Supplementary material

Spectroscopic investigations, computational analysis and molecular docking to SAR-Cov-2 target study of 5,8-quinolinedione attached to betulin derivatives

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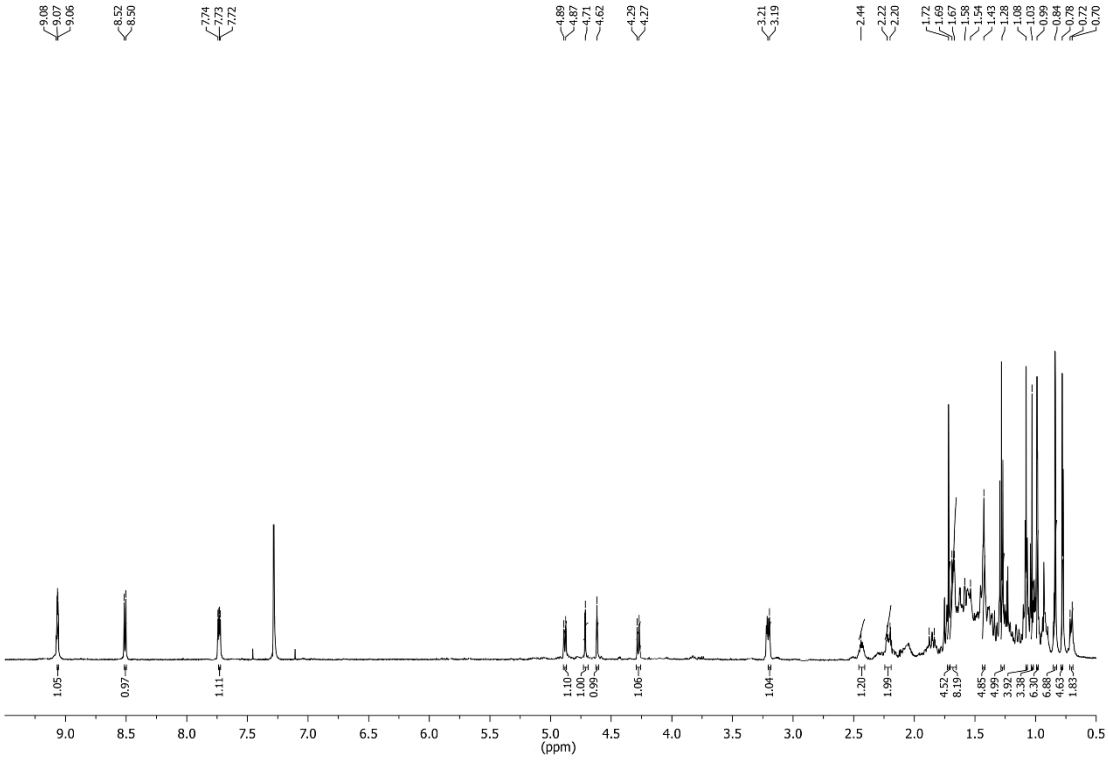
Fig. S1. The experimental (a.) and calculated (b) ^{1}H NMR chemical shifts of hybrid **1**.

a.



b.

