Supporting Information

Synthesis, Computational Study and Glycosidase Inhibitory Activity of Polyhydroxylated Conidine Alkaloids - A Bicyclic Iminosugar

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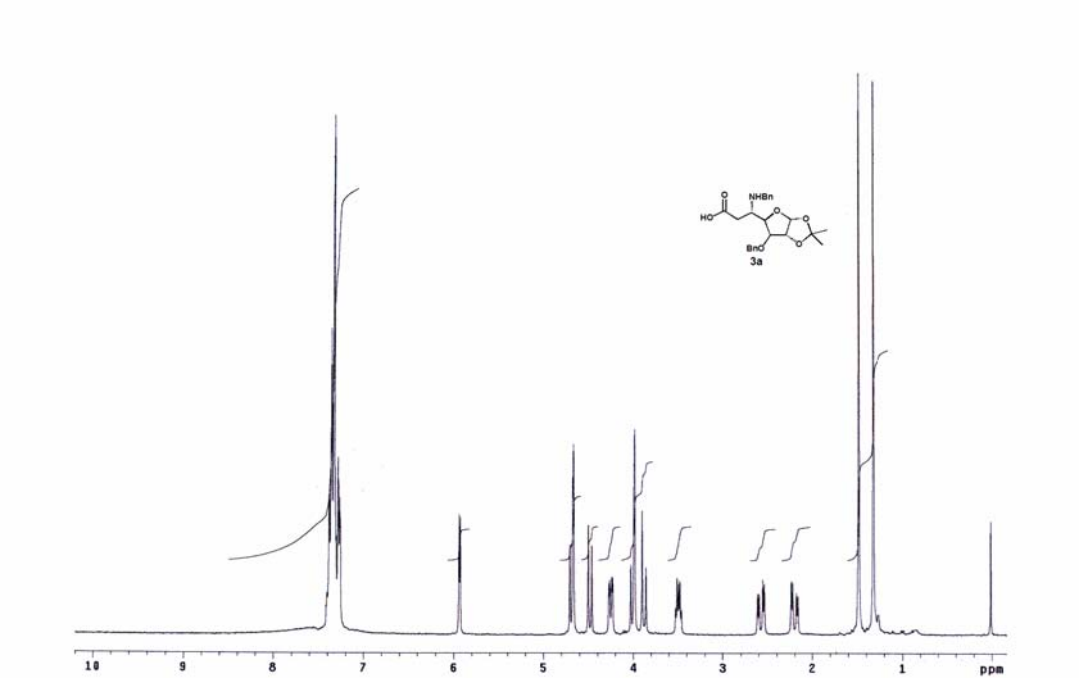


