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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 based 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 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-isoporphine 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; Gonzalez-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 electronegativities $\chi(G)$ (Santana et al., 2006b; Santana et al., 2008) values.

$$\chi(G) = \sum_{j=1}^{n} p_{i}(\chi_{j}) \cdot \chi_{j}$$ (1)

It is possible to consider isolated atoms ($k = 0$) in the estimation of the molecular properties $\chi(G)$. In this case the probabilities $p_{i}(\chi_{j})$ 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 $p_{i}(\chi_{j})$ 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 electronegativities $\chi(G)$ values:

$$\chi(G) = [p_{i}(\chi_{1}) \cdot p_{i}(\chi_{2}) \cdots p_{i}(\chi_{m})] = \sum_{j=1}^{n} p_{i}(\chi_{j}) \cdot \chi_{j}$$ (2)
Where, from left to right, the first term is $k/g_{302}$, which is the average molecular polarizability of the molecule considering the effects of all the atoms placed at distance $k$ over every atomic polarizability $/g_302$. The vector on the left-hand side of the equation contains the probabilities $0p(/g_{548})$ 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 $0p(/g_{548})$ and $1p_{ij}$ are easily calculated from atomic electronegativities ($/g_{548}$) and the chemical bonding information:

$$0p_{ij} = \frac{X_j}{\sum_k X_k} \quad (3) \quad 1p_{ij} = \frac{\delta_{ij} \cdot X_j}{\sum_k \delta_{ik} \cdot X_k} \quad (4)$$

The only difference is that in the probabilities $0p(/g_{548})$ 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 $\delta_{ij}$. 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 $\xi_k$ and HINT Potentials $\mu_k$; 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):

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

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 ($r_{ij} = k \cdot r_{cut-off}$). 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 $R_j$ in the protein structure. However, for the sake of simplicity, a truncation or cut-off function $\alpha_{ij}$ 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 $r_{ij} < r_{cut-off}$). Otherwise, the interaction is banished ($\alpha_{ij} = 0$). The relationship $\alpha_{ij}$ may be visualized in the form of a protein structure complex network. In this network the nodes are the $C_{o}$ 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 $r_j = (x, y, z)$ coordinates of the $C_{o}$ 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 \( r_{\text{max}} \) 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 \( r_{\text{max}} \)). Consequently, we can calculate different \( \alpha_k \) and \( \mu_k \) 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) \( \times \) 5regions \( \times \) 6(higher order considered) = 30 \( (\alpha_k \text{ values}) = 30 \) 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:

\[
S_{\text{DTP}} = \sum_{k=0}^{5} b(G_k) \chi(G) + \sum_{k=0}^{5} b(R_k) \xi(R) + b \quad (6)
\]

We can used 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. \( S_{\text{DTP}} \) 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 \( S_{\text{DTP}} \) 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; Rodríguez-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 ISM 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 (\( \mu \)), absolute hardness (\( \eta \)), electron affinity (EA), and electrophilicity (\( \omega \)) are well defined quantities that conveniently rationalize
molecular reactivity and chemical bonding (Parr et al., 1978). The electronic chemical potential $\mu$ is the natural descriptor of the direction of charge transfer during a chemical interaction (Parr and Pearson, 1983). The descriptor $\eta$ is related to the resistance of the system to charge transfer. A good approximation based on Koopman’s theorem allows $\mu$ and $\eta$ 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):

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

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

In where $\varepsilon_L$ and $\varepsilon_H$ are the energies of the LUMO and HOMO levels, respectively. The link with classical structural chemistry is achieved by making $\mu = -\chi$, where $\chi$ 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 $\chi$ and EA widely used according to Eqs. 3 and 4:

