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Conformational study of glycal-type neuraminidase inhibitors[‡]

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Conformational study of glycal-type neuraminidase inhibitors

The conformational flexibility of two glycal-type neuraminidase inhibitors has been studied, using several molecular modeling techniques. In agreement with the experimental data available, an intramolecular hydrogen bond, representing a key structural feature that controls the conformer distribution in solution, has been identified. The contribution of each substituent on the overall equilibrium was evaluated using simplified derivatives. Additionally, four methods for estimating NMR coupling constants from dihedral angles were evaluated and the Haasnoot method was found to be appropriate for this class of sugars. These results should allow a better understanding of the structural parameters governing physico-chemical properties of glycal-like compounds.

Keywords: molecular modeling; quantum chemistry; molecular dynamics; conformational analysis; neuraminidase inhibitors

Introduction

The Influenza neuraminidase (NA) enzyme is one of the validated targets against influenza viruses.^[1,2] Two NA inhibitors are currently present on the market, oseltamivir phosphate (Tamiflu[®])^[3] and zanamivir (Relenza[®]).^[4] However, resistance phenomena observed during the last few years, especially for Tamiflu[®],^[5-9] and the poor biodisponibility of Relenza[®] make research for novel anti-viral molecules a priority. In this context, we have been interested in the development and the synthesis of Relenza-type compounds modified at the C4 or C6 position.^[10-12] In this work, a combination of several molecular modeling techniques^[13] (conformational analysis, molecular dynamics and quantum chemistry calculations) has been used to obtain insight into the flexibility of two influenza neuraminidase inhibitors (Figure 1) previously described,^[10,14,15] presenting a scaffold similar to zanamivir. Glycal-type compounds are known to be conformationally flexible.^[16-26] With these systems the 3J values of the coupling constants in the $^1\text{H-NMR}$ spectra are often diagnostic of the

conformational equilibrium between the two ${}^6\text{H}_5$ ("all-equatorial") and ${}^5\text{H}_6$ ("all-axial") half-chair conformations. In our synthesis of zanamivir congeners,^[10] we were surprised by the value of the $J_{4,5}$ coupling constant at room temperature in **1** (4.5 Hz)^[10] compared to the same J value in Neu5Ac2en (DANA) **2** (8.5 Hz),^[14,15] since the two compounds only differ by the nature of the side chain at C6. Our aim of this study was to explain how the substituent change on C6 might be responsible for the differences observed experimentally in the NMR coupling constants.

Insert Figure 1 here

Materials and Methods

Conformational Analysis

Three-dimensional structures of the compounds used in this study were generated using CORINA software.^[27] The conformational analysis was carried out using MacroModel with the OPLS_2005 force field and the "Mixed torsional/Large-scale low-mode conformational sampling" procedure.^[28] This is a hybrid technique that combines broad Monte Carlo sampling of torsional space^[29] with local low frequency eigenvector sampling in the vicinity of the current conformation.^[30] After 500,000 steps using an energy window of 42 kJ/mol, a number of 1043 and 1176 unique conformers were obtained for compounds **1** and **2**, respectively.

Molecular Dynamics

Molecular dynamics simulations were performed using GROMACS 4.0.7 software package^[31] with the OPLS-AA force field.^[32,33] Force field topologies of compounds **1** and **2** were generated using an in-house developed script. The system was constructed by positioning the molecule in a cubic periodic box of TIP4P waters, with a minimum

distance of 1.0 nm on each side, then energy-minimized until convergence using a steepest descent algorithm to remove close contacts of water molecules with the solute. Molecular dynamics with position restraints on the solute atoms were then performed for 200 ps to relax the water molecules around the solute, followed by the production run of 250 ns. During the position restraints and production runs, the Parinello-Rahman method^[34] was used for pressure coupling, and the temperature was coupled using the Nosé-Hoover method^[35,36] at 300 K. Electrostatics were calculated with the particle mesh Ewald method.^[37,38] The P-LINCS algorithm^[39] was used to constrain bond lengths, and a time step of 2 fs was used throughout. All simulations were performed using constant temperature, pressure, and number of particles (NPT) and periodic boundary conditions. The cut-off distance for Lennard-Jones interactions and electrostatic interactions were both set at 1.0 nm. Root-mean-square deviation (RMSD) conformational clustering was performed using the *g_cluster* module from GROMACS and a 0.05 Å cut-off value.

Graphics were plotted using the XmGrace package^[40] and images for compounds **1-7** were generated using Chimera.^[41]

Quantum chemistry

The geometries of the compounds **1-7** ("all-equatorial" and "all-axial" conformations), as well as those of the corresponding intermediates and transition states for the conformer interconversion reaction, were optimized in gas-phase using the Gaussian 09 package^[42] with the Becke's three-parameter hybrid exchange functional (B3LYP)^[43,44] and the 6-31+G(d,p) basis set. Subsequent vibrational frequency calculations confirmed that these conformations were local minima and maxima, respectively. IRC calculations were carried out to confirm that the transition states are directly connected to the neighboring minima on the reaction path. Unfortunately, these calculations were

unsuccessful for all compounds using the default SCF and integration grid values. Increasing the accuracy to *irc=(vtight,stepsize=2)* and *int(grid=ultrafine)* led to successful results only for the simplest derivatives **4**, **6** and **7**. Under these conditions, it is worth noting that these latter compounds are characterized by relatively high negative frequency values (ranging from -99 to -115, see Supplementary Information), whereas all other compounds present low negative frequency values (ranging from -23 to -74), which might explain why the IRC calculations were not successful in these cases. Finally, we validated all the transition states by visual inspection in GaussView5 and by geometry optimization of the structures with amplitudes +1 and -1 extracted from Display Vibrations/Manual Displacement menu.

Results and discussion

A combined approach of conformational analysis, molecular dynamics and quantum chemistry calculations allowed the assessment of the conformational flexibility for compounds **1** and **2** (Figure 2). The most stable structures present half-chair conformations with the substituents on C4, C5 and C6 in either an equatorial (conformations **A**) or an axial position (conformations **B**).

Insert Figure 2 here

Extended molecular dynamics (MD) simulations (5 μ s overall) of compounds **1** and **2** in explicit water were performed to explore their conformational flexibility, in complement to the conformational analysis implemented in MacroModel, which uses an implicit solvent. The distribution of ring dihedral angles and the evolution of these angles over time were plotted and show characteristic values for "all-axial" and "all-equatorial" conformations (see Supporting Information). The conformational change

from "all-axial" to "all-equatorial" could be observed in some cases, for both compounds **1** and **2**, but the reverse process never occurred (Table 1). This behavior, in contradiction with the quantum calculations which predict that these conformational changes are equally probable (see below), might be explained by the fact that the force field parameters for sugars were mainly fitted on saturated systems and are probably biased towards the "all-equatorial" conformation. In any case, these MD simulations should be considered only qualitatively, for the assessment of ligand conformations in water, and not quantitatively, for the evaluation of energy barrier for the conformer interconversion process, the quantum calculations being more appropriate for this latter task.

Reduced structural ensembles of representative conformations present during the simulations were generated using root-mean-square deviation (RMSD) conformational clustering and the number of clusters obtained in each case is shown in Table 1. The clustering analysis indicates that compound **1** is represented by a relatively important number of clusters, which implies a high degree of flexibility in solution. In contrast, compound **2** shows fewer clusters, suggesting a good conformational stability in water. This behavior might be explained by the presence of additional stabilizing intramolecular hydrogen bonds compared to compound **1**. These intramolecular hydrogen bonds have been evidenced *in vacuo* (quantum chemistry calculations) and in solution (molecular dynamics simulations), and they can coexist with the intermolecular solute-solvent interactions.^[45]

Insert Table 1 here

The geometries of compounds **1** and **2** (**A** and **B** conformations) were then optimized and transition states and intermediates for the conformer interconversion process identified (Figures 2 and 3). An interesting structural feature of compounds **1**

and **2** revealed by this study is the presence of intramolecular hydrogen bonds. Both equatorial conformers show strong hydrogen bonds between the OH substituent on C4 and the carbonyl oxygen of the acetyl substituent on C5, with an additional interaction between the nitrogen atom of the acetyl substituent on C5 and the OH group on C8 in the case of **2** (Figure 2, Table 2). The situation is different for the axial conformers, where compound **1** presents no hydrogen bonds and compound **2** shows a strong hydrogen bond between the OH substituent on C4 and the OH group on C7 (Figure 2, Table 2).

Insert Table 2 here

The transition states 1TS and 2TS' correspond to the rotation of the *N*-acetyl group and breaking of the hydrogen bond between this group and the OH substituent in position 4. The transition states 1TS' and 2TS'' correspond to the dihydropyran ring conformational interconversion, which flips the C5 and C6 atoms up and down, whereas all other ring atoms are rigid. In the case of compound **2**, there is an additional transition state (2TS), involving the rotation of the substituent on C6 and breaking of the hydrogen bond between this group and the *N*-acetyl moiety. The overall activation barriers differ by about 2 kcal/mol and are in the range 10-12 kcal/mol, which makes in both cases the conformer interexchange possible at room temperature.

Insert Figure 3 here

In order to better understand the details of this conformer interconversion process, which is relatively complex, we have studied the behavior of simpler members of the glycal family (Figure 4). Compound **3** represents the common core of **1** and **2**, compound **7** is completely unsubstituted in the positions 4, 5 and 6, whereas compounds **4**, **5** and **6** bear only one substituent, in the positions 4, 5 or 6, respectively.

Insert Figure 4 here

Similarly to **1** and **2**, the geometries of "all-equatorial" and "all-axial" conformers were optimized, as well as the transition states and (in the case of **3**) the intermediates in the conformer interconversion process (Figures 5 and 6). The conformer **3A** shows a hydrogen bond between the 4-OH and 5-NAc substituents, which is one common feature of compounds **1** and **2**, whereas all other conformers are devoided of any hydrogen bond (Figure 5).

Insert Figure 5 here

The reaction path for compound **3** is very similar to the calculated path for **1**, with two transition states, one for the *N*-acetyl group rotation (**3TS**) and one for the ring conformational change (**3TS'**), although the overall energy barrier is somewhat lower. In the absence of internal hydrogen bonds, compounds **4-7** present only one transition state, which corresponds to the ring conformational change (Figure 6).

Insert Figure 6 here

Without substituents on C4, C5 and C6, the two half-chair conformations of compound **7** have the same energy and an equal amount of these conformations is expected in solution. The situation is different for compounds **4-7**: the 4-OH and 5-NAc substituents stabilize the "all-axial" conformation, whereas the 6-Me substituent stabilizes the "all-equatorial" conformation. Compound **3**, which combines the influences of all the three substituents, has the "all-equatorial" conformer stabilized, although to a less extent than **6**.

The study of simplified derivatives **3-7** showed that substituents in different positions can have opposite influences in stabilizing the ring conformers. Moreover, the

influences of the dihydropyran ring substituents seem not to be additive. The nature and the geometry of substituents on C4, C5 and C6 seem to be the key features that govern the conformer distribution in solution and therefore, a careful choice of these substituents might allow the fine-tuning of physico-chemical properties for these compounds.

The conformer ratio for compounds **1** and **2** was evaluated using the Boltzmann distribution function from the minimized energies of the "all-equatorial" and "all-axial" conformers and compared with the experimental data (Tables 3-5). Although the energy differences are relatively small (less than 1 kcal/mol), the corresponding conformational distributions are significantly different, in agreement with the distinct behavior experimentally observed.

Insert Tables 3-5 here

Four different methods were employed to estimate the NMR vicinal coupling constants ($^3J_{\text{H-C-C-H}}$) starting from the equatorial and axial conformations of compounds **1** and **2**. The relationship between the dihedral angle and the coupling constant observed from ^1H NMR spectra can be calculated using the Karplus equation^[46], where J_0 has a value of 14 ($90^\circ < \theta < 180^\circ$) or 10 ($0^\circ < \theta < 90^\circ$), and $K = 0$:

$$^3J_{\text{HH}} = J_0 * \cos^2\theta - K$$

An alternative method for calculating vicinal coupling constants is given by the Durette-Horton equation:^[47]

$$^3J_{\text{HH}} = 7.8 - \cos\theta + 5.6 * \cos 2\theta$$

However, these two methods do not seem to be adapted for the evaluation of glycal-like systems, as values of 0.9-9.9 Hz and 2.5-10.6 Hz for $^3J_{\text{H6-H5}}$ are calculated

respectively, whereas the experimentally measured value is outside this range (10.9 Hz).

