

SUPPLEMENTARY INFORMATION

REGULAR ARTICLE

Quantum chemical study of hydrogen-bonded complexes of serine with water and H₂O₂

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Table S1: Geometrical parameters of **I**, **II**, **III** and **IV** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	I		II		III		IV	
	L1	L2	L1	L2	L1	L2	L1	L2
C2-O1	1.211	1.221	1.211	1.221	1.211	1.221	1.215	1.224
O3-C2	1.339	1.347	1.356	1.363	1.353	1.360	1.338	1.347
C4-C2	1.543	1.540	1.523	1.520	1.523	1.521	1.539	1.537
N5-C4	1.471	1.473	1.460	1.464	1.464	1.468	1.472	1.474
H6-O3	0.986	0.988	0.971	0.974	0.971	0.974	0.986	0.988
H7-C4	1.101	1.104	1.098	1.101	1.106	1.108	1.100	1.103
C8-C4	1.533	1.530	1.547	1.542	1.542	1.537	1.542	1.538
H9-N5	1.015	1.018	1.016	1.019	1.017	1.021	1.015	1.019
H10-N5	1.019	1.023	1.019	1.023	1.015	1.018	1.018	1.022
H11-C8	1.098	1.101	1.096	1.099	1.095	1.098	1.107	1.109
H12-C8	1.098	1.100	1.106	1.108	1.105	1.106	1.099	1.101
O13-C8	1.427	1.434	1.413	1.421	1.416	1.424	1.412	1.420
H14-O13	0.966	0.969	0.971	0.973	0.971	0.974	0.973	0.974
O3-C2-O1	122.93	123.01	122.84	123.37	122.89	123.44	122.36	122.39
C4-C2-O1	123.07	123.00	125.15	125.06	124.99	125.13	123.10	123.16
N5-C4-C2	108.93	108.45	113.52	113.53	109.12	108.66	109.18	108.82
H6-O3-C2	104.91	103.89	107.31	106.26	107.06	106.02	105.09	104.11
H7-C4-C2	105.55	106.29	108.52	109.26	105.68	106.62	105.61	106.16
C8-C4-C2	110.43	109.17	109.86	108.80	112.07	110.35	110.89	110.31
H9-N5-C4	111.86	111.07	111.24	110.51	110.54	110.01	111.86	111.02
H10-N5-C4	109.63	108.55	109.78	108.67	111.74	110.85	111.49	110.51
H11-C8-C4	109.76	110.11	110.56	110.71	110.96	111.09	108.86	108.75
H12-C8-C4	109.35	109.67	108.91	108.58	107.89	108.32	108.74	108.82
O13-C8-C4	111.14	110.08	110.11	109.93	110.80	109.76	112.80	112.63
H14-O13-C8	108.11	106.69	105.74	104.56	105.71	104.57	106.53	105.51
C4-C2-O1-O3	-179.2	-179.6	-178.0	-177.1	177.9	178.2	-179.3	-179.4
N5-C4-C2-O3	18.8	21.6	165.8	164.3	-173.4	-172.9	17.1	19.0
H6-O3-C2-C4	-5.5	-6.4	177.5	176.7	-179.4	-179.9	-4.3	-4.6
H7-C4-C2-O3	-97.4	-95.0	44.4	41.8	64.4	63.7	-99.0	-97.6
C8-C4-C2-O3	145.6	147.0	-72.7	-75.7	-52.8	-54.5	144.4	145.4
H9-N5-C4-C2	-148.9	-153.4	-81.5	-79.9	-21.6	-27.5	-146.8	-151.2
H10-N5-C4-C2	91.6	88.8	36.2	35.9	-143.1	-147.2	92.8	90.2
H11-C8-C4-C2	57.8	60.5	61.5	61.7	53.7	57.7	-61.1	-59.0
H12-C8-C4-C2	177.2	-179.4	-57.6	-57.7	172.4	177.3	178.3	-176.6
O13-C8-C4-C2	-65.8	-62.8	-179.6	-179.5	-65.7	-61.0	63.2	65.2
H14-O13-C8-C4	80.4	79.1	44.4	44.3	-46.1	-47.0	-52.8	-54.6

Table S2: Geometrical parameters of **I-A** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.216	1.226	H12-C8-C4-C2	178.0	177.3
O3-C2	1.332	1.340	O13-C8-C4-C2	-64.2	-65.5
C4-C2	1.545	1.540	H14-O13-C8-C4	69.0	69.6
N5-C4	1.481	1.483	O15-H6-O3-C2	-61.1	-56.0
H6-O3	0.992	0.992	H16-O15-H6-N5	-11.9	-14.7
H7-C4	1.102	1.105	H17-O15-H16-H6	116.1	117.0
C8-C4	1.535	1.533			
H9-N5	1.019	1.023			
H10-N5	1.020	1.024			
H11-C8	1.101	1.103			
H12-C8	1.099	1.101			
O13-C8	1.420	1.428			
H14-O13	0.970	0.972			
O15-H6	1.724	1.725			
H16-O15	0.991	0.990			
H17-O15	0.964	0.965			
O3-C2-O1	120.63	120.79			
C4-C2-O1	121.35	121.64			
N5-C4-C2	110.22	109.48			
H6-O3-C2	113.81	111.75			
H7-C4-C2	107.06	107.62			
C8-C4-C2	110.20	109.74			
H9-N5-C4	108.49	107.74			
H10-N5-C4	108.55	107.56			
H11-C8-C4	109.49	109.76			
H12-C8-C4	109.00	109.12			
O13-C8-C4	112.10	111.35			
H14-O13-C8	105.76	104.71			
O15-H6-O3	170.08	170.45			
H16-O15-H6	84.29	84.55			
H17-O15-H16	107.32	106.43			
C4-C2-O1-O3	-179.0	-179.4			
N5-C4-C2-O3	59.0	62.1			
H6-O3-C2-C4	-4.5	-2.9			
H7-C4-C2-O3	-57.2	-54.5			
C8-C4-C2-O3	-175.1	-173.3			
H9-N5-C4-C2	-178.8	178.6			
H10-N5-C4-C2	67.1	66.1			
H11-C8-C4-C2	60.0	58.5			

Table S3: Geometrical parameters of **II-A** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.212	1.222	H12-C8-C4-C2	-72.1	-71.9
O3-C2	1.354	1.361	O13-C8-C4-C2	163.6	163.9
C4-C2	1.524	1.522	H14-O13-C8-C4	74.6	76.0
N5-C4	1.469	1.472	H15-N5-C4-C2	155.4	152.5
H6-O3	0.971	0.974	O16-H15-N5-C4	-35.8	-39.5
H7-C4	1.097	1.100	H17-O16-H15-N5	150.5	157.4
C8-C4	1.552	1.546			
H9-N5	1.018	1.021			
H10-N5	1.021	1.025			
H11-C8	1.097	1.100			
H12-C8	1.104	1.107			
O13-C8	1.408	1.416			
H14-O13	0.977	0.978			
H15-N5	1.880	1.874			
O16-H15	0.987	0.987			
H17-O16	0.963	0.965			
O3-C2-O1	122.84	123.37			
C4-C2-O1	124.93	124.77			
N5-C4-C2	111.70	111.73			
H6-O3-C2	107.32	106.29			
H7-C4-C2	108.53	109.15			
C8-C4-C2	109.45	108.39			
H9-N5-C4	109.95	109.40			
H10-N5-C4	108.46	107.47			
H11-C8-C4	108.76	108.84			
H12-C8-C4	108.55	108.40			
O13-C8-C4	112.53	112.34			
H14-O13-C8	109.26	108.01			
H15-N5-C4	115.27	115.26			
O16-H15-N5	159.81	158.77			
H17-O16-H15	106.55	105.73			
C4-C2-O1-O3	-178.2	-177.6			
N5-C4-C2-O3	162.2	160.6			
H6-O3-C2-C4	177.3	176.6			
H7-C4-C2-O3	41.9	39.2			
C8-C4-C2-O3	-74.1	-77.2			
H9-N5-C4-C2	-75.4	-75.2			
H10-N5-C4-C2	39.2	38.1			
H11-C8-C4-C2	45.3	45.8			

Table S4: Geometrical parameters of **III-A** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.212	1.221	H12-C8-C4-C2	-175.4	-171.2
O3-C2	1.349	1.357	O13-C8-C4-C2	-51.2	-47.3
C4-C2	1.521	1.520	H14-O13-C8-C4	-75.2	-78.1
N5-C4	1.473	1.475	H15-N5-C4-C2	96.0	94.5
H6-O3	0.970	0.973	O16-H15-N5-C4	26.3	26.0
H7-C4	1.105	1.107	H17-O16-H15-N5	-143.0	-146.9
C8-C4	1.546	1.541			
H9-N5	1.019	1.022			
H10-N5	1.016	1.019			
H11-C8	1.097	1.099			
H12-C8	1.103	1.105			
O13-C8	1.410	1.420			
H14-O13	0.977	0.978			
H15-N5	1.877	1.867			
O16-H15	0.987	0.986			
H17-O16	0.964	0.965			
O3-C2-O1	123.13	123.74			
C4-C2-O1	124.77	124.95			
N5-C4-C2	108.82	108.58			
H6-O3-C2	107.18	106.18			
H7-C4-C2	105.79	106.69			
C8-C4-C2	111.38	109.36			
H9-N5-C4	109.26	108.78			
H10-N5-C4	110.38	109.76			
H11-C8-C4	108.66	108.91			
H12-C8-C4	107.76	108.38			
O13-C8-C4	113.35	112.03			
H14-O13-C8	108.97	107.63			
H15-N5-C4	114.67	114.17			
O16-H15-N5	162.25	162.16			
H17-O16-H15	106.16	105.32			
C4-C2-O1-O3	177.8	178.3			
N5-C4-C2-O3	-177.3	-177.0			
H6-O3-C2-C4	179.5	178.7			
H7-C4-C2-O3	62.5	61.6			
C8-C4-C2-O3	-53.3	-55.1			
H9-N5-C4-C2	-25.3	-27.7			
H10-N5-C4-C2	-143.8	-144.9			
H11-C8-C4-C2	67.8	70.9			

Table S5: Geometrical parameters of **IV-A** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.218	1.227	H12-C8-C4-C2	-174.9	-174.6
O3-C2	1.332	1.342	O13-C8-C4-C2	67.2	67.7
C4-C2	1.535	1.531	H14-O13-C8-C4	-43.0	-42.4
N5-C4	1.474	1.476	O15-H6-O3-C2	-128.0	-143.3
H6-O3	0.989	0.990	H16-O15-H6-N5	-11.9	-10.1
H7-C4	1.100	1.103	H17-O15-H16-H6	117.4	118.1
C8-C4	1.548	1.544			
H9-N5	1.019	1.023			
H10-N5	1.018	1.022			
H11-C8	1.105	1.108			
H12-C8	1.100	1.103			
O13-C8	1.410	1.420			
H14-O13	0.972	0.973			
O15-H6	1.752	1.752			
H16-O15	0.983	0.983			
H17-O15	0.964	0.966			
O3-C2-O1	120.59	120.92			
C4-C2-O1	118.15	118.78			
N5-C4-C2	114.80	114.22			
H6-O3-C2	115.80	114.17			
H7-C4-C2	104.97	105.57			
C8-C4-C2	107.62	106.73			
H9-N5-C4	110.07	109.67			
H10-N5-C4	109.03	108.36			
H11-C8-C4	109.43	109.13			
H12-C8-C4	108.65	108.88			
O13-C8-C4	112.46	112.33			
H14-O13-C8	107.80	107.48			
O15-H6-O3	174.04	173.78			
H16-O15-H6	82.00	82.13			
H17-O15-H16	107.51	106.59			
C4-C2-O1-O3	178.1	176.5			
N5-C4-C2-O3	-12.6	-21.6			
H6-O3-C2-C4	-9.8	-8.2			
H7-C4-C2-O3	-136.5	-146.7			
C8-C4-C2-O3	110.0	99.0			
H9-N5-C4-C2	-69.7	-63.4			
H10-N5-C4-C2	174.6	-178.0			
H11-C8-C4-C2	-57.4	-56.8			