Figure 1S: ^{1}H NMR (300 MHz, $CDCl_3$) Spectrum of compound **3a**

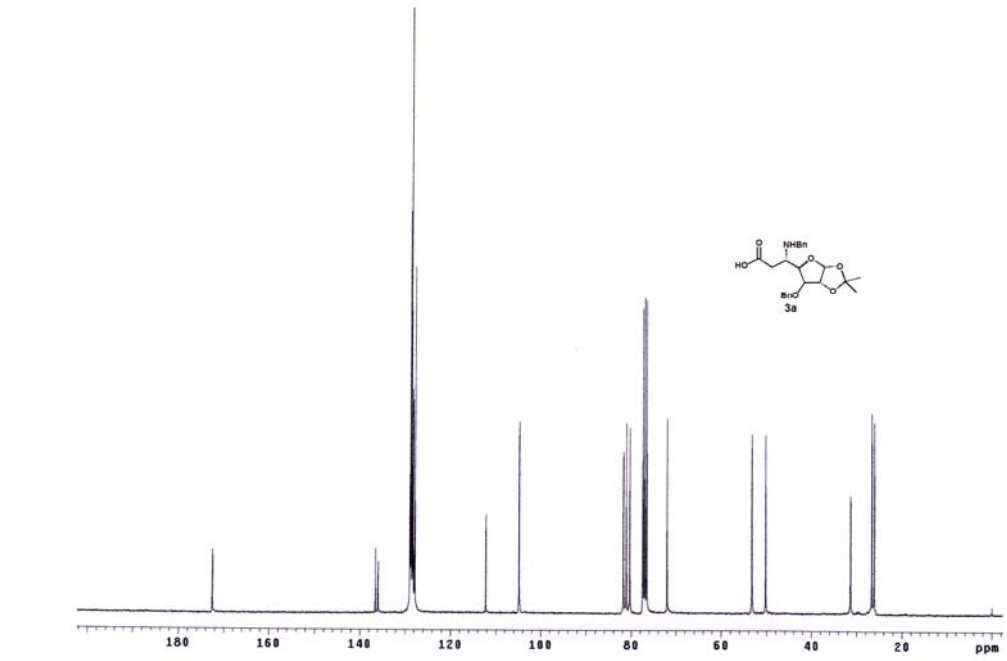


Figure 2S: ^{13}C NMR (75 MHz, $CDCl_3$) Spectrum of compound **3a**

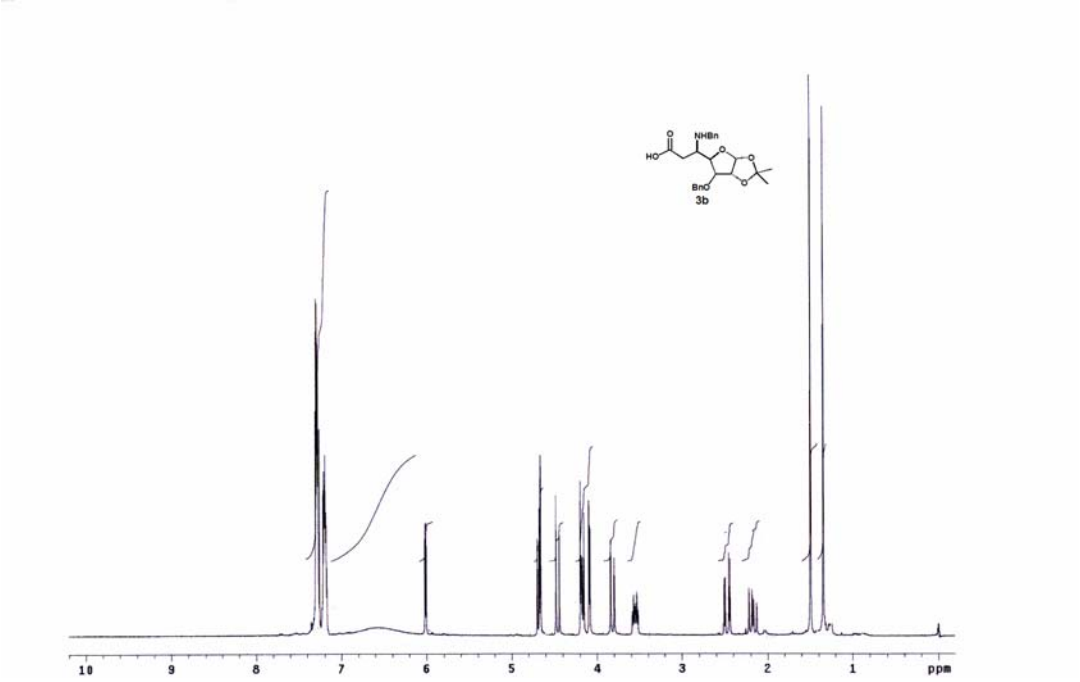


Figure 3S: ^{1}H NMR (300 MHz, $CDCl_3$) Spectrum of compound **3b**

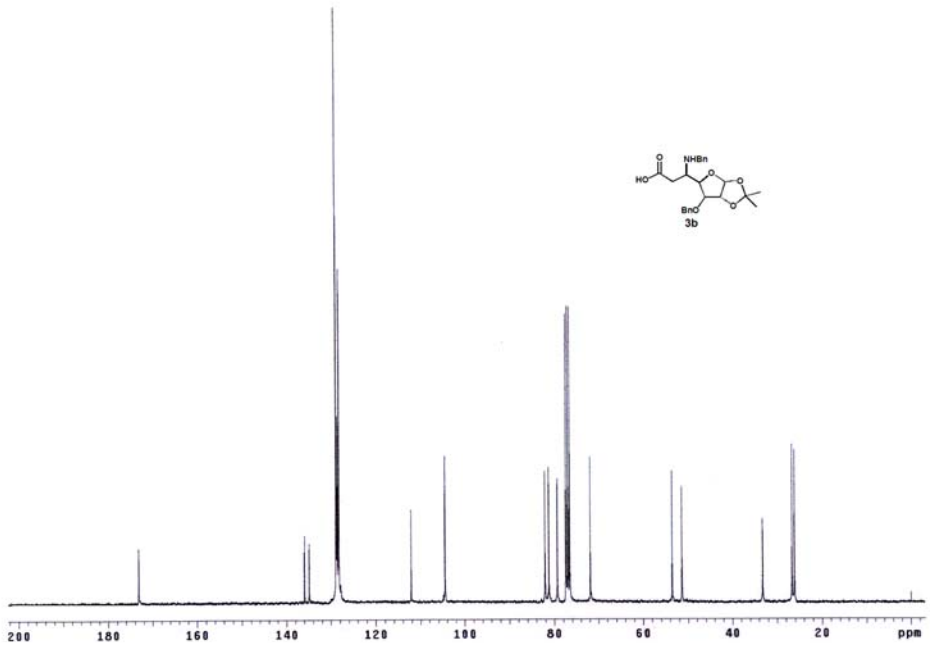


Figure 4S: ^{13}C NMR (75 MHz, $CDCl_3$) Spectrum of compound **3b**

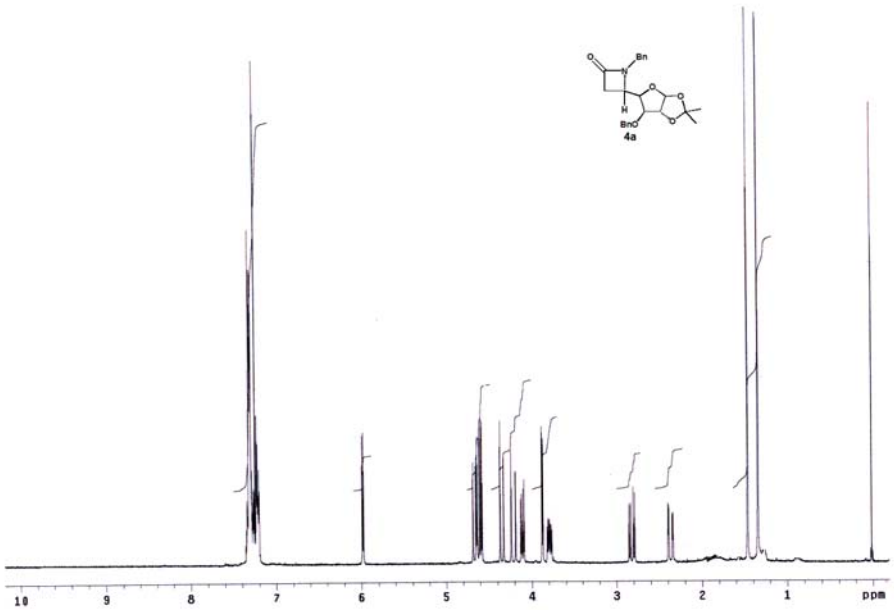


Figure 5S: ^{1}H NMR (300 MHz, $CDCl_3$) Spectrum of compound **4a**

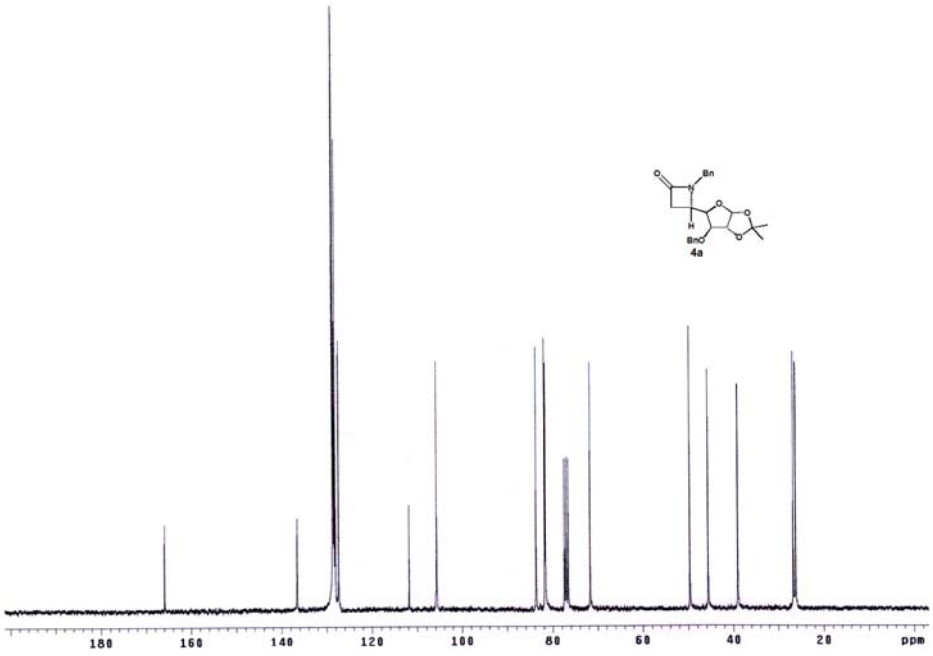


Figure 6S: ^{13}C NMR (75 MHz, $CDCl_3$) Spectrum of compound **4a**

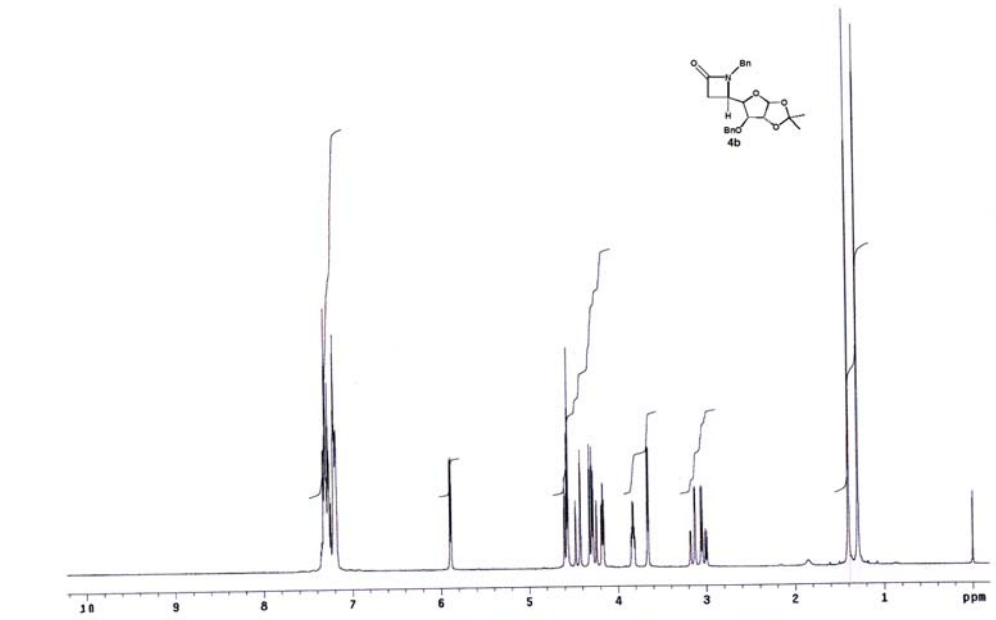


Figure 7S: ^{1}H NMR (300 MHz, $CDCl_3$) Spectrum of compound **4b**

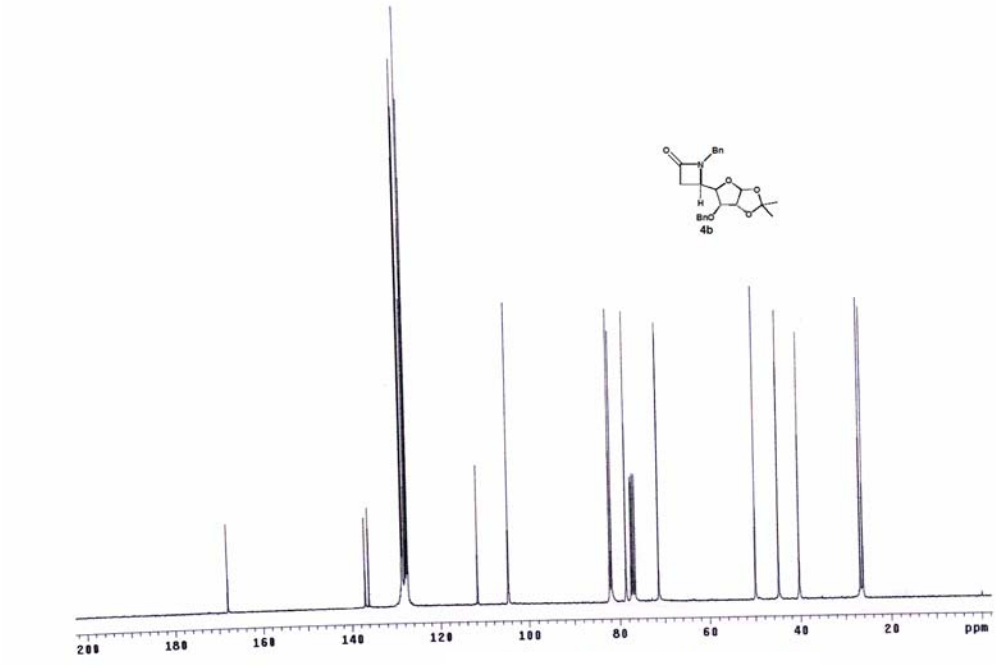


Figure 8S: ^{13}C NMR (75 MHz, $CDCl_3$) Spectrum of compound **4b**

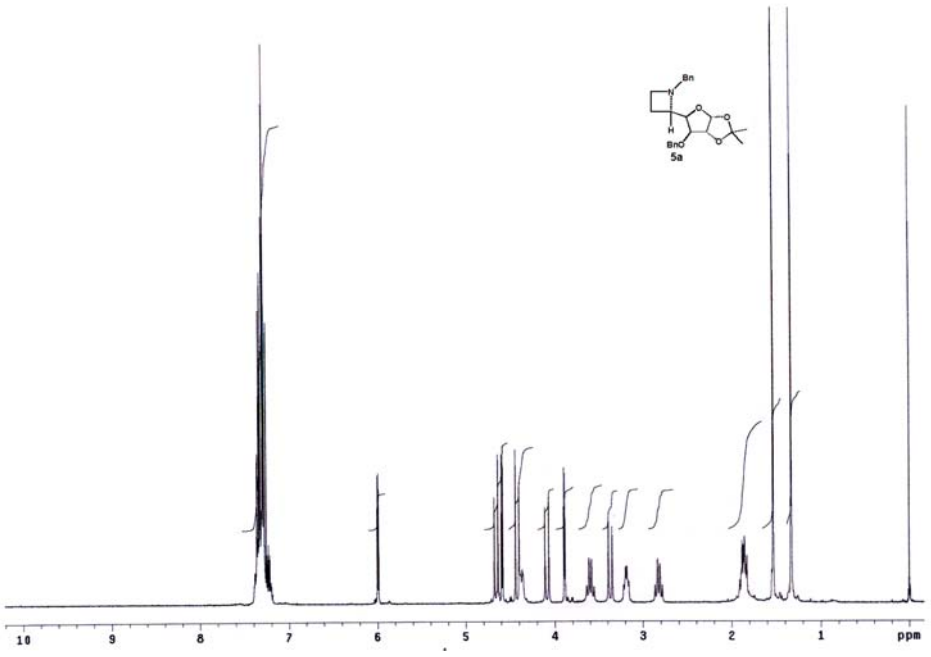


Figure 9S: ^{1}H NMR (300 MHz, $CDCl_3$) Spectrum of compound **5a**

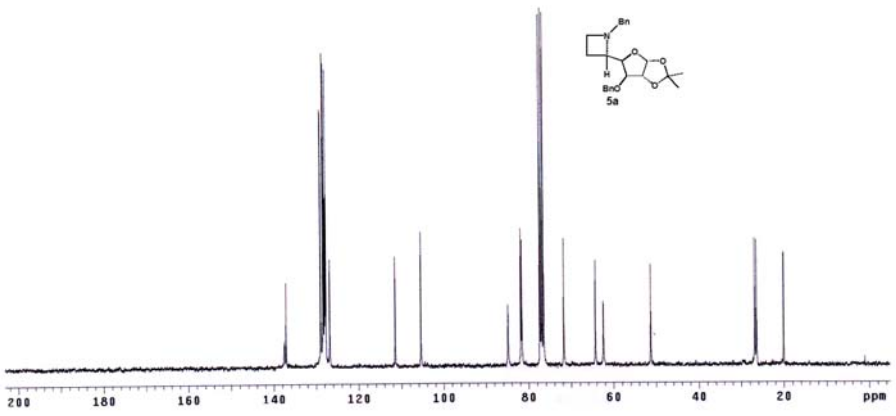


Figure 10S: ^{13}C NMR (75 MHz, $CDCl_3$) Spectrum of compound **5a**

