1	1	0.00
DB01170	Guanethidine	1HOF	1	1	0.00
DB01170	Guanethidine	1HOF	1	1	0.00
DB01034	Cerulenin	1HNK	1	1	0.00
DB01034	Cerulenin	1G5X	1	1	0.00
DB01329	Cefoperazone	1HA2	1	1	0.00
DB01328	Cefonicid	1HA2	1	1	0.00
DB00172	L-Proline	1TJC	1	1	0.00
DB00172	L-Proline	1MZW	1	1	0.00
DB01327	Cefazolin	1HA2	1	1	0.00
DB00456	Cefalotin	1HA2	1	1	0.00
DB00456	Cefalotin	1XGJ	1	1	0.00
DB00172	L-Proline	1CWM	1	1	0.00
DB01136	Carvedilol	1R5S	1	1	0.00

DB01197	Captopril	1HA2	1	1	0.00
DB01197	Captopril	1UZF	1	1	0.00
DB00284	Acarbose	1B2Y	1	1	0.00
DB00722	Lisinopril	1UZF	1	1	0.00
DB00142	L-Glutamic Acid	1YAE	1	1	0.00
DB00142	L-Glutamic Acid	1YAE	1	1	0.00
DB00142	L-Glutamic Acid	1XHY	1	1	0.00
DB00277	Theophylline	1TB5	1	1	0.00
DB01030	Topotecan	1A36	1	1	0.00
DB00752	Tranylcypromine	1O5W	1	1	0.00
DB00993	Azathioprine	1BZY	1	1	0.00
DB01088	Iloprost	1BDA	1	0	0.77
DB00142	L-Glutamic Acid	1WVJ	1	1	0.00
DB00224	Indinavir	1MU2	1	1	0.07
DB00659	Acamprosate	1ISS	1	1	0.00
DB00791	Uracil mustard	1BNA	1	1	0.00
DB00945	Aspirin	1Y38	1	1	0.00
DB01247	Isocarboxazid	1O5W	1	1	0.00
DB01247	Isocarboxazid	2BK3	1	1	0.00
DB00142	L-Glutamic Acid	1L1F	1	1	0.00
DB00142	L-Glutamic Acid	1L1F	1	1	0.00
DB00142	L-Glutamic Acid	1PB7	1	1	0.00
DB00142	L-Glutamic Acid	1L9X	1	1	0.00
DB00142	L-Glutamic Acid	1OHY	1	1	0.00
DB01169	Arsenic trioxide	2IL6	1	1	0.00
DB00276	Amsacrine	1BYW	1	1	0.00
DB00067	Vasopressin	1YTV	1	1	0.00
DB01009	Ketoprofen	1ILQ	1	1	0.00
DB00182	Amphetamine	1HOF	1	1	0.00
DB00233	Aminosalicylic Acid	1Y38	1	1	0.00
DB00513	Aminocaproic Acid	1KI0	1	1	0.00
DB00437	Allopurinol	1V97	1	1	0.00
DB00518	Albendazole	1SA1	1	1	0.00
DB00495	Zidovudine	1VRU	1	1	0.00
DB00128	L-Aspartic Acid	1C0B	1	1	0.00
DB00128	L-Aspartic Acid	1RTU	1	1	0.00
DB00909	Zonisamide	1CZM	1	1	0.00
DB01259	Lapatinib	1S78	1	1	0.00
DB00125	L-Arginine	1PQ3	1	1	0.00
DB00128	L-Aspartic Acid	1Q7L	1	1	0.00
DB01097	Leflunomide	1D3H	1	1	0.00
DB00151	L-Cysteine	1AJS	1	1	0.00
DB00155	L-Citrulline	1FVO	1	1	0.00
DB00155	L-Citrulline	1TLL	1	1	0.00

DB00128	L-Aspartic Acid	1AJS	1	1	0.00
DB00640	Adenosine	1A8M	1	1	0.00
DB00555	Lamotrigine	1BYY	1	1	0.00
DB00709	Lamivudine	1VRU	1	1	0.00
DB00160	L-Alanine	1H0C	1	1	0.00
DB00160	L-Alanine	1OHY	1	1	0.00
DB01172	Kanamycin	1P87	1	1	0.01
DB01064	Isoproterenol	1PBW	1	1	0.00
DB00451	Levothyroxine	1NAV	1	1	0.00
DB00451	Levothyroxine	1Y0X	1	1	0.00
DB00142	L-Glutamic Acid	1AJS	1	1	0.00
DB00951	Isoniazid	1OHY	1	1	0.00
DB00677	Isoflurophate	1P0Q	1	1	0.00
DB00753	Isoflurane	1EXB	1	1	0.00
DB00753	Isoflurane	1WVJ	1	1	0.00
DB01598	Imipenem	3BLM	1	1	0.00
DB00710	Ibandronate	1YV5	1	1	0.00
DB01611	Hydroxychloroquine	1BNA	1	1	0.00
DB00774	Hydroflumethiazide	1MO8	1	1	0.00
DB00142	L-Glutamic Acid	1ISS	1	1	0.00
DB00130	L-Glutamine	1FIE	1	1	0.00
DB00774	Hydroflumethiazide	1T9N	1	1	0.00
DB00601	Linezolid	1EMI	1	1	0.00
DB00279	Liothyronine	1NAV	1	1	0.00
DB00279	Liothyronine	1Y0X	1	1	0.00
DB00279	Liothyronine	1KED	1	1	0.00
DB00774	Hydroflumethiazide	1CZM	1	1	0.00
DB00167	L-Isoleucine	1KTA	1	1	0.00
DB00149	L-Leucine	1KTA	1	1	0.00
DB00134	L-Methionine	1B6A	1	1	0.00
DB04948	Lofexidine	1HOF	1	1	0.00
DB04948	Lofexidine	1HOF	1	1	0.00
DB01206	Lomustine	1BNA	1	1	0.00
DB00999	Hydrochlorothiazide	1T9N	1	1	0.00
DB00999	Hydrochlorothiazide	1CZM	1	1	0.00
DB00129	L-Ornithine	1PQ3	1	1	0.00
DB00129	L-Ornithine	1OAT	1	1	0.00
DB00129	L-Ornithine	1FVO	1	1	0.00
DB01275	Hydralazine	1PU4	1	1	0.00
DB00941	Hexafluronium bromide	1P0Q	1	1	0.00
DB00172	L-Proline	2RMC	1	1	0.00
DB01159	Halothane	1LN6	1	1	0.00
DB01159	Halothane	1GP2	1	1	0.00
DB00133	L-Serine	1JBQ	1	1	0.00

DB00133	L-Serine	1H0C	1	1	0.00
DB00150	L-Tryptophan	1MB2	1	1	0.00
DB00135	L-Tyrosine	1Q11	1	1	0.00
DB01159	Halothane	1U4E	1	1	0.00
DB01159	Halothane	1E79	1	1	0.00
DB00256	Lymecycline	1P87	1	1	0.16
DB00256	Lymecycline	2TRT	1	1	0.00
DB01018	Guanfacine	1HOF	1	1	0.00
DB00742	Mannitol	1BNA	1	1	0.00
DB00226	Guanadrel Sulfate	1HOF	1	1	0.00
DB00226	Guanadrel Sulfate	1HOF	1	1	0.00
DB00629	Guanabenz	1HOF	1	1	0.00
DB00145	Glycine	1BJ4	1	1	0.00
DB00145	Glycine	1T3E	1	1	0.00
DB00145	Glycine	3JDW	1	1	0.00
DB01016	Glibenclamide	1XMI	1	1	0.00
DB00406	Gentian Violet	1BNA	1	1	0.00
DB00798	Gentamicin	1EMI	1	1	0.01
DB00317	Gefitinib	1IVO	1	1	0.00
DB01042	Melphalan	1BNA	1	1	0.00
DB01044	Gatifloxacin	1HA2	1	1	0.00
DB00743	Gadobenate Dimeglumine	1HA2	1	1	0.00
DB00947	Fulvestrant	1R5K	1	1	0.00
DB00452	Framycetin	1EMI	1	1	0.00
DB00158	Folic Acid	1L9X	1	1	0.00
DB01033	Mercaptopurine	1BZY	1	1	0.00
DB00588	Fluticasone Propionate	1NHZ	1	1	0.00
DB00563	Methotrexate	1HA2	1	1	0.00
DB00588	Fluticasone Propionate	1CJY	1	1	0.00
DB01028	Methoxyflurane	1HKO	1	1	0.00
DB01028	Methoxyflurane	1WVJ	1	1	0.00
DB00232	Methyclothiazide	1CZM	1	1	0.00
DB00232	Methyclothiazide	1T9N	1	1	0.00
DB00232	Methyclothiazide	1MO8	1	1	0.00
DB00968	Methyldopa	1HOF	1	1	0.00
DB00712	Flurbiprofen	1HA2	1	1	0.00
DB00846	Flurandrenolide	1CJY	1	1	0.00
DB01185	Fluoxymesterone	1BP3	1	1	0.00
DB01185	Fluoxymesterone	1R5K	1	1	0.00
DB01388	Mibefradil	1VYT	1	1	0.00
DB00544	Fluorouracil	1T0U	1	1	0.00
DB01055	Mimosine	1BJ4	1	1	0.00
DB00544	Fluorouracil	1GTE	1	1	0.00
DB01017	Minocycline	1P87	1	1	0.53

DB01017	Minocycline	1IBC	1	1	0.00
DB01017	Minocycline	1J3S	1	1	0.00
DB01017	Minocycline	9ILB	1	1	0.00
DB01017	Minocycline	1TZI	1	1	0.00
DB00648	Mitotane	1L6V	1	1	0.00
DB00648	Mitotane	1F5F	1	1	0.00
DB01047	Fluocinonide	1CJY	1	1	0.00
DB00180	Flunisolide	1NHZ	1	1	0.00
DB00764	Mometasone	1NHZ	1	1	0.00
DB00663	Flumethasone Pivalate	1NHZ	1	1	0.00
DB00157	NADH	1HSO	1	1	0.00
DB00157	NADH	1HSZ	1	1	0.00
DB00157	NADH	1MC5	1	1	0.00
DB00157	NADH	1D1S	1	1	0.00
DB00157	NADH	1MRQ	1	1	0.00
DB00157	NADH	1IHI	1	1	0.00
DB00157	NADH	1T40	1	1	0.00
DB00157	NADH	1DIA	1	1	0.00
DB01073	Fludarabine	1YVL	1	1	0.00
DB00157	NADH	1QYX	1	1	0.00
DB00157	NADH	1L1F	1	1	0.00
DB00157	NADH	1L1F	1	1	0.00
DB00157	NADH	1J0X	1	1	0.00
DB00157	NADH	1T5P	1	1	0.00
DB00157	NADH	1I10	1	1	0.00
DB00157	NADH	1I0Z	1	1	0.00
DB00157	NADH	1MLD	1	1	0.00
DB00157	NADH	1PT9	1	1	0.00
DB00157	NADH	1S3A	1	1	0.00
DB00157	NADH	1UMK	1	1	0.00
DB00157	NADH	1NI4	1	1	0.00
DB00157	NADH	1NI4	1	1	0.00
DB00157	NADH	1BI9	1	1	0.00
DB00157	NADH	1SG0	1	1	0.00
DB00800	Fenoldopam	1HOF	1	1	0.00
DB00800	Fenoldopam	1HOF	1	1	0.00
DB01039	Fenofibrate	1K7L	1	1	0.00
DB01280	Nelarabine	1BNA	1	1	0.00
DB00903	Ethacrynic acid	1MO8	1	1	0.00
DB00994	Neomycin	1EMI	1	1	0.00
DB00994	Neomycin	1P87	1	1	0.01
DB00903	Ethacrynic acid	1HA2	1	1	0.00
DB00955	Netilmicin	1EMI	1	1	0.00
DB00955	Netilmicin	1P87	1	1	0.04

DB01196	Estramustine	1R5K	1	1	0.00
DB00336	Nitrofurazone	1GET	1	1	0.00
DB00228	Enflurane	1WVJ	1	1	0.00
DB00368	Norepinephrine	1HOF	1	1	0.00
DB00368	Norepinephrine	1HOF	1	1	0.00
DB00228	Enflurane	1E79	1	1	0.00
DB00879	Emtricitabine	1VRU	1	1	0.00
DB01057	Echothiophate Iodide	1P0Q	1	1	0.00
DB06262	Droxidopa	1HOF	1	1	0.00
DB06262	Droxidopa	1HOF	1	1	0.00
DB00254	Doxycycline	1EMI	1	1	0.00
DB00997	Doxorubicin	1BNA	1	1	0.00
DB01093	Dimethyl sulfoxide	1IIH	1	1	0.00
DB01093	Dimethyl sulfoxide	1EYD	1	1	0.00
DB01093	Dimethyl sulfoxide	1R6K	1	1	0.00
DB00595	Oxytetracycline	1EMI	1	1	0.00
DB00282	Pamidronate	1YV5	1	1	0.00
DB00213	Pantoprazole	1MO8	1	1	0.00
DB01093	Dimethyl sulfoxide	2BIU	1	1	0.00
DB01421	Paromomycin	1EMI	1	1	0.00
DB00487	Pefloxacin	1CB6	1	1	0.00
DB00738	Pentamidine	1BNA	1	1	0.00
DB00738	Pentamidine	1QVU	1	1	0.00
DB01093	Dimethyl sulfoxide	1QZ2	1	1	0.00
DB01093	Dimethyl sulfoxide	1BNA	1	1	0.00
DB01093	Dimethyl sulfoxide	1BP3	1	1	0.00
DB00780	Phenelzine	2BK3	1	1	0.00
DB01093	Dimethyl sulfoxide	1JZ2	1	1	0.00
DB01093	Dimethyl sulfoxide	1KTO	1	1	0.00
DB01093	Dimethyl sulfoxide	1P1R	1	1	0.00
DB00861	Diflunisal	1KED	1	1	0.00
DB00890	Dienestrol	1R5K	1	1	0.00
DB00337	Pimecrolimus	1J4I	1	1	0.16
DB01100	Pimozide	1BYW	1	1	0.00
DB00236	Pipobroman	1BNA	1	1	0.00
DB00266	Dicumarol	1YB5	1	1	0.00
DB00266	Dicumarol	1KBQ	1	1	0.00
DB01144	Dichlorphenamide	1CZM	1	1	0.00
DB01119	Diazoxide	1MO8	1	1	0.00
DB01119	Diazoxide	1T9N	1	1	0.00
DB01119	Diazoxide	1CZM	1	1	0.00
DB01234	Dexamethasone	1VMC	1	1	0.00
DB01234	Dexamethasone	1SVC	1	1	0.00
DB01366	Procaterol	9ILB	1	1	0.00

DB01366	Procaterol	1A8M	1	1	0.00
DB01123	Proflavine	1HAG	1	1	0.00
DB00837	Progabide	1SS2	1	1	0.00
DB01189	Desflurane	1EXB	1	1	0.00
DB01189	Desflurane	1E79	1	1	0.00
DB00339	Pyrazinamide	1KPH	1	1	0.00
DB00618	Demeclocycline	1EMI	1	1	0.00
DB00944	Demecarium bromide	1P0Q	1	1	0.00
DB00114	Pyridoxal Phosphate	1AJS	1	1	0.00
DB00114	Pyridoxal Phosphate	1KTA	1	1	0.00
DB00819	Acetazolamide	1RJ6	1	1	0.00
DB01262	Decitabine	1BNA	1	1	0.00
DB00694	Daunorubicin	1BNA	1	1	0.00
DB00114	Pyridoxal Phosphate	1P5J	1	1	0.00
DB00114	Pyridoxal Phosphate	1OAT	1	1	0.00
DB00114	Pyridoxal Phosphate	1BJ4	1	1	0.00
DB00114	Pyridoxal Phosphate	1H0C	1	1	0.00
DB00165	Pyridoxine	1RFV	1	1	0.00
DB00165	Pyridoxine	1HA2	1	1	0.00
DB01254	Dasatinib	1OPL	1	1	0.00
DB01103	Quinacrine	1CJY	1	1	0.00
DB00987	Cytarabine	1HA2	1	1	0.00
DB00987	Cytarabine	8ICK	1	1	0.00
DB01325	Quinethazone	1CZM	1	1	0.00
DB01325	Quinethazone	1T9N	1	1	0.00
DB00606	Cyclothiazide	1WVJ	1	1	0.00
DB00606	Cyclothiazide	1ZNC	1	1	0.00
DB00606	Cyclothiazide	1CZM	1	1	0.00
DB00148	Creatine	1QK1	1	1	0.00
DB00148	Creatine	1CRK	1	1	0.00
DB02709	Resveratrol	1KED	1	1	0.00
DB00811	Ribavirin	1BNA	1	1	0.00
DB00140	Riboflavin	1Q9S	1	1	0.00
DB00148	Creatine	1G0W	1	1	0.00
DB01147	Cloxacillin	1HA2	1	1	0.00
DB00758	Clopidogrel	1G1S	1	1	0.00
DB00758	Clopidogrel	1TQN	1	1	0.00
DB01068	Clonazepam	1HA2	1	1	0.00
DB00453	Clomocycline	1P87	1	1	0.16
DB00118	S-Adenosylmethionine	1JBQ	1	1	0.00
DB00118	S-Adenosylmethionine	1R74	1	1	0.00
DB00173	Adenine	1OD4	1	1	0.00
DB00173	Adenine	1ORE	1	1	0.00
DB00173	Adenine	1D6A	1	1	0.00

DB00173	Adenine	1J1S	1	1	0.00
DB01104	Sertraline	1TQN	1	1	0.00
DB01236	Sevoflurane	1E79	1	1	0.00
DB01236	Sevoflurane	1WVJ	1	1	0.00
DB01236	Sevoflurane	1EXB	1	1	0.00
DB00173	Adenine	1HQC	1	1	0.00
DB00173	Adenine	1D1P	1	1	0.00
DB00173	Adenine	1YXM	1	1	0.00
DB00173	Adenine	1QD2	1	1	0.00
DB00173	Adenine	2AAI	1	1	0.00
DB00173	Adenine	1SD2	1	1	0.00
DB00882	Clomifene	1R5K	1	1	0.00
DB00636	Clofibrate	1K7L	1	1	0.00
DB00720	Clodronate	1A5Y	1	1	0.00
DB00720	Clodronate	1OKC	1	1	0.00
DB00720	Clodronate	1OKC	1	1	0.00
DB00515	Cisplatin	1BNA	1	1	0.00
DB00604	Cisapride	1BYW	1	1	0.00
DB01261	Sitagliptin	2BGR	1	1	0.00
DB00537	Ciprofloxacin	1OYE	1	1	0.00
DB00398	Sorafenib	1UWJ	1	1	0.00
DB01597	Cilastatin	1ITU	1	1	0.00
DB00269	Chlorotrianisene	1R5K	1	1	0.00
DB00880	Chlorothiazide	1ZNC	1	1	0.00
DB01082	Streptomycin	1P87	1	1	0.01
DB00428	Streptozocin	1BNA	1	1	0.00
DB00576	Sulfamethizole	1HA2	1	1	0.00
DB00605	Sulindac	1GXD	1	1	0.00
DB00605	Sulindac	4Q21	1	1	0.00
DB00605	Sulindac	1Y0S	1	1	0.00
DB00880	Chlorothiazide	1CZM	1	1	0.00
DB00608	Chloroquine	1A8M	1	1	0.00
DB00446	Chloramphenicol	1UT1	1	1	0.00
DB00291	Chlorambucil	1BNA	1	1	0.00
DB00482	Celecoxib	2BIY	1	1	0.00
DB01331	Cefoxitin	1YMX	1	1	0.00
DB01136	Carvedilol	1TZI	1	1	0.00
DB00262	Carmustine	1BWC	1	1	0.00
DB00958	Carboplatin	1HA2	1	1	0.00
DB00958	Carboplatin	1BNA	1	1	0.00
DB01101	Capecitabine	1GTE	1	1	0.00
DB00887	Bumetanide	1XMI	1	1	0.00
DB00300	Tenofovir	1VRU	1	1	0.00
DB00484	Brimonidine	1HOF	1	1	0.00

DB00484	Brimonidine	1HOF	1	1	0.00
DB00759	Tetracycline	1EMI	1	1	0.00
DB00759	Tetracycline	1P87	1	1	0.32
DB00116	Tetrahydrofolic acid	1S3I	1	1	0.00
DB00116	Tetrahydrofolic acid	1P4R	1	1	0.00
DB00116	Tetrahydrofolic acid	1BJ4	1	1	0.00
DB01128	Bicalutamide	2IL6	1	1	0.00
DB01128	Bicalutamide	1E3G	1	1	0.00
DB01393	Bezafibrate	1K7L	1	1	0.00
DB00352	Thioguanine	1BZY	1	1	0.00
DB01393	Bezafibrate	1HWL	1	1	0.00
DB00560	Tigecycline	1P87	1	1	0.21
DB01133	Tiludronate	1A5Y	1	1	0.00
DB00217	Bethanidine	1HOF	1	1	0.00
DB00217	Bethanidine	1HOF	1	1	0.00
DB00697	Tizanidine	1HOF	1	1	0.00
DB00684	Tobramycin	1EMI	1	1	0.00
DB00562	Benzthiazide	1ZNC	1	1	0.00
DB00562	Benzthiazide	1CZM	1	1	0.00
DB00522	Bentiromide	1N8S	1	1	0.00
DB00436	Bendroflumethiazide	1ZNC	1	1	0.00
DB00436	Bendroflumethiazide	1CZM	1	1	0.00
DB00181	Baclofen	1SS2	1	1	0.00
DB00656	Trazodone	1HOF	1	1	0.00
DB01117	Atovaquone	1D3H	1	1	0.00
DB01076	Atorvastatin	1A8M	1	1	0.00
DB01076	Atorvastatin	1X86	1	1	0.00
DB01076	Atorvastatin	1C5G	1	1	0.00
DB01076	Atorvastatin	1I7I	1	1	0.00
DB00384	Triamterene	1I5H	1	1	0.00
DB01021	Trichlormethiazide	1CZM	1	1	0.00
DB01021	Trichlormethiazide	1ZNC	1	1	0.00
DB01021	Trichlormethiazide	1MO8	1	1	0.00
DB01076	Atorvastatin	1TQN	1	1	0.00
DB01076	Atorvastatin	1LJ7	1	1	0.00
DB01076	Atorvastatin	1HWL	1	1	0.00
DB00637	Astemizole	1TQN	1	1	0.00
DB00964	Apraclonidine	1HOF	1	1	0.00
DB01427	Amrinone	1A8M	1	1	0.00
DB01427	Amrinone	1TB5	1	1	0.00
DB00381	Amlodipine	1CZM	1	1	0.00
DB01118	Amiodarone	1BYW	1	1	0.00
DB00594	Amiloride	1VJA	1	1	0.00
DB01080	Vigabatrin	1OHY	1	1	0.00

DB00594	Amiloride	1I5H	1	1	0.00
DB00479	Amikacin	1P87	1	1	0.01
DB01143	Amifostine	1EW2	1	1	0.00
DB00288	Amcinonide	1NHZ	1	1	0.00
DB00630	Alendronate	1YV5	1	1	0.00
DB00171	Adenosine triphosphate	1OPL	1	1	0.00
DB00126	Vitamin C	1BNA	1	1	0.00
DB00126	Vitamin C	1OJO	1	1	0.00
DB00126	Vitamin C	1TJC	1	1	0.00
DB00126	Vitamin C	1MNZ	1	1	0.00
DB00171	Adenosine triphosphate	1Z6T	1	1	0.00
DB00171	Adenosine triphosphate	1OKC	1	1	0.00
DB00131	Adenosine monophosphate	1KPF	1	1	0.00
DB00131	Adenosine monophosphate	1FTA	1	1	0.00
DB00131	Adenosine monophosphate	1PTW	1	1	0.00
DB00131	Adenosine monophosphate	1TB5	1	1	0.00
DB00943	Zalcitabine	1VRU	1	1	0.00
DB00744	Zileuton	1ILQ	1	1	0.00
DB00131	Adenosine monophosphate	1W0H	1	1	0.00
DB00151	L-Cysteine	1JBQ	1	1	0.00
DB01048	Abacavir	1VRU	1	1	0.00
DB00641	Simvastatin	2BIY	0	0	0.94
DB00173	Adenine	1H2W	0	0	1.00
DB00173	Adenine	1IRU	0	0	0.97
DB00858	Dromostanolone	1HA2	0	0	0.98
DB00173	Adenine	1DON	0	0	0.95
DB00133	L-Serine	1P87	0	0	0.92
DB01097	Leflunomide	1P87	0	0	1.00
DB01213	Fomepizole	1BDA	0	0	0.79
DB00151	L-Cysteine	1DON	0	0	0.95
DB00858	Dromostanolone	1GGL	0	0	0.98
DB01045	Rifampin	1J3S	0	0	0.81
DB00131	Adenosine monophosphate	1DON	0	0	0.94
DB00858	Dromostanolone	1EII	0	0	0.99
DB00909	Zonisamide	1IRU	0	0	0.98
DB00909	Zonisamide	1IRU	0	0	0.98
DB00828	Fosfomycin	1P87	0	0	0.99
DB00151	L-Cysteine	1P87	0	0	0.94
DB00616	Candoxatril	1L6J	0	0	0.81
DB00115	Cyanocobalamin	1N2Z	0	0	0.92
DB00858	Dromostanolone	1EXX	0	0	0.99
DB00171	Adenosine triphosphate	1IRU	0	0	0.97
DB00171	Adenosine triphosphate	1IRU	0	0	0.97
DB00492	Fosinopril	1P87	0	0	0.99

DB00492	Fosinopril	1HWL	0	0	0.92
DB00492	Fosinopril	1KG3	0	0	0.98
DB00518	Albendazole	1P87	0	0	0.99
DB00492	Fosinopril	1I9B	0	0	0.92
DB00492	Fosinopril	1MF1	0	0	0.98
DB00492	Fosinopril	1OKC	0	0	0.98
DB00492	Fosinopril	1OKC	0	0	0.98
DB00858	Dromostanolone	1EXX	0	0	0.99
DB00492	Fosinopril	1L6V	0	0	0.98
DB00492	Fosinopril	1HSZ	0	0	0.91
DB00858	Dromostanolone	1BBS	0	0	0.88
DB00492	Fosinopril	1OF7	0	0	0.98
DB00492	Fosinopril	1HOF	0	0	0.99
DB00492	Fosinopril	1HOF	0	0	0.99
DB00492	Fosinopril	2BK3	0	0	0.92
DB00492	Fosinopril	1Q7L	0	0	0.98
DB00492	Fosinopril	1UZF	0	0	0.97
DB00492	Fosinopril	1UZF	0	0	0.97
DB00492	Fosinopril	1AJS	0	0	0.92
DB00492	Fosinopril	1LT8	0	0	0.92
DB00492	Fosinopril	1KTA	0	0	0.92
DB00492	Fosinopril	1DIA	0	0	0.98
DB00492	Fosinopril	1T9N	0	0	0.98
DB00492	Fosinopril	1ZNC	0	0	0.88
DB00492	Fosinopril	1CP3	0	0	0.98
DB00492	Fosinopril	1RFN	0	0	0.88
DB00492	Fosinopril	1P0S	0	0	0.88
DB00492	Fosinopril	1TQN	0	0	0.97
DB00492	Fosinopril	1BNA	0	0	0.88
DB00492	Fosinopril	1X9N	0	0	0.92
DB00492	Fosinopril	1A36	0	0	0.92
DB00492	Fosinopril	1R5K	0	0	0.92
DB00492	Fosinopril	1YV5	0	0	0.98
DB00492	Fosinopril	1VRU	0	0	0.92
DB00492	Fosinopril	1NHZ	0	0	0.98
DB00492	Fosinopril	1GET	0	0	0.91
DB00492	Fosinopril	1J0X	0	0	0.97
DB00492	Fosinopril	1T5P	0	0	0.97
DB00909	Zonisamide	1P87	0	0	0.99
DB00492	Fosinopril	1BZY	0	0	0.92
DB00762	Irinotecan	1GTE	0	0	0.90
DB00492	Fosinopril	1M1X	0	0	0.92
DB00492	Fosinopril	1QU2	0	0	0.92
DB00492	Fosinopril	1N7D	0	0	0.92

DB00492	Fosinopril	1B6A	0	0	0.99
DB00492	Fosinopril	1DMT	0	0	0.92
DB00492	Fosinopril	1OC3	0	0	0.96
DB00492	Fosinopril	1I7I	0	0	0.97
DB00492	Fosinopril	1JYD	0	0	0.98
DB00115	Cyanocobalamin	1YTV	0	0	0.85
DB00492	Fosinopril	1BYW	0	0	0.98
DB00492	Fosinopril	1TJC	0	0	0.98
DB00492	Fosinopril	1HAG	0	0	0.88
DB00492	Fosinopril	1G1S	0	0	0.97
DB00492	Fosinopril	1XDK	0	0	0.91
DB00492	Fosinopril	1LBD	0	0	0.97
DB00492	Fosinopril	1UHL	0	0	0.97
DB00492	Fosinopril	1RTU	0	0	0.99
DB00492	Fosinopril	1BJ4	0	0	0.98
DB00492	Fosinopril	1HA2	0	0	0.97
DB00492	Fosinopril	1F5F	0	0	0.98
DB00492	Fosinopril	1Y4E	0	0	0.99
DB00492	Fosinopril	1MO8	0	0	0.98
DB00492	Fosinopril	1WAP	0	0	0.99
DB00492	Fosinopril	1X86	0	0	0.98
DB00492	Fosinopril	1SA1	0	0	0.97
DB00518	Albendazole	1IRU	0	0	0.98
DB00492	Fosinopril	1A8M	0	0	0.98
DB00858	Dromostanolone	1S78	0	0	0.97
DB00780	Phenelzine	1IRU	0	0	0.97
DB00780	Phenelzine	1IRU	0	0	0.97
DB00115	Cyanocobalamin	1A8M	0	0	0.95
DB00858	Dromostanolone	1MO8	0	0	0.98
DB00858	Dromostanolone	1G1S	0	0	0.98
DB00858	Dromostanolone	1OPL	0	0	0.92
DB00858	Dromostanolone	1WD8	0	0	0.99
DB00858	Dromostanolone	1H2W	0	0	1.00
DB00115	Cyanocobalamin	1SA1	0	0	0.93
DB00858	Dromostanolone	1SQN	0	0	0.98
DB00858	Dromostanolone	1BYW	0	0	0.99
DB00630	Alendronate	1H2W	0	0	1.00
DB00802	Alfentanil	1EMI	0	0	0.96
DB00802	Alfentanil	1P87	0	0	1.00
DB00802	Alfentanil	1F8U	0	0	0.79
DB00744	Zileuton	1IRU	0	0	0.97
DB00641	Simvastatin	1GXD	0	0	0.93
DB00641	Simvastatin	1KG3	0	0	0.92
DB00802	Alfentanil	1HOF	0	0	0.93

DB00802	Alfentanil	1UZF	0	0	0.79
DB00802	Alfentanil	1H6I	0	0	0.88
DB00802	Alfentanil	1P4R	0	0	0.98
DB00641	Simvastatin	1F8U	0	0	0.91
DB00802	Alfentanil	1T9N	0	0	0.82
DB01006	Letrozole	1K2H	0	1	0.33
DB00802	Alfentanil	2CBR	0	0	0.87
DB00802	Alfentanil	1P0Q	0	0	0.77
DB00802	Alfentanil	1TQN	0	0	0.80
DB00802	Alfentanil	1BP3	0	0	0.80
DB00802	Alfentanil	1MQB	0	1	0.64
DB00641	Simvastatin	1OD4	0	0	0.95
DB00802	Alfentanil	1QKM	0	0	0.83
DB00802	Alfentanil	1YV5	0	0	0.88
DB00802	Alfentanil	1WVJ	0	0	0.85
DB00802	Alfentanil	1ILQ	0	0	0.94
DB00802	Alfentanil	1B6A	0	0	0.90
DB00802	Alfentanil	1EH6	0	0	0.87
DB00802	Alfentanil	1I7I	0	0	0.75
DB00802	Alfentanil	1BYW	0	0	0.89
DB00858	Dromostanolone	1PBW	0	0	0.98
DB00858	Dromostanolone	1I7I	0	0	0.98
DB00802	Alfentanil	1G1S	0	0	0.74
DB00802	Alfentanil	1R6K	0	0	0.79
DB00616	Candoxatril	2IL6	0	0	0.91
DB00802	Alfentanil	1SG0	0	0	0.80
DB00744	Zileuton	1P87	0	0	0.98
DB00744	Zileuton	1P87	0	0	0.98
DB00802	Alfentanil	1HA2	0	0	0.77
DB00858	Dromostanolone	1K7L	0	0	0.92
DB00858	Dromostanolone	1B2Y	0	0	0.98
DB00858	Dromostanolone	1FVO	0	0	0.98
DB00858	Dromostanolone	1OAT	0	0	0.92
DB00858	Dromostanolone	1TLL	0	0	0.98
DB00858	Dromostanolone	1AMO	0	0	0.99
DB00858	Dromostanolone	1QR6	0	0	0.98
DB00858	Dromostanolone	1PT9	0	0	0.98
DB00858	Dromostanolone	1Y6R	0	0	0.98
DB00858	Dromostanolone	1EH6	0	0	0.99
DB00495	Zidovudine	1IRU	0	0	0.98
DB00858	Dromostanolone	1ISS	0	0	0.93
DB00858	Dromostanolone	1L6J	0	0	0.98
DB00115	Cyanocobalamin	1JNM	0	0	0.91
DB00115	Cyanocobalamin	1WAP	0	0	0.97

DB00858	Dromostanolone	1D1P	0	0	0.98
DB00583	L-Carnitine	1P87	0	0	1.00
DB00452	Framycetin	1IRU	0	0	0.68
DB00115	Cyanocobalamin	1BYY	0	0	0.98
DB01089	Deserpidine	1A5Y	0	0	0.90
DB00947	Fulvestrant	1IRU	0	0	1.00
DB00115	Cyanocobalamin	1G91	0	0	0.93
DB00614	Furazolidone	1P87	0	0	1.00
DB00858	Dromostanolone	1QU2	0	0	0.93
DB01089	Deserpidine	1SA1	0	0	0.88
DB01089	Deserpidine	1KGI	0	0	0.89
DB00115	Cyanocobalamin	1HA2	0	0	0.90
DB00128	L-Aspartic Acid	1DON	0	0	0.97
DB00858	Dromostanolone	1BZY	0	0	0.93
DB00115	Cyanocobalamin	1H0C	0	0	0.92
DB00858	Dromostanolone	1OJO	0	0	0.94
DB00858	Dromostanolone	1ODW	0	0	0.99
DB00115	Cyanocobalamin	1SG0	0	0	0.94
DB00091	Cyclosporine	1HNK	0	0	1.00
DB00115	Cyanocobalamin	1QD2	0	0	0.95
DB00858	Dromostanolone	1UYL	0	0	0.98
DB00802	Alfentanil	1DON	0	0	0.98
DB00802	Alfentanil	1BYY	0	0	0.97
DB00802	Alfentanil	1KED	0	0	0.81
DB00558	Zanamivir	1DON	0	0	0.94
DB00802	Alfentanil	1VYT	0	0	0.82
DB01258	Aliskiren	1EMI	0	0	0.92
DB00616	Candoxatril	1WVJ	0	0	0.89
DB01189	Desflurane	1P87	0	0	1.00
DB00307	Bexarotene	1DON	0	0	0.98
DB00128	L-Aspartic Acid	1IRU	0	0	0.98
DB01258	Aliskiren	1HOF	0	0	0.80
DB01258	Aliskiren	1HOF	0	0	0.80
DB01258	Aliskiren	1O5W	0	0	0.96
DB00304	Desogestrel	1C0B	0	0	0.74
DB00304	Desogestrel	1IRU	0	0	0.98
DB00926	Etretinate	1JBQ	0	1	0.55
DB00616	Candoxatril	1HE5	0	0	0.90
DB01258	Aliskiren	2CBR	0	0	0.76
DB00616	Candoxatril	1QKM	0	0	0.87
DB00115	Cyanocobalamin	1EXX	0	0	0.95
DB00115	Cyanocobalamin	1EXX	0	0	0.95
DB00858	Dromostanolone	3JDW	0	0	0.98
DB00115	Cyanocobalamin	1G1S	0	0	0.91

DB00616	Candoxatril	1TLL	0	0	0.81
DB01258	Aliskiren	1YV5	0	0	0.77
DB01034	Cerulenin	1K2H	0	1	0.56
DB00304	Desogestrel	1BYW	0	1	0.55
DB00396	Progesterone	1T5P	0	0	0.90
DB00304	Desogestrel	1DON	0	0	0.98
DB01258	Aliskiren	1ODW	0	0	0.77
DB00396	Progesterone	1ODW	0	0	0.94
DB00115	Cyanocobalamin	1HAG	0	0	0.81
DB00304	Desogestrel	1BYY	0	0	0.87
DB01089	Deserpidine	1JNM	0	0	0.84
DB00616	Candoxatril	1GTE	0	0	0.86
DB00170	Menadione	1DON	0	0	0.98
DB01258	Aliskiren	1BYW	0	0	0.78
DB00115	Cyanocobalamin	1SQN	0	0	0.95
DB00170	Menadione	1H2W	0	0	1.00
DB00616	Candoxatril	1F4J	0	0	0.87
DB00616	Candoxatril	1T9N	0	0	0.87
DB01258	Aliskiren	1EYD	0	0	0.75
DB01219	Dantrolene	1DON	0	0	0.97
DB01083	Orlistat	1HOF	0	0	0.99
DB00128	L-Aspartic Acid	1IRU	0	0	0.98
DB00858	Dromostanolone	1AGS	0	0	0.98
DB00115	Cyanocobalamin	1I7I	0	0	0.93
DB00641	Simvastatin	1ORE	0	0	0.95
DB00641	Simvastatin	1MF1	0	0	0.93
DB01089	Deserpidine	1Y0X	0	0	0.92
DB00523	Alitretinoin	1P87	0	0	1.00
DB00091	Cyclosporine	1F8U	0	0	0.99
DB00091	Cyclosporine	1OF7	0	0	1.00
DB01089	Deserpidine	1MO8	0	0	0.91
DB01045	Rifampin	1NHZ	0	0	0.89
DB00858	Dromostanolone	1YAE	0	0	0.99
DB00091	Cyclosporine	1HOF	0	0	0.99
DB00858	Dromostanolone	1XHY	0	0	0.99
DB01089	Deserpidine	1F5F	0	0	0.92
DB01089	Deserpidine	1BJ4	0	0	0.89
DB01078	Deslanoside	1ORE	0	0	0.98
DB00091	Cyclosporine	1OIZ	0	0	0.99
DB00858	Dromostanolone	1WVJ	0	0	0.98
DB00655	Estrone	1K2H	0	0	0.98
DB01078	Deslanoside	1D1S	0	0	0.96
DB00858	Dromostanolone	1L1F	0	0	0.98
DB00935	Oxymetazoline	1P87	0	0	0.99

DB00935	Oxymetazoline	1P87	0	0	0.99
DB00641	Simvastatin	1OKC	0	0	0.93
DB00091	Cyclosporine	1E3G	0	0	0.99
DB00641	Simvastatin	1OKC	0	0	0.93
DB00858	Dromostanolone	1R5S	0	0	0.98
DB00091	Cyclosporine	1UZF	0	0	0.99
DB00943	Zalcitabine	1P87	0	0	0.97
DB00943	Zalcitabine	1P87	0	0	0.97
DB00091	Cyclosporine	1Q2P	0	0	0.99
DB00091	Cyclosporine	1CZM	0	0	0.99
DB00858	Dromostanolone	1SS2	0	0	0.98
DB00858	Dromostanolone	1HE5	0	0	0.99
DB00858	Dromostanolone	1J4I	0	0	0.99
DB00858	Dromostanolone	1XKT	0	0	0.98
DB00858	Dromostanolone	1YV5	0	0	0.99
DB00858	Dromostanolone	1R5K	0	0	0.93
DB00858	Dromostanolone	1IVO	0	0	0.92
DB00858	Dromostanolone	1HD7	0	0	0.99
DB01392	Yohimbine	1DON	0	0	0.98
DB00858	Dromostanolone	1A36	0	0	0.93
DB00858	Dromostanolone	1VMC	0	0	0.99
DB00858	Dromostanolone	1BNA	0	0	0.88
DB00858	Dromostanolone	1ITU	0	0	0.93
DB00858	Dromostanolone	1D3H	0	0	0.98
DB00858	Dromostanolone	1PWG	0	0	0.93
DB00858	Dromostanolone	1TQN	0	0	0.98
DB00091	Cyclosporine	1P0Q	0	0	0.99
DB00858	Dromostanolone	1TQN	0	0	0.98
DB00858	Dromostanolone	1KPH	0	0	0.92
DB00091	Cyclosporine	1JBQ	0	0	1.00
DB00091	Cyclosporine	1CJY	0	0	0.99
DB00858	Dromostanolone	1G0W	0	0	0.98
DB00858	Dromostanolone	1P0S	0	0	0.88
DB00858	Dromostanolone	1Z6J	0	0	0.88
DB00091	Cyclosporine	1FYC	0	0	0.99
DB00858	Dromostanolone	1P0Q	0	0	0.98
DB00858	Dromostanolone	1PEH	0	0	0.95
DB00614	Furazolidone	1IRU	0	0	0.98
DB00091	Cyclosporine	1KFD	0	0	0.99
DB00858	Dromostanolone	1JNM	0	0	0.97
DB00858	Dromostanolone	1UTQ	0	0	0.88
DB00858	Dromostanolone	1S5O	0	0	0.98
DB00091	Cyclosporine	1HD7	0	0	0.99
DB00858	Dromostanolone	1T9N	0	0	0.98

DB00858	Dromostanolone	1CZM	0	0	0.98
DB00858	Dromostanolone	1KED	0	0	0.98
DB00858	Dromostanolone	1UWJ	0	0	0.98
DB00858	Dromostanolone	1K6R	0	0	0.99
DB00858	Dromostanolone	1W6F	0	0	0.92
DB00858	Dromostanolone	1PQ3	0	0	0.98
DB00091	Cyclosporine	1YV5	0	0	1.00
DB00858	Dromostanolone	1UZF	0	0	0.98
DB00858	Dromostanolone	1UZF	0	0	0.98
DB00858	Dromostanolone	1I5H	0	0	0.99
DB00858	Dromostanolone	1HOF	0	0	0.99
DB00091	Cyclosporine	1Q6U	0	0	0.99
DB00858	Dromostanolone	1HOF	0	0	0.99
DB00858	Dromostanolone	1EW2	0	0	0.98
DB00170	Menadione	1P87	0	0	1.00
DB00858	Dromostanolone	1XF0	0	0	0.99
DB00858	Dromostanolone	1IHI	0	0	0.93
DB00743	Gadobenate Dimeglumine	1H2W	0	0	1.00
DB00858	Dromostanolone	1HSO	0	0	0.92
DB00858	Dromostanolone	1ODC	0	0	0.98
DB00858	Dromostanolone	1OHY	0	0	0.98
DB00858	Dromostanolone	1HWL	0	0	0.93
DB01045	Rifampin	1Z8L	0	0	0.87
DB00858	Dromostanolone	1P87	0	0	1.00
DB00858	Dromostanolone	1EMI	0	0	0.99
DB00091	Cyclosporine	1VRU	0	0	0.99
DB01078	Deslanoside	1MRQ	0	0	0.99
DB00091	Cyclosporine	1NHZ	0	0	0.99
DB00091	Cyclosporine	1L1F	0	0	0.99
DB01078	Deslanoside	1HOF	0	0	0.98
DB00254	Doxycycline	1DON	0	0	0.97
DB00091	Cyclosporine	1WVJ	0	0	0.99
DB00858	Dromostanolone	1SA1	0	0	0.98
DB00091	Cyclosporine	1ODW	0	0	1.00
DB00858	Dromostanolone	1A5Y	0	0	0.98
DB00091	Cyclosporine	1QVU	0	0	0.99
DB00674	Galantamine	1P87	0	0	1.00
DB01392	Yohimbine	1P87	0	0	0.99
DB00370	Mirtazapine	1P87	0	0	1.00
DB00616	Candoxatril	1SVC	0	0	0.78
DB00137	Xanthophyll	1T0U	0	0	0.91
DB00137	Xanthophyll	1A8M	0	0	0.94
DB00137	Xanthophyll	2TRT	0	0	0.91
DB00137	Xanthophyll	1P49	0	0	0.92

DB00137	Xanthophyll	1HA2	0	0	0.88
DB00137	Xanthophyll	1BI9	0	0	0.89
DB00137	Xanthophyll	1OPL	0	0	0.70
DB00137	Xanthophyll	1SQN	0	0	0.92
DB00137	Xanthophyll	1ZBQ	0	0	0.92
DB00137	Xanthophyll	2RMC	0	0	0.72
DB00137	Xanthophyll	1ILQ	0	0	0.97
DB00137	Xanthophyll	2IL6	0	0	0.94
DB00137	Xanthophyll	1WVJ	0	0	0.93
DB00137	Xanthophyll	1NHZ	0	0	0.93
DB00137	Xanthophyll	1QKM	0	0	0.92
DB00137	Xanthophyll	1R5K	0	0	0.73
DB00137	Xanthophyll	1KFD	0	0	0.92
DB00137	Xanthophyll	8ICK	0	0	0.93
DB01123	Proflavine	1P87	0	0	0.96
DB00137	Xanthophyll	1FYC	0	0	0.91
DB00137	Xanthophyll	1CJY	0	1	0.65
DB00137	Xanthophyll	1JBQ	0	0	0.95
DB00137	Xanthophyll	1LJ7	0	0	0.95
DB04967	Lucanthone	1DON	0	0	0.98
DB00137	Xanthophyll	1P0Q	0	0	0.90
DB00137	Xanthophyll	1T9R	0	0	0.91
DB00137	Xanthophyll	1TB5	0	0	0.70
DB00137	Xanthophyll	1Q2P	0	0	0.93
DB00137	Xanthophyll	1E3G	0	0	0.93
DB00137	Xanthophyll	2BK3	0	0	0.72
DB00137	Xanthophyll	1HOF	0	0	0.96
DB00137	Xanthophyll	1OF7	0	0	0.95
DB00137	Xanthophyll	1F8U	0	0	0.91
DB00137	Xanthophyll	1OHY	0	0	0.91
DB00137	Xanthophyll	1W0H	0	0	0.95
DB00523	Alitretinoin	1O5W	0	1	0.55
DB00641	Simvastatin	1HSO	0	1	0.66
DB00946	Phenprocoumon	1P87	0	0	1.00
DB00946	Phenprocoumon	1P87	0	0	1.00
DB01225	Enoxaparin	1DON	0	0	0.98
DB01045	Rifampin	1L1F	0	0	0.80
DB00091	Cyclosporine	1ILQ	0	0	1.00
DB01045	Rifampin	1HIG	0	0	0.86
DB00091	Cyclosporine	1MLD	0	0	0.99
DB00696	Ergotamine	1P87	0	0	0.97
DB00091	Cyclosporine	2RMC	0	0	0.99
DB00091	Cyclosporine	1C4C	0	0	0.99
DB00616	Candoxatril	1RGY	0	0	0.87

DB00091	Cyclosporine	1BYW	0	0	0.99
DB00291	Chlorambucil	1P87	0	0	0.99
DB00608	Chloroquine	1P87	0	0	0.99
DB00608	Chloroquine	1P87	0	0	0.99
DB00608	Chloroquine	1IRU	0	0	0.99
DB00616	Candoxatril	1E79	0	0	0.85
DB00608	Chloroquine	1DON	0	0	0.99
DB00091	Cyclosporine	1SQN	0	0	0.99
DB01045	Rifampin	1MZW	0	0	0.89
DB00091	Cyclosporine	1S78	0	0	0.99
DB00091	Cyclosporine	1BI9	0	0	0.99
DB01045	Rifampin	1I7I	0	0	0.85
DB01078	Deslanoside	1HOF	0	0	0.98
DB01045	Rifampin	1BYW	0	0	0.92
DB01045	Rifampin	1SQN	0	0	0.89
DB00091	Cyclosporine	1HA2	0	0	0.99
DB00091	Cyclosporine	1YVL	0	0	0.99
DB00880	Chlorothiazide	1IRU	0	0	0.99
DB00641	Simvastatin	1HSZ	0	1	0.66
DB00091	Cyclosporine	1Y0X	0	0	0.99
DB01042	Melphalan	1P87	0	0	0.94
DB00091	Cyclosporine	1KED	0	0	0.99
DB00091	Cyclosporine	1TZI	0	0	0.99
DB00682	Warfarin	1P87	0	0	1.00
DB00682	Warfarin	1P87	0	0	1.00
DB00880	Chlorothiazide	1IRU	0	0	0.99
DB00880	Chlorothiazide	1DON	0	0	0.98
DB04967	Lucanthone	1BDA	0	0	0.87
DB00163	Vitamin E	1VYT	0	0	0.99
DB00163	Vitamin E	1AUT	0	0	0.96
DB00163	Vitamin E	1UJW	0	0	0.96
DB00163	Vitamin E	1YTV	0	0	0.97
DB00163	Vitamin E	1SA1	0	0	0.99
DB00163	Vitamin E	1SA1	0	0	0.99
DB00163	Vitamin E	1IIH	0	0	0.99
DB00163	Vitamin E	1KED	0	0	0.99
DB00091	Cyclosporine	1VYT	0	0	0.99
DB00163	Vitamin E	1MO8	0	0	0.99
DB00163	Vitamin E	1BYY	0	0	1.00
DB00163	Vitamin E	1G91	0	0	0.99
DB00163	Vitamin E	1JQI	0	0	0.97
DB00163	Vitamin E	1BJ4	0	0	0.99
DB00163	Vitamin E	1OLM	0	0	0.99
DB00163	Vitamin E	1SG0	0	0	0.99

DB00163	Vitamin E	1F8Q	0	0	0.99
DB00163	Vitamin E	1LBD	0	0	0.99
DB00163	Vitamin E	1EXX	0	0	0.99
DB00163	Vitamin E	1XDK	0	0	0.97
DB00163	Vitamin E	1BBS	0	0	0.96
DB00163	Vitamin E	1YB5	0	0	0.97
DB00163	Vitamin E	1RFV	0	0	0.99
DB00163	Vitamin E	1HAG	0	0	0.96
DB00163	Vitamin E	1SQN	0	0	0.99
DB00163	Vitamin E	1EXB	0	0	0.99
DB00163	Vitamin E	1KI0	0	0	0.99
DB00163	Vitamin E	1I7I	0	0	0.99
DB00163	Vitamin E	1Y0S	0	0	0.99
DB00163	Vitamin E	1OC3	0	0	0.99
DB00163	Vitamin E	1CWM	0	0	0.99
DB00163	Vitamin E	1OAT	0	0	0.97
DB00163	Vitamin E	1OAT	0	0	0.97
DB00163	Vitamin E	1S3A	0	0	0.99
DB00163	Vitamin E	1QR6	0	0	0.99
DB00163	Vitamin E	1L6J	0	0	0.99
DB00163	Vitamin E	1SPJ	0	0	0.96
DB00163	Vitamin E	1ODW	0	0	0.99
DB00163	Vitamin E	3JDW	0	0	0.99
DB00163	Vitamin E	1WVJ	0	0	0.99
DB00163	Vitamin E	1L1F	0	0	0.99
DB00163	Vitamin E	1Z8L	0	0	0.99
DB00163	Vitamin E	1NHZ	0	0	0.99
DB00163	Vitamin E	1J4I	0	0	0.99
DB00163	Vitamin E	1FE3	0	0	0.99
DB00163	Vitamin E	1VJB	0	0	0.99
DB00163	Vitamin E	1R5K	0	0	0.97
DB00163	Vitamin E	1IVO	0	0	0.97
DB00163	Vitamin E	1UT1	0	0	0.97
DB00163	Vitamin E	1A36	0	0	0.97
DB00163	Vitamin E	1BNA	0	0	0.96
DB00163	Vitamin E	1CJY	0	0	0.96
DB00163	Vitamin E	1TQN	0	0	0.99
DB00163	Vitamin E	1J3S	0	0	0.99
DB00163	Vitamin E	1XMI	0	0	0.98
DB00163	Vitamin E	1P0S	0	0	0.96
DB00163	Vitamin E	1P0Q	0	0	0.99
DB00163	Vitamin E	1F4J	0	0	0.99
DB00163	Vitamin E	1ZNC	0	0	0.96
DB00163	Vitamin E	1CZM	0	0	0.99

