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Deeper insight into properties of the newly synthetized macrocycles as drugs receptors – some preliminary quantum chemical studies.

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Table S1

Comparison of selected vibrations observed in the B3LYP/6-31G(d,p) calculated IR spectra in vacuo (frequencies ν scaled by 0.961) with experimental peaks.

Abbreviations: OOP = out-of-plane; gluc – glucose units connected with urea fragments; gluc' – subsequent glucose units; sciss – scissors; deform - deformation

Host A			**Host B**			**Host C**			**Experiment**
ν [cm^{-1}]	***Intens* [km/mol]**	**Modes**	**ν [cm^{-1}]**	***Intens* [km/mol]**	**Modes**	**ν [cm^{-1}]**	***Intens* [km/mol]**	**Modes**	
450	*208*	CCOH torsion, NH OOP bend	**541**	*140*	CCOH torsion, NH OOP bend	**506**	*62*	CCOH torsion, NH OOP bend, crown CH_2 rock	
528	*174*	CCOH torsion	**544**	*150*	CCOH torsion				
589	*114*	CCOH torsion	**554**	*115*	CCOH torsion, C-OH stretch, OCH bend, C6'H_2 wag	**596**	*96*	CCOH torsion, NH OOP bend	**568**
			609	*114*	CCOH torsion	**606**	*64*	CCOH torsion	
658	*110*	CCOH torsion, NH OOP bend							**637**
677	*142*	CCOH torsion, NH OOP bend							
696	*145*	CCOH torsion, NH OOP bend, CH_2 rock, CH OOP bend, gluc deform							

707	*99*	CCOH torsion
712	*62*	CCOH torsion, NH OOP bend
750	*71*	CCOH torsion, NH OOP bend
704	*204*	CCOH torsion, NH OOP bend
726		
769	*103*	CCOH torsion, CCH bend, C6'H_2 rock
766		
774	*89*	CCOH torsion, CCH bend, crown CH_2 rock
875	*81*	CCOH torsion, gluc' deform
824	*111*	CCOH torsion, CCH bend, C6'H_2 rock
895		
957	*134*	gluc deform (CO & CC stretch, C6'H_2 rock, COH & CCH bend)
935	*127*	CCOH torsion, C6'H_2 & C6H_2 rock, CCH bend, gluc'CO stretch, gluc' deform
943	*64*	gluc'C-O-Cgluc sym stretch, gluc deform (CC &C5C6 stretch), gluc' CCH bend
970	*157, 154*	gluc & gluc' deform (CO & CC stretch, C6'H_2 rock, COH & CCH bend)
967	*77*	glucCN & glucCO stretch, crown CH_2, rock, gluc COH bend
986	*121*	gluc' deform, C6'-OH stretch & bend, C6'H_2 rock, gluc CCH bend
991	*143*	C6'-OH stretch, gluc' deform, C2'OH bend
1012	*77*	C5C6, C2-OH & C3-OH stretch, gluc deform (CC stretch, CCH bend), CC2'H bend, C3'OH bend

			1014	*87*	C4'-OH stretch, gluc' deform (CC stretch, CCH bend), $C6'H_2$ rock, glucC-O-Cgluc' stretch,			
1020	*413*	crown CN stretch, C-OH stretch, CCH bend				**1019**	*165*	gluc' deform (COC asym stretch, $C6'H_2$ rock, COH & CCH bend)
			1021	*214*	C4'-OH stretch, gluc' deform (COC asym stretch), glucC-O-Cgluc' strech, C3-OH stretch, gluc deform	**1023**	*272*	C5'C6' stretch, COH & CCH bend
			1024	*169*	C6'-OH & C4'-OH stretch, gluc' deform (COC asym stretch), glucC-O-Cgluc' strech, C3-OH stretch, gluc deform, COH bend	**1024**	*142*	glucCN stretch, crown deform (CN CC stretch, CH_2 twist), gluc' COH bend
						1029	*187*	C2'-OH stretch, C6-OH stretch & bend, C3'OH & C6'OH bend

1028	
1075	

1035	*182*	glucCN stretch, crown deform (CC stretch), gluc deform & CCH bend
1038	*134*	C3-OH & C6-OH stretch, COH bend, gluc' & gluc deform (CC stretch, CCH bend)
1041	*105*	C3'-OH, C4'-OH & C6'-OH stretch, gluc' deform (CCC & CCH bend), C6OH bend
1044	*133*	gluc' C-OH stretch, COH bend, gluc' deform (CC stretch, CCH bend)
1047	*142*	gluc CCH bend, COH bend, gluc & gluc' deform, gluc (CO stretch)
1048	*199*	C6'-OH & C4'-OH stretch, gluc' deform (COC asym stretch), glucC-O-Cgluc' strech, C3-OH stretch, gluc deform, C6-OH stretch
1055	*213*	glucC-O-Cgluc' stretch, gluc & gluc' C-OH stretch, gluc & gluc' deform (CC stretch, CCH bend)
1056	*462*	gluc C-OH stretch, glucC-O stretch, gluc'C-OH & CCH bend, CNH bend, crown CH_2 twist & rock
1062	*171, 126*	gluc' C-O asym stretch, C-OH stretch, gluc & gluc' COH & CCH bend, crown CH_2 twist
1063	*297*	crown COC asym stretch, gluc C-OH stretch, gluc' COH & CCH bend