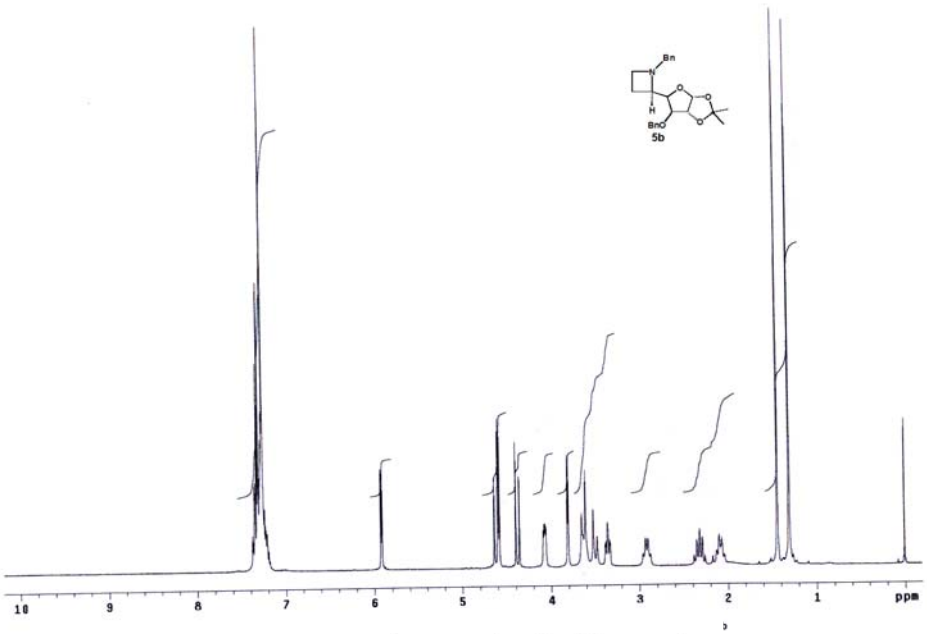


Figure 11S: ^{1}H NMR (300 MHz, $CDCl_3$) Spectrum of compound **5b**

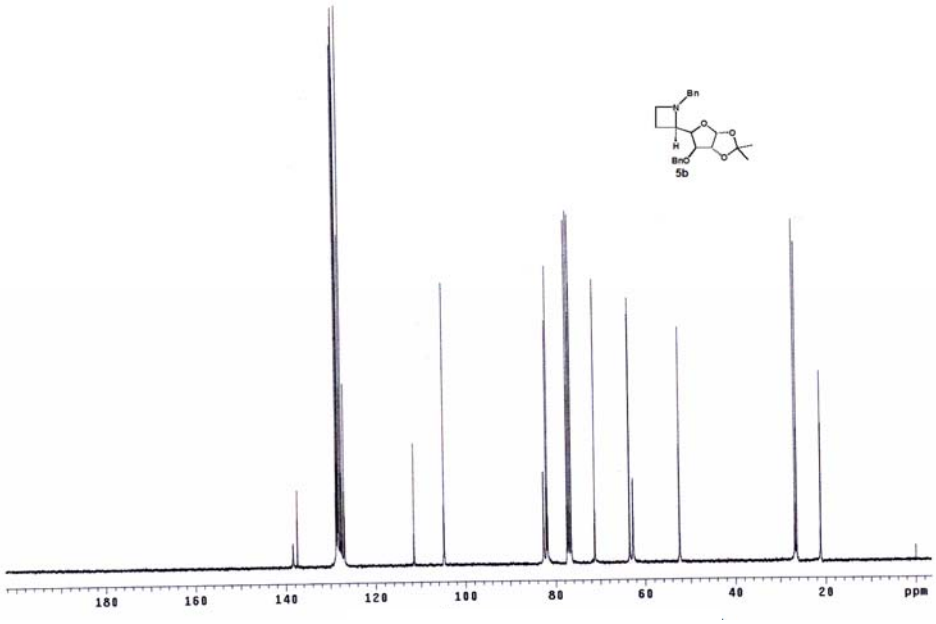


Figure 12S: ^{13}C NMR (75 MHz, $CDCl_3$) Spectrum of compound **5b**

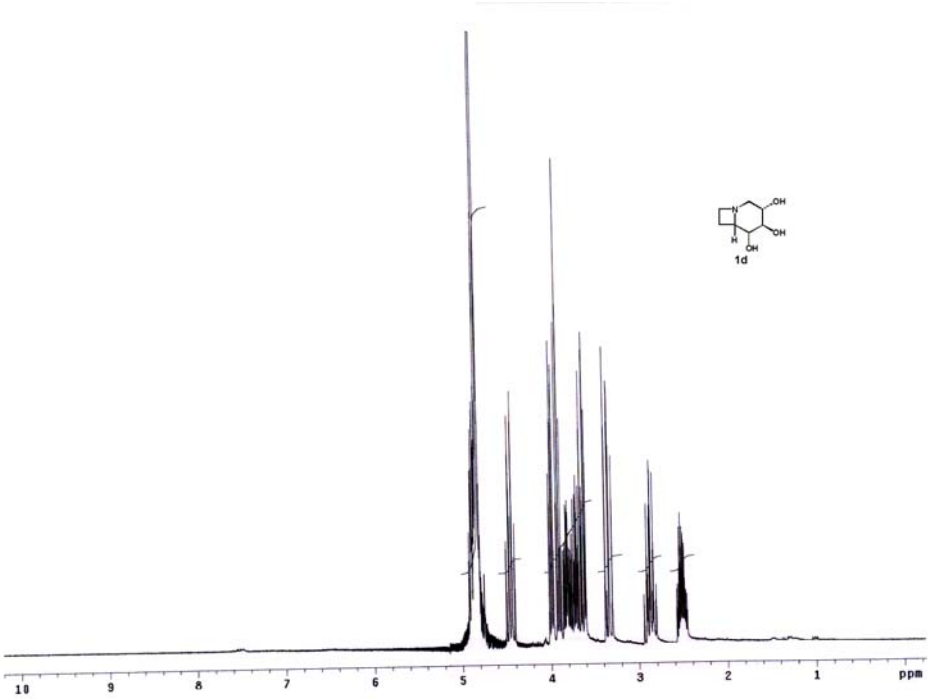


Figure 13S: ^{1}H NMR (300 MHz, D_2O) Spectrum of compound **1d**

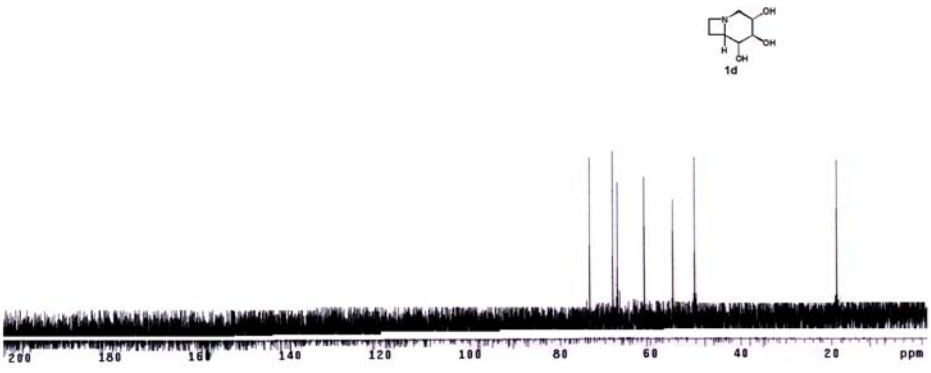


Figure 14S: ^{13}C NMR (75 MHz, D_2O) Spectrum of compound **1d**

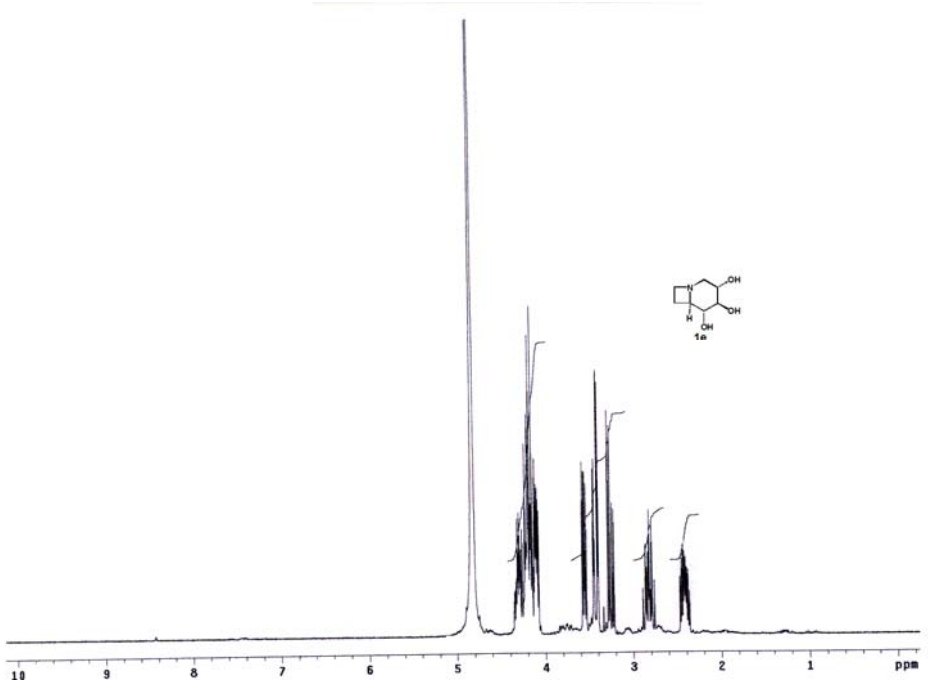


Figure 15S: ^{1}H NMR (300 MHz, D_2O) Spectrum of compound **1e**

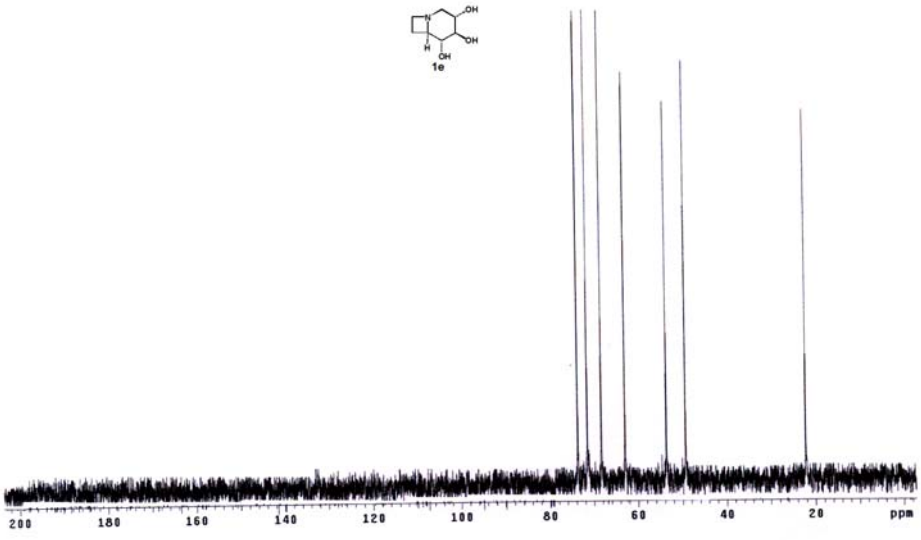


Figure 16S: ^{13}C NMR (75 MHz, D_2O) Spectrum of compound **1e**

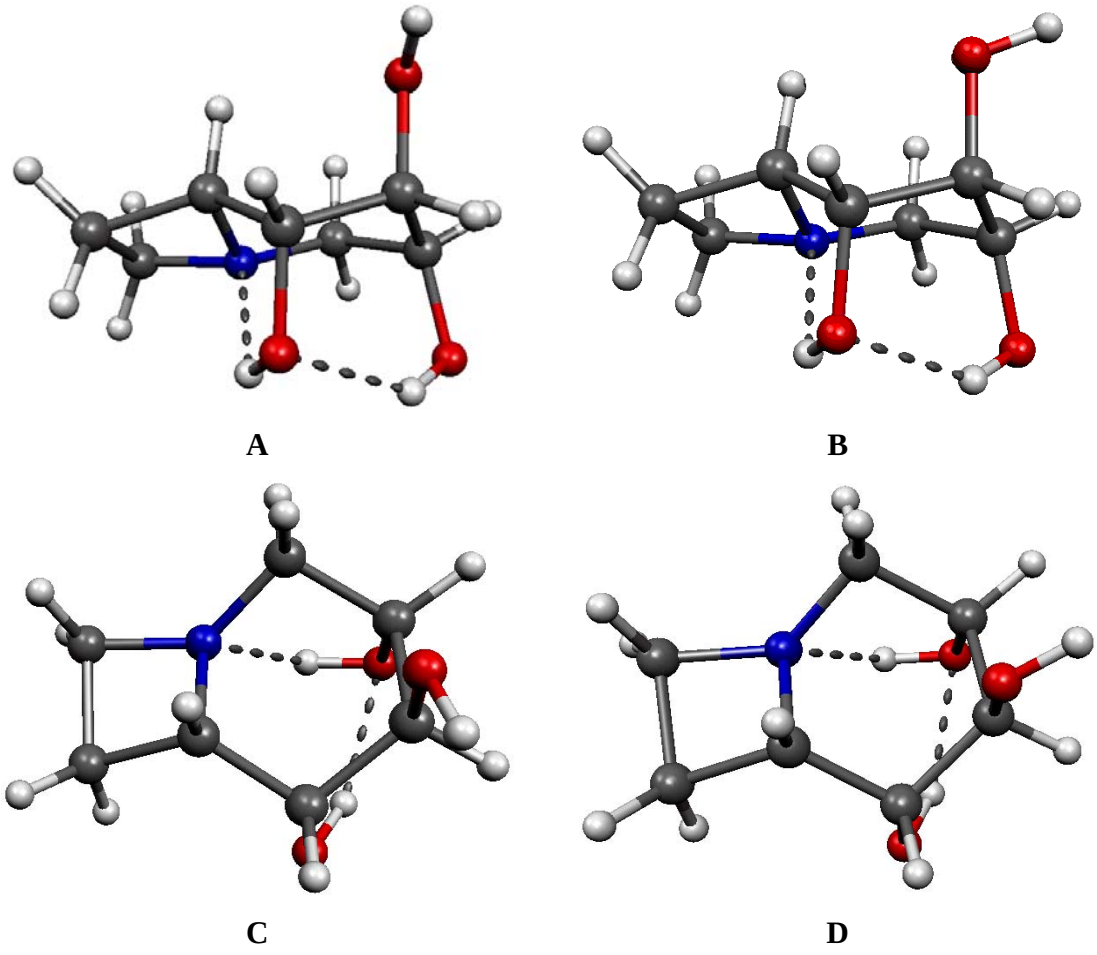
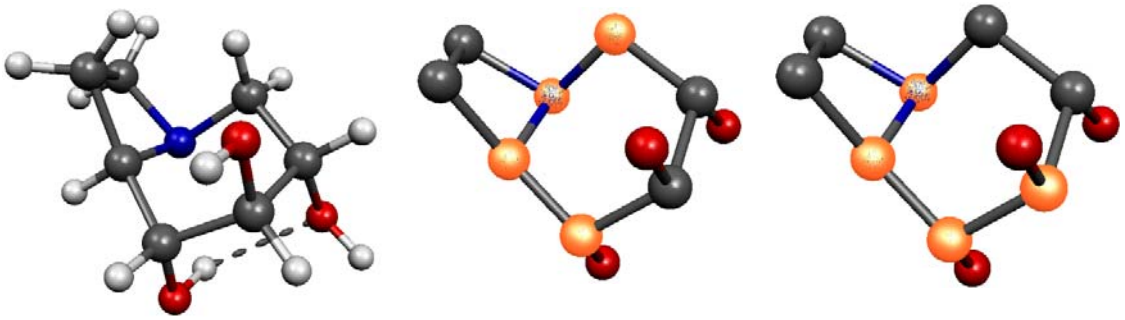


Figure 17S: Hydrogen bonding patterns in hydroxyl groups of **1d**

Depending on the different hydrogen bonding patterns in the constrained form the 4 conformers “A”, “B”, “C”, and “D” have been considered. In “A” and “B” conformers the C4-OH is directed towards the lone pair of the nitrogen whereas it is accepting the