A third method used in this study is given by the Bothner-By equation^[48], which represents a slight modification of the previous equation, but which provides more realistic values for ${}^3J_{H_6-H_5}$ (2.6-11.0 Hz):

$${}^3J_{HH} = 7 - \cos\theta + 5*\cos2\theta$$

The last method makes use of the Haasnoot equation^[49], which takes into account the Huggins electronegativities^[50] of the neighboring atoms and for which two cases can be distinguished. When four substituents are present on the central atoms of the dihedral angle (${}^3J_{H_6-H_5}$ and ${}^3J_{H_5-H_4}$), the following equation can be used:

$${}^3J_{HH} = 13.24*\cos^2\theta - 0.91*\cos\theta + \sum\Delta\chi\{0.53 - 2.41*\cos^2(\theta + 15.5*|\Delta\chi|)\}, \text{ where } \Delta\chi = \Delta\chi^{\alpha\text{-substituent}} - 0.19\Delta\chi^{\beta\text{-substituent}}$$

If only three substituents are present (${}^3J_{H_4-H_3}$), the equation to be used is slightly different:

$${}^3J_{HH} = 13.22*\cos^2\theta - 0.99*\cos\theta + \sum\Delta\chi\{0.57 - 2.46*\cos^2(\theta + 19.9*|\Delta\chi|)\}, \text{ where } \Delta\chi = \Delta\chi^{\alpha\text{-substituent}}$$

The coupling constants calculated for the equatorial and axial conformers using the four methods presented above were subsequently used to evaluate the conformer distribution using the linear regression fit against the experimentally measured values of the coupling constants. The first two methods provided unrealistic results and the Bothner-By method gave relatively poor correlation, whereas the Haasnoot method provided very good results for both compounds included in this study (Table 5). From these data, it seems that the inclusion of neighboring substituents' electronegativities is critical for the reliable prediction of the ${}^3J_{HH}$ NMR coupling constants, and therefore the

Haasnoot method appears to be the most appropriate for evaluating glycal-like compounds.

A fifth method used in this study, developed by Roush *et al.*,^[51] correlates directly the $^3J_{\text{H6-H5}}$ coupling constants with the conformer distribution in solution. However, in our hands this method provided conformer distribution values that are quite different compared to the Boltzmann distributions (Table 5).

Conclusion

In this work, the conformational flexibility of two glycal-type neuraminidase inhibitors has been evaluated, using different molecular modeling techniques (conformational analysis, molecular dynamics and quantum chemistry calculations). We have shown that, in agreement with the experimental data available, compound **2** behaves very differently in solution compared with compound **1**, and this behavior is mainly due to the presence of an additional strong intramolecular hydrogen bond between the nitrogen atom of the acetyl group and the OH group on C8. This hydrogen bond seems to represent the key structural feature that allows the fine-tuning of conformer stabilization, thus controlling the conformer distribution in solution. Several simplified derivatives of **1** and **2** were also studied and the contribution of each substituent on the overall conformational equilibrium evaluated. Additionally, four different methods for the estimation of NMR coupling constants from dihedral angles were evaluated and only one, the method described by Haasnoot *et al.*,^[49] gave very good results and therefore seems to be the most appropriate for the analysis of this class of sugars. The results presented here should allow a better understanding of the structural parameters governing the physico-chemical properties of glycal-like compounds.

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Table 1. Overview of molecular dynamics simulations performed in this study.

Compound	Conformer	Simulation time (ns)	Number of clusters	Remarks
1	1A	5*250	34	Conformationally stable
	1B	5*250	44	Conformational change 1B → 1A observed in 2 simulations
2	2A	5*250	7	Conformationally stable
	2B	5*250	6	Conformational change 2B → 2A observed in 1 simulation

Table 2. Hydrogen bonds (X–H...Y) identified in the structures of compounds **1** and **2**.

Compound	Conformation	X–Y distance (Å)	X–H...Y angle (deg.)
1	1A	2.78	157
	1B	-	-
2	2A	2.73 (O–H...O)	158 (O–H...O)
		2.87 (N–H...O)	155 (N–H...O)
	2B	2.76	153

Table 3. Dihedral angles measured on representative "all-equatorial" (**A**) and "all-axial" (**B**) conformations for compounds **1** and **2**, after geometry optimization using Gaussian^[42].

	Compound 1		Compound 2	
	1A	1B	2A	2B
θ_{H6-H5} (deg.)	0.4	70.6	3.9	72.7
θ_{H5-H4} (deg.)	24.0	96.3	20.9	102.5
θ_{H4-H3} (deg.)	71.6	53.7	73.0	46.3

Table 4. NMR coupling constants for representative "all-equatorial" (**A**) and "all-axial" (**B**) conformations of compounds **1** and **2** calculated using four different methods compared with experimental values.

Compound or conformer	Method used for 3J calculation	Calculated values		Experimental values ^[10]	Calculated values		Experimental values ^[14,15]
		1A	1B	1	2A	2B	2
$^3J_{H6-H5}$ (Hz)	Karplus	10.0	1.1	8	9.9	0.9	10.9
	Durette-Horton	9.8	2.5		10.6	2.5	
	Bothner-By	11.0	2.8		11.0	2.6	
	Haasnoot	11.7	1.2		12.1	0.9	
$^3J_{H5-H4}$ (Hz)	Karplus	8.3	0.2	4.5	8.7	0.6	8.5
	Durette-Horton	7.9	1.8		8.2	2.2	
	Bothner-By	9.4	2.2		9.8	2.7	
	Haasnoot	9.4	0.3		9.8	0.8	
$^3J_{H4-H3}$ (Hz)	Karplus	1.0	3.5	4.5	0.8	4.8	2.3
	Durette-Horton	2.0	3.6		1.9	4.5	
	Bothner-By	2.7	4.9		2.6	6.1	
	Haasnoot	2.0	4.1		1.8	5.6	

Table 5. Comparison of conformer distribution for compounds **1** and **2** estimated from NMR coupling constants (using five different methods) and from quantum chemistry energy calculations.

Method used for A/B ratio calculation	Method used for NMR coupling constants calculation	Compound 1		Compound 2	
		A/B ratio	R ² coefficient	A/B ratio	R ² coefficient
Linear regression of calculated against experimental NMR coupling constants	Karplus ^[46]	62/38	0.867	- ^a	- ^a
	Durette-Horton ^[47]	59/41	0.853	- ^a	- ^a
	Bothner-By ^[48]	48/52	0.894	93/7	0.990
	Haasnoot ^[49]	55/45	0.935	88/12	0.999
From experimental $^3J_{H6-H5}$ NMR coupling constants using the Roush method ^[51]	-	63/37	-	93/7	-
Boltzmann distribution from quantum calculations	-	53/47	-	83/17	-

^a Unrealistic values are obtained from the linear regression fit

Figure 1. Chemical structures of neuraminidase inhibitors **1** and **2** used in this study, and the "all-equatorial" (**A**, ${}^6\text{H}_5$) and "all-axial" (**B**, ${}^5\text{H}_6$) half-chair conformations that these compounds can adopt.

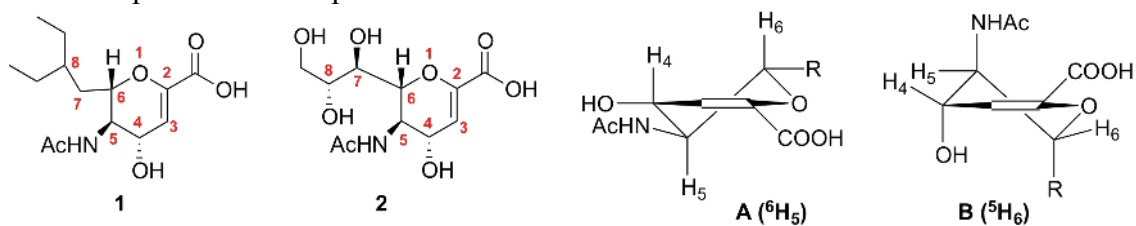


Figure 2. Three-dimensional representation of compounds **1** and **2** as "all-equatorial" (**A**) and "all-axial" (**B**) conformers, generated by conformational analysis and molecular dynamics simulations, followed by geometry optimization. Only hydrogen atoms involved in hydrogen bonds are shown.

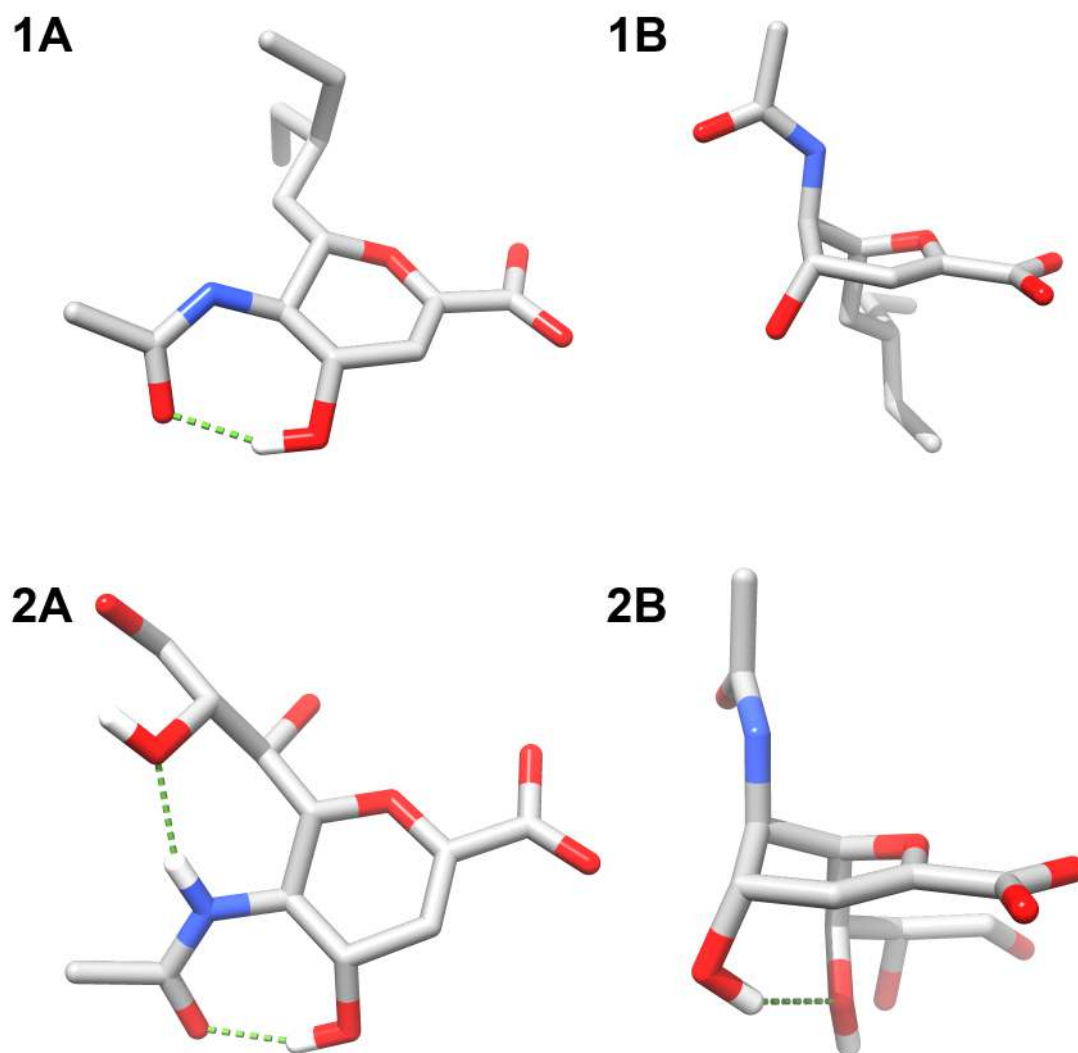


Figure 3. Energy diagram for the "all-equatorial" (A) and "all-axial" (B) conformer interconversion of compounds 1 and 2.

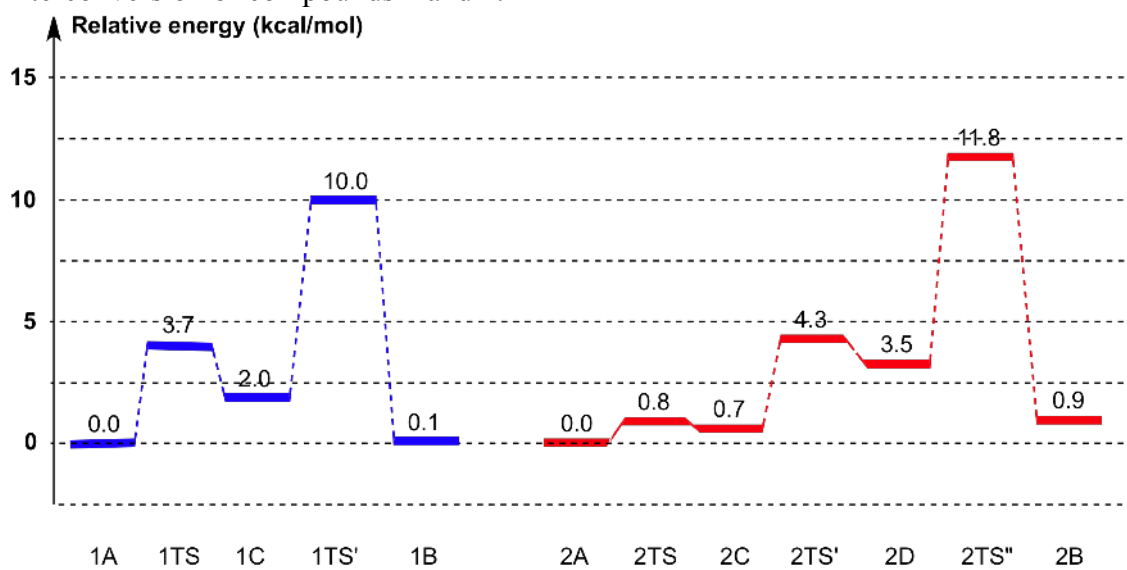


Figure 4. Chemical structures of simplified derivatives 3-7.