Table S6: Geometrical parameters of **I-B** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.212	1.222	H12-C8-C4-C2	177.4	-179.1
O3-C2	1.339	1.348	O13-C8-C4-C2	-65.6	-62.5
C4-C2	1.543	1.538	H14-O13-C8-C4	78.6	77.4
N5-C4	1.469	1.471	O15-H9-N5-H10	173.4	153.5
H6-O3	0.990	0.991	H16-O15-H9-N5	-140.7	-131.1
H7-C4	1.101	1.103	H17-O15-H16-H9	156.6	148.1
C8-C4	1.532	1.529			
H9-N5	1.018	1.020			
H10-N5	1.018	1.022			
H11-C8	1.098	1.101			
H12-C8	1.097	1.100			
O13-C8	1.428	1.435			
H14-O13	0.966	0.969			
O15-H9	2.120	2.165			
H16-O15	0.964	0.966			
H17-O15	0.964	0.966			
O3-C2-O1	123.08	123.07			
C4-C2-O1	123.43	123.33			
N5-C4-C2	109.00	108.68			
H6-O3-C2	103.97	103.03			
H7-C4-C2	105.70	106.73			
C8-C4-C2	110.44	109.32			
H9-N5-C4	111.60	109.68			
H10-N5-C4	109.87	108.98			
H11-C8-C4	109.74	110.12			
H12-C8-C4	109.28	109.49			
O13-C8-C4	111.43	110.46			
H14-O13-C8	107.99	106.56			
O15-H9-N5	165.17	143.92			
H16-O15-H9	131.82	132.15			
H17-O15-H16	105.17	104.07			
C4-C2-O1-O3	-179.5	-179.7			
N5-C4-C2-O3	17.2	20.1			
H6-O3-C2-C4	-5.4	-6.3			
H7-C4-C2-O3	-98.9	-96.2			
C8-C4-C2-O3	144.3	145.9			
H9-N5-C4-C2	-145.6	-150.2			
H10-N5-C4-C2	93.6	90.9			
H11-C8-C4-C2	58.1	60.8			

Table S7: Geometrical parameters of **II-B** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.216	1.225	H12-C8-C4-C2	-59.3	-58.6
O3-C2	1.351	1.358	O13-C8-C4-C2	178.8	179.7
C4-C2	1.526	1.522	H14-O13-C8-C4	40.5	40.6
N5-C4	1.454	1.459	O15-H9-N5-C4	83.0	62.6
H6-O3	0.971	0.974	H16-O15-H9-N5	143.0	131.4
H7-C4	1.100	1.102	H17-O15-H16-O1	-6.7	-8.9
C8-C4	1.546	1.542			
H9-N5	1.017	1.021			
H10-N5	1.018	1.022			
H11-C8	1.095	1.098			
H12-C8	1.107	1.109			
O13-C8	1.413	1.421			
H14-O13	0.971	0.974			
O15-H9	2.297	2.205			
H16-O15	0.963	0.971			
H17-O15	0.972	0.965			
O3-C2-O1	121.93	122.54			
C4-C2-O1	125.82	125.85			
N5-C4-C2	114.62	114.54			
H6-O3-C2	107.51	106.44			
H7-C4-C2	106.60	107.66			
C8-C4-C2	111.32	109.94			
H9-N5-C4	112.02	110.54			
H10-N5-C4	110.61	109.29			
H11-C8-C4	110.77	110.91			
H12-C8-C4	108.97	108.71			
O13-C8-C4	109.99	109.70			
H14-O13-C8	105.75	104.51			
O15-H9-N5	134.94	139.62			
H16-O15-H9	171.64	160.87			
H17-O15-H16	106.03	105.20			
C4-C2-O1-O3	179.9	-178.7			
N5-C4-C2-O3	-178.8	-182.0			
H6-O3-C2-C4	-179.2	179.6			
H7-C4-C2-O3	61.3	56.8			
C8-C4-C2-O3	-55.2	-60.3			
H9-N5-C4-C2	-69.1	-70.5			
H10-N5-C4-C2	48.9	45.4			
H11-C8-C4-C2	59.7	60.8			

Table S8: Geometrical parameters of **III-B** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.215	1.223	H12-C8-C4-C2	173.7	178.6
O3-C2	1.349	1.357	O13-C8-C4-C2	-64.4	-59.7
C4-C2	1.521	1.519	H14-O13-C8-C4	-44.2	-44.5
N5-C4	1.460	1.464	O15-H9-N5-C4	70.8	65.7
H6-O3	0.971	0.974	H16-O15-H9-N5	-28.1	-12.5
H7-C4	1.107	1.108	H17-O15-H16-O1	-145.4	-156.6
C8-C4	1.542	1.538			
H9-N5	1.020	1.025			
H10-N5	1.015	1.020			
H11-C8	1.095	1.097			
H12-C8	1.105	1.106			
O13-C8	1.416	1.424			
H14-O13	0.971	0.974			
O15-H9	2.160	2.205			
H16-O15	0.972	0.973			
H17-O15	0.963	0.965			
O3-C2-O1	121.88	122.53			
C4-C2-O1	126.37	126.44			
N5-C4-C2	110.47	109.82			
H6-O3-C2	107.23	106.20			
H7-C4-C2	105.18	106.47			
C8-C4-C2	111.19	109.10			
H9-N5-C4	113.36	112.24			
H10-N5-C4	110.28	109.26			
H11-C8-C4	111.08	111.21			
H12-C8-C4	107.79	108.22			
O13-C8-C4	110.74	109.68			
H14-O13-C8	105.70	104.54			
O15-H9-N5	170.00	166.77			
H16-O15-H9	73.13	75.55			
H17-O15-H16	105.50	104.77			
C4-C2-O1-O3	177.9	178.9			
N5-C4-C2-O3	-173.5	-175.5			
H6-O3-C2-C4	-178.9	179.9			
H7-C4-C2-O3	62.8	59.4			
C8-C4-C2-O3	-53.6	-58.1			
H9-N5-C4-C2	-38.7	-45.5			
H10-N5-C4-C2	-159.7	-164.2			
H11-C8-C4-C2	55.1	59.1			

Table S9: Geometrical parameters of **IV-B** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.217	1.226	H12-C8-C4-C2	-179.0	-177.9
O3-C2	1.337	1.345	O13-C8-C4-C2	63.4	64.8
C4-C2	1.535	1.532	H14-O13-C8-C4	-59.1	-60.5
N5-C4	1.469	1.471	H15-O1-C2-C4	93.5	91.9
H6-O3	0.984	0.986	O16-H15-O1-C2	-23.6	-18.7
H7-C4	1.101	1.105	H17-O16-H15-O3	108.5	97.1
C8-C4	1.538	1.535			
H9-N5	1.015	1.019			
H10-N5	1.019	1.023			
H11-C8	1.102	1.104			
H12-C8	1.098	1.101			
O13-C8	1.418	1.425			
H14-O13	0.970	0.972			
H15-O1	2.473	2.376			
O16-H15	0.967	0.969			
H17-O16	0.964	0.966			
O3-C2-O1	121.72	121.81			
C4-C2-O1	124.09	124.00			
N5-C4-C2	107.64	107.25			
H6-O3-C2	105.18	104.06			
H7-C4-C2	105.49	105.94			
C8-C4-C2	111.95	111.36			
H9-N5-C4	111.76	110.94			
H10-N5-C4	110.14	108.87			
H11-C8-C4	109.30	109.32			
H12-C8-C4	108.50	108.62			
O13-C8-C4	112.35	112.06			
H14-O13-C8	106.44	105.42			
H15-O1-C2	83.02	81.39			
O16-H15-O1	131.08	131.00			
H17-O16-H15	104.91	103.80			
C4-C2-O1-O3	-179.5	-179.6			
N5-C4-C2-O3	29.8	31.9			
H6-O3-C2-C4	-9.8	-10.5			
H7-C4-C2-O3	-85.2	-83.5			
C8-C4-C2-O3	157.8	159.2			
H9-N5-C4-C2	-160.1	-163.4			
H10-N5-C4-C2	79.4	77.5			
H11-C8-C4-C2	-61.3	-60.0			

Table S10: Geometrical parameters of **I-C** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.217	1.226	H12-C8-C4-C2	172.2	172.7
O3-C2	1.331	1.339	O13-C8-C4-C2	-69.8	-69.6
C4-C2	1.542	1.539	H14-O13-C8-C4	97.2	99.3
N5-C4	1.472	1.474	O15-H14-O13-C8	-6.9	-4.2
H6-O3	0.991	0.994	H16-O15-H14-O13	-150.4	-156.2
H7-C4	1.101	1.104	H17-O15-H16-O1	-14.5	-14.0
C8-C4	1.536	1.533			
H9-N5	1.015	1.018			
H10-N5	1.020	1.023			
H11-C8	1.098	1.101			
H12-C8	1.100	1.102			
O13-C8	1.419	1.428			
H14-O13	0.977	0.978			
O15-H14	1.872	1.858			
H16-O15	0.964	0.965			
H17-O15	0.976	0.975			
O3-C2-O1	122.32	122.60			
C4-C2-O1	123.73	123.34			
N5-C4-C2	108.29	108.21			
H6-O3-C2	104.19	103.08			
H7-C4-C2	105.19	105.87			
C8-C4-C2	111.99	110.66			
H9-N5-C4	112.01	111.38			
H10-N5-C4	109.01	108.08			
H11-C8-C4	109.84	110.17			
H12-C8-C4	108.33	108.78			
O13-C8-C4	110.77	109.55			
H14-O13-C8	107.79	106.50			
O15-H14-O13	159.99	159.31			
H16-O15-H14	124.27	124.55			
H17-O15-H16	105.84	105.04			
C4-C2-O1-O3	-178.3	-178.5			
N5-C4-C2-O3	15.4	13.9			
H6-O3-C2-C4	-4.8	-3.8			
H7-C4-C2-O3	-100.7	-103.1			
C8-C4-C2-O3	141.5	138.3			
H9-N5-C4-C2	-144.7	-146.3			
H10-N5-C4-C2	95.7	95.3			
H11-C8-C4-C2	54.1	53.6			