hydrogen bond from the C2O-H. The conformer “A” differ in the orientation of the –OH at C3 position compared to “B”. The reverse hydrogen bonding pattern is considered in “C” and “D” conformers.



1e d(C2-N1 –C6 –C5) d(C4-C5-C6-N1)

Figure 18S: The selected angles in **1e** are scanned to check the minimum energy structure these enantiomers.

In order to obtain minimum energy conformers the two dihedral angles (C2-N1–C6 –C5 and C4-C5-C6-N1) were scanned. These dihedral angle (the atoms highlighted in Figure 18S) are scanned from –80° to +80° at HF/3-21G(d) level of theory. The energy profiles for the scans of aforementioned dihedral angles have been shown in **1e**_X1 and **1e**_X2 (X = "A", "B", "C", or "D"), respectively. The energy of the lowest energy conformers has been chosen as a reference.

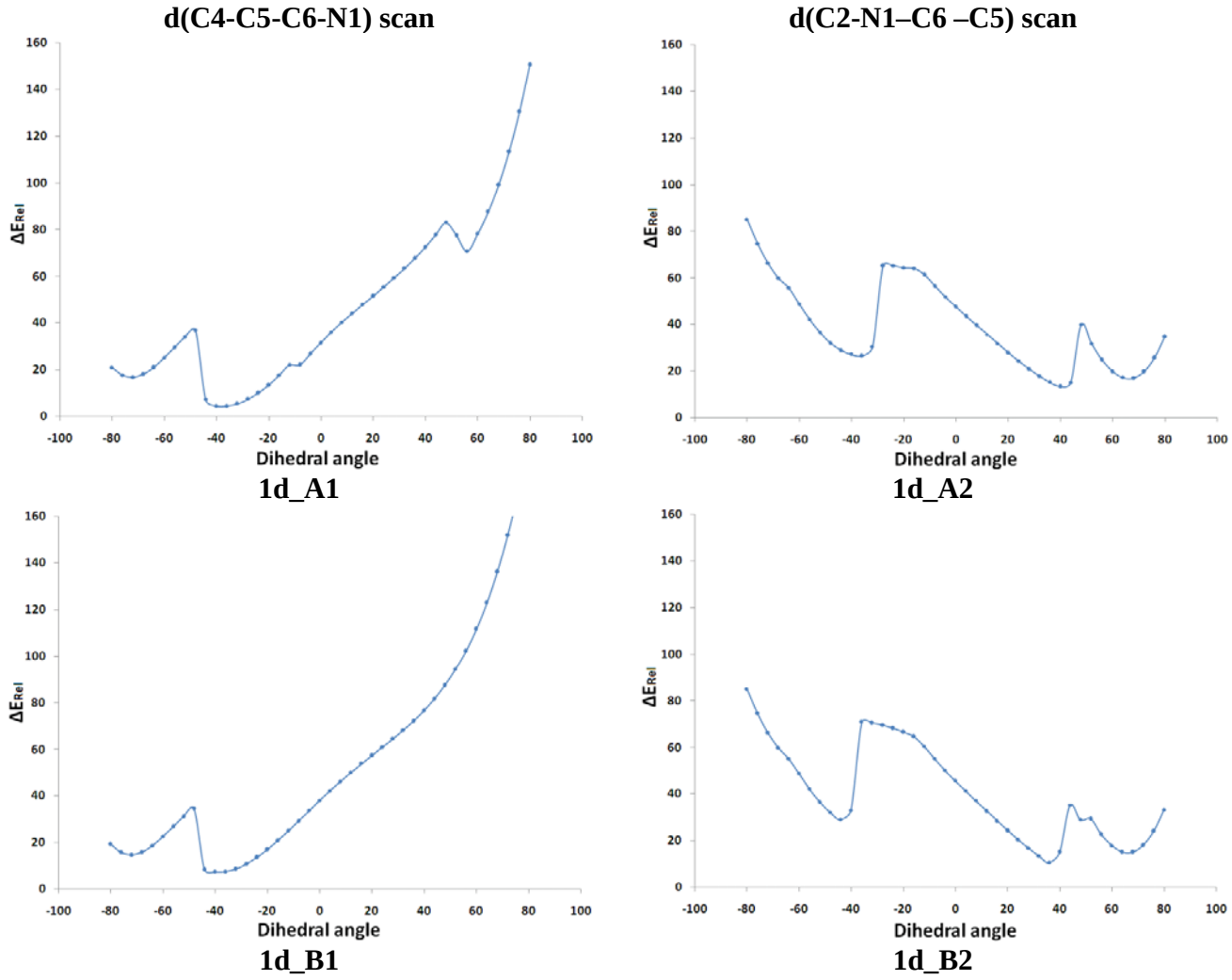


Figure 19S: Relative energy profiles for the conformers of **1d** with different hydrogen bonding pattern as a function of dihedral angle. The minimum energy conformer amongst all the profiles is considered as a reference.