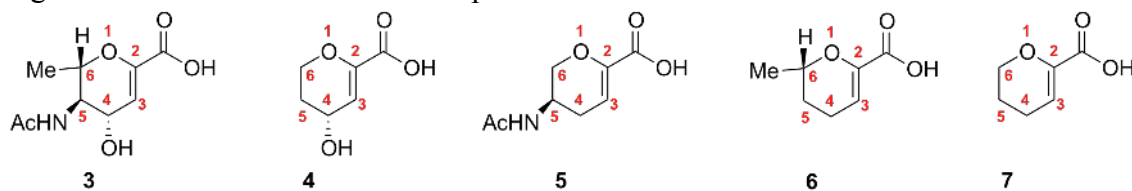
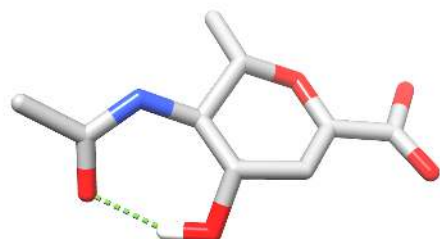
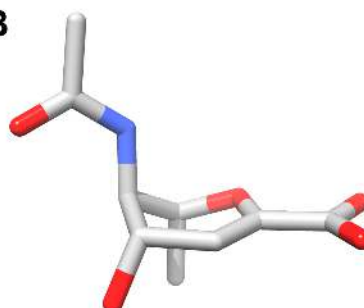


Figure 5. Three-dimensional representation of simplified derivatives **3-7** as "all-equatorial" (**A**) and "all-axial" (**B**) conformers, after geometry optimization. Only hydrogen atoms involved in hydrogen bonds are shown.

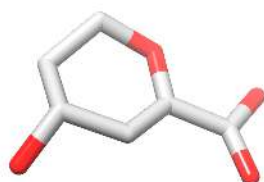
3A



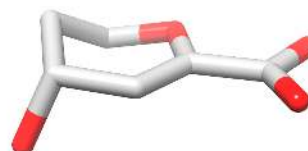
3B



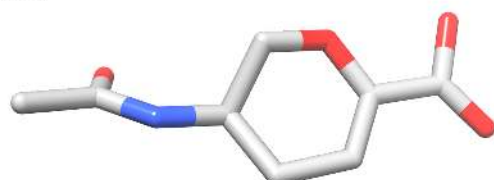
4A



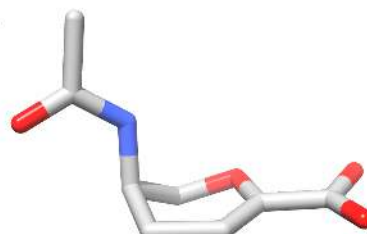
4B



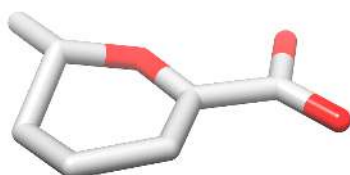
5A



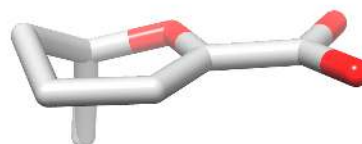
5B



6A



6B



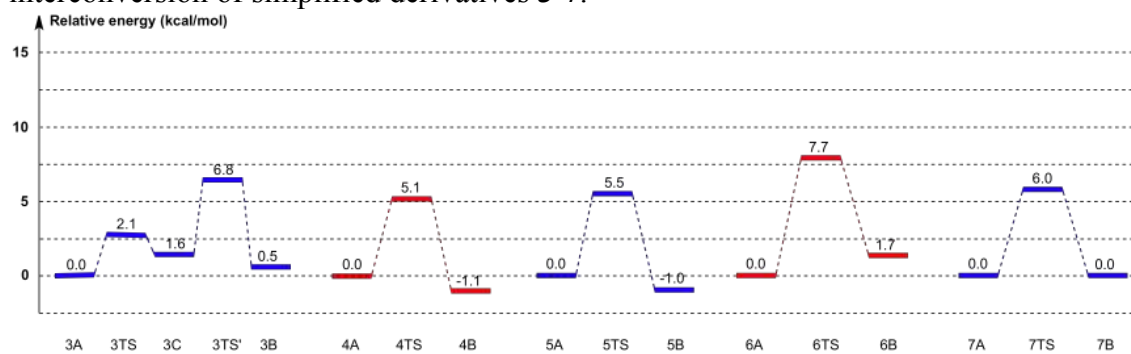
7A



7B



Figure 6. Energy diagram for the "all-equatorial" (A) and "all-axial" (B) conformer interconversion of simplified derivatives **3-7**.



Supporting Information

Conformational study of glycal-type neuraminidase inhibitors

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Theoretical data for compound 1A :

Final Energy in Hartrees: HF=-978.3002685 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.142081	-2.627449	2.206467
2	6	0	-2.681116	-1.378288	1.493534
3	6	0	-2.410009	-1.283227	-0.027394
4	6	0	-0.907103	-1.239575	-0.381971
5	6	0	-0.125665	-0.070763	0.225085
6	6	0	1.358457	-0.024720	-0.200118
7	7	0	2.015215	-1.255953	0.256246
8	6	0	3.241261	-1.672360	-0.164863
9	6	0	3.702193	-3.027954	0.333104
10	8	0	3.946538	-0.995111	-0.919671
11	6	0	2.061989	1.246849	0.347814
12	8	0	3.170976	1.638063	-0.447766
13	6	0	1.121628	2.417440	0.379414
14	6	0	-0.183294	2.304837	0.098030
15	6	0	-1.072887	3.501391	0.057731
16	8	0	-2.352980	3.198406	-0.258149
17	8	0	-0.701547	4.636740	0.281517
18	8	0	-0.805732	1.122288	-0.191605
19	6	0	-3.127241	-2.410888	-0.804331
20	6	0	-3.245519	-2.178578	-2.317116
21	1	0	-0.166406	-0.100482	1.326952
22	1	0	1.412475	0.011747	-1.295184
23	1	0	2.397265	1.022404	1.376429
24	1	0	-1.048973	-2.698884	2.152256
25	1	0	-2.552340	-3.549589	1.781860
26	1	0	-2.408961	-2.608399	3.268440
27	1	0	-3.768298	-1.334439	1.638448
28	1	0	-2.286437	-0.482321	1.988863
29	1	0	-2.845406	-0.332272	-0.358908
30	1	0	-0.435881	-2.182409	-0.080056
31	1	0	-0.790732	-1.173443	-1.469656
32	1	0	1.523494	-1.841146	0.916193
33	1	0	4.683380	-2.915025	0.801222
34	1	0	3.014115	-3.493908	1.043668
35	1	0	3.824174	-3.690058	-0.529251
36	1	0	3.651829	0.827996	-0.712491
37	1	0	1.534028	3.397917	0.585366
38	1	0	-2.623732	-3.370945	-0.624073
39	1	0	-4.138550	-2.518074	-0.389673
40	1	0	-2.270103	-2.161274	-2.814436
41	1	0	-3.833051	-2.974949	-2.786504
42	1	0	-3.743808	-1.226062	-2.531722
43	1	0	-2.836288	4.041922	-0.268393

	1 A	2 A	3 A
Frequencies --	22.4713	31.4626	41.7372
Red. masses --	3.2270	6.4843	5.3710
Frc consts --	0.0010	0.0038	0.0055
IR Inten --	0.4424	0.3230	5.3400

Theoretical data for compound 1TS :

Final Energy in Hartrees: HF = -978.2943184 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.543430	-2.037900	2.094680
2	6	0	-2.719798	-0.574895	1.663033
3	6	0	-2.675300	-0.302106	0.139733
4	6	0	-1.330980	-0.693554	-0.515080
5	6	0	-0.091918	-0.007085	0.052596
6	6	0	1.231676	-0.388915	-0.656555
7	7	0	1.405487	-1.835968	-0.799661
8	6	0	2.068589	-2.699463	0.028009
9	6	0	2.083678	-4.151447	-0.423781
10	8	0	2.628596	-2.353376	1.068517
11	6	0	2.400636	0.328427	0.054900
12	8	0	3.626462	0.168239	-0.651556
13	6	0	2.066593	1.789065	0.150982
14	6	0	0.806186	2.234013	0.079907
15	6	0	0.442627	3.686416	0.171724
16	8	0	-0.882802	3.942307	0.086366
17	8	0	1.254004	4.572056	0.308984
18	8	0	-0.295097	1.422801	-0.095882
19	6	0	-3.860189	-0.972904	-0.593019
20	6	0	-4.131849	-0.440306	-2.006654
21	1	0	0.008490	-0.212339	1.126985
22	1	0	1.186783	0.010899	-1.676893
23	1	0	2.510524	-0.086993	1.061165
24	1	0	-2.624864	-2.126432	3.182980
25	1	0	-3.307727	-2.687552	1.655423
26	1	0	-1.563117	-2.437727	1.812460
27	1	0	-1.962671	0.040276	2.165209
28	1	0	-3.685749	-0.209657	2.035234
29	1	0	-2.799538	0.782706	0.015593
30	1	0	-1.184690	-1.775292	-0.417087
31	1	0	-1.372651	-0.473508	-1.589298
32	1	0	1.036763	-2.232397	-1.651097
33	1	0	1.635391	-4.763394	0.363874
34	1	0	1.553325	-4.333301	-1.362625
35	1	0	3.123599	-4.471388	-0.533374
36	1	0	4.063342	-0.618019	-0.296126
37	1	0	2.869276	2.503041	0.292261
38	1	0	-1.358279	3.098966	-0.013819
39	1	0	-3.702032	-2.059088	-0.637971
40	1	0	-4.763298	-0.823952	0.013366
41	1	0	-5.023183	-0.911853	-2.433942
42	1	0	-3.302376	-0.635950	-2.694557
43	1	0	-4.304154	0.642428	-1.994411

	1	2	3
	A	A	A
Frequencies --	-61.7339	20.7064	35.6559
Red. masses --	7.0178	3.2958	1.4627
Frc consts --	0.0158	0.0008	0.0011
IR Inten --	13.8189	0.3306	1.7797

Theoretical data for compound 1C :

Final Energy in Hartrees: HF = -978.2970991 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.969899	-0.721917	2.119602
2	6	0	2.000893	-1.778312	1.567702
3	6	0	1.843693	-1.828811	0.028502
4	6	0	1.328900	-0.507308	-0.584898
5	6	0	0.012403	0.015899	-0.021998
6	6	0	-0.520990	1.282102	-0.731698
7	7	0	0.454916	2.367597	-0.846898
8	6	0	1.091820	2.960493	0.209402
9	6	0	2.037926	4.097688	-0.135998
10	8	0	0.918418	2.591794	1.370102
11	6	0	-1.826187	1.751510	-0.052998
12	8	0	-2.521382	2.695113	-0.875398
13	6	0	-2.728194	0.573915	0.169702
14	6	0	-2.284601	-0.686288	0.078002
15	6	0	-3.175907	-1.881783	0.258702
16	8	0	-2.546414	-3.072686	0.150102
17	8	0	-4.361707	-1.804476	0.481002
18	8	0	-0.982803	-1.032095	-0.196598
19	6	0	3.150790	-2.281818	-0.662498
20	6	0	2.989888	-2.732217	-2.121098
21	1	0	0.091904	0.211399	1.051802
22	1	0	-0.777691	0.999704	-1.758498
23	1	0	-1.575984	2.215208	0.910702
24	1	0	3.051499	-0.815918	3.207602
25	1	0	3.977999	-0.837423	1.706502
26	1	0	2.631105	0.298085	1.911302
27	1	0	1.015794	-1.631306	2.027902
28	1	0	2.331488	-2.772614	1.896102
29	1	0	1.092989	-2.604307	-0.180798
30	1	0	2.082605	0.274288	-0.440098
31	1	0	1.208200	-0.631407	-1.668098
32	1	0	0.643718	2.718996	-1.773498
33	1	0	3.045825	3.823982	0.189102
34	1	0	2.062628	4.346488	-1.200598
35	1	0	1.741731	4.983190	0.432902
36	1	0	-2.146477	3.571511	-0.720898
37	1	0	-3.773493	0.746320	0.396802
38	1	0	-1.601113	-2.911692	-0.018998
39	1	0	3.895795	-1.476222	-0.611898
40	1	0	3.568386	-3.116721	-0.084598
41	1	0	3.939386	-3.106923	-2.518198
42	1	0	2.664693	-1.917416	-2.776698
43	1	0	2.253683	-3.540513	-2.205798

	1	2	3
	A	A	A
Frequencies --	16.4745	35.0440	48.1026
Red. masses --	3.3444	5.0518	3.9361
Frc consts --	0.0005	0.0037	0.0054
IR Inten --	0.3543	1.0613	0.7655

Theoretical data for compound 1TS' :