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

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

Recently the global $\omega$ 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 $\omega$ 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, $\chi$, and global $\omega$ 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, $\varepsilon_L$ and $\varepsilon_H$, respectively (Parr et al., 1989). With these quantities at hand, $\chi$ and $\omega$ 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 \( r_{in} = 15 \) Å and \( r_{out} = 17 \) Å. 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 \( r_{out} = 17 \) Å (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 \textit{vacuo} at 300 K and 1000 optimization steps, thus obtaining MDTs with 100 potential energy \( E_j \) (\( j = 1, 2, 3, \ldots, 100 \)) 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, \( \Delta r \), is the maximum allowed atomic displacement used in the generation of trial configurations. The default value of \( r \) in HyperChem is 0.05 Å (Froimowitz, 1993). For most organic molecules, this will result in an ACCR of about 0.5 Å, 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 reported\(^{11-14}\). 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 μg/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% \( \text{CO}_2 \) 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 deshydrogenases in viable cells.\(^{44}\) The cell lines 5000 HeLa, Gal-43, WI-38 and J-774 (adherent cells) in 200μl medium were seeded in each well of 96-well plates. Cells were first incubated 24h, then, the medium was removed and replaced by 200μl/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 100μl of DMEM.
(without serum) containing 10µl of MTT (3mg/ml in PBS). After 5 min in the incubator, the medium containing MTT was removed, and 100µl of DMSO were added to each well.

The samples for line HL-60 at 50000 cells (non-adherent cells) in 100µl medium were seeded in each well of 96-well plates. A volume of 100µl 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 10µl MTT (5mg/ml in PBS) added to each well. After 2h in the incubator, the reaction was stopped by adding 100µl of 0.04M HCl in 2-propanol. 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 3.1µg/ml to 100µg/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 ± 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 Jensen with modifications described by Benoit et al. (1995). The cultures were synchronized every 48 h by 5% D-sorbitol lysis (Merck, Darmstadt, Germany). The FcB1-Columbia strain was considered as chloroquine-resistant strain (chloroquine IC50: 145 nM). In vitro antimalarial activity testing was performed by [3H]-hypoxanthine incorporation as described by Desjardins et al. (1979) with modifications.

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 µl of rehidratation 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 distained 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 3 mg/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 65:65-4086-2-2:1has 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 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 the other models have 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 $k^G(G)_{\text{query}}$ 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 $k^R(R)_{\text{query}}$ for each query protein. MIND-BEST have also an internal database with all information related to names, DB codes, PDB code, $k^G(G)_{\text{FDA}}$, $k^R(R)_{\text{FDA}}$ 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/chembldb/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 $k^G(G)$ values of the $i^{th}$ query drugs $k^G(G)_{\text{query}}$ and $s^{th}$ FDA approved drugs $k^G(G)_{\text{FDA}}$. The server use a similar procedure to calculate protein-protein similarity $P_{\text{F-Q}}$ 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 $P_{\text{F-Q}}$ scores. Last, and based on the same idea this server determines similarity between $r^{th} + u^{th}$ DTPs in query list vs. $s^{th}$ and $v^{th}$ DTPs in FDA list using a DTP-DTP similarity score $D_{\text{F-D}}$. For pairs already present in FDA list $D_{\text{F-D}}(\%) = 100$ % 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.

$$\text{DDS}_{\text{F-Q}}(\%) = 100 \times \frac{\sum [ k^G(G)_{\text{F}} - k^G(G)_{\text{Q}} ]}{\sum k^G(G)_{\text{Q}}}$$ (12)

$$\text{PPS}_{\text{F-Q}}(\%) = 100 \times \frac{\sum [ k^R(R)_{\text{F}} - k^R(R)_{\text{Q}} ]}{\sum k^R(R)_{\text{Q}}}$$ (13)
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 \( S_{\text{pred}} \) 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 \( S_{\text{pred}} \) 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 \( \mu \)M)(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.
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 IC₅₀ values of the eight compounds and chloroquine are listed in Table 4.