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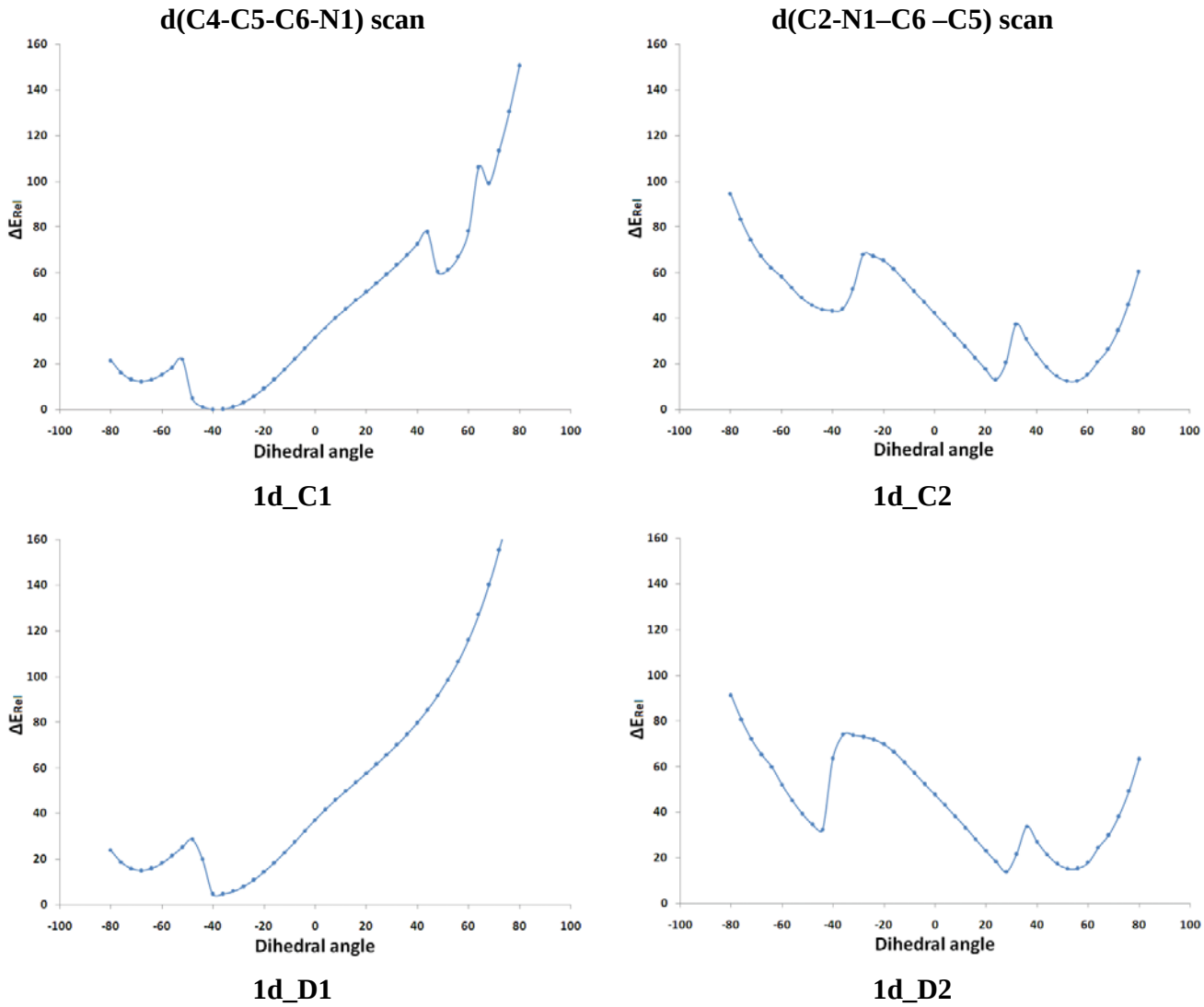


Figure 19S: Relative energy profiles for the conformers of **1d** with different hydrogen bonding pattern as a function of dihedral angle. The minimum energy conformer amongst all the profiles is considered as a reference. (Contd.)

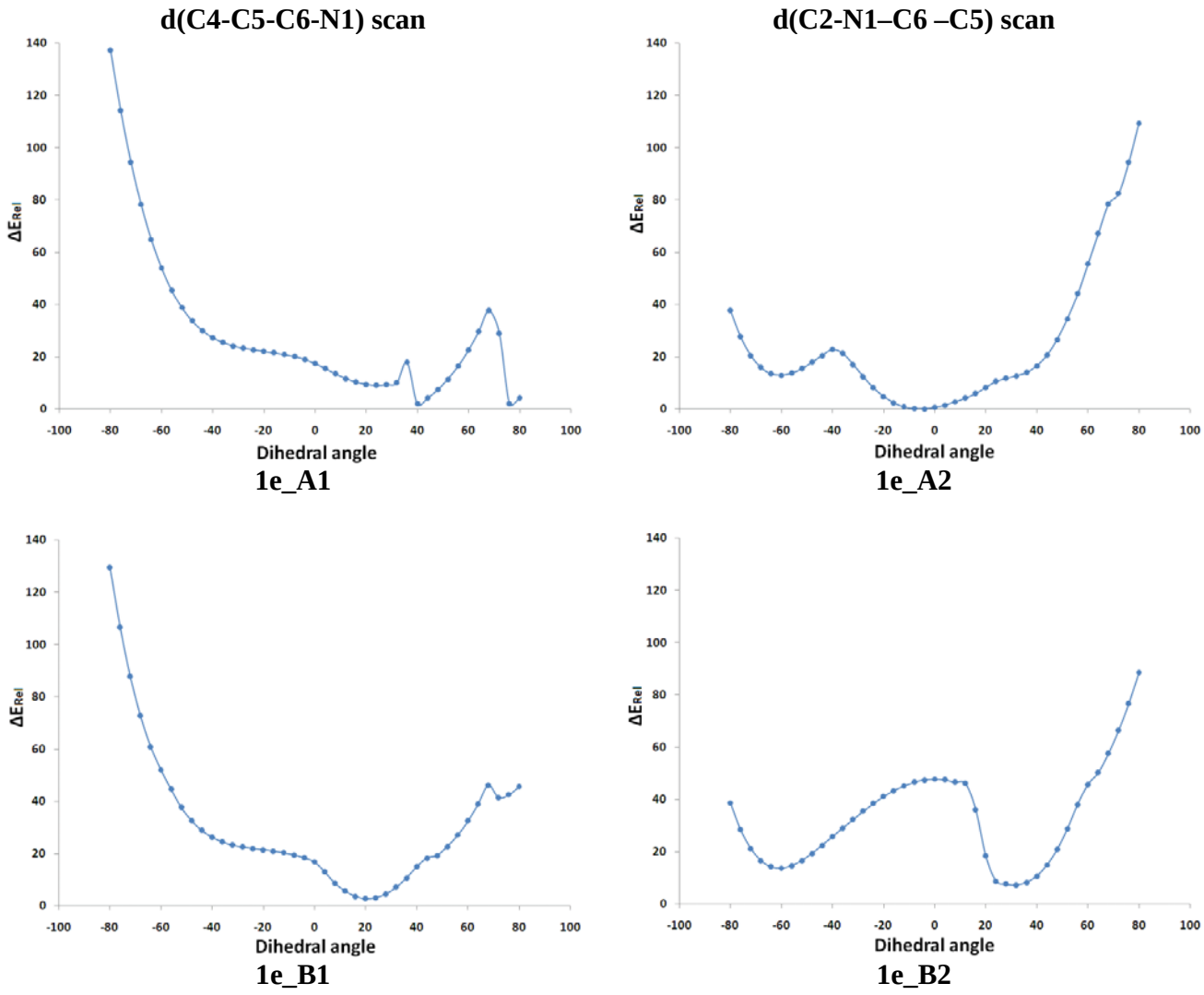


Figure 20S: Relative energy profiles for the conformers of **1e** with different hydrogen bonding pattern as a function of dihedral angle. The minimum energy conformer amongst all the profiles is considered as a reference.

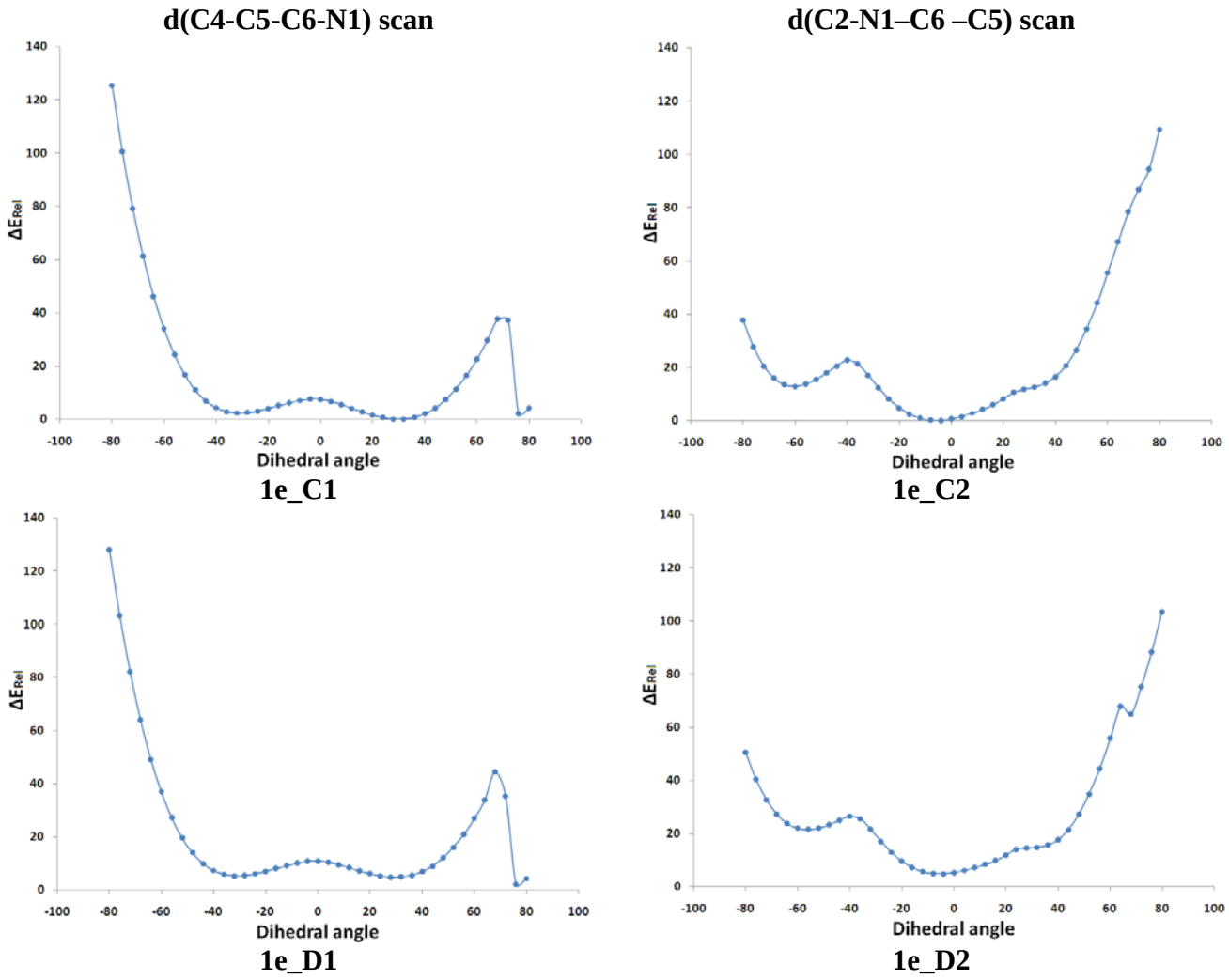


Figure 20S: Relative energy profiles for the conformers of **1e** with different hydrogen bonding pattern as a function of dihedral angle. The minimum energy conformer amongst all the profiles is considered as a reference. (Contd.)