Final Energy in Hartrees: HF = -978.2843704 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.340223	-3.385637	-0.801057
2	6	0	2.447842	-1.927243	-1.270731
3	6	0	2.480640	-0.851356	-0.157550
4	6	0	1.209115	-0.831281	0.716155
5	6	0	-0.122431	-0.657479	-0.036306
6	6	0	-1.321273	-0.610681	0.958517
7	7	0	-2.472857	-1.410670	0.522881
8	6	0	-3.302357	-1.072910	-0.515816
9	6	0	-4.404922	-2.067832	-0.837290
10	8	0	-3.169320	-0.024904	-1.139734
11	6	0	-1.732071	0.826428	1.418273
12	8	0	-1.647491	0.943994	2.849634
13	6	0	-0.908782	1.911009	0.802949
14	6	0	-0.197745	1.714149	-0.312444
15	6	0	0.498768	2.821115	-1.047619
16	8	0	1.119330	2.432793	-2.184374
17	8	0	0.513708	3.971283	-0.673587
18	8	0	-0.055002	0.491295	-0.914520
19	6	0	3.750143	-0.975089	0.716368
20	6	0	4.061989	0.255598	1.578987
21	1	0	-0.283802	-1.489876	-0.723876
22	1	0	-0.972753	-1.102650	1.869588
23	1	0	-2.768491	0.991910	1.100881
24	1	0	2.346991	-4.065634	-1.659560
25	1	0	3.176309	-3.668407	-0.153104
26	1	0	1.413992	-3.574801	-0.246209
27	1	0	1.620992	-1.711485	-1.959442
28	1	0	3.362655	-1.815882	-1.867026
29	1	0	2.544905	0.119044	-0.668622
30	1	0	1.140512	-1.770173	1.282213
31	1	0	1.292251	-0.034745	1.463878
32	1	0	-2.616352	-2.301418	0.974920
33	1	0	-4.284340	-2.398103	-1.872972
34	1	0	-4.417722	-2.944233	-0.182929
35	1	0	-5.368614	-1.555808	-0.768066
36	1	0	-2.497543	0.698630	3.236036
37	1	0	-0.961553	2.906388	1.227018
38	1	0	0.969849	1.477925	-2.306636
39	1	0	3.672138	-1.860961	1.361296
40	1	0	4.604161	-1.158955	0.050848
41	1	0	5.009153	0.123096	2.112689
42	1	0	3.290366	0.444881	2.332411
43	1	0	4.152248	1.157513	0.962541

	1	2	3
	A	A	A
Frequencies --	-27.1927	32.5496	36.2328
Red. masses --	5.8326	3.3604	4.7213
Frc consts --	0.0025	0.0021	0.0037
IR Inten --	0.5501	0.6714	1.8328

Theoretical data for compound 1B :

Final Energy in Hartrees: HF = -978.3001577 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.827448	-2.593988	-1.636178
2	6	0	2.608979	-2.433979	-0.716551
3	6	0	2.491008	-1.067208	-0.004494
4	6	0	1.124590	-0.929897	0.706145
5	6	0	-0.057233	-0.691433	-0.240611
6	6	0	-1.435669	-0.737951	0.432926
7	7	0	-2.471258	-0.741710	-0.596790
8	6	0	-3.719679	-1.242527	-0.352817
9	6	0	-4.708965	-1.170456	-1.501454
10	8	0	-4.018185	-1.734080	0.735578
11	6	0	-1.638339	0.450354	1.411049
12	8	0	-1.093500	0.182363	2.709392
13	6	0	-1.003493	1.697335	0.874427
14	6	0	-0.239005	1.689674	-0.231674
15	6	0	0.305516	2.965600	-0.787977
16	8	0	1.109577	2.776061	-1.857558
17	8	0	0.058931	4.066321	-0.335261
18	8	0	0.089601	0.574244	-0.946048
19	6	0	3.650845	-0.834444	0.989571
20	6	0	3.806018	0.615463	1.468996
21	1	0	-0.043801	-1.426069	-1.050320
22	1	0	-1.535553	-1.669173	0.997248
23	1	0	-2.719656	0.617031	1.502122
24	1	0	4.772681	-2.556388	-1.086288
25	1	0	3.793847	-3.556524	-2.158066
26	1	0	3.852928	-1.804746	-2.397112
27	1	0	1.706360	-2.609084	-1.315975
28	1	0	2.621651	-3.227537	0.045574
29	1	0	2.552092	-0.281908	-0.772503
30	1	0	0.919460	-1.847024	1.275087
31	1	0	1.151235	-0.124777	1.443887
32	1	0	-2.277751	-0.275480	-1.472447
33	1	0	-4.304825	-0.694250	-2.399149
34	1	0	-5.029729	-2.186120	-1.750089
35	1	0	-5.593199	-0.619299	-1.169668
36	1	0	-1.704220	-0.405170	3.176458
37	1	0	-1.178071	2.641333	1.376484
38	1	0	1.402723	3.659557	-2.138454
39	1	0	3.515477	-1.498175	1.856504
40	1	0	4.592213	-1.139862	0.520023
41	1	0	3.966420	1.292326	0.621433
42	1	0	2.927811	0.972230	2.016913
43	1	0	4.667191	0.712564	2.138891

	1 A	2 A	3 A
Frequencies --	10.0220	32.2525	38.3486
Red. masses --	3.5314	4.2326	4.8934
Frc consts --	0.0002	0.0026	0.0042
IR Inten --	0.0753	0.0693	0.1242

Theoretical data for compound 2A :

Final Energy in Hartrees: HF= -1086.017505 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	3.581607	-2.371672	0.354449
2	6	0	3.778071	-1.132678	-0.155901
3	6	0	2.530586	-0.320847	-0.190446
4	6	0	2.519962	0.954477	-0.594722
5	6	0	1.290791	1.819497	-0.535533
6	8	0	1.684173	3.021672	0.102317
7	6	0	0.136771	1.094335	0.211065
8	7	0	-1.182925	1.638507	-0.118289
9	6	0	-1.606535	2.870858	0.261816
10	6	0	-3.054237	3.204110	-0.039282
11	8	0	-0.868699	3.693492	0.821310
12	6	0	0.150180	-0.410946	-0.125362
13	6	0	-0.945040	-1.250640	0.621260
14	8	0	-0.412065	-2.371736	1.307388
15	6	0	-2.001463	-1.792938	-0.352613
16	8	0	-2.592466	-0.683755	-1.043800
17	6	0	-3.089103	-2.589203	0.358594
18	8	0	-4.059702	-2.899633	-0.652335
19	8	0	1.409409	-0.984567	0.246411
20	8	0	4.862243	-0.737591	-0.533389
21	1	0	0.941580	2.027855	-1.562685
22	1	0	0.316294	1.213423	1.288311
23	1	0	-1.443776	-0.596180	1.351217
24	1	0	-1.500587	-2.450429	-1.078322
25	1	0	0.040565	-0.535792	-1.212451
26	1	0	4.448012	-2.812748	0.347672
27	1	0	3.447461	1.410275	-0.920537
28	1	0	0.870565	3.469724	0.420567
29	1	0	-1.849970	1.014704	-0.567796
30	1	0	-3.556480	3.447165	0.901604
31	1	0	-3.085471	4.099348	-0.666487
32	1	0	-3.592866	2.393560	-0.536152
33	1	0	0.556777	-2.319028	1.277513
34	1	0	-3.392051	-1.016933	-1.480479
35	1	0	-2.659470	-3.494890	0.797104
36	1	0	-3.540828	-1.976606	1.151615
37	1	0	-4.815176	-3.348830	-0.254742

	1 A	2 A	3 A
Frequencies --	26.0081	37.1993	44.3198
Red. masses --	6.7105	5.3376	5.1404
Frc consts --	0.0027	0.0044	0.0059
IR Inten --	1.7884	0.6596	0.8600

Theoretical data for compound 2TS :

Final Energy in Hartrees: HF= -1086.0161907 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	2.695901	-3.119149	0.212980
2	6	0	3.244033	-1.948761	-0.191369
3	6	0	2.264317	-0.826377	-0.204221
4	6	0	2.635732	0.428486	-0.484590
5	6	0	1.691278	1.595221	-0.434871
6	8	0	2.354063	2.624008	0.280085
7	6	0	0.340051	1.195936	0.217597
8	7	0	-0.769546	2.050594	-0.225161
9	6	0	-0.890635	3.368872	0.088873
10	6	0	-2.165104	4.054157	-0.361656
11	8	0	-0.019311	3.984725	0.712943
12	6	0	-0.056674	-0.246048	-0.144626
13	6	0	-1.295335	-0.764823	0.640054
14	8	0	-0.926942	-1.424774	1.836842
15	6	0	-2.179829	-1.640400	-0.259031
16	8	0	-2.623833	-0.776585	-1.313141
17	6	0	-3.375420	-2.218179	0.486371
18	8	0	-4.188102	-2.852038	-0.512010
19	8	0	0.983562	-1.195214	0.121026
20	8	0	4.413595	-1.839519	-0.498932
21	1	0	1.475883	1.926211	-1.466753
22	1	0	0.453336	1.289311	1.304837
23	1	0	-1.905295	0.094290	0.940519
24	1	0	-1.590239	-2.469586	-0.679885
25	1	0	-0.270746	-0.283783	-1.221361
26	1	0	3.412400	-3.776236	0.198471
27	1	0	3.675477	0.626427	-0.716654
28	1	0	1.681726	3.295285	0.518606
29	1	0	-1.502076	1.622944	-0.779217
30	1	0	-2.710571	4.387367	0.526369
31	1	0	-1.900406	4.945098	-0.936878
32	1	0	-2.818297	3.415148	-0.961533
33	1	0	-0.082840	-1.877061	1.676802
34	1	0	-3.344628	-1.235558	-1.770807
35	1	0	-3.035337	-2.934288	1.241632
36	1	0	-3.931433	-1.408790	0.980732
37	1	0	-5.006081	-3.171066	-0.112292

	1	2	3
	A	A	A
Frequencies --	-23.6031	32.2352	44.3804
Red. masses --	6.4733	5.4791	7.8504
Frc consts --	0.0021	0.0034	0.0091
IR Inten --	0.4721	0.7710	0.8693

Theoretical data for compound 2C :

Final Energy in Hartrees: HF=-1086.016375 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	1.522231	3.716970	0.274500
2	6	0	0.228842	3.689024	-0.124681
3	6	0	-0.330020	2.308716	-0.181371
4	6	0	-1.618885	2.085195	-0.464580
5	6	0	-2.231459	0.714403	-0.456626
6	8	0	-3.447033	0.815151	0.266787
7	6	0	-1.262356	-0.330570	0.158004
8	7	0	-1.549840	-1.693793	-0.305918
9	6	0	-2.654173	-2.405086	0.052967
10	6	0	-2.721414	-3.838523	-0.434348
11	8	0	-3.554859	-1.921263	0.746458
12	6	0	0.201519	-0.027100	-0.212753
13	6	0	1.227905	-0.901333	0.541919
14	8	0	1.393662	-0.455956	1.877814
15	6	0	2.563051	-0.968691	-0.216337
16	8	0	2.270734	-1.586426	-1.472986
17	6	0	3.611516	-1.778688	0.537008
18	8	0	4.732540	-1.885864	-0.351957
19	8	0	0.577012	1.321349	0.106692
20	8	0	-0.399269	4.692420	-0.395816
21	1	0	-2.434595	0.405972	-1.498113
22	1	0	-1.379530	-0.299274	1.247580
23	1	0	0.842365	-1.923937	0.608895
24	1	0	2.953352	0.047156	-0.380401
25	1	0	0.334720	-0.165254	-1.294705
26	1	0	1.783657	4.653372	0.287631
27	1	0	-2.265753	2.930682	-0.666318
28	1	0	-3.719252	-0.090275	0.521687
29	1	0	-0.891370	-2.129437	-0.938299
30	1	0	-2.712852	-4.499811	0.437291
31	1	0	-3.672157	-3.989740	-0.951766
32	1	0	-1.898599	-4.116486	-1.098309
33	1	0	1.444698	0.513069	1.856225
34	1	0	3.120455	-1.825588	-1.873242
35	1	0	3.885052	-1.269268	1.466851
36	1	0	3.210979	-2.774472	0.775456
37	1	0	5.400404	-2.465277	0.033811

	1	2	3
	A	A	A
Frequencies --	22.3026	31.6165	45.5108
Red. masses --	6.2387	5.8925	7.0568
Frc consts --	0.0018	0.0035	0.0086
IR Inten --	0.4392	0.9123	1.5439

Theoretical data for compound 2TS' :

Final Energy in Hartrees: HF= -1086.0106485 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	3.463435	-2.165252	-0.616907
2	6	0	3.666294	-0.978150	0.009180
3	6	0	2.485930	-0.078861	-0.070086
4	6	0	2.430592	1.095592	0.574062
5	6	0	1.209836	1.940464	0.411778
6	8	0	1.167743	2.904623	1.455668
7	6	0	-0.024082	0.999376	0.463290
8	7	0	-1.304675	1.688031	0.311872
9	6	0	-1.619963	2.607880	-0.646598
10	6	0	-3.073352	3.054569	-0.669495
11	8	0	-0.796483	3.074656	-1.436345
12	6	0	0.099419	-0.159121	-0.558404
13	6	0	-0.535602	-1.495108	-0.104746
14	8	0	-0.253772	-2.496112	-1.075313
15	6	0	-2.062139	-1.482675	0.063323
16	8	0	-2.390457	-0.746635	1.249376
17	6	0	-2.620770	-2.900917	0.185889
18	8	0	-3.999270	-2.735357	0.557915
19	8	0	1.474353	-0.513699	-0.885929
20	8	0	4.705876	-0.703443	0.574550
21	1	0	1.230560	2.439054	-0.564434
22	1	0	-0.036623	0.587325	1.476293
23	1	0	-0.093834	-1.767542	0.868111
24	1	0	-2.528074	-1.000536	-0.809347
25	1	0	-0.338037	0.148992	-1.512628
26	1	0	4.285510	-2.673481	-0.512591
27	1	0	3.245550	1.422509	1.207927
28	1	0	0.569371	3.613890	1.186761
29	1	0	-2.058545	1.254989	0.832871
30	1	0	-3.107034	4.142170	-0.561370
31	1	0	-3.496149	2.811353	-1.648752
32	1	0	-3.687519	2.597017	0.110619
33	1	0	0.691999	-2.430242	-1.282555
34	1	0	-3.270408	-1.057562	1.519257
35	1	0	-2.524116	-3.428429	-0.766133
36	1	0	-2.075292	-3.451040	0.964286
37	1	0	-4.382997	-3.593233	0.775293