Table 4 comes about here

Compound 8 exhibited the strongest antiplasmodial activity (IC₅₀ = 1.45 μM), whereas 5 exhibited a lower activity (IC₅₀ ~ 10 μM), 2, 4 and 6 had a moderate effect (IC₅₀ ~ 50μM) and 1, 3 and 7 possessed a very low activity (IC₅₀ > 80 μM). 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 (IC₅₀ = 0.58 μM, INDO, chloroquine resistant strain of P. falciparum)(Munoz et al., 1999). In addition, liriodenine (11), an oxoaporphine alkaloid was found to be active against P. falciparum (IC₅₀ = 25.1 μM, 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 (IC₅₀ = 189.2 μM, 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:

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

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

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 $I(L) = (active\ compounds)/(total\ compounds)$ 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 $\chi$. 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 $\chi$ 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 $c = 1.6 \mu g/mL$ 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 $\omega$ 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, $\chi$
and \( \rho \) 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 o xoaporphine 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 x 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 McL-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 Plasmspein 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 1 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.

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.

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 (Ms) 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 $\xi_k$ and $\mu_k$ 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 $\xi_k$ and $\mu_k$ 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 $\alpha$-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 $\xi_k$ and $\mu_k$ 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 $\beta$-Tubulin (in nematodes, cestodes and trematodes) (Roos et al., 1995).
8. Clorsulon, target Phosphoglycerate kinase and mutase (Schulman et al., 1982).

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 server 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 (Agüero-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.
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


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.


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$_{50}$ (μM) of oxoisoaporphine derivatives 1-8.

**Figure 8.** (A) Map of multivariate relationships between drug cellular inhibition and the electronic properties (EA) and $\chi$. (B) Back-projection maps for 6 and 8 at c = 1.6 μg/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
## Tables

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

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DTPs: Drug-Target Pairs for compounds with high affinity; nDTPs: Drug-Target Pair for compounds with non-affinity.
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<sup>a</sup> Structural Indices: Drugs Total or Group Electronegativity (χ), Protein Total or Region Electrostatic Potential (ξ), Similarity (S), Gibbs Free energy (∆G), Physicochemical 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).<sup>b</sup> Dimension of the structures parameters: 1D-structure, 2D-Structure and 3D structure;<sup>c</sup> Types of drug targets: prot. (all types of proteins), MR (Membrane Receptor protein), Enz. (Enzymes).<sup>d</sup> Method: MARCH-INSIDE (MI), Bipartite Local Model (BLM), Drug-Target Likeness (DTL), pKa values for protein ligand complexes (PROPKA), comparative interaction fingerprint analysis (ColIFA), Negative Training Data (NTD), Ligand-Based drug design (LBDD), Quantum Mechanics (QM), Molecular Mechanics + Generalized Born Surface Area theory (GBSA).<sup>e</sup> N- Number of cases used to seek the model.<sup>f</sup> Nv- Number of variables in the model.<sup>g</sup> 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).<sup>h</sup> Accuracy (Ac).<sup>i</sup> Parameter used in the accuracy. * This work.
Table 3. Cytotoxic activities IC$_{50}$ (μM) of oxoisoaporphine derivatives 1-8 upon several cell lines

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Table 4. Antiplasmodial activities of 1 – 8.

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<td>2</td>
<td>51.78 ± 5.37</td>
</tr>
<tr>
<td>3</td>
<td>82.35 ± 12.66</td>
</tr>
<tr>
<td>4</td>
<td>59.38 ± 2.45</td>
</tr>
<tr>
<td>5</td>
<td>10.62 ± 2.77</td>
</tr>
<tr>
<td>6</td>
<td>44.96 ± 7.65</td>
</tr>
<tr>
<td>7</td>
<td>93.13 ± 11.69</td>
</tr>
<tr>
<td>8$^c$</td>
<td>1.45 ± 0.56</td>
</tr>
<tr>
<td>CQ$^c$</td>
<td>0.097</td>
</tr>
</tbody>
</table>

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

$^b$ Mean ± S.D.