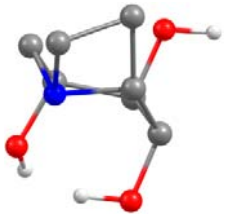
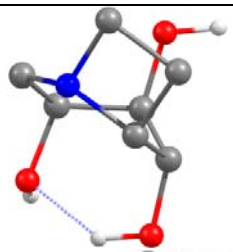
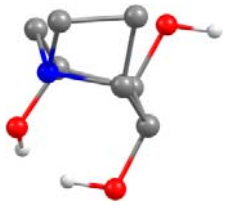
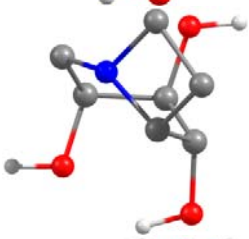
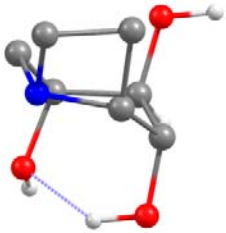
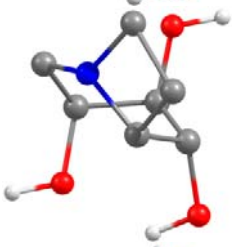
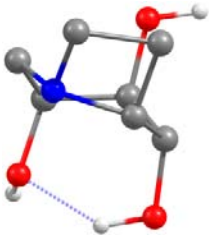
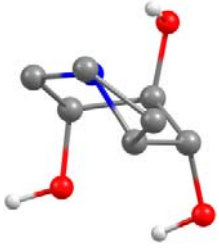
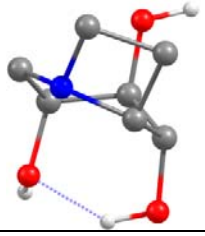
Conformer name	Scan Point No.	D1	Ring conformer	Conformer name	Scan Point No.	D1	Ring conformer
1d_A101	01	-80.0		1d_A125	25	16.0	
1d_A205	05	-64.0		1d_A130	30	36.0	
1d_A110	10	-44.0		1d_A135	35	56.0	
1d_A115	15	-24.0		1d_A141	41	80.0	
1d_A120	20	-4.0					

Figure 21S: Different ring conformations along the scan of dihedral angle C4-C5-C6-N1 (D1).

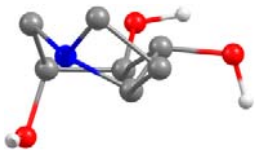
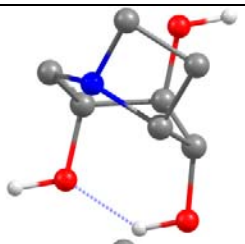
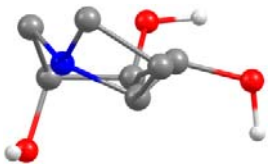
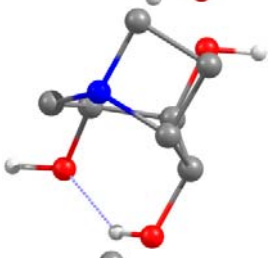
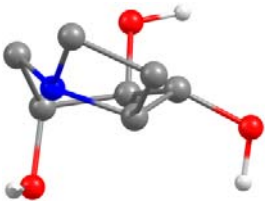
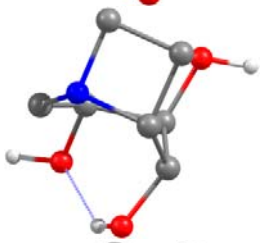
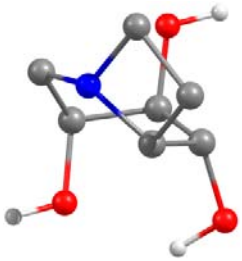
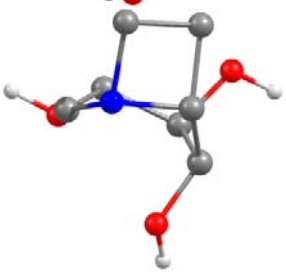
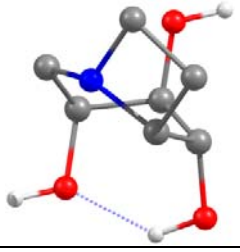
Conformer name	Scan Point No.	D2	Ring conformer	Conformer name	Scan Point No.	D2	Ring conformer
1e_A201	01	-80.0		1e_A225	25	16.0	
1e_A205	05	-64.0		1e_A230	30	36.0	
1e_A210	10	-44.0		1e_A235	35	56.0	
1e_A215	15	-24.0		1e_A241	41	80.0	
1e_A220	20	-4.0					

Figure 22S: Different ring conformations along the scan of dihedral angle C2-N1–C6–C5 (D2).

Table 2S: B3LYP/6-31G(d,p) calculated relative stabilization of energies of **1e** and **1e** conformers (local minima on scan).

1d	ΔE_{Rel}	**1e**	ΔE_{Rel}	ΔE^*
A103	1.5	A127	10.4	18.1
A112	2.0	A131	7.3	15.0
A119	1.8	A140	1.2	9.0
A135	18.3	A206	0.0	7.7
A204	1.5	A220	7.3	15.0
A211	9.2	B126	7.7	15.5
A230	9.3	B139	29.4	37.1
B103	0.0	B206	2.5	10.3
B112	6.4	B229	10.7	18.4
B205	0.0	C113	2.9	10.6
B212	6.3	C128	7.3	15.0
B232	9.3	C140	1.2	9.0
C104	0.4	C206	0.0	7.7
C111	1.8	C220	7.3	15.0
C133	18.3	D113	4.9	12.6
C138	18.3	D128	10.5	18.2
C208	0.4	D140	1.2	9.0
C215	1.8	D207	8.1	15.8
C232	18.5	D220	10.5	18.2
D104	2.7	D238	21.2	28.9
D111	4.4			
D208	2.7			
D214	4.4			
D232	10.5			

* The relative energies of conformers of **1e** are calculated with reference to minimum energy conformers of **1d**.

It has been observed that the some of the local minima (conformers) located on the different dihedral scan possess be same in the geometry as well as energetically.

Table 3S: B3LYP/6-31G(d,p) stabilization energies (ΔE_{Rel}, in kJ mol^{-1}) and Boltzmann contribution (BC in %) of the minima along the dihedral scan.

1d						**1e**					
	Gas phase		SCRF-PCM		Ring Config		Gas phase		SCRF-PCM		Ring Config
	ΔE_{Rel}	BC	ΔE_{Rel}	BC			ΔE_{Rel}	BC	ΔE_{Rel}	BC	
A103	1.5	13.8	11.4	0.4	$^{6}C_{3}$	A127	10.4	0.6	8.4	1.6	^{4}HC
A112	2.0	11.3	0.0	36.5	$^{N}C_{4}$	A131	7.3	2.0	9.2	1.2	$^{3}TB_{6}$
A119	1.8	12.3	0.9	25.4	$^{N}C_{4}$	A140	1.2	23.6	11.9	0.4	$^{N}TB_{5}$
A135	18.3	0.0	26.2	0.0	$^{N}TB_{4}$	**A206**	**0.0**	**38.3**	**0.0**	**48.2**	$^{\mathbf{3}}\mathbf{TB_{5}}$
A211	9.2	0.6	4.6	5.7	$^{N}C_{4}$	B126	7.7	1.7	7.4	2.4	$^{N}TB_{4}$
B103	0.0	25.3	11.4	0.4	$^{6}C_{3}$	B139	29.4	0.0	29.3	0.0	$^{N}TB_{4}$
B112	6.4	1.9	5.0	4.9	$^{N}C_{4}$	B206	2.5	14.0	2.3	19.1	$^{2}TB_{5}$
C104	0.4	21.6	12.3	0.3	$^{N}C_{4}$	B229	10.7	0.5	6.0	4.3	$^{2}TB_{5}$
C232	**16.6**	**0.1**	**13.1**	**0.2**	$^{\mathbf{3}}\mathbf{HC}$	C113	2.9	11.9	9.4	1.1	$^{3}TC_{6}$
D111	4.4	4.3	1.1	23.4	$^{N}C_{4}$	D113	4.9	5.3	12.3	0.3	$^{2}TC_{5}$
D208	2.7	8.5	7.9	1.5	$^{N}C_{4}$	D128	10.5	0.6	10.3	0.8	$^{N}TB_{4}$
D232	10.5	0.4	8.5	1.2	$^{2}TB_{5}$	D207	8.1	1.5	2.3	19.1	$^{2}TB_{5}$
						D238	21.2	0.0	8.6	1.5	$^{2}TB_{5}$

Only one conformers have been reported out of the conformers having same ΔE_{Rel} values and the geometry.

Table 4S: Calculated ^{1}H NMR spectra of **1e** and **1e** conformers.