Table S11: Geometrical parameters of **II-C** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.224	1.232	H12-C8-C4-C2	-57.5	-57.6
O3-C2	1.336	1.344	O13-C8-C4-C2	-179.4	-179.4
C4-C2	1.523	1.520	H14-O13-C8-C4	43.9	43.7
N5-C4	1.461	1.464	O15-H6-O3-C2	8.5	7.3
H6-O3	0.992	0.992	H16-O15-H6-O3	-11.3	-10.9
H7-C4	1.097	1.100	H17-O15-H16-O1	131.1	133.1
C8-C4	1.547	1.542			
H9-N5	1.015	1.019			
H10-N5	1.019	1.023			
H11-C8	1.096	1.098			
H12-C8	1.106	1.108			
O13-C8	1.413	1.421			
H14-O13	0.971	0.973			
O15-H6	1.765	1.766			
H16-O15	0.976	0.976			
H17-O15	0.964	0.965			
O3-C2-O1	123.73	124.34			
C4-C2-O1	123.43	123.32			
N5-C4-C2	113.87	113.92			
H6-O3-C2	108.51	107.52			
H7-C4-C2	108.37	109.13			
C8-C4-C2	109.62	108.55			
H9-N5-C4	111.16	110.44			
H10-N5-C4	109.73	108.55			
H11-C8-C4	110.51	110.64			
H12-C8-C4	108.89	108.57			
O13-C8-C4	110.16	109.99			
H14-O13-C8	105.60	104.49			
O15-H6-O3	157.38	158.77			
H16-O15-H6	85.44	86.67			
H17-O15-H16	106.57	105.69			
C4-C2-O1-O3	-177.9	-177.0			
N5-C4-C2-O3	164.4	163.2			
H6-O3-C2-C4	177.5	176.6			
H7-C4-C2-O3	42.8	40.5			
C8-C4-C2-O3	-74.1	-76.8			
H9-N5-C4-C2	-82.0	-80.0			
H10-N5-C4-C2	35.6	35.7			
H11-C8-C4-C2	61.7	61.7			

Table S12: Geometrical parameters of **III-C** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.224	1.231	H12-C8-C4-C2	171.5	176.5
O3-C2	1.333	1.341	O13-C8-C4-C2	-66.7	-61.8
C4-C2	1.522	1.521	H14-O13-C8-C4	-45.6	-46.7
N5-C4	1.464	1.467	O15-H6-O3-C2	4.8	3.5
H6-O3	0.992	0.992	H16-O15-H6-O3	-7.3	-6.7
H7-C4	1.105	1.107	H17-O15-H16-O1	127.5	128.1
C8-C4	1.542	1.537			
H9-N5	1.016	1.020			
H10-N5	1.014	1.018			
H11-C8	1.095	1.097			
H12-C8	1.104	1.106			
O13-C8	1.416	1.425			
H14-O13	0.971	0.974			
O15-H6	1.760	1.764			
H16-O15	0.977	0.976			
H17-O15	0.964	0.966			
O3-C2-O1	123.72	124.36			
C4-C2-O1	123.46	123.53			
N5-C4-C2	109.62	109.13			
H6-O3-C2	108.30	107.28			
H7-C4-C2	105.62	106.57			
C8-C4-C2	111.68	109.96			
H9-N5-C4	110.46	109.91			
H10-N5-C4	111.69	110.82			
H11-C8-C4	110.84	110.98			
H12-C8-C4	107.99	108.43			
O13-C8-C4	110.74	109.67			
H14-O13-C8	105.55	104.38			
O15-H6-O3	158.12	159.38			
H16-O15-H6	85.06	85.70			
H17-O15-H16	106.29	105.33			
C4-C2-O1-O3	178.1	178.6			
N5-C4-C2-O3	-174.9	-173.9			
H6-O3-C2-C4	-179.6	179.6			
H7-C4-C2-O3	62.6	62.4			
C8-C4-C2-O3	-54.3	-55.5			
H9-N5-C4-C2	-21.8	-27.3			
H10-N5-C4-C2	-143.2	-147.0			
H11-C8-C4-C2	52.7	56.8			

Table S13: Geometrical parameters of **II-D** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.211	1.221	H12-C8-C4-C2	-53.5	-53.2
O3-C2	1.354	1.362	O13-C8-C4-C2	-174.5	-173.9
C4-C2	1.522	1.519	H14-O13-C8-C4	43.0	42.6
N5-C4	1.461	1.465	H15-O13-C8-C4	-64.9	-63.5
H6-O3	0.971	0.974	O16-H15-O13-C8	34.6	30.0
H7-C4	1.097	1.100	H17-O16-H15-O13	-175.2	-173.7
C8-C4	1.549	1.545			
H9-N5	1.015	1.018			
H10-N5	1.018	1.022			
H11-C8	1.094	1.098			
H12-C8	1.103	1.106			
O13-C8	1.423	1.431			
H14-O13	0.975	0.978			
H15-O13	1.904	1.887			
O16-H15	0.976	0.977			
H17-O16	0.963	0.964			
O3-C2-O1	122.93	123.40			
C4-C2-O1	125.09	125.15			
N5-C4-C2	113.06	113.16			
H6-O3-C2	107.34	106.29			
H7-C4-C2	108.78	109.45			
C8-C4-C2	109.85	108.78			
H9-N5-C4	111.24	110.50			
H10-N5-C4	110.08	109.11			
H11-C8-C4	110.82	110.97			
H12-C8-C4	109.78	109.52			
O13-C8-C4	109.23	109.00			
H14-O13-C8	104.46	103.35			
H15-O13-C8	104.48	100.39			
O16-H15-O13	157.72	156.44			
H17-O16-H15	105.84	105.04			
C4-C2-O1-O3	-177.9	-177.1			
N5-C4-C2-O3	171.2	170.5			
H6-O3-C2-C4	178.0	177.3			
H7-C4-C2-O3	49.4	47.7			
C8-C4-C2-O3	-67.8	-69.9			
H9-N5-C4-C2	-90.9	-89.2			
H10-N5-C4-C2	27.5	27.5			
H11-C8-C4-C2	66.9	67.6			

Table S14: Geometrical parameters of **III-D** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.209	1.218	H12-C8-C4-C2	173.7	178.2
O3-C2	1.364	1.373	O13-C8-C4-C2	-64.4	-60.1
C4-C2	1.519	1.518	H14-O13-C8-C4	-47.2	-47.6
N5-C4	1.465	1.470	H15-O3-H6-C2	-139.2	-138.2
H6-O3	0.971	0.974	O16-H15-O3-C2	7.8	12.8
H7-C4	1.104	1.106	H17-O16-H15-O3	-177.2	-177.9
C8-C4	1.544	1.537			
H9-N5	1.017	1.021			
H10-N5	1.015	1.019			
H11-C8	1.095	1.097			
H12-C8	1.104	1.106			
O13-C8	1.416	1.426			
H14-O13	0.971	0.974			
H15-O3	2.115	2.065			
O16-H15	0.968	0.970			
H17-O16	0.964	0.965			
O3-C2-O1	121.87	122.35			
C4-C2-O1	125.73	125.89			
N5-C4-C2	109.08	108.47			
H6-O3-C2	106.62	105.64			
H7-C4-C2	106.22	107.01			
C8-C4-C2	111.60	110.14			
H9-N5-C4	110.75	110.16			
H10-N5-C4	111.38	110.34			
H11-C8-C4	111.16	111.32			
H12-C8-C4	107.64	108.11			
O13-C8-C4	110.84	109.75			
H14-O13-C8	105.74	104.55			
H15-O3-H6	124.46	128.09			
O16-H15-O3	150.07	149.80			
H17-O16-H15	105.59	104.74			
C4-C2-O1-O3	178.6	178.6			
N5-C4-C2-O3	-176.2	-173.0			
H6-O3-C2-C4	179.5	179.8			
H7-C4-C2-O3	60.9	63.1			
C8-C4-C2-O3	-56.2	-55.1			
H9-N5-C4-C2	-21.1	-28.8			
H10-N5-C4-C2	-142.2	-148.0			
H11-C8-C4-C2	55.2	59.0			

Table S15: Geometrical parameters of **IV-D** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.216	1.226	H12-C8-C4-C2	-179.3	-178.1
O3-C2	1.335	1.344	O13-C8-C4-C2	62.5	64.0
C4-C2	1.536	1.534	H14-O13-C8-C4	-51.7	-52.6
N5-C4	1.469	1.472	O15-H7-C4-C2	-121.0	-126.66
H6-O3	0.986	0.988	H16-O15-H7-C4	133.93	142.81
H7-C4	1.099	1.102	H17-O15-H16-O13	-1.3	-3.1
C8-C4	1.540	1.537			
H9-N5	1.015	1.018			
H10-N5	1.018	1.021			
H11-C8	1.104	1.107			
H12-C8	1.097	1.100			
O13-C8	1.423	1.432			
H14-O13	0.975	0.977			
O15-H7	2.477	2.363			
H16-O15	0.963	0.965			
H17-O15	0.976	0.977			
O3-C2-O1	122.38	122.38			
C4-C2-O1	122.90	123.04			
N5-C4-C2	109.43	109.10			
H6-O3-C2	105.00	103.90			
H7-C4-C2	106.00	106.61			
C8-C4-C2	110.62	110.08			
H9-N5-C4	111.51	110.67			
H10-N5-C4	111.86	110.95			
H11-C8-C4	109.69	109.54			
H12-C8-C4	109.00	109.05			
O13-C8-C4	112.12	112.03			
H14-O13-C8	105.91	104.97			
O15-H7-C4	129.87	128.41			
H16-O15-H7	157.94	157.85			
H17-O15-H16	105.94	105.08			
C4-C2-O1-O3	-179.2	-179.3			
N5-C4-C2-O3	17.8	18.6			
H6-O3-C2-C4	-4.4	-4.4			
H7-C4-C2-O3	-98.5	-98.1			
C8-C4-C2-O3	145.1	144.9			
H9-N5-C4-C2	-146.7	-149.8			
H10-N5-C4-C2	92.6	91.3			
H11-C8-C4-C2	-60.7	-59.1			

Table S16: Geometrical parameters of **III-E** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.210	1.220	H12-C8-C4-C2	170.8	175.5
O3-C2	1.351	1.360	O13-C8-C4-C2	-68.1	-63.6
C4-C2	1.523	1.521	H14-O13-C8-C4	-42.5	-42.7
N5-C4	1.463	1.467	H15-O13-H14-C8	-117.7	-104.2
H6-O3	0.971	0.974	O16-H15-O13-C8	27.3	16.9
H7-C4	1.105	1.107	H17-O16-H15-O13	-168.6	-176.6
C8-C4	1.540	1.535			
H9-N5	1.017	1.020			
H10-N5	1.014	1.018			
H11-C8	1.094	1.097			
H12-C8	1.102	1.104			
O13-C8	1.424	1.434			
H14-O13	0.974	0.977			
H15-O13	1.902	1.899			
O16-H15	0.974	0.975			
H17-O16	0.963	0.964			
O3-C2-O1	123.04	123.53			
C4-C2-O1	124.83	125.02			
N5-C4-C2	108.96	108.50			
H6-O3-C2	107.16	106.09			
H7-C4-C2	105.64	106.59			
C8-C4-C2	112.43	110.80			
H9-N5-C4	110.62	110.21			
H10-N5-C4	111.84	110.92			
H11-C8-C4	111.43	111.61			
H12-C8-C4	108.56	109.11			
O13-C8-C4	109.91	108.93			
H14-O13-C8	105.10	103.76			
H15-O13-H14	111.65	110.17			
O16-H15-O13	167.19	157.77			
H17-O16-H15	105.20	104.64			
C4-C2-O1-O3	177.7	178.2			
N5-C4-C2-O3	-172.5	-172.0			
H6-O3-C2-C4	-178.8	-179.3			
H7-C4-C2-O3	65.2	64.4			
C8-C4-C2-O3	-52.1	-53.9			
H9-N5-C4-C2	-23.5	-29.9			
H10-N5-C4-C2	-145.4	-150.2			
H11-C8-C4-C2	51.1	54.9			