DB00163	Vitamin E	1PTW	0	0	0.98
DB00163	Vitamin E	1DIA	0	0	0.99
DB00163	Vitamin E	1YMX	0	0	0.99
DB00163	Vitamin E	1E79	0	0	0.99
DB00163	Vitamin E	1AJS	0	0	0.97
DB00163	Vitamin E	1UZF	0	0	0.99
DB00163	Vitamin E	1E3G	0	0	0.99
DB00163	Vitamin E	1HOF	0	0	0.99
DB00163	Vitamin E	1HOF	0	0	0.99
DB00163	Vitamin E	1EW2	0	0	0.99
DB00163	Vitamin E	1T40	0	0	0.96
DB00163	Vitamin E	1HT0	0	0	0.97
DB00163	Vitamin E	1HSZ	0	0	0.97
DB00163	Vitamin E	1OKC	0	0	0.99
DB00163	Vitamin E	1F8U	0	0	0.99
DB00163	Vitamin E	2BIY	0	0	0.99
DB00163	Vitamin E	1HNK	0	0	0.99
DB00163	Vitamin E	1HWL	0	0	0.97
DB00163	Vitamin E	1P87	0	0	1.00
DB00163	Vitamin E	1EMI	0	0	1.00
DB00163	Vitamin E	1EMI	0	0	1.00
DB01065	Melatonin	1DON	0	0	0.98
DB00172	L-Proline	1P87	0	0	0.99
DB01078	Deslanoside	1XQ8	0	0	0.96
DB01045	Rifampin	1EXX	0	0	0.91
DB01065	Melatonin	1IRU	0	0	0.98
DB01078	Deslanoside	1O5W	0	0	0.99
DB01065	Melatonin	1IRU	0	0	0.98
DB01045	Rifampin	1C0B	0	0	0.95
DB01078	Deslanoside	1E3G	0	0	0.98
DB01045	Rifampin	1HA2	0	0	0.80
DB00511	Acetyldigitoxin	1OHY	0	0	0.99
DB01045	Rifampin	1BYY	0	0	0.97
DB00126	Vitamin C	1DON	0	0	0.97
DB00511	Acetyldigitoxin	1F8U	0	0	0.99
DB00511	Acetyldigitoxin	1HSO	0	0	0.97
DB00511	Acetyldigitoxin	1HOF	0	0	0.99
DB01034	Cerulenin	1P87	0	0	0.99
DB04839	Cyproterone	1P87	0	0	0.99
DB01034	Cerulenin	1P87	0	0	0.99
DB01045	Rifampin	1Y4E	0	0	0.96
DB01065	Melatonin	1P87	0	0	0.99
DB00641	Simvastatin	1MC5	0	1	0.66
DB01045	Rifampin	1SA1	0	0	0.87

DB04839	Cyproterone	1IRU	0	0	0.99
DB01045	Rifampin	1T0U	0	0	0.85
DB01236	Sevoflurane	1IRU	0	0	1.00
DB04839	Cyproterone	1DON	0	0	0.99
DB00439	Cerivastatin	1H2W	0	0	1.00
DB00227	Lovastatin	1SA1	0	0	0.86
DB00351	Megestrol	1SA1	0	1	0.64
DB00351	Megestrol	1KED	0	1	0.67
DB00926	Etretinate	1SS2	0	1	0.45
DB00227	Lovastatin	1MO8	0	0	0.89
DB00227	Lovastatin	1Y4E	0	0	0.97
DB00351	Megestrol	1EYD	0	0	0.78
DB00227	Lovastatin	1Q9S	0	0	0.91
DB00926	Etretinate	1L9X	0	1	0.46
DB00858	Dromostanolone	1YTV	0	0	0.92
DB00351	Megestrol	1MO8	0	0	0.72
DB00227	Lovastatin	1UHL	0	0	0.84
DB00858	Dromostanolone	1VYT	0	0	0.98
DB00227	Lovastatin	1EXX	0	0	0.91
DB00217	Bethanidine	1H2W	0	0	1.00
DB01395	Drospirenone	1S3I	0	0	0.95
DB00191	Phentermine	1P87	0	0	0.99
DB00227	Lovastatin	1SQN	0	0	0.88
DB00227	Lovastatin	1BYW	0	0	0.92
DB00227	Lovastatin	1JYD	0	0	0.91
DB00351	Megestrol	1DON	0	0	0.98
DB00351	Megestrol	1F5F	0	0	0.75
DB01395	Drospirenone	1HWL	0	0	0.75
DB00227	Lovastatin	1Y0S	0	0	0.76
DB00641	Simvastatin	1D1S	0	1	0.65
DB01395	Drospirenone	1OHY	0	0	0.95
DB00114	Pyridoxal Phosphate	1IRU	0	0	0.97
DB01045	Rifampin	1G0W	0	0	0.88
DB01395	Drospirenone	1F8U	0	0	0.94
DB00114	Pyridoxal Phosphate	1IRU	0	0	0.97
DB01395	Drospirenone	1HSZ	0	0	0.74
DB00227	Lovastatin	1CWM	0	0	0.91
DB00351	Megestrol	1H0C	0	1	0.66
DB01395	Drospirenone	1OF7	0	0	0.96
DB00351	Megestrol	1RTU	0	0	0.87
DB01395	Drospirenone	1EW2	0	0	0.95
DB00523	Alitretinoin	1UMK	0	1	0.55
DB00351	Megestrol	1UHL	0	1	0.60
DB01395	Drospirenone	1E3G	0	0	0.95

DB00351	Megestrol	1EXX	0	0	0.75
DB01395	Drospirenone	1UZF	0	0	0.94
DB00487	Pefloxacin	1DON	0	0	0.99
DB00227	Lovastatin	1ODW	0	0	0.92
DB00641	Simvastatin	1OF7	0	0	0.95
DB00227	Lovastatin	1XKT	0	0	0.84
DB01395	Drospirenone	1E79	0	0	0.94
DB00616	Candoxatril	1UZF	0	0	0.85
DB00351	Megestrol	1G1S	0	1	0.55
DB00641	Simvastatin	1MRQ	0	0	0.95
DB00351	Megestrol	1SQN	0	0	0.68
DB00351	Megestrol	1C5G	0	0	0.68
DB01395	Drospirenone	1XGJ	0	0	0.77
DB00227	Lovastatin	1QYE	0	0	0.92
DB01395	Drospirenone	1TB5	0	0	0.75
DB01395	Drospirenone	1CZM	0	0	0.95
DB00351	Megestrol	1JYD	0	0	0.76
DB01244	Bepridil	1TEV	0	0	0.70
DB01395	Drospirenone	1T9N	0	0	0.95
DB00641	Simvastatin	1XF0	0	0	0.95
DB01395	Drospirenone	1ZNC	0	1	0.62
DB00115	Cyanocobalamin	1K7L	0	0	0.84
DB01244	Bepridil	1A8M	0	1	0.67
DB00227	Lovastatin	2BGR	0	0	0.86
DB00115	Cyanocobalamin	1YXM	0	0	0.85
DB00227	Lovastatin	1P0Q	0	0	0.84
DB00351	Megestrol	1L6J	0	1	0.57
DB00227	Lovastatin	1T9R	0	0	0.88
DB00227	Lovastatin	1T9N	0	0	0.88
DB00115	Cyanocobalamin	1CWM	0	0	0.95
DB00227	Lovastatin	1CZM	0	0	0.88
DB00523	Alitretinoin	1DON	0	0	0.98
DB00641	Simvastatin	1HOF	0	0	0.96
DB00227	Lovastatin	1DIA	0	0	0.87
DB00351	Megestrol	1ILQ	0	0	0.89
DB00641	Simvastatin	1HOF	0	0	0.96
DB00351	Megestrol	2IL6	0	0	0.77
DB00227	Lovastatin	1UZF	0	0	0.86
DB01395	Drospirenone	3CBS	0	0	0.96
DB00351	Megestrol	1ODW	0	0	0.78
DB00227	Lovastatin	1HOF	0	0	0.94
DB00351	Megestrol	1T5P	0	1	0.65
DB00227	Lovastatin	1EW2	0	0	0.88
DB00351	Megestrol	1BWC	0	1	0.65

DB01045	Rifampin	1T9N	0	0	0.88
DB01395	Drospirenone	1T9R	0	0	0.96
DB01395	Drospirenone	1P0Q	0	0	0.94
DB01395	Drospirenone	1XU9	0	0	0.95
DB00351	Megestrol	1NHZ	0	0	0.70
DB00126	Vitamin C	1P87	0	0	0.96
DB00126	Vitamin C	1P87	0	0	0.96
DB00227	Lovastatin	1OKC	0	0	0.89
DB01395	Drospirenone	1CRK	0	0	0.86
DB00128	L-Aspartic Acid	1P87	0	0	0.99
DB00641	Simvastatin	1XQ8	0	0	0.75
DB00114	Pyridoxal Phosphate	1DON	0	0	0.94
DB00227	Lovastatin	1ORE	0	0	0.92
DB00351	Megestrol	1SS2	0	0	0.71
DB00641	Simvastatin	1OIZ	0	0	0.87
DB00641	Simvastatin	1O5W	0	0	0.99
DB00641	Simvastatin	2BK3	0	0	0.70
DB00641	Simvastatin	1E3G	0	0	0.93
DB00641	Simvastatin	1R4L	0	0	0.70
DB00641	Simvastatin	1UZF	0	0	0.91
DB00641	Simvastatin	1JVQ	0	0	0.68
DB01244	Bepidil	1X86	0	1	0.63
DB00641	Simvastatin	1J1S	0	0	0.92
DB00162	Vitamin A	1DON	0	0	0.98
DB00641	Simvastatin	1H6I	0	0	0.94
DB00641	Simvastatin	1PQ3	0	0	0.92
DB00162	Vitamin A	1RTU	0	1	0.40
DB00641	Simvastatin	1AJS	0	0	0.68
DB01244	Bepidil	1BDA	0	0	0.93
DB00641	Simvastatin	1E79	0	0	0.91
DB00641	Simvastatin	1JZ2	0	0	0.93
DB00641	Simvastatin	1LT8	0	0	0.69
DB00227	Lovastatin	1P87	0	0	1.00
DB00351	Megestrol	1QKM	0	0	0.68
DB00641	Simvastatin	1YMX	0	0	0.87
DB00227	Lovastatin	1EMI	0	0	0.97
DB00641	Simvastatin	1K6R	0	0	0.96
DB00873	Loteprednol Etabonate	1V97	0	0	0.69
DB00162	Vitamin A	1IRU	0	0	0.98
DB00162	Vitamin A	1H2W	0	0	1.00
DB00641	Simvastatin	1REW	0	0	0.90
DB00641	Simvastatin	1KTA	0	1	0.67
DB01244	Bepidil	1MO8	0	1	0.64
DB00641	Simvastatin	1TB5	0	1	0.67

DB00641	Simvastatin	1PTW	0	0	0.74
DB00162	Vitamin A	1Y38	0	1	0.52
DB00641	Simvastatin	1S5O	0	0	0.92
DB00926	Etretinate	1PB7	0	1	0.46
DB00641	Simvastatin	1CP3	0	0	0.92
DB01244	Bepridil	1HA2	0	1	0.53
DB01244	Bepridil	1BJ4	0	1	0.59
DB00641	Simvastatin	1F4J	0	0	0.92
DB00873	Loteprednol Etabonate	1TEV	0	1	0.61
DB00641	Simvastatin	1I9R	0	0	0.91
DB00641	Simvastatin	2CBR	0	0	0.94
DB00641	Simvastatin	1T9R	0	0	0.92
DB00162	Vitamin A	1UMK	0	0	0.85
DB00641	Simvastatin	1D6G	0	0	0.95
DB00873	Loteprednol Etabonate	1A5Y	0	1	0.53
DB00641	Simvastatin	1P0Q	0	0	0.90
DB01244	Bepridil	1EXX	0	0	0.68
DB00641	Simvastatin	1FIE	0	0	0.70
DB00616	Candoxatril	1E3G	0	0	0.89
DB01244	Bepridil	1BYW	0	0	0.74
DB00641	Simvastatin	1LJ7	0	0	0.95
DB00873	Loteprednol Etabonate	1IIH	0	1	0.51
DB00162	Vitamin A	1ILQ	0	1	0.43
DB00873	Loteprednol Etabonate	1VMC	0	0	0.74
DB00641	Simvastatin	1G0W	0	0	0.92
DB00616	Candoxatril	1HOF	0	0	0.94
DB00926	Etretinate	1IBC	0	1	0.55
DB00641	Simvastatin	1CRK	0	0	0.81
DB00641	Simvastatin	1QK1	0	0	0.90
DB00641	Simvastatin	1JBQ	0	0	0.95
DB00616	Candoxatril	1HOF	0	0	0.94
DB01244	Bepridil	1D1P	0	1	0.56
DB00641	Simvastatin	1XMI	0	0	0.77
DB00641	Simvastatin	1OCZ	0	0	0.90
DB00641	Simvastatin	1PO5	0	0	0.90
DB00641	Simvastatin	1TQN	0	0	0.91
DB00162	Vitamin A	1GCN	0	1	0.54
DB01244	Bepridil	1ODW	0	0	0.72
DB00641	Simvastatin	1EA1	0	0	0.91
DB00873	Loteprednol Etabonate	1LBD	0	1	0.52
DB00641	Simvastatin	1PWG	0	0	0.69
DB00641	Simvastatin	1D3H	0	0	0.93
DB00396	Progesterone	1ILQ	0	0	0.97
DB00641	Simvastatin	1BP3	0	0	0.90

DB01244	Bepridil	3JDW	0	1	0.60
DB00641	Simvastatin	1ITU	0	0	0.70
DB01244	Bepridil	1NHZ	0	1	0.63
DB00926	Etretinate	1WVJ	0	1	0.45
DB00641	Simvastatin	1EI1	0	1	0.67
DB00396	Progesterone	1P5J	0	0	0.93
DB00926	Etretinate	1YAE	0	1	0.47
DB01244	Bepridil	1D3H	0	1	0.65
DB00873	Loteprednol Etabonate	1CWM	0	1	0.60
DB00641	Simvastatin	1UW0	0	0	0.94
DB00641	Simvastatin	8ICK	0	0	0.93
DB01264	Darunavir	1H2W	0	0	1.00
DB00873	Loteprednol Etabonate	1TYE	0	0	0.91
DB00641	Simvastatin	1A36	0	0	0.70
DB00641	Simvastatin	1HD7	0	0	0.94
DB00351	Megestrol	1EA1	0	1	0.64
DB00351	Megestrol	1P0Q	0	1	0.61
DB01244	Bepridil	1CZM	0	1	0.62
DB00633	Dexmedetomidine	1P87	0	0	1.00
DB00641	Simvastatin	1MQB	0	0	0.85
DB01244	Bepridil	1I2W	0	0	0.73
DB00188	Bortezomib	1IRU	0	0	0.98
DB00641	Simvastatin	1IVO	0	1	0.67
DB00351	Megestrol	2CBR	0	0	0.76
DB00641	Simvastatin	1R5K	0	0	0.69
DB00351	Megestrol	1CP3	0	1	0.66
DB00641	Simvastatin	1QKM	0	0	0.92
DB01244	Bepridil	1UZF	0	1	0.55
DB00873	Loteprednol Etabonate	1NHZ	0	1	0.53
DB01244	Bepridil	1E3G	0	1	0.63
DB01418	Acenocoumarol	1DON	0	0	0.98
DB00641	Simvastatin	1XKT	0	0	0.90
DB00506	Norgestrel	1VMC	0	1	0.66
DB00641	Simvastatin	1FE3	0	0	0.94
DB00641	Simvastatin	1QZ2	0	1	0.64
DB00641	Simvastatin	1Q6U	0	0	0.89
DB00873	Loteprednol Etabonate	1HE5	0	1	0.59
DB00162	Vitamin A	1HOF	0	1	0.37
DB00162	Vitamin A	1HOF	0	1	0.37
DB00351	Megestrol	1CZM	0	0	0.70
DB01244	Bepridil	1HOF	0	0	0.83
DB00165	Pyridoxine	1P87	0	0	0.97
DB01244	Bepridil	1HOF	0	0	0.83
DB00188	Bortezomib	1IRU	0	0	0.98

DB00641	Simvastatin	1U4E	0	0	0.92
DB00506	Norgestrel	1Y4E	0	0	0.84
DB00641	Simvastatin	1VRU	0	0	0.68
DB00641	Simvastatin	1L9X	0	0	0.93
DB01244	Bepridil	1OF7	0	0	0.71
DB00162	Vitamin A	1P87	0	0	1.00
DB00162	Vitamin A	1EMI	0	1	0.60
DB00162	Vitamin A	1EMI	0	1	0.60
DB00641	Simvastatin	1R5S	0	0	0.93
DB01395	Drospirenone	1JBQ	0	0	0.97
DB01395	Drospirenone	1FYC	0	0	0.95
DB01395	Drospirenone	1BNA	0	1	0.62
DB01395	Drospirenone	1IVO	0	0	0.74
DB00361	Vinorelbine	1VYT	0	0	0.98
DB00361	Vinorelbine	1T0U	0	0	0.98
DB00361	Vinorelbine	1SA1	0	0	0.98
DB00361	Vinorelbine	1BYY	0	0	0.99
DB00361	Vinorelbine	1F5F	0	0	0.98
DB00361	Vinorelbine	1C0B	0	0	0.99
DB00361	Vinorelbine	1UHL	0	0	0.97
DB00361	Vinorelbine	1OPL	0	0	0.94
DB00361	Vinorelbine	1K2H	0	0	1.00
DB00361	Vinorelbine	1SQN	0	0	0.98
DB00361	Vinorelbine	1BYW	0	0	0.98
DB00361	Vinorelbine	1KI0	0	0	0.98
DB00361	Vinorelbine	1JYD	0	0	0.98
DB00361	Vinorelbine	1CWM	0	0	0.98
DB00361	Vinorelbine	1N8S	0	0	0.92
DB00361	Vinorelbine	1I0Z	0	0	0.94
DB00361	Vinorelbine	9ILB	0	0	0.98
DB00361	Vinorelbine	1M1X	0	0	0.94
DB00361	Vinorelbine	1Z8L	0	0	0.98
DB00361	Vinorelbine	1MU2	0	0	0.94
DB00361	Vinorelbine	1R5K	0	0	0.94
DB00361	Vinorelbine	1BNA	0	0	0.92
DB00361	Vinorelbine	1FYC	0	0	0.98
DB00361	Vinorelbine	1P0Q	0	0	0.97
DB00361	Vinorelbine	2CBR	0	0	0.98
DB00361	Vinorelbine	1T9N	0	0	0.98
DB00361	Vinorelbine	1KTA	0	0	0.94
DB00361	Vinorelbine	1KTO	0	0	0.98
DB00361	Vinorelbine	1E79	0	0	0.98
DB00361	Vinorelbine	1UZF	0	0	0.98
DB00361	Vinorelbine	1HOF	0	0	0.99

DB00361	Vinorelbine	1EW2	0	0	0.98
DB00361	Vinorelbine	2T40	0	0	0.92
DB00361	Vinorelbine	1KG3	0	0	0.98
DB00361	Vinorelbine	1P87	0	0	0.99
DB00351	Megestrol	1REW	0	1	0.60
DB00541	Vincristine	1YTV	0	0	0.93
DB00541	Vincristine	1VJA	0	0	0.91
DB00541	Vincristine	1TEV	0	0	0.98
DB00541	Vincristine	1SA1	0	0	0.97
DB00541	Vincristine	1VMC	0	0	0.98
DB00541	Vincristine	1UHL	0	0	0.97
DB00541	Vincristine	1LBD	0	0	0.96
DB00541	Vincristine	1S78	0	0	0.96
DB00541	Vincristine	1G1S	0	0	0.96
DB00541	Vincristine	1SQN	0	0	0.98
DB00541	Vincristine	1BYW	0	0	0.98
DB00541	Vincristine	1LSZ	0	0	0.98
DB00541	Vincristine	1I10	0	0	0.97
DB00541	Vincristine	1TYE	0	0	0.99
DB00541	Vincristine	1WVJ	0	0	0.98
DB00541	Vincristine	1NHZ	0	0	0.98
DB00541	Vincristine	1R5S	0	0	0.98
DB00541	Vincristine	1BDF	0	0	0.93
DB00541	Vincristine	1BNA	0	0	0.91
DB00541	Vincristine	1CJY	0	0	0.92
DB00541	Vincristine	1XU9	0	0	0.98
DB00541	Vincristine	1CP3	0	0	0.97
DB00541	Vincristine	1ZNC	0	0	0.91
DB00541	Vincristine	1TB5	0	0	0.92
DB00541	Vincristine	1KTA	0	0	0.93
DB00541	Vincristine	1UZF	0	0	0.97
DB00541	Vincristine	1R4L	0	0	0.93
DB00541	Vincristine	1I5H	0	0	0.98
DB00541	Vincristine	1HOF	0	0	0.98
DB00541	Vincristine	1XF0	0	0	0.98
DB00541	Vincristine	1F8U	0	0	0.97
DB00541	Vincristine	1GXD	0	0	0.98
DB00541	Vincristine	1HWL	0	0	0.93
DB00191	Phentermine	1IRU	0	0	0.98
DB00115	Cyanocobalamin	1OAT	0	0	0.84
DB00541	Vincristine	1EMI	0	0	0.99
DB00852	Pseudoephedrine	1DON	0	0	0.98
DB00570	Vinblastine	1TEV	0	0	0.98
DB00570	Vinblastine	1A5Y	0	0	0.98

DB00570	Vinblastine	1MB2	0	0	0.93
DB00570	Vinblastine	1WAP	0	0	0.99
DB00873	Loteprednol Etabonate	1TQN	0	1	0.46
DB00570	Vinblastine	1VMC	0	0	0.99
DB00570	Vinblastine	1MO8	0	0	0.98
DB00570	Vinblastine	1F5F	0	0	0.98
DB00570	Vinblastine	1HA2	0	0	0.97
DB00570	Vinblastine	1UHL	0	0	0.97
DB00570	Vinblastine	1LBD	0	0	0.97
DB00570	Vinblastine	1EXX	0	0	0.98
DB00570	Vinblastine	1NI4	0	0	0.94
DB00570	Vinblastine	1OPL	0	0	0.94
DB00570	Vinblastine	1HAG	0	0	0.93
DB00570	Vinblastine	1SQN	0	0	0.98
DB00570	Vinblastine	1BYW	0	0	0.98
DB00570	Vinblastine	1K7L	0	0	0.94
DB00570	Vinblastine	1FVO	0	0	0.97
DB00570	Vinblastine	1N7D	0	0	0.95
DB00570	Vinblastine	1ILQ	0	0	0.99
DB00570	Vinblastine	1ODW	0	0	0.98
DB00570	Vinblastine	1T5P	0	0	0.98
DB00570	Vinblastine	1NHZ	0	0	0.98
DB00570	Vinblastine	1R5S	0	0	0.98
DB00570	Vinblastine	1SS2	0	0	0.98
DB00570	Vinblastine	1VRU	0	0	0.95
DB00570	Vinblastine	1YV5	0	0	0.98
DB00570	Vinblastine	1R5K	0	0	0.95
DB00570	Vinblastine	1UW0	0	0	0.98
DB00570	Vinblastine	1X9N	0	0	0.95
DB00570	Vinblastine	1CJY	0	0	0.94
DB00570	Vinblastine	1TQN	0	0	0.97
DB00570	Vinblastine	1D6G	0	0	0.98
DB00570	Vinblastine	2CBR	0	0	0.98
DB00570	Vinblastine	1ZNC	0	0	0.93
DB00570	Vinblastine	1T9N	0	0	0.98
DB00570	Vinblastine	1DIA	0	0	0.98
DB00570	Vinblastine	1KTA	0	0	0.95
DB00570	Vinblastine	1E79	0	0	0.98
DB00570	Vinblastine	1AJS	0	0	0.94
DB00570	Vinblastine	1UZF	0	0	0.98
DB00570	Vinblastine	1UZF	0	0	0.98
DB00570	Vinblastine	1Q7L	0	0	0.98
DB00570	Vinblastine	2BK3	0	0	0.95
DB00570	Vinblastine	1I5H	0	0	0.98

DB00570	Vinblastine	1XQ8	0	0	0.95
DB00570	Vinblastine	1HOF	0	0	0.99
DB00570	Vinblastine	1HOF	0	0	0.99
DB00570	Vinblastine	1P1R	0	0	0.97
DB00570	Vinblastine	1OKC	0	0	0.98
DB00570	Vinblastine	1OHY	0	0	0.98
DB01244	Bepiridil	1F8U	0	1	0.55
DB01395	Drospirenone	1QYX	0	0	0.96
DB00351	Megestrol	1PQ3	0	0	0.70
DB01430	Almitrine	1P87	0	0	0.99
DB00132	Alpha-Linolenic Acid	1EMI	0	1	0.51
DB00641	Simvastatin	1NHZ	0	0	0.93
DB00641	Simvastatin	1PB7	0	0	0.94
DB01395	Drospirenone	1QKM	0	0	0.95
DB00873	Loteprednol Etabonate	1LJ7	0	1	0.64
DB00873	Loteprednol Etabonate	1XU9	0	1	0.51
DB00641	Simvastatin	1L1F	0	0	0.90
DB00641	Simvastatin	1L1F	0	0	0.90
DB01045	Rifampin	1KTO	0	0	0.86
DB00641	Simvastatin	1WVJ	0	0	0.93
DB00641	Simvastatin	1XHY	0	0	0.94
DB00115	Cyanocobalamin	1E71	0	0	0.93
DB00641	Simvastatin	1YAE	0	0	0.94
DB00873	Loteprednol Etabonate	1D6G	0	0	0.70
DB00641	Simvastatin	1YAE	0	0	0.94
DB00188	Bortezomib	1DON	0	0	0.97
DB00873	Loteprednol Etabonate	1T9R	0	1	0.56
DB00641	Simvastatin	1GET	0	1	0.65
DB00641	Simvastatin	1BWC	0	0	0.92
DB01244	Bepiridil	1P87	0	0	1.00
DB00641	Simvastatin	1J0X	0	0	0.91
DB00641	Simvastatin	3JDW	0	0	0.92
DB00641	Simvastatin	4Q21	0	0	0.94
DB00641	Simvastatin	1GP2	0	1	0.65
DB00351	Megestrol	1H6I	0	0	0.76
DB00641	Simvastatin	1T5P	0	0	0.91
DB00641	Simvastatin	1KPF	0	0	0.95
DB00641	Simvastatin	1HQC	0	0	0.71
DB00641	Simvastatin	1QVU	0	1	0.67
DB00351	Megestrol	1UZF	0	1	0.63
DB00641	Simvastatin	1F0Y	0	1	0.67
DB00641	Simvastatin	1BZY	0	0	0.70
DB01080	Vigabatrin	1P87	0	0	0.98
DB00641	Simvastatin	1M1X	0	0	0.71

DB00641	Simvastatin	1MQ8	0	0	0.68
DB00641	Simvastatin	9ILB	0	0	0.95
DB00488	Altretamine	1P87	0	0	1.00
DB00191	Phentermine	1DON	0	0	0.98
DB00562	Benzthiazide	1DON	0	0	0.99
DB00859	Penicillamine	1P87	0	0	0.94
DB00351	Megestrol	1UZF	0	1	0.63
DB00641	Simvastatin	1HUL	0	0	0.96
DB00488	Altretamine	1O5W	0	1	0.48
DB01158	Bretylum	1P87	0	0	0.99
DB00873	Loteprednol Etabonate	3BLM	0	1	0.56
DB00865	Benzphetamine	1BDA	0	0	0.93
DB04690	Camptothecin	1P87	0	0	1.00
DB01158	Bretylum	1DON	0	0	0.99
DB01395	Drospirenone	1XKT	0	0	0.94
DB00641	Simvastatin	1ILQ	0	0	0.97
DB00641	Simvastatin	1QU2	0	0	0.68
DB00351	Megestrol	1O5W	0	0	0.97
DB00865	Benzphetamine	1DON	0	0	0.98
DB00115	Cyanocobalamin	1L6J	0	0	0.91
DB01564	Calusterone	1UAE	0	0	0.78
DB00884	Risedronate	1IRU	0	0	0.97
DB00351	Megestrol	1HOF	0	0	0.85
DB00351	Megestrol	1HOF	0	0	0.85
DB01045	Rifampin	1UZF	0	0	0.86
DB00873	Loteprednol Etabonate	1E3G	0	1	0.52
DB01564	Calusterone	1IIH	0	0	0.77
DB00873	Loteprednol Etabonate	1I5H	0	1	0.59
DB00819	Acetazolamide	1DON	0	0	0.97
DB00351	Megestrol	1L6V	0	0	0.74
DB01564	Calusterone	1MO8	0	0	0.80
DB01564	Calusterone	1DON	0	0	0.98
DB00884	Risedronate	1DON	0	0	0.94
DB00641	Simvastatin	1W7N	0	0	0.92
DB01395	Drospirenone	1J4I	0	0	0.97
DB01395	Drospirenone	1QZ2	0	0	0.71
DB01045	Rifampin	1UZF	0	0	0.86
DB01564	Calusterone	1HA2	0	0	0.70
DB01564	Calusterone	1RTU	0	0	0.91
DB01045	Rifampin	1HOF	0	0	0.93
DB00926	Etretinate	4Q21	0	1	0.53
DB00503	Ritonavir	1EMI	0	0	0.86
DB00661	Verapamil	1VYT	0	0	0.95
DB00661	Verapamil	1YTV	0	0	0.75

DB00661	Verapamil	1TZI	0	1	0.63
DB00661	Verapamil	1A8M	0	0	0.96
DB00661	Verapamil	1KGI	0	0	0.95
DB00661	Verapamil	1Y0X	0	0	0.96
DB00661	Verapamil	1NAV	0	0	0.96
DB00661	Verapamil	1MO8	0	0	0.96
DB00661	Verapamil	1BYY	0	0	0.99
DB00661	Verapamil	1YVL	0	0	0.95
DB00661	Verapamil	1F5F	0	0	0.96
DB00661	Verapamil	1H0C	0	0	0.95
DB00661	Verapamil	1BJ4	0	0	0.95
DB00661	Verapamil	1Q9S	0	0	0.97
DB00661	Verapamil	1UHL	0	0	0.94
DB00661	Verapamil	1EXX	0	0	0.96
DB00661	Verapamil	1EXX	0	0	0.96
DB00661	Verapamil	1BI9	0	0	0.93
DB00661	Verapamil	1BXS	0	1	0.63
DB00661	Verapamil	1S78	0	0	0.93
DB00661	Verapamil	1G1S	0	0	0.93
DB00661	Verapamil	1RV7	0	0	0.97
DB00661	Verapamil	1TJC	0	0	0.96
DB00661	Verapamil	1BYW	0	0	0.97
DB00661	Verapamil	1EXB	0	0	0.93
DB00661	Verapamil	1K7L	0	0	0.73
DB00661	Verapamil	2BIU	0	0	0.97
DB00661	Verapamil	1NRL	0	0	0.74
DB00661	Verapamil	1SVC	0	0	0.93
DB00661	Verapamil	1L6J	0	0	0.93
DB00661	Verapamil	2IL6	0	0	0.96
DB00661	Verapamil	1BZY	0	0	0.78
DB00661	Verapamil	1ODW	0	0	0.97
DB00661	Verapamil	1R75	0	0	0.94
DB00661	Verapamil	1AGS	0	0	0.95
DB00661	Verapamil	1WVJ	0	0	0.96
DB00661	Verapamil	1L1F	0	0	0.94
DB00661	Verapamil	1PB7	0	0	0.96
DB00661	Verapamil	1NHZ	0	0	0.95
DB00661	Verapamil	1VRU	0	0	0.75
DB00661	Verapamil	1FTA	0	0	0.96
DB00661	Verapamil	1FE3	0	0	0.96
DB00661	Verapamil	1XKT	0	0	0.94
DB00661	Verapamil	1R5K	0	0	0.76
DB00661	Verapamil	1IVO	0	0	0.75
DB00661	Verapamil	1UT1	0	0	0.75

DB00661	Verapamil	1BDF	0	0	0.77
DB00661	Verapamil	1BNA	0	1	0.63
DB00661	Verapamil	1F0X	0	0	0.74
DB00661	Verapamil	1GTE	0	0	0.95
DB00661	Verapamil	1JBQ	0	0	0.97
DB00661	Verapamil	1T9R	0	0	0.96
DB00661	Verapamil	1F4J	0	0	0.95
DB00661	Verapamil	1T9N	0	0	0.95
DB00661	Verapamil	1CZM	0	0	0.95
DB00661	Verapamil	1UWJ	0	0	0.95
DB00661	Verapamil	1Q2P	0	0	0.96
DB00661	Verapamil	1E79	0	0	0.94
DB00661	Verapamil	1AJS	0	0	0.76
DB00661	Verapamil	1JVQ	0	0	0.76
DB00661	Verapamil	1UZF	0	0	0.94
DB00661	Verapamil	1E3G	0	0	0.95
DB00661	Verapamil	2BK3	0	0	0.78
DB00661	Verapamil	1BV8	0	0	0.96
DB00661	Verapamil	1HOF	0	0	0.98
DB00661	Verapamil	1HOF	0	0	0.98
DB00661	Verapamil	1EW2	0	0	0.95
DB00661	Verapamil	1OF7	0	0	0.97
DB00661	Verapamil	1D1S	0	0	0.73
DB00661	Verapamil	1OKC	0	0	0.96
DB00661	Verapamil	1ODC	0	0	0.94
DB00661	Verapamil	1HWL	0	0	0.76
DB00661	Verapamil	1P87	0	0	1.00
DB00661	Verapamil	1EMI	0	0	0.99
DB00641	Simvastatin	1CB6	0	0	0.70
DB00926	Etretinate	1P4R	0	0	0.90
DB01395	Drospirenone	1U4E	0	0	0.95
DB01395	Drospirenone	1VRU	0	0	0.75
DB01395	Drospirenone	1WVJ	0	0	0.96
DB00692	Phentolamine	1P87	0	0	0.99
DB00641	Simvastatin	1I0Z	0	0	0.68
DB01395	Drospirenone	1XHY	0	0	0.96
DB00692	Phentolamine	1P87	0	0	0.99
DB00873	Loteprednol Etabonate	1HOF	0	0	0.76
DB00648	Mitotane	1P87	0	0	1.00
DB01395	Drospirenone	1GET	0	0	0.72
DB01395	Drospirenone	1ODW	0	0	0.97
DB00483	Gallamine Triethiodide	1DON	0	0	0.99
DB01395	Drospirenone	9ILB	0	0	0.96
DB01395	Drospirenone	1ILQ	0	0	0.98

DB00926	Etretinate	3BLM	0	1	0.46
DB00484	Brimonidine	1H2W	0	0	1.00
DB00503	Ritonavir	1HOF	0	0	0.69
DB00843	Donepezil	1A8M	0	1	0.60
DB00351	Megestrol	1OD4	0	0	0.77
DB00154	gamma-Homolinolenic acid	1OF7	0	1	0.51
DB00843	Donepezil	1WAP	0	0	0.82
DB00503	Ritonavir	1HOF	0	0	0.69
DB00843	Donepezil	1F5F	0	1	0.61
DB00926	Etretinate	1PQ3	0	1	0.46
DB01219	Dantrolene	1P87	0	0	1.00
DB00154	gamma-Homolinolenic acid	1HOF	0	0	0.68
DB00484	Brimonidine	1DON	0	0	0.99
DB00641	Simvastatin	1D1P	0	0	0.91
DB00843	Donepezil	1EXX	0	1	0.61
DB00862	Vardenafil	1V97	0	0	0.76
DB00926	Etretinate	1ODW	0	1	0.54
DB00351	Megestrol	1KG3	0	0	0.68
DB00862	Vardenafil	1A5Y	0	1	0.62
DB00862	Vardenafil	1SA1	0	1	0.55
DB00351	Megestrol	1OHY	0	1	0.66
DB00862	Vardenafil	1IIH	0	1	0.59
DB00873	Loteprednol Etabonate	1ORE	0	1	0.65
DB00862	Vardenafil	1LBD	0	1	0.59
DB00584	Enalapril	1H2W	0	0	1.00
DB00616	Candoxatril	1EXB	0	0	0.79
DB00873	Loteprednol Etabonate	1HNK	0	0	0.70
DB01194	Brinzolamide	1P87	0	0	0.99
DB00367	Levonorgestrel	2BIU	0	1	0.54
DB00862	Vardenafil	1CWM	0	0	0.68
DB00641	Simvastatin	1P5J	0	0	0.94
DB00873	Loteprednol Etabonate	1EMI	0	0	0.88
DB00511	Acetyldigitoxin	2BK3	0	0	0.98
DB00862	Vardenafil	1NHZ	0	1	0.62
DB00641	Simvastatin	1LSZ	0	0	0.95
DB00862	Vardenafil	1FE3	0	0	0.70
DB00862	Vardenafil	1YV5	0	0	0.70
DB01328	Cefonicid	1P87	0	0	0.96
DB00862	Vardenafil	1GTE	0	1	0.58
DB00862	Vardenafil	1FYC	0	1	0.60
DB00364	Sucralfate	1P87	0	0	0.99
DB00862	Vardenafil	1HKO	0	0	0.71
DB00351	Megestrol	1P87	0	0	1.00
DB00862	Vardenafil	1T9R	0	1	0.63

DB00477	Chlorpromazine	1IRU	0	0	0.99
DB00862	Vardenafil	3BLM	0	1	0.65
DB00862	Vardenafil	1UZF	0	1	0.54
DB00862	Vardenafil	1E3G	0	1	0.62
DB00862	Vardenafil	1HOF	0	0	0.81
DB00862	Vardenafil	1HOF	0	0	0.81
DB00169	Cholecalciferol	1EMI	0	0	0.99
DB00862	Vardenafil	1ORE	0	0	0.72
DB00862	Vardenafil	1OHY	0	1	0.58
DB00862	Vardenafil	1HNK	0	0	0.77
DB01122	Ambenonium	1P87	0	0	0.98
DB00364	Sucralfate	1P87	0	0	0.99
DB00169	Cholecalciferol	1P87	0	0	1.00
DB00367	Levonorgestrel	1BYW	0	1	0.57
DB00616	Candoxatril	1G1S	0	0	0.80
DB00154	gamma-Homolinolenic acid	3CBS	0	1	0.49
DB00154	gamma-Homolinolenic acid	1T9R	0	1	0.45
DB01259	Lapatinib	1DON	0	0	0.99
DB00154	gamma-Homolinolenic acid	1JBQ	0	1	0.54
DB00926	Etretinate	1TYE	0	0	0.89
DB00154	gamma-Homolinolenic acid	1YV5	0	1	0.51
DB00641	Simvastatin	5MDH	0	1	0.67
DB00594	Amiloride	1IRU	0	0	0.98
DB00594	Amiloride	1IRU	0	0	0.98
DB00594	Amiloride	1DON	0	0	0.93
DB00169	Cholecalciferol	1HWL	0	0	0.81
DB00513	Aminocaproic Acid	1P87	0	0	1.00
DB00154	gamma-Homolinolenic acid	1HE5	0	1	0.48
DB00551	Acetohydroxamic Acid	1P87	0	0	1.00
DB00154	gamma-Homolinolenic acid	1WVJ	0	1	0.44
DB00843	Donepezil	1SQN	0	1	0.51
DB00843	Donepezil	1BYW	0	1	0.67
DB00154	gamma-Homolinolenic acid	1YAE	0	1	0.46
DB01406	Danazol	1VMC	0	1	0.55
DB00154	gamma-Homolinolenic acid	1ODW	0	1	0.53
DB01045	Rifampin	1ORE	0	0	0.92
DB01406	Danazol	1DON	0	0	0.98
DB00154	gamma-Homolinolenic acid	1BYW	0	1	0.55
DB00616	Candoxatril	1EXX	0	0	0.90
DB00616	Candoxatril	1Q9S	0	0	0.91
DB00169	Cholecalciferol	1OHY	0	0	0.95
DB00616	Candoxatril	1BJ4	0	0	0.87
DB00364	Sucralfate	1GCN	0	1	0.50
DB00154	gamma-Homolinolenic acid	1EXX	0	1	0.47

DB00154	gamma-Homolinolenic acid	1EXX	0	1	0.47
DB00616	Candoxatril	1HA2	0	0	0.81
DB00848	Levamisole	1P87	0	0	1.00
DB00616	Candoxatril	1G91	0	0	0.86
DB00154	gamma-Homolinolenic acid	1A8M	0	1	0.47
DB00396	Progesterone	1B6A	0	0	0.95
DB01044	Gatifloxacin	1P87	0	0	0.96
DB01044	Gatifloxacin	1DON	0	0	0.99
DB00843	Donepezil	1HUL	0	0	0.75
DB00843	Donepezil	1T5P	0	1	0.48
DB01327	Cefazolin	1DON	0	0	0.98
DB00169	Cholecalciferol	1HSO	0	0	0.79
DB00169	Cholecalciferol	1HOF	0	0	0.98
DB01078	Deslanoside	1Z6T	0	0	0.98
DB00780	Phenelzine	1P87	0	0	0.98
DB00351	Megestrol	1EMI	0	0	0.93
DB00616	Candoxatril	1BYY	0	0	0.97
DB00130	L-Glutamine	1IRU	0	0	0.97
DB01078	Deslanoside	1PQ3	0	0	0.97
DB00253	Medrysone	1SA1	0	0	0.80
DB00253	Medrysone	1Y0X	0	0	0.87
DB00641	Simvastatin	1MLD	0	1	0.64
DB00115	Cyanocobalamin	5MDH	0	0	0.85
DB00169	Cholecalciferol	1HOF	0	0	0.98
DB00843	Donepezil	1WVJ	0	1	0.58
DB00843	Donepezil	1NHZ	0	1	0.55
DB00903	Ethacrynic acid	1P87	0	0	1.00
DB00843	Donepezil	1YV5	0	1	0.64
DB00169	Cholecalciferol	1O5W	0	0	0.99
DB01031	Ethinamate	1P87	0	0	0.99
DB00511	Acetyldigoxin	1W7N	0	0	0.99
DB01078	Deslanoside	1E79	0	0	0.98
DB00253	Medrysone	1F5F	0	0	0.87
DB00253	Medrysone	1HA2	0	0	0.77
DB00843	Donepezil	1T9R	0	1	0.58
DB01236	Sevoflurane	1DON	0	0	0.98
DB01078	Deslanoside	1RGY	0	0	0.98
DB00253	Medrysone	1UHL	0	0	0.78
DB00253	Medrysone	1EXX	0	0	0.87
DB00843	Donepezil	1T9N	0	1	0.52
DB00313	Valproic Acid	1P87	0	0	1.00
DB00317	Gefitinib	1P87	0	0	1.00
DB00641	Simvastatin	1PU4	0	0	0.69
DB01586	Ursodeoxycholic acid	1A8M	0	0	0.90

DB00843	Donepezil	1CZM	0	1	0.54
DB01586	Ursodeoxycholic acid	1SLM	0	0	0.87
DB01586	Ursodeoxycholic acid	1MO8	0	0	0.88
DB01586	Ursodeoxycholic acid	1HA2	0	0	0.80
DB01586	Ursodeoxycholic acid	1BJ4	0	0	0.86
DB01586	Ursodeoxycholic acid	1UHL	0	0	0.82
DB01586	Ursodeoxycholic acid	1EXX	0	0	0.90
DB01078	Deslanoside	1ZNC	0	0	0.96
DB01586	Ursodeoxycholic acid	1R6K	0	0	0.83
DB01586	Ursodeoxycholic acid	1BYW	0	0	0.91
DB01586	Ursodeoxycholic acid	1I7I	0	0	0.81
DB01586	Ursodeoxycholic acid	1OC3	0	0	0.77
DB01078	Deslanoside	1JBQ	0	0	0.99
DB01586	Ursodeoxycholic acid	1B6A	0	0	0.93
DB00641	Simvastatin	1ISS	0	1	0.68
DB01078	Deslanoside	1CJY	0	0	0.96
DB00253	Medrysone	1R6K	0	0	0.79
DB00115	Cyanocobalamin	1I0Z	0	0	0.85
DB01586	Ursodeoxycholic acid	2BGR	0	0	0.84
DB01586	Ursodeoxycholic acid	1D3H	0	0	0.87
DB01586	Ursodeoxycholic acid	1JBQ	0	0	0.91
DB00253	Medrysone	1RFV	0	0	0.83
DB01586	Ursodeoxycholic acid	1T9R	0	0	0.85
DB01586	Ursodeoxycholic acid	1CZM	0	0	0.87
DB01586	Ursodeoxycholic acid	1UZF	0	0	0.84
DB01586	Ursodeoxycholic acid	1HOF	0	0	0.93
DB01586	Ursodeoxycholic acid	1HOF	0	0	0.93
DB01586	Ursodeoxycholic acid	1OF7	0	0	0.91
DB01586	Ursodeoxycholic acid	1OKC	0	0	0.88
DB01586	Ursodeoxycholic acid	1F8U	0	0	0.84
DB01586	Ursodeoxycholic acid	1GXD	0	0	0.88
DB01586	Ursodeoxycholic acid	2BIY	0	0	0.89
DB01078	Deslanoside	2BGR	0	0	0.98
DB01586	Ursodeoxycholic acid	1EMI	0	0	0.97
DB00364	Sucralfate	1IRU	0	0	0.98
DB00169	Cholecalciferol	1J1S	0	0	0.95
DB00169	Cholecalciferol	1Z6T	0	0	0.95
DB00094	Urofollitropin	1DON	0	0	0.97
DB01078	Deslanoside	1UW0	0	0	0.98
DB01078	Deslanoside	1R5K	0	0	0.96
DB00169	Cholecalciferol	1JZ2	0	0	0.95
DB00169	Cholecalciferol	1XGJ	0	0	0.82
DB00503	Ritonavir	1ILQ	0	0	0.77
DB01078	Deslanoside	1VRU	0	0	0.96

DB00253	Medrysone	1EXB	0	0	0.74
DB01393	Bezafibrate	1P87	0	0	0.97
DB00253	Medrysone	1Y38	0	0	0.95
DB01078	Deslanoside	1L9X	0	0	0.97
DB00511	Acetyldigitoxin	1UZF	0	0	0.99
DB00165	Pyridoxine	1IRU	0	0	0.97
DB00926	Etretinate	1HUL	0	1	0.66
DB00115	Cyanocobalamin	1CB6	0	0	0.87
DB00926	Etretinate	1ILQ	0	0	0.74
DB00511	Acetyldigitoxin	1E79	0	0	0.99
DB00511	Acetyldigitoxin	1DIA	0	0	0.99
DB01078	Deslanoside	1ODW	0	0	0.98
DB00115	Cyanocobalamin	2IL6	0	0	0.95
DB00253	Medrysone	1B2Y	0	0	0.82
DB00926	Etretinate	1FYC	0	1	0.43
DB01254	Dasatinib	1DON	0	0	0.99
DB00926	Etretinate	1D3H	0	1	0.45
DB00503	Ritonavir	1B6A	0	1	0.67
DB01327	Cefazolin	1P87	0	0	0.99
DB00843	Donepezil	1HOF	0	0	0.78
DB00253	Medrysone	2BAT	0	0	0.81
DB01601	Lopinavir	1DON	0	0	0.98
DB00253	Medrysone	1LSZ	0	0	0.89
DB00641	Simvastatin	1EH6	0	0	0.94
DB00253	Medrysone	1P5J	0	0	0.86
DB00396	Progesterone	3JDW	0	0	0.91
DB01045	Rifampin	1EMI	0	0	0.97
DB00503	Ritonavir	1BYW	0	1	0.62
DB00641	Simvastatin	1Y6R	0	0	0.92
DB00926	Etretinate	1QYE	0	1	0.55
DB00253	Medrysone	1HIG	0	0	0.81
DB01236	Sevoflurane	1P87	0	0	1.00
DB00576	Sulfamethizole	1P87	0	0	0.98
DB00576	Sulfamethizole	1P87	0	0	0.98
DB00253	Medrysone	1TYE	0	0	0.97
DB00843	Donepezil	1OF7	0	1	0.64
DB00717	Norethindrone	1Y38	0	1	0.67
DB00987	Cytarabine	1DON	0	0	0.96
DB00503	Ritonavir	1EII	0	1	0.65
DB00791	Uracil mustard	1DON	0	0	0.98
DB00843	Donepezil	1OKC	0	1	0.57
DB00843	Donepezil	1OD4	0	1	0.64
DB00253	Medrysone	1KPF	0	0	0.90
DB00843	Donepezil	1EMI	0	0	0.89

DB01395	Drospirenone	1E71	0	0	0.94
DB00641	Simvastatin	1E71	0	0	0.91
DB01395	Drospirenone	1KBQ	0	0	0.71
DB01395	Drospirenone	1CWM	0	0	0.96
DB01395	Drospirenone	1CYN	0	0	0.96
DB01395	Drospirenone	1YXM	0	0	0.77
DB01395	Drospirenone	1K7L	0	0	0.73
DB00253	Medrysone	1UYL	0	0	0.86
DB01395	Drospirenone	1BYW	0	0	0.97
DB01395	Drospirenone	1SQN	0	0	0.95
DB00648	Mitotane	1DON	0	0	0.99
DB00253	Medrysone	1YV5	0	0	0.88
DB01395	Drospirenone	1K2H	0	0	1.00
DB00253	Medrysone	1QKM	0	0	0.83
DB01395	Drospirenone	1HAG	0	1	0.62
DB00641	Simvastatin	1PT9	0	0	0.90
DB01395	Drospirenone	1I4L	0	0	0.94
DB01395	Drospirenone	1S78	0	0	0.93
DB01395	Drospirenone	1UHL	0	0	0.94
DB00253	Medrysone	1PO5	0	0	0.77
DB00115	Cyanocobalamin	1T3E	0	0	0.86
DB01395	Drospirenone	1Q9S	0	0	0.97
DB01406	Danazol	1IRU	0	0	0.98
DB00253	Medrysone	1CZM	0	0	0.83
DB01171	Moclobemide	1P87	0	0	0.99
DB01171	Moclobemide	1P87	0	0	0.99
DB00641	Simvastatin	1QR6	0	0	0.91
DB01406	Danazol	1IRU	0	0	0.98
DB01395	Drospirenone	1BJ4	0	0	0.95
DB01048	Abacavir	1IRU	0	0	0.98
DB06267	Udenafil	1A8M	0	0	0.75
DB06267	Udenafil	1KED	0	0	0.68
DB06267	Udenafil	1P49	0	0	0.68
DB06267	Udenafil	1HA2	0	1	0.58
DB06267	Udenafil	1QD2	0	0	0.75
DB06267	Udenafil	1EXX	0	0	0.76
DB00253	Medrysone	1UZF	0	0	0.80
DB06267	Udenafil	1TJC	0	0	0.73
DB06267	Udenafil	1BYW	0	0	0.80
DB01078	Deslanoside	1F0Y	0	0	0.96
DB00119	Pyruvic acid	1P87	0	0	1.00
DB06267	Udenafil	1YAE	0	0	0.73
DB06267	Udenafil	1NHZ	0	0	0.71
DB00232	Methyclothiazide	1P87	0	0	0.98

DB00253	Medrysone	1E3G	0	0	0.84
DB06267	Udenafil	1QKM	0	0	0.69
DB00253	Medrysone	1I5H	0	0	0.86
DB06267	Udenafil	1D3H	0	0	0.71
DB01078	Deslanoside	1NRL	0	0	0.96
DB06267	Udenafil	3CBS	0	0	0.77
DB06267	Udenafil	1T9N	0	0	0.69
DB00253	Medrysone	1HOF	0	0	0.92
DB06267	Udenafil	1CZM	0	0	0.70
DB00169	Cholecalciferol	1ZNC	0	0	0.71
DB00169	Cholecalciferol	1UTQ	0	0	0.71
DB06267	Udenafil	3BLM	0	0	0.73
DB06267	Udenafil	1UZF	0	1	0.64
DB06267	Udenafil	1E3G	0	0	0.71
DB06267	Udenafil	1HOF	0	0	0.85
DB06267	Udenafil	1MRQ	0	0	0.80
DB06267	Udenafil	1OHY	0	1	0.66
DB06267	Udenafil	1EMI	0	0	0.93
DB06267	Udenafil	1S3I	0	1	0.65
DB01259	Lapatinib	1P87	0	0	0.99
DB00232	Methyclothiazide	1P87	0	0	0.98
DB00641	Simvastatin	1S3A	0	0	0.90
DB00511	Acetyldigitoxin	1QVU	0	0	0.98
DB01078	Deslanoside	1KI0	0	0	0.98
DB01199	Tubocurarine	1DON	0	0	0.98
DB01601	Lopinavir	1HUL	0	0	0.71
DB00616	Candoxatril	1Y0X	0	0	0.90
DB00537	Ciprofloxacin	1DON	0	0	0.99
DB00511	Acetyldigitoxin	1GET	0	0	0.98
DB00641	Simvastatin	1AMO	0	0	0.94
DB00692	Phentolamine	1IRU	0	0	0.98
DB00604	Cisapride	1P87	0	0	0.95
DB00641	Simvastatin	1YOV	0	0	0.93
DB00926	Etretinate	1P5J	0	1	0.49
DB01199	Tubocurarine	1UMK	0	0	0.90
DB01601	Lopinavir	1J4I	0	1	0.65
DB01199	Tubocurarine	1ILQ	0	1	0.63
DB00621	Oxandrolone	1SA1	0	0	0.76
DB00641	Simvastatin	2BAT	0	0	0.91
DB00601	Linezolid	1P87	0	0	0.99
DB00926	Etretinate	1O5W	0	0	0.95
DB01395	Drospirenone	1HA2	0	0	0.94
DB01395	Drospirenone	1Y4E	0	0	0.99
DB00641	Simvastatin	1TLL	0	0	0.90