	1	2	3
	A	A	A
Frequencies --	-37.9861	20.9175	44.0866
Red. masses --	7.1312	6.1671	5.8704
Frc consts --	0.0061	0.0016	0.0067
IR Inten --	4.3113	0.2863	0.1021

Theoretical data for compound 2D :

Final Energy in Hartrees: HF= -1086.0118575 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	1.298346	-3.706847	-0.048313
2	6	0	2.284339	-2.803703	-0.254496
3	6	0	1.814771	-1.393236	-0.131790
4	6	0	2.672651	-0.366665	-0.235418
5	6	0	2.236155	1.057593	-0.072962
6	8	0	3.222316	1.732821	0.714906
7	6	0	0.853619	1.095354	0.611600
8	7	0	0.286587	2.443920	0.659586
9	6	0	0.008883	3.226174	-0.431771
10	6	0	-0.633050	4.571446	-0.134779
11	8	0	0.262795	2.872554	-1.580760
12	6	0	-0.087352	0.063788	-0.047417
13	6	0	-1.469156	-0.017756	0.611222
14	8	0	-1.360589	-0.404923	1.979989
15	6	0	-2.422848	-0.949250	-0.155417
16	8	0	-2.526160	-0.435775	-1.480215
17	6	0	-3.801346	-1.010739	0.495478
18	8	0	-4.605091	-1.828045	-0.367437
19	8	0	0.475010	-1.262753	0.105270
20	8	0	3.429957	-3.123979	-0.502390
21	1	0	2.159274	1.534001	-1.057968
22	1	0	1.004189	0.797978	1.653229
23	1	0	-1.905032	0.986061	0.612129
24	1	0	-2.000030	-1.965154	-0.176889
25	1	0	-0.202209	0.273769	-1.115540
26	1	0	1.706913	-4.583660	-0.145984
27	1	0	3.717878	-0.572964	-0.431651
28	1	0	3.129990	2.682865	0.566663
29	1	0	0.015338	2.788640	1.568345
30	1	0	-0.026158	5.357252	-0.592412
31	1	0	-1.616405	4.598190	-0.613339
32	1	0	-0.749725	4.782659	0.931930
33	1	0	-0.825938	-1.213691	2.009088
34	1	0	-3.252641	-0.910571	-1.910647
35	1	0	-3.730331	-1.443152	1.499394
36	1	0	-4.220400	0.003410	0.566104
37	1	0	-5.523492	-1.805536	-0.073459

	1	2	3
	A	A	A
Frequencies --	35.9167	38.3385	45.8667
Red. masses --	5.4270	6.1976	5.4499
Frc consts --	0.0041	0.0054	0.0068
IR Inten --	0.4152	0.2878	2.1554

Theoretical data for compound 2TS'' :

Final Energy in Hartrees: HF= -1085.9986171 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	2.187554	-2.803379	-1.427218
2	6	0	2.674299	-2.134328	-0.351568
3	6	0	1.824057	-0.968846	0.023892
4	6	0	1.960665	-0.364216	1.211077
5	6	0	1.155587	0.831159	1.601363
6	8	0	0.703844	0.630948	2.951943
7	6	0	-0.055131	1.111865	0.650525
8	7	0	-0.028215	2.464506	0.081606
9	6	0	1.005759	2.969624	-0.667348
10	6	0	0.790986	4.359635	-1.240325
11	8	0	2.039938	2.337733	-0.854463
12	6	0	-0.297457	0.012981	-0.421899
13	6	0	-1.219088	-1.137036	0.043278
14	8	0	-1.348402	-2.090920	-1.013592
15	6	0	-2.656153	-0.737735	0.417708
16	8	0	-3.414367	-1.917175	0.702099
17	6	0	-3.400082	0.085013	-0.642263
18	8	0	-4.724060	0.366319	-0.211497
19	8	0	0.906198	-0.607643	-0.918722
20	8	0	3.676237	-2.477900	0.240344
21	1	0	1.819446	1.702618	1.561321
22	1	0	-0.926558	1.106636	1.308037
23	1	0	-0.772378	-1.621183	0.924181
24	1	0	-2.648735	-0.173781	1.356537
25	1	0	-0.727256	0.474728	-1.312841
26	1	0	2.798353	-3.541138	-1.594252
27	1	0	2.705824	-0.728749	1.907543
28	1	0	0.648433	1.486239	3.397521
29	1	0	-0.867195	3.019136	0.169514
30	1	0	1.650120	4.982379	-0.978777
31	1	0	0.760345	4.284540	-2.331573
32	1	0	-0.125442	4.845107	-0.893344
33	1	0	-0.461656	-2.312851	-1.337634
34	1	0	-3.163485	-2.580604	0.038907
35	1	0	-2.918175	1.056436	-0.799123
36	1	0	-3.398131	-0.454331	-1.600046
37	1	0	-5.092187	-0.469270	0.114999

	1	2	3
	A	A	A
Frequencies --	-27.0664	37.6809	40.7982
Red. masses --	5.7888	6.0423	6.6307
Frc consts --	0.0025	0.0051	0.0065
IR Inten --	0.7593	0.0812	2.0377

Theoretical data for compound 2B :

Final Energy in Hartrees: HF= -1086.0160349 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	1.327397	2.635492	-1.701399
2	6	0	0.516698	2.944093	-0.661899
3	6	0	-0.109304	1.745294	-0.025799
4	6	0	-0.876904	1.879695	1.070401
5	6	0	-1.512305	0.692495	1.742301
6	8	0	-0.888505	0.372995	2.978701
7	6	0	-1.538906	-0.501805	0.762001
8	7	0	-2.652806	-0.331303	-0.169399
9	6	0	-3.181608	-1.382703	-0.866799
10	6	0	-4.323907	-1.053401	-1.810499
11	8	0	-2.758409	-2.529503	-0.728799
12	6	0	-0.215307	-0.659106	-0.022999
13	6	0	0.956993	-1.256108	0.768701
14	8	0	1.464894	-0.310408	1.712801
15	6	0	2.109592	-1.783509	-0.104999
16	8	0	3.081191	-2.251710	0.836001
17	6	0	2.755993	-0.763510	-1.042299
18	8	0	3.999492	-1.364311	-1.445899
19	8	0	0.163395	0.575693	-0.671299
20	8	0	0.329499	4.087093	-0.294899
21	1	0	-2.549805	0.927597	2.005901
22	1	0	-1.715008	-1.422504	1.323801
23	1	0	0.559692	-2.131707	1.303901
24	1	0	1.734191	-2.629109	-0.700199
25	1	0	-0.415808	-1.353506	-0.843299
26	1	0	1.667098	3.482291	-2.037599
27	1	0	-0.997902	2.869095	1.494901
28	1	0	0.059694	0.221793	2.798801
29	1	0	-2.962705	0.606697	-0.382399
30	1	0	-4.598406	0.005199	-1.815599
31	1	0	-4.042008	-1.355802	-2.822999
32	1	0	-5.195908	-1.646600	-1.521399
33	1	0	2.293293	-0.691609	2.050001
34	1	0	3.915591	-2.346911	0.348901
35	1	0	2.115693	-0.573109	-1.908499
36	1	0	2.931794	0.181690	-0.517799
37	1	0	4.532293	-0.715712	-1.920999

	1	2	3
	A	A	A
Frequencies --	29.7006	39.4068	49.1798
Red. masses --	4.9379	5.4471	10.9286
Frc consts --	0.0026	0.0050	0.0156
IR Inten --	0.4655	0.5008	2.0664

Theoretical data for compound 3A :

Final Energy in Hartrees: HF = -781.7194156 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.239058	2.699872	-0.292742
2	6	0	0.129528	1.338074	0.283460
3	6	0	-0.809857	0.188696	-0.138002
4	7	0	-2.166944	0.505547	0.324615
5	6	0	-3.289480	-0.151513	-0.079200
6	6	0	-4.611030	0.399821	0.418358
7	8	0	-3.247321	-1.140426	-0.817791
8	6	0	-0.301528	-1.172176	0.408736
9	8	0	-0.751690	-2.273392	-0.364694
10	6	0	1.199982	-1.225714	0.398541
11	6	0	1.962702	-0.164028	0.104794
12	6	0	3.447629	-0.277903	0.019255
13	8	0	4.048940	0.886085	-0.314296
14	8	0	4.065644	-1.304437	0.222789
15	8	0	1.470783	1.085833	-0.157321
16	1	0	0.151607	1.383623	1.386107
17	1	0	-0.821342	0.124883	-1.233287
18	1	0	-0.663542	-1.268312	1.448336
19	1	0	-1.198276	3.060459	0.089255
20	1	0	-0.297050	2.649307	-1.384188
21	1	0	-2.282831	1.275276	0.967844
22	1	0	-5.165695	-0.405588	0.906530
23	1	0	-4.506485	1.238468	1.112141
24	1	0	-5.197483	0.725195	-0.445964
25	1	0	-1.682793	-2.105947	-0.615197
26	1	0	1.676122	-2.181598	0.581317
27	1	0	5.002028	0.698297	-0.353801
28	1	0	0.530175	3.427024	-0.020097

	1	2	3
	A	A	A
Frequencies --	30.5263	50.5430	58.0496
Red. masses --	5.8892	9.2431	3.9152
Frc consts --	0.0032	0.0139	0.0078
IR Inten --	0.0885	0.8529	8.9625

Theoretical data for compound 3TS :

Final Energy in Hartrees: HF = -781.7160383 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.485709	2.548029	0.020783
2	6	0	-0.042233	1.211639	-0.477336
3	6	0	0.802003	-0.002514	-0.039025
4	7	0	2.173616	0.118681	-0.520967
5	6	0	3.280693	-0.027300	0.279538
6	6	0	4.619857	0.202349	-0.398591
7	8	0	3.197854	-0.322763	1.467796
8	6	0	0.158447	-1.314431	-0.532177
9	8	0	0.626156	-2.452482	0.188159
10	6	0	-1.332064	-1.265189	-0.371898
11	6	0	-1.981823	-0.123816	-0.098004
12	6	0	-3.460406	-0.118606	0.115784
13	8	0	-3.947339	1.106265	0.410296
14	8	0	-4.162357	-1.107676	0.037766
15	8	0	-1.387711	1.098195	0.026097
16	1	0	-0.112606	1.218969	-1.578713
17	1	0	0.854465	-0.029613	1.053753
18	1	0	0.406941	-1.440194	-1.602179
19	1	0	1.472398	2.756949	-0.400079
20	1	0	0.564059	2.545073	1.112080
21	1	0	2.316782	0.317110	-1.501974
22	1	0	5.262721	-0.660666	-0.207937
23	1	0	4.547759	0.366881	-1.477535
24	1	0	5.096195	1.073344	0.061434
25	1	0	1.579084	-2.367832	0.335227
26	1	0	-1.894975	-2.187740	-0.446667
27	1	0	-4.904458	0.995920	0.540759
28	1	0	-0.197599	3.347765	-0.276748

	1	2	3
	A	A	A
Frequencies --	-74.6194	41.8396	49.7637
Red. masses --	4.2687	5.5764	9.7734
Frc consts --	0.0140	0.0058	0.0143
IR Inten --	20.5460	1.5634	1.4728

Theoretical data for compound 3C :

Final Energy in Hartrees: HF = -781.7167761 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.658963	-2.402890	-0.223373
2	6	0	-0.040803	-1.065711	-0.597027
3	6	0	-0.794536	0.162308	-0.043620
4	7	0	-2.181708	0.210275	-0.488609
5	6	0	-3.252939	-0.100115	0.319983
6	6	0	-4.615568	-0.050922	-0.350173
7	8	0	-3.122700	-0.389372	1.503070
8	6	0	-0.067955	1.455403	-0.456419
9	8	0	-0.487880	2.579447	0.312221
10	6	0	1.411228	1.300771	-0.271638
11	6	0	1.980456	0.098457	-0.090303
12	6	0	3.451803	-0.018511	0.145348
13	8	0	3.856204	-1.292294	0.336793
14	8	0	4.214024	0.927967	0.166757
15	8	0	1.311030	-1.088181	-0.087606
16	1	0	0.033431	-0.976371	-1.693950
17	1	0	-0.818540	0.101970	1.048432
18	1	0	-0.280775	1.652430	-1.524456
19	1	0	-1.652245	-2.505801	-0.667954
20	1	0	-0.752160	-2.494590	0.862075
21	1	0	-2.358552	0.365582	-1.472364
22	1	0	-5.264534	0.612673	0.227277
23	1	0	-4.586867	0.290375	-1.389102
24	1	0	-5.057775	-1.050960	-0.315953
25	1	0	-1.452216	2.641734	0.258525
26	1	0	2.032643	2.187819	-0.257439
27	1	0	4.815280	-1.254900	0.491845
28	1	0	-0.027502	-3.215171	-0.593219