Table S17: Geometrical parameters of **IV-F** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.213	1.222	H12-C8-C4-C2	-177.6	-176.4
O3-C2	1.344	1.354	O13-C8-C4-C2	64.3	65.9
C4-C2	1.536	1.534	H14-O13-C8-C4	-55.1	-56.8
N5-C4	1.468	1.472	H15-O3-C2-O1	89.4	86.3
H6-O3	0.989	0.991	O16-H15-O3-C2	61.2	57.9
H7-C4	1.101	1.104	H17-O16-H15-H10	-172.4	-174.9
C8-C4	1.541	1.537			
H9-N5	1.014	1.018			
H10-N5	1.019	1.023			
H11-C8	1.104	1.105			
H12-C8	1.098	1.101			
O13-C8	1.415	1.424			
H14-O13	0.971	0.973			
H15-O3	2.429	2.323			
O16-H15	0.967	0.969			
H17-O16	0.964	0.965			
O3-C2-O1	121.97	121.91			
C4-C2-O1	123.92	124.09			
N5-C4-C2	108.37	108.11			
H6-O3-C2	104.42	103.36			
H7-C4-C2	105.87	106.26			
C8-C4-C2	110.81	110.35			
H9-N5-C4	112.04	111.16			
H10-N5-C4	110.96	109.75			
H11-C8-C4	108.86	108.64			
H12-C8-C4	108.61	108.67			
O13-C8-C4	112.57	112.33			
H14-O13-C8	106.51	105.48			
H15-O3-C2	92.48	87.29			
O16-H15-O3	120.99	121.11			
H17-O16-H15	105.38	104.57			
C4-C2-O1-O3	179.8	179.9			
N5-C4-C2-O3	18.2	20.1			
H6-O3-C2-C4	-2.3	-3.5			
H7-C4-C2-O3	-97.7	-96.2			
C8-C4-C2-O3	145.6	146.8			
H9-N5-C4-C2	-155.9	-157.8			
H10-N5-C4-C2	82.0	82.1			
H11-C8-C4-C2	-60.1	-58.5			

Table S18: Geometrical parameters of **IV-G** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.221	1.230	H12-C8-C4-C2	-179.5	-178.2
O3-C2	1.329	1.337	O13-C8-C4-C2	61.9	63.4
C4-C2	1.536	1.534	H14-O13-C8-C4	-46.6	-48.1
N5-C4	1.473	1.476	H15-O1-C2-O3	111.2	110.6
H6-O3	0.991	0.993	O16-H15-O1-C2	11.2	10.0
H7-C4	1.098	1.101	H17-O16-H15-H7	172.0	168.1
C8-C4	1.544	1.541			
H9-N5	1.014	1.017			
H10-N5	1.017	1.021			
H11-C8	1.108	1.110			
H12-C8	1.098	1.101			
O13-C8	1.410	1.418			
H14-O13	0.971	0.973			
H15-O1	2.123	2.144			
O16-H15	0.969	0.970			
H17-O16	0.963	0.965			
O3-C2-O1	122.44	122.47			
C4-C2-O1	122.58	122.67			
N5-C4-C2	109.14	108.90			
H6-O3-C2	104.21	103.13			
H7-C4-C2	105.73	106.07			
C8-C4-C2	110.34	109.78			
H9-N5-C4	112.11	111.28			
H10-N5-C4	112.03	111.18			
H11-C8-C4	108.69	108.66			
H12-C8-C4	108.30	108.43			
O13-C8-C4	113.58	113.27			
H14-O13-C8	107.42	106.14			
H15-O1-C2	100.18	95.89			
O16-H15-O1	125.57	138.80			
H17-O16-H15	105.43	104.61			
C4-C2-O1-O3	179.9	179.7			
N5-C4-C2-O3	4.6	6.2			
H6-O3-C2-C4	0.4	0.2			
H7-C4-C2-O3	-113.8	-112.4			
C8-C4-C2-O3	129.1	130.1			
H9-N5-C4-C2	-130.9	-135.0			
H10-N5-C4-C2	107.6	105.3			
H11-C8-C4-C2	-62.6	-60.9			

Table S19: Geometrical parameters of **I-H** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.217	1.227	H12-C8-C4-C2	174.2	177.4
O3-C2	1.330	1.338	O13-C8-C4-C2	-69.5	-66.5
C4-C2	1.543	1.539	H14-O13-C8-C4	85.8	83.4
N5-C4	1.472	1.474	H15-O1-C2-O3	153.2	144.9
H6-O3	0.992	0.994	O16-H15-O1-C2	13.8	11.0
H7-C4	1.100	1.102	H17-O16-H15-H7	-148.0	-150.6
C8-C4	1.536	1.532			
H9-N5	1.014	1.017			
H10-N5	1.018	1.022			
H11-C8	1.096	1.098			
H12-C8	1.097	1.100			
O13-C8	1.430	1.438			
H14-O13	0.965	0.968			
H15-O1	1.890	1.928			
O16-H15	0.975	0.975			
H17-O16	0.963	0.964			
O3-C2-O1	122.39	122.63			
C4-C2-O1	123.38	123.04			
N5-C4-C2	108.63	108.36			
H6-O3-C2	104.11	103.00			
H7-C4-C2	105.65	106.32			
C8-C4-C2	111.26	109.58			
H9-N5-C4	112.29	111.45			
H10-N5-C4	109.85	108.99			
H11-C8-C4	110.40	110.48			
H12-C8-C4	108.72	109.25			
O13-C8-C4	110.91	109.97			
H14-O13-C8	108.85	107.50			
H15-O1-C2	117.64	108.00			
O16-H15-O1	161.46	155.31			
H17-O16-H15	105.58	104.75			
C4-C2-O1-O3	-179.6	-180.0			
N5-C4-C2-O3	7.9	10.2			
H6-O3-C2-C4	-1.0	-1.5			
H7-C4-C2-O3	-109.8	-108.3			
C8-C4-C2-O3	133.3	134.1			
H9-N5-C4-C2	-138.5	-143.2			
H10-N5-C4-C2	100.6	97.6			
H11-C8-C4-C2	55.3	57.7			

Table S20: Geometrical parameters of **II-I** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.209	1.219	H12-C8-C4-C2	-58.8	-58.9
O3-C2	1.365	1.373	O13-C8-C4-C2	179.4	179.6
C4-C2	1.522	1.519	H14-O13-C8-C4	45.8	45.6
N5-C4	1.460	1.465	H15-O3-H6-C2	149.5	140.4
H6-O3	0.972	0.975	O16-H15-O3-C2	159.4	-79.39
H7-C4	1.098	1.100	H17-O16-H7-C4	-167.0	-170.8
C8-C4	1.549	1.544			
H9-N5	1.016	1.019			
H10-N5	1.019	1.023			
H11-C8	1.096	1.098			
H12-C8	1.105	1.108			
O13-C8	1.413	1.422			
H14-O13	0.970	0.973			
H15-O3	2.084	2.058			
O16-H15	0.967	0.968			
H17-O16	0.964	0.965			
O3-C2-O1	122.04	122.51			
C4-C2-O1	125.49	125.26			
N5-C4-C2	113.30	113.20			
H6-O3-C2	107.14	106.03			
H7-C4-C2	108.64	109.53			
C8-C4-C2	110.11	109.01			
H9-N5-C4	111.38	110.67			
H10-N5-C4	109.89	108.67			
H11-C8-C4	111.11	111.20			
H12-C8-C4	108.66	108.24			
O13-C8-C4	109.82	109.54			
H14-O13-C8	105.95	104.85			
H15-O3-H6	110.80	113.79			
O16-H15-O3	158.28	154.85			
H17-O16-H7	96.54	102.21			
C4-C2-O1-O3	-178.5	-177.8			
N5-C4-C2-O3	161.3	155.8			
H6-O3-C2-C4	176.7	175.7			
H7-C4-C2-O3	40.1	33.5			
C8-C4-C2-O3	-77.2	-84.6			
H9-N5-C4-C2	-79.3	-76.9			
H10-N5-C4-C2	38.7	39.3			
H11-C8-C4-C2	60.5	61.0			

Table S21: Geometrical parameters of **II-J** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.210	1.221	H12-C8-C4-C2	-55.6	-56.0
O3-C2	1.355	1.363	O13-C8-C4-C2	-176.8	-177.0
C4-C2	1.525	1.522	H14-O13-C8-C4	41.2	40.5
N5-C4	1.460	1.464	H15-O13-C8-C4	162.9	154.81
H6-O3	0.972	0.975	O16-H15-O13-C8	-25.9	-16.1
H7-C4	1.098	1.101	H17-O16-H15-O13	164.8	176.2
C8-C4	1.546	1.540			
H9-N5	1.016	1.020			
H10-N5	1.019	1.023			
H11-C8	1.095	1.098			
H12-C8	1.104	1.106			
O13-C8	1.422	1.432			
H14-O13	0.974	0.977			
H15-O13	1.906	1.900			
O16-H15	0.975	0.975			
H17-O16	0.963	0.964			
O3-C2-O1	123.12	123.61			
C4-C2-O1	125.06	125.06			
N5-C4-C2	113.60	113.68			
H6-O3-C2	107.44	106.36			
H7-C4-C2	108.44	109.11			
C8-C4-C2	109.85	108.89			
H9-N5-C4	111.35	110.60			
H10-N5-C4	109.97	108.83			
H11-C8-C4	110.96	111.21			
H12-C8-C4	109.56	109.44			
O13-C8-C4	109.27	109.06			
H14-O13-C8	105.11	103.84			
H15-O13-C8	109.84	98.44			
O16-H15-O13	168.23	157.71			
H17-O16-H15	105.17	104.67			
C4-C2-O1-O3	-178.2	-177.5			
N5-C4-C2-O3	167.4	166.8			
H6-O3-C2-C4	177.6	176.8			
H7-C4-C2-O3	46.1	44.5			
C8-C4-C2-O3	-71.2	-73.3			
H9-N5-C4-C2	-82.0	-79.1			
H10-N5-C4-C2	36.0	37.0			
H11-C8-C4-C2	64.5	64.5			

Table S22: Geometrical parameters of **IV-K** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.216	1.215	H12-C8-C4-C2	-178.7	184.2
O3-C2	1.336	1.335	O13-C8-C4-C2	62.7	65.9
C4-C2	1.539	1.534	H14-O13-C8-C4	-50.8	-54.6
N5-C4	1.469	1.465	O15-H9-N5-H10	160.2	142.5
H6-O3	0.990	0.985	H16-O15-H9-N5	78.2	101.4
H7-C4	1.100	1.095	H17-O15-H16-H9	172.6	-173.0
C8-C4	1.540	1.532			
H9-N5	1.021	1.021			
H10-N5	1.017	1.017			
H11-C8	1.107	1.102			
H12-C8	1.098	1.094			
O13-C8	1.413	1.412			
H14-O13	0.973	0.968			
O15-H9	2.090	2.139			
H16-O15	0.964	0.961			
H17-O15	0.964	0.961			
O3-C2-O1	122.59	123.07			
C4-C2-O1	123.35	122.95			
N5-C4-C2	109.32	109.25			
H6-O3-C2	104.08	103.23			
H7-C4-C2	105.78	106.32			
C8-C4-C2	110.77	110.60			
H9-N5-C4	111.48	109.46			
H10-N5-C4	111.60	111.07			
H11-C8-C4	108.89	108.98			
H12-C8-C4	108.67	108.52			
O13-C8-C4	112.92	112.56			
H14-O13-C8	106.52	105.05			
O15-H9-N5	167.08	145.36			
H16-O15-H9	123.55	125.47			
H17-O15-H16	105.23	103.97			
C4-C2-O1-O3	-179.4	-179.0			
N5-C4-C2-O3	14.6	18.2			
H6-O3-C2-C4	-3.9	-4.7			
H7-C4-C2-O3	-101.7	-98.0			
C8-C4-C2-O3	141.7	145.3			
H9-N5-C4-C2	-142.6	-147.5			
H10-N5-C4-C2	96.0	92.8			
H11-C8-C4-C2	-61.5	-58.3			