DB00926	Etretinate	1HOF	0	0	0.69
DB00253	Medrysone	1F8U	0	0	0.79
DB00621	Oxandrolone	1BYY	0	0	0.96
DB01395	Drospirenone	1MO8	0	0	0.96
DB00926	Etretinate	1HOF	0	0	0.69
DB00641	Simvastatin	1OAT	0	1	0.66
DB00641	Simvastatin	1FVO	0	0	0.88
DB01601	Lopinavir	1P4R	0	0	0.91
DB00926	Etretinate	1XF0	0	1	0.55
DB00115	Cyanocobalamin	1WVJ	0	0	0.94
DB01395	Drospirenone	1KED	0	0	0.95
DB01395	Drospirenone	1SA1	0	0	0.94
DB01395	Drospirenone	1TEV	0	0	0.96
DB01395	Drospirenone	1VJA	0	1	0.62
DB01395	Drospirenone	1VYT	0	0	0.95
DB00989	Rivastigmine	1EMI	0	1	0.44
DB00989	Rivastigmine	1P87	0	0	1.00
DB00641	Simvastatin	1B2Y	0	0	0.92
DB00197	Troglitazone	1DON	0	0	0.98
DB00378	Dydrogesterone	1EMI	0	0	0.95
DB00378	Dydrogesterone	1OHY	0	0	0.75
DB00378	Dydrogesterone	1F8U	0	0	0.72
DB00510	Divalproex sodium	1P87	0	0	0.98
DB00253	Medrysone	1P87	0	0	1.00
DB00641	Simvastatin	1CYN	0	0	0.94
DB00615	Rifabutin	1YTV	0	0	0.92
DB01123	Proflavine	1IRU	0	0	0.97
DB00692	Phentolamine	1DON	0	0	0.98
DB00926	Etretinate	1MRQ	0	1	0.55
DB00641	Simvastatin	2BIU	0	0	0.95
DB00641	Simvastatin	1OC3	0	0	0.87
DB00822	Disulfiram	1DON	0	0	0.98
DB00253	Medrysone	1EMI	0	0	0.96
DB00615	Rifabutin	1TZI	0	0	0.91
DB00641	Simvastatin	1ZBQ	0	0	0.93
DB00641	Simvastatin	1K7L	0	1	0.65
DB00621	Oxandrolone	1F5F	0	0	0.83
DB00641	Simvastatin	1Y0S	0	0	0.85
DB00615	Rifabutin	1Q11	0	0	0.97
DB01171	Moclobemide	1DON	0	0	0.99
DB00396	Progesterone	1J0X	0	0	0.92
DB00641	Simvastatin	1PBW	0	0	0.90
DB00603	Medroxyprogesterone	1A5Y	0	0	0.83
DB00603	Medroxyprogesterone	1SA1	0	0	0.80

DB00603	Medroxyprogesterone	1SA1	0	0	0.80
DB00641	Simvastatin	1Y38	0	0	0.98
DB00378	Dydrogesterone	1O5W	0	0	0.98
DB00691	Moexipril	1EMI	0	1	0.66
DB00691	Moexipril	1P87	0	0	0.99
DB01601	Lopinavir	1HOF	0	0	0.68
DB01601	Lopinavir	1HOF	0	0	0.68
DB01406	Danazol	1Y38	0	0	0.72
DB00621	Oxandrolone	1H0C	0	0	0.77
DB00616	Candoxatril	1X86	0	0	0.88
DB00641	Simvastatin	1KI0	0	0	0.91
DB00396	Progesterone	1PT9	0	0	0.89
DB00641	Simvastatin	1C5G	0	0	0.92
DB00511	Acetyldigoxin	1CZM	0	0	0.99
DB00691	Moexipril	1P4R	0	0	0.77
DB00926	Etretinate	1OF7	0	1	0.52
DB00621	Oxandrolone	1GGL	0	0	0.75
DB00819	Acetazolamide	1P87	0	0	0.99
DB00621	Oxandrolone	1SQN	0	0	0.78
DB00621	Oxandrolone	1Y6R	0	0	0.79
DB00641	Simvastatin	1BYW	0	0	0.95
DB00621	Oxandrolone	1B6A	0	0	0.88
DB00169	Cholecalciferol	1FIE	0	0	0.82
DB00197	Troglitazone	1P87	0	0	0.99
DB00615	Rifabutin	1A5Y	0	0	0.97
DB00641	Simvastatin	1SQN	0	0	0.92
DB00621	Oxandrolone	1ODW	0	0	0.86
DB00621	Oxandrolone	4Q21	0	0	0.85
DB00603	Medroxyprogesterone	1KGI	0	0	0.82
DB01108	Trilostane	1DON	0	0	0.98
DB00603	Medroxyprogesterone	1JNM	0	0	0.73
DB00621	Oxandrolone	1L1F	0	0	0.74
DB00621	Oxandrolone	1NHZ	0	0	0.80
DB00115	Cyanocobalamin	1NHZ	0	0	0.94
DB00397	Phenylpropanolamine	1P87	0	0	0.98
DB01108	Trilostane	1H2W	0	0	1.00
DB00115	Cyanocobalamin	1L9X	0	0	0.91
DB00691	Moexipril	1GCN	0	1	0.56
DB01103	Quinacrine	1P87	0	0	0.99
DB00115	Cyanocobalamin	1FE3	0	0	0.96
DB00621	Oxandrolone	1TQN	0	0	0.75
DB00603	Medroxyprogesterone	1NAV	0	0	0.86
DB00621	Oxandrolone	1QK1	0	0	0.73
DB00603	Medroxyprogesterone	1MO8	0	0	0.84

DB00621	Oxandrolone	1S5O	0	0	0.78
DB00621	Oxandrolone	1T9N	0	0	0.78
DB00621	Oxandrolone	1UZF	0	0	0.75
DB00621	Oxandrolone	1E3G	0	0	0.80
DB00977	Ethinyl Estradiol	1IRU	0	0	0.98
DB00641	Simvastatin	1TJC	0	0	0.93
DB00977	Ethinyl Estradiol	1IRU	0	0	0.98
DB00621	Oxandrolone	1HOF	0	0	0.90
DB00621	Oxandrolone	1HOF	0	0	0.90
DB00115	Cyanocobalamin	1XKT	0	0	0.92
DB00115	Cyanocobalamin	1A36	0	0	0.87
DB00616	Candoxatril	1F8U	0	0	0.85
DB00783	Estradiol	1P87	0	0	0.99
DB00115	Cyanocobalamin	1BNA	0	0	0.81
DB00615	Rifabutin	1SA1	0	0	0.97
DB00621	Oxandrolone	1F8U	0	0	0.75
DB00621	Oxandrolone	1OHY	0	0	0.77
DB01108	Trilostane	1P87	0	0	0.99
DB01108	Trilostane	1EMI	0	0	0.73
DB01083	Orlistat	1EW2	0	0	0.99
DB00641	Simvastatin	1H2W	0	0	1.00
DB00615	Rifabutin	1MB2	0	0	0.91
DB01096	Oxamniquine	1IRU	0	0	0.98
DB01225	Enoxaparin	1IRU	0	0	0.98
DB00115	Cyanocobalamin	1OCZ	0	0	0.91
DB00115	Cyanocobalamin	1XMI	0	0	0.89
DB01120	Gliclazide	1P87	0	0	0.99
DB00977	Ethinyl Estradiol	1BDA	0	0	0.82
DB00641	Simvastatin	1IRU	0	0	0.99
DB00615	Rifabutin	1WAP	0	0	0.99
DB01028	Methoxyflurane	1P87	0	0	1.00
DB00169	Cholecalciferol	1JBQ	0	0	0.97
DB00115	Cyanocobalamin	1KPH	0	0	0.84
DB00115	Cyanocobalamin	1P0Q	0	0	0.92
DB00691	Moexipril	1IRU	0	0	0.98
DB00691	Moexipril	1IRU	0	0	0.98
DB00513	Aminocaproic Acid	1H2W	0	0	1.00
DB00691	Moexipril	1WD8	0	1	0.57
DB00115	Cyanocobalamin	1F4J	0	0	0.94
DB01021	Trichlormethiazide	1IRU	0	0	0.99
DB01021	Trichlormethiazide	1IRU	0	0	0.99
DB00311	Ethoxzolamide	1P87	0	0	1.00
DB00311	Ethoxzolamide	1P87	0	0	1.00
DB04967	Lucanthone	1P87	0	0	1.00

DB00709	Lamivudine	1P87	0	0	0.97
DB00169	Cholecalciferol	1TQN	0	0	0.94
DB00641	Simvastatin	1IRU	0	0	0.99
DB00115	Cyanocobalamin	1IBC	0	0	0.96
DB00311	Ethoxzolamide	1IRU	0	0	0.98
DB00311	Ethoxzolamide	1DON	0	0	0.98
DB00691	Moexipril	1DON	0	0	0.98
DB00513	Aminocaproic Acid	1BDA	0	0	0.79
DB00169	Cholecalciferol	1CJY	0	0	0.75
DB00823	Ethynodiol Diacetate	1P87	0	0	1.00
DB00823	Ethynodiol Diacetate	1P87	0	0	1.00
DB00641	Simvastatin	1WD8	0	0	0.98
DB00511	Acetyldigitoxin	1L6J	0	0	0.98
DB00926	Etretinate	1HE5	0	1	0.49
DB00396	Progesterone	1SVC	0	0	0.87
DB00764	Mometasone	1P87	0	0	0.97
DB01118	Amiodarone	1P87	0	0	1.00
DB00641	Simvastatin	1OPL	0	1	0.66
DB00115	Cyanocobalamin	1PTW	0	0	0.86
DB00641	Simvastatin	1G1S	0	0	0.88
DB00115	Cyanocobalamin	1TB5	0	0	0.85
DB00641	Simvastatin	1NI4	0	1	0.67
DB00641	Simvastatin	1NI4	0	1	0.67
DB00641	Simvastatin	1I4L	0	0	0.91
DB00115	Cyanocobalamin	1KTA	0	0	0.85
DB00115	Cyanocobalamin	1E79	0	0	0.93
DB00115	Cyanocobalamin	1UZF	0	0	0.93
DB00641	Simvastatin	1S78	0	0	0.88
DB00115	Cyanocobalamin	1UZF	0	0	0.93
DB00615	Rifabutin	1Y4E	0	0	0.99
DB00641	Simvastatin	1XDK	0	1	0.66
DB00641	Simvastatin	1EXX	0	0	0.94
DB00615	Rifabutin	1F5F	0	0	0.98
DB00641	Simvastatin	1LBD	0	0	0.91
DB00115	Cyanocobalamin	2BK3	0	0	0.85
DB00641	Simvastatin	1UHL	0	0	0.90
DB00615	Rifabutin	1UHL	0	0	0.96
DB00926	Etretinate	1ORE	0	1	0.55
DB00115	Cyanocobalamin	1O5W	0	0	0.99
DB00989	Rivastigmine	1H2W	0	0	1.00
DB00615	Rifabutin	1LBD	0	0	0.95
DB00641	Simvastatin	1CRB	0	0	0.94
DB00321	Amitriptyline	1DON	0	0	0.98
DB00641	Simvastatin	1EII	0	0	0.95

DB00641	Simvastatin	1LN6	0	0	0.91
DB00641	Simvastatin	1C0B	0	0	0.97
DB00511	Acetyldigitoxin	1AUT	0	0	0.97
DB00641	Simvastatin	1QD2	0	0	0.94
DB00989	Rivastigmine	1BDA	0	0	0.93
DB00641	Simvastatin	1F8Q	0	0	0.94
DB00115	Cyanocobalamin	1HOF	0	0	0.96
DB00115	Cyanocobalamin	1HOF	0	0	0.96
DB00641	Simvastatin	2AAI	0	0	0.97
DB00641	Simvastatin	1OLM	0	0	0.89
DB00553	Methoxsalen	1P87	0	0	1.00
DB00115	Cyanocobalamin	1HT0	0	0	0.84
DB00641	Simvastatin	1H0C	0	0	0.92
DB00412	Rosiglitazone	1P87	0	0	1.00
DB00506	Norgestrel	1Q9S	0	1	0.54
DB00823	Ethinodiol Diacetate	1MRQ	0	1	0.58
DB00511	Acetyldigitoxin	1N2Z	0	0	0.99
DB00115	Cyanocobalamin	1OKC	0	0	0.94
DB00641	Simvastatin	1HA2	0	0	0.89
DB00115	Cyanocobalamin	1F8U	0	0	0.93
DB00727	Nitroglycerin	1P87	0	0	1.00
DB00822	Disulfiram	1P87	0	0	1.00
DB00115	Cyanocobalamin	2BIY	0	0	0.95
DB00822	Disulfiram	1P87	0	0	1.00
DB00615	Rifabutin	1EXX	0	0	0.98
DB00954	Dirithromycin	1VYT	0	0	0.99
DB00954	Dirithromycin	2KAU	0	0	0.98
DB00115	Cyanocobalamin	1EMI	0	0	0.98
DB00115	Cyanocobalamin	1EMI	0	0	0.98
DB00954	Dirithromycin	1A5Y	0	0	0.99
DB00384	Triamterene	1IRU	0	0	0.97
DB00954	Dirithromycin	1KED	0	0	0.99
DB00145	Glycine	1P87	0	0	0.98
DB00145	Glycine	1P87	0	0	0.98
DB00145	Glycine	1H2W	0	0	1.00
DB00145	Glycine	1IRU	0	0	0.97
DB00954	Dirithromycin	1JNM	0	0	0.99
DB00823	Ethinodiol Diacetate	1EW2	0	1	0.46
DB00629	Guanabenz	1H2W	0	0	1.00
DB00629	Guanabenz	1IRU	0	0	0.99
DB00603	Medroxyprogesterone	1YVL	0	0	0.79
DB00764	Mometasone	1DON	0	0	0.99
DB00148	Creatine	1H2W	0	0	1.00
DB00226	Guanadrel Sulfate	1P87	0	0	0.96

DB00226	Guanadrel Sulfate	1DON	0	0	0.99
DB00148	Creatine	1P87	0	0	0.94
DB00954	Dirithromycin	1MO8	0	0	0.99
DB00605	Sulindac	1P87	0	0	0.99
DB00954	Dirithromycin	1YVL	0	0	0.99
DB01009	Ketoprofen	1BDA	0	0	0.78
DB01009	Ketoprofen	1IRU	0	0	0.98
DB01009	Ketoprofen	1IRU	0	0	0.98
DB00954	Dirithromycin	1HA2	0	0	0.99
DB00954	Dirithromycin	1H0C	0	0	0.99
DB01009	Ketoprofen	1P87	0	0	1.00
DB01009	Ketoprofen	1P87	0	0	1.00
DB00823	Ethinodiol Diacetate	1HOF	0	0	0.72
DB00615	Rifabutin	1XDK	0	0	0.92
DB00603	Medroxyprogesterone	1F5F	0	0	0.86
DB01172	Kanamycin	1DON	0	0	0.93
DB00410	Mupirocin	1OHY	0	0	0.75
DB00410	Mupirocin	1OKC	0	0	0.80
DB01103	Quinacrine	1IRU	0	0	0.99
DB01103	Quinacrine	1IRU	0	0	0.99
DB00603	Medroxyprogesterone	1H0C	0	0	0.81
DB00823	Ethinodiol Diacetate	1HOF	0	0	0.72
DB00603	Medroxyprogesterone	1BJ4	0	0	0.82
DB00605	Sulindac	1P87	0	0	0.99
DB00823	Ethinodiol Diacetate	1BV8	0	1	0.50
DB00396	Progesterone	1B2Y	0	0	0.91
DB00755	Tretinoin	1DON	0	0	0.98
DB00410	Mupirocin	1OF7	0	0	0.85
DB01089	Deserpidine	1V97	0	0	0.94
DB00970	Dactinomycin	1EMI	0	0	1.00
DB00169	Cholecalciferol	1A36	0	0	0.82
DB00603	Medroxyprogesterone	1LBD	0	0	0.81
DB00603	Medroxyprogesterone	1EXX	0	0	0.86
DB00926	Etretinate	1EH6	0	1	0.50
DB00286	Conjugated Estrogens	1DON	0	0	0.98
DB00957	Norgestimate	1EMI	0	0	0.94
DB00926	Etretinate	1AMO	0	1	0.47
DB00823	Ethinodiol Diacetate	1K6R	0	1	0.65
DB00410	Mupirocin	1E3G	0	0	0.80
DB00755	Tretinoin	1IRU	0	0	0.98
DB00755	Tretinoin	1IRU	0	0	0.98
DB01406	Danazol	1ILQ	0	1	0.64
DB00865	Benzphetamine	1P87	0	0	1.00
DB01028	Methoxyflurane	1P87	0	0	1.00

DB00603	Medroxyprogesterone	1TJC	0	0	0.85
DB00823	Ethinodiol Diacetate	1CZM	0	1	0.45
DB00641	Simvastatin	1DON	0	0	0.98
DB00410	Mupirocin	1UZF	0	0	0.74
DB00410	Mupirocin	1CZM	0	0	0.79
DB00641	Simvastatin	1SD2	0	0	0.93
DB00410	Mupirocin	1T9N	0	0	0.77
DB00603	Medroxyprogesterone	1SQN	0	0	0.82
DB00823	Ethinodiol Diacetate	1S5O	0	1	0.46
DB00506	Norgestrel	2BIU	0	1	0.54
DB00615	Rifabutin	1BXS	0	0	0.91
DB00641	Simvastatin	1Y4E	0	0	0.98
DB00436	Bendroflumethiazide	1DON	0	0	0.99
DB00410	Mupirocin	1D6G	0	0	0.86
DB00615	Rifabutin	1NI4	0	0	0.92
DB00926	Etretinate	1CWM	0	1	0.50
DB00823	Ethinodiol Diacetate	1JBQ	0	1	0.58
DB00603	Medroxyprogesterone	1EXB	0	0	0.73
DB00436	Bendroflumethiazide	1H2W	0	0	1.00
DB00511	Acetyldigitoxin	1A8M	0	0	0.99
DB00169	Cholecalciferol	1IVO	0	0	0.79
DB00881	Quinapril	1P87	0	0	0.99
DB00506	Norgestrel	1TYE	0	0	0.88
DB00970	Dactinomycin	1GXD	0	0	0.99
DB00336	Nitrofurazone	1DON	0	0	0.95
DB04948	Lofexidine	1P87	0	0	0.99
DB04948	Lofexidine	1P87	0	0	0.99
DB00641	Simvastatin	1MO8	0	0	0.93
DB00655	Estrone	1P87	0	0	1.00
DB00256	Lymecycline	1H2W	0	0	1.00
DB00603	Medroxyprogesterone	1C5G	0	0	0.82
DB00823	Ethinodiol Diacetate	1D3H	0	1	0.49
DB00410	Mupirocin	1JBQ	0	0	0.86
DB00655	Estrone	1P87	0	0	1.00
DB01096	Oxamniquine	1P87	0	0	0.98
DB00511	Acetyldigitoxin	1Z6J	0	0	0.97
DB00970	Dactinomycin	1ORE	0	0	0.99
DB00603	Medroxyprogesterone	2BIU	0	0	0.88
DB01096	Oxamniquine	1P87	0	0	0.98
DB01078	Deslanoside	1WD8	0	0	0.99
DB00410	Mupirocin	1QKM	0	0	0.77
DB00410	Mupirocin	1YV5	0	0	0.85
DB00603	Medroxyprogesterone	1B2Y	0	0	0.81
DB00511	Acetyldigitoxin	1XMI	0	0	0.98

DB00410	Mupirocin	1J4I	0	0	0.87
DB01078	Deslanoside	1HAG	0	0	0.96
DB00641	Simvastatin	1VMC	0	0	0.96
DB00410	Mupirocin	1YAE	0	0	0.81
DB00410	Mupirocin	1ODW	0	0	0.85
DB00641	Simvastatin	1SLM	0	0	0.93
DB00957	Norgestimate	1P87	0	0	1.00
DB01078	Deslanoside	1BBS	0	0	0.96
DB00970	Dactinomycin	1P1R	0	0	0.99
DB00410	Mupirocin	1B6A	0	0	0.88
DB00603	Medroxyprogesterone	9ILB	0	0	0.88
DB01078	Deslanoside	1BXS	0	0	0.96
DB00926	Etretinate	1MZW	0	1	0.51
DB00603	Medroxyprogesterone	1HIG	0	0	0.80
DB00410	Mupirocin	1B2Y	0	0	0.73
DB00641	Simvastatin	1EYD	0	0	0.95
DB00603	Medroxyprogesterone	1ODW	0	0	0.88
DB01119	Diazoxide	1DON	0	0	0.99
DB00641	Simvastatin	1NAV	0	0	0.94
DB00410	Mupirocin	1I7I	0	0	0.71
DB00603	Medroxyprogesterone	1WVJ	0	0	0.85
DB00410	Mupirocin	1SQN	0	0	0.79
DB00603	Medroxyprogesterone	1WVJ	0	0	0.85
DB01078	Deslanoside	1SG0	0	0	0.98
DB00410	Mupirocin	1H2W	0	0	1.00
DB01078	Deslanoside	1HA2	0	0	0.97
DB00641	Simvastatin	1Y0X	0	0	0.94
DB00641	Simvastatin	1X86	0	0	0.93
DB00736	Esomeprazole	1IRU	0	0	0.98
DB00266	Dicumarol	1P87	0	0	0.99
DB00603	Medroxyprogesterone	1L1F	0	0	0.78
DB00641	Simvastatin	1KED	0	0	0.92
DB00755	Tretinoin	1P87	0	0	1.00
DB00641	Simvastatin	1SA1	0	0	0.91
DB01170	Guanethidine	1DON	0	0	0.98
DB00981	Physostigmine	1P87	0	0	1.00
DB00410	Mupirocin	1EXX	0	0	0.83
DB00410	Mupirocin	1GGL	0	0	0.75
DB00410	Mupirocin	1C0B	0	0	0.92
DB00410	Mupirocin	1HA2	0	1	0.65
DB00410	Mupirocin	1F5F	0	0	0.83
DB00410	Mupirocin	1MO8	0	0	0.80
DB00410	Mupirocin	1SLM	0	0	0.77
DB00374	Treprostinil	1DON	0	0	0.98

DB00823	Ethynodiol Diacetate	1YV5	0	1	0.56
DB00410	Mupirocin	1VYT	0	0	0.71
DB00954	Dirithromycin	1UHL	0	0	0.99
DB01018	Guanfacine	1H2W	0	0	1.00
DB00823	Ethynodiol Diacetate	1FE3	0	1	0.55
DB01218	Halofantrine	1P87	0	0	1.00
DB00378	Dydrogesterone	1CZM	0	0	0.77
DB01218	Halofantrine	1DON	0	0	0.99
DB00374	Treprostinil	1K2H	0	0	0.97
DB00954	Dirithromycin	1EXX	0	0	0.99
DB00954	Dirithromycin	1BBS	0	0	0.98
DB00378	Dydrogesterone	1T9N	0	0	0.76
DB00954	Dirithromycin	1I4L	0	0	0.99
DB00641	Simvastatin	1SA1	0	0	0.91
DB00378	Dydrogesterone	1G0W	0	0	0.73
DB00641	Simvastatin	1A8M	0	0	0.94
DB00584	Enalapril	1O5W	0	1	0.55
DB01121	Phenacemide	1DON	0	0	0.96
DB00954	Dirithromycin	1EXB	0	0	0.99
DB00926	Etretinate	2BIY	0	1	0.47
DB00954	Dirithromycin	1I7I	0	0	0.99
DB00378	Dydrogesterone	1YV5	0	0	0.83
DB00378	Dydrogesterone	1L9X	0	0	0.80
DB00954	Dirithromycin	1B6A	0	0	0.99
DB00954	Dirithromycin	9ILB	0	0	0.99
DB00378	Dydrogesterone	1L1F	0	0	0.73
DB00378	Dydrogesterone	1BWC	0	0	0.74
DB00970	Dactinomycin	1HOF	0	0	0.99
DB00641	Simvastatin	1Q11	0	0	0.92
DB01159	Halothane	1P87	0	0	1.00
DB01159	Halothane	1IRU	0	0	1.00
DB00378	Dydrogesterone	1HUL	0	0	0.89
DB00954	Dirithromycin	1T3E	0	0	0.98
DB00926	Etretinate	1Y38	0	0	0.80
DB01159	Halothane	1IRU	0	0	1.00
DB01159	Halothane	1DON	0	0	0.98
DB00954	Dirithromycin	1L1F	0	0	0.99
DB00378	Dydrogesterone	1W7N	0	0	0.76
DB00378	Dydrogesterone	1L6J	0	1	0.67
DB00641	Simvastatin	1UAE	0	0	0.93
DB00954	Dirithromycin	1VRU	0	0	0.98
DB00970	Dactinomycin	1O5W	0	0	1.00
DB00954	Dirithromycin	1XWD	0	0	0.98
DB00954	Dirithromycin	1QKM	0	0	0.99

DB00954	Dirithromycin	1R5K	0	0	0.98
DB01078	Deslanoside	1MO8	0	0	0.98
DB01078	Deslanoside	1MB2	0	0	0.96
DB00954	Dirithromycin	1UT1	0	0	0.98
DB00954	Dirithromycin	1BDF	0	0	0.98
DB00954	Dirithromycin	1F0X	0	0	0.98
DB00954	Dirithromycin	1RFN	0	0	0.98
DB00374	Treprostinil	1P87	0	0	0.96
DB00954	Dirithromycin	1CZM	0	0	0.99
DB00954	Dirithromycin	1KTA	0	0	0.98
DB00970	Dactinomycin	1UZF	0	0	0.99
DB00526	Oxaliplatin	1IRU	0	0	0.97
DB00954	Dirithromycin	1E79	0	0	0.99
DB00823	Ethynodiol Diacetate	1SS2	0	1	0.49
DB00823	Ethynodiol Diacetate	1NHZ	0	1	0.46
DB00584	Enalapril	1P87	0	0	0.99
DB00823	Ethynodiol Diacetate	1WVJ	0	1	0.49
DB00954	Dirithromycin	1AJS	0	0	0.98
DB00970	Dactinomycin	1E79	0	0	0.99
DB00954	Dirithromycin	1UZF	0	0	0.99
DB00823	Ethynodiol Diacetate	1YAE	0	1	0.50
DB00954	Dirithromycin	1E3G	0	0	0.99
DB00954	Dirithromycin	1BV8	0	0	0.99
DB00954	Dirithromycin	1HOF	0	0	0.99
DB00542	Benazepril	1IRU	0	0	0.98
DB00954	Dirithromycin	1OKC	0	0	0.99
DB00542	Benazepril	1IRU	0	0	0.98
DB00210	Adapalene	1P87	0	0	1.00
DB00970	Dactinomycin	1TB5	0	0	0.99
DB00881	Quinapril	1IRU	0	0	0.98
DB00169	Cholecalciferol	1YV5	0	0	0.97
DB00954	Dirithromycin	1F8U	0	0	0.99
DB00926	Etretinate	1BYW	0	1	0.56
DB00210	Adapalene	1P87	0	0	1.00
DB00169	Cholecalciferol	1J4I	0	0	0.97
DB00641	Simvastatin	2KAU	0	1	0.67
DB00954	Dirithromycin	1EMI	0	0	0.99
DB01092	Ouabain	1IRU	0	0	0.98
DB00270	Isradipine	1UMK	0	1	0.44
DB00169	Cholecalciferol	4Q21	0	0	0.96
DB00823	Ethynodiol Diacetate	1ODW	0	1	0.58
DB04575	Quinestrol	1EMI	0	0	0.92
DB04575	Quinestrol	1OHY	0	1	0.61
DB00879	Emtricitabine	1H2W	0	0	1.00

DB00926	Etretinate	1RV7	0	1	0.53
DB01121	Phenacemide	1IRU	0	0	0.97
DB04575	Quinestrol	1MF1	0	1	0.65
DB00926	Etretinate	1K2H	0	0	1.00
DB00378	Dydrogesterone	1MZW	0	0	0.82
DB04575	Quinestrol	1HOF	0	0	0.82
DB00256	Lymecycline	1DON	0	0	0.99
DB04575	Quinestrol	1UZF	0	1	0.57
DB00378	Dydrogesterone	1I7I	0	1	0.66
DB04575	Quinestrol	1H6I	0	0	0.72
DB04575	Quinestrol	1CZM	0	1	0.64
DB00169	Cholecalciferol	1GP2	0	0	0.79
DB01121	Phenacemide	1IRU	0	0	0.97
DB04575	Quinestrol	1T9N	0	1	0.62
DB00641	Simvastatin	1T0U	0	0	0.91
DB00641	Simvastatin	1YTV	0	1	0.67
DB00378	Dydrogesterone	1EXB	0	1	0.66
DB04575	Quinestrol	1CP3	0	1	0.60
DB00834	Mifepristone	1VYT	0	0	0.76
DB00641	Simvastatin	1N2Z	0	0	0.90
DB00970	Dactinomycin	1T9N	0	0	0.99
DB04575	Quinestrol	2CBR	0	0	0.71
DB04575	Quinestrol	1T9R	0	1	0.65
DB04575	Quinestrol	1QKM	0	1	0.63
DB01194	Brinzolamide	1DON	0	0	0.98
DB04575	Quinestrol	1FE3	0	0	0.72
DB04575	Quinestrol	1NHZ	0	1	0.65
DB00834	Mifepristone	1TEV	0	0	0.84
DB00641	Simvastatin	1KXP	0	0	0.68
DB00665	Nilutamide	1P87	0	0	1.00
DB00603	Medroxyprogesterone	1PB7	0	0	0.86
DB04575	Quinestrol	1YAE	0	0	0.68
DB00616	Candoxatril	1OHY	0	0	0.86
DB00615	Rifabutin	1HAG	0	0	0.91
DB00834	Mifepristone	1X86	0	0	0.79
DB00970	Dactinomycin	1S5O	0	0	0.99
DB00615	Rifabutin	1K2H	0	0	0.98
DB04575	Quinestrol	1ODW	0	0	0.74
DB01089	Deserpidine	1E3G	0	0	0.90
DB04575	Quinestrol	1QLZ	0	1	0.65
DB00957	Norgestimate	1HNK	0	0	0.84
DB00834	Mifepristone	2TRT	0	0	0.77
DB00970	Dactinomycin	1IBC	0	0	0.99
DB00834	Mifepristone	1SLM	0	0	0.79

DB01166	Cilostazol	1O5W	0	0	0.85
DB00276	Amsacrine	1H2W	0	0	1.00
DB04575	Quinestrol	1B2Y	0	1	0.61
DB00926	Etretinate	1G5X	0	1	0.47
DB04575	Quinestrol	1C5G	0	1	0.63
DB04575	Quinestrol	1SQN	0	1	0.62
DB04575	Quinestrol	1BP3	0	1	0.57
DB00449	Dipivefrin	1BYY	0	1	0.59
DB00926	Etretinate	1EXX	0	1	0.48
DB00926	Etretinate	1LPJ	0	1	0.49
DB00926	Etretinate	1CRB	0	1	0.47
DB00834	Mifepristone	1F5F	0	0	0.83
DB00449	Dipivefrin	1K2H	0	0	0.99
DB00970	Dactinomycin	1CJY	0	0	0.98
DB00970	Dactinomycin	1BNA	0	0	0.98
DB01064	Isoproterenol	1P87	0	0	0.93
DB00199	Erythromycin	1VYT	0	0	0.98
DB00926	Etretinate	1F8Q	0	1	0.50
DB00199	Erythromycin	1KXP	0	0	0.96
DB04575	Quinestrol	1F5F	0	0	0.70
DB00926	Etretinate	1P87	0	0	1.00
DB01006	Letrozole	1P87	0	0	1.00
DB00970	Dactinomycin	1R5K	0	0	0.99
DB00970	Dactinomycin	1FTA	0	0	0.99
DB00641	Simvastatin	1VYT	0	0	0.92
DB00641	Simvastatin	1V97	0	0	0.96
DB00951	Isoniazid	1DON	0	0	0.95
DB00834	Mifepristone	1HA2	0	0	0.71
DB00970	Dactinomycin	1VRU	0	0	0.99
DB00302	Tranexamic Acid	1BDA	0	0	0.81
DB04575	Quinestrol	1X86	0	1	0.65
DB00970	Dactinomycin	1L9X	0	0	0.99
DB00834	Mifepristone	1LN6	0	0	0.74
DB00511	Acetyldigitoxin	1SVC	0	0	0.98
DB04575	Quinestrol	1IIH	0	1	0.62
DB00169	Cholecalciferol	1ILQ	0	0	0.98
DB00641	Simvastatin	1G5X	0	0	0.93
DB00877	Sirolimus	1EMI	0	0	1.00
DB00877	Sirolimus	1HNK	0	0	0.99
DB00823	Ethinodiol Diacetate	1ILQ	0	0	0.77
DB00199	Erythromycin	1SA1	0	0	0.98
DB02709	Resveratrol	1P87	0	0	0.97
DB00951	Isoniazid	1H2W	0	0	1.00
DB01093	Dimethyl sulfoxide	1IRU	0	0	0.98

DB01093	Dimethyl sulfoxide	1IRU	0	0	0.98
DB01093	Dimethyl sulfoxide	1H2W	0	0	1.00
DB01093	Dimethyl sulfoxide	1P87	0	0	0.99
DB01325	Quinethazone	1P87	0	0	0.94
DB00703	Methazolamide	1P87	0	0	1.00
DB00970	Dactinomycin	1NHZ	0	0	0.99
DB00286	Conjugated Estrogens	1P87	0	0	1.00
DB00823	Ethinodiol Diacetate	1B6A	0	1	0.63
DB00834	Mifepristone	1EXX	0	0	0.83
DB00173	Adenine	1P87	0	0	0.98
DB00926	Etretinate	1F5F	0	1	0.49
DB00877	Sirolimus	1F8U	0	0	0.99
DB00926	Etretinate	1DON	0	0	0.98
DB00823	Ethinodiol Diacetate	1EH6	0	1	0.53
DB00926	Etretinate	1SD2	0	1	0.49
DB00199	Erythromycin	1MO8	0	0	0.98
DB00603	Medroxyprogesterone	1L9X	0	0	0.84
DB00390	Digoxin	1VYT	0	0	0.97
DB00823	Ethinodiol Diacetate	1AMO	0	1	0.51
DB00390	Digoxin	1VJA	0	0	0.95
DB00720	Clodronate	1DON	0	0	0.98
DB00199	Erythromycin	1DON	0	0	0.98
DB00390	Digoxin	1SA1	0	0	0.98
DB00390	Digoxin	1WAP	0	0	0.99
DB00390	Digoxin	1DON	0	0	0.98
DB00390	Digoxin	1BJ4	0	0	0.98
DB00603	Medroxyprogesterone	1SS2	0	0	0.84
DB00390	Digoxin	1RTU	0	0	0.99
DB01564	Calusterone	1Y38	0	0	0.94
DB00603	Medroxyprogesterone	1FTA	0	0	0.86
DB00603	Medroxyprogesterone	1YV5	0	0	0.88
DB00390	Digoxin	1BXS	0	0	0.95
DB00390	Digoxin	1NI4	0	0	0.95
DB00390	Digoxin	1G1S	0	0	0.97
DB00390	Digoxin	1HAG	0	0	0.95
DB00390	Digoxin	1SQN	0	0	0.98
DB02709	Resveratrol	1P87	0	0	0.97
DB00456	Cefalotin	1P87	0	0	0.99
DB00603	Medroxyprogesterone	1QYE	0	0	0.89
DB00615	Rifabutin	1SQN	0	0	0.97
DB01564	Calusterone	1LSZ	0	0	0.86
DB00390	Digoxin	1BYW	0	0	0.98
DB00390	Digoxin	1PBW	0	0	0.97
DB00390	Digoxin	1Y0S	0	0	0.97

DB00390	Digoxin	1W7N	0	0	0.97
DB00390	Digoxin	2IL6	0	0	0.98
DB00877	Sirolimus	1HSZ	0	0	0.98
DB00877	Sirolimus	1D1S	0	0	0.98
DB00199	Erythromycin	1JQI	0	0	0.96
DB00459	Acitretin	1P87	0	0	1.00
DB00877	Sirolimus	1HOF	0	0	0.99
DB00877	Sirolimus	1HOF	0	0	0.99
DB00615	Rifabutin	1BYW	0	0	0.98
DB00877	Sirolimus	1UZF	0	0	0.99
DB00519	Trandolapril	2AAI	0	1	0.66
DB00199	Erythromycin	1HA2	0	0	0.97
DB00877	Sirolimus	1RGY	0	0	0.99
DB00877	Sirolimus	1T9N	0	0	0.99
DB00877	Sirolimus	1T9R	0	0	0.99
DB00390	Digoxin	1BWC	0	0	0.97
DB00823	Ethynodiol Diacetate	1RV7	0	1	0.56
DB00001	Lepirudin	1UJW	0	0	0.97
DB01564	Calusterone	1NHZ	0	0	0.79
DB00199	Erythromycin	1H0C	0	0	0.98
DB00823	Ethynodiol Diacetate	1EII	0	1	0.60
DB00957	Norgestimate	1F8U	0	1	0.67
DB00519	Trandolapril	1Y38	0	0	0.77
DB00390	Digoxin	1YAE	0	0	0.98
DB00001	Lepirudin	1YTV	0	0	0.97
DB00390	Digoxin	1NHZ	0	0	0.98
DB00823	Ethynodiol Diacetate	1F5F	0	1	0.53
DB00390	Digoxin	1GCN	0	0	0.99
DB00823	Ethynodiol Diacetate	1MO8	0	1	0.48
DB00957	Norgestimate	1ORE	0	0	0.81
DB00390	Digoxin	1VRU	0	0	0.96
DB00519	Trandolapril	1ILQ	0	0	0.70
DB00390	Digoxin	1YV5	0	0	0.98
DB00877	Sirolimus	1P0S	0	0	0.98
DB00615	Rifabutin	1KI0	0	0	0.97
DB00877	Sirolimus	1LJ7	0	0	0.99
DB00615	Rifabutin	1JYD	0	0	0.98
DB00390	Digoxin	1BNA	0	0	0.95
DB00001	Lepirudin	1A8M	0	0	0.97
DB00199	Erythromycin	1LN6	0	0	0.98
DB00390	Digoxin	1GTE	0	0	0.97
DB00390	Digoxin	1PO5	0	0	0.97
DB00390	Digoxin	1LJ7	0	0	0.98
DB00615	Rifabutin	1Y0S	0	0	0.95

DB00199	Erythromycin	1EXX	0	0	0.99
DB00001	Lepirudin	1SA1	0	0	0.97
DB00390	Digoxin	1ZNC	0	0	0.95
DB00390	Digoxin	1CZM	0	0	0.98
DB00845	Clofazimine	1P87	0	0	0.99
DB00823	Ethinodiol Diacetate	1A8M	0	1	0.51
DB01564	Calusterone	1FYC	0	0	0.77
DB00519	Trandolapril	1K6R	0	1	0.58
DB00199	Erythromycin	1RFV	0	0	0.98
DB00169	Cholecalciferol	5MDH	0	0	0.80
DB00390	Digoxin	1TB5	0	0	0.95
DB00390	Digoxin	1KTA	0	0	0.95
DB01564	Calusterone	1J3S	0	0	0.68
DB00519	Trandolapril	1HOF	0	1	0.62
DB00390	Digoxin	1UZF	0	0	0.97
DB01564	Calusterone	1HKO	0	0	0.84
DB00542	Benazepril	1P87	0	0	0.99
DB00390	Digoxin	1UZF	0	0	0.97
DB01262	Decitabine	1P87	0	0	0.92
DB00603	Medroxyprogesterone	1D3H	0	0	0.84
DB00542	Benazepril	1P87	0	0	0.99
DB00603	Medroxyprogesterone	1JBQ	0	0	0.89
DB01564	Calusterone	1T9R	0	0	0.79
DB00603	Medroxyprogesterone	1T9N	0	0	0.82
DB00390	Digoxin	2BK3	0	0	0.95
DB00390	Digoxin	1HOF	0	0	0.98
DB00390	Digoxin	1HOF	0	0	0.98
DB06692	Aprotinin	1EMI	0	0	0.97
DB06692	Aprotinin	1EMI	0	0	0.97
DB06692	Aprotinin	1P87	0	0	0.87
DB06692	Aprotinin	1HWL	0	0	0.96
DB06692	Aprotinin	1HNK	0	0	0.97
DB06692	Aprotinin	1OHY	0	0	0.97
DB06692	Aprotinin	1F8U	0	0	0.97
DB06692	Aprotinin	1ORE	0	0	0.97
DB06692	Aprotinin	1OKC	0	0	0.97
DB06692	Aprotinin	1OF7	0	0	0.97
DB06692	Aprotinin	1HOF	0	0	0.97
DB06692	Aprotinin	1HOF	0	0	0.97
DB06692	Aprotinin	2BK3	0	0	0.97
DB06692	Aprotinin	1E3G	0	0	0.97
DB06692	Aprotinin	1JVQ	0	0	0.97
DB06692	Aprotinin	1AJS	0	0	0.97
DB06692	Aprotinin	1Q2P	0	0	0.97

DB06692	Aprotinin	1UWJ	0	0	0.97
DB06692	Aprotinin	1DIA	0	0	0.97
DB06692	Aprotinin	1TB5	0	0	0.97
DB06692	Aprotinin	1CZM	0	0	0.97
DB06692	Aprotinin	1T9N	0	0	0.97
DB06692	Aprotinin	1F4J	0	0	0.97
DB06692	Aprotinin	1T9R	0	0	0.97
DB06692	Aprotinin	1P0S	0	0	0.96
DB06692	Aprotinin	1XU9	0	0	0.97
DB06692	Aprotinin	1JBQ	0	0	0.97
DB06692	Aprotinin	1XMI	0	0	0.96
DB00539	Toremifene	1P87	0	0	0.99
DB00390	Digoxin	1P1R	0	0	0.97
DB00390	Digoxin	1OHY	0	0	0.98
DB01564	Calusterone	1T9N	0	0	0.77
DB00834	Mifepristone	1R6K	0	0	0.74
DB00390	Digoxin	1EMI	0	0	0.99
DB01396	Digitoxin	1YTV	0	0	0.96
DB01396	Digitoxin	1T0U	0	0	0.98
DB01396	Digitoxin	1SA1	0	0	0.98
DB01396	Digitoxin	2TRT	0	0	0.98
DB01396	Digitoxin	1Y4E	0	0	0.99
DB01396	Digitoxin	1BYY	0	0	0.99
DB01564	Calusterone	3BLM	0	0	0.81
DB00615	Rifabutin	1K7L	0	0	0.92
DB01396	Digitoxin	1F5F	0	0	0.98
DB00756	Hexachlorophene	1P87	0	0	1.00
DB01396	Digitoxin	1HA2	0	0	0.97
DB01396	Digitoxin	1BJ4	0	0	0.98
DB01396	Digitoxin	1C0B	0	0	0.99
DB01396	Digitoxin	1NI4	0	0	0.96
DB00603	Medroxyprogesterone	1Q2P	0	0	0.84
DB00941	Hexafluronium bromide	1P87	0	0	1.00
DB01396	Digitoxin	1NI4	0	0	0.96
DB01396	Digitoxin	1HAG	0	0	0.96
DB01396	Digitoxin	1IRU	0	0	1.00
DB01275	Hydralazine	1P87	0	0	0.98
DB01396	Digitoxin	1SQN	0	0	0.98
DB01396	Digitoxin	1BYW	0	0	0.99
DB00677	Isoflurophate	1DON	0	0	0.99
DB00603	Medroxyprogesterone	1UZF	0	0	0.79
DB01396	Digitoxin	1ZBQ	0	0	0.98
DB01396	Digitoxin	1NRL	0	0	0.96
DB01396	Digitoxin	1UMK	0	0	1.00

DB00999	Hydrochlorothiazide	1IRU	0	0	0.99
DB01396	Digitoxin	1LSZ	0	0	0.99
DB01564	Calusterone	1HOF	0	0	0.90
DB01564	Calusterone	1HOF	0	0	0.90
DB00603	Medroxyprogesterone	1E3G	0	0	0.84
DB00603	Medroxyprogesterone	1Q7L	0	0	0.85
DB01564	Calusterone	1OF7	0	0	0.84
DB00133	L-Serine	1IRU	0	0	0.97
DB00615	Rifabutin	1CYN	0	0	0.97
DB00134	L-Methionine	1P87	0	0	0.98
DB00877	Sirolimus	1J3S	0	0	0.99
DB00511	Acetyldigitoxin	1BNA	0	0	0.97
DB00273	Topiramate	1BYY	0	1	0.66
DB01564	Calusterone	1ORE	0	0	0.85
DB00877	Sirolimus	1TQN	0	0	0.99
DB00149	L-Leucine	1DON	0	0	0.97
DB01564	Calusterone	1F8U	0	0	0.73
DB00615	Rifabutin	1CWM	0	0	0.97
DB01564	Calusterone	1OHY	0	0	0.76
DB01396	Digitoxin	1CB6	0	0	0.97
DB01564	Calusterone	1HNK	0	0	0.88
DB01396	Digitoxin	2IL6	0	0	0.98
DB01396	Digitoxin	1MQ8	0	0	0.96
DB01396	Digitoxin	1M1X	0	0	0.96
DB00199	Erythromycin	1IRU	0	0	1.00
DB04573	Estriol	1DON	0	0	0.98
DB00150	L-Tryptophan	1P87	0	0	0.95
DB01564	Calusterone	1EMI	0	0	0.95
DB01245	Decamethonium	1UJW	0	0	0.70
DB01245	Decamethonium	1A8M	0	0	0.96
DB00603	Medroxyprogesterone	1O5W	0	0	0.98
DB01396	Digitoxin	1QVU	0	0	0.96
DB00149	L-Leucine	1P87	0	0	0.98
DB01396	Digitoxin	1UYL	0	0	0.98
DB00273	Topiramate	1UMK	0	0	0.82
DB01245	Decamethonium	1IIH	0	0	0.95
DB01396	Digitoxin	1AGS	0	0	0.98
DB01245	Decamethonium	1X86	0	0	0.95
DB01396	Digitoxin	1BWC	0	0	0.98
DB01245	Decamethonium	1MO8	0	0	0.95
DB00167	L-Isoleucine	1IRU	0	0	0.98
DB01396	Digitoxin	1XHY	0	0	0.98
DB01396	Digitoxin	1WVJ	0	0	0.98
DB00603	Medroxyprogesterone	1BV8	0	0	0.85

DB00282	Pamidronate	1DON	0	0	0.89
DB01245	Decamethonium	1SD2	0	0	0.96
DB01396	Digitoxin	1NHZ	0	0	0.98
DB01089	Deserpidine	1RTU	0	0	0.96
DB01245	Decamethonium	1EXX	0	0	0.96
DB01396	Digitoxin	1QKM	0	0	0.98
DB01245	Decamethonium	1BXS	0	1	0.60
DB00615	Rifabutin	1NRL	0	0	0.92
DB01245	Decamethonium	1S78	0	0	0.92
DB00294	Etonogestrel	1P87	0	0	1.00
DB01245	Decamethonium	1SQN	0	0	0.95
DB00294	Etonogestrel	1P87	0	0	1.00
DB01396	Digitoxin	1A36	0	0	0.97
DB01245	Decamethonium	1C5G	0	0	0.95
DB01396	Digitoxin	8ICK	0	0	0.98
DB01396	Digitoxin	1GTE	0	0	0.98
DB01396	Digitoxin	1CJY	0	0	0.96
DB01396	Digitoxin	1JBQ	0	0	0.99
DB01396	Digitoxin	1P0S	0	0	0.96
DB00877	Sirolimus	2BGR	0	0	0.99
DB01245	Decamethonium	1Y0S	0	0	0.89
DB01089	Deserpidine	1EXX	0	0	0.92
DB00603	Medroxyprogesterone	1HOF	0	0	0.92
DB00150	L-Tryptophan	1H2W	0	0	1.00
DB00877	Sirolimus	1BNA	0	0	0.98
DB00926	Etretinate	1EYD	0	1	0.55
DB01396	Digitoxin	1I9R	0	0	0.98
DB00626	Bacitracin	1VJA	0	0	0.93
DB01396	Digitoxin	1CP3	0	0	0.98
DB00169	Cholecalciferol	1C4C	0	0	0.94
DB00603	Medroxyprogesterone	1HOF	0	0	0.92
DB01396	Digitoxin	1ZNC	0	0	0.96
DB00294	Etonogestrel	1HOF	0	1	0.57
DB01245	Decamethonium	1ISS	0	0	0.74
DB00294	Etonogestrel	1HOF	0	1	0.57
DB01396	Digitoxin	1T9N	0	0	0.98
DB01245	Decamethonium	1PU4	0	0	0.75
DB00626	Bacitracin	1WAP	0	0	0.99
DB00877	Sirolimus	1R5K	0	0	0.98
DB00877	Sirolimus	1FE3	0	0	0.99
DB01396	Digitoxin	1TB5	0	0	0.96
DB01396	Digitoxin	1KTA	0	0	0.96
DB01396	Digitoxin	1W6F	0	0	0.96
DB00167	L-Isoleucine	1P87	0	0	0.98

DB01245	Decamethonium	1NHZ	0	0	0.95
DB01396	Digitoxin	1JVQ	0	0	0.96
DB00273	Topiramate	1P87	0	0	1.00
DB00273	Topiramate	1P87	0	0	1.00
DB00626	Bacitracin	1F5F	0	0	0.98
DB00769	Hydrocortamate	1EMI	0	0	0.98
DB01396	Digitoxin	1UZF	0	0	0.98
DB06692	Aprotinin	1OCZ	0	0	0.97
DB06692	Aprotinin	1CJY	0	0	0.96
DB06692	Aprotinin	1GTE	0	0	0.97
DB06692	Aprotinin	1F0X	0	0	0.96
DB06692	Aprotinin	1KFD	0	0	0.97
DB06692	Aprotinin	1HD7	0	0	0.97
DB06692	Aprotinin	1IVO	0	0	0.96
DB06692	Aprotinin	1VJ5	0	0	0.96
DB06692	Aprotinin	1QKM	0	0	0.97
DB06692	Aprotinin	1XKT	0	0	0.97
DB06692	Aprotinin	1FTA	0	0	0.97
DB06692	Aprotinin	1VRU	0	0	0.96
DB06692	Aprotinin	1L1F	0	0	0.97
DB00684	Tobramycin	1H2W	0	0	0.99
DB06692	Aprotinin	1L1F	0	0	0.97
DB06692	Aprotinin	1WVJ	0	0	0.97
DB06692	Aprotinin	1XHY	0	0	0.97
DB06692	Aprotinin	1ODW	0	0	0.97
DB06692	Aprotinin	1BZY	0	0	0.96
DB06692	Aprotinin	1L6J	0	0	0.97
DB06692	Aprotinin	1QR6	0	0	0.97
DB00769	Hydrocortamate	1HWL	0	0	0.80
DB06692	Aprotinin	1UMK	0	0	0.97
DB06692	Aprotinin	1DMT	0	0	0.96
DB06692	Aprotinin	1CYN	0	0	0.97
DB06692	Aprotinin	2RMC	0	0	0.96
DB06692	Aprotinin	1I7I	0	0	0.97
DB06692	Aprotinin	1KI0	0	0	0.97
DB06692	Aprotinin	1BYW	0	0	0.97
DB06692	Aprotinin	1SQN	0	0	0.97
DB06692	Aprotinin	1OPL	0	0	0.96
DB06692	Aprotinin	1G1S	0	0	0.97
DB06692	Aprotinin	1S78	0	0	0.97
DB06692	Aprotinin	1BXS	0	0	0.96
DB06692	Aprotinin	1XDK	0	0	0.96
DB06692	Aprotinin	1EXX	0	0	0.97
DB06692	Aprotinin	1UHL	0	0	0.97