	1d								1e					
	A103	A112	A119	A211	B103	C104	D111	D208	A140	A206	B206	C113	D113	D207
H-2a	2.76	2.55	2.35	2.45	2.75	2.72	2.35	2.65	2.46	2.84	2.53	2.85	2.81	2.87
H-2e	2.65	3.00	2.97	2.90	2.74	2.79	3.07	2.81	3.25	2.67	3.06	3.25	3.47	2.63
H-3	3.71	4.02	4.07	3.61	3.55	3.91	3.96	3.52	4.50	3.83	4.11	4.29	4.10	3.67
H-4	4.03	4.12	4.24	4.25	4.02	4.04	4.23	3.93	3.73	3.55	3.92	4.13	4.08	3.64
H-5	3.64	3.59	3.57	4.02	3.84	3.51	3.71	3.68	3.84	3.88	4.18	3.49	3.66	3.90
H-6	3.62	3.88	3.86	3.87	3.55	3.38	3.77	3.43	3.45	3.38	3.36	4.21	4.17	3.34
H-7a	1.77	2.16	2.16	2.30	1.77	1.64	2.17	1.70	2.05	2.03	1.97	3.12	3.09	1.96
H-7e	2.17	2.22	2.22	1.81	2.18	2.28	2.23	2.18	2.07	2.35	1.95	2.06	2.08	2.36
H-8a	3.21	3.79	3.85	3.91	3.21	3.19	3.84	3.16	2.96	3.68	2.96	3.69	3.66	3.65
H-8e	3.05	3.35	3.33	3.34	3.06	3.15	3.33	3.05	3.19	3.34	3.19	2.63	2.64	3.33

Table 5S: Calculated coupling constants (in Hz) of the **1d** and **1e** protons.

	1d		**1e**	
	Expt	Calc. **A112 (C232)**	Expt	Calc. **A206**
H-2a	11.0	1.37 (**9.11**)	6.0	3.45
H-2e	5.0	3.27 (**4.20**)	3.3	1.41
H-3		3.68, 3.27, 1.37 (9.11, 4.20,7.52)		3.45, 1.41, 2.43
H-4	6.9, 6.9	3.51, 3.68 (**7.52,7.33**)	8.2, 4.8	5.68, 2.43
H-5	6.9, 6.0	4.19, 3.51 (**7.33,7.64**)		9.51, 5.68
H-6		1.26, 7.28, 4.19 (7.64, 6.01, 9.61)		7.72, 2.66, 9.51
H-7a		1.41, 7.62, 1.26 (9.61, 8.97, 8.51)		6.52, 8.45, 7.72
H-7e		7.58, 6.52, 7.28 (6.01, 1.04, 5.49)		9.56, 3.18, 2.66
H-8a	10.0, 4.7	7.62, 6.51 (**8.97, 1.04**)		8.45, 3.18
H-8e	10.0, 8.8	7.58, 1.41 (**8.51, 5.49**)		6.52, 9.56

Table 6S: Atomic coordinates in selected conformers of **1d** optimized in water using SCRF_PCM model.

1d_A103				1d_A112		
N	0.970884	0.787949	0.001569	N	0.963080	0.667547	_0.957918
C	2.420501	0.881045	_0.277956	C	2.073873	0.888556	_0.003636
C	2.503590	_0.652221	_0.008764	C	2.377524	_0.630452	_0.072481
C	0.994045	_0.644253	_0.346929	C	0.957503	_0.792525	_0.673764
C	_0.164904	_1.303391	0.380913	C	_0.123185	_1.273777	0.326072
C	_1.453205	_0.663917	_0.224722	C	_1.478439	_0.593562	0.026440
C	_1.439859	0.891737	_0.195126	C	_1.341879	0.942707	0.061832
C	_0.099045	1.514045	_0.662003	C	_0.282377	1.423655	_0.936855
O	_0.101910	_1.054427	1.787622	O	0.218674	_1.077883	1.700626
O	_1.615659	_1.050180	_1.587056	O	_1.964508	_0.928598	_1.269684
O	_1.819580	1.369907	1.096101	O	_0.964710	1.379029	1.382731
H	2.641799	1.116154	_1.332008	H	2.848043	1.577191	_0.367300
H	2.978900	1.563795	0.371541	H	1.761409	1.211519	0.999125
H	2.706734	_0.875362	1.042378	H	2.553943	_1.133135	0.878146
H	3.155001	_1.245758	_0.652596	H	3.168145	_0.875087	_0.785850
H	0.860400	_0.806627	_1.430681	H	0.869448	_1.401344	_1.585085
H	_0.202008	_2.392298	0.234227	H	_0.239943	_2.360394	0.197931
H	_2.315482	_0.984279	0.380855	H	_2.193054	_0.898897	0.809750
H	_2.228384	1.228056	_0.879914	H	_2.309580	1.387658	_0.213940
H	_0.020239	1.446733	_1.763051	H	_0.740855	1.369757	_1.933333
H	_0.092927	2.573107	_0.381314	H	_0.055203	2.477728	_0.740705
H	0.442986	_0.246582	1.889355	H	0.013061	_0.143865	1.896489
H	_1.680434	_2.029795	_1.616556	H	_2.090035	_1.901808	_1.298921
H	_1.312080	0.876544	1.760962	H	_1.740715	1.249842	1.974089
1d_A119				1d_A211			
N	0.947131	0.685758	_0.956793	N	0.932376	0.775484	_0.897219
C	2.062602	0.880760	_0.002490	C	2.055764	0.913763	0.055766
C	2.369168	_0.634428	_0.121884	C	2.378512	_0.582863	_0.182722
C	0.940702	_0.780872	_0.707195	C	0.942147	_0.703623	_0.760826
C	_0.128146	_1.286763	0.294725	C	_0.124253	_1.294506	0.191339
C	_1.483204	_0.586045	0.042953	C	_1.483805	_0.590431	_0.007732
C	_1.338735	0.945033	0.108402	C	_1.355421	0.933462	0.190785
C	_0.297049	1.440657	_0.906790	C	_0.318063	1.517859	_0.784635
O	0.239006	_1.150591	1.669651	O	0.174884	_1.139470	1.588181
O	_1.998812	_0.879089	_1.250463	O	_1.974053	_0.798938	_1.327697
O	_0.991259	1.255488	1.467758	O	_1.078170	1.254630	1.556339
H	2.832553	1.584295	_0.346047	H	2.814672	1.648760	_0.243369
H	1.752843	1.167474	1.011986	H	1.755707	1.118723	1.092387
H	2.562966	_1.166382	0.809154	H	2.625671	_1.183064	0.695637
H	3.148557	_0.852512	_0.855895	H	3.143121	_0.734904	_0.947912
H	0.838673	_1.366579	_1.632100	H	0.843081	_1.223310	_1.724553
H	_0.258835	_2.366357	0.127014	H	_0.241773	_2.366330	_0.038507
H	_2.180872	_0.901977	0.835291	H	_2.184096	_0.980762	0.747678
H	_2.313361	1.394073	_0.141270	H	_2.330160	1.384369	_0.042691
H	_0.774235	1.399684	_1.895744	H	_0.787261	1.559874	_1.777687
H	_0.063393	2.495802	_0.712632	H	_0.089923	2.548351	_0.489297
H	0.025872	_0.232313	1.922850	H	0.943576	_1.700748	1.824859
H	_2.149699	_1.847396	_1.298418	H	_2.103901	_1.764290	_1.450269
H	_0.794494	2.215378	1.531464	H	_0.465923	0.573202	1.887831

1d_B103			1d_C104		
N	0.967637	0.788834	0.006485	N	0.997137	0.756482	0.040224
C	2.415858	0.893820	_0.276308	C	2.452627	0.774755	_0.204993
C	2.508273	_0.642020	_0.025659	C	2.410906	_0.780754	_0.096129
C	0.998200	_0.638243	_0.361908	C	0.922330	_0.620308	_0.476060
C	_0.155495	_1.314217	0.361249	C	_0.299636	_1.349959	0.068965
C	_1.446601	_0.676191	_0.227496	C	_1.532378	_0.459327	_0.285699
C	_1.442931	0.882918	_0.169841	C	_1.334130	1.031391	0.097137
C	_0.109822	1.518294	_0.640273	C	_0.037252	1.625480	_0.488255
O	_0.087279	_1.078168	1.770216	O	_0.236741	_1.626328	1.465818
O	_1.545859	_1.143057	_1.569827	O	_1.798802	_0.480680	_1.684253
O	_1.815065	1.337728	1.133612	O	_1.307586	1.140422	1.530095
H	2.633506	1.143576	_1.327731	H	2.722796	1.099661	_1.223660
H	2.972043	1.571318	0.380626	H	3.042285	1.340330	0.524843
H	2.714435	_0.876447	1.022376	H	2.534532	_1.119063	0.935507
H	3.161699	_1.223896	_0.678025	H	3.048480	_1.355529	_0.770557
H	0.866695	_0.787235	_1.447732	H	0.831313	_0.619341	_1.579839
H	_0.191990	_2.398764	0.197456	H	_0.422445	_2.320692	_0.433328
H	_2.304532	_1.014478	0.374548	H	_2.393552	_0.833931	0.290792
H	_2.240748	1.234666	_0.838882	H	_2.206890	1.589226	_0.266259
H	_0.040762	1.463020	_1.742692	H	_0.080076	1.639282	_1.591362
H	_0.104813	2.574228	_0.348061	H	0.086742	2.654984	_0.131217
H	0.457431	_0.270834	1.878970	H	_0.496992	_0.813580	1.928691
H	_2.406494	_0.839618	_1.930701	H	_2.029196	_1.401735	_1.931649
H	_1.309185	0.824435	1.783856	H	_0.366728	1.250027	1.783390
1d_D111				1d_D208			
N	0.940188	0.699463	_0.953676	N	0.943572	0.794086	0.032914
C	2.056974	0.894782	_0.000006	C	2.394640	0.920395	_0.225940
C	2.377071	_0.615999	_0.137421	C	2.481269	_0.631109	_0.111223
C	0.947669	_0.769687	_0.717547	C	0.975388	_0.596451	_0.460106
C	_0.111660	_1.293616	0.284385	C	_0.167321	_1.370406	0.177916
C	_1.473136	_0.611096	0.044017	C	_1.473147	_0.613153	_0.217449
C	_1.344464	0.925807	0.121817	C	_1.427279	0.934734	_0.014582
C	_0.312806	1.439775	_0.893785	C	_0.131621	1.573743	_0.556555
O	0.257321	_1.154196	1.658469	O	_0.026716	_1.495093	1.587822
O	_1.931645	_1.008255	_1.243173	O	_1.695911	_0.923065	_1.593748
O	_0.999025	1.235099	1.482985	O	_1.623745	1.276157	1.357887
H	2.818505	1.610719	_0.336059	H	2.623940	1.261702	_1.248570
H	1.746892	1.164468	1.018889	H	2.944916	1.535585	0.494224
H	2.587270	_1.158297	0.783978	H	2.665558	_0.957397	0.915758
H	3.151445	_0.814950	_0.882398	H	3.145098	_1.155413	_0.801006
H	0.844042	_1.349111	_1.646126	H	0.851114	_0.635538	_1.557549
H	_0.231455	_2.371842	0.111654	H	_0.246229	_2.389596	_0.221786
H	_2.163263	_0.942402	0.836143	H	_2.289383	_0.995576	0.415062
H	_2.325052	1.370561	_0.121226	H	_2.290181	1.350838	_0.554852
H	_0.791982	1.396999	_1.881591	H	_0.116975	1.544225	_1.660969
H	_0.090896	2.496635	_0.695371	H	_0.086194	2.621109	_0.236716
H	0.027627	_0.240975	1.913741	H	0.348520	_0.656938	1.921977
H	_2.836538	_0.647201	_1.364863	H	_2.546265	_0.511941	_1.860061
H	_0.768999	2.188175	1.543953	H	_0.749535	1.259834	1.796038

Table 7S: Atomic coordinates in selected conformers of **1e** optimized in water using SCRF_PCM model.