1075	*91*	gluc & gluc' C-OH stretch & bend, gluc & gluc' deform (CC & CO stretch, CCH bend)
1090	*134*	C5-C6 & C6-OH stretch, CN stretch, gluc deform, gluc' COH bend
1092	*112*	C5'-C6' & C6'-OH stretch, gluc' deform (CCC & CCH bend), gluc' COH bend
1108	*105*	C4'OH bend, C1'C2' stretch, C2OH bend, CN stretch, crown CH_2 rock

1090	*125*	C5'-C6' & C6'-OH stretch, gluc' deform (CCC & CCH bend), gluc' COH bend
1095	*160*	C5-C6 & C6-OH stretch, gluc deform (CO stretch), CNH bend, crown CH_2 rock
1107	*91*	gluc deform (CO stretch, CCH bend), C6-OH bend, $C6H_2$ twist, CNH bend
1109	*109*	C2-OH stretch, crown deform, gluc deform
1111	*153*	crown COC asym stretch, crown CH_2 rock and twist, gluc CCH bend
1143	*259*	gluc'C-O-Cgluc asym stretch, C5'C6' stretch, gluc' deform (COC sciss, CCH bend)

1075	*143*	C3-OH stretch, COH & CCH bend, gluc deform
1076	*149*	C5-C6 & C6-OH stretch, glucCN stretch, gluc' CC stretch, C2'OH bend,
1083	*123*	C2'-OH stretch, COH, OCH & CCH bends, $C6H_2$ rock
1110	*131*	gluc CC stretch, CNH bend, COH bends, crown CH_2 rock,
1111	*115*	gluc CC & CO asym stretch, CNH bend, COH bends, $C6H_2$ rock,
1139	*157*	gluc'C-O-Cgluc asym stretch, gluc' deform, COH & CCH bend

1116

1163	*99*	CN stretch, crown CH_2 twist & rock, C4'OH bend						**1166**
1169	*47*	CN stretch, crown CH_2 twist & rock				**1174**	*97*	C2OH & C6'OH bend, CCH bend
1192	*113*	C4'OH & C6'OH bend, C6'H_2 twist, CCH bend	**1185**	*27*	crown CN & CC stretch, crown CH_2 twist	**1183**	*101*	C6OH, C6'OH & C4'OH bend, CCH bend
1227	*410*	C2OH bend, CNH bend, crownN-C stretch, crown CH_2 twist, C6H_2 twist	**1228**	*95*	crown C-NH stretch & bend, crown CH_2 twist, gluc COH bend			
						1244	*84*	C2'OH, C3'OH & C4'OH bend, crown CH_2 twist, gluc' CCH bend, **1288**
			1310	*67*	CCH & CNH bend, crown CH_2 twist	**1308**	*54*	COH, CCH & CNH bend, crown CH_2 twist **1315**
1378	*97*	C2OH & CC2H bend, crown CH_2 wag, CCH bend,	**1372**	*79*	C3'OH bend, crown CH_2 wag	**1356**	*87*	C6OH, C2OH bend, CCH bend, crown CH_2 twist **1359**
1424	*87*	C4'OH & OC4'H bend, gluc CH bend, C6'H_2 sciss	**1415**	*100*	C6OH, C4'OH & C2'OH bend and corresponding OCH bend	**1427**	*153*	C2'OH, C4'OH & C2OH bend, CCH bend **1418**
1434	*88*	C6'OH bend, C6'H_2 wag, C2'OH bend, gluc' CH bend				**1442**	*104*	C2'OH & C2OH bend, C6'H_2 sciss, crown CH_2 sciss **1458**