DB06692	Aprotinin	1SG0	0	0	0.97
DB06692	Aprotinin	1BJ4	0	0	0.97
DB06692	Aprotinin	1H0C	0	0	0.97
DB06692	Aprotinin	1F5F	0	0	0.97
DB06692	Aprotinin	1G91	0	0	0.97
DB06692	Aprotinin	1MO8	0	0	0.97
DB06692	Aprotinin	1P49	0	0	0.97
DB06692	Aprotinin	1Y0X	0	0	0.97
DB06692	Aprotinin	1BDA	0	0	0.89
DB06692	Aprotinin	1TRN	0	0	0.96
DB06692	Aprotinin	1A8M	0	0	0.97
DB06692	Aprotinin	1TZI	0	0	0.96
DB06692	Aprotinin	1N2Z	0	0	0.97
DB00769	Hydrocortamate	1OHY	0	0	0.94
DB06692	Aprotinin	1VYT	0	0	0.97
DB00769	Hydrocortamate	1OKC	0	0	0.95
DB00769	Hydrocortamate	1HSZ	0	0	0.78
DB00769	Hydrocortamate	2T40	0	0	0.72
DB00769	Hydrocortamate	1HOF	0	0	0.97
DB00769	Hydrocortamate	1E3G	0	0	0.95
DB00769	Hydrocortamate	1UZF	0	0	0.93
DB01396	Digitoxin	1R4L	0	0	0.96
DB00769	Hydrocortamate	1KTO	0	0	0.94
DB00769	Hydrocortamate	1XGJ	0	0	0.81
DB00769	Hydrocortamate	1CZM	0	0	0.94
DB00769	Hydrocortamate	1T9N	0	0	0.94
DB00769	Hydrocortamate	1I9R	0	0	0.93
DB00769	Hydrocortamate	1P0Q	0	0	0.92
DB00769	Hydrocortamate	1P0S	0	0	0.71
DB00769	Hydrocortamate	1J3S	0	0	0.92
DB00769	Hydrocortamate	1R5K	0	0	0.81
DB00769	Hydrocortamate	1NHZ	0	0	0.95
DB00769	Hydrocortamate	1HIG	0	0	0.93
DB00769	Hydrocortamate	1I0Z	0	0	0.80
DB00769	Hydrocortamate	1B6A	0	0	0.97
DB00769	Hydrocortamate	1DMT	0	0	0.81
DB00769	Hydrocortamate	1OC3	0	0	0.90
DB00769	Hydrocortamate	1I7I	0	0	0.92
DB00769	Hydrocortamate	1EXB	0	0	0.90
DB00769	Hydrocortamate	1BYW	0	0	0.96
DB00769	Hydrocortamate	1IRU	0	0	0.99
DB00769	Hydrocortamate	1OPL	0	0	0.78
DB00769	Hydrocortamate	1LPJ	0	0	0.96
DB00769	Hydrocortamate	1C0B	0	0	0.98

DB00769	Hydrocortamate	1HA2	0	0	0.91
DB00769	Hydrocortamate	1F5F	0	0	0.95
DB00769	Hydrocortamate	1MO8	0	0	0.95
DB00769	Hydrocortamate	1VMC	0	0	0.97
DB01396	Digitoxin	2BK3	0	0	0.96
DB01396	Digitoxin	1O5W	0	0	1.00
DB00769	Hydrocortamate	1A8M	0	0	0.95
DB00769	Hydrocortamate	1T0U	0	0	0.93
DB00769	Hydrocortamate	1YTV	0	0	0.79
DB00603	Medroxyprogesterone	1F8U	0	0	0.79
DB00603	Medroxyprogesterone	1OHY	0	0	0.81
DB01245	Decamethonium	1GCN	0	0	0.98
DB01396	Digitoxin	1HOF	0	0	0.99
DB00603	Medroxyprogesterone	1P87	0	0	1.00
DB00697	Tizanidine	1P87	0	0	0.97
DB01396	Digitoxin	1HOF	0	0	0.99
DB00147	Pyridoxal	1P87	0	0	0.99
DB01396	Digitoxin	1ORE	0	0	0.99
DB01396	Digitoxin	1QON	0	0	0.98
DB00741	Hydrocortisone	1P87	0	0	0.97
DB00615	Rifabutin	1YOV	0	0	0.97
DB01396	Digitoxin	1OHY	0	0	0.98
DB01396	Digitoxin	1HWL	0	0	0.96
DB00926	Etretinate	1Y0X	0	1	0.49
DB00834	Mifepristone	1RFV	0	0	0.79
DB00603	Medroxyprogesterone	1EMI	0	0	0.96
DB00775	Tirofiban	1Y4E	0	0	0.73
DB00775	Tirofiban	1BYY	0	0	0.79
DB00970	Dactinomycin	1YAE	0	0	0.99
DB00626	Bacitracin	1HA2	0	0	0.96
DB00819	Acetazolamide	1P87	0	0	0.99
DB00877	Sirolimus	1NHZ	0	0	0.99
DB00970	Dactinomycin	1ODW	0	0	0.99
DB00970	Dactinomycin	1F0Y	0	0	0.99
DB01396	Digitoxin	1EMI	0	0	0.99
DB01245	Decamethonium	1R5K	0	0	0.74
DB01245	Decamethonium	1VJ5	0	1	0.60
DB00877	Sirolimus	1ODW	0	0	0.99
DB00775	Tirofiban	1K2H	0	0	0.99
DB00775	Tirofiban	1IRU	0	0	0.98
DB00775	Tirofiban	1IRU	0	0	0.98
DB00970	Dactinomycin	1ISS	0	0	0.99
DB00926	Etretinate	1BDA	0	0	0.93
DB00970	Dactinomycin	1B6A	0	0	0.99

DB00775	Tirofiban	1Y38	0	0	0.70
DB00834	Mifepristone	1IRU	0	0	0.99
DB00834	Mifepristone	1SQN	0	0	0.78
DB00970	Dactinomycin	1PBW	0	0	0.99
DB00834	Mifepristone	1C5G	0	0	0.78
DB00834	Mifepristone	1Y0S	0	1	0.59
DB00970	Dactinomycin	1Y38	0	0	1.00
DB00626	Bacitracin	1UHL	0	0	0.97
DB00834	Mifepristone	1ZBQ	0	0	0.79
DB01136	Carvedilol	1P87	0	0	0.97
DB00834	Mifepristone	1UMK	0	0	0.98
DB01136	Carvedilol	1P87	0	0	0.97
DB00834	Mifepristone	1E71	0	0	0.75
DB00626	Bacitracin	1XDK	0	0	0.94
DB00872	Conivaptan	1P87	0	0	0.99
DB01245	Decamethonium	1F0X	0	0	0.72
DB00970	Dactinomycin	1BYW	0	0	0.99
DB00970	Dactinomycin	1BP3	0	0	0.99
DB00262	Carmustine	1IRU	0	0	0.99
DB00262	Carmustine	1IRU	0	0	0.99
DB00877	Sirolimus	1SVC	0	0	0.99
DB00775	Tirofiban	1GCN	0	1	0.65
DB01245	Decamethonium	1EA1	0	0	0.94
DB00834	Mifepristone	1W7N	0	0	0.77
DB00834	Mifepristone	1ILQ	0	0	0.92
DB01089	Deserpidine	1BI9	0	0	0.84
DB01245	Decamethonium	1JBQ	0	0	0.97
DB01245	Decamethonium	1T9R	0	0	0.95
DB01100	Pimozide	1DON	0	0	0.99
DB04573	Estriol	1P87	0	0	0.97
DB00877	Sirolimus	1OAT	0	0	0.98
DB01394	Colchicine	1BDA	0	0	0.87
DB01245	Decamethonium	2CBR	0	0	0.96
DB01394	Colchicine	1DON	0	0	0.98
DB01089	Deserpidine	1I4L	0	0	0.87
DB00970	Dactinomycin	1BXS	0	0	0.98
DB01245	Decamethonium	1CP3	0	0	0.94
DB01089	Deserpidine	1SQN	0	0	0.89
DB00818	Propofol	1P87	0	0	1.00
DB01089	Deserpidine	1SVC	0	0	0.83
DB01245	Decamethonium	1CZM	0	0	0.95
DB01132	Pioglitazone	1P87	0	0	1.00
DB00834	Mifepristone	1ODW	0	0	0.85
DB00970	Dactinomycin	1EXX	0	0	0.99

DB00970	Dactinomycin	1HA2	0	0	0.99
DB00626	Bacitracin	1SQN	0	0	0.98
DB00626	Bacitracin	1BYW	0	0	0.98
DB00626	Bacitracin	1JYD	0	0	0.98
DB00877	Sirolimus	1CWM	0	0	0.99
DB00970	Dactinomycin	1F5F	0	0	0.99
DB01089	Deserpidine	1TLL	0	0	0.86
DB00970	Dactinomycin	1MB2	0	0	0.98
DB00970	Dactinomycin	1SA1	0	0	0.99
DB00626	Bacitracin	1OAT	0	0	0.94
DB00775	Tirofiban	1P87	0	0	0.98
DB00775	Tirofiban	1EMI	0	0	0.75
DB00677	Isoflurophate	1P87	0	0	1.00
DB00626	Bacitracin	1ILQ	0	0	0.99
DB00605	Sulindac	1H2W	0	0	1.00
DB00790	Perindopril	1BYY	0	0	0.89
DB00834	Mifepristone	3JDW	0	0	0.78
DB00877	Sirolimus	2RMC	0	0	0.98
DB00834	Mifepristone	1AGS	0	0	0.78
DB00626	Bacitracin	1T5P	0	0	0.97
DB00626	Bacitracin	1FE3	0	0	0.98
DB00615	Rifabutin	1LSZ	0	0	0.98
DB00790	Perindopril	1IRU	0	0	0.98
DB00615	Rifabutin	1N7D	0	0	0.93
DB00790	Perindopril	1MZW	0	1	0.56
DB01173	Orphenadrine	1O5W	0	1	0.44
DB00834	Mifepristone	1XHY	0	0	0.82
DB00790	Perindopril	1ILQ	0	0	0.78
DB00834	Mifepristone	1WVJ	0	0	0.81
DB00790	Perindopril	1ODW	0	1	0.62
DB00779	Nalidixic Acid	1K2H	0	1	0.61
DB00615	Rifabutin	1ILQ	0	0	0.99
DB01132	Pioglitazone	1DON	0	0	0.98
DB00834	Mifepristone	1J4I	0	0	0.87
DB00626	Bacitracin	1YV5	0	0	0.98
DB00626	Bacitracin	1X9N	0	0	0.94
DB00626	Bacitracin	1BNA	0	0	0.93
DB00877	Sirolimus	1K7L	0	0	0.98
DB00877	Sirolimus	1EXB	0	0	0.99
DB00834	Mifepristone	1QKM	0	0	0.78
DB00615	Rifabutin	9ILB	0	0	0.98
DB01089	Deserpidine	2IL6	0	0	0.92
DB00932	Tipranavir	1P87	0	0	0.99
DB00834	Mifepristone	1DYT	0	0	0.69

DB00615	Rifabutin	1M1X	0	0	0.92
DB00615	Rifabutin	1TYE	0	0	0.99
DB00834	Mifepristone	1D3H	0	0	0.80
DB01089	Deserpidine	1ODW	0	0	0.93
DB00834	Mifepristone	1JBQ	0	0	0.86
DB00626	Bacitracin	1CJY	0	0	0.94
DB00834	Mifepristone	1P0Q	0	0	0.72
DB00877	Sirolimus	1WD8	0	0	1.00
DB00834	Mifepristone	1T9N	0	0	0.78
DB01169	Arsenic trioxide	1DON	0	0	0.97
DB00877	Sirolimus	1OPL	0	0	0.98
DB00615	Rifabutin	1ODW	0	0	0.98
DB00615	Rifabutin	1T5P	0	0	0.97
DB00834	Mifepristone	1UZF	0	0	0.74
DB00834	Mifepristone	1E3G	0	0	0.80
DB00774	Hydroflumethiazide	1H2W	0	0	1.00
DB00774	Hydroflumethiazide	1DON	0	0	0.98
DB00615	Rifabutin	1WVJ	0	0	0.97
DB00945	Aspirin	1P87	0	0	1.00
DB00945	Aspirin	1P87	0	0	1.00
DB01611	Hydroxychloroquine	1P87	0	0	0.97
DB01611	Hydroxychloroquine	1P87	0	0	0.97
DB00626	Bacitracin	1HKO	0	0	0.97
DB01040	Hydroxystilbamidine Isethionate	1DON	0	0	0.98
DB00615	Rifabutin	1PB7	0	0	0.97
DB00834	Mifepristone	1O5W	0	0	0.98
DB00877	Sirolimus	1XDK	0	0	0.98
DB00834	Mifepristone	1HOF	0	0	0.90
DB00834	Mifepristone	1HOF	0	0	0.90
DB01245	Decamethonium	1UZF	0	0	0.94
DB00626	Bacitracin	1P0S	0	0	0.93
DB00877	Sirolimus	1EXX	0	0	0.99
DB01183	Naloxone	1IRU	0	0	0.98
DB00834	Mifepristone	1ORE	0	0	0.86
DB00834	Mifepristone	1GXD	0	0	0.81
DB00753	Isoflurane	1P87	0	0	1.00
DB00753	Isoflurane	1P87	0	0	1.00
DB00834	Mifepristone	1OHY	0	0	0.76
DB00834	Mifepristone	1W0H	0	0	0.88
DB00615	Rifabutin	1L9X	0	0	0.96
DB00834	Mifepristone	1EMI	0	0	0.95
DB01247	Isocarboxazid	1IRU	0	0	0.98
DB01247	Isocarboxazid	1H2W	0	0	1.00
DB00378	Dydrogesterone	1SQN	0	0	0.75

DB00378	Dydrogesterone	1TJC	0	0	0.78
DB01247	Isocarboxazid	1P87	0	0	0.99
DB01245	Decamethonium	1O5W	0	0	0.99
DB00762	Irinotecan	1N2Z	0	0	0.88
DB00626	Bacitracin	1CP3	0	0	0.97
DB00762	Irinotecan	1Q11	0	0	0.90
DB00762	Irinotecan	1A8M	0	0	0.93
DB00762	Irinotecan	1WAP	0	0	0.97
DB00762	Irinotecan	1MO8	0	0	0.92
DB00762	Irinotecan	1H0C	0	0	0.90
DB00762	Irinotecan	1UHL	0	0	0.88
DB00762	Irinotecan	1H2W	0	0	1.00
DB00762	Irinotecan	1BYW	0	0	0.94
DB00762	Irinotecan	1YOV	0	0	0.91
DB00762	Irinotecan	1E71	0	0	0.89
DB00762	Irinotecan	1LSZ	0	0	0.94
DB00762	Irinotecan	1P5J	0	0	0.93
DB00762	Irinotecan	1MQ8	0	1	0.62
DB00762	Irinotecan	1TYE	0	0	0.98
DB00762	Irinotecan	1R74	0	0	0.89
DB00762	Irinotecan	1BWC	0	0	0.90
DB00762	Irinotecan	1J4I	0	0	0.95
DB00762	Irinotecan	1XKT	0	0	0.88
DB00762	Irinotecan	1A36	0	1	0.64
DB00877	Sirolimus	1SG0	0	0	0.99
DB01394	Colchicine	1UMK	0	1	0.63
DB00877	Sirolimus	1HA2	0	0	0.99
DB00762	Irinotecan	1OCZ	0	0	0.87
DB00762	Irinotecan	1CZM	0	0	0.91
DB00626	Bacitracin	1CZM	0	0	0.97
DB00626	Bacitracin	1KTA	0	0	0.94
DB00762	Irinotecan	1R4L	0	1	0.64
DB00762	Irinotecan	1E3G	0	0	0.91
DB00762	Irinotecan	1O5W	0	0	0.99
DB00762	Irinotecan	1I5H	0	0	0.93
DB00762	Irinotecan	1HOF	0	0	0.96
DB00762	Irinotecan	1HOF	0	0	0.96
DB00762	Irinotecan	1F8U	0	0	0.89
DB00762	Irinotecan	1OHY	0	0	0.90
DB00762	Irinotecan	1HWL	0	1	0.62
DB00762	Irinotecan	1P87	0	0	1.00
DB00626	Bacitracin	1PQ3	0	0	0.97
DB00615	Rifabutin	1SS2	0	0	0.97
DB00615	Rifabutin	1HE5	0	0	0.97

DB00877	Sirolimus	1MO8	0	0	0.99
DB01029	Irbesartan	1BYY	0	1	0.49
DB00615	Rifabutin	1FE3	0	0	0.98
DB00378	Dydrogesterone	1BI9	0	1	0.65
DB00506	Norgestrel	1O5W	0	0	0.94
DB00118	S-Adenosylmethionine	1DON	0	0	0.97
DB00877	Sirolimus	1IIH	0	0	0.99
DB00626	Bacitracin	1UZF	0	0	0.97
DB00605	Sulindac	1DON	0	0	0.99
DB01173	Orphenadrine	1P87	0	0	1.00
DB00506	Norgestrel	1HOF	0	0	0.68
DB00615	Rifabutin	1YV5	0	0	0.98
DB01245	Decamethonium	1HOF	0	0	0.98
DB00626	Bacitracin	1Q7L	0	0	0.97
DB00626	Bacitracin	2BK3	0	0	0.94
DB00877	Sirolimus	1SA1	0	0	0.99
DB00506	Norgestrel	1HOF	0	0	0.68
DB00615	Rifabutin	1R5K	0	0	0.93
DB00877	Sirolimus	1TZI	0	0	0.98
DB00877	Sirolimus	1V97	0	0	0.99
DB00626	Bacitracin	1EW2	0	0	0.97
DB01245	Decamethonium	1T40	0	1	0.60
DB01083	Orlistat	1UJW	0	0	0.97
DB00626	Bacitracin	1MRQ	0	0	0.98
DB00378	Dydrogesterone	1LBD	0	0	0.77
DB01147	Cloxacillin	1P87	0	0	0.97
DB00378	Dydrogesterone	1UHL	0	0	0.70
DB01147	Cloxacillin	1P87	0	0	0.97
DB00169	Cholecalciferol	1I7I	0	0	0.93
DB00758	Clopidogrel	1H2W	0	0	1.00
DB00169	Cholecalciferol	1BYW	0	0	0.97
DB00236	Pipobroman	1DON	0	0	0.99
DB00575	Clonidine	1DON	0	0	0.99
DB00378	Dydrogesterone	1OLM	0	1	0.64
DB00575	Clonidine	1IRU	0	0	0.99
DB00378	Dydrogesterone	1HA2	0	0	0.70
DB00575	Clonidine	1P87	0	0	0.99
DB00906	Tiagabine	1P87	0	0	1.00
DB00626	Bacitracin	1OD4	0	0	0.98
DB00626	Bacitracin	1F8U	0	0	0.97
DB00615	Rifabutin	1QYE	0	0	0.98
DB00378	Dydrogesterone	1EYD	0	0	0.84
DB00378	Dydrogesterone	1NAV	0	0	0.80
DB00626	Bacitracin	1HWL	0	0	0.94

DB00378	Dydrogesterone	1N2Z	0	0	0.71
DB01083	Orlistat	1A5Y	0	0	0.99
DB01068	Clonazepam	1IRU	0	0	0.99
DB00615	Rifabutin	1UW0	0	0	0.97
DB00001	Lepirudin	1JNM	0	0	0.97
DB00001	Lepirudin	1BDA	0	0	0.91
DB00707	Porfimer	1EMI	0	0	0.97
DB00926	Etretinate	1TEV	0	1	0.51
DB00615	Rifabutin	1BNA	0	0	0.91
DB01388	Mibefradil	1P87	0	0	0.99
DB00984	Nandrolone	1EMI	0	0	0.98
DB00142	L-Glutamic Acid	1IRU	0	0	0.98
DB00984	Nandrolone	1HOF	0	0	0.96
DB00984	Nandrolone	1HOF	0	0	0.96
DB00142	L-Glutamic Acid	1IRU	0	0	0.98
DB00984	Nandrolone	1O5W	0	0	0.99
DB00169	Cholecalciferol	1IRU	0	0	0.99
DB00142	L-Glutamic Acid	1H2W	0	0	1.00
DB00207	Azithromycin	1UAE	0	0	0.99
DB00615	Rifabutin	1GTE	0	0	0.96
DB00790	Perindopril	1HOF	0	0	0.72
DB01261	Sitagliptin	1P87	0	0	1.00
DB00553	Methoxsalen	1K2H	0	1	0.32
DB00926	Etretinate	1V97	0	1	0.60
DB00207	Azithromycin	1SA1	0	0	0.98
DB00707	Porfimer	1F8U	0	0	0.86
DB00169	Cholecalciferol	1BBS	0	0	0.71
DB01083	Orlistat	1A8M	0	0	0.99
DB00169	Cholecalciferol	1UHL	0	0	0.94
DB01196	Estramustine	1DON	0	0	0.99
DB00339	Pyrazinamide	1DON	0	0	0.96
DB00637	Astemizole	1P87	0	0	0.99
DB00637	Astemizole	1IRU	0	0	0.99
DB00637	Astemizole	1IRU	0	0	0.99
DB01072	Atazanavir	1EMI	0	0	0.81
DB00768	Olopatadine	1BDA	0	0	0.84
DB00001	Lepirudin	1F5F	0	0	0.97
DB00001	Lepirudin	1HA2	0	0	0.98
DB01072	Atazanavir	1O5W	0	0	0.91
DB00481	Raloxifene	1P87	0	0	0.98
DB00481	Raloxifene	1P87	0	0	0.98
DB00511	Acetyldigitoxin	1QKM	0	0	0.99
DB00511	Acetyldigitoxin	1L9X	0	0	0.99
DB00169	Cholecalciferol	1HA2	0	0	0.93

DB00870	Suprofen	1P87	0	0	1.00
DB00641	Simvastatin	1P87	0	0	1.00
DB00001	Lepirudin	1Q9S	0	0	0.97
DB00001	Lepirudin	1EXX	0	0	0.97
DB00641	Simvastatin	1P87	0	0	1.00
DB00783	Estradiol	1DON	0	0	0.98
DB00984	Nandrolone	1Q2P	0	0	0.91
DB00352	Thioguanine	1P87	0	0	0.96
DB01083	Orlistat	1P87	0	0	1.00
DB00984	Nandrolone	1T9N	0	0	0.90
DB00641	Simvastatin	1EMI	0	0	0.98
DB01083	Orlistat	1KED	0	0	0.99
DB00984	Nandrolone	1T9R	0	0	0.92
DB01083	Orlistat	1JNM	0	0	0.99
DB00984	Nandrolone	1P0Q	0	0	0.87
DB00169	Cholecalciferol	1F5F	0	0	0.96
DB00641	Simvastatin	1EMI	0	0	0.98
DB00984	Nandrolone	1LJ7	0	0	0.94
DB00984	Nandrolone	1JBQ	0	0	0.94
DB01245	Decamethonium	1OKC	0	0	0.95
DB00506	Norgestrel	1P87	0	0	1.00
DB00006	Bivalirudin	1TZI	0	0	0.96
DB00006	Bivalirudin	1SA1	0	0	0.98
DB00984	Nandrolone	1QYE	0	0	0.94
DB00616	Candoxatril	1P87	0	0	0.98
DB00001	Lepirudin	1R6K	0	0	0.97
DB00001	Lepirudin	1SQN	0	0	0.97
DB00294	Etonogestrel	1ILQ	0	1	0.64
DB00279	Liothyronine	1DON	0	0	0.98
DB00984	Nandrolone	1FTA	0	0	0.92
DB00006	Bivalirudin	1Y4E	0	0	0.99
DB01196	Estramustine	1P87	0	0	0.99
DB00506	Norgestrel	1EMI	0	0	0.84
DB00169	Cholecalciferol	1SLM	0	0	0.95
DB00984	Nandrolone	1NHZ	0	0	0.91
DB00506	Norgestrel	1EMI	0	0	0.84
DB00294	Etonogestrel	1UMK	0	0	0.91
DB00887	Bumetanide	1P87	0	0	0.98
DB00984	Nandrolone	1PB7	0	0	0.92
DB00984	Nandrolone	1WVJ	0	0	0.92
DB00169	Cholecalciferol	1SA1	0	0	0.95
DB00006	Bivalirudin	1BYY	0	0	0.99
DB00224	Indinavir	1O5W	0	0	0.92
DB00224	Indinavir	1HOF	0	1	0.61

DB01089	Deserpidine	1WVJ	0	0	0.91
DB00984	Nandrolone	1WVJ	0	0	0.92
DB01222	Budesonide	1V97	0	0	0.80
DB00001	Lepirudin	1Y0S	0	0	0.97
DB00224	Indinavir	1EMI	0	0	0.82
DB00001	Lepirudin	1NRL	0	0	0.97
DB00984	Nandrolone	1ODW	0	0	0.93
DB00001	Lepirudin	1SVC	0	0	0.98
DB00001	Lepirudin	1ISS	0	0	0.97
DB00001	Lepirudin	3JDW	0	0	0.97
DB00707	Porfimer	1EW2	0	0	0.87
DB00984	Nandrolone	1YXL	0	0	0.94
DB00001	Lepirudin	1AGS	0	0	0.97
DB00984	Nandrolone	1BI9	0	0	0.85
DB00984	Nandrolone	1BJ4	0	0	0.90
DB00984	Nandrolone	1HA2	0	0	0.87
DB00984	Nandrolone	1MO8	0	0	0.91
DB00984	Nandrolone	1JNM	0	0	0.85
DB00984	Nandrolone	1SA1	0	0	0.89
DB00984	Nandrolone	1SA1	0	0	0.89
DB00001	Lepirudin	1NHZ	0	0	0.97
DB01222	Budesonide	1KED	0	1	0.65
DB01050	Ibuprofen	1BDA	0	0	0.83
DB00957	Norgestimate	1V97	0	0	0.84
DB00277	Theophylline	1P87	0	0	1.00
DB01222	Budesonide	1F5F	0	0	0.73
DB01245	Decamethonium	1MF1	0	0	0.95
DB00294	Etonogestrel	1WD8	0	0	0.71
DB00707	Porfimer	1HOF	0	0	0.93
DB00255	Diethylstilbestrol	1H2W	0	0	1.00
DB00957	Norgestimate	1A5Y	0	0	0.73
DB06148	Mianserin	1H2W	0	0	1.00
DB00707	Porfimer	1HOF	0	0	0.93
DB01041	Thalidomide	1BDA	0	0	0.78
DB00308	Ibutilide	1P87	0	0	0.99
DB00001	Lepirudin	1VRU	0	0	0.97
DB00707	Porfimer	1OIZ	0	0	0.81
DB01222	Budesonide	2AAI	0	0	0.85
DB00006	Bivalirudin	1H0C	0	0	0.98
DB00006	Bivalirudin	1C0B	0	0	0.99
DB00001	Lepirudin	1VJ5	0	0	0.97
DB00957	Norgestimate	1SA1	0	0	0.68
DB00308	Ibutilide	1O5W	0	0	0.83
DB00006	Bivalirudin	1BXS	0	0	0.96

DB00707	Porfimer	1UZF	0	0	0.86
DB00294	Etonogestrel	1DON	0	0	0.98
DB00006	Bivalirudin	1OPL	0	0	0.96
DB00707	Porfimer	1E79	0	0	0.86
DB00294	Etonogestrel	1VMC	0	1	0.55
DB00957	Norgestimate	1SA1	0	0	0.68
DB00001	Lepirudin	1IVO	0	0	0.97
DB01222	Budesonide	1EXX	0	0	0.73
DB01245	Decamethonium	1GXD	0	0	0.95
DB00957	Norgestimate	1IIIH	0	0	0.71
DB00006	Bivalirudin	1BP3	0	0	0.98
DB00957	Norgestimate	1KED	0	0	0.70
DB00957	Norgestimate	1NAV	0	0	0.76
DB00957	Norgestimate	1MO8	0	0	0.75
DB00615	Rifabutin	1PWG	0	0	0.93
DB00006	Bivalirudin	1BYW	0	0	0.98
DB01245	Decamethonium	2BIY	0	0	0.96
DB00001	Lepirudin	1BNA	0	0	0.97
DB00001	Lepirudin	1D3H	0	0	0.97
DB00006	Bivalirudin	1PBW	0	0	0.98
DB00006	Bivalirudin	1NRL	0	0	0.96
DB01083	Orlistat	1MO8	0	0	0.99
DB00957	Norgestimate	1HA2	0	1	0.63
DB01497	Etorphine	1EMI	0	0	0.84
DB00220	Nelfinavir	1EMI	0	0	0.85
DB00220	Nelfinavir	1HOF	0	1	0.67
DB00707	Porfimer	1DIA	0	0	0.87
DB00220	Nelfinavir	1O5W	0	0	0.93
DB00619	Imatinib	1P87	0	0	0.99
DB00001	Lepirudin	1XMI	0	0	0.97
DB01083	Orlistat	1HA2	0	0	0.99
DB01088	Iloprost	1A8M	0	1	0.62
DB00001	Lepirudin	1JBQ	0	0	0.97
DB00006	Bivalirudin	1HIG	0	0	0.98
DB01088	Iloprost	1NAV	0	1	0.60
DB01088	Iloprost	1F5F	0	1	0.63
DB00001	Lepirudin	1DIA	0	0	0.97
DB00001	Lepirudin	1K6R	0	0	0.97
DB01088	Iloprost	1LPJ	0	1	0.64
DB01497	Etorphine	1HOF	0	0	0.68
DB00707	Porfimer	1PTW	0	0	0.70
DB00707	Porfimer	1CZM	0	0	0.89
DB01083	Orlistat	1H0C	0	0	0.99
DB00001	Lepirudin	1UZF	0	0	0.97

DB01088	Iloprost	1BYW	0	0	0.68
DB00006	Bivalirudin	1M1X	0	0	0.96
DB01088	Iloprost	1MZW	0	1	0.61
DB01088	Iloprost	1CYN	0	1	0.62
DB00001	Lepirudin	1HOF	0	0	0.97
DB01041	Thalidomide	1P87	0	0	1.00
DB00001	Lepirudin	1XF0	0	0	0.97
DB00001	Lepirudin	1IHI	0	0	0.97
DB01088	Iloprost	1PB7	0	1	0.60
DB00001	Lepirudin	1F8U	0	0	0.97
DB01083	Orlistat	1LPJ	0	0	0.99
DB00001	Lepirudin	1GXD	0	0	0.97
DB00707	Porfimer	1IBC	0	0	0.93
DB00001	Lepirudin	1HWL	0	0	0.97
DB01072	Atazanavir	1IRU	0	0	0.98
DB01072	Atazanavir	1IRU	0	0	0.98
DB01011	Metyrapone	1DON	0	0	0.98
DB00707	Porfimer	1GTE	0	0	0.85
DB01083	Orlistat	1UHL	0	0	0.99
DB00957	Norgestimate	1SG0	0	0	0.69
DB00001	Lepirudin	1P87	0	0	0.93
DB01072	Atazanavir	1DON	0	0	0.98
DB00006	Bivalirudin	1YAE	0	0	0.98
DB01083	Orlistat	1EXX	0	0	0.99
DB00870	Suprofen	1DON	0	0	0.98
DB01076	Atorvastatin	1H2W	0	0	1.00
DB01076	Atorvastatin	1IRU	0	0	0.99
DB01076	Atorvastatin	1IRU	0	0	0.99
DB01076	Atorvastatin	1DON	0	0	0.99
DB00957	Norgestimate	1LBD	0	0	0.70
DB00006	Bivalirudin	1YAE	0	0	0.98
DB00572	Atropine	1P87	0	0	1.00
DB00707	Porfimer	1DYT	0	0	0.85
DB00707	Porfimer	1R5K	0	0	0.71
DB00707	Porfimer	1FE3	0	0	0.92
DB00622	Nicardipine	1BYY	0	1	0.56
DB01083	Orlistat	1BI9	0	0	0.99
DB00707	Porfimer	1YAE	0	0	0.90
DB00199	Erythromycin	1BYW	0	0	0.99
DB00957	Norgestimate	1EXX	0	0	0.78
DB00572	Atropine	1O5W	0	1	0.42
DB00707	Porfimer	3JDW	0	0	0.88
DB00707	Porfimer	1ILQ	0	0	0.95
DB00199	Erythromycin	2BIU	0	0	0.99

DB00707	Porfimer	1SVC	0	0	0.77
DB00207	Azithromycin	1Y0X	0	0	0.99
DB00707	Porfimer	1C5G	0	0	0.88
DB00707	Porfimer	1BYW	0	0	0.92
DB01089	Deserpidine	1E79	0	0	0.88
DB00707	Porfimer	1LBD	0	0	0.80
DB00707	Porfimer	1UHL	0	0	0.84
DB00615	Rifabutin	1CJY	0	0	0.92
DB00707	Porfimer	2AAI	0	0	0.95
DB00707	Porfimer	1HA2	0	0	0.80
DB00707	Porfimer	1SLM	0	0	0.88
DB00707	Porfimer	1X86	0	0	0.88
DB00199	Erythromycin	1EH6	0	0	0.99
DB00006	Bivalirudin	1VRU	0	0	0.96
DB00616	Candoxatril	1A5Y	0	0	0.88
DB00957	Norgestimate	1EW2	0	0	0.73
DB00178	Ramipril	1P87	0	0	0.99
DB00220	Nelfinavir	1Y4E	0	0	0.82
DB00178	Ramipril	1P87	0	0	0.99
DB00006	Bivalirudin	1U4E	0	0	0.98
DB01083	Orlistat	1G1S	0	0	0.99
DB01083	Orlistat	1XWS	0	0	0.99
DB00790	Perindopril	1P87	0	0	0.99
DB00790	Perindopril	1EMI	0	0	0.87
DB01411	Pranlukast	1P87	0	0	0.99
DB01083	Orlistat	1TJC	0	0	0.99
DB01245	Decamethonium	1P87	0	0	1.00
DB01083	Orlistat	1SQN	0	0	0.99
DB00643	Mebendazole	1DON	0	0	0.97
DB01245	Decamethonium	1P87	0	0	1.00
DB00806	Pentoxifylline	1BDA	0	0	0.93
DB00207	Azithromycin	1HA2	0	0	0.98
DB00957	Norgestimate	1SQN	0	0	0.71
DB00643	Mebendazole	1IRU	0	0	0.98
DB00210	Adapalene	1IRU	0	0	0.98
DB01216	Finasteride	1EMI	0	0	0.96
DB00572	Atropine	1DON	0	0	0.98
DB00957	Norgestimate	1BYW	0	0	0.82
DB00006	Bivalirudin	1R5K	0	0	0.97
DB00006	Bivalirudin	8ICK	0	0	0.98
DB00957	Norgestimate	1HOF	0	0	0.87
DB01216	Finasteride	1P87	0	0	0.99
DB00615	Rifabutin	1HKO	0	0	0.97
DB00207	Azithromycin	1H0C	0	0	0.98

DB00643	Mebendazole	1P87	0	0	0.99
DB00262	Carmustine	1P87	0	0	0.99
DB00995	Auranofin	1EMI	0	0	0.99
DB00995	Auranofin	1P87	0	0	1.00
DB00995	Auranofin	1P87	0	0	1.00
DB00995	Auranofin	1OHY	0	0	0.96
DB00995	Auranofin	1F8U	0	0	0.95
DB00995	Auranofin	1OKC	0	0	0.97
DB00995	Auranofin	1OKC	0	0	0.97
DB00995	Auranofin	1HSO	0	0	0.79
DB00995	Auranofin	1HSZ	0	0	0.80
DB00995	Auranofin	1OF7	0	0	0.97
DB00995	Auranofin	1HOF	0	0	0.98
DB00995	Auranofin	1HOF	0	0	0.98
DB00995	Auranofin	1E3G	0	0	0.96
DB00926	Etretinate	1W0H	0	1	0.60
DB00995	Auranofin	1UZF	0	0	0.96
DB00995	Auranofin	1E79	0	0	0.96
DB00615	Rifabutin	1P0S	0	0	0.91
DB00995	Auranofin	1K6R	0	0	0.98
DB00995	Auranofin	1TB5	0	0	0.81
DB00995	Auranofin	1T9N	0	0	0.96
DB00995	Auranofin	1S5O	0	0	0.96
DB00995	Auranofin	1P0Q	0	0	0.95
DB00995	Auranofin	1Z6J	0	0	0.70
DB00995	Auranofin	1LJ7	0	0	0.97
DB00995	Auranofin	1HKO	0	0	0.97
DB00759	Tetracycline	1DON	0	0	0.97
DB00995	Auranofin	1TQN	0	0	0.96
DB00995	Auranofin	1FYC	0	0	0.96
DB00995	Auranofin	1BNA	0	0	0.70
DB00995	Auranofin	1A36	0	0	0.82
DB00995	Auranofin	1QYX	0	0	0.97
DB00995	Auranofin	1R5K	0	0	0.81
DB00995	Auranofin	1VJB	0	0	0.96
DB00995	Auranofin	1XKT	0	0	0.95
DB00995	Auranofin	1VRU	0	0	0.81
DB00995	Auranofin	1NHZ	0	0	0.96
DB00995	Auranofin	1GET	0	0	0.79
DB00995	Auranofin	3JDW	0	0	0.96
DB00995	Auranofin	9ILB	0	0	0.97
DB00995	Auranofin	1N7D	0	0	0.82
DB00995	Auranofin	1TLL	0	0	0.95
DB00995	Auranofin	1SVC	0	0	0.94

DB00995	Auranofin	1OAT	0	0	0.80
DB00995	Auranofin	1FVO	0	0	0.94
DB00995	Auranofin	2RMC	0	0	0.82
DB00995	Auranofin	1MZW	0	0	0.97
DB00995	Auranofin	1Y0S	0	0	0.92
DB00995	Auranofin	1BYW	0	0	0.97
DB00995	Auranofin	1HAG	0	0	0.70
DB00995	Auranofin	1OPL	0	0	0.79
DB00995	Auranofin	1EXX	0	0	0.97
DB00995	Auranofin	1EXX	0	0	0.97
DB00995	Auranofin	1HA2	0	0	0.95
DB00995	Auranofin	1F5F	0	0	0.97
DB00995	Auranofin	1MO8	0	0	0.97
DB00995	Auranofin	1NAV	0	0	0.97
DB00995	Auranofin	1IIH	0	0	0.96
DB00995	Auranofin	1TRN	0	0	0.70
DB00995	Auranofin	1SA1	0	0	0.96
DB00995	Auranofin	1A8M	0	0	0.97
DB00995	Auranofin	1TZI	0	0	0.70
DB00995	Auranofin	1VYT	0	0	0.96
DB01083	Orlistat	1OKC	0	0	0.99
DB01216	Finasteride	1OHY	0	0	0.78
DB00207	Azithromycin	1EXX	0	0	0.99
DB00957	Norgestimate	1OC3	0	1	0.58
DB01216	Finasteride	1F8U	0	0	0.77
DB01083	Orlistat	1EXB	0	0	0.99
DB01088	Iloprost	1HOF	0	0	0.75
DB00957	Norgestimate	1CWM	0	0	0.78
DB00207	Azithromycin	1RFV	0	0	0.98
DB01088	Iloprost	1P87	0	0	0.99
DB01088	Iloprost	1EMI	0	0	0.89
DB01083	Orlistat	1KI0	0	0	0.99
DB01216	Finasteride	1L6V	0	0	0.84
DB01216	Finasteride	1EW2	0	0	0.81
DB01083	Orlistat	1Y38	0	0	1.00
DB01083	Orlistat	1I7I	0	0	0.99
DB01216	Finasteride	1HOF	0	0	0.91
DB00159	Icosapent	1BDA	0	0	0.85
DB00006	Bivalirudin	1BNA	0	0	0.96
DB01180	Rescinnamine	1YTV	0	0	0.75
DB00934	Maprotiline	1P87	0	0	1.00
DB01216	Finasteride	1O5W	0	0	0.98
DB00006	Bivalirudin	1J3S	0	0	0.98
DB00742	Mannitol	1DON	0	0	0.96

DB00615	Rifabutin	2CBR	0	0	0.98
DB01089	Deserpidine	1L1F	0	0	0.87
DB01216	Finasteride	1UZF	0	0	0.77
DB00530	Erlotinib	1H2W	0	0	1.00
DB00199	Erythromycin	1EMI	0	0	0.99
DB00882	Clomifene	1P87	0	0	0.99
DB00615	Rifabutin	1CP3	0	0	0.97
DB01180	Rescinnamine	1SA1	0	0	0.94
DB00006	Bivalirudin	1ZNC	0	0	0.96
DB00006	Bivalirudin	1T9N	0	0	0.98
DB00622	Nicardipine	1H2W	0	0	1.00
DB01216	Finasteride	1UZF	0	0	0.77
DB01180	Rescinnamine	1MO8	0	0	0.95
DB00624	Testosterone	1EYD	0	1	0.59
DB01168	Procarbazine	1P87	0	0	0.98
DB00624	Testosterone	1DON	0	0	0.98
DB00624	Testosterone	1F5F	0	1	0.55
DB00006	Bivalirudin	1TB5	0	0	0.96
DB00624	Testosterone	1EII	0	1	0.62
DB00199	Erythromycin	1OYE	0	0	0.96
DB00006	Bivalirudin	1KTA	0	0	0.96
DB00464	Sodium Tetradecyl Sulfate	1P87	0	0	1.00
DB00615	Rifabutin	1T9N	0	0	0.97
DB00199	Erythromycin	1OKC	0	0	0.98
DB00624	Testosterone	1WD8	0	0	0.82
DB00624	Testosterone	1IRU	0	0	0.98
DB01200	Bromocriptine	1DON	0	0	0.99
DB01180	Rescinnamine	1F5F	0	0	0.96
DB01180	Rescinnamine	1SG0	0	0	0.94
DB01180	Rescinnamine	1UHL	0	0	0.93
DB00199	Erythromycin	1HOF	0	0	0.99
DB01083	Orlistat	1P87	0	0	1.00
DB00199	Erythromycin	1HOF	0	0	0.99
DB01216	Finasteride	1RGY	0	0	0.79
DB00199	Erythromycin	1W6F	0	0	0.97
DB00624	Testosterone	1ILQ	0	0	0.77
DB00624	Testosterone	1ODW	0	1	0.59
DB00199	Erythromycin	1P4R	0	0	0.99
DB00207	Azithromycin	1Y38	0	0	0.99
DB00207	Azithromycin	2BAT	0	0	0.98
DB00624	Testosterone	1GCN	0	0	0.82
DB00624	Testosterone	1J4I	0	1	0.64
DB00624	Testosterone	1FE3	0	1	0.57
DB00207	Azithromycin	1P5J	0	0	0.99

DB00199	Erythromycin	1T9N	0	0	0.98
DB00957	Norgestimate	3JDW	0	0	0.71
DB00936	Salicylic acid	1BDA	0	0	0.89
DB01180	Rescinnamine	1EXX	0	0	0.96
DB00199	Erythromycin	1ZNC	0	0	0.96
DB00199	Erythromycin	2CBR	0	0	0.99
DB00199	Erythromycin	1T9R	0	0	0.98
DB00207	Azithromycin	1TYE	0	0	0.99
DB00199	Erythromycin	1TQN	0	0	0.98
DB00624	Testosterone	1LJ7	0	1	0.60
DB00199	Erythromycin	1BP3	0	0	0.97
DB01216	Finasteride	1REW	0	0	0.73
DB01083	Orlistat	1K7L	0	0	0.98
DB00624	Testosterone	2CBR	0	1	0.56
DB00199	Erythromycin	1R5K	0	0	0.97
DB01222	Budesonide	1P87	0	0	0.99
DB01180	Rescinnamine	1HAG	0	1	0.64
DB00199	Erythromycin	1YV5	0	0	0.99
DB00615	Rifabutin	1CZM	0	0	0.97
DB00396	Progesterone	1QKM	0	0	0.91
DB00624	Testosterone	1H6I	0	1	0.56
DB00396	Progesterone	1VJB	0	0	0.90
DB00284	Acarbose	1H2W	0	0	1.00
DB00199	Erythromycin	1ISS	0	0	0.96
DB01180	Rescinnamine	1SQN	0	0	0.94
DB00624	Testosterone	1O5W	0	0	0.95
DB00624	Testosterone	1HOF	0	0	0.71
DB00624	Testosterone	1HOF	0	0	0.71
DB00624	Testosterone	1OF7	0	1	0.58
DB01216	Finasteride	1CZM	0	0	0.81
DB06144	Sertindole	1DON	0	0	0.99
DB01216	Finasteride	1TQN	0	0	0.76
DB00367	Levonorgestrel	1ODW	0	1	0.55
DB00624	Testosterone	1P87	0	0	1.00
DB00624	Testosterone	1EMI	0	0	0.86
DB00916	Metronidazole	1P87	0	0	1.00
DB01180	Rescinnamine	1BYW	0	0	0.96
DB00255	Diethylstilbestrol	1P87	0	0	0.99
DB01083	Orlistat	1MZW	0	0	0.99
DB00615	Rifabutin	1KTA	0	0	0.93
DB01222	Budesonide	1P87	0	0	0.99
DB00615	Rifabutin	1XGJ	0	0	0.93
DB00142	L-Glutamic Acid	1P87	0	0	0.99
DB02638	Terlipressin	1IRU	0	0	0.70

DB00207	Azithromycin	1UYL	0	0	0.99
DB00207	Azithromycin	1BWC	0	0	0.98
DB00717	Norethindrone	1HOF	0	1	0.51
DB01180	Rescinnamine	1K7L	0	0	0.73
DB00142	L-Glutamic Acid	1P87	0	0	0.99
DB00159	Icosapent	1K2H	0	0	0.98
DB00203	Sildenafil	1DON	0	0	0.98
DB00618	Demeclocycline	1DON	0	0	0.98
DB00511	Acetyldigitoxin	1K7L	0	0	0.98
DB00511	Acetyldigitoxin	1I7I	0	0	0.99
DB01083	Orlistat	1N8S	0	0	0.97
DB00511	Acetyldigitoxin	1I4L	0	0	0.99
DB00864	Tacrolimus	1G5X	0	0	0.99
DB00864	Tacrolimus	1HNK	0	0	0.99
DB01083	Orlistat	1NRL	0	0	0.98
DB00511	Acetyldigitoxin	1BI9	0	0	0.99
DB01089	Deserpidine	1EMI	0	0	0.98
DB00511	Acetyldigitoxin	1LBD	0	0	0.98
DB00864	Tacrolimus	1GXD	0	0	0.99
DB00511	Acetyldigitoxin	1UHL	0	0	0.99
DB01083	Orlistat	1N7D	0	0	0.98
DB00864	Tacrolimus	1F8U	0	0	0.99
DB01197	Captopril	1P87	0	0	0.99
DB01083	Orlistat	1ILQ	0	0	1.00
DB00122	Choline	1P87	0	0	1.00
DB00150	L-Tryptophan	1DON	0	0	0.96
DB00957	Norgestimate	1AGS	0	0	0.71
DB00994	Neomycin	1DON	0	0	0.75
DB01089	Deserpidine	1PB7	0	0	0.91
DB01083	Orlistat	1M1X	0	0	0.98
DB00203	Sildenafil	1IRU	0	0	0.98
DB00203	Sildenafil	1IRU	0	0	0.98
DB01083	Orlistat	1ODW	0	0	0.99
DB00342	Terfenadine	1BYY	0	0	0.74
DB00339	Pyrazinamide	1H2W	0	0	1.00
DB00864	Tacrolimus	1MRQ	0	0	0.99
DB00342	Terfenadine	1IRU	0	0	0.98
DB01083	Orlistat	1UYL	0	0	0.99
DB01083	Orlistat	3JDW	0	0	0.99
DB01083	Orlistat	1WVJ	0	0	0.99
DB01083	Orlistat	1L1F	0	0	0.99
DB01083	Orlistat	1NHZ	0	0	0.99
DB01083	Orlistat	1VRU	0	0	0.98
DB00615	Rifabutin	1AJS	0	0	0.92

DB01089	Deserpidine	1SS2	0	0	0.91
DB00203	Sildenafil	1YXL	0	1	0.50
DB01497	Etorphine	1BYW	0	1	0.59
DB01083	Orlistat	1YV5	0	0	0.99
DB01083	Orlistat	1R5K	0	0	0.98
DB00615	Rifabutin	1Z6T	0	0	0.97
DB00511	Acetyldigitoxin	1SG0	0	0	0.99
DB01083	Orlistat	1BDF	0	0	0.98
DB01497	Etorphine	1K2H	0	0	0.99
DB01083	Orlistat	8ICK	0	0	0.99
DB00864	Tacrolimus	1IHI	0	0	0.98
DB01083	Orlistat	1BNA	0	0	0.97
DB00511	Acetyldigitoxin	1OLM	0	0	0.99
DB00864	Tacrolimus	1HOF	0	0	0.99
DB00864	Tacrolimus	1OIZ	0	0	0.99
DB01083	Orlistat	1PWG	0	0	0.98
DB00203	Sildenafil	1ILQ	0	0	0.70
DB01083	Orlistat	1TQN	0	0	0.99
DB00864	Tacrolimus	1E3G	0	0	0.99
DB01089	Deserpidine	1P87	0	0	1.00
DB01083	Orlistat	1P0S	0	0	0.97
DB00175	Pravastatin	1K2H	0	0	0.93
DB01083	Orlistat	1ZNC	0	0	0.97
DB01083	Orlistat	1T9N	0	0	0.99
DB00006	Bivalirudin	1E79	0	0	0.98
DB00548	Azelaic Acid	1P87	0	0	1.00
DB00511	Acetyldigitoxin	1F5F	0	0	0.99
DB00511	Acetyldigitoxin	1MO8	0	0	0.99
DB00511	Acetyldigitoxin	1X86	0	0	0.99
DB01083	Orlistat	1KTA	0	0	0.98
DB01083	Orlistat	1REW	0	0	0.99
DB01216	Finasteride	1YV5	0	0	0.86
DB01083	Orlistat	1AJS	0	0	0.98
DB01216	Finasteride	1XKT	0	0	0.74
DB01083	Orlistat	1D6A	0	0	0.97
DB01083	Orlistat	1JVQ	0	0	0.98
DB01216	Finasteride	1NHZ	0	0	0.82
DB00006	Bivalirudin	1AJS	0	0	0.96
DB01083	Orlistat	1UZF	0	0	0.99
DB01216	Finasteride	1WVJ	0	0	0.83
DB01083	Orlistat	1Q7L	0	0	0.99
DB01083	Orlistat	2BK3	0	0	0.98
DB01216	Finasteride	1R75	0	0	0.76
DB01367	Rasagiline	1BDA	0	0	0.84

DB01216	Finasteride	1ILQ	0	0	0.93
DB00615	Rifabutin	1UZF	0	0	0.96
DB00615	Rifabutin	1UZF	0	0	0.96
DB04840	Debrisoquin	1DON	0	0	0.97
DB00864	Tacrolimus	1UZF	0	0	0.99
DB01216	Finasteride	2BIU	0	0	0.87
DB00459	Acitretin	1BDA	0	0	0.84
DB01216	Finasteride	1C4C	0	0	0.77
DB01089	Deserpidine	1QKM	0	0	0.89
DB01216	Finasteride	1EXB	0	0	0.69
DB00212	Remikiren	1EMI	0	0	0.94
DB01089	Deserpidine	1QYE	0	0	0.93
DB00212	Remikiren	1HNK	0	0	0.86
DB00212	Remikiren	1F8U	0	0	0.71
DB00006	Bivalirudin	1UZF	0	0	0.98
DB00853	Temozolomide	1IRU	0	0	0.98
DB00957	Norgestimate	1WVJ	0	0	0.75
DB00212	Remikiren	1OF7	0	0	0.83
DB00212	Remikiren	1HOF	0	0	0.86
DB01216	Finasteride	1BYW	0	0	0.87
DB00006	Bivalirudin	1UZF	0	0	0.98
DB00212	Remikiren	1BV8	0	0	0.75
DB00212	Remikiren	1UZF	0	0	0.71
DB00212	Remikiren	1CZM	0	0	0.76
DB01083	Orlistat	1BV8	0	0	0.99
DB00212	Remikiren	1T9R	0	0	0.69
DB00006	Bivalirudin	1O5W	0	0	0.99
DB00212	Remikiren	1HKO	0	0	0.77
DB00212	Remikiren	1FYC	0	0	0.70
DB01083	Orlistat	1HOF	0	0	0.99
DB01216	Finasteride	1XWS	0	0	0.81
DB00006	Bivalirudin	1HOF	0	0	0.99
DB01089	Deserpidine	1GTE	0	0	0.89
DB00207	Azithromycin	1EMI	0	0	0.99
DB00207	Azithromycin	1HWL	0	0	0.97
DB00207	Azithromycin	1OHY	0	0	0.98
DB00006	Bivalirudin	1P1R	0	0	0.98
DB00207	Azithromycin	1E3G	0	0	0.99
DB00006	Bivalirudin	1KG3	0	0	0.98
DB00207	Azithromycin	1UZF	0	0	0.98
DB01216	Finasteride	1EXX	0	0	0.85
DB01089	Deserpidine	1JBQ	0	0	0.93
DB00207	Azithromycin	1E79	0	0	0.98
DB00853	Temozolomide	1P87	0	0	0.99