$^c$ CQ, chloroquine; positive control for *Plasmodium falciparum* inhibition.
<table>
<thead>
<tr>
<th>Parameter</th>
<th>%</th>
<th>class</th>
<th>low</th>
<th>high</th>
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<td><strong>Training series</strong></td>
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<td></td>
<td></td>
<td></td>
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<tr>
<td>Sensitivity</td>
<td>73.7</td>
<td>low</td>
<td>87</td>
<td>31</td>
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<tr>
<td>Specificity</td>
<td>76.7</td>
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<tr>
<td>Accuracy</td>
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<td></td>
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<tr>
<td><strong>Validation series</strong></td>
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<td></td>
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<tr>
<td>Sensitivity</td>
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<td>24</td>
<td>8</td>
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<td>Specificity</td>
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<td>high</td>
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<tr>
<td>Accuracy</td>
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</table>
Table 6. Non-interaction c-level values for 8 compounds vs. selected proteins of *P. falciparum*

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<tbody>
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<td></td>
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<td>3</td>
<td>4</td>
<td>5</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>1QNG</td>
<td>0.77</td>
<td>0.95</td>
<td>0.83</td>
<td>0.36</td>
<td>0.58</td>
<td>0.74</td>
<td>0.80</td>
<td>0.63</td>
</tr>
<tr>
<td>1LDG</td>
<td>0.89</td>
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<td>1.00</td>
<td>0.97</td>
<td>0.99</td>
<td>0.99</td>
<td>0.99</td>
<td>0.98</td>
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<tr>
<td>3EWC</td>
<td>0.86</td>
<td>0.94</td>
<td>0.81</td>
<td>0.18</td>
<td>0.50</td>
<td>0.74</td>
<td>0.74</td>
<td>0.58</td>
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<tr>
<td>2AAW</td>
<td>0.89</td>
<td>0.96</td>
<td>0.84</td>
<td>0.27</td>
<td>0.51</td>
<td>0.69</td>
<td>0.73</td>
<td>1.00</td>
</tr>
<tr>
<td>1NHG</td>
<td>0.90</td>
<td>0.95</td>
<td>0.88</td>
<td>0.33</td>
<td>0.59</td>
<td>0.76</td>
<td>0.79</td>
<td>1.00</td>
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<td>3LT2</td>
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<td>0.88</td>
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<td>1.00</td>
<td>1.00</td>
<td>0.79</td>
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<td>0.49</td>
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<td>0.76</td>
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<td>0.92</td>
<td>0.77</td>
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<td>0.50</td>
<td>0.76</td>
<td>0.78</td>
<td>0.62</td>
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<td>1CET</td>
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<td>0.97</td>
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<td>0.99</td>
<td>0.99</td>
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<td>1.00</td>
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<td>0.44</td>
<td>0.58</td>
<td>0.72</td>
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<td>0.51</td>
<td>0.69</td>
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<td>0.74</td>
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<td>0.64</td>
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<td>1.00</td>
<td>1.00</td>
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<td>0.99</td>
<td>0.26</td>
<td>0.57</td>
<td>0.68</td>
<td>0.71</td>
<td>0.21</td>
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<tr>
<td>1CJB</td>
<td>0.51</td>
<td>0.95</td>
<td>0.81</td>
<td>0.35</td>
<td>0.59</td>
<td>0.76</td>
<td>1.00</td>
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<tr>
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<td>0.76</td>
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<td>0.89</td>
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<td>0.99</td>
<td>0.99</td>
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<td>1.00</td>
<td>1.00</td>
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<td>0.50</td>
<td>0.71</td>
<td>0.68</td>
<td>0.46</td>
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</table>
Table 7. Comparative cytotoxicity table for aporphines compounds.