	1	2	3
	A	A	A
Frequencies --	43.3550	45.7869	52.9325
Red. masses --	4.9078	5.8914	4.1922
Frc consts --	0.0054	0.0073	0.0069
IR Inten --	1.3218	4.5777	0.3466

Theoretical data for compound 3TS' :

Final Energy in Hartrees: HF = -781.7084934 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.273770	-1.540127	1.687843
2	6	0	-0.091486	-1.100301	0.270455
3	6	0	-0.947145	0.200271	0.253051
4	7	0	-2.105135	0.105009	-0.633673
5	6	0	-3.344940	-0.285749	-0.188624
6	6	0	-4.412607	-0.440595	-1.257316
7	8	0	-3.583023	-0.483558	0.999337
8	6	0	-0.133867	1.485403	-0.081246
9	8	0	-0.503950	2.585276	0.745949
10	6	0	1.345801	1.293893	0.018246
11	6	0	1.882556	0.098784	-0.269050
12	6	0	3.359137	-0.097675	-0.329814
13	8	0	3.712478	-1.386089	-0.532743
14	8	0	4.171135	0.800140	-0.212789
15	8	0	1.110150	-0.995263	-0.542433
16	1	0	-0.656509	-1.893232	-0.224303
17	1	0	-1.360282	0.331868	1.255442
18	1	0	-0.346657	1.743779	-1.134707
19	1	0	-0.638787	-1.754400	2.252663
20	1	0	0.828077	-0.761605	2.221122
21	1	0	-1.943428	0.133764	-1.631551
22	1	0	-5.266032	0.189177	-0.992151
23	1	0	-4.072009	-0.177671	-2.262861
24	1	0	-4.759274	-1.478115	-1.257465
25	1	0	-1.438740	2.785610	0.600129
26	1	0	1.977099	2.144924	0.242131
27	1	0	4.684104	-1.401983	-0.563041
28	1	0	0.886738	-2.444647	1.650469

	1	2	3
	A	A	A
Frequencies --	-34.2984	21.9337	51.9748
Red. masses --	5.0362	5.9415	4.6353
Frc consts --	0.0035	0.0017	0.0074
IR Inten --	0.8853	7.0860	2.3672

Theoretical data for compound 3B :

Final Energy in Hartrees: HF = -781.7186536 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.686899	2.152428	1.600675
2	6	0	0.076897	0.764219	1.421569
3	6	0	-1.029147	0.679460	0.361472
4	7	0	-1.684166	-0.621748	0.457790
5	6	0	-2.953886	-0.818355	-0.009465
6	6	0	-3.512583	-2.222032	0.133607
7	8	0	-3.608289	0.097612	-0.507413
8	6	0	-0.468574	0.911535	-1.068143
9	8	0	-0.390012	2.304278	-1.397586
10	6	0	0.895373	0.307563	-1.212110
11	6	0	1.557782	-0.219028	-0.167437
12	6	0	2.877200	-0.892888	-0.364898
13	8	0	3.432068	-1.318828	0.790771
14	8	0	3.406239	-1.048732	-1.448091
15	8	0	1.109645	-0.214732	1.122269
16	1	0	-0.324620	0.417205	2.378228
17	1	0	-1.787043	1.442202	0.561265
18	1	0	-1.149701	0.413305	-1.770255
19	1	0	-0.086909	2.855952	1.924703
20	1	0	1.118940	2.536075	0.674991
21	1	0	-1.142874	-1.407637	0.791075
22	1	0	-2.810551	-2.929672	0.583471
23	1	0	-4.416539	-2.177039	0.747659
24	1	0	-3.805538	-2.586379	-0.854920
25	1	0	-1.279362	2.610795	-1.624169
26	1	0	1.359636	0.272005	-2.190300
27	1	0	4.275874	-1.738062	0.550801
28	1	0	1.460858	2.109299	2.371707

	1	2	3
	A	A	A
Frequencies --	42.3509	47.4959	58.3532
Red. masses --	4.8127	7.3181	3.1848
Frc consts --	0.0051	0.0097	0.0064
IR Inten --	0.8317	1.1110	5.6500

Theoretical data for compound 4A :

Final Energy in Hartrees: HF = -534.3670502 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.955360	1.814094	0.257298
2	6	0	-2.025574	0.870263	-0.280016
3	6	0	-1.833978	-0.528972	0.325046
4	8	0	-2.551865	-1.540419	-0.390243
5	6	0	-0.378771	-0.894754	0.278120
6	6	0	0.583239	0.023899	0.079244
7	6	0	2.015633	-0.389499	-0.015270
8	8	0	2.849543	0.644254	-0.260989
9	8	0	2.404785	-1.534584	0.110452
10	8	0	0.373764	1.363782	-0.062702
11	1	0	-1.025400	1.907945	1.350697
12	1	0	-1.942056	0.791668	-1.369665
13	1	0	-2.172418	-0.526543	1.375031
14	1	0	-3.498209	-1.420480	-0.235106
15	1	0	-0.094594	-1.935253	0.379682
16	1	0	3.743940	0.266606	-0.311681
17	1	0	-3.018991	1.271199	-0.045654
18	1	0	-1.033228	2.810411	-0.181979

	1	2	3
	A	A	A
Frequencies --	53.0511	111.4331	136.9818
Red. masses --	8.5722	4.3396	5.3073
Frc consts --	0.0142	0.0317	0.0587
IR Inten --	1.2966	8.6301	0.5972

Theoretical data for compound 4TS :

Final Energy in Hartrees: HF = -534.3589057 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.819195	1.820370	0.265534
2	6	0	2.070599	0.910230	0.230658
3	6	0	1.787491	-0.497884	-0.351387
4	8	0	2.691809	-1.477916	0.159117
5	6	0	0.390424	-0.937570	-0.052836
6	6	0	-0.595934	-0.030320	-0.136067
7	6	0	-2.026989	-0.405225	0.033851
8	8	0	-2.860210	0.658799	-0.000891
9	8	0	-2.419674	-1.546216	0.188792
10	8	0	-0.334725	1.281941	-0.419521
11	1	0	0.999060	2.780282	-0.220191
12	1	0	2.434012	0.759049	1.251883
13	1	0	1.886197	-0.448065	-1.449202
14	1	0	3.576041	-1.302732	-0.188391
15	1	0	0.179489	-1.975880	0.171741
16	1	0	-3.758784	0.305269	0.111757
17	1	0	2.877735	1.384110	-0.339653
18	1	0	0.519930	2.007506	1.303568

	1	2	3
	A	A	A
Frequencies --	-99.1045	56.5361	112.4554
Red. masses --	1.8357	8.2658	4.2883
Frc consts --	0.0106	0.0156	0.0320
IR Inten --	1.6107	1.0176	6.1502

Theoretical data for compound 4B :

Final Energy in Hartrees: HF = -534.3688084 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.118916	1.586863	-0.308663
2	6	0	-2.017344	0.783164	0.623127
3	6	0	-1.786114	-0.718571	0.389753
4	8	0	-2.458786	-1.189686	-0.793329
5	6	0	-0.320726	-0.993920	0.224779
6	6	0	0.576393	-0.002622	0.064987
7	6	0	2.039354	-0.306740	0.003825
8	8	0	2.800687	0.791274	-0.189671
9	8	0	2.507659	-1.423070	0.116348
10	8	0	0.270851	1.317547	-0.042612
11	1	0	-1.231249	2.664270	-0.176804
12	1	0	-3.067284	1.039769	0.442214
13	1	0	-2.150503	-1.286138	1.258760
14	1	0	-3.397860	-1.303188	-0.591591
15	1	0	0.038215	-2.015404	0.252610
16	1	0	3.722972	0.484425	-0.209657
17	1	0	-1.787622	1.035602	1.665954
18	1	0	-1.325829	1.323108	-1.354222

	1	2	3
	A	A	A
Frequencies --	54.3431	109.0751	127.8473
Red. masses --	8.2021	4.7196	5.3046
Frc consts --	0.0143	0.0331	0.0511
IR Inten --	2.0783	2.7099	1.9749

Theoretical data for compound 5A :

Final Energy in Hartrees: HF = -667.1778869 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.209906	-0.769966	-0.716999
2	6	0	-0.916133	0.298275	0.133060
3	7	0	-2.295303	0.480230	-0.297434
4	6	0	-3.335459	-0.252695	0.216032
5	6	0	-4.712360	0.073099	-0.336294
6	8	0	-3.166344	-1.114226	1.073455
7	6	0	-0.133634	1.616252	0.061009
8	6	0	1.346265	1.356618	0.096255
9	6	0	1.862654	0.121511	-0.033166
10	6	0	3.333120	-0.103141	0.087545
11	8	0	3.686309	-1.395153	-0.079403
12	8	0	4.141176	0.778026	0.313880
13	8	0	1.130169	-1.006220	-0.263928
14	1	0	-0.176156	-0.454276	-1.770454
15	1	0	-0.949883	-0.064081	1.164657
16	1	0	-0.391531	2.164529	-0.859578
17	1	0	-2.488303	1.161105	-1.018219
18	1	0	-5.354425	0.386746	0.491587
19	1	0	-4.708529	0.855628	-1.100667
20	1	0	-5.144363	-0.837928	-0.759405
21	1	0	2.036107	2.176432	0.259198
22	1	0	4.651890	-1.431395	0.027646
23	1	0	-0.422224	2.271623	0.892078
24	1	0	-0.723222	-1.729133	-0.641493

	1	2	3
	Å	Å	Å
Frequencies --	27.8783	47.9963	54.5326
Red. masses --	4.5935	3.3672	1.6761
Frc consts --	0.0021	0.0046	0.0029
IR Inten --	7.2726	3.1523	2.9213

Theoretical data for compound 5TS :

Final Energy in Hartrees: HF = -667.169153 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.145089	-1.046829	-0.029154
2	6	0	-0.934523	0.274840	0.205749
3	7	0	-2.245891	0.262343	-0.431757
4	6	0	-3.382547	-0.144567	0.218803
5	6	0	-4.663279	-0.102113	-0.596694
6	8	0	-3.371779	-0.514653	1.389654
7	6	0	-0.129130	1.512814	-0.248813
8	6	0	1.325256	1.362894	0.084091
9	6	0	1.895126	0.167237	-0.135017
10	6	0	3.349046	-0.070434	0.082500
11	8	0	3.715337	-1.352060	-0.137743
12	8	0	4.136305	0.793249	0.421867
13	8	0	1.165673	-0.884286	-0.615970
14	1	0	-0.683360	-1.694790	-0.722623
15	1	0	-1.134182	0.358800	1.276005
16	1	0	-0.224300	1.613091	-1.342587
17	1	0	-2.306315	0.503881	-1.411164
18	1	0	-5.383111	0.539622	-0.081192
19	1	0	-4.525018	0.264958	-1.617794
20	1	0	-5.088984	-1.108820	-0.633076
21	1	0	1.919172	2.183239	0.467938
22	1	0	4.673117	-1.395005	0.023563
23	1	0	-0.560299	2.415780	0.191200
24	1	0	-0.018932	-1.578202	0.920773

	1	2	3
	A	A	A
Frequencies --	-40.8111	25.7654	60.1037
Red. masses --	3.3505	5.8318	5.0825
Frc consts --	0.0033	0.0023	0.0108
IR Inten --	3.1614	7.5693	2.4598

Theoretical data for compound 5B :

Final Energy in Hartrees: HF = -667.1794514 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.026325	-0.802772	1.617646
2	6	0	1.039937	-0.966328	0.535855
3	7	0	1.650423	0.332103	0.268615
4	6	0	2.935174	0.451078	-0.185624
5	6	0	3.423592	1.866289	-0.440331
6	8	0	3.655624	-0.528325	-0.368619
7	6	0	0.382482	-1.581597	-0.717836
8	6	0	-0.979684	-0.992572	-0.954779
9	6	0	-1.590470	-0.209517	-0.047405
10	6	0	-2.907488	0.423255	-0.339117
11	8	0	-3.368238	1.182131	0.679904
12	8	0	-3.515132	0.284263	-1.383908
13	8	0	-1.067542	0.091769	1.185736
14	1	0	0.377837	-0.357251	2.528345
15	1	0	1.835963	-1.624363	0.894261
16	1	0	1.029569	-1.417147	-1.586376
17	1	0	1.071086	1.155857	0.355296
18	1	0	2.674736	2.634814	-0.228968
19	1	0	4.306517	2.047590	0.178981
20	1	0	3.734297	1.946760	-1.485793
21	1	0	-1.499275	-1.173831	-1.889106
22	1	0	-4.219965	1.546848	0.385319
23	1	0	0.307477	-2.672219	-0.601640
24	1	0	-0.472215	-1.777493	1.854023