Table S23: Geometrical parameters of **IV-L** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.218	1.217	H12-C8-C4-C2	-176.9	-174.9
O3-C2	1.332	1.333	O13-C8-C4-C2	64.9	67.0
C4-C2	1.536	1.532	H14-O13-C8-C4	-55.0	-57.5
N5-C4	1.471	1.467	H15-O1-C2-C4	179.3	158.4
H6-O3	0.988	0.984	O16-H15-O1-C2	-170.5	-15.6
H7-C4	1.100	1.096	H17-O16-H15-O3	5.7	21.41
C8-C4	1.542	1.534			
H9-N5	1.015	1.014			
H10-N5	1.018	1.018			
H11-C8	1.106	1.101			
H12-C8	1.098	1.093			
O13-C8	1.411	1.409			
H14-O13	0.971	0.967			
H15-O1	1.987	2.076			
O16-H15	0.971	0.968			
H17-O16	0.963	0.960			
O3-C2-O1	122.28	122.51			
C4-C2-O1	122.94	122.87			
N5-C4-C2	108.79	108.54			
H6-O3-C2	104.85	103.89			
H7-C4-C2	105.67	106.01			
C8-C4-C2	111.05	110.52			
H9-N5-C4	111.97	111.38			
H10-N5-C4	111.59	111.05			
H11-C8-C4	109.01	108.86			
H12-C8-C4	108.49	108.43			
O13-C8-C4	112.89	112.46			
H14-O13-C8	107.21	105.70			
H15-O1-C2	126.71	110.14			
O16-H15-O1	177.43	161.41			
H17-O16-H15	104.51	102.13			
C4-C2-O1-O3	-179.4	-179.8			
N5-C4-C2-O3	15.8	17.6			
H6-O3-C2-C4	-3.9	-3.9			
H7-C4-C2-O3	-100.5	-99.2			
C8-C4-C2-O3	142.9	144.3			
H9-N5-C4-C2	-144.7	-147.5			
H10-N5-C4-C2	94.6	92.8			
H11-C8-C4-C2	-59.6	-57.4			

Table S24: Geometrical parameters of **I-A'** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.215	1.225	H10-N5-C4-C2	66.0	64.0
O3-C2	1.333	1.340	H11-C8-C4-C2	60.0	58.9
C4-C2	1.546	1.542	H12-C8-C4-C2	178.2	177.8
N5-C4	1.481	1.483	O13-C8-C4-C2	-64.1	-65.0
H6-O3	0.988	0.989	H14-O13-C8-C4	71.1	71.8
H7-C4	1.102	1.106	O15-H6-O3-C2	-64.3	-73.1
C8-C4	1.535	1.532	H16-O15-H6-N5	-7.6	-6.8
H9-N5	1.019	1.023	O17-O15-H16-H6	101.6	93.1
H10-N5	1.020	1.024	H18-O17-H16-O15	-69.2	-69.8
H11-C8	1.100	1.102			
H12-C8	1.099	1.101			
O13-C8	1.420	1.427			
H14-O13	0.969	0.971			
O15-H6	1.775	1.758			
H16-O15	1.004	1.007			
O17-O15	1.452	1.474			
H18-O17	0.969	0.971			
O3-C2-O1	120.55	120.74			
C4-C2-O1	121.00	121.15			
N5-C4-C2	110.87	110.25			
H6-O3-C2	114.28	112.46			
H7-C4-C2	106.79	107.36			
C8-C4-C2	110.05	109.52			
H9-N5-C4	108.64	108.06			
H10-N5-C4	108.74	107.96			
H11-C8-C4	109.53	109.81			
H12-C8-C4	109.01	109.15			
O13-C8-C4	111.93	111.09			
H14-O13-C8	106.06	104.95			
O15-H6-O3	170.01	168.04			
H16-O15-H6	81.17	80.90			
O17-O15-H16	101.92	99.23			
H18-O17-H16	113.93	112.25			
C4-C2-O1-O3	-178.4	-178.9			
N5-C4-C2-O3	54.2	56.2			
H6-O3-C2-C4	-5.4	-3.8			
H7-C4-C2-O3	-62.2	-60.7			
C8-C4-C2-O3	-179.8	-179.2			
H9-N5-C4-C2	-179.6	177.2			

Table S25: Geometrical parameters of **II-A'** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.212	1.222	H10-N5-C4-C2	33.3	33.4
O3-C2	1.352	1.360	H11-C8-C4-C2	44.8	43.6
C4-C2	1.524	1.521	H12-C8-C4-C2	-72.7	-74.0
N5-C4	1.472	1.474	O13-C8-C4-C2	162.8	161.4
H6-O3	0.971	0.974	H14-O13-C8-C4	71.4	70.2
H7-C4	1.097	1.100	H15-N5-C4-C2	155.8	157.2
C8-C4	1.552	1.547	O16-H15-N5-C4	-18.3	1.5
H9-N5	1.018	1.021	O17-O16-H15-N5	119.4	85.1
H10-N5	1.021	1.024	H18-O17-O16-H15	117.5	118.5
H11-C8	1.096	1.100			
H12-C8	1.104	1.108			
O13-C8	1.408	1.416			
H14-O13	0.974	0.976			
H15-N5	1.770	1.740			
O16-H15	1.001	1.003			
O17-O16	1.453	1.475			
H18-O17	0.968	0.971			
O3-C2-O1	123.03	123.50			
C4-C2-O1	124.64	124.62			
N5-C4-C2	111.15	111.21			
H6-O3-C2	107.46	106.39			
H7-C4-C2	108.76	109.34			
C8-C4-C2	109.60	108.63			
H9-N5-C4	110.10	109.63			
H10-N5-C4	108.33	107.60			
H11-C8-C4	108.92	109.04			
H12-C8-C4	108.54	108.24			
O13-C8-C4	112.55	112.53			
H14-O13-C8	109.70	108.51			
H15-N5-C4	115.34	114.10			
O16-H15-N5	167.56	168.38			
O17-O16-H15	101.07	98.16			
H18-O17-O16	100.60	98.96			
C4-C2-O1-O3	-178.1	-177.5			
N5-C4-C2-O3	162.6	161.2			
H6-O3-C2-C4	177.3	176.7			
H7-C4-C2-O3	42.2	39.9			
C8-C4-C2-O3	-73.9	-76.7			
H9-N5-C4-C2	-81.6	-80.7			

Table S26: Geometrical parameters of **III-A'** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.211	1.221	H10-N5-C4-C2	-132.7	-141.6
O3-C2	1.349	1.356	H11-C8-C4-C2	65.2	69.3
C4-C2	1.522	1.520	H12-C8-C4-C2	-177.5	-172.4
N5-C4	1.476	1.477	O13-C8-C4-C2	-53.6	-48.6
H6-O3	0.971	0.973	H14-O13-C8-C4	-80.9	-81.8
H7-C4	1.104	1.107	H15-N5-C4-C2	107.3	100.8
C8-C4	1.545	1.540	O16-H15-N5-C4	4.5	27.3
H9-N5	1.020	1.023	O17-O16-H15-N5	85.8	57.7
H10-N5	1.015	1.019	H18-O17-O16-H15	119.3	120.5
H11-C8	1.096	1.099			
H12-C8	1.101	1.104			
O13-C8	1.413	1.422			
H14-O13	0.973	0.975			
H15-N5	1.761	1.735			
O16-H15	1.003	1.006			
O17-O16	1.454	1.476			
H18-O17	0.968	0.971			
O3-C2-O1	123.19	123.80			
C4-C2-O1	124.67	124.83			
N5-C4-C2	108.92	108.46			
H6-O3-C2	107.24	106.20			
H7-C4-C2	106.02	106.76			
C8-C4-C2	111.33	109.60			
H9-N5-C4	108.79	108.79			
H10-N5-C4	110.58	109.93			
H11-C8-C4	108.65	108.80			
H12-C8-C4	108.01	108.65			
O13-C8-C4	112.86	111.68			
H14-O13-C8	108.52	107.27			
H15-N5-C4	114.57	113.85			
O16-H15-N5	169.16	167.94			
O17-O16-H15	100.54	97.96			
H18-O17-O16	100.65	98.92			
C4-C2-O1-O3	178.3	178.3			
N5-C4-C2-O3	-177.4	-176.2			
H6-O3-C2-C4	179.2	178.9			
H7-C4-C2-O3	62.8	62.8			
C8-C4-C2-O3	-53.0	-54.0			
H9-N5-C4-C2	-14.5	-23.9			

Table S27: Geometrical parameters of **IV-A'** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.215	1.225	H10-N5-C4-C2	175.8	178.7
O3-C2	1.336	1.344	H11-C8-C4-C2	-56.4	-55.8
C4-C2	1.534	1.531	H12-C8-C4-C2	-174.2	-174
N5-C4	1.478	1.480	O13-C8-C4-C2	68.6	69.1
H6-O3	0.985	0.989	H14-O13-C8-C4	-45.8	-46.4
H7-C4	1.099	1.102	O15-H6-O3-C2	-72.4	-109.4
C8-C4	1.548	1.544	H16-O15-H6-N5	-3.2	-1.4
H9-N5	1.019	1.022	O17-O15-H16-H6	101.5	96.2
H10-N5	1.019	1.022	H18-O17-O15-H16	121.3	121.2
H11-C8	1.103	1.104			
H12-C8	1.100	1.102			
O13-C8	1.412	1.422			
H14-O13	0.970	0.972			
O15-H6	1.804	1.790			
H16-O15	1.000	1.002			
O17-O15	1.452	1.474			
H18-O17	0.969	0.971			
O3-C2-O1	120.68	120.85			
C4-C2-O1	118.50	119.08			
N5-C4-C2	114.57	114.10			
H6-O3-C2	114.96	113.47			
H7-C4-C2	105.10	105.63			
C8-C4-C2	107.67	106.91			
H9-N5-C4	109.95	109.45			
H10-N5-C4	108.97	108.28			
H11-C8-C4	109.68	109.60			
H12-C8-C4	108.66	108.77			
O13-C8-C4	112.12	111.72			
H14-O13-C8	108.58	107.80			
O15-H6-O3	176.07	166.85			
H16-O15-H6	78.16	77.33			
O17-O15-H16	101.27	98.86			
H18-O17-O15	100.65	99.06			
C4-C2-O1-O3	177.3	176.1			
N5-C4-C2-O3	-21.6	-26.8			
H6-O3-C2-C4	-10.0	-7.3			
H7-C4-C2-O3	-144.9	-151.1			
C8-C4-C2-O3	101.1	94.4			
H9-N5-C4-C2	-68.5	-66.6			