1474	*86*	crown CH_2 sciss	**1467 -1495**	*16-23*	crown CH_2 sciss	**1460 -1481**	*5-89*	crown CH_2 sciss	
1485	*108*	crown CH_2 sciss							
1521	*602*	CNH & NCH bend, CNC asym stretch, crown CH_2 sciss	**1501**	*404*	CNH & NCH bend, CNC asym stretch, crown CH_2 sciss	**1484**	*468*	CNH & NCH bend, CNC asym stretch, crown CH_2 sciss	
1525	*290*	CNH & NCH bend, CNC asym stretch, crown CH_2 sciss	**1547**	*462*	CNH & NCH bend, CNC asym stretch, crown CH bend	**1495**	*423*	CNH & NCH bend, CNC asym stretch, crown CH_2 sciss	**1541**
1710	*394*	C=O stretch, CNH bend, NCH bend, crown CH_2 sciss	**1596**	*440*	C=O stretch, CNH bend, NCH bend, crown CH_2 sciss	**1637**	*472*	C=O stretch, CNH bend, NCH bend, crown CH_2 sciss	**1636**
1711	*200*	C=O stretch, CNH bend, NCH bend, crown CH_2 sciss	**1651**	*299*	C=O stretch, CNH bend, NCH bend, crown CH_2 sciss	**1641**	*239*	C=O stretch, CNH bend, NCH bend, crown CH_2 sciss	
2874 -3032	*3-91*	C-H stretch	**2841 -3091**	*2-157*	C-H stretch	**2861 -3059**	*2-67*	C-H stretch	**2881 2920**
			3250	*811*	OH stretch				
						3300	*291*	NH stretch, OH stretch	
						3315	*626*	NH stretch, OH stretch	
3333	*338*	OH stretch	**3323**	*635*	OH stretch				
			3366	*135*	NH stretch	**3351**	*602*	OH stretch	
			3367	*383*	OH stretch				

			3385	*595*	OH stretch					
3394	*1227*	OH stretch	**3395**	*1221*	OH stretch	**3395**	*63*	OH stretch		
3404	*1094*	OH stretch				**3402**	*1172*	OH stretch		
						3408	*442*	OH stretch		
			3426	*207*	OH stretch				**3420**	
3433	*289*	OH stretch	**3430**	*478*	OH stretch					
3445	*184*	OH stretch				**3445**	*18*	NH stretch		
3456	*241*	OH stretch								
3473	*155*	NH stretch, OH stretch								
3488	*111*	NH stretch, OH stretch				**3488**	*424*	OH stretch		
			3516	*35*	NH stretch					
			3541	*146*	OH stretch					
3549	*170*	OH stretch	**3543**	*346*	OH stretch					
3552	*137*	OH stretch				**3554**	*110*	NH stretch		
3558	*472*	OH stretch	**3554**	*126*	OH stretch					
3570	*354*	OH stretch								
3575	*108*	OH stretch								
						3590	*168*	OH stretch		
						3617	*124*	OH stretch		

Table S2

Values of changes $\Delta\delta$ in ^{1}H scaled chemical shifts [ppm] computed in vacuo and in water for each specified atom in the aspirin and the host molecule upon formation of complex 1:1 compared to experimental data. The changes are calculated as $\Delta\delta=\delta_{complex}-\delta_{substrate}$, in the pairs shown in columns. Averaged values are also included. Last column contains our experimental values obtained in D2O.

	Calc. VACUO			**Calc. WATER**			**EXP**
Aspirin	**A′-Asp.**	**B′- Asp.**	**C′- Asp.**	**A′- Asp.**	**B′- Asp.**	**C′- Asp.**	
H-3_{as}	-0.017	-0.099	1.468	-0.008	-0.012	1.165	-0.0206
H-4_{as}	-0.037	-0.055	0.916	-0.081	-0.053	0.445	-0.0333
H-5_{as}	0.032	1.080	0.130	-0.093	0.664	-0.030	-0.0206
H-6_{as}	-0.357	0.078	-0.572	-0.487	-0.062	-0.581	-0.0490
H-9_{as}	0.300	2.177	0.262	0.230	1.474	-0.050	
H-9_{as}	0.569	0.278	0.393	0.198	0.046	-0.218	
H-9_{as}	-0.336	-0.589	-0.755	-0.150	-0.429	-0.621	
Averaged H-9_{as} (CH_3)	0.178	0.622	-0.033	0.093	0.364	-0.296	-0.0107
Host	**A′-A**	**B′-B**	**C′-C**	**A′-A**	**B′-B**	**C′-C**	
H-1	0.097	0.590	0.434	0.003	0.664	0.469	-0.0022
H-1	-0.295	0.041	0.016	-0.283	-0.093	0.020	-0.0022
H-1’	-0.130	0.002	-0.264	0.084	-0.028	-0.024	-0.0031
H-1’	-0.054	-1.046	-0.800	-0.069	-0.906	0.206	-0.0031
H-6a	-0.075	-0.009	-0.021	-0.026	0.013	-0.199	-0.0020
H-6a	0.049	-0.272	-0.187	0.082	-0.243	-0.057	-0.0020
H-6b	-0.107	0.058	0.260	-0.070	0.074	0.339	-0.0020
H-6b	-0.085	0.075	-0.423	0.079	-0.037	-0.316	-0.0020
Averaged values for host:							
H-1	-0.099	0.316	0.225	-0.140	0.285	0.244	-0.0022
H-1’	-0.092	-0.522	-0.532	0.007	-0.467	0.091	-0.0031
H-6a	-0.013	-0.140	-0.104	0.028	-0.115	-0.128	-0.0020
H-6b	-0.096	0.066	-0.082	0.005	0.019	0.012	-0.0020