	1	2	3
	A	A	A
Frequencies --	28.4601	48.4263	54.9798
Red. masses --	5.8829	6.6168	5.6907
Frc consts --	0.0028	0.0091	0.0101
IR Inten --	4.5063	0.3131	5.8310

Theoretical data for compound 6A :

Final Energy in Hartrees: HF = -498.4738783 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.450158	-1.733933	0.011884
2	6	0	-1.623220	-0.509036	-0.341709
3	6	0	-2.082880	0.777779	0.348123
4	6	0	-1.180807	1.954933	-0.055090
5	6	0	0.258007	1.525578	-0.091455
6	6	0	0.615905	0.230249	-0.022366
7	6	0	2.055053	-0.157322	0.017846
8	8	0	2.245090	-1.494647	0.075292
9	8	0	2.979653	0.634665	0.004269
10	8	0	-0.257132	-0.818277	0.024956
11	1	0	-1.630242	-0.353883	-1.432127
12	1	0	-2.038860	0.623462	1.433508
13	1	0	-1.478046	2.352921	-1.036459
14	1	0	-3.483066	-1.602862	-0.326666
15	1	0	-2.454751	-1.896170	1.094586
16	1	0	1.050776	2.262860	-0.148734
17	1	0	3.207271	-1.629729	0.105764
18	1	0	-2.037321	-2.625626	-0.468155
19	1	0	-1.299921	2.787691	0.649707
20	1	0	-3.128136	0.977914	0.089032

	1	2	3
	A	A	A
Frequencies --	56.2493	104.0554	163.0077
Red. masses --	7.4951	4.2899	3.1803
Frc consts --	0.0140	0.0274	0.0498
IR Inten --	2.1360	3.1780	0.2893

Theoretical data for compound **6TS** :

Final Energy in Hartrees: HF = -498.4616404 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.447916	-1.742071	0.938715
2	6	0	-1.541159	-0.892054	-0.329606
3	6	0	-2.368698	0.405620	-0.132338
4	6	0	-1.524198	1.708507	-0.078704
5	6	0	-0.079686	1.466656	0.240584
6	6	0	0.502481	0.330253	-0.172914
7	6	0	1.955362	0.080082	0.030638
8	8	0	2.348453	-1.146322	-0.383662
9	8	0	2.728887	0.886304	0.515530
10	8	0	-0.197053	-0.642493	-0.831322
11	1	0	-1.983175	-1.492058	-1.128806
12	1	0	-2.932063	0.308311	0.801641
13	1	0	-1.567147	2.202890	-1.060678
14	1	0	-2.448245	-2.052569	1.259772
15	1	0	-0.989857	-1.178610	1.758797
16	1	0	0.518726	2.210355	0.753818
17	1	0	3.304788	-1.194419	-0.216251
18	1	0	-0.848604	-2.637384	0.751478
19	1	0	-3.109989	0.494554	-0.932558
20	1	0	-1.963852	2.417054	0.630174

	1	2	3
	A	A	A
Frequencies --	-115.7088	58.0864	81.5945
Red. masses --	1.9283	7.3575	4.3578
Frc consts --	0.0152	0.0146	0.0171
IR Inten --	0.1869	1.9778	1.7228

Theoretical data for compound 6B :

Final Energy in Hartrees: HF = -498.4711274 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.963787	-1.325277	1.060159
2	6	0	-1.576971	-0.874971	-0.348806
3	6	0	-2.129552	0.498751	-0.750013
4	6	0	-1.501815	1.618274	0.094880
5	6	0	-0.025412	1.390019	0.236924
6	6	0	0.539601	0.206455	-0.066304
7	6	0	2.017436	0.029860	0.031365
8	8	0	2.428693	-1.214892	-0.299070
9	8	0	2.792180	0.905686	0.370599
10	8	0	-0.133045	-0.903293	-0.488867
11	1	0	-1.912965	-1.626619	-1.069469
12	1	0	-3.220770	0.494070	-0.654740
13	1	0	-1.685274	2.594203	-0.371494
14	1	0	-3.054220	-1.388775	1.147511
15	1	0	-1.597927	-0.632434	1.823838
16	1	0	0.628062	2.185994	0.575245
17	1	0	3.396475	-1.212536	-0.207919
18	1	0	-1.542468	-2.312918	1.267112
19	1	0	-1.973392	1.673429	1.087275
20	1	0	-1.897142	0.666900	-1.807889

	1	2	3
	A	A	A
Frequencies --	57.0748	84.7187	163.3301
Red. masses --	7.4717	4.2507	2.7462
Frc consts --	0.0143	0.0180	0.0432
IR Inten --	2.2147	1.5659	0.4173

Theoretical data for compound 7A :

Final Energy in Hartrees: HF = -459.1503584 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.625841	-1.240837	0.311071
2	6	0	2.445571	-0.145859	-0.366339
3	6	0	1.918907	1.234814	0.057645
4	6	0	0.416385	1.231555	0.100137
5	6	0	-0.299982	0.094687	0.020169
6	6	0	-1.789775	0.137757	-0.016324
7	8	0	-2.355806	-1.087372	-0.089375
8	8	0	-2.446816	1.162224	0.013105
9	8	0	0.234003	-1.161182	-0.042499
10	1	0	1.705663	-1.162268	1.405078
11	1	0	2.361251	-0.262920	-1.453132
12	1	0	2.320859	1.517847	1.041619
13	1	0	-0.132240	2.164060	0.170147
14	1	0	-3.316507	-0.941141	-0.115093
15	1	0	3.502985	-0.265042	-0.105712
16	1	0	1.939316	-2.241648	0.007248
17	1	0	2.265956	2.009055	-0.638153

	1	2	3
	A	A	A
Frequencies --	61.7523	112.5726	205.7987
Red. masses --	6.5814	3.8480	5.8010
Frc consts --	0.0148	0.0287	0.1448
IR Inten --	2.4310	3.0964	1.9780

Theoretical data for compound 7TS :

Final Energy in Hartrees: HF = -459.1407397 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.521325	-1.315329	0.247513
2	6	0	-2.504824	-0.121171	0.296848
3	6	0	-1.892747	1.181978	-0.275849
4	6	0	-0.419848	1.266938	-0.005831
5	6	0	0.307243	0.144117	-0.128278
6	6	0	1.785595	0.136740	0.038008
7	8	0	2.326034	-1.099267	-0.057441
8	8	0	2.456198	1.133275	0.238073
9	8	0	-0.282698	-1.047417	-0.451275
10	1	0	-1.946020	-2.171762	-0.278749
11	1	0	-2.790506	0.051693	1.339766
12	1	0	-2.039202	1.192824	-1.366220
13	1	0	0.071118	2.198570	0.249448
14	1	0	3.284894	-0.985784	0.055344
15	1	0	-3.423452	-0.360747	-0.248713
16	1	0	-1.255680	-1.632295	1.263667
17	1	0	-2.421990	2.055137	0.116146

	1	2	3
	A	A	A
Frequencies --	-104.3344	63.5480	111.9685
Red. masses --	1.6939	6.5381	4.1944
Frc consts --	0.0109	0.0156	0.0310
IR Inten --	0.7152	2.5944	3.5470

Theoretical data for compound 7B :

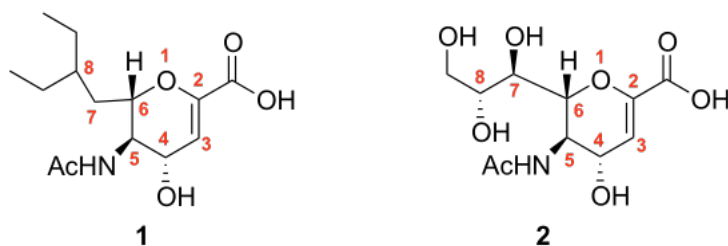
Final Energy in Hartrees: HF = -459.1503584 (B3LYP/6-31+G(D,P))

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.625620	-1.240674	0.311650
2	6	0	-2.445725	-0.146072	-0.366053
3	6	0	-1.918951	1.234719	0.057244
4	6	0	-0.416385	1.231606	0.099778
5	6	0	0.300096	0.094841	0.019991
6	6	0	1.789805	0.137755	-0.016328
7	8	0	2.355668	-1.087436	-0.089809
8	8	0	2.446897	1.162173	0.013778
9	8	0	-0.234062	-1.161123	-0.042834
10	1	0	-1.939120	-2.241709	0.008607
11	1	0	-3.503075	-0.265131	-0.105106
12	1	0	-2.266194	2.008756	-0.638932
13	1	0	0.132030	2.164226	0.169955
14	1	0	3.316370	-0.941217	-0.115186
15	1	0	-2.361697	-0.263734	-1.452801
16	1	0	-1.704992	-1.161393	1.405647
17	1	0	-2.320673	1.518235	1.041043

	1	2	3
	A	A	A
Frequencies --	61.8406	112.5290	205.7833
Red. masses --	6.5800	3.8483	5.7981
Frc consts --	0.0148	0.0287	0.1447
IR Inten --	2.4335	3.0972	1.9714

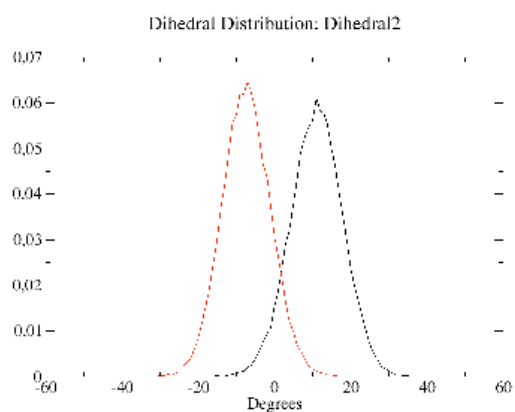
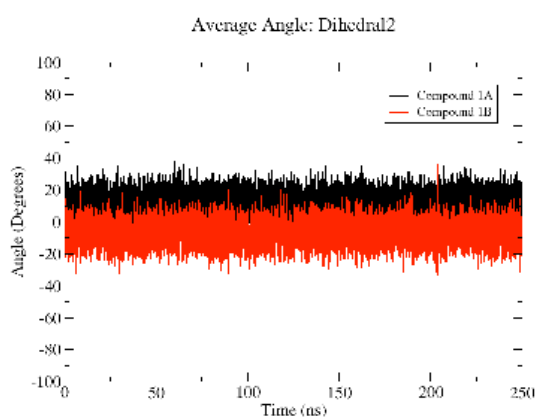
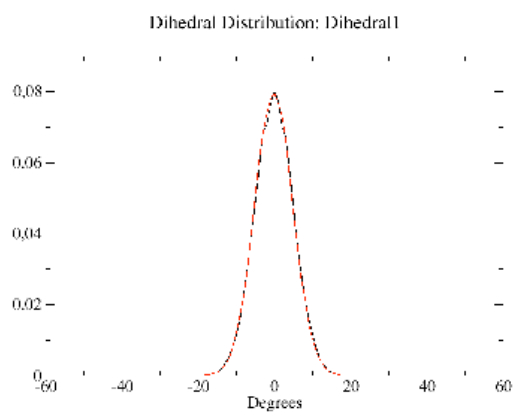
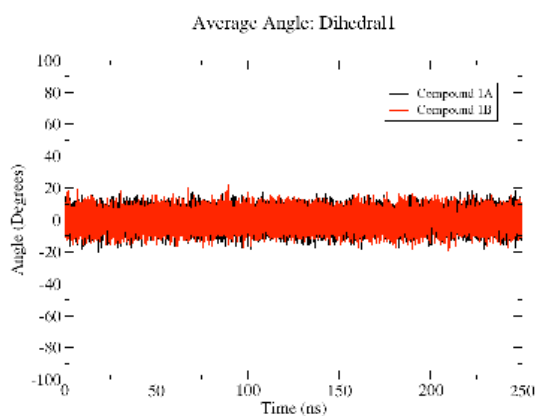
Dihedral angles plots and distributions for compounds 1 and 2 from molecular dynamics simulations