<table>
<thead>
<tr>
<th>Organism</th>
<th>Compound</th>
<th>2e</th>
<th>3e</th>
<th>6e</th>
<th>8e</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parasite</td>
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<td>51.78</td>
<td>82.35</td>
<td>44.96</td>
<td>1.45</td>
</tr>
<tr>
<td>PDB Parasite</td>
<td>2Z8W</td>
<td>2Z8W</td>
<td>2PSS</td>
<td>2ANL</td>
<td></td>
</tr>
<tr>
<td>Protein</td>
<td>AMA1</td>
<td>AMA 1</td>
<td>Spermidine synth</td>
<td>Plasmepsin IV</td>
<td></td>
</tr>
<tr>
<td>NL-MB Score</td>
<td>0.220574</td>
<td>0.270574</td>
<td>0.056099</td>
<td>0.205199</td>
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</tr>
<tr>
<td>BLAST Score</td>
<td>49.7</td>
<td>49.7</td>
<td>273</td>
<td>180</td>
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<tr>
<td>Human</td>
<td>Mel-43</td>
<td>2.7</td>
<td>4.7</td>
<td>26.3</td>
<td>16.4</td>
</tr>
<tr>
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<td>WI-38</td>
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<td>19.6</td>
<td>4.5</td>
<td>16</td>
</tr>
<tr>
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<td>2CD0</td>
<td>2005</td>
<td>3D91</td>
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<tr>
<td>Protein</td>
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<td>λ-6 Ig</td>
<td>Spermidine synth</td>
<td>Renin</td>
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<td>NL-MB Score</td>
<td>0.000024</td>
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</table>

AMA1 = Apical membrane antigen 1; λ-6 Ig = lambda-VI iminoglutuline; NL-MB = Non Linear Mind Best; Mel-43 and WI-38 are cancer cell lines.
Table 8. Top-20 template proteins in *G. lamblia* found by MASCOT search

<table>
<thead>
<tr>
<th>Protein</th>
<th>Accession</th>
<th>Mass</th>
<th>Score</th>
<th>Function</th>
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<tr>
<td>1</td>
<td>gi159116163</td>
<td>99431</td>
<td>421</td>
<td>Hypothetical protein GL50803_16507</td>
</tr>
<tr>
<td>2</td>
<td>gi121999104</td>
<td>89668</td>
<td>82</td>
<td>DNA topoisomerase III</td>
</tr>
<tr>
<td>3</td>
<td>gi83593171</td>
<td>46301</td>
<td>73</td>
<td>O-acetylserine sulfhydrylase</td>
</tr>
<tr>
<td>4</td>
<td>gi152970457</td>
<td>32953</td>
<td>72</td>
<td>putative transcriptional regulator (LysR family)</td>
</tr>
<tr>
<td>5</td>
<td>gi148256476</td>
<td>22222</td>
<td>67</td>
<td>hypothetical protein BBta</td>
</tr>
<tr>
<td>6</td>
<td>gi160878692</td>
<td>47367</td>
<td>65</td>
<td>GTP-binding protein HflX</td>
</tr>
<tr>
<td>7</td>
<td>gi19697420</td>
<td>11743</td>
<td>63</td>
<td>hypothetical protein Oryza sativa</td>
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<tr>
<td>8</td>
<td>gi66044158</td>
<td>46312</td>
<td>63</td>
<td>outer membrane porin syringae B728a]</td>
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<td>9</td>
<td>gi168003694</td>
<td>13992</td>
<td>62</td>
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<td>10</td>
<td>gi168017259</td>
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<td>gi116749322</td>
<td>109448</td>
<td>61</td>
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<td>12</td>
<td>gi1002271</td>
<td>11977</td>
<td>61</td>
<td>envelope glycoprotein, v3 region</td>
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<tr>
<td>13</td>
<td>gi116330615</td>
<td>19688</td>
<td>60</td>
<td>Transcriptional regulator</td>
</tr>
<tr>
<td>14</td>
<td>gi168048940</td>
<td>14081</td>
<td>60</td>
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<td>31855</td>
<td>59</td>
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<td>20</td>
<td>gi78048009</td>
<td>44141</td>
<td>59</td>
<td>filamentous phage Cf1c related protein</td>
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Table 9. MASCOT, MM/MD, and QSAR results for new peptides