DB00853	Temozolomide	1P87	0	0	0.99
DB00212	Remikiren	1NHZ	0	0	0.77
DB00976	Telithromycin	1KXP	0	0	0.99
DB00976	Telithromycin	1YTV	0	0	0.99
DB00976	Telithromycin	1SA1	0	0	0.99
DB00976	Telithromycin	1SA1	0	0	0.99
DB00976	Telithromycin	1MO8	0	0	0.99
DB00976	Telithromycin	1Y4E	0	0	1.00
DB00976	Telithromycin	1HA2	0	0	0.99
DB00976	Telithromycin	1H0C	0	0	0.99
DB00976	Telithromycin	1LN6	0	0	0.99
DB00976	Telithromycin	1UHL	0	0	0.99
DB00976	Telithromycin	1EXX	0	0	1.00
DB00976	Telithromycin	1RFV	0	0	0.99
DB00976	Telithromycin	1HAG	0	0	0.99
DB00976	Telithromycin	1IRU	0	0	1.00
DB00976	Telithromycin	1IRU	0	0	1.00
DB00976	Telithromycin	1BYW	0	0	1.00
DB00976	Telithromycin	1Y38	0	0	1.00
DB00976	Telithromycin	1NRL	0	0	0.99
DB00976	Telithromycin	1YOV	0	0	0.99
DB00976	Telithromycin	1LSZ	0	0	1.00
DB00976	Telithromycin	1W7N	0	0	0.99
DB00976	Telithromycin	1ILQ	0	0	1.00
DB00976	Telithromycin	1HIG	0	0	0.99
DB00976	Telithromycin	1MQ8	0	0	0.99
DB00976	Telithromycin	1TYE	0	0	1.00
DB00976	Telithromycin	1ODW	0	0	1.00
DB00976	Telithromycin	1UYL	0	0	0.99
DB00976	Telithromycin	1GP2	0	0	0.99
DB00976	Telithromycin	1BWC	0	0	0.99
DB00976	Telithromycin	1NHZ	0	0	0.99
DB00976	Telithromycin	1J4I	0	0	1.00
DB00976	Telithromycin	1YV5	0	0	1.00
DB00976	Telithromycin	1R5K	0	0	0.99
DB00976	Telithromycin	1MQB	0	0	0.99
DB00976	Telithromycin	8ICK	0	0	0.99
DB00976	Telithromycin	1BNA	0	0	0.99
DB00976	Telithromycin	1CJY	0	0	0.99
DB00976	Telithromycin	1TQN	0	0	0.99
DB00976	Telithromycin	1J3S	0	0	0.99
DB00976	Telithromycin	1JBQ	0	0	1.00
DB00976	Telithromycin	1PEH	0	0	0.99
DB00976	Telithromycin	1I9R	0	0	0.99

DB00976	Telithromycin	1CP3	0	0	0.99
DB00976	Telithromycin	1ZNC	0	0	0.99
DB00976	Telithromycin	1KTA	0	0	0.99
DB00976	Telithromycin	1REW	0	0	0.99
DB00976	Telithromycin	1Z6T	0	0	0.99
DB00976	Telithromycin	1JVQ	0	0	0.99
DB00976	Telithromycin	1UZF	0	0	0.99
DB00976	Telithromycin	1R4L	0	0	0.99
DB00976	Telithromycin	2BK3	0	0	0.99
DB00976	Telithromycin	1O5W	0	0	1.00
DB00976	Telithromycin	1HOF	0	0	1.00
DB00976	Telithromycin	1HSZ	0	0	0.99
DB00976	Telithromycin	1OKC	0	0	0.99
DB00976	Telithromycin	1F8U	0	0	0.99
DB00976	Telithromycin	1OHY	0	0	0.99
DB00976	Telithromycin	1HWL	0	0	0.99
DB00212	Remikiren	1CWM	0	0	0.81
DB00864	Tacrolimus	1JVQ	0	0	0.98
DB00976	Telithromycin	1EMI	0	0	1.00
DB01216	Finasteride	1Q9S	0	0	0.86
DB00212	Remikiren	1SQN	0	0	0.76
DB00006	Bivalirudin	1EMI	0	0	0.99
DB01089	Deserpidine	1P0Q	0	0	0.86
DB01058	Praziquantel	1EMI	0	0	0.75
DB01058	Praziquantel	1P87	0	0	1.00
DB00212	Remikiren	1LBD	0	1	0.64
DB00864	Tacrolimus	1E79	0	0	0.99
DB00212	Remikiren	1MO8	0	0	0.77
DB01216	Finasteride	1BJ4	0	0	0.80
DB01400	Neostigmine	1BDA	0	0	0.93
DB00212	Remikiren	1IIH	0	0	0.71
DB01606	Tazobactam	1IRU	0	0	0.98
DB00858	Dromostanolone	1F5F	0	0	0.99
DB01089	Deserpidine	1T9R	0	0	0.90
DB00396	Progesterone	1HD7	0	0	0.93
DB00959	Methylprednisolone	1H2W	0	0	1.00
DB00864	Tacrolimus	1CZM	0	0	0.99
DB00212	Remikiren	1SA1	0	0	0.72
DB00864	Tacrolimus	1T9N	0	0	0.99
DB00212	Remikiren	1A8M	0	0	0.81
DB00864	Tacrolimus	1T9R	0	0	0.99
DB00957	Norgestimate	1NHZ	0	0	0.74
DB00551	Acetohydroxamic Acid	1BDA	0	0	0.73
DB01216	Finasteride	1HA2	0	0	0.72

DB00212	Remikiren	1VYT	0	1	0.67
DB00864	Tacrolimus	1FIE	0	0	0.98
DB04794	Bifonazole	1DON	0	0	0.98
DB00711	Diethylcarbamazine	1EMI	0	1	0.59
DB00711	Diethylcarbamazine	1EMI	0	1	0.59
DB01058	Praziquantel	1HOF	0	1	0.55
DB00864	Tacrolimus	1I0E	0	0	0.98
DB00864	Tacrolimus	1CRK	0	0	0.98
DB01089	Deserpidine	1Q2P	0	0	0.90
DB01180	Rescinnamine	1EMI	0	0	0.99
DB00717	Norethindrone	1P87	0	0	1.00
DB00864	Tacrolimus	1XMI	0	0	0.98
DB01606	Tazobactam	1P87	0	0	1.00
DB00890	Dienestrol	1H2W	0	0	1.00
DB00207	Azithromycin	1ZNC	0	0	0.97
DB01216	Finasteride	1MO8	0	0	0.82
DB00864	Tacrolimus	1TQN	0	0	0.99
DB01216	Finasteride	1Y0X	0	0	0.85
DB00615	Rifabutin	1E3G	0	0	0.97
DB01180	Rescinnamine	1P87	0	0	1.00
DB00751	Epinastine	1P87	0	0	0.99
DB01033	Mercaptopurine	1P87	0	0	0.99
DB00717	Norethindrone	1EMI	0	0	0.73
DB01083	Orlistat	1F8U	0	0	0.99
DB01033	Mercaptopurine	1P87	0	0	0.99
DB00799	Tazarotene	1DON	0	0	0.98
DB00957	Norgestimate	1SS2	0	0	0.74
DB00615	Rifabutin	1Q7L	0	0	0.97
DB00180	Flunisolide	1IRU	0	0	0.99
DB00304	Desogestrel	1P87	0	0	1.00
DB00180	Flunisolide	1IRU	0	0	0.99
DB00957	Norgestimate	1J4I	0	0	0.84
DB00957	Norgestimate	1FE3	0	0	0.79
DB01180	Rescinnamine	1HWL	0	0	0.76
DB04840	Debrisoquin	1P87	0	0	0.98
DB01180	Rescinnamine	1F8U	0	0	0.93
DB00304	Desogestrel	1P87	0	0	1.00
DB01180	Rescinnamine	1OKC	0	0	0.95
DB00396	Progesterone	1TQN	0	0	0.90
DB00799	Tazarotene	1IRU	0	0	0.98
DB01047	Fluocinonide	1P87	0	0	0.99
DB01047	Fluocinonide	1IRU	0	0	0.99
DB00615	Rifabutin	1O5W	0	0	0.99
DB00864	Tacrolimus	1BNA	0	0	0.97

DB00864	Tacrolimus	1A36	0	0	0.98
DB01047	Fluocinonide	1DON	0	0	0.99
DB00615	Rifabutin	1I5H	0	0	0.97
DB00864	Tacrolimus	1R5K	0	0	0.98
DB00864	Tacrolimus	1QKM	0	0	0.99
DB00396	Progesterone	1JBQ	0	0	0.94
DB00396	Progesterone	1QK1	0	0	0.89
DB00396	Progesterone	1I0E	0	0	0.74
DB00864	Tacrolimus	1YV5	0	0	0.99
DB00864	Tacrolimus	1XKT	0	0	0.99
DB00368	Norepinephrine	1DON	0	0	0.94
DB00864	Tacrolimus	1L9X	0	0	0.99
DB00544	Fluorouracil	1DON	0	0	0.98
DB00396	Progesterone	1PEH	0	0	0.70
DB00864	Tacrolimus	1NHZ	0	0	0.99
DB00367	Levonorgestrel	1HKO	0	1	0.54
DB00304	Desogestrel	1HOF	0	1	0.66
DB00489	Sotalol	1P87	0	0	0.98
DB00957	Norgestimate	1YV5	0	0	0.80
DB00864	Tacrolimus	1Z8L	0	0	0.99
DB01083	Orlistat	1OD4	0	0	0.99
DB00957	Norgestimate	1VJB	0	1	0.67
DB00615	Rifabutin	1BV8	0	0	0.97
DB01180	Rescinnamine	1MRQ	0	0	0.96
DB00864	Tacrolimus	1WVJ	0	0	0.99
DB00864	Tacrolimus	1QVU	0	0	0.98
DB01185	Fluoxymesterone	1IRU	0	0	0.99
DB01185	Fluoxymesterone	1DON	0	0	0.99
DB00367	Levonorgestrel	1HOF	0	0	0.68
DB00864	Tacrolimus	1BZY	0	0	0.98
DB01180	Rescinnamine	1EW2	0	0	0.95
DB00367	Levonorgestrel	1HOF	0	0	0.68
DB00615	Rifabutin	1HOF	0	0	0.98
DB00864	Tacrolimus	1ILQ	0	0	0.99
DB01113	Papaverine	1P87	0	0	1.00
DB00864	Tacrolimus	1SPJ	0	0	0.97
DB00712	Flurbiprofen	1IRU	0	0	0.99
DB00367	Levonorgestrel	1P87	0	0	1.00
DB00957	Norgestimate	1QYX	0	0	0.74
DB01180	Rescinnamine	1HOF	0	0	0.97
DB00615	Rifabutin	1HOF	0	0	0.98
DB00615	Rifabutin	1EW2	0	0	0.97
DB00588	Fluticasone Propionate	1P87	0	0	1.00
DB00588	Fluticasone Propionate	1DON	0	0	0.99

DB00864	Tacrolimus	1MLD	0	0	0.98
DB00615	Rifabutin	1P1R	0	0	0.96
DB00615	Rifabutin	1OKC	0	0	0.97
DB00367	Levonorgestrel	1EMI	0	0	0.84
DB00367	Levonorgestrel	1EMI	0	0	0.84
DB00864	Tacrolimus	1L6J	0	0	0.99
DB00396	Progesterone	1T9N	0	0	0.91
DB01095	Fluvastatin	1P87	0	0	0.90
DB00396	Progesterone	1PTW	0	1	0.67
DB00396	Progesterone	1I2W	0	0	0.94
DB00459	Acitretin	1K2H	0	0	0.97
DB00396	Progesterone	1RL0	0	0	0.92
DB00957	Norgestimate	2BGR	0	1	0.66
DB00396	Progesterone	1UZF	0	0	0.89
DB00799	Tazarotene	1P87	0	0	1.00
DB00864	Tacrolimus	1E71	0	0	0.99
DB00864	Tacrolimus	1PT9	0	0	0.99
DB00207	Azithromycin	1CJY	0	0	0.97
DB01213	Fomepizole	1P87	0	0	1.00
DB00957	Norgestimate	1FYC	0	0	0.71
DB00957	Norgestimate	1TQN	0	1	0.67
DB00864	Tacrolimus	1OAT	0	0	0.98
DB00864	Tacrolimus	1NRL	0	0	0.98
DB00396	Progesterone	1HOF	0	0	0.96
DB00957	Norgestimate	1HKO	0	0	0.80
DB00992	Methyl aminolevulinate	1DON	0	0	0.98
DB00957	Norgestimate	1LJ7	0	0	0.81
DB00615	Rifabutin	1OD4	0	0	0.98
DB00396	Progesterone	1HOF	0	0	0.96
DB00615	Rifabutin	1F8U	0	0	0.97
DB00848	Levamisole	1K2H	0	0	0.77
DB00615	Rifabutin	1OHY	0	0	0.97
DB00396	Progesterone	1ORE	0	0	0.94
DB00615	Rifabutin	1HWL	0	0	0.93
DB00957	Norgestimate	1P0Q	0	1	0.64
DB00926	Etretinate	1FE3	0	1	0.51
DB00615	Rifabutin	1EMI	0	0	0.99
DB00957	Norgestimate	1T9R	0	0	0.73
DB00396	Progesterone	1GXD	0	0	0.92
DB00864	Tacrolimus	1C4C	0	0	0.99
DB00864	Tacrolimus	1YXM	0	0	0.98
DB00396	Progesterone	1OHY	0	0	0.91
DB00511	Acetyldigitoxin	1EH6	0	0	0.99
DB01180	Rescinnamine	1UZF	0	0	0.93

DB01182	Propafenone	1P87	0	0	0.99
DB00864	Tacrolimus	1KI0	0	0	0.99
DB00396	Progesterone	1P87	0	0	1.00
DB00635	Prednisone	1P87	0	0	0.99
DB00957	Norgestimate	1UWJ	0	0	0.71
DB00635	Prednisone	1P87	0	0	0.99
DB01182	Propafenone	1P87	0	0	0.99
DB01089	Deserpidine	1F8U	0	0	0.87
DB00396	Progesterone	1EMI	0	0	0.98
DB01180	Rescinnamine	1E79	0	0	0.93
DB00864	Tacrolimus	1EXB	0	0	0.99
DB00957	Norgestimate	3BLM	0	0	0.76
DB04690	Camptothecin	1K2H	0	0	0.79
DB00957	Norgestimate	1E79	0	1	0.67
DB00864	Tacrolimus	1SQN	0	0	0.99
DB00864	Tacrolimus	1TJC	0	0	0.99
DB00864	Tacrolimus	1RFV	0	0	0.99
DB00957	Norgestimate	1UZF	0	1	0.67
DB00992	Methyl aminolevulinate	1IRU	0	0	0.98
DB00304	Desogestrel	1K6R	0	1	0.60
DB00339	Pyrazinamide	1P87	0	0	0.99
DB00396	Progesterone	1KED	0	0	0.90
DB00396	Progesterone	1MO8	0	0	0.92
DB00396	Progesterone	1BYY	0	0	0.98
DB00864	Tacrolimus	1R6K	0	0	0.99
DB00210	Adapalene	1O5W	0	1	0.60
DB00228	Enflurane	1P87	0	0	1.00
DB00396	Progesterone	1HA2	0	0	0.89
DB00957	Norgestimate	1E3G	0	0	0.74
DB00864	Tacrolimus	1BI9	0	0	0.99
DB01418	Acenocoumarol	1P87	0	0	1.00
DB00396	Progesterone	1GGL	0	0	0.89
DB06144	Sertindole	1P87	0	0	0.99
DB01222	Budesonide	1BYW	0	0	0.77
DB00396	Progesterone	1R5S	0	0	0.92
DB00864	Tacrolimus	1EXX	0	0	0.99
DB00837	Progabide	1IRU	0	0	0.99
DB04794	Bifonazole	1P87	0	0	1.00
DB01222	Budesonide	1C5G	0	1	0.64
DB00864	Tacrolimus	1LBD	0	0	0.99
DB00864	Tacrolimus	1UHL	0	0	0.99
DB00122	Choline	1DON	0	0	0.98
DB00203	Sildenafil	1QYE	0	1	0.51
DB00396	Progesterone	1CRB	0	0	0.93

DB01222	Budesonide	3JDW	0	1	0.64
DB00675	Tamoxifen	1P87	0	0	1.00
DB01128	Bicalutamide	1P87	0	0	1.00
DB00864	Tacrolimus	1F8Q	0	0	0.99
DB00864	Tacrolimus	2AAI	0	0	0.99
DB01222	Budesonide	1YAE	0	0	0.70
DB00207	Azithromycin	1BNA	0	0	0.97
DB00396	Progesterone	1BI9	0	0	0.86
DB01222	Budesonide	1J4I	0	0	0.79
DB01180	Rescinnamine	1RGY	0	0	0.94
DB00396	Progesterone	1L1F	0	0	0.90
DB00864	Tacrolimus	1HA2	0	0	0.99
DB00203	Sildenafil	1JBQ	0	1	0.51
DB00396	Progesterone	1WVJ	0	0	0.92
DB00955	Netilmicin	1DON	0	0	0.97
DB00864	Tacrolimus	1YVL	0	0	0.99
DB00396	Progesterone	1G1S	0	0	0.87
DB00864	Tacrolimus	1MO8	0	0	0.99
DB00806	Pentoxifylline	1P87	0	0	1.00
DB01393	Bezafibrate	1P87	0	0	0.97
DB00864	Tacrolimus	1EYD	0	0	0.99
DB01180	Rescinnamine	1TB5	0	0	0.75
DB00864	Tacrolimus	1KED	0	0	0.99
DB00159	Icosapent	1P87	0	0	1.00
DB00864	Tacrolimus	1A8M	0	0	0.99
DB01180	Rescinnamine	1CZM	0	0	0.95
DB01406	Danazol	1EMI	0	0	0.77
DB01406	Danazol	1P87	0	0	1.00
DB01180	Rescinnamine	1P0Q	0	0	0.93
DB01180	Rescinnamine	1JBQ	0	0	0.96
DB01032	Probenecid	1P87	0	0	1.00
DB00992	Methyl aminolevulinate	1P87	0	0	1.00
DB00864	Tacrolimus	2KAU	0	0	0.98
DB01222	Budesonide	3CBS	0	0	0.74
DB00304	Desogestrel	1JBQ	0	1	0.54
DB00864	Tacrolimus	1T0U	0	0	0.99
DB01180	Rescinnamine	1BNA	0	1	0.64
DB01180	Rescinnamine	1A36	0	0	0.77
DB01406	Danazol	1HOF	0	1	0.57
DB00091	Cyclosporine	1HWL	0	0	0.99
DB00199	Erythromycin	1WVJ	0	0	0.98
DB00308	Ibutilide	1Y4E	0	1	0.60
DB01180	Rescinnamine	1R5K	0	0	0.76
DB01180	Rescinnamine	1VJB	0	0	0.93

DB04942	Tamibarotene	1P87	0	0	0.99
DB00232	Methyclothiazide	1IRU	0	0	0.99
DB01222	Budesonide	1IBC	0	0	0.77
DB00622	Nicardipine	1EMI	0	1	0.46
DB00957	Norgestimate	1HOF	0	0	0.87
DB01222	Budesonide	1CZM	0	1	0.67
DB00820	Tadalafil	1BDA	0	0	0.86
DB00738	Pentamidine	1DON	0	0	0.97
DB01406	Danazol	1HOF	0	1	0.57
DB00199	Erythromycin	1WVJ	0	0	0.98
DB00228	Enflurane	1IRU	0	0	1.00
DB00199	Erythromycin	9ILB	0	0	0.99
DB00396	Progesterone	1H2W	0	0	1.00
DB00199	Erythromycin	2IL6	0	0	0.99
DB00203	Sildenafil	1EMI	0	0	0.81
DB00837	Progabide	1P87	0	0	0.95
DB00837	Progabide	1P87	0	0	0.95
DB00396	Progesterone	1SQN	0	0	0.91
DB01222	Budesonide	1UZF	0	1	0.60
DB01180	Rescinnamine	1VRU	0	0	0.76
DB00199	Erythromycin	1W7N	0	0	0.98
DB00396	Progesterone	1Y0S	0	0	0.81
DB00396	Progesterone	1BYW	0	0	0.94
DB01222	Budesonide	1Q7L	0	0	0.68
DB00616	Candoxatril	1V97	0	0	0.93
DB01180	Rescinnamine	1SS2	0	0	0.95
DB00199	Erythromycin	1D1P	0	0	0.98
DB00616	Candoxatril	1EMI	0	0	0.97
DB01348	Spirapril	1P87	0	0	0.99
DB01348	Spirapril	1P87	0	0	0.99
DB01222	Budesonide	1HOF	0	0	0.82
DB01089	Deserpidine	1OF7	0	0	0.93
DB00203	Sildenafil	1P87	0	0	1.00
DB00396	Progesterone	1I7I	0	0	0.87
DB01222	Budesonide	1HOF	0	0	0.82
DB01083	Orlistat	1MF1	0	0	0.99
DB01089	Deserpidine	1HOF	0	0	0.95
DB01180	Rescinnamine	3JDW	0	0	0.94
DB01180	Rescinnamine	9ILB	0	0	0.96
DB01180	Rescinnamine	1MZW	0	0	0.96
DB01222	Budesonide	1EW2	0	1	0.65

Validation

DB00926	Etretinate	1EXX	1	1	0.48
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DB00163	Vitamin E	1OIZ	1	0	0.99
DB00107	Oxytocin	1H2W	1	0	1.00
DB01396	Digitoxin	1MO8	1	0	0.98
DB00492	Fosinopril	1UZF	1	0	0.97
DB00624	Testosterone	1F5F	1	1	0.55
DB00615	Rifabutin	1QYE	1	0	0.98
DB00570	Vinblastine	1SA1	1	0	0.98
DB01497	Etorphine	1D6G	1	1	0.62
DB00513	Aminocaproic Acid	1BDA	1	0	0.79
DB01245	Decamethonium	1F8U	1	0	0.94
DB00661	Verapamil	1CZM	1	0	0.95
DB01216	Finasteride	1E3G	1	0	0.82
DB00188	Bortezomib	1IRU	1	0	0.98
DB00154	gamma-Homolinolenic acid	1FE3	1	1	0.50
DB00641	Simvastatin	1CP3	1	0	0.92
DB06692	Aprotinin	1SPJ	1	0	0.96
DB00976	Telithromycin	1EMI	1	0	1.00
DB00873	Loteprednol Etabonate	1NHZ	1	1	0.53
DB00641	Simvastatin	1HIG	1	0	0.91
DB00957	Norgestimate	1SQN	1	0	0.71
DB00641	Simvastatin	1L6J	1	0	0.89
DB01083	Orlistat	1N8S	1	0	0.97
DB01076	Atorvastatin	1DON	1	0	0.99
DB01406	Danazol	1DON	1	0	0.98
DB00006	Bivalirudin	1HAG	1	0	0.96
DB00970	Dactinomycin	1BNA	1	0	0.98
DB00864	Tacrolimus	1J4I	1	0	0.99
DB00834	Mifepristone	1SQN	1	0	0.78
DB01395	Drospirenone	1SQN	1	0	0.95
DB00641	Simvastatin	1SLM	1	0	0.93
DB00858	Dromostanolone	1BP3	1	0	0.98
DB01601	Lopinavir	1ODW	1	1	0.61
DB00203	Sildenafil	1T9R	1	1	0.39
DB00162	Vitamin A	1JYD	1	1	0.20
DB00926	Etretinate	1UHL	1	1	0.32
DB00162	Vitamin A	1LPJ	1	1	0.19
DB01058	Praziquantel	1AGS	1	1	0.24
DB00396	Progesterone	1R5K	1	1	0.58
DB00641	Simvastatin	1TZI	1	1	0.55
DB00641	Simvastatin	1HAG	1	1	0.55
DB00364	Sucalfate	1HA2	1	1	0.09
DB00321	Amitriptyline	1HOF	1	1	0.04
DB00220	Nelfinavir	1ODW	1	1	0.60
DB00224	Indinavir	1ODW	1	1	0.53

DB00162	Vitamin A	1GGL	1	1	0.11
DB06148	Mianserin	1HOF	1	1	0.02
DB00799	Tazarotene	1EXX	1	1	0.05
DB00675	Tamoxifen	1QKM	1	1	0.02
DB00989	Rivastigmine	1P0Q	1	1	0.05
DB00273	Topiramate	1YAE	1	1	0.16
DB00865	Benzphetamine	1HOF	1	1	0.01
DB00572	Atropine	1Y38	1	1	0.12
DB00717	Norethindrone	1SQN	1	1	0.23
DB00253	Medrysone	1CJY	1	1	0.31
DB01400	Neostigmine	1F8U	1	1	0.01
DB00975	Dipyridamole	1T9R	1	1	0.25
DB00210	Adapalene	1LBD	1	1	0.04
DB04575	Quinestrol	1R5K	1	1	0.16
DB01108	Trilostane	1QKM	1	1	0.25
DB01199	Tubocurarine	1F8U	1	1	0.24
DB00691	Moexipril	1UZF	1	1	0.14
DB00523	Alitretinoin	1LBD	1	1	0.03
DB01232	Saquinavir	1HA2	1	1	0.09
DB00696	Ergotamine	1HOF	1	1	0.15
DB00308	Ibutilide	1BYW	1	1	0.26
DB00736	Esomeprazole	1MO8	1	1	0.00
DB00806	Pentoxifylline	1TB5	1	1	0.00
DB01113	Papaverine	1TB5	1	1	0.00
DB00655	Estrone	1P49	1	1	0.01
DB00775	Tirofiban	1G1S	1	1	0.16
DB00159	Icosapent	1Y0S	1	1	0.01
DB00981	Physostigmine	1F8U	1	1	0.01
DB00755	Tretinoin	1EXX	1	1	0.04
DB00755	Tretinoin	1UHL	1	1	0.02
DB00094	Urofollitropin	1XWD	1	1	0.01
DB00459	Acitretin	1EXX	1	1	0.01
DB00459	Acitretin	1UHL	1	1	0.01
DB00848	Levamisole	1HA2	1	1	0.00
DB01392	Yohimbine	1HOF	1	1	0.06
DB00633	Dexmedetomidine	1HOF	1	1	0.00
DB00583	L-Carnitine	1S5O	1	1	0.00
DB00818	Propofol	1HA2	1	1	0.00
DB00704	Naltrexone	1A8M	1	1	0.02
DB00119	Pyruvic acid	1OHY	1	1	0.00
DB00749	Etodolac	1HA2	1	1	0.00
DB01132	Pioglitazone	1I7I	1	1	0.00
DB00210	Adapalene	1XDK	1	1	0.00
DB00692	Phentolamine	1GCN	1	1	0.00

DB00532	Mephenytoin	1HA2	1	1	0.00
DB01166	Cilostazol	1TB5	1	1	0.01
DB01120	Gliclazide	1HA2	1	1	0.00
DB00934	Maprotiline	2BK3	1	1	0.00
DB04967	Lucanthone	1BNA	1	1	0.00
DB01109	Heparin	1P0S	1	1	0.00
DB00741	Hydrocortisone	1F5F	1	1	0.14
DB01008	Busulfan	1BNA	1	1	0.00
DB02638	Terlipressin	1YTV	1	1	0.00
DB00540	Nortriptyline	1HA2	1	1	0.00
DB00542	Benazepril	1UZF	1	1	0.01
DB00374	Treprostinil	1G91	1	1	0.09
DB00655	Estrone	1R5K	1	1	0.00
DB00584	Enalapril	1UZF	1	1	0.02
DB01225	Enoxaparin	1HAG	1	1	0.00
DB00523	Alitretinoin	1XDK	1	1	0.00
DB01258	Aliskiren	1BBS	1	1	0.20
DB00783	Estradiol	1NRL	1	1	0.00
DB00238	Nevirapine	1VRU	1	1	0.00
DB00651	Dyphylline	1PTW	1	1	0.00
DB00869	Dorzolamide	1T9N	1	1	0.00
DB00191	Phentermine	1O5W	1	1	0.00
DB01031	Ethinamate	1T9N	1	1	0.00
DB00311	Ethoxzolamide	1CZM	1	1	0.00
DB01411	Pranlukast	1DYT	1	1	0.00
DB01411	Pranlukast	1A8M	1	1	0.00
DB00035	Desmopressin	1YTV	1	1	0.00
DB04840	Debrisoquin	1HOF	1	1	0.00
DB00481	Raloxifene	1QKM	1	1	0.00
DB01367	Rasagiline	2BK3	1	1	0.00
DB00872	Conivaptan	1YTV	1	1	0.00
DB00916	Metronidazole	1BNA	1	1	0.00
DB00703	Methazolamide	1CZM	1	1	0.00
DB01001	Salbutamol	1ILQ	1	1	0.00
DB01213	Fomepizole	1HSZ	1	1	0.00
DB01418	Acenocoumarol	1HA2	1	1	0.00
DB00170	Menadione	1HAG	1	1	0.00
DB00170	Menadione	1Z6J	1	1	0.00
DB00464	Sodium Tetradecyl Sulfate	1AUT	1	1	0.00
DB01065	Melatonin	1R5K	1	1	0.00
DB01065	Melatonin	1XQ8	1	1	0.00
DB00122	Choline	1PEH	1	1	0.00
DB00919	Spectinomycin	1P87	1	0	0.75
DB00786	Marimastat	1SLM	1	1	0.00

DB01034	Cerulenin	1XKT	1	1	0.00
DB01170	Guanethidine	1HOF	1	1	0.00
DB04942	Tamibarotene	1XDK	1	1	0.00
DB00172	L-Proline	2BIU	1	1	0.00
DB00456	Cefalotin	1PWG	1	1	0.00
DB01136	Carvedilol	1BYW	1	1	0.00
DB00172	L-Proline	1CYN	1	1	0.00
DB01197	Captopril	1MO8	1	1	0.00
DB00722	Lisinopril	1UZF	1	1	0.00
DB01197	Captopril	1UZF	1	1	0.00
DB04690	Camptothecin	1A36	1	1	0.00
DB01041	Thalidomide	1A8M	1	1	0.00
DB00142	L-Glutamic Acid	1YAE	1	1	0.00
DB00142	L-Glutamic Acid	1XHY	1	1	0.00
DB00560	Tigecycline	1EMI	1	1	0.02
DB00302	Tranexamic Acid	1KI0	1	1	0.00
DB00619	Imatinib	1OPL	1	1	0.00
DB00909	Zonisamide	1BYY	1	1	0.00
DB00142	L-Glutamic Acid	1WVJ	1	1	0.00
DB00142	L-Glutamic Acid	1Z8L	1	1	0.00
DB00945	Aspirin	1YXL	1	1	0.00
DB01009	Ketoprofen	1HA2	1	1	0.00
DB00701	Amprenavir	1ODW	1	1	0.01
DB00518	Albendazole	1SA1	1	1	0.00
DB00682	Warfarin	1HAG	1	1	0.00
DB01006	Letrozole	1R5K	1	1	0.00
DB00128	L-Aspartic Acid	1MF1	1	1	0.00
DB00151	L-Cysteine	1EH6	1	1	0.00
DB01259	Lapatinib	1IVO	1	1	0.00
DB00155	L-Citrulline	1WD8	1	1	0.00
DB00128	L-Aspartic Acid	1LSZ	1	1	0.00
DB00709	Lamivudine	1BNA	1	1	0.00
DB01172	Kanamycin	1EMI	1	1	0.00
DB00451	Levothyroxine	1HA2	1	1	0.00
DB00451	Levothyroxine	1KGI	1	1	0.00
DB00951	Isoniazid	1W6F	1	1	0.00
DB00142	L-Glutamic Acid	1KTA	1	1	0.00
DB00677	Isoflurophate	1F8U	1	1	0.00
DB00753	Isoflurane	1E79	1	1	0.00
DB01040	Hydroxystilbamidine Isethionate	1BNA	1	1	0.00
DB00774	Hydroflumethiazide	1ZNC	1	1	0.00
DB00130	L-Glutamine	1W7N	1	1	0.00
DB00279	Liothyronine	1HA2	1	1	0.00
DB00279	Liothyronine	1Y0X	1	1	0.00

DB00999	Hydrochlorothiazide	1ZNC	1	1	0.00
DB00134	L-Methionine	1LT8	1	1	0.00
DB04948	Lofexidine	1HOF	1	1	0.00
DB00129	L-Ornithine	3JDW	1	1	0.00
DB01275	Hydralazine	1TJC	1	1	0.00
DB00756	Hexachlorophene	1F0X	1	1	0.00
DB01159	Halothane	1HA2	1	1	0.00
DB00133	L-Serine	1P5J	1	1	0.00
DB01159	Halothane	1WVJ	1	1	0.00
DB00150	L-Tryptophan	1WAP	1	1	0.00
DB01218	Halofantrine	1BYW	1	1	0.00
DB00256	Lymecycline	1EMI	1	1	0.00
DB00653	Magnesium Sulfate	1VYT	1	1	0.00
DB00226	Guanadrel Sulfate	1HOF	1	1	0.00
DB00145	Glycine	1H0C	1	1	0.00
DB00888	Mechlorethamine	1BNA	1	1	0.00
DB00145	Glycine	1R75	1	1	0.00
DB00798	Gentamicin	1P87	1	1	0.05
DB00441	Gemcitabine	1TEV	1	1	0.00
DB00695	Furosemide	1MO8	1	1	0.00
DB00452	Framycetin	1P87	1	1	0.01
DB00569	Fondaparinux sodium	1JVQ	1	1	0.00
DB01095	Fluvastatin	1HWL	1	1	0.00
DB01028	Methoxyflurane	1E79	1	1	0.00
DB01028	Methoxyflurane	1EXB	1	1	0.00
DB00232	Methyclothiazide	1ZNC	1	1	0.00
DB00499	Flutamide	1E3G	1	1	0.00
DB00551	Acetohydroxamic Acid	2KAU	1	1	0.00
DB01185	Fluoxymesterone	1F5F	1	1	0.00
DB01185	Fluoxymesterone	1E3G	1	1	0.00
DB01017	Minocycline	1EMI	1	1	0.00
DB01017	Minocycline	1CP3	1	1	0.00
DB01017	Minocycline	1L6J	1	1	0.00
DB00324	Fluorometholone	1CJY	1	1	0.00
DB00305	Mitomycin	1BNA	1	1	0.00
DB01171	Moclobemide	1O5W	1	1	0.00
DB00180	Flunisolide	1CJY	1	1	0.00
DB00157	NADH	1HWL	1	1	0.00
DB00157	NADH	1HT0	1	1	0.00
DB00157	NADH	1OF7	1	1	0.00
DB00157	NADH	1XF0	1	1	0.00
DB00157	NADH	1XU9	1	1	0.00
DB00157	NADH	1HE5	1	1	0.00
DB00157	NADH	1BWC	1	1	0.00

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DB00157	NADH	1F0Y	1	1	0.00
DB00157	NADH	5MDH	1	1	0.00
DB00157	NADH	1QR6	1	1	0.00
DB00157	NADH	1ZBQ	1	1	0.00
DB00157	NADH	1BXS	1	1	0.00
DB00157	NADH	1JQI	1	1	0.00
DB00800	Fenoldopam	1HOF	1	1	0.00
DB01196	Estramustine	1QKM	1	1	0.00
DB00228	Enflurane	1EXB	1	1	0.00
DB00665	Nilutamide	1E3G	1	1	0.00
DB00368	Norepinephrine	1HOF	1	1	0.00
DB00625	Efavirenz	1VRU	1	1	0.00
DB06262	Droxidopa	1HOF	1	1	0.00
DB00254	Doxycycline	1P87	1	1	0.28
DB00510	Divalproex sodium	1OHY	1	1	0.00
DB00526	Oxaliplatin	1BNA	1	1	0.00
DB01093	Dimethyl sulfoxide	1KED	1	1	0.00
DB00842	Oxazepam	1HA2	1	1	0.00
DB01093	Dimethyl sulfoxide	1C5G	1	1	0.00
DB00859	Penicillamine	1IBC	1	1	0.00
DB01093	Dimethyl sulfoxide	1J4I	1	1	0.00
DB01121	Phenacemide	1BYY	1	1	0.00
DB00780	Phenelzine	1PU4	1	1	0.00
DB01093	Dimethyl sulfoxide	1UTQ	1	1	0.00
DB01093	Dimethyl sulfoxide	1XF0	1	1	0.00
DB00861	Diflunisal	1HA2	1	1	0.00
DB00255	Diethylstilbestrol	1R5K	1	1	0.00
DB00900	Didanosine	1VRU	1	1	0.00
DB00586	Diclofenac	1KED	1	1	0.00
DB01119	Diazoxide	1ZNC	1	1	0.00
DB01168	Procarbazine	1BNA	1	1	0.00
DB01123	Proflavine	1BNA	1	1	0.00
DB01234	Dexamethasone	1NHZ	1	1	0.00
DB01189	Desflurane	1WVJ	1	1	0.00
DB00618	Demeclocycline	1P87	1	1	0.16
DB00339	Pyrazinamide	1XKT	1	1	0.00
DB00114	Pyridoxal Phosphate	1OHY	1	1	0.00
DB00114	Pyridoxal Phosphate	1JBQ	1	1	0.00
DB00944	Demecarium bromide	1F8U	1	1	0.01
DB00819	Acetazolamide	1JD0	1	1	0.00
DB00114	Pyridoxal Phosphate	1W7N	1	1	0.00
DB00114	Pyridoxal Phosphate	1OAT	1	1	0.00
DB00165	Pyridoxine	1JBQ	1	1	0.00
DB01254	Dasatinib	1MQB	1	1	0.00

DB01103	Quinacrine	1BNA	1	1	0.00
DB04839	Cyproterone	1E3G	1	1	0.00
DB01325	Quinethazone	1ZNC	1	1	0.00
DB00606	Cyclothiazide	1T9N	1	1	0.00
DB00531	Cyclophosphamide	1BNA	1	1	0.00
DB00148	Creatine	3JDW	1	1	0.00
DB02709	Resveratrol	1SG0	1	1	0.00
DB00140	Riboflavin	1HE5	1	1	0.00
DB00148	Creatine	1I0E	1	1	0.00
DB01147	Cloxacillin	1XGJ	1	1	0.00
DB00884	Risedronate	1YV5	1	1	0.00
DB00575	Clonidine	1HOF	1	1	0.00
DB01098	Rosuvastatin	1HWL	1	1	0.00
DB00173	Adenine	1KG3	1	1	0.00
DB00173	Adenine	1RL0	1	1	0.00
DB06144	Sertindole	1BYW	1	1	0.00
DB00173	Adenine	1BNA	1	1	0.00
DB00173	Adenine	1Y6R	1	1	0.00
DB00173	Adenine	1F8Q	1	1	0.00
DB00453	Clomocycline	1EMI	1	1	0.00
DB00845	Clofazimine	1BNA	1	1	0.00
DB00720	Clodronate	1OKC	1	1	0.00
DB00242	Cladribine	1BNA	1	1	0.00
DB00537	Ciprofloxacin	1HA2	1	1	0.00
DB00477	Chlorpromazine	1HA2	1	1	0.00
DB01082	Streptomycin	1EMI	1	1	0.00
DB00880	Chlorothiazide	1T9N	1	1	0.00
DB00605	Sulindac	2T40	1	1	0.00
DB00605	Sulindac	1HA2	1	1	0.00
DB00608	Chloroquine	1AGS	1	1	0.00
DB00439	Cerivastatin	1HWL	1	1	0.00
DB01331	Cefoxitin	1I2W	1	1	0.00
DB00535	Cefdinir	1MYP	1	1	0.00
DB00262	Carmustine	1BNA	1	1	0.00
DB00853	Temozolomide	1BNA	1	1	0.00
DB01200	Bromocriptine	1TQN	1	1	0.00
DB00484	Brimonidine	1HOF	1	1	0.00
DB01158	Bretylum	1MO8	1	1	0.00
DB00759	Tetracycline	1QLZ	1	1	0.00
DB00116	Tetrahydrofolic acid	1DIA	1	1	0.00
DB01128	Bicalutamide	1QKM	1	1	0.00
DB00352	Thioguanine	1BNA	1	1	0.00
DB01393	Bezafibrate	1LJ7	1	1	0.00
DB00932	Tipranavir	1ODW	1	1	0.00

DB00217	Bethanidine	1HOF	1	1	0.00
DB00684	Tobramycin	1P87	1	1	0.01
DB00443	Betamethasone	1NHZ	1	1	0.00
DB00562	Benzthiazide	1T9N	1	1	0.00
DB00539	Toremifene	1R5K	1	1	0.00
DB00436	Bendroflumethiazide	1T9N	1	1	0.00
DB00355	Aztreonam	1RGY	1	1	0.00
DB00752	Tranylcypromine	2BK3	1	1	0.00
DB00928	Azacididine	1BNA	1	1	0.00
DB01076	Atorvastatin	1TZI	1	1	0.00
DB01076	Atorvastatin	1K7L	1	1	0.00
DB01021	Trichlormethiazide	1T9N	1	1	0.00
DB01076	Atorvastatin	1I9R	1	1	0.00
DB00637	Astemizole	1BYW	1	1	0.00
DB00278	Argatroban	1HAG	1	1	0.00
DB00276	Amsacrine	1BNA	1	1	0.00
DB00512	Vancomycin	1BNA	1	1	0.00
DB00194	Vidarabine	1BNA	1	1	0.00
DB00594	Amiloride	1Y4E	1	1	0.00
DB00479	Amikacin	1EMI	1	1	0.00
DB01122	Ambenonium	1F8U	1	1	0.00
DB01430	Almitrine	1MO8	1	1	0.00
DB00171	Adenosine triphosphate	1YOV	1	1	0.00
DB00126	Vitamin C	1E71	1	1	0.00
DB00131	Adenosine monophosphate	1XWS	1	1	0.00
DB00131	Adenosine monophosphate	1BNA	1	1	0.00
DB00558	Zanamivir	2BAT	1	1	0.00
DB00131	Adenosine monophosphate	1ORE	1	1	0.00
DB00399	Zoledronate	1YV5	1	1	0.00
DB01213	Fomepizole	1DON	0	0	0.97
DB00173	Adenine	1IRU	0	0	0.97
DB00304	Desogestrel	1IRU	0	0	0.98
DB00858	Dromostanolone	1SG0	0	0	0.98
DB00133	L-Serine	1P87	0	0	0.92
DB00531	Cyclophosphamide	1H2W	0	0	1.00
DB01319	Fosamprenavir	1DON	0	0	0.98
DB00828	Fosfomycin	1P87	0	0	0.99
DB00909	Zonisamide	1IRU	0	0	0.98
DB00151	L-Cysteine	1P87	0	0	0.94
DB00531	Cyclophosphamide	1P87	0	0	0.99
DB00115	Cyanocobalamin	1AUT	0	0	0.81
DB00858	Dromostanolone	1LBD	0	0	0.98
DB00171	Adenosine triphosphate	1IRU	0	0	0.97
DB00492	Fosinopril	1EMI	0	0	0.99

DB00171	Adenosine triphosphate	1DON	0	0	0.96
DB00492	Fosinopril	1OHY	0	0	0.98
DB00492	Fosinopril	1OD4	0	0	0.98
DB00492	Fosinopril	1OKC	0	0	0.98
DB00492	Fosinopril	1HSO	0	0	0.91
DB00858	Dromostanolone	1BYY	0	0	1.00
DB00858	Dromostanolone	1XDK	0	0	0.92
DB00155	L-Citrulline	1H2W	0	0	1.00
DB00492	Fosinopril	1HI	0	0	0.92
DB00492	Fosinopril	1O5W	0	0	1.00
DB00492	Fosinopril	1E3G	0	0	0.98
DB00492	Fosinopril	1JVQ	0	0	0.92
DB00492	Fosinopril	1REW	0	0	0.97
DB00492	Fosinopril	1CZM	0	0	0.98
DB00492	Fosinopril	1S5O	0	0	0.98
DB00492	Fosinopril	1Z6J	0	0	0.88
DB00492	Fosinopril	1CJY	0	0	0.90
DB00492	Fosinopril	8ICK	0	0	0.98
DB00492	Fosinopril	1QKM	0	0	0.98
DB00492	Fosinopril	1SS2	0	0	0.98
DB00492	Fosinopril	1BWC	0	0	0.98
DB00492	Fosinopril	1ODW	0	0	0.98
DB00492	Fosinopril	1ILQ	0	0	0.99
DB00492	Fosinopril	1LSZ	0	0	0.98
DB00492	Fosinopril	1NRL	0	0	0.91
DB00492	Fosinopril	1Y38	0	0	0.99
DB00492	Fosinopril	1SQN	0	0	0.98
DB00492	Fosinopril	1XWS	0	0	0.98
DB00492	Fosinopril	1EXX	0	0	0.98
DB00492	Fosinopril	1C0B	0	0	0.99
DB00492	Fosinopril	1H0C	0	0	0.97
DB00492	Fosinopril	1DON	0	0	0.98
DB00492	Fosinopril	1SLM	0	0	0.98
DB00492	Fosinopril	1KED	0	0	0.98
DB00492	Fosinopril	1VJA	0	0	0.88
DB00115	Cyanocobalamin	1Q11	0	0	0.94
DB00858	Dromostanolone	1I4L	0	0	0.98
DB00518	Albendazole	1DON	0	0	0.98
DB00858	Dromostanolone	1HAG	0	0	0.88
DB00858	Dromostanolone	1BP3	0	0	0.98
DB00744	Zileuton	1DON	0	0	0.97
DB00802	Alfentanil	1P87	0	0	1.00
DB00641	Simvastatin	1OHY	0	0	0.92
DB00744	Zileuton	1IRU	0	0	0.97

DB00802	Alfentanil	1HOF	0	0	0.93
DB00802	Alfentanil	1PQ3	0	0	0.85
DB00641	Simvastatin	1I9B	0	0	0.68
DB00802	Alfentanil	1CZM	0	0	0.83
DB00858	Dromostanolone	1C5G	0	0	0.98
DB00802	Alfentanil	1JBQ	0	0	0.89
DB01045	Rifampin	1YV5	0	0	0.92
DB00641	Simvastatin	1OYE	0	0	0.68
DB00802	Alfentanil	1XKT	0	0	0.78
DB00802	Alfentanil	1D1P	0	0	0.80
DB00802	Alfentanil	1QR6	0	0	0.81
DB00802	Alfentanil	1RV7	0	0	0.88
DB00802	Alfentanil	1F5F	0	0	0.86
DB00858	Dromostanolone	1Y0S	0	0	0.97
DB00858	Dromostanolone	1NRL	0	0	0.92
DB00858	Dromostanolone	1SVC	0	0	0.97
DB00858	Dromostanolone	1S3A	0	0	0.98
DB00858	Dromostanolone	1MYP	0	0	0.94
DB00858	Dromostanolone	1B6A	0	0	0.99
DB00858	Dromostanolone	1MLD	0	0	0.91
DB00115	Cyanocobalamin	1MB2	0	0	0.81
DB00583	L-Carnitine	1P87	0	0	1.00
DB00115	Cyanocobalamin	1MO8	0	0	0.94
DB01089	Deserpidine	1A8M	0	0	0.92
DB00115	Cyanocobalamin	1YVL	0	0	0.89
DB00616	Candoxatril	1R75	0	0	0.84
DB00858	Dromostanolone	1ILQ	0	0	0.99
DB00858	Dromostanolone	1HQC	0	0	0.94
DB00115	Cyanocobalamin	1BJ4	0	0	0.94
DB00495	Zidovudine	1P87	0	0	0.99
DB00802	Alfentanil	1Y0X	0	0	0.86
DB01189	Desflurane	1P87	0	0	1.00
DB00091	Cyclosporine	1OHY	0	0	0.99
DB01258	Aliskiren	1HOF	0	0	0.80
DB00926	Etretinate	1HKO	0	1	0.56
DB00616	Candoxatril	1NHZ	0	0	0.88
DB00858	Dromostanolone	1R74	0	0	0.98
DB00616	Candoxatril	1XKT	0	0	0.83
DB00304	Desogestrel	1RTU	0	0	0.70
DB00115	Cyanocobalamin	1LBD	0	0	0.90
DB00532	Mephenytoin	1P87	0	0	1.00
DB00115	Cyanocobalamin	1I4L	0	0	0.93
DB01089	Deserpidine	1X86	0	0	0.90
DB01258	Aliskiren	1GCN	0	0	0.85

DB01078	Deslanoside	1EMI	0	0	0.99
DB01078	Deslanoside	1F8U	0	0	0.98
DB00926	Etretinate	1LJ7	0	1	0.55
DB04967	Lucanthone	1H2W	0	0	1.00
DB00115	Cyanocobalamin	1TJC	0	0	0.95
DB00616	Candoxatriol	1T9R	0	0	0.86
DB00128	L-Aspartic Acid	1IRU	0	0	0.98
DB00304	Desogestrel	1Y38	0	0	0.79
DB00523	Alitretinoin	1P87	0	0	1.00
DB00858	Dromostanolone	1BWC	0	0	0.98
DB01089	Deserpidine	1P49	0	0	0.89
DB00091	Cyclosporine	1HOF	0	0	0.99
DB01089	Deserpidine	1HA2	0	0	0.86
DB00858	Dromostanolone	1WVJ	0	0	0.98
DB00091	Cyclosporine	2BK3	0	0	0.99
DB00858	Dromostanolone	1NHZ	0	0	0.98
DB00641	Simvastatin	1OKC	0	0	0.93
DB00091	Cyclosporine	1UZF	0	0	0.99
DB00858	Dromostanolone	1VRU	0	0	0.92
DB00858	Dromostanolone	1FE3	0	0	0.99
DB00858	Dromostanolone	1QKM	0	0	0.98
DB00858	Dromostanolone	1MQB	0	0	0.97
DB00858	Dromostanolone	1EI1	0	0	0.92
DB00858	Dromostanolone	1BP3	0	0	0.98
DB00858	Dromostanolone	1CJY	0	0	0.90
DB00858	Dromostanolone	2TRT	0	0	0.98
DB00091	Cyclosporine	1T9R	0	0	0.99
DB00858	Dromostanolone	1JBQ	0	0	0.99
DB01392	Yohimbine	1K2H	0	0	0.97
DB00091	Cyclosporine	1HKO	0	0	0.99
DB00858	Dromostanolone	1XU9	0	0	0.98
DB00858	Dromostanolone	1RFN	0	0	0.88
DB00091	Cyclosporine	1BNA	0	0	0.99
DB00858	Dromostanolone	1D6G	0	0	0.99
DB00858	Dromostanolone	1ZNC	0	0	0.88
DB00091	Cyclosporine	1R5K	0	0	0.99
DB00858	Dromostanolone	1DIA	0	0	0.98
DB00858	Dromostanolone	1E79	0	0	0.98
DB00858	Dromostanolone	1H6I	0	0	0.99
DB00858	Dromostanolone	1E3G	0	0	0.98
DB00614	Furazolidone	1DON	0	0	0.98
DB00858	Dromostanolone	1HOF	0	0	0.99
DB01017	Minocycline	1DON	0	0	0.98
DB00091	Cyclosporine	1FTA	0	0	0.99

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DB00858	Dromostanolone	1T40	0	0	0.88
DB00858	Dromostanolone	1MRQ	0	0	0.99
DB00170	Menadione	1P87	0	0	1.00
DB01045	Rifampin	1PB7	0	0	0.91
DB00858	Dromostanolone	1I9B	0	0	0.93
DB00858	Dromostanolone	1SA1	0	0	0.98
DB00858	Dromostanolone	1P87	0	0	1.00
DB00858	Dromostanolone	1EMI	0	0	0.99
DB01078	Deslanoside	1P1R	0	0	0.97
DB00091	Cyclosporine	1PB7	0	0	0.99
DB00091	Cyclosporine	1AGS	0	0	0.99
DB01392	Yohimbine	1P87	0	0	0.99
DB00858	Dromostanolone	1TEV	0	0	0.99
DB00641	Simvastatin	1L6V	0	0	0.94
DB00674	Galantamine	1P87	0	0	1.00
DB00091	Cyclosporine	2IL6	0	0	0.99
DB00137	Xanthophyll	1VYT	0	0	0.91
DB00137	Xanthophyll	1A5Y	0	0	0.92
DB01123	Proflavine	1P87	0	0	0.96
DB00137	Xanthophyll	1Y0X	0	0	0.94
DB00137	Xanthophyll	1MO8	0	0	0.93
DB00137	Xanthophyll	1S78	0	0	0.86
DB00137	Xanthophyll	1BYW	0	0	0.95
DB00137	Xanthophyll	1CWM	0	0	0.94
DB00137	Xanthophyll	1ODW	0	0	0.95
DB00137	Xanthophyll	1VRU	0	0	0.72
DB00137	Xanthophyll	1UT1	0	0	0.72
DB00137	Xanthophyll	1HKO	0	0	0.94
DB00137	Xanthophyll	1IBC	0	0	0.95
DB00137	Xanthophyll	1UZF	0	0	0.91
DB00137	Xanthophyll	1HOF	0	0	0.96
DB00137	Xanthophyll	1ORE	0	0	0.95
DB00137	Xanthophyll	1HNK	0	0	0.96
DB01078	Deslanoside	1HOF	0	0	0.98
DB00751	Epinastine	1DON	0	0	0.97
DB00682	Warfarin	1BDA	0	0	0.80
DB00926	Etretinate	1T9R	0	1	0.46
DB00696	Ergotamine	1P87	0	0	0.97
DB00616	Candoxatril	1PTW	0	1	0.63
DB00091	Cyclosporine	1QR6	0	0	0.99
DB00091	Cyclosporine	1YXL	0	0	0.99
DB00091	Cyclosporine	1OPL	0	0	0.99
DB01045	Rifampin	1EXB	0	0	0.77
DB00091	Cyclosporine	2AAI	0	0	1.00