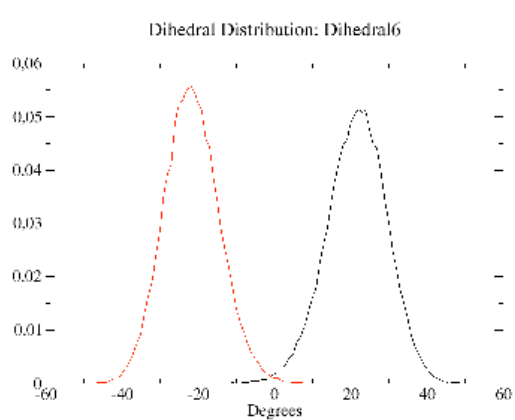
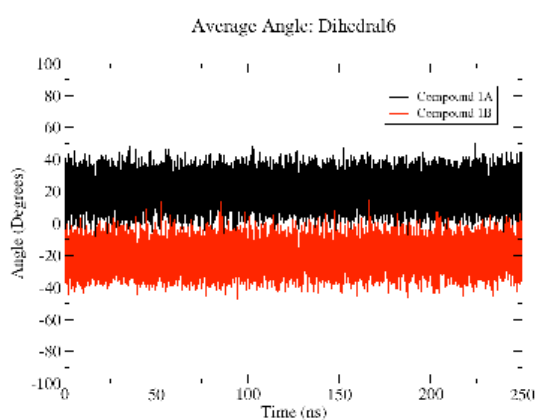
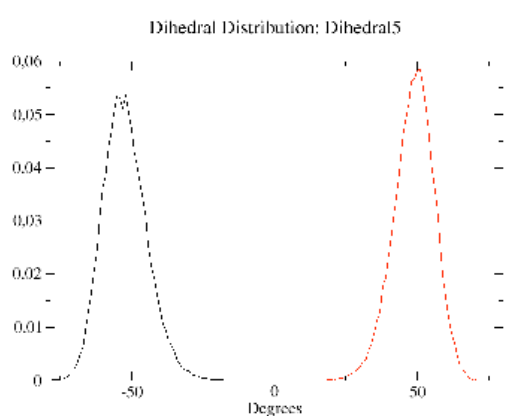
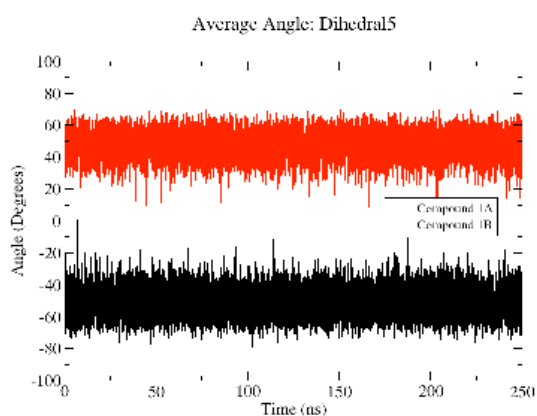
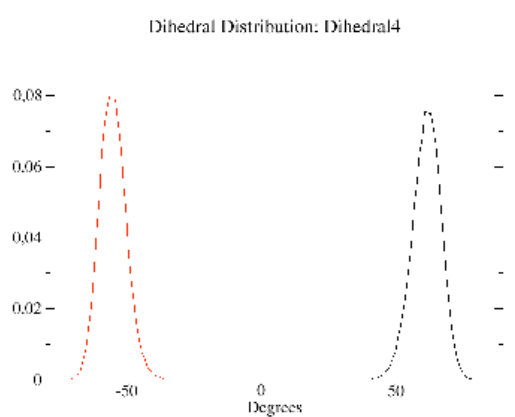
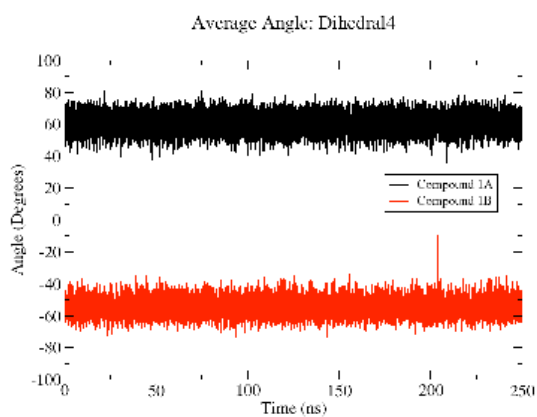
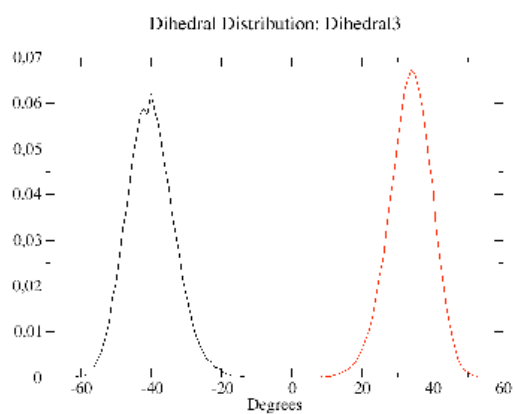
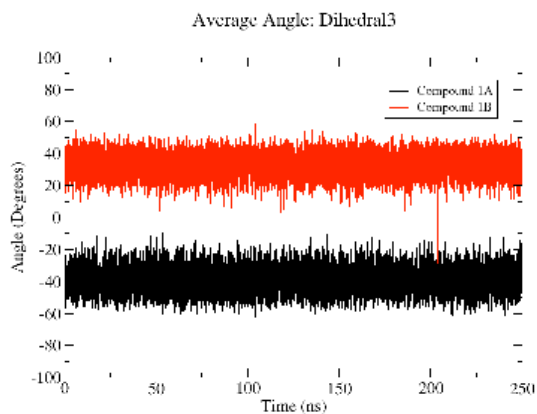


Legend :

- Dihedral 1: 1 – 2 – 3 – 4
- Dihedral 2: 2 – 3 – 4 – 5
- Dihedral 3: 3 – 4 – 5 – 6
- Dihedral 4: 4 – 5 – 6 – 1
- Dihedral 5: 5 – 6 – 1 – 2
- Dihedral 6: 6 – 1 – 2 – 3

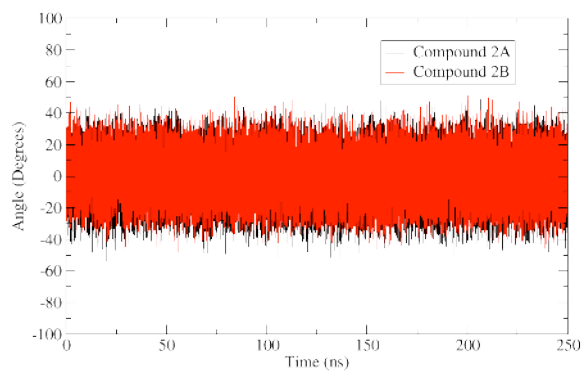
Compound 1



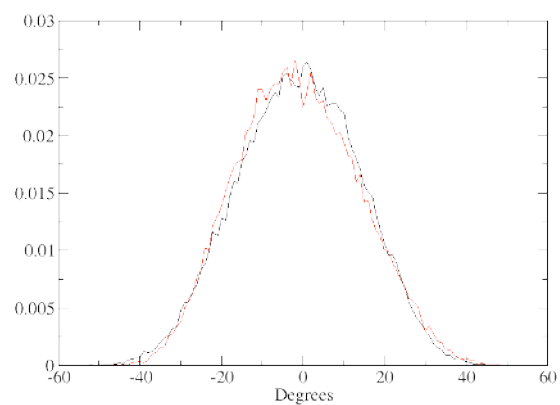


Compound 2

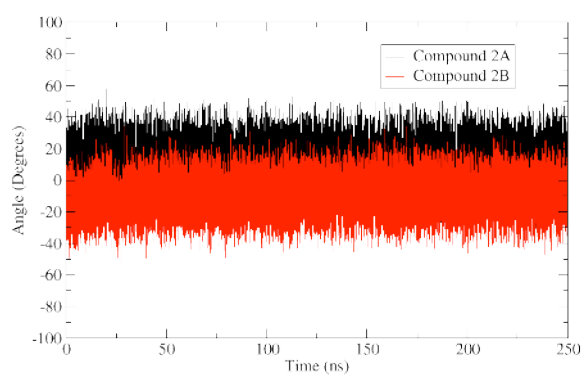
Average Angle: Dihedral1



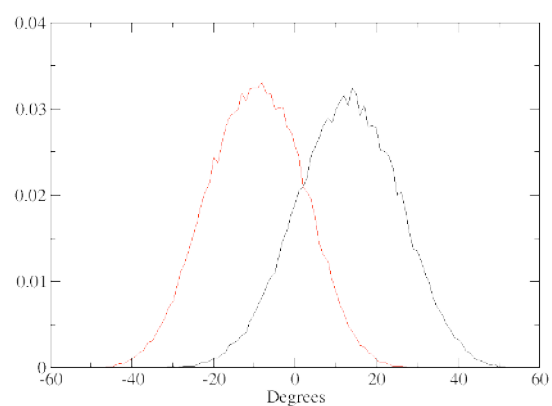
Dihedral Distribution: Dihedral1



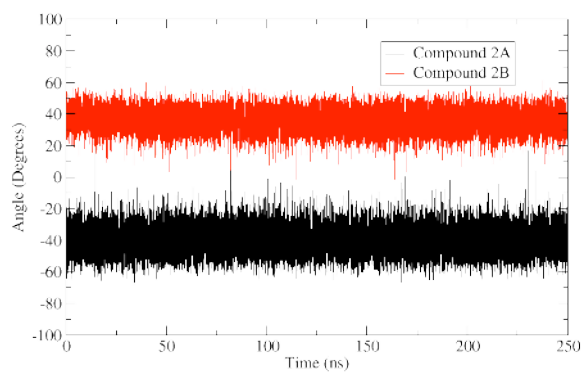
Average Angle: Dihedral2



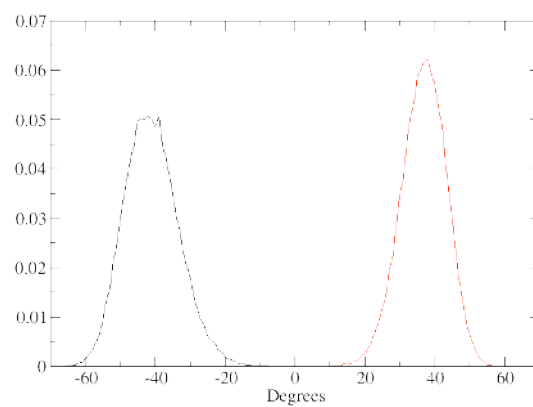
Dihedral Distribution: Dihedral2



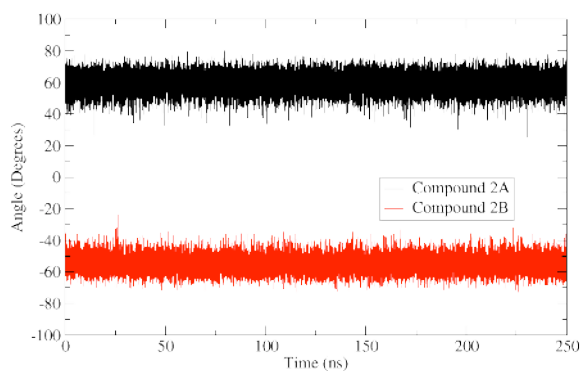
Average Angle: Dihedral3



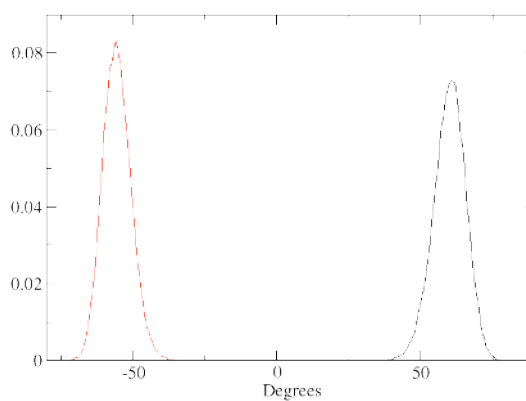
Dihedral Distribution: Dihedral3



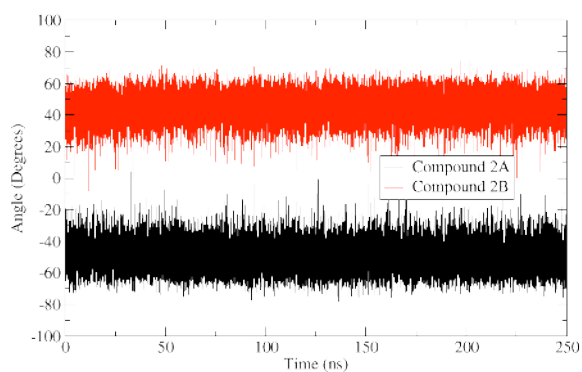
Average Angle: Dihedral4



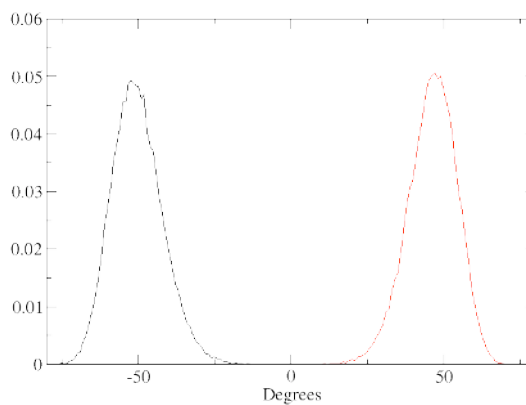
Dihedral Distribution: Dihedral4



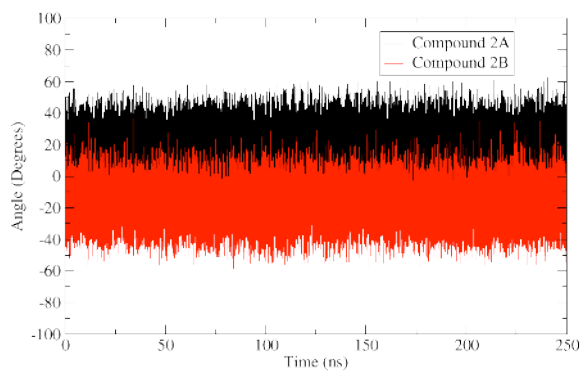
Average Angle: Dihedral5



Dihedral Distribution: Dihedral5



Average Angle: Dihedral6



Dihedral Distribution: Dihedral6