1e_A140				1e_A206			
N	1.081830	_0.706474	0.123807	N	_1.203831	_0.943275	0.050591
C	2.519921	_0.580312	_0.186925	C	_2.455293	_0.499084	_0.617090
C	2.340043	0.960982	_0.060524	C	_2.387758	0.850087	0.142336
C	0.844163	0.671029	_0.344097	C	_0.967797	0.436097	0.596688
C	_0.391862	1.260916	0.351201	C	0.211192	1.132623	_0.080089
C	_1.274032	0.062139	0.829455	C	1.485796	0.275917	0.054148
C	_1.282343	_1.080210	_0.215752	C	1.186864	_1.247147	_0.038952
C	0.144093	_1.689923	_0.390038	C	_0.127230	_1.494327	_0.779109
O	_1.116087	2.154857	_0.490918	O	0.408716	2.466603	0.381937
O	_0.859981	_0.424584	2.101843	O	2.425545	0.597710	_0.968434
O	_1.766435	_0.476452	_1.420724	O	1.146032	_1.836889	1.262245
H	3.196374	_1.093637	0.504917	H	_2.347407	_0.391229	_1.706518
H	2.763037	_0.875800	_1.220974	H	_3.322186	_1.139836	_0.417553
H	2.874542	1.593452	_0.771760	H	_3.105190	0.938165	0.961580
H	2.513175	1.311063	0.961129	H	_2.436166	1.751588	_0.473459
H	0.672861	0.702504	_1.436351	H	_0.804688	0.434046	1.686356
H	_0.114770	1.834123	1.245476	H	_0.000070	1.234747	_1.154004
H	_2.298808	0.434052	0.947859	H	1.920672	0.450191	1.053409
H	_1.975399	_1.864919	0.120223	H	2.022367	_1.709308	_0.580698
H	0.234342	_2.626142	0.173068	H	_0.072154	_1.027882	_1.778244
H	0.302751	_1.922180	_1.459380	H	_0.288897	_2.569358	_0.927208
H	_1.465506	1.608755	_1.217144	H	0.595627	2.422494	1.345858
H	0.084666	_0.654545	1.987182	H	2.538852	1.571241	_0.968635
H	_1.819945	_1.159693	_2.122424	H	0.209074	_1.906320	1.531398
1e_B206				1e_C113			
N	_1.191938	_0.970778	0.054544	N	_1.085936	0.773113	_0.718042
C	_2.444605	_0.542463	_0.619656	C	_2.493688	0.584601	_0.222800
C	_2.417615	0.789217	0.170320	C	_2.158947	_0.836929	0.283461
C	_0.980187	0.409557	0.606654	C	_0.905151	_0.730195	_0.613292
C	0.179051	1.137425	_0.073697	C	0.458925	_1.287251	_0.193001
C	1.467471	0.310731	0.057845	C	1.205884	_0.383280	0.811440
C	1.214266	_1.218662	_0.059097	C	1.162767	1.079799	0.346293
C	_0.105943	_1.505909	_0.772929	C	_0.280928	1.562678	0.231942
O	0.433194	2.416853	0.506616	O	1.290528	_1.523110	_1.334578
O	2.409170	0.672238	_0.951412	O	0.628565	_0.413964	2.112034
O	1.243429	_1.850739	1.222149	O	1.873958	1.123046	_0.897660
H	_2.322278	_0.405181	_1.704447	H	_2.816773	1.324940	0.517091
H	_3.300076	_1.206839	_0.449666	H	_3.203801	0.589374	_1.058514
H	_3.129146	0.829549	0.998335	H	_2.867341	_1.642888	0.067326
H	_2.510799	1.702599	_0.424023	H	_1.903382	_0.847461	1.345779
H	_0.802370	0.414052	1.692467	H	_1.114114	_1.155392	_1.604725
H	_0.035052	1.246373	_1.149340	H	0.296168	_2.271574	0.270927
H	1.882960	0.492268	1.061940	H	2.255789	_0.714521	0.834570
H	2.049677	_1.634765	_0.636078	H	1.672126	1.703207	1.097970
H	_0.074404	_1.057341	_1.781603	H	_0.690716	1.545002	1.254567
H	_0.237961	_2.587687	_0.900518	H	_0.289737	2.613499	_0.092020
H	_0.219508	3.055412	0.151213	H	1.573705	_0.637923	_1.630648
H	2.551797	1.639904	_0.883265	H	0.698850	_1.333752	2.446494
H	0.329747	_1.879095	1.567718	H	1.713200	1.991380	_1.325151

1e_D113			1e_D207		
N	_1.113924	0.692757 _0.727106	N	_1.160943	_1.000229 0.042652
C	_2.516540	0.493113 _0.218885	C	_2.394826	_0.588377 _0.674320
C	_2.124614	_0.864452 0.408744	C	_2.420566	0.732580 0.134451
C	_0.889025	_0.794763 _0.515401	C	_0.985581	0.382779 0.594892
C	0.500715	_1.287130 _0.087304	C	0.152887	1.154628 _0.073541
C	1.272511	_0.279545 0.785729	C	1.471629	0.363263 0.017920
C	1.127659	1.143414 0.207677	C	1.248397	_1.179845 0.007812
C	_0.339845	1.544428 0.195026	C	_0.038590	_1.532902 _0.734946
O	1.297148	_1.625690 _1.228614	O	0.260971	2.481456 0.431276
O	0.763994	_0.350524 2.113017	O	2.265922	0.776807 _1.091954
O	1.720641	1.145396 _1.105277	O	1.234596	_1.704718 1.337551
H	_2.871877	1.284604 0.449251	H	_2.232177	_0.432501 _1.751531
H	_3.218305	0.392841 _1.055078	H	_3.242699	_1.271834 _0.547709
H	_2.806319	_1.710442 0.278044	H	_3.150950	0.737396 0.947005
H	_1.856321	_0.770800 1.464243	H	_2.518729	1.655501 _0.442141
H	_1.107308	_1.293401 _1.469285	H	_0.823413	0.387822 1.684738
H	0.371206	_2.214891 0.486559	H	_0.071907	1.272339 _1.143035
H	2.334368	_0.569556 0.754649	H	1.965929	0.605812 0.973164
H	1.682419	1.848873 0.846907	H	2.109676	_1.627931 _0.507702
H	_0.689133	1.485222 1.237513	H	0.016150	_1.110869 _1.753860
H	_0.448843	2.589512 _0.123962	H	_0.140824	_2.620971 _0.835508
H	1.600898	_0.772569 _1.590620	H	0.452325	2.416516 1.392423
H	1.283158	0.270702 2.669677	H	3.165783	0.406182 _0.970013
H	1.084101	1.526766 _1.744688	H	0.305429	_1.836975 1.607012

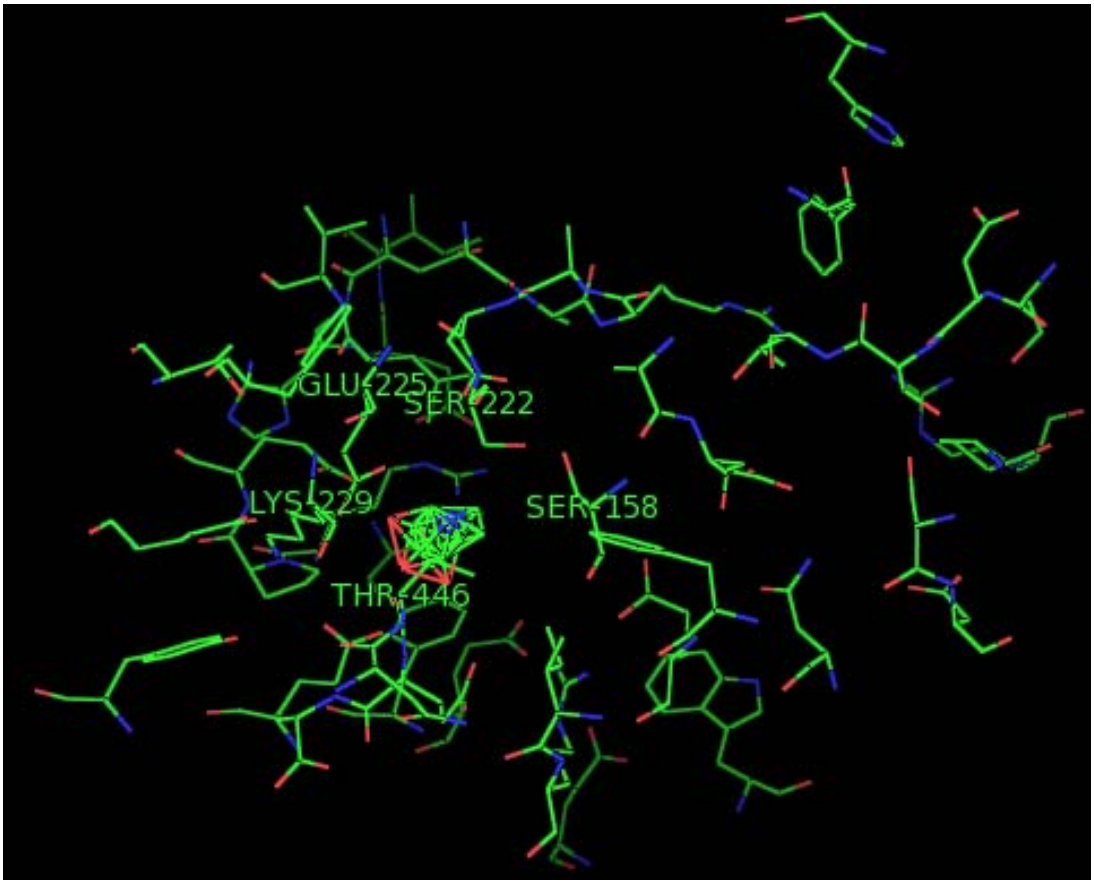


Figure 23S: Binding of **1e** to mannosidase active pocket. A docking grid of 60 Å (0.375 spacing) was computed around the binding site of apo-mannosidase (PDB: 1FO3). **1e** placed in different locations outside the grid consistently docked well into the binding site. (As estimated by Autodock runs using 2,500,000 energy evaluations over 100 GA runs)