DB00091	Cyclosporine	1P49	0	0	0.99
DB01045	Rifampin	1IRU	0	0	0.99
DB00091	Cyclosporine	1A5Y	0	0	0.99
DB00163	Vitamin E	1V97	0	0	0.99
DB00163	Vitamin E	1N2Z	0	0	0.99
DB00163	Vitamin E	1A8M	0	0	0.99
DB00163	Vitamin E	1TRN	0	0	0.96
DB00163	Vitamin E	1SD2	0	0	0.99
DB00163	Vitamin E	1HA2	0	0	0.99
DB00163	Vitamin E	2AAI	0	0	1.00
DB00163	Vitamin E	1UHL	0	0	0.99
DB00163	Vitamin E	1EXX	0	0	0.99
DB00163	Vitamin E	1I4L	0	0	0.99
DB00163	Vitamin E	1G1S	0	0	0.99
DB00163	Vitamin E	1BYW	0	0	0.99
DB00163	Vitamin E	1PBW	0	0	0.99
DB00163	Vitamin E	1K7L	0	0	0.97
DB00163	Vitamin E	1NRL	0	0	0.97
DB00163	Vitamin E	1DMT	0	0	0.97
DB00163	Vitamin E	1PT9	0	0	0.99
DB00163	Vitamin E	9ILB	0	0	0.99
DB00163	Vitamin E	1WVJ	0	0	0.99
DB00163	Vitamin E	1L1F	0	0	0.99
DB00163	Vitamin E	1VRU	0	0	0.97
DB00163	Vitamin E	1XKT	0	0	0.99
DB00163	Vitamin E	1VJ5	0	0	0.96
DB00163	Vitamin E	1HD7	0	0	0.99
DB00163	Vitamin E	2BGR	0	0	0.99
DB00163	Vitamin E	1TQN	0	0	0.99
DB00163	Vitamin E	1LJ7	0	0	0.99
DB00163	Vitamin E	1T9R	0	0	0.99
DB00163	Vitamin E	1T9N	0	0	0.99
DB00163	Vitamin E	1TB5	0	0	0.97
DB00163	Vitamin E	3BLM	0	0	0.99
DB00163	Vitamin E	1JVQ	0	0	0.97
DB00163	Vitamin E	1O5W	0	0	1.00
DB00163	Vitamin E	1HOF	0	0	0.99
DB00163	Vitamin E	1XF0	0	0	0.99
DB00163	Vitamin E	1OKC	0	0	0.99
DB00163	Vitamin E	1OHY	0	0	0.99
DB00163	Vitamin E	1G5X	0	0	0.99
DB00163	Vitamin E	1W0H	0	0	0.99
DB00269	Chlorotrianisene	1IRU	0	0	0.99
DB01045	Rifampin	1G1S	0	0	0.81

DB00616	Candoxatril	1UZF	0	0	0.85
DB01065	Melatonin	1IRU	0	0	0.98
DB00641	Simvastatin	1HT0	0	1	0.66
DB00172	L-Proline	1P87	0	0	0.99
DB01078	Deslanoside	1I5H	0	0	0.98
DB01219	Dantrolene	1IRU	0	0	0.98
DB01045	Rifampin	1LPJ	0	0	0.92
DB00511	Acetyldigitoxin	1HWL	0	0	0.98
DB01045	Rifampin	1F5F	0	0	0.91
DB00511	Acetyldigitoxin	1OKC	0	0	0.99
DB04839	Cyproterone	1P87	0	0	0.99
DB00227	Lovastatin	1VYT	0	0	0.87
DB01065	Melatonin	1P87	0	0	0.99
DB00227	Lovastatin	1NAV	0	0	0.90
DB00351	Megestrol	1WAP	0	0	0.89
DB00126	Vitamin C	1H2W	0	0	1.00
DB00227	Lovastatin	1HA2	0	0	0.83
DB00115	Cyanocobalamin	1Y0S	0	0	0.90
DB00227	Lovastatin	1EXX	0	0	0.91
DB00351	Megestrol	1Y4E	0	0	0.93
DB00227	Lovastatin	1K2H	0	0	1.00
DB00227	Lovastatin	1KI0	0	0	0.86
DB00269	Chlorotrianisene	1DON	0	0	0.99
DB01395	Drospirenone	1EMI	0	0	0.99
DB01395	Drospirenone	1KG3	0	0	0.95
DB00114	Pyridoxal Phosphate	1IRU	0	0	0.97
DB00351	Megestrol	1HA2	0	1	0.59
DB00641	Simvastatin	1P1R	0	0	0.92
DB01395	Drospirenone	1HT0	0	0	0.73
DB00227	Lovastatin	9ILB	0	0	0.92
DB01395	Drospirenone	1HOF	0	0	0.98
DB00351	Megestrol	1C0B	0	0	0.89
DB00227	Lovastatin	3JDW	0	0	0.88
DB01395	Drospirenone	1AJS	0	0	0.75
DB00351	Megestrol	1XWS	0	0	0.69
DB00227	Lovastatin	1VJB	0	0	0.86
DB00351	Megestrol	1BYW	0	0	0.79
DB00641	Simvastatin	1IHI	0	0	0.68
DB01395	Drospirenone	1DIA	0	0	0.95
DB00351	Megestrol	1Y38	0	0	0.91
DB01395	Drospirenone	1JD0	0	1	0.62
DB01045	Rifampin	1I9R	0	0	0.85
DB00540	Nortriptyline	1P87	0	0	1.00
DB00641	Simvastatin	1EW2	0	0	0.93

DB00227	Lovastatin	1FYC	0	0	0.87
DB00115	Cyanocobalamin	1C4C	0	0	0.93
DB00227	Lovastatin	2CBR	0	0	0.91
DB01244	Bepridil	1KGI	0	1	0.62
DB01395	Drospirenone	2CBR	0	0	0.96
DB00227	Lovastatin	1E79	0	0	0.86
DB00227	Lovastatin	1HOF	0	0	0.94
DB00351	Megestrol	1J0X	0	1	0.67
DB01395	Drospirenone	1D6G	0	0	0.97
DB01395	Drospirenone	1I0E	0	0	0.86
DB00641	Simvastatin	1HOF	0	0	0.96
DB00128	L-Aspartic Acid	1P87	0	0	0.99
DB00351	Megestrol	1GCN	0	0	0.91
DB00641	Simvastatin	1I5H	0	0	0.94
DB00641	Simvastatin	1Q7L	0	0	0.93
DB00641	Simvastatin	1UZF	0	0	0.91
DB00162	Vitamin A	1BDA	0	0	0.93
DB00641	Simvastatin	1RL0	0	0	0.92
DB00162	Vitamin A	1BYY	0	0	0.70
DB00641	Simvastatin	1Z6T	0	0	0.92
DB00641	Simvastatin	1W6F	0	1	0.66
DB01244	Bepridil	1WAP	0	0	0.86
DB00641	Simvastatin	1KTO	0	0	0.92
DB00641	Simvastatin	3BLM	0	0	0.93
DB00351	Megestrol	1YV5	0	0	0.77
DB00641	Simvastatin	1P4R	0	0	0.99
DB00511	Acetyldigitoxin	1O5W	0	0	1.00
DB00162	Vitamin A	1WD8	0	1	0.50
DB00641	Simvastatin	1DIA	0	0	0.92
DB00641	Simvastatin	1CZM	0	0	0.93
DB00641	Simvastatin	1T9N	0	0	0.92
DB01045	Rifampin	1CZM	0	0	0.89
DB00641	Simvastatin	1IBC	0	0	0.95
DB01244	Bepridil	1SD2	0	0	0.68
DB01244	Bepridil	1EXX	0	0	0.68
DB00351	Megestrol	8ICK	0	0	0.68
DB00641	Simvastatin	3CBS	0	0	0.94
DB00641	Simvastatin	1PEH	0	0	0.78
DB00873	Loteprednol Etabonate	1A8M	0	1	0.58
DB01236	Sevoflurane	1IRU	0	0	1.00
DB01244	Bepridil	1R6K	0	1	0.54
DB00641	Simvastatin	1XU9	0	0	0.93
DB00616	Candoxatril	1HOF	0	0	0.94
DB00396	Progesterone	1HQC	0	0	0.68

DB00641	Simvastatin	1I0E	0	0	0.78
DB00641	Simvastatin	1KPH	0	1	0.67
DB00616	Candoxatril	1EW2	0	0	0.87
DB01244	Bepridil	1P5J	0	0	0.68
DB00641	Simvastatin	1J3S	0	0	0.89
DB00641	Simvastatin	1TQN	0	0	0.91
DB00641	Simvastatin	1GTE	0	0	0.92
DB00873	Loteprednol Etabonate	1EXX	0	1	0.58
DB01244	Bepridil	1T5P	0	1	0.56
DB01244	Bepridil	1YAE	0	1	0.67
DB00641	Simvastatin	1F0X	0	1	0.66
DB00396	Progesterone	1D1P	0	0	0.90
DB00873	Loteprednol Etabonate	1BYW	0	1	0.65
DB00641	Simvastatin	1X9N	0	1	0.67
DB00641	Simvastatin	1KFD	0	0	0.92
DB01244	Bepridil	1JBQ	0	0	0.73
DB00926	Etretinate	1YAE	0	1	0.47
DB01234	Dexamethasone	1H2W	0	0	1.00
DB01244	Bepridil	1P0Q	0	1	0.52
DB00351	Megestrol	1TQN	0	1	0.64
DB00641	Simvastatin	1DYT	0	0	0.89
DB00351	Megestrol	3CBS	0	0	0.76
DB00641	Simvastatin	1YV5	0	0	0.95
DB00873	Loteprednol Etabonate	1R5S	0	1	0.55
DB01244	Bepridil	1HOF	0	0	0.83
DB00351	Megestrol	1T9N	0	0	0.68
DB00641	Simvastatin	1J4I	0	0	0.95
DB00641	Simvastatin	1XWD	0	0	0.68
DB00162	Vitamin A	1O5W	0	0	0.85
DB00162	Vitamin A	1HOF	0	1	0.37
DB00873	Loteprednol Etabonate	1J4I	0	0	0.69
DB00165	Pyridoxine	1P87	0	0	0.97
DB00641	Simvastatin	1SS2	0	0	0.93
DB00162	Vitamin A	1P87	0	0	1.00
DB01395	Drospirenone	1HKO	0	0	0.97
DB01395	Drospirenone	1BDF	0	0	0.76
DB00641	Simvastatin	1GCN	0	0	0.98
DB00361	Vinorelbine	1YTV	0	0	0.94
DB00361	Vinorelbine	1Y4E	0	0	0.99
DB00361	Vinorelbine	1HA2	0	0	0.97
DB00361	Vinorelbine	1EXX	0	0	0.98
DB00361	Vinorelbine	1IRU	0	0	0.99
DB00361	Vinorelbine	1EXB	0	0	0.97
DB00361	Vinorelbine	1K7L	0	0	0.93

DB00361	Vinorelbine	1NRL	0	0	0.93
DB00361	Vinorelbine	1HIG	0	0	0.98
DB00361	Vinorelbine	1NHZ	0	0	0.98
DB00361	Vinorelbine	1QYE	0	0	0.99
DB00361	Vinorelbine	1J3S	0	0	0.97
DB00361	Vinorelbine	1I9R	0	0	0.98
DB00361	Vinorelbine	1XGJ	0	0	0.94
DB00361	Vinorelbine	1UZF	0	0	0.98
DB00361	Vinorelbine	1HOF	0	0	0.99
DB00361	Vinorelbine	1OD4	0	0	0.98
DB00361	Vinorelbine	1EMI	0	0	0.99
DB00541	Vincristine	1TZI	0	0	0.91
DB00541	Vincristine	1Q11	0	0	0.97
DB00541	Vincristine	1HA2	0	0	0.96
DB00541	Vincristine	1XDK	0	0	0.93
DB00541	Vincristine	1IRU	0	0	0.99
DB00541	Vincristine	1YOV	0	0	0.98
DB00541	Vincristine	1MQ8	0	0	0.93
DB00541	Vincristine	1PB7	0	0	0.98
DB00541	Vincristine	1R5K	0	0	0.93
DB00541	Vincristine	1GTE	0	0	0.97
DB00541	Vincristine	1D6G	0	0	0.98
DB00541	Vincristine	1CZM	0	0	0.98
DB00541	Vincristine	3BLM	0	0	0.98
DB00541	Vincristine	2BK3	0	0	0.93
DB00541	Vincristine	1HOF	0	0	0.98
DB00541	Vincristine	1KG3	0	0	0.97
DB00570	Vinblastine	1SA1	0	0	0.98
DB00570	Vinblastine	1Y4E	0	0	0.99
DB00570	Vinblastine	1Q9S	0	0	0.98
DB00570	Vinblastine	1EXX	0	0	0.98
DB00570	Vinblastine	1G1S	0	0	0.97
DB00570	Vinblastine	1BP3	0	0	0.97
DB00570	Vinblastine	1EXB	0	0	0.97
DB00570	Vinblastine	1SVC	0	0	0.97
DB00570	Vinblastine	1F0Y	0	0	0.95
DB00570	Vinblastine	1BWC	0	0	0.98
DB00570	Vinblastine	1L9X	0	0	0.98
DB00570	Vinblastine	1HE5	0	0	0.98
DB00570	Vinblastine	1IVO	0	0	0.94
DB00570	Vinblastine	1BNA	0	0	0.93
DB00570	Vinblastine	1POS	0	0	0.93
DB00570	Vinblastine	1CP3	0	0	0.98
DB00570	Vinblastine	1CZM	0	0	0.98

DB00570	Vinblastine	1XGJ	0	0	0.95
DB00570	Vinblastine	1Z6T	0	0	0.98
DB00570	Vinblastine	1E3G	0	0	0.98
DB00570	Vinblastine	1O5W	0	0	1.00
DB00570	Vinblastine	1BV8	0	0	0.98
DB00570	Vinblastine	1T40	0	0	0.93
DB00570	Vinblastine	1F8U	0	0	0.98
DB00570	Vinblastine	1EMI	0	0	0.99
DB01395	Drospirenone	1R5K	0	0	0.75
DB00132	Alpha-Linolenic Acid	1P87	0	0	1.00
DB01244	Bepridil	1GXD	0	1	0.65
DB00641	Simvastatin	1Z8L	0	0	0.92
DB00506	Norgestrel	1BYY	0	0	0.88
DB00641	Simvastatin	1WVJ	0	0	0.93
DB00115	Cyanocobalamin	1DMT	0	0	0.87
DB00641	Simvastatin	1XHY	0	0	0.94
DB00641	Simvastatin	1YAE	0	0	0.94
DB00641	Simvastatin	1AGS	0	0	0.92
DB00873	Loteprednol Etabonate	1CZM	0	1	0.52
DB00641	Simvastatin	1R74	0	0	0.91
DB00641	Simvastatin	1UYL	0	0	0.94
DB00641	Simvastatin	1ODW	0	0	0.95
DB00641	Simvastatin	1OJO	0	0	0.71
DB00132	Alpha-Linolenic Acid	1BYY	0	1	0.62
DB00641	Simvastatin	1TYE	0	0	0.98
DB01080	Vigabatrin	1P87	0	0	0.98
DB00641	Simvastatin	1HIG	0	0	0.91
DB00641	Simvastatin	2IL6	0	0	0.94
DB01564	Calusterone	1VYT	0	0	0.75
DB00484	Brimonidine	1P87	0	0	0.97
DB01395	Drospirenone	1FE3	0	0	0.96
DB01564	Calusterone	1SA1	0	0	0.74
DB01564	Calusterone	1P49	0	0	0.76
DB01564	Calusterone	1LBD	0	0	0.76
DB01045	Rifampin	1HOF	0	0	0.93
DB00661	Verapamil	1AUT	0	1	0.63
DB00661	Verapamil	1A5Y	0	0	0.95
DB00661	Verapamil	1JNM	0	0	0.92
DB00661	Verapamil	1P49	0	0	0.95
DB00661	Verapamil	1G91	0	0	0.95
DB00661	Verapamil	1HA2	0	0	0.94
DB00661	Verapamil	1SG0	0	0	0.95
DB00661	Verapamil	1LBD	0	0	0.95
DB00661	Verapamil	1XDK	0	0	0.74

DB00661	Verapamil	1BBS	0	1	0.63
DB00661	Verapamil	1WD8	0	0	0.99
DB00661	Verapamil	1SQN	0	0	0.95
DB00661	Verapamil	1YXL	0	0	0.97
DB00661	Verapamil	1N8S	0	1	0.63
DB00661	Verapamil	1DMT	0	0	0.76
DB00661	Verapamil	9ILB	0	0	0.97
DB00661	Verapamil	1T3E	0	0	0.75
DB00661	Verapamil	1WVJ	0	0	0.96
DB00661	Verapamil	1L1F	0	0	0.94
DB00661	Verapamil	1SS2	0	0	0.96
DB00661	Verapamil	1HE5	0	0	0.96
DB00661	Verapamil	1QKM	0	0	0.95
DB00661	Verapamil	1QYE	0	0	0.97
DB00661	Verapamil	1KFD	0	0	0.95
DB00661	Verapamil	2BGR	0	0	0.94
DB00661	Verapamil	1P0Q	0	0	0.94
DB00661	Verapamil	1ZNC	0	1	0.63
DB00661	Verapamil	1PTW	0	0	0.81
DB00661	Verapamil	1RGY	0	0	0.95
DB00661	Verapamil	1PQ3	0	0	0.96
DB00661	Verapamil	1UZF	0	0	0.94
DB00661	Verapamil	1O5W	0	0	0.99
DB00661	Verapamil	1HOF	0	0	0.98
DB00661	Verapamil	1MRQ	0	0	0.97
DB00661	Verapamil	1OKC	0	0	0.96
DB00661	Verapamil	1OHY	0	0	0.95
DB00661	Verapamil	1EMI	0	0	0.99
DB00873	Loteprednol Etabonate	1HOF	0	0	0.76
DB00351	Megestrol	1OKC	0	0	0.72
DB01395	Drospirenone	1Q6U	0	0	0.93
DB00641	Simvastatin	1I10	0	0	0.92
DB01395	Drospirenone	1NHZ	0	0	0.95
DB01395	Drospirenone	1YAE	0	0	0.96
DB00648	Mitotane	1P87	0	0	1.00
DB01055	Mimosine	1DON	0	0	0.96
DB01395	Drospirenone	1TYE	0	0	0.99
DB00926	Etretinate	1K6R	0	1	0.61
DB00869	Dorzolamide	1P87	0	0	0.99
DB00154	gamma-Homolinolenic acid	1EMI	0	0	0.84
DB00926	Etretinate	1UYL	0	1	0.47
DB00503	Ritonavir	1HOF	0	0	0.69
DB00843	Donepezil	1MO8	0	1	0.57
DB00873	Loteprednol Etabonate	1XF0	0	1	0.64

ACCEPTED MANUSCRIPT

DB00616	Candoxatril	2BIU	0	0	0.91
DB00641	Simvastatin	1N7D	0	0	0.69
DB00351	Megestrol	1F8U	0	1	0.63
DB00862	Vardenafil	1F5F	0	0	0.68
DB00584	Enalapril	1K2H	0	0	0.98
DB00862	Vardenafil	1EXX	0	1	0.67
DB00873	Loteprednol Etabonate	1OD4	0	1	0.62
DB00862	Vardenafil	1BYW	0	0	0.73
DB00367	Levonorgestrel	1Y38	0	0	0.80
DB01006	Letrozole	1BDA	0	0	0.91
DB00477	Chlorpromazine	1P87	0	0	1.00
DB00364	Sucralfate	1EMI	0	1	0.59
DB00351	Megestrol	1P87	0	0	1.00
DB00862	Vardenafil	1TQN	0	1	0.55
DB00862	Vardenafil	1LJ7	0	0	0.72
DB00862	Vardenafil	1T9N	0	1	0.59
DB00862	Vardenafil	1E79	0	1	0.55
DB00862	Vardenafil	1HOF	0	0	0.81
DB00169	Cholecalciferol	1EMI	0	0	0.99
DB00862	Vardenafil	1F8U	0	1	0.54
DB00862	Vardenafil	1P87	0	0	1.00
DB00641	Simvastatin	1QLZ	0	0	0.93
DB00169	Cholecalciferol	1P87	0	0	1.00
DB00396	Progesterone	1L6J	0	0	0.87
DB00594	Amiloride	1IRU	0	0	0.98
DB00513	Aminocaproic Acid	1P87	0	0	1.00
DB01166	Cilostazol	1UMK	0	0	0.85
DB00843	Donepezil	1JYD	0	1	0.63
DB00154	gamma-Homolinolenic acid	1EH6	0	1	0.48
DB00616	Candoxatril	1EXX	0	0	0.90
DB01406	Danazol	1BYY	0	0	0.82
DB00616	Candoxatril	1RTU	0	0	0.95
DB00154	gamma-Homolinolenic acid	1QD2	0	1	0.48
DB00616	Candoxatril	1F5F	0	0	0.90
DB01044	Gatifloxacin	1P87	0	0	0.96
DB00843	Donepezil	1ILQ	0	0	0.82
DB00169	Cholecalciferol	1F8U	0	0	0.94
DB00115	Cyanocobalamin	1MLD	0	0	0.84
DB01078	Deslanoside	1UZF	0	0	0.98
DB00780	Phenelzine	1P87	0	0	0.98
DB00169	Cholecalciferol	1HOF	0	0	0.98
DB00253	Medrysone	1A8M	0	0	0.86
DB00396	Progesterone	4Q21	0	0	0.94
DB00843	Donepezil	1BWC	0	1	0.50

DB00253	Medrysone	1MO8	0	0	0.85
DB00843	Donepezil	1SS2	0	1	0.57
DB00903	Ethacrynic acid	1P87	0	0	1.00
DB00903	Ethacrynic acid	1DON	0	0	0.99
DB00130	L-Glutamine	1IRU	0	0	0.97
DB00926	Etretinate	9ILB	0	1	0.53
DB01031	Ethinamate	1P87	0	0	0.99
DB01078	Deslanoside	1AJS	0	0	0.96
DB00253	Medrysone	1H0C	0	0	0.81
DB01254	Dasatinib	1P87	0	0	0.90
DB00641	Simvastatin	1L6J	0	0	0.89
DB00843	Donepezil	1S5O	0	1	0.55
DB00313	Valproic Acid	1P87	0	0	1.00
DB00396	Progesterone	1MYP	0	1	0.64
DB01078	Deslanoside	1T9N	0	0	0.98
DB01586	Ursodeoxycholic acid	1SD2	0	0	0.87
DB01586	Ursodeoxycholic acid	1C0B	0	0	0.95
DB00169	Cholecalciferol	1E3G	0	0	0.96
DB01586	Ursodeoxycholic acid	1SQN	0	0	0.87
DB01586	Ursodeoxycholic acid	1Y0S	0	0	0.74
DB00977	Ethinyl Estradiol	1P87	0	0	1.00
DB01078	Deslanoside	1TQN	0	0	0.97
DB01586	Ursodeoxycholic acid	1XMI	0	1	0.65
DB01586	Ursodeoxycholic acid	1P0Q	0	0	0.82
DB00115	Cyanocobalamin	1I10	0	0	0.94
DB01586	Ursodeoxycholic acid	1T9N	0	0	0.86
DB01586	Ursodeoxycholic acid	1E3G	0	0	0.88
DB00253	Medrysone	1G1S	0	0	0.74
DB01586	Ursodeoxycholic acid	1OKC	0	0	0.88
DB01586	Ursodeoxycholic acid	1OHY	0	0	0.85
DB01586	Ursodeoxycholic acid	1P87	0	0	0.99
DB00641	Simvastatin	1B6A	0	0	0.96
DB00169	Cholecalciferol	1H6I	0	0	0.96
DB01078	Deslanoside	1BNA	0	0	0.96
DB01078	Deslanoside	1YV5	0	0	0.98
DB00253	Medrysone	1I7I	0	0	0.76
DB00165	Pyridoxine	1IRU	0	0	0.97
DB00511	Acetyldigitoxin	1JVQ	0	0	0.98
DB01078	Deslanoside	1R5S	0	0	0.98
DB00843	Donepezil	1Q7L	0	1	0.60
DB00364	Sucralfate	1DON	0	0	0.98
DB01045	Rifampin	1KG3	0	0	0.88
DB01348	Spirapril	1Y4E	0	1	0.58
DB00115	Cyanocobalamin	9ILB	0	0	0.96

DB00169	Cholecalciferol	1T9N	0	0	0.95
DB01236	Sevoflurane	1P87	0	0	1.00
DB00253	Medrysone	1ILQ	0	0	0.94
DB00843	Donepezil	1HOF	0	0	0.78
DB00641	Simvastatin	1MYP	0	0	0.72
DB00253	Medrysone	1ODW	0	0	0.88
DB00843	Donepezil	1OHY	0	1	0.51
DB00456	Cefalotin	1DON	0	0	0.98
DB01395	Drospirenone	1QLZ	0	0	0.95
DB01395	Drospirenone	1UMK	0	0	0.99
DB01395	Drospirenone	1ZBQ	0	0	0.95
DB01395	Drospirenone	1I7I	0	0	0.93
DB00253	Medrysone	1BWC	0	0	0.81
DB01055	Mimosine	1IRU	0	0	0.97
DB01395	Drospirenone	1TJC	0	0	0.96
DB01395	Drospirenone	1RFV	0	0	0.96
DB00616	Candoxatril	1MO8	0	0	0.89
DB00511	Acetyldigoxin	1SPJ	0	0	0.97
DB01406	Danazol	1WD8	0	0	0.71
DB01395	Drospirenone	1XDK	0	0	0.73
DB00641	Simvastatin	1KBQ	0	1	0.64
DB01395	Drospirenone	1QD2	0	0	0.96
DB00791	Uracil mustard	1P87	0	0	1.00
DB00253	Medrysone	1H6I	0	0	0.87
DB06267	Udenafil	1UAE	0	0	0.70
DB06267	Udenafil	1X86	0	0	0.70
DB06267	Udenafil	1BJ4	0	0	0.68
DB06267	Udenafil	1EXX	0	0	0.76
DB06267	Udenafil	1SQN	0	0	0.69
DB06267	Udenafil	1ZBQ	0	0	0.70
DB00119	Pyruvic acid	1P87	0	0	1.00
DB00926	Etretinate	1QYX	0	1	0.45
DB06267	Udenafil	1HUL	0	0	0.85
DB06267	Udenafil	1WVJ	0	0	0.72
DB06267	Udenafil	1Q6U	0	1	0.57
DB00253	Medrysone	1O5W	0	0	0.98
DB06267	Udenafil	1J3S	0	1	0.57
DB01078	Deslanoside	1SVC	0	0	0.97
DB06267	Udenafil	1P0Q	0	1	0.61
DB00169	Cholecalciferol	1P0S	0	0	0.71
DB06267	Udenafil	1UZF	0	1	0.64
DB06267	Udenafil	1Q7L	0	0	0.72
DB06267	Udenafil	1F8U	0	1	0.64
DB06267	Udenafil	1EMI	0	0	0.93

DB01259	Lapatinib	1P87	0	0	0.99
DB00641	Simvastatin	1UMK	0	0	0.99
DB01199	Tubocurarine	1BYY	0	0	0.80
DB00692	Phentolamine	1IRU	0	0	0.98
DB00511	Acetyldigitoxin	1NHZ	0	0	0.99
DB00253	Medrysone	1HOF	0	0	0.92
DB01078	Deslanoside	1BYW	0	0	0.98
DB00641	Simvastatin	1DMT	0	0	0.69
DB00621	Oxandrolone	1MO8	0	0	0.81
DB00989	Rivastigmine	1EMI	0	1	0.44
DB01395	Drospirenone	1DON	0	0	0.98
DB01123	Proflavine	1IRU	0	0	0.97
DB00641	Simvastatin	1SVC	0	0	0.88
DB00926	Etretinate	1HOF	0	0	0.69
DB00641	Simvastatin	1NRL	0	1	0.66
DB01199	Tubocurarine	1P87	0	0	0.98
DB01395	Drospirenone	1X86	0	0	0.95
DB01395	Drospirenone	1A8M	0	0	0.96
DB01395	Drospirenone	1TZI	0	1	0.62
DB06262	Droxidopa	1DON	0	0	0.92
DB00989	Rivastigmine	1P87	0	0	1.00
DB00253	Medrysone	1OHY	0	0	0.81
DB00378	Dydrogesterone	1MRQ	0	0	0.84
DB00204	Dofetilide	1P87	0	0	0.99
DB00641	Simvastatin	1CWM	0	0	0.94
DB00510	Divalproex sodium	1P87	0	0	0.98
DB00615	Rifabutin	1VYT	0	0	0.96
DB00253	Medrysone	1P87	0	0	1.00
DB00641	Simvastatin	1C4C	0	0	0.91
DB00641	Simvastatin	1YXM	0	0	0.70
DB00615	Rifabutin	1VJA	0	0	0.91
DB00641	Simvastatin	1I7I	0	0	0.89
DB01601	Lopinavir	1HOF	0	0	0.68
DB00603	Medroxyprogesterone	1A8M	0	0	0.86
DB00641	Simvastatin	1JYD	0	0	0.94
DB00378	Dydrogesterone	1UZF	0	0	0.72
DB00621	Oxandrolone	1HA2	0	0	0.72
DB00691	Moexipril	1P87	0	0	0.99
DB00304	Desogestrel	1GCN	0	0	0.78
DB00616	Candoxatril	1OKC	0	0	0.89
DB01083	Orlistat	1HOF	0	0	0.99
DB00603	Medroxyprogesterone	1SA1	0	0	0.80
DB01601	Lopinavir	1EMI	0	0	0.86
DB00641	Simvastatin	1EXB	0	0	0.88

DB00115	Cyanocobalamin	1PB7	0	0	0.95
DB00511	Acetyldigitoxin	1T9N	0	0	0.99
DB01206	Lomustine	1DON	0	0	0.99
DB00621	Oxandrolone	1KI0	0	0	0.74
DB00621	Oxandrolone	1ILQ	0	0	0.92
DB00615	Rifabutin	1A8M	0	0	0.98
DB00621	Oxandrolone	1R75	0	0	0.75
DB00603	Medroxyprogesterone	1Y0X	0	0	0.86
DB00397	Phenylpropanolamine	1P87	0	0	0.98
DB00641	Simvastatin	1BP3	0	0	0.90
DB00621	Oxandrolone	1R5S	0	0	0.81
DB00621	Oxandrolone	1HD7	0	0	0.83
DB00115	Cyanocobalamin	1VRU	0	0	0.86
DB00621	Oxandrolone	1TQN	0	0	0.75
DB00621	Oxandrolone	1P0Q	0	0	0.73
DB00367	Levonorgestrel	1BYY	0	0	0.88
DB00603	Medroxyprogesterone	1BYY	0	0	0.97
DB00621	Oxandrolone	1YMX	0	1	0.66
DB00621	Oxandrolone	1HOF	0	0	0.90
DB00115	Cyanocobalamin	1R5K	0	0	0.86
DB00621	Oxandrolone	1ORE	0	0	0.86
DB00511	Acetyldigitoxin	1IBC	0	0	0.99
DB00115	Cyanocobalamin	2BGR	0	0	0.94
DB01096	Oxamniquine	1DON	0	0	0.98
DB00641	Simvastatin	1RV7	0	0	0.95
DB01225	Enoxaparin	1IRU	0	0	0.98
DB00115	Cyanocobalamin	1JBQ	0	0	0.96
DB00691	Moexipril	1Y38	0	1	0.59
DB00615	Rifabutin	1JNM	0	0	0.96
DB01120	Gliclazide	1P87	0	0	0.99
DB01021	Trichlormethiazide	1DON	0	0	0.98
DB00115	Cyanocobalamin	1T9R	0	0	0.92
DB00691	Moexipril	1IRU	0	0	0.98
DB04948	Lofexidine	1H2W	0	0	1.00
DB00169	Cholecalciferol	1J3S	0	0	0.93
DB01021	Trichlormethiazide	1IRU	0	0	0.99
DB00691	Moexipril	1BYY	0	0	0.72
DB00396	Progesterone	1TLL	0	0	0.89
DB00641	Simvastatin	1IRU	0	0	0.99
DB00115	Cyanocobalamin	1CZM	0	0	0.94
DB00823	Ethinodiol Diacetate	1EMI	0	0	0.86
DB00169	Cholecalciferol	1BNA	0	0	0.71
DB00233	Aminosalicylic Acid	1P87	0	0	0.99
DB00641	Simvastatin	1XWS	0	0	0.93

DB01118	Amiodarone	1P87	0	0	1.00
DB00115	Cyanocobalamin	1DIA	0	0	0.93
DB00641	Simvastatin	1RFV	0	0	0.92
DB00641	Simvastatin	1YB5	0	1	0.66
DB00823	Ethynodiol Diacetate	1OF7	0	1	0.56
DB00115	Cyanocobalamin	1AJS	0	0	0.84
DB00641	Simvastatin	1R6K	0	0	0.91
DB00615	Rifabutin	1MO8	0	0	0.97
DB00641	Simvastatin	1BI9	0	0	0.89
DB04967	Lucanthone	1P87	0	0	1.00
DB00641	Simvastatin	1EXX	0	0	0.94
DB00321	Amitriptyline	1UMK	0	1	0.32
DB00115	Cyanocobalamin	1E3G	0	0	0.95
DB00615	Rifabutin	1HA2	0	0	0.95
DB00641	Simvastatin	1LPJ	0	0	0.94
DB00641	Simvastatin	1GGL	0	0	0.91
DB00989	Rivastigmine	1BYY	0	1	0.55
DB00182	Amphetamine	1P87	0	0	0.99
DB00641	Simvastatin	1RTU	0	0	0.97
DB00115	Cyanocobalamin	1HOF	0	0	0.96
DB00641	Simvastatin	1SG0	0	0	0.92
DB00115	Cyanocobalamin	1T40	0	0	0.81
DB00615	Rifabutin	1EXX	0	0	0.98
DB00641	Simvastatin	1BJ4	0	0	0.92
DB00115	Cyanocobalamin	1OKC	0	0	0.94
DB01048	Abacavir	1DON	0	0	0.98
DB00822	Disulfiram	1EMI	0	1	0.38
DB00182	Amphetamine	1DON	0	0	0.97
DB00954	Dirithromycin	1TZI	0	0	0.98
DB00115	Cyanocobalamin	1HWL	0	0	0.86
DB00823	Ethynodiol Diacetate	1XF0	0	1	0.58
DB00954	Dirithromycin	1A8M	0	0	0.99
DB00954	Dirithromycin	1NAV	0	0	0.99
DB00226	Guanadrel Sulfate	1P87	0	0	0.96
DB00226	Guanadrel Sulfate	1IRU	0	0	0.99
DB00148	Creatine	1P87	0	0	0.94
DB00160	L-Alanine	1P87	0	0	0.98
DB00954	Dirithromycin	1F5F	0	0	0.99
DB00954	Dirithromycin	1C0B	0	0	0.99
DB00410	Mupirocin	1EMI	0	0	0.95
DB00603	Medroxyprogesterone	1HA2	0	0	0.76
DB00823	Ethynodiol Diacetate	1HOF	0	0	0.72
DB00410	Mupirocin	1F8U	0	0	0.74
DB00252	Phenytoin	1P87	0	0	0.99

DB00823	Ethinodiol Diacetate	1E3G	0	1	0.46
DB00926	Etretinate	1OD4	0	1	0.52
DB00511	Acetyldigitoxin	1A5Y	0	0	0.99
DB00603	Medroxyprogesterone	1UHL	0	0	0.77
DB00957	Norgestimate	1EMI	0	0	0.94
DB00615	Rifabutin	1BI9	0	0	0.96
DB00641	Simvastatin	1F5F	0	0	0.94
DB00823	Ethinodiol Diacetate	1PQ3	0	1	0.49
DB00603	Medroxyprogesterone	1BI9	0	0	0.75
DB00410	Mupirocin	1HOF	0	0	0.87
DB00755	Tretinoin	1IRU	0	0	0.98
DB01103	Quinacrine	1DON	0	0	0.99
DB00865	Benzphetamine	1P87	0	0	1.00
DB00410	Mupirocin	1P4R	0	0	0.97
DB00616	Candoxatril	1KED	0	0	0.88
DB00506	Norgestrel	1BYW	0	1	0.57
DB00641	Simvastatin	1BYY	0	0	0.98
DB00603	Medroxyprogesterone	1BYW	0	0	0.89
DB00436	Bendroflumethiazide	1IRU	0	0	0.99
DB00970	Dactinomycin	1F8U	0	0	0.99
DB00641	Simvastatin	1P49	0	0	0.92
DB00603	Medroxyprogesterone	1YXL	0	0	0.88
DB00506	Norgestrel	1ODW	0	1	0.55
DB00511	Acetyldigitoxin	1FIE	0	0	0.98
DB00410	Mupirocin	1FE3	0	0	0.85
DB00410	Mupirocin	1WVJ	0	0	0.80
DB00705	Delavirdine	1P87	0	0	0.98
DB00926	Etretinate	1CYN	0	1	0.49
DB00603	Medroxyprogesterone	2IL6	0	0	0.87
DB01078	Deslanoside	1NI4	0	0	0.96
DB00410	Mupirocin	1PT9	0	0	0.71
DB00641	Simvastatin	2TRT	0	0	0.92
DB01119	Diazoxide	1P87	0	0	0.99
DB00252	Phenytoin	1H2W	0	0	1.00
DB01078	Deslanoside	1UHL	0	0	0.98
DB00603	Medroxyprogesterone	1AGS	0	0	0.82
DB00823	Ethinodiol Diacetate	1HD7	0	1	0.51
DB00410	Mupirocin	1BP3	0	1	0.66
DB00755	Tretinoin	1O5W	0	1	0.55
DB00641	Simvastatin	1Y0X	0	0	0.94
DB00641	Simvastatin	1WAP	0	0	0.97
DB01078	Deslanoside	1F5F	0	0	0.98
DB00603	Medroxyprogesterone	1L1F	0	0	0.78
DB00665	Nilutamide	1DON	0	0	0.99

DB00755	Tretinoin	1P87	0	0	1.00
DB00641	Simvastatin	1IIH	0	0	0.92
DB00410	Mupirocin	1I4L	0	0	0.74
DB00659	Acamprosate	1P87	0	0	1.00
DB00641	Simvastatin	1SA1	0	0	0.91
DB00410	Mupirocin	1UHL	0	0	0.70
DB00410	Mupirocin	1BJ4	0	0	0.78
DB00410	Mupirocin	1BYY	0	0	0.95
DB00926	Etretinate	2BIU	0	1	0.54
DB00954	Dirithromycin	1BXS	0	0	0.98
DB00954	Dirithromycin	1TJC	0	0	0.99
DB00378	Dydrogesterone	1IBC	0	0	0.84
DB00970	Dactinomycin	1HOF	0	0	0.99
DB00926	Etretinate	1GXD	0	1	0.45
DB00378	Dydrogesterone	1JBQ	0	0	0.84
DB00378	Dydrogesterone	1QKM	0	0	0.76
DB00954	Dirithromycin	1N8S	0	0	0.98
DB00378	Dydrogesterone	1PB7	0	0	0.80
DB00641	Simvastatin	1A5Y	0	0	0.93
DB01159	Halothane	1P87	0	0	1.00
DB00954	Dirithromycin	1ODW	0	0	0.99
DB01159	Halothane	1IRU	0	0	1.00
DB00954	Dirithromycin	1NHZ	0	0	0.99
DB00954	Dirithromycin	1J4I	0	0	0.99
DB00926	Etretinate	1JYD	0	1	0.51
DB00954	Dirithromycin	1IVO	0	0	0.98
DB00954	Dirithromycin	1BNA	0	0	0.98
DB00954	Dirithromycin	1ZNC	0	0	0.98
DB00970	Dactinomycin	1E3G	0	0	0.99
DB00374	Treprostinil	1P87	0	0	0.96
DB00954	Dirithromycin	1P4R	0	0	1.00
DB01078	Deslanoside	1YTV	0	0	0.96
DB00134	L-Methionine	1DON	0	0	0.97
DB00584	Enalapril	1P87	0	0	0.99
DB01427	Amrinone	1P87	0	0	0.98
DB00954	Dirithromycin	1JVQ	0	0	0.98
DB00970	Dactinomycin	1KTO	0	0	0.99
DB00954	Dirithromycin	1O5W	0	0	1.00
DB00276	Amsacrine	1P87	0	0	0.99
DB00954	Dirithromycin	1OF7	0	0	0.99
DB01089	Deserpidine	1UZF	0	0	0.87
DB00169	Cholecalciferol	1R5K	0	0	0.81
DB00641	Simvastatin	1TEV	0	0	0.94
DB00957	Norgestimate	1P87	0	0	1.00

DB00954	Dirithromycin	1HWL	0	0	0.98
DB00881	Quinapril	1DON	0	0	0.98
DB00926	Etretinate	1HNK	0	1	0.61
DB00169	Cholecalciferol	1L1F	0	0	0.94
DB00926	Etretinate	1TJC	0	1	0.44
DB00134	L-Methionine	1IRU	0	0	0.98
DB04575	Quinestrol	1P87	0	0	1.00
DB00378	Dydrogesterone	1SVC	0	1	0.66
DB04575	Quinestrol	1OF7	0	0	0.73
DB00615	Rifabutin	1G1S	0	0	0.95
DB04575	Quinestrol	1UZF	0	1	0.57
DB01083	Orlistat	1L6V	0	0	0.99
DB04575	Quinestrol	1F4J	0	1	0.63
DB04575	Quinestrol	1D6G	0	0	0.78
DB04575	Quinestrol	1JBQ	0	0	0.75
DB04575	Quinestrol	1YV5	0	0	0.73
DB00970	Dactinomycin	1ZNC	0	0	0.98
DB01064	Isoproterenol	1DON	0	0	0.97
DB04575	Quinestrol	1WVJ	0	1	0.67
DB00834	Mifepristone	1A8M	0	0	0.83
DB00834	Mifepristone	1JNM	0	1	0.67
DB04575	Quinestrol	1BYW	0	0	0.75
DB00926	Etretinate	1EXX	0	1	0.48
DB04575	Quinestrol	1H2W	0	0	1.00
DB00834	Mifepristone	1MO8	0	0	0.81
DB00970	Dactinomycin	1TQN	0	0	0.99
DB00957	Norgestimate	1OHY	0	0	0.70
DB00169	Cholecalciferol	1ODW	0	0	0.97
DB00926	Etretinate	1P87	0	0	1.00
DB04575	Quinestrol	1GGL	0	1	0.58
DB00970	Dactinomycin	1X9N	0	0	0.99
DB00752	Tranlycypromine	1P87	0	0	0.99
DB00926	Etretinate	2AAI	0	0	0.70
DB04575	Quinestrol	1BYY	0	0	0.93
DB00970	Dactinomycin	1U4E	0	0	0.99
DB00199	Erythromycin	1A8M	0	0	0.99
DB00834	Mifepristone	1BJ4	0	0	0.77
DB00641	Simvastatin	1MNZ	0	0	0.70
DB00449	Dipivefrin	1P87	0	0	0.99
DB00817	Rosoxacin	1DON	0	0	0.98
DB00511	Acetyldigitoxin	1CWM	0	0	0.99
DB01093	Dimethyl sulfoxide	1DON	0	0	0.98
DB01093	Dimethyl sulfoxide	1IRU	0	0	0.99
DB01093	Dimethyl sulfoxide	1P87	0	0	0.99

DB00970	Dactinomycin	1R5S	0	0	0.99
DB00603	Medroxyprogesterone	1NHZ	0	0	0.84
DB00390	Digoxin	1KXP	0	0	0.95
DB00199	Erythromycin	1BYY	0	0	0.99
DB00390	Digoxin	1JNM	0	0	0.97
DB00390	Digoxin	1HA2	0	0	0.97
DB01564	Calusterone	1BYW	0	0	0.85
DB00390	Digoxin	1XDK	0	0	0.95
DB00603	Medroxyprogesterone	1QKM	0	0	0.82
DB00615	Rifabutin	1IRU	0	0	0.99
DB00390	Digoxin	1RFV	0	0	0.97
DB00337	Pimecrolimus	1DON	0	0	0.99
DB00390	Digoxin	1IRU	0	0	0.99
DB00834	Mifepristone	1EXX	0	0	0.83
DB01564	Calusterone	1CWM	0	0	0.83
DB00456	Cefalotin	1P87	0	0	0.99
DB00390	Digoxin	1JYD	0	0	0.98
DB01173	Orphenadrine	1BDA	0	0	0.93
DB00302	Tranexamic Acid	1P87	0	0	1.00
DB00390	Digoxin	1N7D	0	0	0.95
DB00877	Sirolimus	1ORE	0	0	0.99
DB00390	Digoxin	1T5P	0	0	0.98
DB00877	Sirolimus	1HOF	0	0	0.99
DB00199	Erythromycin	1F5F	0	0	0.99
DB00877	Sirolimus	1E3G	0	0	0.99
DB00877	Sirolimus	1TB5	0	0	0.98
DB00823	Ethynodiol Diacetate	1H2W	0	0	1.00
DB00459	Acitretin	1P87	0	0	1.00
DB00615	Rifabutin	1EXB	0	0	0.95
DB00199	Erythromycin	1SG0	0	0	0.98
DB00390	Digoxin	1XHY	0	0	0.98
DB00173	Adenine	1P87	0	0	0.98
DB00823	Ethynodiol Diacetate	1BYY	0	0	0.90
DB00390	Digoxin	1SS2	0	0	0.98
DB00877	Sirolimus	1D6G	0	0	0.99
DB00519	Trandolapril	1HUL	0	1	0.62
DB00390	Digoxin	1R5K	0	0	0.96
DB00001	Lepirudin	2KAU	0	0	0.97
DB00615	Rifabutin	1Y38	0	0	0.99
DB00957	Norgestimate	1OKC	0	0	0.75
DB00877	Sirolimus	1HKO	0	0	0.99
DB00390	Digoxin	1CJY	0	0	0.95
DB01564	Calusterone	1KFD	0	0	0.76
DB00390	Digoxin	1POS	0	0	0.95

DB00199	Erythromycin	1XDK	0	0	0.96
DB01564	Calusterone	1TQN	0	0	0.74
DB00390	Digoxin	1PTW	0	0	0.96
DB01136	Carvedilol	1H2W	0	0	1.00
DB00519	Trandolapril	1HOF	0	1	0.62
DB00390	Digoxin	1LT8	0	0	0.96
DB00001	Lepirudin	1X86	0	0	0.97
DB01564	Calusterone	1LJ7	0	0	0.85
DB00519	Trandolapril	1HNK	0	1	0.57
DB00519	Trandolapril	1EMI	0	0	0.81
DB00703	Methazolamide	1P87	0	0	1.00
DB00390	Digoxin	1E3G	0	0	0.98
DB00603	Medroxyprogesterone	1TQN	0	0	0.80
DB01564	Calusterone	1P0Q	0	0	0.71
DB00603	Medroxyprogesterone	1T9R	0	0	0.83
DB00390	Digoxin	1HOF	0	0	0.98
DB06692	Aprotinin	1W0H	0	0	0.97
DB00539	Toremifene	1H2W	0	0	1.00
DB06692	Aprotinin	1G5X	0	0	0.97
DB06692	Aprotinin	1GXD	0	0	0.97
DB06692	Aprotinin	1OKC	0	0	0.97
DB06692	Aprotinin	1HOF	0	0	0.97
DB06692	Aprotinin	1O5W	0	0	0.97
DB06692	Aprotinin	1UZF	0	0	0.97
DB06692	Aprotinin	1E79	0	0	0.97
DB06692	Aprotinin	1KTA	0	0	0.96
DB06692	Aprotinin	1PTW	0	0	0.97
DB06692	Aprotinin	1ZNC	0	0	0.96
DB06692	Aprotinin	1P0Q	0	0	0.97
DB06692	Aprotinin	1LJ7	0	0	0.97
DB06692	Aprotinin	1HKO	0	0	0.97
DB00390	Digoxin	1OD4	0	0	0.98
DB00603	Medroxyprogesterone	1CZM	0	0	0.83
DB01564	Calusterone	1DIA	0	0	0.75
DB01396	Digitoxin	1VYT	0	0	0.98
DB01396	Digitoxin	1A8M	0	0	0.98
DB01396	Digitoxin	1MO8	0	0	0.98
DB00749	Etodolac	1P87	0	0	0.99
DB01396	Digitoxin	1DON	0	0	0.98
DB00756	Hexachlorophene	1P87	0	0	1.00
DB01396	Digitoxin	1H0C	0	0	0.98
DB00951	Isoniazid	1P87	0	0	0.98
DB00756	Hexachlorophene	1DON	0	0	0.98
DB01396	Digitoxin	1UHL	0	0	0.98

DB00603	Medroxyprogesterone	1E79	0	0	0.80
DB01396	Digitoxin	1OPL	0	0	0.96
DB01564	Calusterone	1UZF	0	0	0.73
DB01396	Digitoxin	1IRU	0	0	1.00
DB01275	Hydralazine	1P87	0	0	0.98
DB01396	Digitoxin	1EXB	0	0	0.97
DB01396	Digitoxin	1YOV	0	0	0.98
DB00157	NADH	1H2W	0	0	1.00
DB00999	Hydrochlorothiazide	1DON	0	0	0.98
DB00603	Medroxyprogesterone	1UZF	0	0	0.79
DB00615	Rifabutin	2RMC	0	0	0.93
DB00134	L-Methionine	1P87	0	0	0.98
DB01564	Calusterone	1OKC	0	0	0.80
DB00511	Acetyldigitoxin	1GTE	0	0	0.99
DB00273	Topiramate	1DON	0	0	0.98
DB00149	L-Leucine	1IRU	0	0	0.98
DB00133	L-Serine	1IRU	0	0	0.97
DB01396	Digitoxin	1P5J	0	0	0.98
DB01396	Digitoxin	1HIG	0	0	0.98
DB01564	Calusterone	1P87	0	0	1.00
DB01245	Decamethonium	1YTV	0	0	0.73
DB01396	Digitoxin	1TYE	0	0	0.99
DB00201	Caffeine	1BDA	0	0	0.92
DB00511	Acetyldigitoxin	1A36	0	0	0.98
DB01396	Digitoxin	1J0X	0	0	0.97
DB00150	L-Tryptophan	1P87	0	0	0.95
DB01245	Decamethonium	1KED	0	0	0.94
DB00169	Cholecalciferol	1L6J	0	0	0.93
DB01245	Decamethonium	1EYD	0	0	0.96
DB01396	Digitoxin	1XHY	0	0	0.98
DB00877	Sirolimus	1FYC	0	0	0.99
DB00615	Rifabutin	1N8S	0	0	0.91
DB01396	Digitoxin	1WVJ	0	0	0.98
DB01245	Decamethonium	1HA2	0	0	0.93
DB00926	Etretinate	1MO8	0	1	0.45
DB01245	Decamethonium	1R6K	0	0	0.94
DB01396	Digitoxin	1R5K	0	0	0.97
DB01245	Decamethonium	1BYW	0	0	0.97
DB01089	Deserpidine	1LBD	0	0	0.88
DB01396	Digitoxin	1BNA	0	0	0.96
DB01396	Digitoxin	1J3S	0	0	0.98
DB01245	Decamethonium	1NRL	0	0	0.72
DB00603	Medroxyprogesterone	1HOF	0	0	0.92
DB01396	Digitoxin	1P0Q	0	0	0.98

DB00626	Bacitracin	1YTV	0	0	0.94
DB00926	Etretinate	1NAV	0	1	0.47
DB01396	Digitoxin	1IBC	0	0	0.99
DB00273	Topiramate	1P4R	0	0	0.71
DB01245	Decamethonium	1L6J	0	0	0.93
DB00626	Bacitracin	1MO8	0	0	0.97
DB00877	Sirolimus	1IVO	0	0	0.98
DB00877	Sirolimus	1VRU	0	0	0.98
DB01396	Digitoxin	1CZM	0	0	0.98
DB01396	Digitoxin	1AJS	0	0	0.96
DB00511	Acetyldigitoxin	1R5K	0	0	0.98
DB00273	Topiramate	1EMI	0	1	0.57
DB00157	NADH	1DON	0	0	0.97
DB01396	Digitoxin	1UZF	0	0	0.98
DB06692	Aprotinin	1FYC	0	0	0.97
DB06692	Aprotinin	1BNA	0	0	0.96
DB06692	Aprotinin	1UT1	0	0	0.96
DB06692	Aprotinin	1R5K	0	0	0.96
DB06692	Aprotinin	1FE3	0	0	0.97
DB00769	Hydrocortamate	1P87	0	0	0.99
DB06692	Aprotinin	1NHZ	0	0	0.97
DB06692	Aprotinin	1WVJ	0	0	0.97
DB06692	Aprotinin	1AGS	0	0	0.97
DB06692	Aprotinin	1CB6	0	0	0.96
DB06692	Aprotinin	1S3A	0	0	0.97
DB06692	Aprotinin	1CWM	0	0	0.97
DB06692	Aprotinin	1K7L	0	0	0.96
DB06692	Aprotinin	1EXB	0	0	0.97
DB06692	Aprotinin	1HAG	0	0	0.96
DB06692	Aprotinin	1I4L	0	0	0.97
DB06692	Aprotinin	1BI9	0	0	0.97
DB06692	Aprotinin	1LBD	0	0	0.97
DB06692	Aprotinin	1OLM	0	0	0.97
DB06692	Aprotinin	1HA2	0	0	0.97
DB06692	Aprotinin	1BYY	0	0	0.97
DB06692	Aprotinin	1NAV	0	0	0.97
DB06692	Aprotinin	1KED	0	0	0.97
DB06692	Aprotinin	1A5Y	0	0	0.97
DB06692	Aprotinin	1AUT	0	0	0.96
DB00769	Hydrocortamate	1F8U	0	0	0.93
DB00769	Hydrocortamate	1OF7	0	0	0.96
DB00769	Hydrocortamate	1HOF	0	0	0.97
DB00769	Hydrocortamate	1D6A	0	0	0.72
DB00769	Hydrocortamate	1KTA	0	0	0.79