Table S28: Geometrical parameters of **I-B'** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.212	1.222	H10-N5-C4-C2	93.6	89.4
O3-C2	1.340	1.348	H11-C8-C4-C2	58.1	61.4
C4-C2	1.543	1.538	H12-C8-C4-C2	177.5	-178.5
N5-C4	1.470	1.472	O13-C8-C4-C2	-65.6	-61.9
H6-O3	0.990	0.991	H14-O13-C8-C4	78.8	77.2
H7-C4	1.101	1.104	O15-H9-N5-C4	51.8	31.0
C8-C4	1.532	1.529	H16-O15-H9-N5	59.6	50.7
H9-N5	1.017	1.020	O17-O15-H16-H9	99.9	95.0
H10-N5	1.019	1.023	H18-O17-O15-H16	110.3	109.7
H11-C8	1.099	1.102			
H12-C8	1.098	1.099			
O13-C8	1.429	1.436			
H14-O13	0.966	0.970			
O15-H9	2.236	2.173			
H16-O15	0.971	0.973			
O17-O15	1.450	1.470			
H18-O17	0.971	0.973			
O3-C2-O1	123.00	123.01			
C4-C2-O1	123.39	123.34			
N5-C4-C2	109.01	108.59			
H6-O3-C2	104.09	103.15			
H7-C4-C2	105.87	106.60			
C8-C4-C2	110.51	109.48			
H9-N5-C4	111.60	110.08			
H10-N5-C4	109.83	108.64			
H11-C8-C4	109.78	110.15			
H12-C8-C4	109.24	109.16			
O13-C8-C4	111.43	110.43			
H14-O13-C8	107.99	106.53			
O15-H9-N5	164.58	157.42			
H16-O15-H9	115.25	117.90			
O17-O15-H16	101.11	99.65			
H18-O17-O15	101.01	99.43			
C4-C2-O1-O3	-179.3	-179.6			
N5-C4-C2-O3	17.6	20.8			
H6-O3-C2-C4	-5.5	-6.4			
H7-C4-C2-O3	-98.5	-95.8			
C8-C4-C2-O3	144.6	146.5			
H9-N5-C4-C2	-145.9	-152.5			

Table S29: Geometrical parameters of **II-B'** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.218	1.228	H10-N5-C4-C2	49.0	42.3
O3-C2	1.349	1.356	H11-C8-C4-C2	59.3	61.0
C4-C2	1.526	1.519	H12-C8-C4-C2	-59.8	-58.5
N5-C4	1.453	1.459	O13-C8-C4-C2	178.3	179.8
H6-O3	0.972	0.975	H14-O13-C8-C4	41.4	41.6
H7-C4	1.100	1.101	H15-O1-C2-O3	-155.6	-118.8
C8-C4	1.547	1.544	O16-H15-O1-C2	3.6	4.8
H9-N5	1.017	1.020	O17-O16-H15-O1	33.5	14.2
H10-N5	1.018	1.022	H18-O17-O16-H15	111.7	115.2
H11-C8	1.095	1.099			
H12-C8	1.107	1.109			
O13-C8	1.413	1.421			
H14-O13	0.972	0.974			
H15-O1	1.846	1.888			
O16-H15	0.981	0.981			
O17-O16	1.452	1.472			
H18-O17	0.969	0.972			
O3-C2-O1	121.64	122.42			
C4-C2-O1	126.16	125.73			
N5-C4-C2	114.97	114.50			
H6-O3-C2	107.65	106.43			
H7-C4-C2	106.71	108.07			
C8-C4-C2	110.85	109.21			
H9-N5-C4	112.20	110.16			
H10-N5-C4	111.14	109.44			
H11-C8-C4	110.76	110.82			
H12-C8-C4	108.93	108.76			
O13-C8-C4	109.98	109.72			
H14-O13-C8	105.86	104.5			
H15-O1-C2	130.58	108.86			
O16-H15-O1	175.06	156.02			
O17-O16-H15	100.60	98.32			
H18-O17-O16	101.12	99.27			
C4-C2-O1-O3	-179.5	-176.7			
N5-C4-C2-O3	177.9	171.1			
H6-O3-C2-C4	180.0	177.7			
H7-C4-C2-O3	57.6	49.5			
C8-C4-C2-O3	-58.6	-67.8			
H9-N5-C4-C2	-70.0	-74.0			

Table S30: Geometrical parameters of **III-B'** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.216	1.224	H10-N5-C4-C2	-162.9	-167.2
O3-C2	1.348	1.356	H11-C8-C4-C2	56.6	60.3
C4-C2	1.520	1.518	H12-C8-C4-C2	175.1	179.7
N5-C4	1.458	1.462	O13-C8-C4-C2	-63.0	-58.4
H6-O3	0.971	0.974	H14-O13-C8-C4	-44.5	-45.1
H7-C4	1.108	1.109	H15-O1-C2-O3	-174.5	-173.3
C8-C4	1.544	1.539	O16-H15-O1-C2	65.8	83.4
H9-N5	1.018	1.022	O17-O16-H15-O1	-25.8	-34.0
H10-N5	1.016	1.020	H18-O17-O16-H15	106.3	102.4
H11-C8	1.095	1.098			
H12-C8	1.105	1.107			
O13-C8	1.415	1.424			
H14-O13	0.971	0.974			
H15-O1	1.859	1.859			
O16-H15	0.980	0.981			
O17-O16	1.451	1.469			
H18-O17	0.969	0.971			
O3-C2-O1	121.82	122.45			
C4-C2-O1	126.46	126.46			
N5-C4-C2	110.18	109.42			
H6-O3-C2	107.39	106.37			
H7-C4-C2	105.58	106.83			
C8-C4-C2	110.66	108.61			
H9-N5-C4	113.44	112.17			
H10-N5-C4	110.54	109.55			
H11-C8-C4	110.98	111.07			
H12-C8-C4	107.73	108.19			
O13-C8-C4	110.87	109.84			
H14-O13-C8	106.04	104.90			
H15-O1-C2	142.17	136.08			
O16-H15-O1	169.05	165.50			
O17-O16-H15	100.36	98.88			
H18-O17-O16	101.20	99.76			
C4-C2-O1-O3	178.3	179.4			
N5-C4-C2-O3	-178.0	-179.7			
H6-O3-C2-C4	179.8	178.4			
H7-C4-C2-O3	57.7	54.7			
C8-C4-C2-O3	-58.6	-62.7			
H9-N5-C4-C2	-41.4	-48.3			

Table S31: Geometrical parameters of **IV-B'** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.220	1.229	H10-N5-C4-C2	86.0	82.8
O3-C2	1.332	1.342	H11-C8-C4-C2	-58.2	-58.6
C4-C2	1.534	1.531	H12-C8-C4-C2	-176.2	-177.9
N5-C4	1.470	1.472	O13-C8-C4-C2	66.4	66.2
H6-O3	0.986	0.988	H14-O13-C8-C4	-60.5	-60.7
H7-C4	1.101	1.105	H15-O1-C2-C4	95.7	85.1
C8-C4	1.539	1.535	O16-H15-O1-C2	-22.9	-4.8
H9-N5	1.015	1.019	O17-O16-H15-O3	-15.0	-10.2
H10-N5	1.018	1.023	H18-O17-O16-H15	103.5	97.3
H11-C8	1.102	1.104			
H12-C8	1.098	1.101			
O13-C8	1.417	1.426			
H14-O13	0.969	0.971			
H15-O1	1.925	1.940			
O16-H15	0.979	0.980			
O17-O16	1.448	1.466			
H18-O17	0.969	0.972			
O3-C2-O1	121.87	121.81			
C4-C2-O1	123.57	123.83			
N5-C4-C2	108.09	107.59			
H6-O3-C2	104.93	103.83			
H7-C4-C2	105.37	105.56			
C8-C4-C2	111.81	111.62			
H9-N5-C4	111.70	110.83			
H10-N5-C4	110.79	109.22			
H11-C8-C4	109.48	109.58			
H12-C8-C4	108.44	108.48			
O13-C8-C4	112.24	111.92			
H14-O13-C8	106.90	105.79			
H15-O1-C2	107.58	102.28			
O16-H15-O1	156.89	152.82			
O17-O16-H15	100.65	99.25			
H18-O17-O16	101.06	99.86			
C4-C2-O1-O3	-178.4	-177.7			
N5-C4-C2-O3	25.2	30.3			
H6-O3-C2-C4	-8.1	-10.3			
H7-C4-C2-O3	-89.8	-84.9			
C8-C4-C2-O3	153.5	158.0			
H9-N5-C4-C2	-153.7	-158.6			

Table S32: Geometrical parameters of **I-C'** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.218	1.226	H10-N5-C4-C2	96.3	95.4
O3-C2	1.329	1.336	H11-C8-C4-C2	54.1	55.3
C4-C2	1.541	1.538	H12-C8-C4-C2	172.4	174.5
N5-C4	1.472	1.474	O13-C8-C4-C2	-69.8	-68.1
H6-O3	0.992	0.995	H14-O13-C8-C4	99.8	100.3
H7-C4	1.101	1.104	H15-O1-C2-O3	-128.7	-135
C8-C4	1.535	1.532	O16-H15-O1-C2	28.3	52.4
H9-N5	1.015	1.018	O17-O16-H15-H7	75.4	81.1
H10-N5	1.019	1.023	H18-O17-O16-H15	96.6	91.7
H11-C8	1.097	1.100			
H12-C8	1.100	1.102			
O13-C8	1.421	1.430			
H14-O13	0.973	0.975			
H15-O1	1.779	1.771			
O16-H15	0.984	0.984			
O17-O16	1.448	1.466			
H18-O17	0.969	0.971			
O3-C2-O1	22.09	122.18			
C4-C2-O1	123.83	123.67			
N5-C4-C2	108.25	108.00			
H6-O3-C2	104.16	103.06			
H7-C4-C2	105.20	105.90			
C8-C4-C2	112.03	110.80			
H9-N5-C4	112.08	111.43			
H10-N5-C4	109.25	108.29			
H11-C8-C4	110.24	110.78			
H12-C8-C4	108.36	108.72			
O13-C8-C4	110.40	109.20			
H14-O13-C8	108.41	107.08			
H15-O1-C2	133.72	132.00			
O16-H15-O1	171.25	169.09			
O17-O16-H15	101.16	99.51			
H18-O17-O16	102.07	100.57			
C4-C2-O1-O3	-177.9	-178.0			
N5-C4-C2-O3	14.2	13.8			
H6-O3-C2-C4	-4.2	-3.8			
H7-C4-C2-O3	-102.0	-103.1			
C8-C4-C2-O3	140.1	138.1			
H9-N5-C4-C2	-143.7	-145.9			

Table S33: Geometrical parameters of **II-C'** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.225	1.234	H10-N5-C4-C2	36.6	36.4
O3-C2	1.332	1.339	H11-C8-C4-C2	61.2	61.3
C4-C2	1.521	1.518	H12-C8-C4-C2	-57.9	-58.1
N5-C4	1.460	1.463	O13-C8-C4-C2	-180.0	-179.9
H6-O3	0.992	0.993	H14-O13-C8-C4	44.3	44.1
H7-C4	1.097	1.100	O15-H6-O3-C2	5.3	2.4
C8-C4	1.548	1.543	O16-H15-H6-O3	9.3	16.8
H9-N5	1.015	1.019	H17-O16-H15-O1	-2.5	-2.8
H10-N5	1.018	1.023	H18-H15-O16-O17	109.1	104.7
H11-C8	1.096	1.099			
H12-C8	1.106	1.108			
O13-C8	1.412	1.420			
H14-O13	0.971	0.973			
O15-H6	1.761	1.751			
O16-O15	1.451	1.468			
H17-O16	0.989	0.987			
H18-H15	0.970	0.972			
O3-C2-O1	123.59	124.07			
C4-C2-O1	123.29	123.16			
N5-C4-C2	114.03	114.06			
H6-O3-C2	109.36	108.08			
H7-C4-C2	108.25	109.00			
C8-C4-C2	109.61	108.52			
H9-N5-C4	111.30	110.57			
H10-N5-C4	110.00	108.83			
H11-C8-C4	110.50	110.63			
H12-C8-C4	108.88	108.58			
O13-C8-C4	110.13	109.94			
H14-O13-C8	105.77	104.61			
O15-H6-O3	171.93	173.55			
O16-H15-H6	106.78	105.86			
H17-O16-H15	100.41	99.26			
H18-H15-O16	101.44	99.94			
C4-C2-O1-O3	-177.9	-177.0			
N5-C4-C2-O3	164.4	163.3			
H6-O3-C2-C4	176.8	175.7			
H7-C4-C2-O3	42.8	40.6			
C8-C4-C2-O3	-73.9	-76.6			
H9-N5-C4-C2	-81.3	-79.6			