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<th>Obs. Mr(expt)</th>
<th>Mr(calc)</th>
<th>δ</th>
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<tr>
<td>kataweyhealakt</td>
<td>965.5</td>
<td>964.5</td>
<td>0.0032</td>
</tr>
<tr>
<td>kdahslyvkpsffghfrl</td>
<td>2309.2</td>
<td>2308.2</td>
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<tr>
<td>kkppapyehlatdeaslslire</td>
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<td>2565.4</td>
<td>0.0073</td>
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<tr>
<td>kkppapyehlatdeaslslireky</td>
<td>1389.7</td>
<td>1388.7</td>
<td>-0.0004</td>
</tr>
<tr>
<td>k_sshgrlnsllsgdfyars</td>
<td>1908.0</td>
<td>1906.9</td>
<td>-0.002</td>
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<tr>
<td>ktgsvtfdlptsvry</td>
<td>1480.8</td>
<td>1479.8</td>
<td>0.0047</td>
</tr>
<tr>
<td>kvfglnpegdenlvflvdgrs</td>
<td>1260.6</td>
<td>1259.6</td>
<td>0.0033</td>
</tr>
<tr>
<td>kwadkyvystks</td>
<td>1879.9</td>
<td>1878.9</td>
<td>-0.0288</td>
</tr>
<tr>
<td>ratypissarg</td>
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<td>1354.7</td>
<td>0.0014</td>
</tr>
<tr>
<td>rfahqlfswdiktdwks</td>
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<td>2532.3</td>
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<td>rlnsllsgdfyars</td>
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<table>
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<th>E₁</th>
<th>E₀</th>
<th>Pred.</th>
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<tr>
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<td>45.71</td>
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<td>0</td>
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<td>47.92</td>
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</table>

* M/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.

<table>
<thead>
<tr>
<th>DB</th>
<th>Drug name</th>
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<th>Protein</th>
<th>OC</th>
<th>PC</th>
<th>Score</th>
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<tr>
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<td>Imatinib</td>
<td>1OPL</td>
<td>ABL1</td>
<td>1</td>
<td>1</td>
<td>0</td>
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<tr>
<td>DB00132</td>
<td>Alpha-Linolenic Acid</td>
<td>1FE3</td>
<td>FABP</td>
<td>1</td>
<td>1</td>
<td>0.15</td>
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<tr>
<td>DB00162</td>
<td>Vitamin A</td>
<td>1BI9</td>
<td>Aldehyde hydrogenase</td>
<td>1</td>
<td>1</td>
<td>0.08</td>
</tr>
<tr>
<td>DB00162</td>
<td>Vitamin A</td>
<td>1CRB</td>
<td>Retinol binding protein</td>
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<td>1</td>
<td>0.18</td>
</tr>
<tr>
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<td>Metalloprotease</td>
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<td>1</td>
<td>0.15</td>
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<td>1UZF</td>
<td>Metalloprotease</td>
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<td>1</td>
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<tr>
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<td>Gamma receptor</td>
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<td>1</td>
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OC=observed class, PC=predicted class, PRO=probability
**TABLE 2SM.** 2,3-dihydrooxoisoaporphine, oxoisoaporphine and oxoaporphine alkaloids Prediction results.

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OC~observed class, PC~predicted class, PRO~Probability.
MARCH-INSIDE (MI)

Drug + Protein + Drug-Protein Complex Physicochemical Indices

Training Set
Statistica
Linear Discriminant Analysis (LDA) & Artificial Neural Networks (ANN)

Validation Set

New Protein Targets Peptides or Drug Candidates

MIDB-PDB Web-Server

Predicting Drug or Drug-Target Candidates
(A) LNN, PNN, MLP1, MLP2

(B) ROC curve

1-Specificity

Sensitivity
Mode 1: Drugs - Standard PDBs

Input drug names

Get FDA-approved PDBs

Mode 2: Drugs - HyperChem ENT file

Input drug names

Get Model FDA-approved Drugs

Upload & evaluate obtained ENT file created with HyperChem V6.0 algorithm (max. 10)

Test Accuracy = 91.36%