DB00769	Hydrocortamate	1S5O	0	0	0.93
DB00769	Hydrocortamate	1RFN	0	0	0.71
DB00769	Hydrocortamate	1BNA	0	0	0.71
DB00769	Hydrocortamate	1Z8L	0	0	0.94
DB00769	Hydrocortamate	1N7D	0	0	0.80
DB00769	Hydrocortamate	1N8S	0	0	0.72
DB00769	Hydrocortamate	1Y38	0	0	0.98
DB00769	Hydrocortamate	1BP3	0	0	0.92
DB00603	Medroxyprogesterone	1L6V	0	0	0.86
DB00769	Hydrocortamate	1UHL	0	0	0.92
DB00769	Hydrocortamate	1BJ4	0	0	0.94
DB00769	Hydrocortamate	1BYY	0	0	0.98
DB01396	Digitoxin	1E3G	0	0	0.98
DB01169	Arsenic trioxide	1P87	0	0	1.00
DB00769	Hydrocortamate	1SLM	0	0	0.94
DB01396	Digitoxin	1I5H	0	0	0.98
DB00769	Hydrocortamate	1TZI	0	0	0.71
DB01396	Digitoxin	1HOF	0	0	0.99
DB01396	Digitoxin	1KG3	0	0	0.98
DB00741	Hydrocortisone	1P87	0	0	0.97
DB00775	Tirofiban	1DON	0	0	0.98
DB01245	Decamethonium	1VRU	0	0	0.73
DB00970	Dactinomycin	1YAE	0	0	0.99
DB00970	Dactinomycin	1ILQ	0	0	1.00
DB00775	Tirofiban	1IRU	0	0	0.98
DB01325	Quinethazone	1DON	0	0	0.99
DB00626	Bacitracin	1SG0	0	0	0.97
DB00834	Mifepristone	1IRU	0	0	0.99
DB00970	Dactinomycin	1OAT	0	0	0.99
DB00834	Mifepristone	1BYW	0	0	0.86
DB01245	Decamethonium	1A36	0	0	0.75
DB00834	Mifepristone	1S3A	0	0	0.71
DB00970	Dactinomycin	1KI0	0	0	0.99
DB00834	Mifepristone	1Y6R	0	0	0.79
DB00877	Sirolimus	1BZY	0	0	0.98
DB00262	Carmustine	1DON	0	0	0.99
DB01245	Decamethonium	2BGR	0	0	0.94
DB00970	Dactinomycin	1HAG	0	0	0.98
DB00262	Carmustine	1P87	0	0	0.99
DB00506	Norgestrel	1D6G	0	1	0.61
DB00834	Mifepristone	2IL6	0	0	0.84
DB01245	Decamethonium	1P0Q	0	0	0.93
DB00908	Quinidine	1P87	0	0	1.00
DB00626	Bacitracin	1G1S	0	0	0.96

DB00150	L-Tryptophan	1IRU	0	0	0.97
DB00779	Nalidixic Acid	1P87	0	0	1.00
DB01089	Deserpidine	1S78	0	0	0.83
DB01245	Decamethonium	1F4J	0	0	0.95
DB01089	Deserpidine	1YXL	0	0	0.93
DB00877	Sirolimus	1NRL	0	0	0.98
DB00970	Dactinomycin	1SG0	0	0	0.99
DB00626	Bacitracin	1EXB	0	0	0.96
DB04573	Estriol	1P87	0	0	0.97
DB00970	Dactinomycin	1MO8	0	0	0.99
DB01121	Phenacemide	1P87	0	0	0.98
DB00775	Tirofiban	1P87	0	0	0.98
DB00834	Mifepristone	1R74	0	0	0.74
DB00626	Bacitracin	1N7D	0	0	0.94
DB00790	Perindopril	1F5F	0	1	0.58
DB00834	Mifepristone	1YAE	0	0	0.82
DB00615	Rifabutin	1AMO	0	0	0.98
DB00626	Bacitracin	1SS2	0	0	0.97
DB00790	Perindopril	1K2H	0	0	0.99
DB00877	Sirolimus	1OC3	0	0	0.99
DB00615	Rifabutin	1I10	0	0	0.97
DB00834	Mifepristone	1NHZ	0	0	0.80
DB00779	Nalidixic Acid	1IRU	0	0	0.98
DB00790	Perindopril	1KPF	0	1	0.66
DB00626	Bacitracin	1R5K	0	0	0.95
DB01245	Decamethonium	1UZF	0	0	0.94
DB00626	Bacitracin	1D3H	0	0	0.97
DB00236	Pipobroman	1P87	0	0	1.00
DB00834	Mifepristone	1YV5	0	0	0.85
DB01183	Naloxone	1P87	0	0	0.98
DB00615	Rifabutin	1MQ8	0	0	0.92
DB00741	Hydrocortisone	1IRU	0	0	0.98
DB00877	Sirolimus	1BYW	0	0	0.99
DB00834	Mifepristone	1GTE	0	0	0.77
DB00615	Rifabutin	1F0Y	0	0	0.93
DB00741	Hydrocortisone	1DON	0	0	0.98
DB00834	Mifepristone	1G0W	0	0	0.76
DB01089	Deserpidine	1AGS	0	0	0.89
DB00834	Mifepristone	1IBC	0	0	0.86
DB00834	Mifepristone	1CZM	0	0	0.79
DB00834	Mifepristone	1DIA	0	0	0.76
DB00615	Rifabutin	1UYL	0	0	0.97
DB00834	Mifepristone	1PQ3	0	0	0.79
DB00877	Sirolimus	1BBS	0	0	0.98

DB00626	Bacitracin	1JBQ	0	0	0.98
DB00118	S-Adenosylmethionine	1H2W	0	0	1.00
DB01050	Ibuprofen	1P87	0	0	1.00
DB00834	Mifepristone	1HOF	0	0	0.90
DB00615	Rifabutin	1NHZ	0	0	0.97
DB00834	Mifepristone	1OF7	0	0	0.85
DB00834	Mifepristone	1F8U	0	0	0.74
DB00877	Sirolimus	1EXX	0	0	0.99
DB01247	Isocarboxazid	1DON	0	0	0.97
DB01247	Isocarboxazid	1IRU	0	0	0.98
DB00378	Dydrogesterone	1BYW	0	0	0.85
DB01247	Isocarboxazid	1P87	0	0	0.99
DB00762	Irinotecan	1SA1	0	0	0.89
DB00762	Irinotecan	1HA2	0	0	0.87
DB00762	Irinotecan	1IRU	0	0	0.99
DB00762	Irinotecan	1YXM	0	1	0.64
DB00626	Bacitracin	1T9N	0	0	0.97
DB00762	Irinotecan	1I10	0	0	0.90
DB00762	Irinotecan	1UYL	0	0	0.92
DB00762	Irinotecan	1L9X	0	0	0.91
DB00762	Irinotecan	1R5K	0	1	0.63
DB00762	Irinotecan	1CP3	0	0	0.90
DB00877	Sirolimus	1JQI	0	0	0.98
DB00626	Bacitracin	1UWJ	0	0	0.97
DB00762	Irinotecan	1UZF	0	0	0.89
DB00762	Irinotecan	2BK3	0	1	0.63
DB00762	Irinotecan	1HOF	0	0	0.96
DB00762	Irinotecan	1XF0	0	0	0.94
DB00762	Irinotecan	2BIY	0	0	0.92
DB00762	Irinotecan	1P87	0	0	1.00
DB01245	Decamethonium	1HOF	0	0	0.98
DB00615	Rifabutin	1VRU	0	0	0.93
DB01388	Mibefradil	1DON	0	0	0.99
DB00615	Rifabutin	1XKT	0	0	0.96
DB00877	Sirolimus	1TRN	0	0	0.98
DB00626	Bacitracin	1UZF	0	0	0.97
DB00035	Desmopressin	1IRU	0	0	0.91
DB00378	Dydrogesterone	1EXX	0	0	0.81
DB00626	Bacitracin	1HOF	0	0	0.98
DB00877	Sirolimus	1YTV	0	0	0.98
DB01083	Orlistat	1YTV	0	0	0.98
DB00378	Dydrogesterone	1LPJ	0	0	0.81
DB00758	Clopidogrel	1P87	0	0	1.00
DB00169	Cholecalciferol	1C5G	0	0	0.95

DB00615	Rifabutin	1QYX	0	0	0.97
DB00626	Bacitracin	1OKC	0	0	0.97
DB00575	Clonidine	1P87	0	0	0.99
DB00790	Perindopril	1HOF	0	0	0.72
DB00906	Tiagabine	1P87	0	0	1.00
DB00378	Dydrogesterone	1MO8	0	0	0.79
DB00626	Bacitracin	1OHY	0	0	0.97
DB00142	L-Glutamic Acid	1DON	0	0	0.97
DB00378	Dydrogesterone	1A8M	0	0	0.81
DB00626	Bacitracin	1EMI	0	0	0.99
DB00926	Etretinate	1A8M	0	1	0.48
DB00651	Dyphylline	1P87	0	0	0.99
DB00615	Rifabutin	1X9N	0	0	0.93
DB01388	Mibefradil	1P87	0	0	0.99
DB00984	Nandrolone	1P87	0	0	1.00
DB00142	L-Glutamic Acid	1IRU	0	0	0.98
DB00984	Nandrolone	1XQ8	0	1	0.65
DB00001	Lepirudin	1SD2	0	0	0.97
DB01029	Irbesartan	1O5W	0	0	0.71
DB00595	Oxytetracycline	1DON	0	0	0.97
DB00207	Azithromycin	1A8M	0	0	0.99
DB00169	Cholecalciferol	1WD8	0	0	0.98
DB01029	Irbesartan	1P87	0	0	1.00
DB00224	Indinavir	1WAP	0	0	0.71
DB00637	Astemizole	1P87	0	0	0.99
DB00637	Astemizole	1DON	0	0	0.99
DB00224	Indinavir	1BY Y	0	0	0.84
DB01245	Decamethonium	1HSZ	0	0	0.72
DB00169	Cholecalciferol	1CRB	0	0	0.96
DB00595	Oxytetracycline	1H2W	0	0	1.00
DB00984	Nandrolone	1UZF	0	0	0.88
DB00641	Simvastatin	1HWL	0	0	0.68
DB00001	Lepirudin	1BJ4	0	0	0.97
DB00001	Lepirudin	1BXS	0	0	0.97
DB00641	Simvastatin	1W0H	0	0	0.96
DB00984	Nandrolone	1CZM	0	0	0.91
DB01083	Orlistat	1EMI	0	0	1.00
DB00944	Demecarium bromide	1P87	0	0	1.00
DB01083	Orlistat	1SA1	0	0	0.99
DB00984	Nandrolone	1CP3	0	0	0.89
DB00184	Nicotine	1P87	0	0	1.00
DB00616	Candoxatril	1P87	0	0	0.98
DB00224	Indinavir	1ILQ	0	0	0.71
DB00006	Bivalirudin	1YTV	0	0	0.96

DB00506	Norgestrel	1P87	0	0	1.00
DB00169	Cholecalciferol	1DON	0	0	0.98
DB00006	Bivalirudin	1MO8	0	0	0.98
DB00001	Lepirudin	1BYW	0	0	0.97
DB00984	Nandrolone	1SS2	0	0	0.92
DB00984	Nandrolone	1L1F	0	0	0.89
DB00887	Bumetanide	1P87	0	0	0.98
DB00224	Indinavir	1HOF	0	1	0.61
DB00984	Nandrolone	1AGS	0	0	0.90
DB01222	Budesonide	1A8M	0	0	0.72
DB00707	Porfimer	1XF0	0	0	0.93
DB00001	Lepirudin	1OAT	0	0	0.97
DB00984	Nandrolone	2IL6	0	0	0.93
DB00001	Lepirudin	1ODW	0	0	0.97
DB00001	Lepirudin	1BWC	0	0	0.97
DB00984	Nandrolone	1LBD	0	0	0.90
DB00984	Nandrolone	1BYY	0	0	0.98
DB00984	Nandrolone	1KGI	0	0	0.91
DB00984	Nandrolone	1A8M	0	0	0.92
DB00615	Rifabutin	1FYC	0	0	0.96
DB00277	Theophylline	1P87	0	0	1.00
DB01083	Orlistat	1WAP	0	0	1.00
DB00707	Porfimer	1HOF	0	0	0.93
DB00308	Ibutilide	1EMI	0	1	0.61
DB01089	Deserpidine	1WVJ	0	0	0.91
DB00957	Norgestimate	1A8M	0	0	0.77
DB00006	Bivalirudin	1HA2	0	0	0.98
DB00001	Lepirudin	1R5K	0	0	0.97
DB00006	Bivalirudin	1EXX	0	0	0.98
DB00006	Bivalirudin	1HAG	0	0	0.96
DB00707	Porfimer	1YMX	0	0	0.81
DB00001	Lepirudin	1DYT	0	0	0.97
DB01245	Decamethonium	1F8U	0	0	0.94
DB00957	Norgestimate	1JNM	0	1	0.59
DB00006	Bivalirudin	1Y38	0	0	0.99
DB01245	Decamethonium	1HWL	0	0	0.74
DB00006	Bivalirudin	1OAT	0	0	0.96
DB01083	Orlistat	1F5F	0	0	0.99
DB00001	Lepirudin	1TQN	0	0	0.97
DB00220	Nelfinavir	1HOF	0	1	0.67
DB00001	Lepirudin	1P0Q	0	0	0.97
DB00001	Lepirudin	1UZF	0	0	0.97
DB01083	Orlistat	1Q9S	0	0	0.99
DB00707	Porfimer	1T9N	0	0	0.88

DB01011	Metyrapone	1BDA	0	0	0.92
DB01088	Iloprost	1TJC	0	1	0.59
DB00001	Lepirudin	1HOF	0	0	0.97
DB00001	Lepirudin	1OF7	0	0	0.97
DB01088	Iloprost	1YV5	0	1	0.66
DB00001	Lepirudin	2BIY	0	0	0.97
DB00006	Bivalirudin	1J0X	0	0	0.97
DB00481	Raloxifene	1DON	0	0	0.98
DB00116	Tetrahydrofolic acid	1DON	0	0	0.97
DB01083	Orlistat	1EXX	0	0	0.99
DB00957	Norgestimate	1XF0	0	0	0.81
DB01076	Atorvastatin	1IRU	0	0	0.99
DB00957	Norgestimate	1UHL	0	1	0.64
DB00001	Lepirudin	1P87	0	0	0.93
DB00199	Erythromycin	1RV7	0	0	0.99
DB00707	Porfimer	1QKM	0	0	0.88
DB00707	Porfimer	1NHZ	0	0	0.89
DB00957	Norgestimate	1EXX	0	0	0.78
DB00707	Porfimer	1BZY	0	0	0.70
DB00707	Porfimer	1TLL	0	0	0.79
DB01083	Orlistat	1BXS	0	0	0.97
DB00707	Porfimer	1KI0	0	0	0.88
DB00622	Nicardipine	1DON	0	0	0.98
DB00199	Erythromycin	1QR6	0	0	0.97
DB00707	Porfimer	1EXX	0	0	0.91
DB00707	Porfimer	1LN6	0	0	0.85
DB00207	Azithromycin	1MO8	0	0	0.99
DB00707	Porfimer	1F5F	0	0	0.91
DB00220	Nelfinavir	1C0B	0	0	0.77
DB00707	Porfimer	1A5Y	0	0	0.88
DB00006	Bivalirudin	1NHZ	0	0	0.98
DB00707	Porfimer	1V97	0	0	0.94
DB00220	Nelfinavir	1BYY	0	0	0.87
DB01168	Procarbazine	1P87	0	0	0.98
DB01083	Orlistat	1HAG	0	0	0.97
DB00790	Perindopril	1EMI	0	0	0.87
DB00957	Norgestimate	1I4L	0	1	0.66
DB00006	Bivalirudin	1FTA	0	0	0.98
DB00615	Rifabutin	1TQN	0	0	0.96
DB00888	Mechlorethamine	1P87	0	0	1.00
DB00696	Ergotamine	1DON	0	0	0.98
DB01245	Decamethonium	1EMI	0	0	0.99
DB00957	Norgestimate	1BP3	0	1	0.66
DB00957	Norgestimate	1HOF	0	0	0.87

DB00572	Atropine	1BDA	0	0	0.85
DB00995	Auranofin	1EMI	0	0	0.99
DB00995	Auranofin	1HNK	0	0	0.98
DB00995	Auranofin	1ORE	0	0	0.97
DB00995	Auranofin	1OKC	0	0	0.97
DB00995	Auranofin	1HT0	0	0	0.79
DB00995	Auranofin	1HOF	0	0	0.98
DB00995	Auranofin	1UZF	0	0	0.96
DB00786	Marimastat	1DON	0	0	0.98
DB00178	Ramipril	1O5W	0	0	0.87
DB00926	Etretinate	1EMI	0	0	0.84
DB01083	Orlistat	1BYW	0	0	0.99
DB00995	Auranofin	3BLM	0	0	0.97
DB00995	Auranofin	1CZM	0	0	0.96
DB00995	Auranofin	1T9R	0	0	0.97
DB00995	Auranofin	1P0S	0	0	0.70
DB00995	Auranofin	1J3S	0	0	0.95
DB00995	Auranofin	1GTE	0	0	0.96
DB00995	Auranofin	1IVO	0	0	0.80
DB00995	Auranofin	1QKM	0	0	0.96
DB00995	Auranofin	1HE5	0	0	0.97
DB00995	Auranofin	1WVJ	0	0	0.97
DB00995	Auranofin	1BZY	0	0	0.83
DB00995	Auranofin	1DMT	0	0	0.81
DB00995	Auranofin	1OAT	0	0	0.80
DB00995	Auranofin	1CWM	0	0	0.97
DB00995	Auranofin	1K7L	0	0	0.79
DB00995	Auranofin	1K2H	0	0	1.00
DB00995	Auranofin	1XDK	0	0	0.80
DB00995	Auranofin	1RTU	0	0	0.98
DB00995	Auranofin	1JQI	0	0	0.80
DB00995	Auranofin	1X86	0	0	0.96
DB00995	Auranofin	1SA1	0	0	0.96
DB00995	Auranofin	1A5Y	0	0	0.96
DB00995	Auranofin	1V97	0	0	0.98
DB00207	Azithromycin	1UHL	0	0	0.98
DB00993	Azathioprine	1P87	0	0	1.00
DB00957	Norgestimate	1MZW	0	0	0.78
DB00615	Rifabutin	1P0Q	0	0	0.96
DB01088	Iloprost	1O5W	0	0	0.95
DB01088	Iloprost	1OKC	0	1	0.58
DB01088	Iloprost	1EMI	0	0	0.89
DB00806	Pentoxifylline	1IRU	0	0	0.98
DB01216	Finasteride	1MF1	0	0	0.81

DB01083	Orlistat	1JYD	0	0	0.99
DB00006	Bivalirudin	1X9N	0	0	0.96
DB01216	Finasteride	1HOF	0	0	0.91
DB00957	Norgestimate	1FVO	0	1	0.59
DB00530	Erlotinib	1IRU	0	0	0.98
DB00530	Erlotinib	1DON	0	0	0.98
DB01011	Metyrapone	1P87	0	0	1.00
DB00916	Metronidazole	1H2W	0	0	1.00
DB00916	Metronidazole	1P87	0	0	1.00
DB00006	Bivalirudin	1I9R	0	0	0.98
DB01180	Rescinnamine	1NAV	0	0	0.95
DB00207	Azithromycin	1EXB	0	0	0.98
DB00624	Testosterone	1BYY	0	0	0.89
DB00006	Bivalirudin	1CZM	0	0	0.98
DB00624	Testosterone	1CRB	0	1	0.53
DB00615	Rifabutin	1ZNC	0	0	0.91
DB00624	Testosterone	1H2W	0	0	1.00
DB00624	Testosterone	1BYW	0	1	0.61
DB01180	Rescinnamine	1HA2	0	0	0.92
DB00957	Norgestimate	9ILB	0	0	0.80
DB00122	Choline	1P87	0	0	1.00
DB00199	Erythromycin	1MC5	0	0	0.96
DB00641	Simvastatin	1S3I	0	0	0.91
DB00199	Erythromycin	2BK3	0	0	0.96
DB00624	Testosterone	2IL6	0	1	0.57
DB01083	Orlistat	1Y0S	0	0	0.99
DB00624	Testosterone	4Q21	0	1	0.58
DB01222	Budesonide	1EMI	0	0	0.92
DB00203	Sildenafil	1EMI	0	0	0.81
DB00207	Azithromycin	1PU4	0	0	0.97
DB00308	Ibutilide	1TYE	0	0	0.68
DB00199	Erythromycin	1RJ6	0	0	0.96
DB00624	Testosterone	1YV5	0	1	0.58
DB01180	Rescinnamine	1EXX	0	0	0.96
DB00199	Erythromycin	1CP3	0	0	0.98
DB00199	Erythromycin	1JBQ	0	0	0.99
DB00382	Tacrine	1H2W	0	0	1.00
DB00207	Azithromycin	1KPF	0	0	0.99
DB00624	Testosterone	1JBQ	0	1	0.60
DB00624	Testosterone	1D6G	0	1	0.65
DB00199	Erythromycin	1BNA	0	0	0.96
DB00199	Erythromycin	1XKT	0	0	0.98
DB01180	Rescinnamine	1K2H	0	0	1.00
DB00624	Testosterone	1HOF	0	0	0.71

DB00615	Rifabutin	1TB5	0	0	0.92
DB01216	Finasteride	1JBQ	0	0	0.87
DB00717	Norethindrone	1O5W	0	0	0.90
DB00199	Erythromycin	1L6J	0	0	0.98
DB00624	Testosterone	1P87	0	0	1.00
DB00255	Diethylstilbestrol	1P87	0	0	0.99
DB00396	Progesterone	1YV5	0	0	0.94
DB01180	Rescinnamine	1Y0S	0	0	0.89
DB01216	Finasteride	8ICK	0	0	0.81
DB01083	Orlistat	2RMC	0	0	0.98
DB01197	Captopril	1P87	0	0	0.99
DB00284	Acarbose	1DON	0	0	0.95
DB00711	Diethylcarbamazine	1BDA	0	0	0.93
DB00207	Azithromycin	1A36	0	0	0.97
DB00308	Ibutilide	1K2H	0	0	0.99
DB00864	Tacrolimus	1HWL	0	0	0.98
DB00511	Acetyldigitoxin	1Y38	0	0	0.99
DB00511	Acetyldigitoxin	1EXX	0	0	0.99
DB00864	Tacrolimus	1OHY	0	0	0.99
DB01083	Orlistat	1AMO	0	0	0.99
DB00511	Acetyldigitoxin	1RTU	0	0	0.99
DB01083	Orlistat	1OHY	0	0	0.99
DB01083	Orlistat	9ILB	0	0	0.99
DB00864	Tacrolimus	1OF7	0	0	0.99
DB01089	Deserpidine	1NHZ	0	0	0.90
DB01083	Orlistat	1T5P	0	0	0.99
DB01196	Estramustine	1P87	0	0	0.99
DB00615	Rifabutin	1E79	0	0	0.96
DB01083	Orlistat	1J0X	0	0	0.99
DB01083	Orlistat	1PB7	0	0	0.99
DB01083	Orlistat	1HE5	0	0	0.99
DB00203	Sildenafil	1BYW	0	1	0.52
DB01400	Neostigmine	1P87	0	0	1.00
DB01083	Orlistat	1QYE	0	0	0.99
DB00957	Norgestimate	1BWC	0	0	0.69
DB01083	Orlistat	1X9N	0	0	0.98
DB00864	Tacrolimus	1HOF	0	0	0.99
DB01083	Orlistat	1CJY	0	0	0.97
DB00342	Terfenadine	1EMI	0	0	0.68
DB00864	Tacrolimus	2BK3	0	0	0.98
DB00511	Acetyldigitoxin	1HA2	0	0	0.98
DB00006	Bivalirudin	1KTO	0	0	0.98
DB01083	Orlistat	1CP3	0	0	0.99
DB01497	Etorphine	1Y4E	0	0	0.83

DB00548	Azelaic Acid	1P87	0	0	1.00
DB01083	Orlistat	1CZM	0	0	0.99
DB00511	Acetyldigitoxin	1EYD	0	0	0.99
DB01216	Finasteride	1QKM	0	0	0.80
DB01083	Orlistat	1XGJ	0	0	0.98
DB01216	Finasteride	1HE5	0	0	0.84
DB01083	Orlistat	1RL0	0	0	0.99
DB00615	Rifabutin	1RL0	0	0	0.96
DB01216	Finasteride	1PB7	0	0	0.84
DB01083	Orlistat	1UZF	0	0	0.99
DB01216	Finasteride	1ODW	0	0	0.87
DB01083	Orlistat	1O5W	0	0	1.00
DB00398	Sorafenib	1P87	0	0	0.99
DB01089	Deserpidine	1FTA	0	0	0.91
DB00615	Rifabutin	1R4L	0	0	0.93
DB00006	Bivalirudin	1JVQ	0	0	0.96
DB00212	Remikiren	1ORE	0	0	0.83
DB00212	Remikiren	1HOF	0	0	0.86
DB00006	Bivalirudin	1E3G	0	0	0.98
DB00212	Remikiren	1E3G	0	0	0.78
DB01216	Finasteride	1TJC	0	0	0.83
DB00212	Remikiren	3BLM	0	0	0.79
DB00751	Epinastine	1P87	0	0	0.99
DB00212	Remikiren	1LJ7	0	0	0.84
DB00864	Tacrolimus	1UZF	0	0	0.99
DB00212	Remikiren	1TQN	0	1	0.67
DB00212	Remikiren	1KFD	0	0	0.76
DB01216	Finasteride	1EXX	0	0	0.85
DB00212	Remikiren	1J4I	0	0	0.85
DB00006	Bivalirudin	1HOF	0	0	0.99
DB00207	Azithromycin	1I5H	0	0	0.99
DB00207	Azithromycin	1PQ3	0	0	0.98
DB00006	Bivalirudin	1GXD	0	0	0.98
DB00976	Telithromycin	1A8M	0	0	1.00
DB00976	Telithromycin	1SLM	0	0	0.99
DB00976	Telithromycin	1DON	0	0	0.98
DB00976	Telithromycin	1C0B	0	0	1.00
DB00976	Telithromycin	1EXX	0	0	1.00
DB00976	Telithromycin	1XWS	0	0	0.99
DB00976	Telithromycin	1IRU	0	0	1.00
DB00976	Telithromycin	1EXB	0	0	0.99
DB00976	Telithromycin	2BAT	0	0	0.99
DB00976	Telithromycin	1P5J	0	0	1.00
DB00976	Telithromycin	9ILB	0	0	1.00

DB00976	Telithromycin	1M1X	0	0	0.99
DB00976	Telithromycin	1KPF	0	0	1.00
DB00976	Telithromycin	1J0X	0	0	0.99
DB00976	Telithromycin	1VRU	0	0	0.99
DB00976	Telithromycin	1QKM	0	0	0.99
DB00976	Telithromycin	1A36	0	0	0.99
DB00976	Telithromycin	1BP3	0	0	0.99
DB00976	Telithromycin	1PO5	0	0	0.99
DB00976	Telithromycin	1FIE	0	0	0.99
DB00976	Telithromycin	1UTQ	0	0	0.99
DB00976	Telithromycin	1CZM	0	0	0.99
DB00976	Telithromycin	1AJS	0	0	0.99
DB00976	Telithromycin	1UZF	0	0	0.99
DB00976	Telithromycin	1E3G	0	0	0.99
DB00976	Telithromycin	1I5H	0	0	1.00
DB00976	Telithromycin	1HSO	0	0	0.99
DB00976	Telithromycin	1KG3	0	0	0.99
DB00976	Telithromycin	1EMI	0	0	1.00
DB01058	Praziquantel	1EMI	0	0	0.75
DB00212	Remikiren	1RV7	0	0	0.83
DB01216	Finasteride	1QD2	0	0	0.85
DB00212	Remikiren	1EXX	0	0	0.81
DB01400	Neostigmine	1IRU	0	0	0.98
DB01400	Neostigmine	1DON	0	0	0.98
DB00864	Tacrolimus	1TB5	0	0	0.98
DB00864	Tacrolimus	1IBC	0	0	0.99
DB01089	Deserpidine	1T9N	0	0	0.89
DB00711	Diethylcarbamazine	1O5W	0	0	0.84
DB00864	Tacrolimus	1LJ7	0	0	0.99
DB01058	Praziquantel	1HOF	0	1	0.55
DB01216	Finasteride	1YVL	0	0	0.74
DB00212	Remikiren	1V97	0	0	0.87
DB00711	Diethylcarbamazine	1P87	0	0	1.00
DB01058	Praziquantel	1O5W	0	0	0.91
DB00864	Tacrolimus	1JBQ	0	0	0.99
DB01180	Rescinnamine	1EMI	0	0	0.99
DB01216	Finasteride	1KED	0	0	0.80
DB00864	Tacrolimus	1D3H	0	0	0.99
DB00957	Norgestimate	1R5S	0	0	0.75
DB01089	Deserpidine	1OHY	0	0	0.89
DB00663	Flumethasone Pivalate	1P87	0	0	0.99
DB00304	Desogestrel	1EMI	0	0	0.83
DB00957	Norgestimate	1HE5	0	0	0.77
DB00615	Rifabutin	2BK3	0	0	0.92

DB01180	Rescinnamine	1OHY	0	0	0.94
DB01047	Fluocinonide	1P87	0	0	0.99
DB00799	Tazarotene	1K2H	0	0	0.99
DB00396	Progesterone	1TQN	0	0	0.90
DB00957	Norgestimate	1XKT	0	1	0.65
DB00864	Tacrolimus	1DYT	0	0	0.99
DB00304	Desogestrel	1MRQ	0	1	0.54
DB00864	Tacrolimus	1VJB	0	0	0.99
DB00396	Progesterone	1CRK	0	0	0.75
DB00532	Mephenytoin	1BDA	0	0	0.84
DB01180	Rescinnamine	1HT0	0	0	0.74
DB00864	Tacrolimus	1Q6U	0	0	0.99
DB00396	Progesterone	1P0Q	0	0	0.89
DB00615	Rifabutin	1XQ8	0	0	0.93
DB00489	Sotalol	1P87	0	0	0.98
DB00864	Tacrolimus	1PB7	0	0	0.99
DB00396	Progesterone	1S5O	0	0	0.92
DB01185	Fluoxymesterone	1H2W	0	0	1.00
DB00864	Tacrolimus	3JDW	0	0	0.99
DB00367	Levonorgestrel	1O5W	0	0	0.94
DB00367	Levonorgestrel	1HOF	0	0	0.68
DB00846	Flurandrenolide	1IRU	0	0	0.99
DB00864	Tacrolimus	1HUL	0	0	0.99
DB00367	Levonorgestrel	1ORE	0	1	0.56
DB01180	Rescinnamine	1HOF	0	0	0.97
DB00864	Tacrolimus	1W7N	0	0	0.99
DB00615	Rifabutin	1HOF	0	0	0.98
DB00367	Levonorgestrel	1P87	0	0	1.00
DB00588	Fluticasone Propionate	1P87	0	0	1.00
DB00615	Rifabutin	1XF0	0	0	0.98
DB00304	Desogestrel	1HOF	0	1	0.66
DB00615	Rifabutin	1ORE	0	0	0.98
DB00799	Tazarotene	1O5W	0	1	0.61
DB00511	Acetyldigitoxin	1V97	0	0	0.99
DB00396	Progesterone	1CZM	0	0	0.91
DB00396	Progesterone	1J1S	0	0	0.91
DB00158	Folic Acid	1P87	0	0	0.95
DB00957	Norgestimate	1D3H	0	0	0.74
DB00396	Progesterone	1E3G	0	0	0.92
DB00864	Tacrolimus	1ISS	0	0	0.98
DB00799	Tazarotene	1P87	0	0	1.00
DB00207	Azithromycin	1PO5	0	0	0.98
DB01213	Fomepizole	1P87	0	0	1.00
DB00864	Tacrolimus	1SVC	0	0	0.98

DB00957	Norgestimate	1J3S	0	1	0.61
DB00675	Tamoxifen	1BDA	0	0	0.93
DB00615	Rifabutin	1KG3	0	0	0.97
DB00864	Tacrolimus	1CWM	0	0	0.99
DB00396	Progesterone	1HOF	0	0	0.96
DB01113	Papaverine	1O5W	0	1	0.48
DB00926	Etretinate	1J4I	0	1	0.60
DB00396	Progesterone	1F8U	0	0	0.89
DB00957	Norgestimate	1CZM	0	0	0.73
DB00926	Etretinate	1YV5	0	1	0.52
DB00540	Nortriptyline	1K2H	0	0	0.83
DB00864	Tacrolimus	1K7L	0	0	0.98
DB00396	Progesterone	1P87	0	0	1.00
DB01180	Rescinnamine	1PQ3	0	0	0.95
DB00675	Tamoxifen	1UMK	0	1	0.46
DB00957	Norgestimate	1K6R	0	0	0.85
DB00768	Olopatadine	1P87	0	0	1.00
DB00396	Progesterone	1VYT	0	0	0.91
DB00864	Tacrolimus	1BYW	0	0	0.99
DB00957	Norgestimate	1UZF	0	1	0.67
DB00864	Tacrolimus	1HAG	0	0	0.97
DB00396	Progesterone	1SA1	0	0	0.90
DB00396	Progesterone	1Y0X	0	0	0.93
DB00122	Choline	1H2W	0	0	1.00
DB00396	Progesterone	1F5F	0	0	0.93
DB00864	Tacrolimus	1BXS	0	0	0.97
DB00837	Progabide	1DON	0	0	0.99
DB00228	Enflurane	1P87	0	0	1.00
DB00396	Progesterone	1EII	0	0	0.94
DB01083	Orlistat	1ORE	0	0	0.99
DB01222	Budesonide	1TJC	0	0	0.70
DB00675	Tamoxifen	1O5W	0	1	0.46
DB00864	Tacrolimus	1EXX	0	0	0.99
DB04794	Bifonazole	1P87	0	0	1.00
DB00864	Tacrolimus	1QD2	0	0	0.99
DB01222	Budesonide	1ILQ	0	0	0.87
DB00396	Progesterone	1NHZ	0	0	0.92
DB01222	Budesonide	1NHZ	0	0	0.68
DB00864	Tacrolimus	1BJ4	0	0	0.99
DB01222	Budesonide	1FE3	0	0	0.75
DB01128	Bicalutamide	1P87	0	0	1.00
DB00957	Norgestimate	1I5H	0	0	0.77
DB01180	Rescinnamine	1UWJ	0	0	0.94
DB00864	Tacrolimus	1SD2	0	0	0.99

ACCEPTED MANUSCRIPT

DB01222	Budesonide	1T9R	0	1	0.64
DB00864	Tacrolimus	1X86	0	0	0.99
DB01180	Rescinnamine	1T9R	0	0	0.95
DB00238	Nevirapine	1P87	0	0	1.00
DB01101	Capecitabine	1P87	0	0	0.92
DB01406	Danazol	1EMI	0	0	0.77
DB01180	Rescinnamine	2BGR	0	0	0.93
DB01406	Danazol	1P87	0	0	1.00
DB00864	Tacrolimus	1TEV	0	0	0.99
DB00772	Malathion	1EMI	0	1	0.57
DB00992	Methyl aminolevulinate	1P87	0	0	1.00
DB01406	Danazol	1HOF	0	1	0.57
DB01180	Rescinnamine	1QYX	0	0	0.95
DB00232	Methyclothiazide	1IRU	0	0	0.99
DB00622	Nicardipine	1EMI	0	1	0.46
DB01180	Rescinnamine	1XKT	0	0	0.93
DB00864	Tacrolimus	1MNZ	0	0	0.98
DB00203	Sildenafil	1O5W	0	0	0.93
DB00199	Erythromycin	1ODW	0	0	0.99
DB00199	Erythromycin	1ILQ	0	0	0.99
DB01406	Danazol	1O5W	0	0	0.92
DB00396	Progesterone	1BP3	0	0	0.90
DB01222	Budesonide	1PQ3	0	1	0.64
DB00396	Progesterone	1KI0	0	0	0.89
DB00396	Progesterone	1YAE	0	0	0.93
DB01180	Rescinnamine	1WVJ	0	0	0.95
DB01222	Budesonide	1HOF	0	0	0.82
DB01089	Deserpidine	1HOF	0	0	0.95
DB01180	Rescinnamine	1OAT	0	0	0.74
DB01348	Spirapril	1O5W	0	0	0.82
DB01222	Budesonide	1XF0	0	0	0.77

OC=observed class, PC=predicted class, PRO=probability

TABLE 2SM. 2,3-dihydrooxoisoaporphine, oxoisoaporphine and oxoaporphine alkaloids Prediction results.

Drugs	PDB Malarial	PC	c-level
1e	1QNG	0	0.93
2e	3C02	0	0.82
3e	3IHZ	1	0.32
4e	1RT9	1	0.43
5e	1RSZ	0	0.79
6e	1CEQ	0	0.86
7e	1CET	0	0.79
8e	2RJI	0	0.87
1e	1LDG	0	1.00
2e	1T25	0	1.00
3e	1T2E	0	0.97
4e	1T24	0	0.99
5e	1T2C	0	1.00
6e	1T26	0	1.00
7e	1YVB	0	0.98
8e	3MMR	0	0.83
1e	3EWC	0	0.91
2e	1QNH	0	0.78
3e	3EWD	1	0.17
4e	2VFA	1	0.35
5e	1VYQ	0	0.79
6e	3GEP	0	0.77
7e	3GGJ	0	0.69
8e	1OKT	0	0.70
1e	2AAW	0	0.94
2e	2VFE	0	0.83
3e	2VFI	1	0.25
4e	2VFF	1	0.37
5e	2VFH	0	0.74
6e	2VFD	0	0.76
7e	3LSY	0	1.00
8e	1NHW	0	0.89
1e	1NHG	0	0.93
2e	1VRW	0	0.88
3e	1NNU	1	0.30
4e	2NQ8	1	0.44
5e	1ZW1	0	0.81
6e	1ZXB	0	0.82
7e	1ZXL	0	1.00
8e	1ZSN	0	0.85
1e	3LT2	0	1.00
2e	2FOI	0	0.88
3e	3LT1	0	1.00
4e	3LT4	0	1.00
5e	3LT0	0	1.00
6e	1T2D	0	0.83
7e	2ANL	1	0.59

8e	1MIQ	0	0.98
1e	2PSS	0	0.90
2e	1ONF	0	0.86
3e	2PT9	1	0.24
4e	2GHU	1	0.34
5e	2Z8W	1	0.34
6e	2Z8V	1	0.36
7e	1CJB	0	0.74
8e	2VFG	0	0.81
1e	3F4B	0	0.94
2e	1J3J	0	0.87
3e	1J3I	1	0.33
4e	1J3K	0	1.00
5e	1T2F	0	0.78
6e	1YXE	0	0.77
7e	3KQX	1	0.67
8e	3KQZ	0	0.86
1e	3KR5	0	0.87
2e	3KR4	0	0.73
3e	1QNG	1	0.31
4e	3C02	1	0.35
5e	3IHZ	0	0.81
6e	1RT9	0	0.81
7e	1RSZ	0	0.74
8e	1CEQ	0	0.91
1e	1CET	0	0.95
2e	2RJI	0	0.86
3e	1LDG	0	0.97
4e	1T25	0	0.99
5e	1T2E	0	1.00
6e	1T24	0	1.00
7e	1T2C	0	1.00
8e	1T26	0	1.00
1e	1YVB	0	1.00
2e	3MMR	0	0.82
3e	3EWC	1	0.27
4e	1QNH	1	0.30
5e	3EWD	1	0.63
6e	2VFA	0	0.75
7e	1VYQ	0	0.74
8e	3GEP	0	0.85
1e	3GGJ	0	0.91
2e	1OKT	1	0.68
3e	2AAW	1	0.33
4e	2VFE	1	0.37
5e	2VFI	0	0.74
6e	2VFF	0	0.76
7e	2VFH	1	0.68
8e	2VFD	0	0.85

1e	3LSY	0	1.00
2e	1NHW	0	0.87
3e	1NHG	1	0.32
4e	1VRW	1	0.46
5e	1NNU	0	0.79
6e	2NQ8	0	0.81
7e	1ZW1	0	0.75
8e	1ZXB	0	0.89
1e	1ZXL	0	1.00
2e	1ZSN	0	0.84
3e	3LT2	0	1.00
4e	2FOI	1	0.46
5e	3LT1	0	1.00
6e	3LT4	0	1.00
7e	3LT0	0	1.00
8e	1T2D	0	0.90
1e	2ANL	0	0.85
2e	1MIQ	0	0.98
3e	2PSS	1	0.24
4e	1ONF	1	0.42
5e	2PT9	0	0.73
6e	2GHU	0	0.74
7e	2Z8W	1	0.31
8e	2Z8V	1	0.45
1e	1CJB	0	0.93
2e	2VFG	0	0.79
3e	3F4B	1	0.32
4e	1J3J	1	0.44
5e	1J3I	0	0.81
6e	1J3K	0	1.00
7e	1T2F	0	0.72
8e	1YXE	0	0.85
1e	3KQX	0	0.90
2e	3KQZ	0	0.84
3e	3KR5	1	0.20
4e	3KR4	1	0.25
5e	1QNG	0	0.80
6e	3C02	0	0.75
7e	3IHZ	0	0.76
8e	1RT9	0	0.88
1e	1RSZ	0	0.93
2e	1CEQ	0	0.90
3e	1CET	1	0.38
4e	2RJI	1	0.41
5e	1LDG	0	1.00
6e	1T25	0	1.00
7e	1T2E	0	1.00
8e	1T24	0	1.00
1e	1T2C	0	1.00

2e	1T26	0	1.00
3e	1YVB	0	0.89
4e	3MMR	1	0.35
5e	3EWC	0	0.76
6e	1QNH	0	0.71
7e	3EWD	1	0.57
8e	2VFA	0	0.84
1e	1VYQ	0	0.93
2e	3GEP	0	0.83
3e	3GGJ	1	0.25
4e	1OKT	1	0.17
5e	2AAW	0	0.82
6e	2VFE	0	0.76
7e	2VFI	1	0.68
8e	2VFF	0	0.84
1e	2VFH	0	0.91
2e	2VFD	0	0.83
3e	3LSY	0	1.00
4e	1NHW	1	0.45
5e	1NHG	0	0.81
6e	1VRW	0	0.82
7e	1NNU	0	0.74
8e	2NQ8	0	0.88
1e	1ZW1	0	0.93
2e	1ZXB	0	0.88
3e	1ZXL	0	1.00
4e	1ZSN	1	0.38
5e	3LT2	0	1.00
6e	2FOI	0	0.82
7e	3LT1	0	1.00
8e	3LT4	0	1.00
1e	3LT0	0	1.00
2e	1T2D	0	0.88
3e	2ANL	1	0.18
4e	1MIQ	0	0.85
5e	2PSS	0	0.73
6e	1ONF	0	0.80
7e	2PT9	1	0.67
8e	2GHU	0	0.83
1e	2Z8W	1	0.57
2e	2Z8V	1	0.43
3e	1CJB	1	0.30
4e	2VFG	1	0.32
5e	3F4B	0	0.81
6e	1J3J	0	0.82
7e	1J3I	0	0.76
8e	1J3K	0	1.00
1e	1T2F	0	0.92
2e	1YXE	0	0.83

3e	3KQX	1	0.23
4e	3KQZ	1	0.40
5e	3KR5	1	0.68
6e	3KR4	1	0.65
7e	1QNG	0	0.75
8e	3C02	0	0.84
1e	3IHZ	0	0.93
2e	1RT9	0	0.86
3e	1RSZ	1	0.29
4e	1CEQ	1	0.54
5e	1CET	0	0.84
6e	2RJI	0	0.80
7e	1LDG	0	1.00
8e	1T25	0	1.00
1e	1T2E	0	1.00
2e	1T24	0	1.00
3e	1T2C	0	0.97
4e	1T26	0	0.99
5e	1YVB	0	0.99
6e	3MMR	0	0.75
7e	3EWC	0	0.71
8e	1QNH	0	0.80
1e	3EWD	0	0.84
2e	2VFA	0	0.82
3e	1VYQ	1	0.30
4e	3GEP	1	0.38
5e	3GGJ	0	0.75
6e	1OKT	1	0.63
7e	2AAW	0	0.77
8e	2VFE	0	0.85
1e	2VFI	0	0.90
2e	2VFF	0	0.83
3e	2VFH	1	0.25
4e	2VFD	1	0.37
5e	3LSY	0	1.00
6e	1NHW	0	0.82
7e	1NHG	0	0.75
8e	1VRW	0	0.89
1e	1NNU	0	0.93
2e	2NQ8	0	0.87
3e	1ZW1	1	0.32
4e	1ZXB	1	0.46
5e	1ZXL	0	1.00
6e	1ZSN	0	0.77
7e	3LT2	0	1.00
8e	2FOI	0	0.89
1e	3LT1	0	1.00
2e	3LT4	0	1.00
3e	3LT0	0	1.00

4e	1T2D	1	0.47
5e	2ANL	1	0.65
6e	1MIQ	0	0.97
7e	2PSS	1	0.67
8e	1ONF	0	0.87
1e	2PT9	0	0.90
2e	2GHU	0	0.81
3e	2Z8W	1	0.07
4e	2Z8V	1	0.09
5e	1CJB	0	0.79
6e	2VFG	0	0.72
7e	3F4B	0	0.76
8e	1J3J	0	0.88
1e	1J3I	0	0.94
2e	1J3K	0	1.00
3e	1T2F	1	0.29
4e	1YXE	1	0.37
5e	3KQX	0	0.73
6e	3KQZ	0	0.78
7e	3KR5	1	0.62
8e	3KR4	0	0.76
1e	1QNG	0	0.93
2e	3C02	0	0.82
3e	3IHZ	1	0.32
4e	1RT9	1	0.43
5e	1RSZ	0	0.79
6e	1CEQ	0	0.86
7e	1CET	0	0.79
8e	2RJI	0	0.87
1e	1LDG	0	1.00
2e	1T25	0	1.00
3e	1T2E	0	0.97
4e	1T24	0	0.99
5e	1T2C	0	1.00
6e	1T26	0	1.00
7e	1YVB	0	0.98
8e	3MMR	0	0.83
1e	3EWC	0	0.91
2e	1QNH	0	0.78
3e	3EWD	1	0.17
4e	2VFA	1	0.35
5e	1VYQ	0	0.79
6e	3GEP	0	0.77
7e	3GGJ	0	0.69
8e	1OKT	0	0.70
1e	2AAW	0	0.94
2e	2VFE	0	0.83
3e	2VFI	1	0.25
4e	2VFF	1	0.37

5e	2VFH	0	0.74
6e	2VFD	0	0.76
7e	3LSY	0	1.00
8e	1NHW	0	0.89
1e	1NHG	0	0.93
2e	1VRW	0	0.88
3e	1NNU	1	0.30
4e	2NQ8	1	0.44
5e	1ZW1	0	0.81
6e	1ZXB	0	0.82
7e	1ZXL	0	1.00
8e	1ZSN	0	0.85
1e	3LT2	0	1.00
2e	2FOI	0	0.88
3e	3LT1	0	1.00
4e	3LT4	0	1.00
5e	3LT0	0	1.00
6e	1T2D	0	0.83
7e	2ANL	1	0.59
8e	1MIQ	0	0.98
1e	2PSS	0	0.90
2e	1ONF	0	0.86
3e	2PT9	1	0.24
4e	2GHU	1	0.34
5e	2Z8W	1	0.34
6e	2Z8V	1	0.36
7e	1CJB	0	0.74
8e	2VFG	0	0.81
1e	3F4B	0	0.94
2e	1J3J	0	0.87
3e	1J3I	1	0.33
4e	1J3K	0	1.00
5e	1T2F	0	0.78
6e	1YXE	0	0.77
7e	3KQX	1	0.67
8e	3KQZ	0	0.86
1e	3KR5	0	0.87
2e	3KR4	0	0.73
3e	1QNG	1	0.31
4e	3C02	1	0.35
5e	3IHZ	0	0.81
6e	1RT9	0	0.81
7e	1RSZ	0	0.74
8e	1CEQ	0	0.91
1e	1CET	0	0.95
2e	2RJI	0	0.86
3e	1LDG	0	0.97
4e	1T25	0	0.99
5e	1T2E	0	1.00

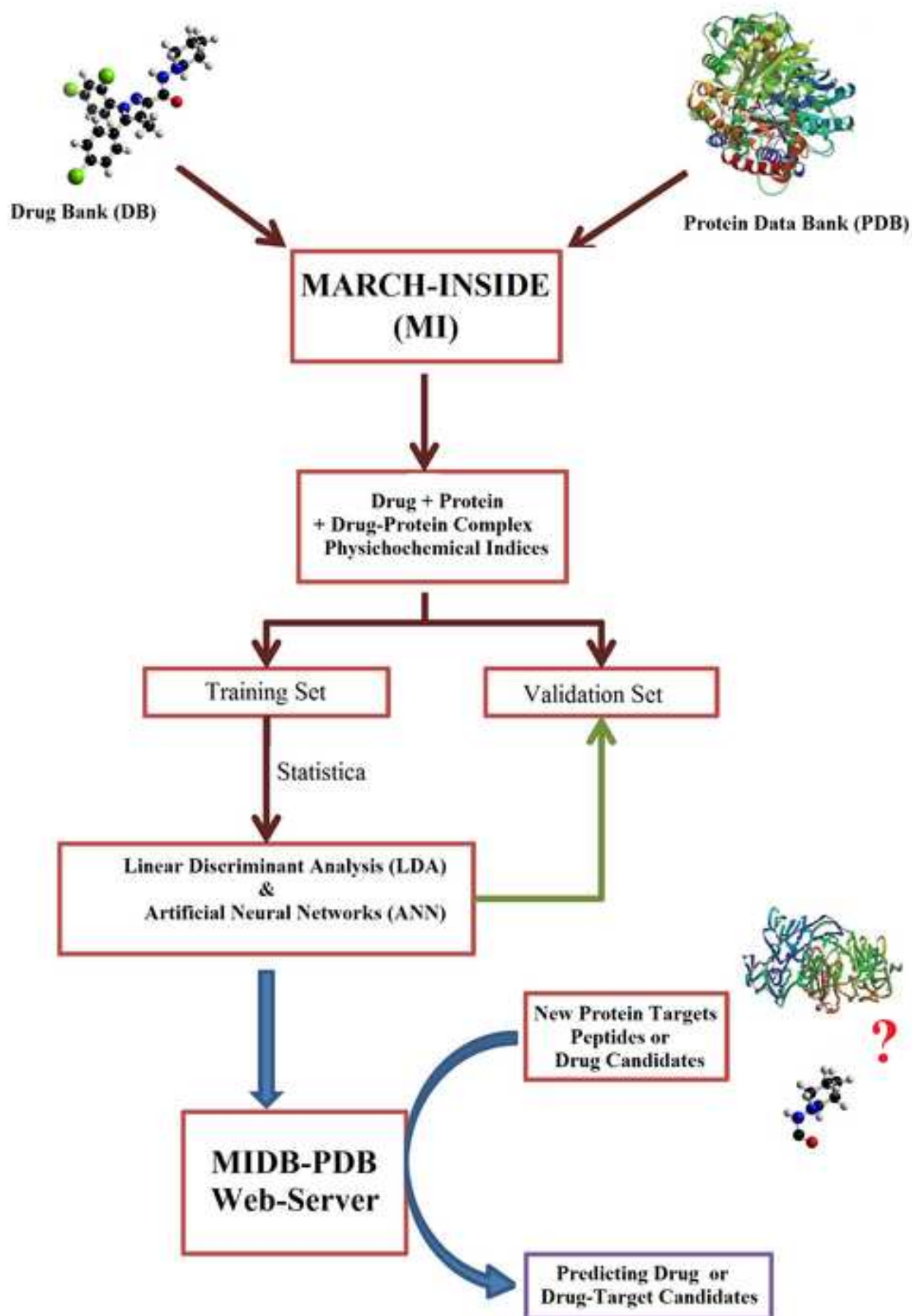
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8e	1T26	0	1.00
1e	1YVB	0	1.00
2e	3MMR	0	0.82
3e	3EWC	1	0.27
4e	1QNH	1	0.30
5e	3EWD	1	0.63
6e	2VFA	0	0.75
7e	1VYQ	0	0.74
8e	3GEP	0	0.85
1e	3GGJ	0	0.91
2e	1OKT	1	0.68
3e	2AAW	1	0.33
4e	2VFE	1	0.37
5e	2VFI	0	0.74
6e	2VFF	0	0.76
7e	2VFH	1	0.68
8e	2VFD	0	0.85
1e	3LSY	0	1.00
2e	1NHW	0	0.87
3e	1NHG	1	0.32
4e	1VRW	1	0.46
5e	1NNU	0	0.79
6e	2NQ8	0	0.81
7e	1ZW1	0	0.75
8e	1ZXB	0	0.89
1e	1ZXL	0	1.00
2e	1ZSN	0	0.84
3e	3LT2	0	1.00
4e	2FOI	1	0.46
5e	3LT1	0	1.00
6e	3LT4	0	1.00
7e	3LT0	0	1.00
8e	1T2D	0	0.90
1e	2ANL	0	0.85
2e	1MIQ	0	0.98
3e	2PSS	1	0.24
4e	1ONF	1	0.42
5e	2PT9	0	0.73
6e	2GHU	0	0.74
7e	2Z8W	1	0.31
8e	2Z8V	1	0.45
1e	1CJB	0	0.93
2e	2VFG	0	0.79
3e	3F4B	1	0.32
4e	1J3J	1	0.44
5e	1J3I	0	0.81
6e	1J3K	0	1.00