Table S34: Geometrical parameters of **II-C1'** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.225	1.234	H10-N5-C4-C2	36.9	36.1
O3-C2	1.337	1.344	H11-C8-C4-C2	61.1	61.6
C4-C2	1.522	1.519	H12-C8-C4-C2	-58.0	-57.8
N5-C4	1.460	1.464	O13-C8-C4-C2	179.9	-179.7
H6-O3	0.988	0.989	H14-O13-C8-C4	44.3	44.0
H7-C4	1.098	1.101	O15-H6-O3-C2	-1.5	6.8
C8-C4	1.548	1.543	H16-O15-H6-O1	4.8	0.7
H9-N5	1.016	1.020	O17-O15-H16-O1	-115.3	-94.2
H10-N5	1.019	1.023	H18-O17-O15-H6	162.7	165.0
H11-C8	1.096	1.099			
H12-C8	1.106	1.108			
O13-C8	1.413	1.421			
H14-O13	0.971	0.974			
O15-H6	1.856	1.851			
H16-O15	0.986	0.987			
O17-O15	1.450	1.472			
H18-O17	0.970	0.972			
O3-C2-O1	123.64	124.31			
C4-C2-O1	123.52	123.32			
N5-C4-C2	113.97	113.96			
H6-O3-C2	108.70	107.65			
H7-C4-C2	108.28	109.03			
C8-C4-C2	109.64	108.55			
H9-N5-C4	111.27	110.50			
H10-N5-C4	109.95	108.75			
H11-C8-C4	110.52	110.65			
H12-C8-C4	108.91	108.59			
O13-C8-C4	110.10	109.93			
H14-O13-C8	105.74	104.57			
O15-H6-O3	153.70	154.66			
H16-O15-H6	81.50	81.11			
O17-O15-H16	102.05	99.23			
H18-O17-O15	100.80	99.29			
C4-C2-O1-O3	-177.9	-177.0			
N5-C4-C2-O3	164.3	163.8			
H6-O3-C2-C4	178.2	177.6			
H7-C4-C2-O3	42.7	41.1			
C8-C4-C2-O3	-74.1	-76.2			
H9-N5-C4-C2	-81.0	-79.9			

Table S35: Geometrical parameters of **III-C'** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.225	1.233	H10-N5-C4-C2	-145.2	-148.9
O3-C2	1.329	1.337	H11-C8-C4-C2	53.8	57.7
C4-C2	1.520	1.519	H12-C8-C4-C2	172.5	177.4
N5-C4	1.463	1.467	O13-C8-C4-C2	-65.5	-60.8
H6-O3	0.992	0.993	H14-O13-C8-C4	-46.5	-47.4
H7-C4	1.106	1.107	O15-H6-O3-C2	-4.7	-13.0
C8-C4	1.542	1.537	O16-O15-H6-O3	21.0	33.0
H9-N5	1.016	1.020	H17-O16-O15-O1	-2.6	-2.6
H10-N5	1.014	1.018	H18-O15-O16-H17	106.2	102.0
H11-C8	1.095	1.097			
H12-C8	1.104	1.106			
O13-C8	1.416	1.424			
H14-O13	0.971	0.973			
O15-H6	1.754	1.745			
O16-O15	1.450	1.468			
H17-O16	0.989	0.988			
H18-O15	0.970	0.972			
O3-C2-O1	123.62	124.16			
C4-C2-O1	123.29	123.35			
N5-C4-C2	109.71	109.18			
H6-O3-C2	109.19	107.88			
H7-C4-C2	105.52	106.55			
C8-C4-C2	111.57	109.74			
H9-N5-C4	110.81	110.21			
H10-N5-C4	111.60	110.72			
H11-C8-C4	110.88	111.00			
H12-C8-C4	107.94	108.41			
O13-C8-C4	110.72	109.64			
H14-O13-C8	105.73	104.56			
O15-H6-O3	172.16	173.58			
O16-O15-H6	106.64	105.78			
H17-O16-O15	100.43	99.29			
H18-O15-O16	101.57	100.03			
C4-C2-O1-O3	178.1	178.7			
N5-C4-C2-O3	-174.0	-173.4			
H6-O3-C2-C4	179.7	178.4			
H7-C4-C2-O3	63.3	62.7			
C8-C4-C2-O3	-53.4	-55.1			
H9-N5-C4-C2	-23.7	-29.1			

Table S36: Geometrical parameters of **III-C1'** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.225	1.233	H10-N5-C4-C2	-144.1	-148.1
O3-C2	1.334	1.342	H11-C8-C4-C2	53.2	57.1
C4-C2	1.521	1.520	H12-C8-C4-C2	171.9	176.7
N5-C4	1.464	1.468	O13-C8-C4-C2	-66.2	-61.6
H6-O3	0.987	0.988	H14-O13-C8-C4	-46.1	-47.0
H7-C4	1.106	1.108	O15-H6-O3-C2	-1.6	6.9
C8-C4	1.543	1.537	H16-O15-H6-O1	3.8	-0.5
H9-N5	1.017	1.020	O17-O15-H16-O1	-113.2	-91.8
H10-N5	1.015	1.019	H18-O17-O15-H6	162.9	165.9
H11-C8	1.095	1.098			
H12-C8	1.105	1.106			
O13-C8	1.416	1.424			
H14-O13	0.971	0.974			
O15-H6	1.854	1.852			
H16-O15	0.986	0.987			
O17-O15	1.450	1.472			
H18-O17	0.970	0.972			
O3-C2-O1	123.66	124.36			
C4-C2-O1	123.50	123.53			
N5-C4-C2	109.67	109.17			
H6-O3-C2	108.51	107.48			
H7-C4-C2	105.50	106.45			
C8-C4-C2	111.70	109.95			
H9-N5-C4	110.70	110.12			
H10-N5-C4	111.62	110.72			
H11-C8-C4	110.87	111.01			
H12-C8-C4	107.89	108.35			
O13-C8-C4	110.77	109.71			
H14-O13-C8	105.73	104.54			
O15-H6-O3	154.10	154.84			
H16-O15-H6	81.36	80.69			
O17-O15-H16	101.97	99.18			
H18-O17-O15	100.76	99.27			
C4-C2-O1-O3	178.0	178.5			
N5-C4-C2-O3	-174.9	-173.9			
H6-O3-C2-C4	-178.3	-178.6			
H7-C4-C2-O3	62.7	62.5			
C8-C4-C2-O3	-54.2	-55.4			
H9-N5-C4-C2	-22.6	-28.4			

Table S37: Geometrical parameters of **II-D'** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.211	1.221	H10-N5-C4-C2	28.5	26.6
O3-C2	1.355	1.361	H11-C8-C4-C2	66.3	68.5
C4-C2	1.521	1.519	H12-C8-C4-C2	-54.3	-52.9
N5-C4	1.461	1.465	O13-C8-C4-C2	-175.0	-173.1
H6-O3	0.971	0.974	H14-O13-C8-C4	42.4	43.8
H7-C4	1.097	1.099	H15-O13-C8-C4	-72.8	-62.2
C8-C4	1.547	1.544	O16-H15-O13-C8	66.6	30.5
H9-N5	1.015	1.018	O17-O16-H15-O13	-44.2	-59.7
H10-N5	1.018	1.022	H18-O17-O16-H15	-115.8	-112.1
H11-C8	1.094	1.096			
H12-C8	1.103	1.106			
O13-C8	1.424	1.435			
H14-O13	0.975	0.979			
H15-O13	1.813	1.798			
O16-H15	0.985	0.987			
O17-O16	1.453	1.474			
H18-O17	0.968	0.971			
O3-C2-O1	122.89	123.45			
C4-C2-O1	125.24	125.10			
N5-C4-C2	113.26	113.08			
H6-O3-C2	107.30	106.23			
H7-C4-C2	108.83	109.19			
C8-C4-C2	110.03	108.83			
H9-N5-C4	111.30	110.53			
H10-N5-C4	110.20	109.11			
H11-C8-C4	111.01	110.89			
H12-C8-C4	109.96	109.68			
O13-C8-C4	109.02	108.80			
H14-O13-C8	104.51	103.03			
H15-O13-C8	113.77	104.39			
O16-H15-O13	173.29	165.53			
O17-O16-H15	100.51	98.40			
H18-O17-O16	100.70	99.25			
C4-C2-O1-O3	-178.0	-177.1			
N5-C4-C2-O3	171.4	171.6			
H6-O3-C2-C4	178.0	177.4			
H7-C4-C2-O3	49.4	48.7			
C8-C4-C2-O3	-67.4	-68.7			
H9-N5-C4-C2	-89.9	-90.0			

Table S38: Geometrical parameters of **III-D'** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.207	1.216	H10-N5-C4-C2	-143.2	-147.9
O3-C2	1.367	1.377	H11-C8-C4-C2	55.6	58.6
C4-C2	1.518	1.516	H12-C8-C4-C2	173.9	177.8
N5-C4	1.465	1.469	O13-C8-C4-C2	-64.2	-60.4
H6-O3	0.972	0.974	H14-O13-C8-C4	-47.4	-47.3
H7-C4	1.104	1.105	H15-O3-C2-O1	135.5	133.5
C8-C4	1.544	1.538	O16-H15-O3-H7	-29.5	-17.6
H9-N5	1.017	1.020	O17-O16-H15-O3	88.8	81.5
H10-N5	1.015	1.018	H18-O17-O16-H15	113.7	113.7
H11-C8	1.094	1.096			
H12-C8	1.104	1.105			
O13-C8	1.416	1.425			
H14-O13	0.971	0.973			
H15-O3	1.989	2.056			
O16-H15	0.975	0.977			
O17-O16	1.452	1.471			
H18-O17	0.969	0.971			
O3-C2-O1	121.74	122.20			
C4-C2-O1	125.96	126.26			
N5-C4-C2	109.08	108.56			
H6-O3-C2	106.72	105.71			
H7-C4-C2	106.32	107.16			
C8-C4-C2	111.53	109.79			
H9-N5-C4	110.94	110.28			
H10-N5-C4	111.40	110.29			
H11-C8-C4	111.15	111.21			
H12-C8-C4	107.57	108.04			
O13-C8-C4	110.80	109.68			
H14-O13-C8	105.85	104.59			
H15-O3-C2	118.77	112.05			
O16-H15-O3	166.23	160.86			
O17-O16-H15	100.62	98.92			
H18-O17-O16	100.92	99.27			
C4-C2-O1-O3	178.6	178.9			
N5-C4-C2-O3	-177.2	-175.1			
H6-O3-C2-C4	179.0	178.9			
H7-C4-C2-O3	60.0	60.9			
C8-C4-C2-O3	-57.2	-57.2			
H9-N5-C4-C2	-21.8	-28.7			