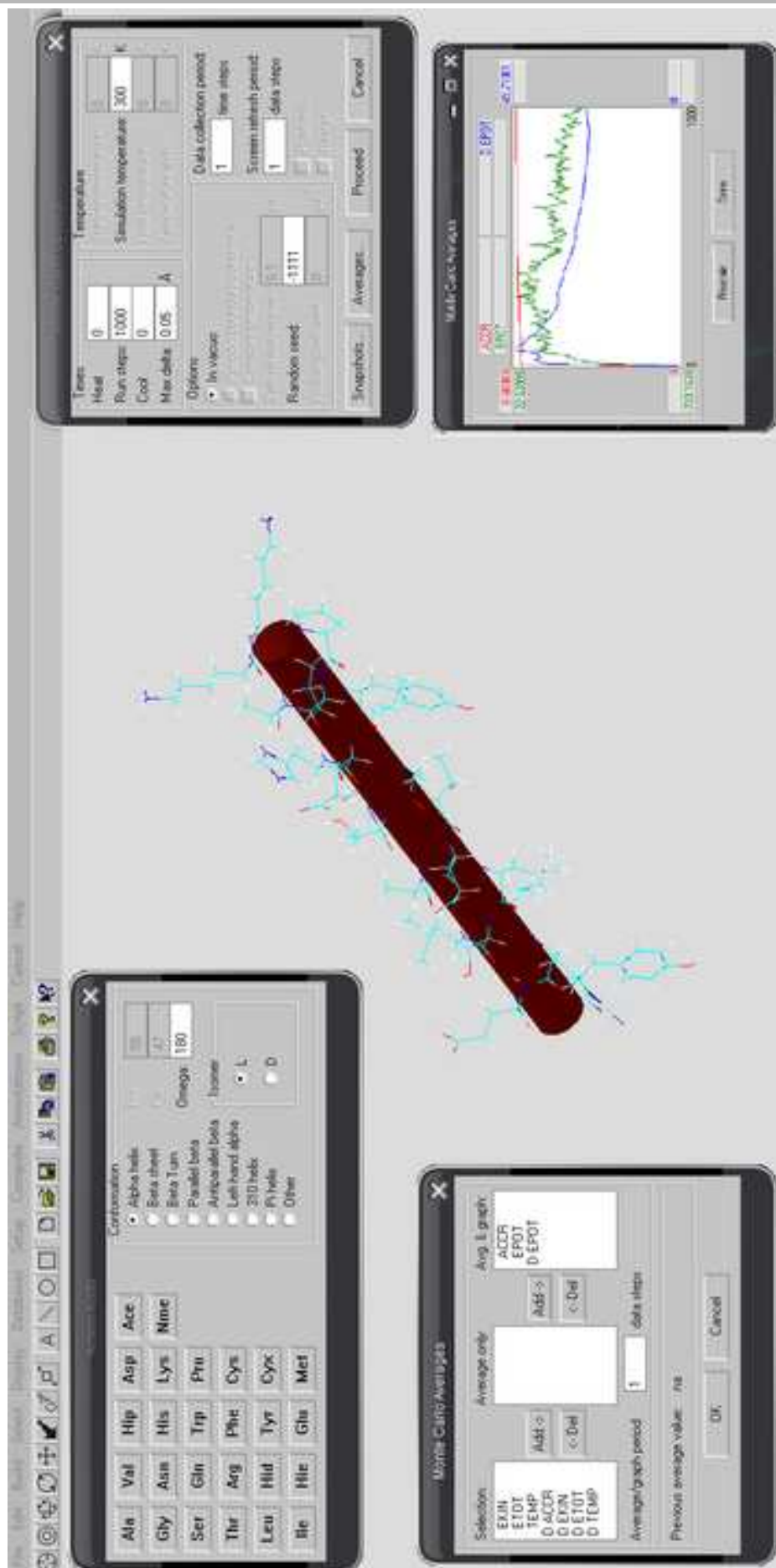
7e	1T2F	0	0.72
8e	1YXE	0	0.85
1e	3KQX	0	0.90
2e	3KQZ	0	0.84
3e	3KR5	1	0.20
4e	3KR4	1	0.25
5e	1QNG	0	0.80
6e	3C02	0	0.75
7e	3IHZ	0	0.76
8e	1RT9	0	0.88
1e	1RSZ	0	0.93
2e	1CEQ	0	0.90
3e	1CET	1	0.38
4e	2RJI	1	0.41
5e	1LDG	0	1.00
6e	1T25	0	1.00
7e	1T2E	0	1.00
8e	1T24	0	1.00
1e	1T2C	0	1.00
2e	1T26	0	1.00
3e	1YVB	0	0.89
4e	3MMR	1	0.35
5e	3EWC	0	0.76
6e	1QNH	0	0.71
7e	3EWD	1	0.57
8e	2VFA	0	0.84
1e	1VYQ	0	0.93
2e	3GEP	0	0.83
3e	3GGJ	1	0.25
4e	1OKT	1	0.17
5e	2AAW	0	0.82
6e	2VFE	0	0.76
7e	2VFI	1	0.68
8e	2VFF	0	0.84
1e	2VFH	0	0.91
2e	2VFD	0	0.83
3e	3LSY	0	1.00
4e	1NHW	1	0.45
5e	1NHG	0	0.81
6e	1VRW	0	0.82
7e	1NNU	0	0.74
8e	2NQ8	0	0.88
1e	1ZW1	0	0.93
2e	1ZXB	0	0.88
3e	1ZXL	0	1.00
4e	1ZSN	1	0.38
5e	3LT2	0	1.00
6e	2FOI	0	0.82
7e	3LT1	0	1.00

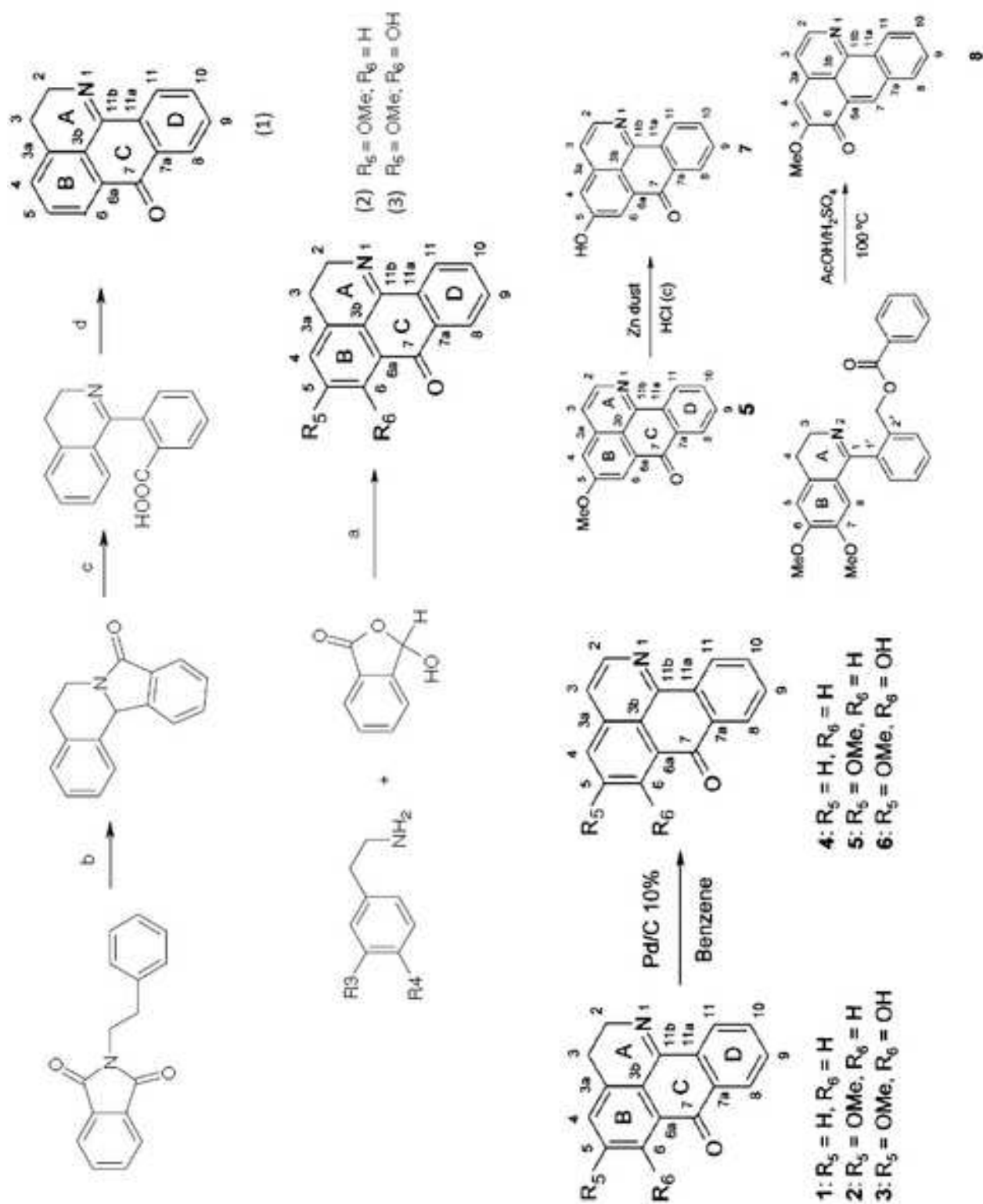
8e	3LT4	0	1.00
1e	3LT0	0	1.00
2e	1T2D	0	0.88
3e	2ANL	1	0.18
4e	1MIQ	0	0.85
5e	2PSS	0	0.73
6e	1ONF	0	0.80
7e	2PT9	1	0.67
8e	2GHU	0	0.83
1e	2Z8W	1	0.57
2e	2Z8V	1	0.43
3e	1CJB	1	0.30
4e	2VFG	1	0.32
5e	3F4B	0	0.81
6e	1J3J	0	0.82
7e	1J3I	0	0.76
8e	1J3K	0	1.00
1e	1T2F	0	0.92
2e	1YXE	0	0.83
3e	3KQX	1	0.23
4e	3KQZ	1	0.40
5e	3KR5	1	0.68
6e	3KR4	1	0.65
7e	1QNG	0	0.75
8e	3C02	0	0.84
1e	3IHZ	0	0.93
2e	1RT9	0	0.86
3e	1RSZ	1	0.29
4e	1CEQ	1	0.54
5e	1CET	0	0.84
6e	2RJI	0	0.80
7e	1LDG	0	1.00
8e	1T25	0	1.00
1e	1T2E	0	1.00
2e	1T24	0	1.00
3e	1T2C	0	0.97
4e	1T26	0	0.99
5e	1YVB	0	0.99
6e	3MMR	0	0.75
7e	3EWC	0	0.71
8e	1QNH	0	0.80
1e	3EWD	0	0.84
2e	2VFA	0	0.82
3e	1VYQ	1	0.30
4e	3GEP	1	0.38
5e	3GGJ	0	0.75
6e	1OKT	1	0.63
7e	2AAW	0	0.77
8e	2VFE	0	0.85

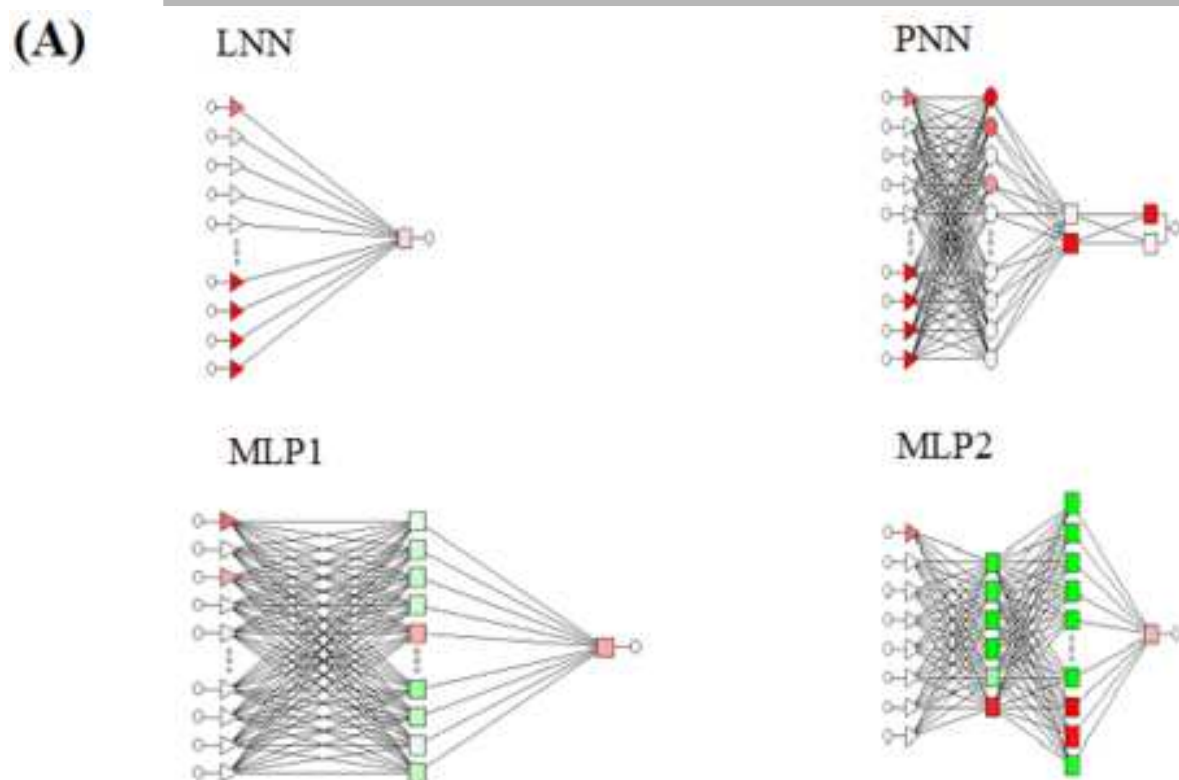
1e	2VFI	0	0.90
2e	2VFF	0	0.83
3e	2VFH	1	0.25
4e	2VFD	1	0.37
5e	3LSY	0	1.00
6e	1NHW	0	0.82
7e	1NHG	0	0.75
8e	1VRW	0	0.89
1e	1NNU	0	0.93
2e	2NQ8	0	0.87
3e	1ZW1	1	0.32
4e	1ZXB	1	0.46
5e	1ZXL	0	1.00
6e	1ZSN	0	0.77
7e	3LT2	0	1.00
8e	2FOI	0	0.89
1e	3LT1	0	1.00
2e	3LT4	0	1.00
3e	3LT0	0	1.00
4e	1T2D	1	0.47
5e	2ANL	1	0.65
6e	1MIQ	0	0.97
7e	2PSS	1	0.67
8e	1ONF	0	0.87
1e	2PT9	0	0.90
2e	2GHU	0	0.81
3e	2Z8W	1	0.07
4e	2Z8V	1	0.09
5e	1CJB	0	0.79
6e	2VFG	0	0.72
7e	3F4B	0	0.76
8e	1J3J	0	0.88
1e	1J3I	0	0.94
2e	1J3K	0	1.00
3e	1T2F	1	0.29
4e	1YXE	1	0.37
5e	3KQX	0	0.73
6e	3KQZ	0	0.78
7e	3KR5	1	0.62
8e	3KR4	0	0.76

OC=observed class, PC=predicted class, PRO=Probability.

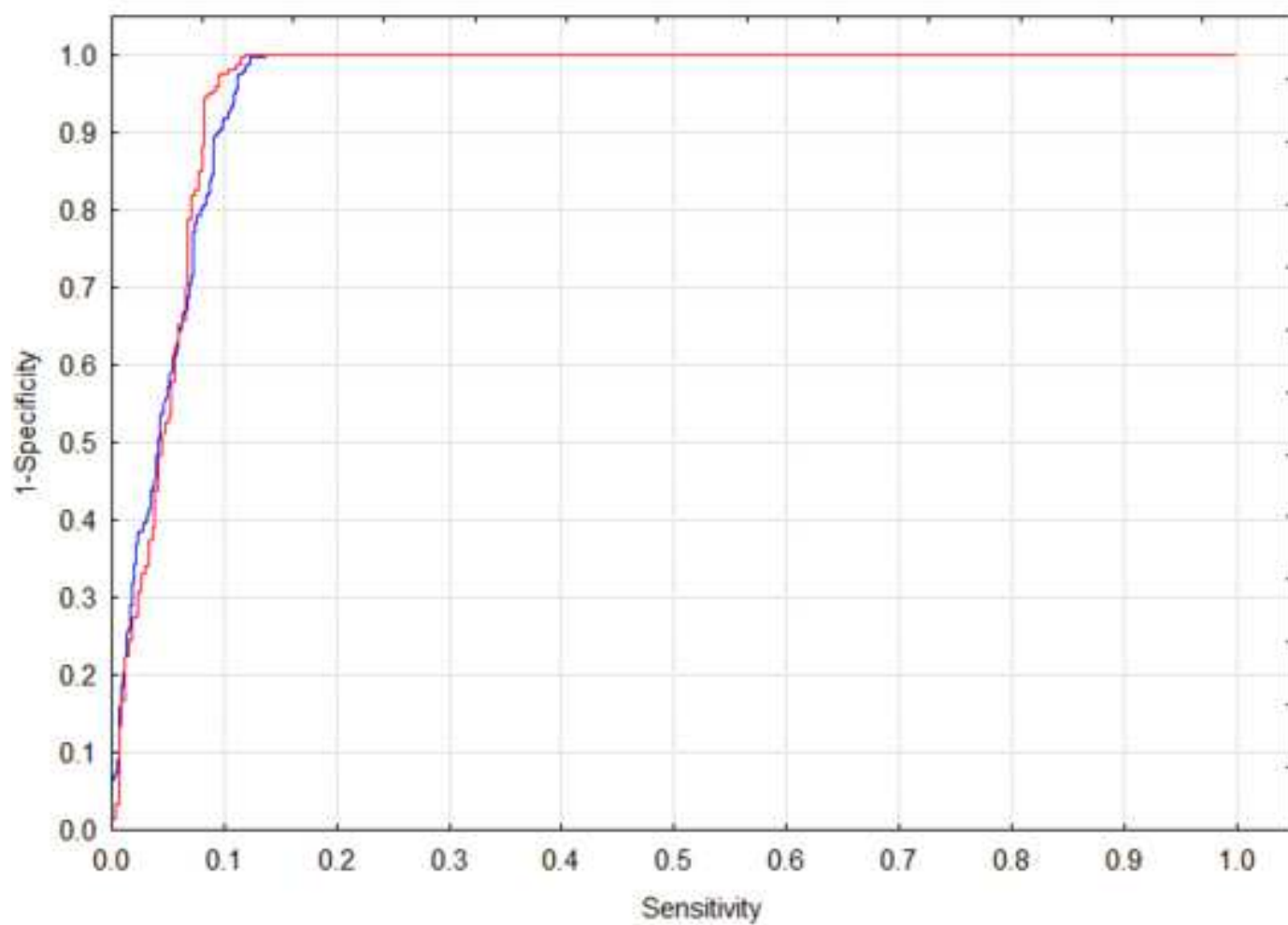


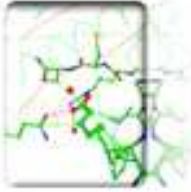






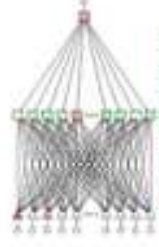
(B) ROC curve





MIND-BEST
MARCH-INSIDE Nested Drug-Bank Exploration & Screening Tool

Tool: MARCH-INSIDE (PY)
Data: RCSB PDB



MLP 20:20-15-11
Test Accuracy = 91.30%
(Training Accuracy = 90.41%)
Programmed by Prado-Prado F. & González-Díaz M.

(A)

Please choose drug and protein names to add to the calculation lists (maximum 10)

Mode 1: Drugs - Standard PDBs

Input drug names:
(Drug name|TAB|SMILE formula)

```

ESR000000
OC1=C2C(=C(C=C2)O)C(=O)C=C1
B1C00001 C=C3 C (O) (CC) C (H) OC4
B100000000 C=C3 C (H) OC1OC (C) C=C2=C(O) C (O) OC
(H) (O) C12
                    
```

Get Model FDA-approved Drugs*
(use Copy-Paste)

Predict*

* access on demand

(B)

Mode 2: Drugs - HyperChem ENT file

Input drug names:
(Drug name|TAB|SMILE formula)

```

ESR000000
OC1=C2C(=C(C=C2)O)C(=O)C=C1
OC1=C(O) (CC) C (H) OC4
B100000000 C=C3 C (H) OC1OC (C) C=C2=C(O) C (O) OC
(H) (O) C12
                    
```

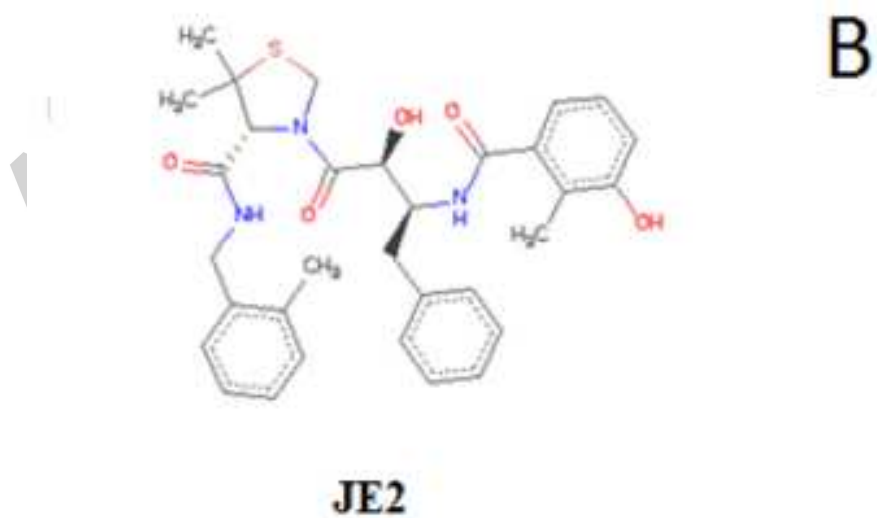
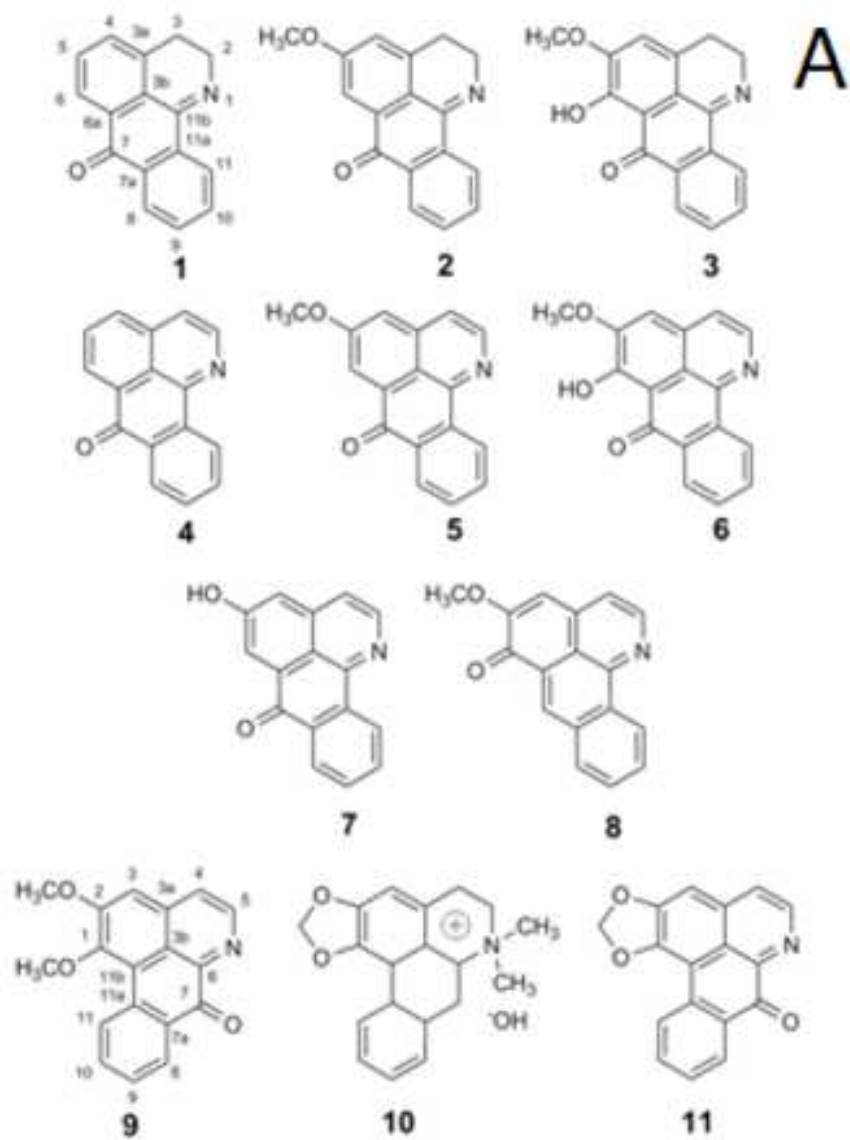
Get Model FDA-approved Drugs*
(use Copy-Paste)

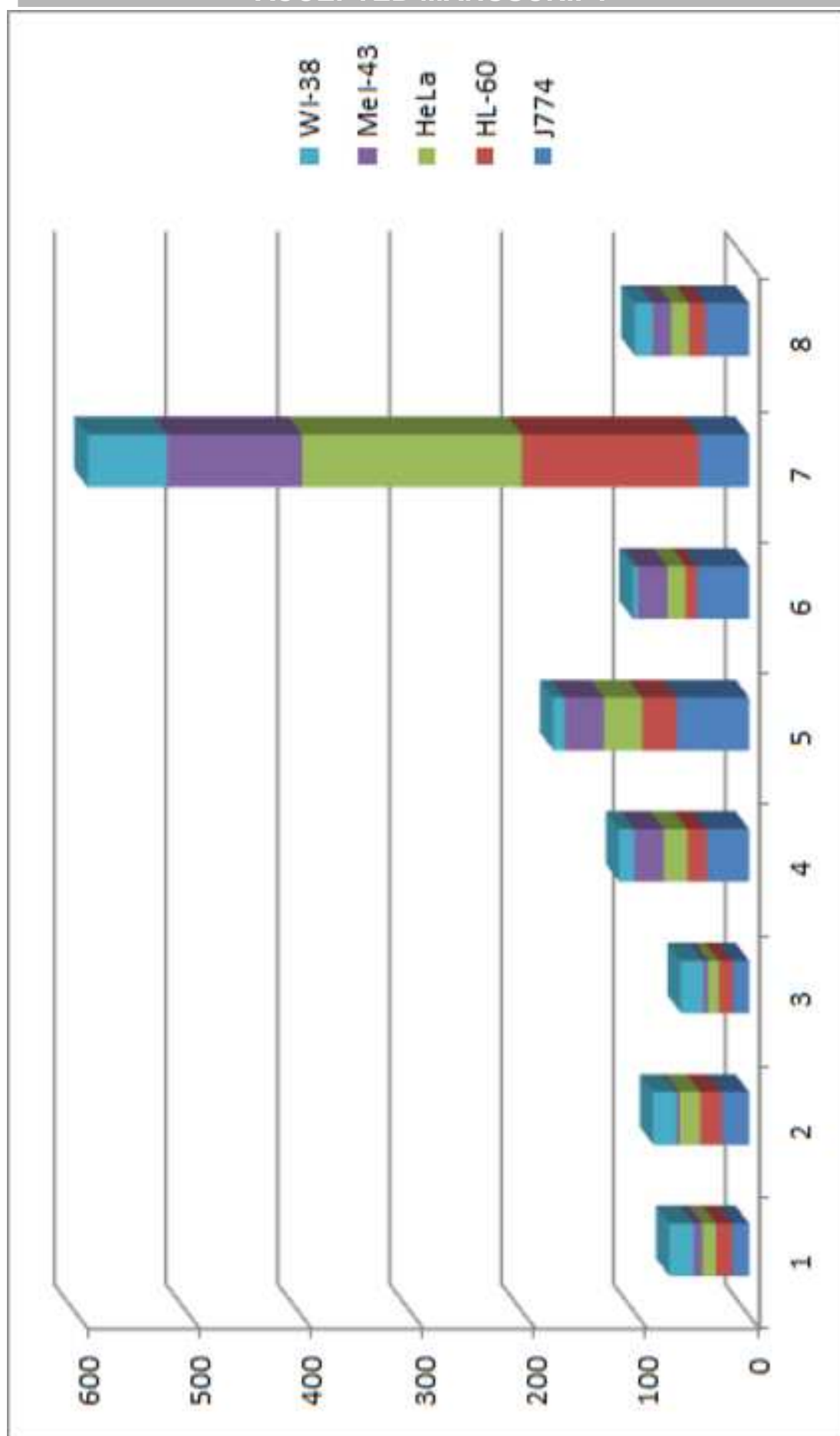
Upload*

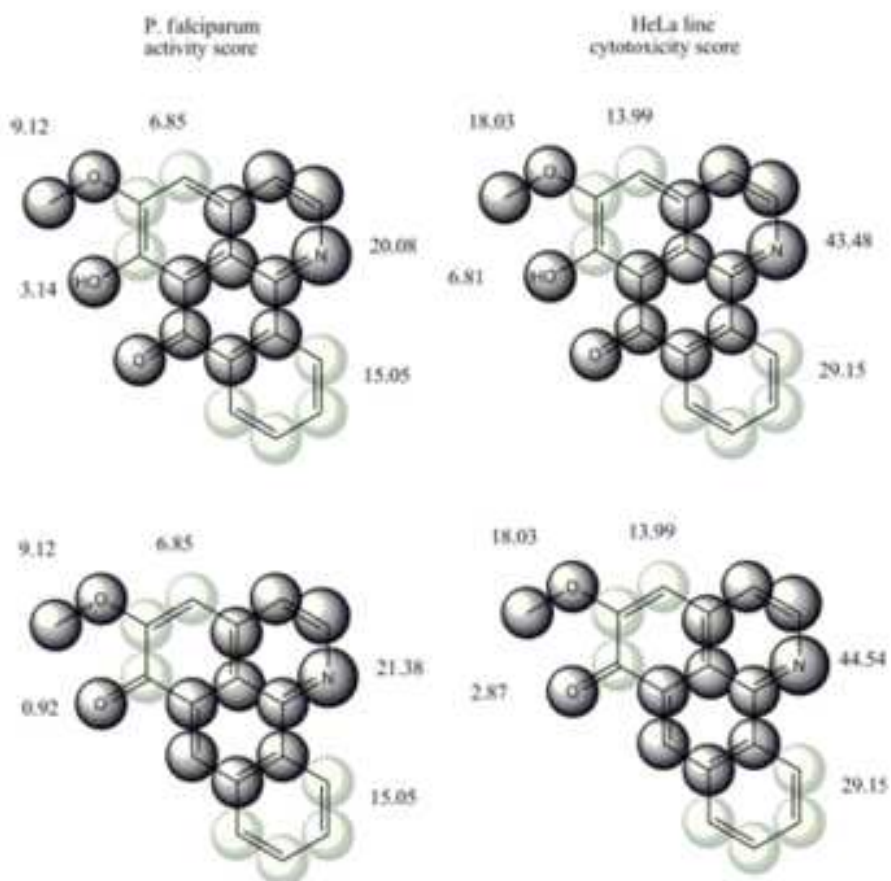
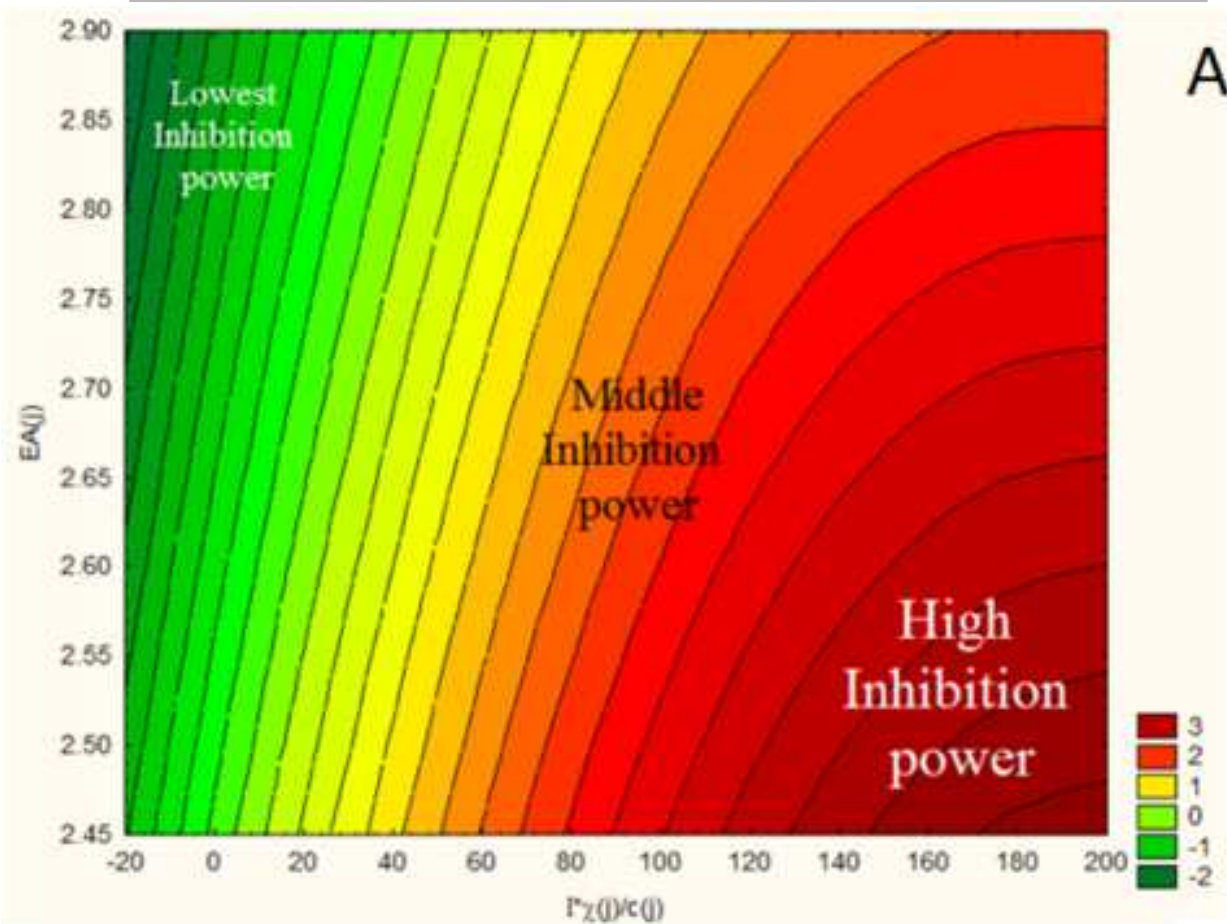
* access on demand

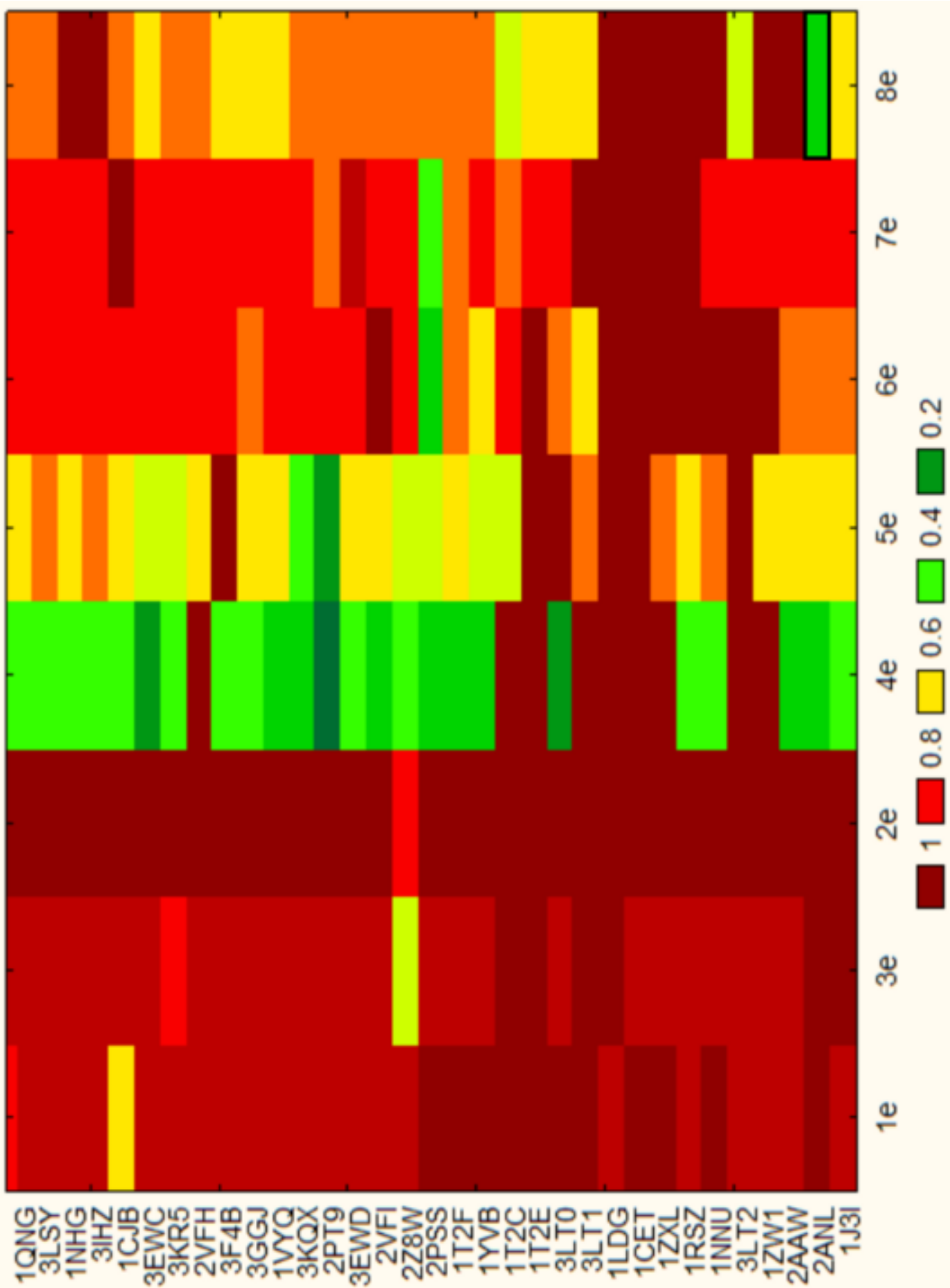
Upload & evaluate one ENT file created with HyperChem MM/MD algorithms (max. 2MB)

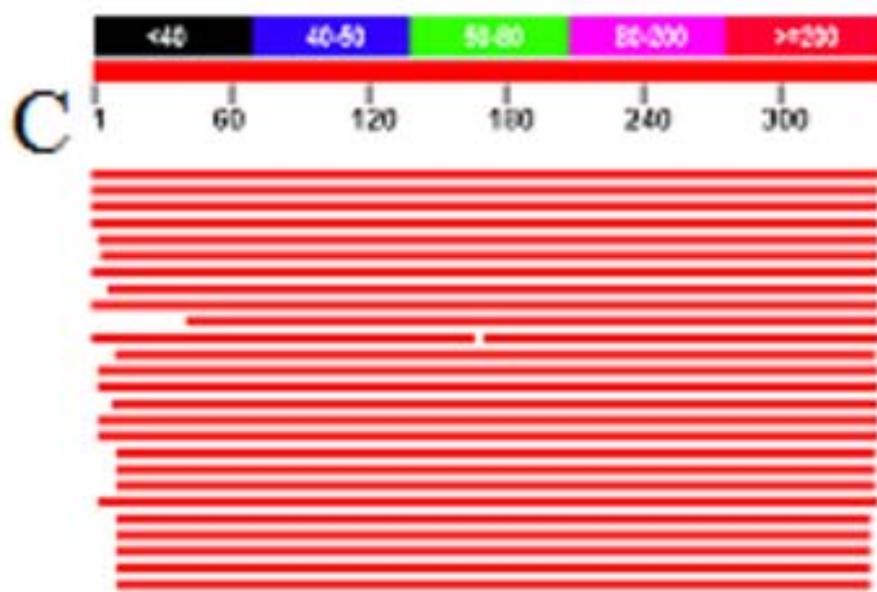
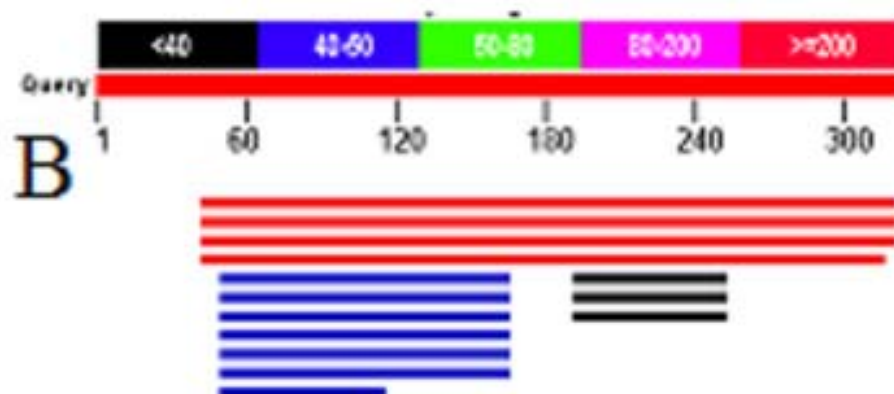
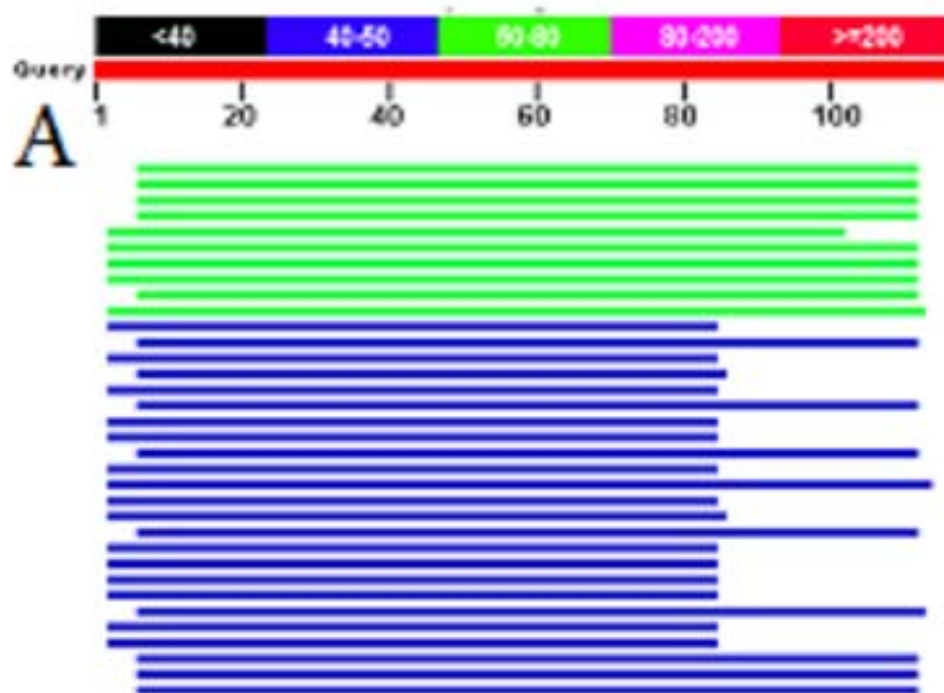
ENT file:

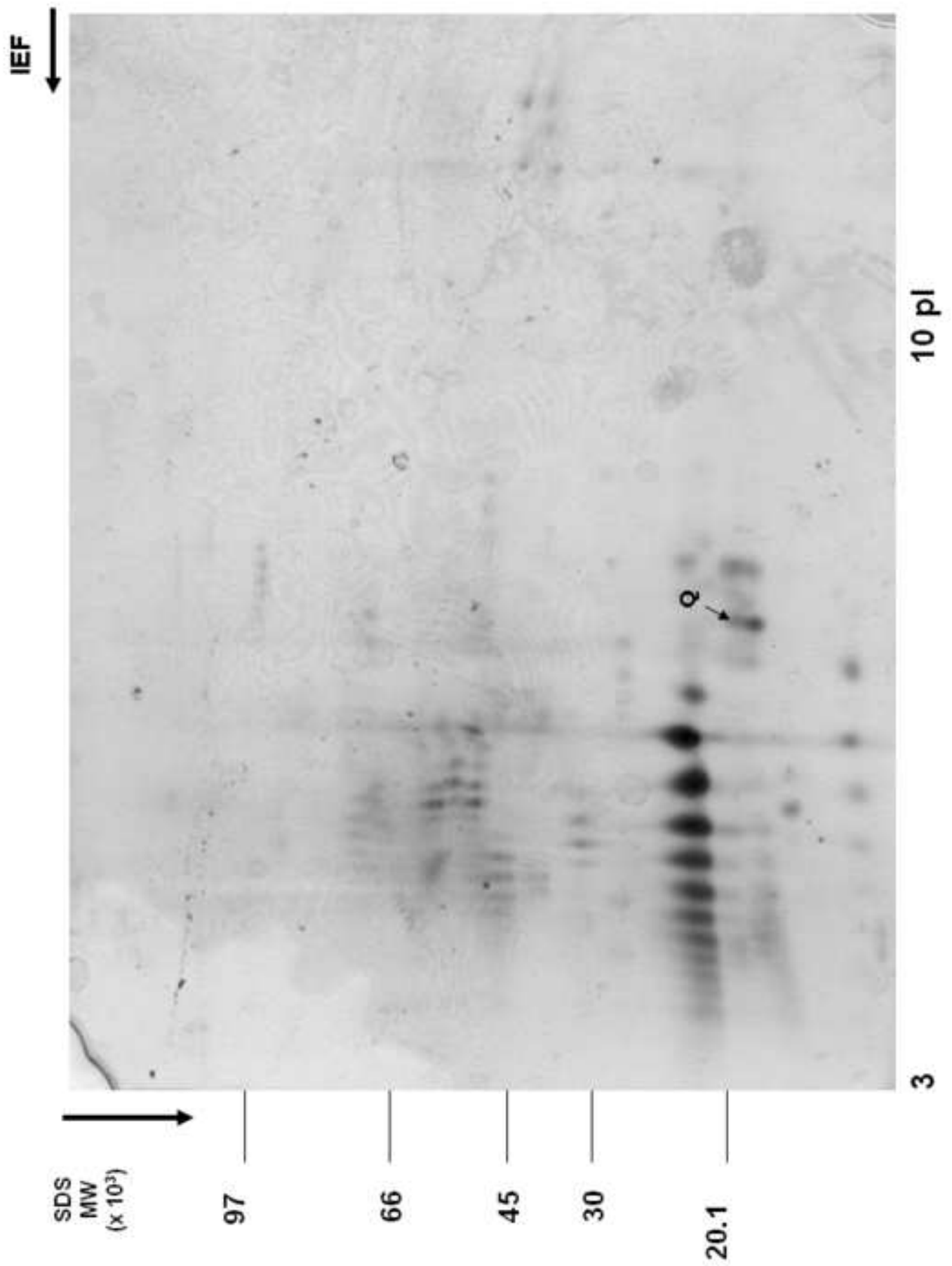




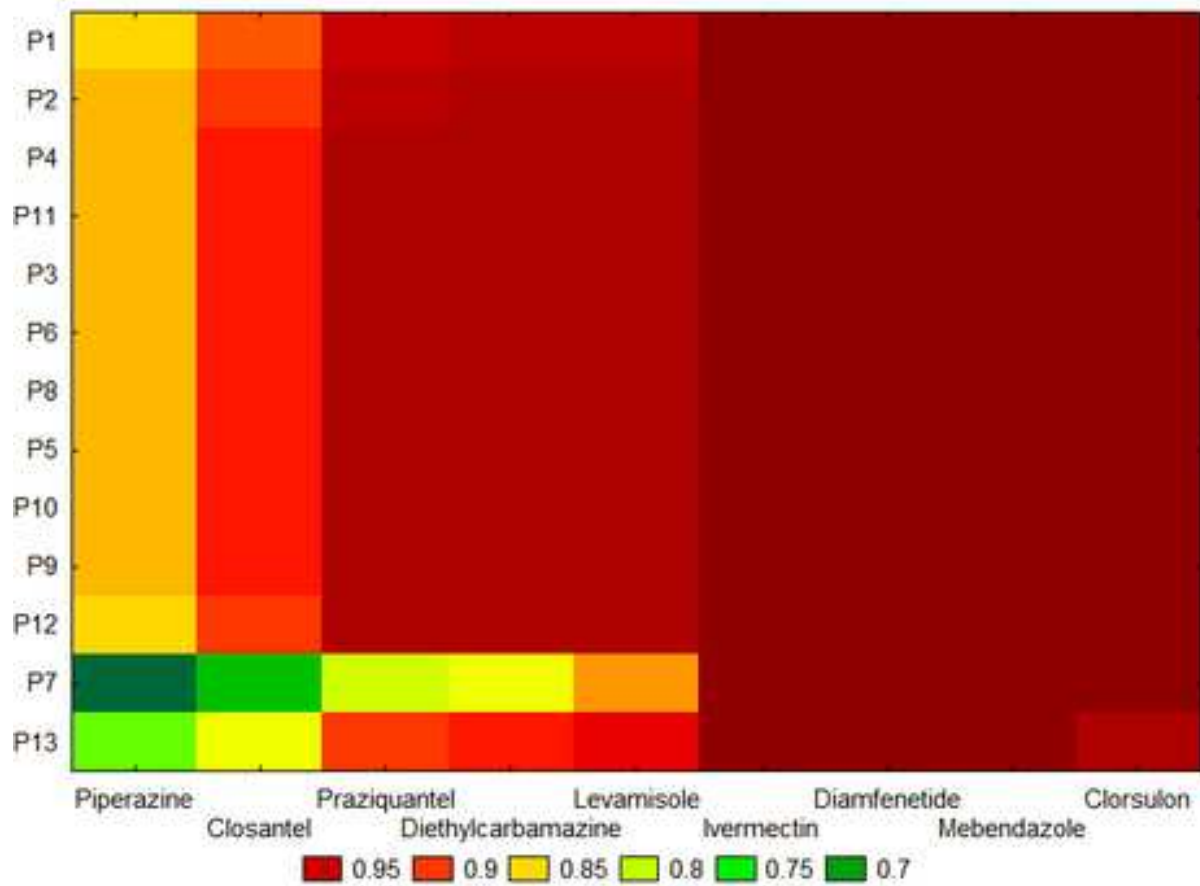








(A)



(B)