Table S39: Geometrical parameters of **IV-D'** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.217	1.226	H10-N5-C4-C2	92.5	90.4
O3-C2	1.334	1.344	H11-C8-C4-C2	-60.3	-57.4
C4-C2	1.537	1.533	H12-C8-C4-C2	-179.6	-177.1
N5-C4	1.469	1.471	O13-C8-C4-C2	62.4	65.2
H6-O3	0.986	0.988	H14-O13-C8-C4	-52.2	-54.9
H7-C4	1.099	1.102	O15-H12-C8-C4	-68.0	-57.8
C8-C4	1.539	1.536	H16-O15-H12-C8	-128.0	-138.6
H9-N5	1.015	1.019	O17-O15-H12-C8	-20.2	-30.5
H10-N5	1.018	1.021	H18-O17-H15-O13	-8.0	-8.9
H11-C8	1.104	1.106			
H12-C8	1.095	1.098			
O13-C8	1.426	1.436			
H14-O13	0.976	0.978			
O15-H12	2.724	2.590			
H16-O15	0.969	0.971			
O17-O15	1.453	1.474			
H18-O17	0.986	0.987			
O3-C2-O1	122.38	122.43			
C4-C2-O1	122.89	122.94			
N5-C4-C2	109.44	109.28			
H6-O3-C2	105.07	103.98			
H7-C4-C2	105.90	106.34			
C8-C4-C2	110.52	109.87			
H9-N5-C4	111.54	110.36			
H10-N5-C4	111.82	110.98			
H11-C8-C4	109.77	109.71			
H12-C8-C4	109.07	109.17			
O13-C8-C4	111.93	111.69			
H14-O13-C8	105.89	104.69			
O15-H12-C8	112.45	107.28			
H16-O15-H12	124.58	123.65			
O17-O15-H12	96.10	99.87			
H18-O17-H15	100.52	98.73			
C4-C2-O1-O3	-179.4	-179.3			
N5-C4-C2-O3	17.4	19.2			
H6-O3-C2-C4	-4.1	-4.4			
H7-C4-C2-O3	-98.8	-97.2			
C8-C4-C2-O3	144.6	145.7			
H9-N5-C4-C2	-146.8	-150.8			

Table S40: Geometrical parameters of **III-E'** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.211	1.220	H10-N5-C4-C2	-144.6	-149.6
O3-C2	1.351	1.359	H11-C8-C4-C2	50.5	54.3
C4-C2	1.524	1.522	H12-C8-C4-C2	170.4	175.0
N5-C4	1.464	1.467	O13-C8-C4-C2	-68.7	-64.3
H6-O3	0.971	0.974	H14-O13-C8-C4	-42.0	-41.8
H7-C4	1.105	1.107	H15-O13-C8-C4	-168.7	-160.1
C8-C4	1.539	1.534	O16-H15-O13-C8	1.1	-2.6
H9-N5	1.017	1.020	O17-O16-H15-O13	-41.0	-39.9
H10-N5	1.014	1.018	H18-O17-O16-H15	-109.3	-109.6
H11-C8	1.093	1.095			
H12-C8	1.102	1.104			
O13-C8	1.426	1.437			
H14-O13	0.974	0.978			
H15-O13	1.816	1.796			
O16-H15	0.983	0.985			
O17-O16	1.452	1.472			
H18-O17	0.969	0.971			
O3-C2-O1	123.08	123.57			
C4-C2-O1	124.78	124.98			
N5-C4-C2	108.95	108.48			
H6-O3-C2	107.19	106.11			
H7-C4-C2	105.68	106.59			
C8-C4-C2	112.48	110.83			
H9-N5-C4	110.56	110.17			
H10-N5-C4	111.84	110.94			
H11-C8-C4	111.83	112.07			
H12-C8-C4	108.68	109.29			
O13-C8-C4	109.59	108.57			
H14-O13-C8	105.06	103.70			
H15-O13-C8	110.82	102.57			
O16-H15-O13	171.77	165.59			
O17-O16-H15	100.41	98.42			
H18-O17-O16	100.86	99.18			
C4-C2-O1-O3	177.9	178.3			
N5-C4-C2-O3	-172.4	-171.9			
H6-O3-C2-C4	-178.8	-179.2			
H7-C4-C2-O3	65.2	64.4			
C8-C4-C2-O3	-52.1	-53.8			
H9-N5-C4-C2	-22.8	-29.4			

Table S41: Geometrical parameters of **IV-F'** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.211	1.223	H10-N5-C4-C2	85.1	82.6
O3-C2	1.348	1.354	H11-C8-C4-C2	-59.4	-58.7
C4-C2	1.536	1.533	H12-C8-C4-C2	-177.0	-176.8
N5-C4	1.469	1.471	O13-C8-C4-C2	65.0	65.7
H6-O3	0.990	0.991	H14-O13-C8-C4	-55.2	-57.3
H7-C4	1.100	1.104	H15-O3-C2-O1	77.0	78.6
C8-C4	1.543	1.537	O16-H15-O3-C2	55.5	49.8
H9-N5	1.014	1.018	O17-O16-H15-H10	41.4	58.6
H10-N5	1.019	1.023	H18-O17-O16-H15	113.2	113.3
H11-C8	1.105	1.105			
H12-C8	1.098	1.101			
O13-C8	1.414	1.424			
H14-O13	0.971	0.972			
H15-O3	2.123	2.316			
O16-H15	0.975	0.975			
O17-O16	1.451	1.471			
H18-O17	0.969	0.971			
O3-C2-O1	121.87	121.69			
C4-C2-O1	124.04	124.21			
N5-C4-C2	108.61	108.03			
H6-O3-C2	104.38	103.46			
H7-C4-C2	106.07	106.26			
C8-C4-C2	110.45	110.48			
H9-N5-C4	111.98	111.09			
H10-N5-C4	111.75	110.50			
H11-C8-C4	108.98	108.72			
H12-C8-C4	108.53	108.58			
O13-C8-C4	112.65	112.31			
H14-O13-C8	106.88	105.54			
H15-O3-C2	98.33	83.43			
O16-H15-O3	144.67	122.94			
O17-O16-H15	48.89	50.37			
H18-O17-O16	109.10	109.08			
C4-C2-O1-O3	179.1	179.5			
N5-C4-C2-O3	14.0	19.9			
H6-O3-C2-C4	-0.6	-4.1			
H7-C4-C2-O3	-102.2	-96.3			
C8-C4-C2-O3	141.1	146.5			
H9-N5-C4-C2	-152.9	-157.3			

Table S42: Geometrical parameters of **IV-G'** at B3LYP/aug-cc-pVDZ (**L1**) and MP2/aug-cc-pVDZ (**L2**) levels. Distances are in Å and angles are in degrees.

Parameters	L1	L2	Parameters	L1	L2
C2-O1	1.220	1.228	H10-N5-C4-C2	98.7	95.6
O3-C2	1.329	1.338	H11-C8-C4-C2	-62.8	-60.4
C4-C2	1.537	1.535	H12-C8-C4-C2	179.7	-178.2
N5-C4	1.470	1.473	O13-C8-C4-C2	61.3	63.6
H6-O3	0.989	0.990	H14-O13-C8-C4	-56.0	-57.7
H7-C4	1.099	1.102	H15-O1-C2-O3	118.9	117.2
C8-C4	1.544	1.540	O16-H15-O1-H7	57.8	58.6
H9-N5	1.014	1.018	O17-O16-H15-O1	54.9	58.7
H10-N5	1.018	1.021	H18-O17-O16-H15	86.6	88.8
H11-C8	1.105	1.107			
H12-C8	1.097	1.100			
O13-C8	1.418	1.427			
H14-O13	0.972	0.975			
H15-O1	2.079	2.039			
O16-H15	0.975	0.975			
O17-O16	1.450	1.470			
H18-O17	0.976	0.978			
O3-C2-O1	122.25	122.28			
C4-C2-O1	123.00	123.04			
N5-C4-C2	109.17	108.87			
H6-O3-C2	104.77	103.79			
H7-C4-C2	105.08	105.40			
C8-C4-C2	111.30	110.68			
H9-N5-C4	112.19	111.34			
H10-N5-C4	112.06	111.16			
H11-C8-C4	109.13	109.00			
H12-C8-C4	108.52	108.66			
O13-C8-C4	113.68	113.53			
H14-O13-C8	107.07	106.09			
H15-O1-C2	119.76	117.28			
O16-H15-O1	152.81	151.29			
O17-O16-H15	101.54	99.83			
H18-O17-O16	100.82	98.72			
C4-C2-O1-O3	-179.3	-179.6			
N5-C4-C2-O3	11.8	14.3			
H6-O3-C2-C4	-2.4	-2.8			
H7-C4-C2-O3	-105.0	-102.6			
C8-C4-C2-O3	137.8	139.6			
H9-N5-C4-C2	-139.8	-144.7			

Table S43: Intra-molecular HB distances in serine conformers and in 1:1 hydrogen bonded complexes of serine-water and serine-HP at MP2/aug-cc-pVDZ (L2) level.

Species	Intra-molecular HB distance (R, Å)		Species	Intra-molecular HB distance (R, Å)		Species	Intra-molecular HB distance (R, Å)		Species	Intra-molecular HB distance (R, Å)	
I	N5...H6	1.904	II	N5...H14	2.232	III	N5...H14	2.267	IV	N5...H6	1.912
	O13...H10	2.478		O1...H10	2.450		O1...H9	2.257		O1...H14	2.024
I-A	O13...H10	2.545	II-A	O1...H10	2.398	III-A	O1...H9	2.245	IV-A	O1...H14	2.154
	O1...H14	2.118									
I-B	N5...H6	1.870	II-B	N5...H14	2.194	III-B	N5...H14	2.257	IV-B	N5...H6	1.956
	O13...H10	2.505		O1...H10	2.521		O1...H9	2.525		O1...H14	2.094
I-C	N5...H6	1.836	II-C	N5...H14	2.223	III-C	N5...H14	2.255	IV-D	N5...H6	1.913
	O13...H10	2.321		O1...H10	2.424		O1...H9	2.240		O1...H14	1.964
I-H	N5...H6	1.833	II-D	N5...H14	2.125	III-D	N5...H14	2.274	IV-F	N5...H6	1.880
	O13...H10	2.388		O1...H10	2.383		O1...H9	2.277		O1...H14	2.059
			II-I	N5...H14	2.246	III-E	N5...H14	2.174	IV-G	N5...H6	1.851
				O1...H10	2.480		O1...H9	2.271		O1...H14	2.017
			II-J	N5...H14	2.147				IV-K	N5...H6	1.879
				O1...H10	2.466					O1...H14	2.032
									IV-L	N5...H6	1.888
										O1...H14	2.067
I-A'	O13...H10	2.566	II-A'	O1...H10	2.343	III-A'	O1...H9	2.211	IV-A'	O1...H14	2.250
	O1...H14	2.160									
I-B'	N5...H6	1.876	II-B'	N5...H14	2.204	III-B'	N5...H14	2.278	IV-B'	N5...H6	1.946
	O13...H10	2.506		O1...H10	2.561		O1...H9	2.559		O1...H14	2.120
I-C'	N5...H6	1.829	II-C'	N5...H14	2.231	III-C'	N5...H14	2.271	IV-D'	N5...H6	1.924
	O13...H10	2.334		O1...H10	2.433		O1...H9	2.253		O1...H14	1.974
			II-D'	N5...H14	2.116	III-D'	N5...H14	2.268	IV-F'	N5...H6	1.879
				O1...H10	2.375		O1...H9	2.292		O1...H14	2.065
						III-E'	N5...H14	2.151	IV-G'	N5...H6	1.883
							O1...H9	2.265		O1...H14	2.074