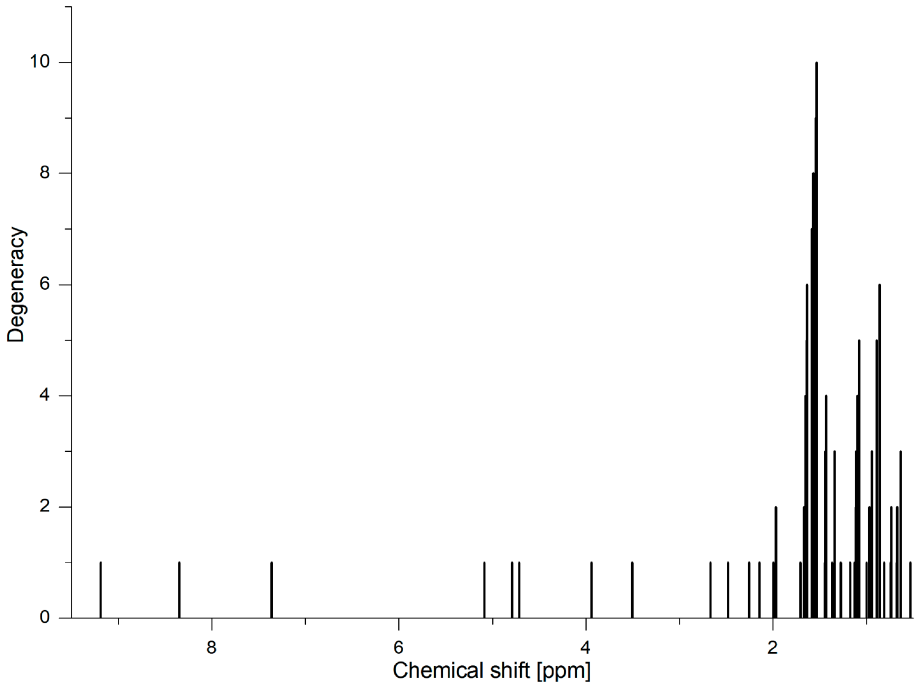
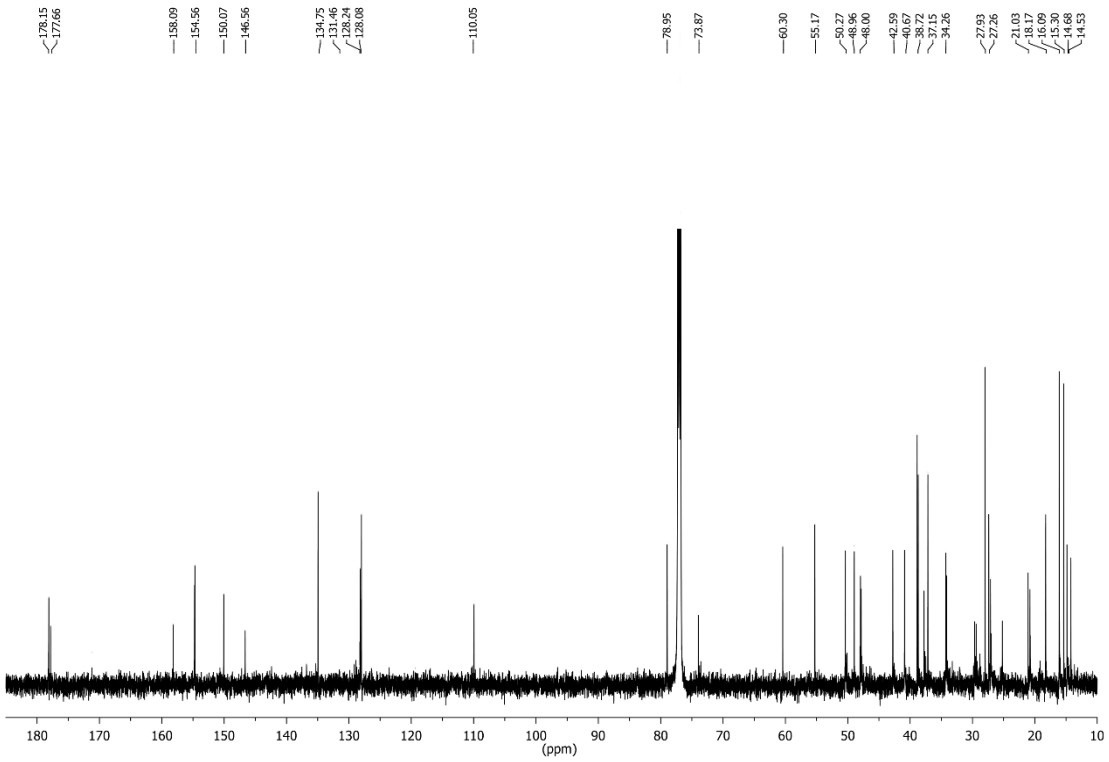


Fig. S2. The experimental (a.) and calculated (b) ^{13}C NMR chemical shifts of hybrid **1**.

a.



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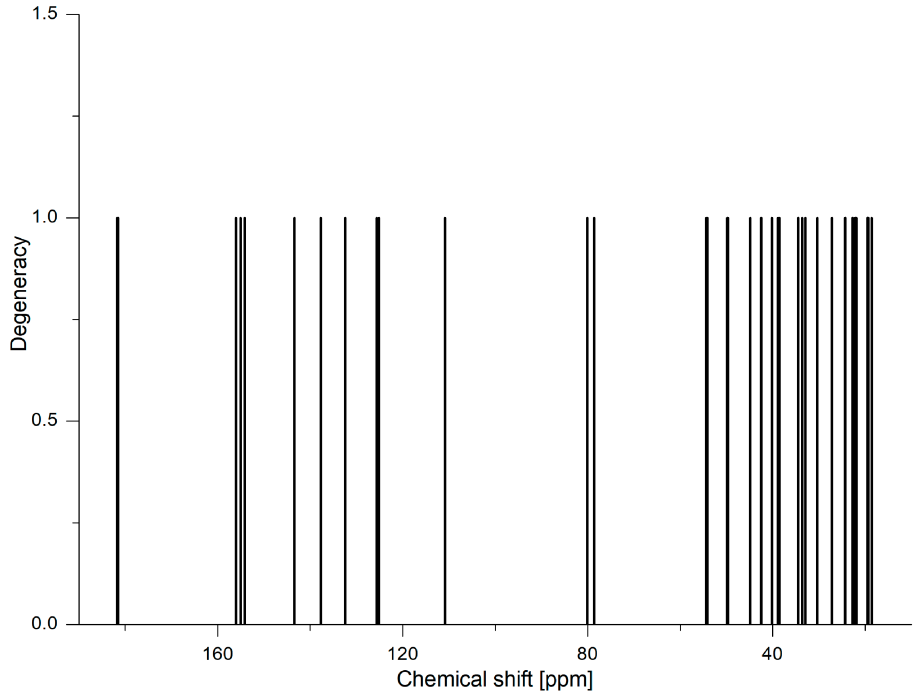
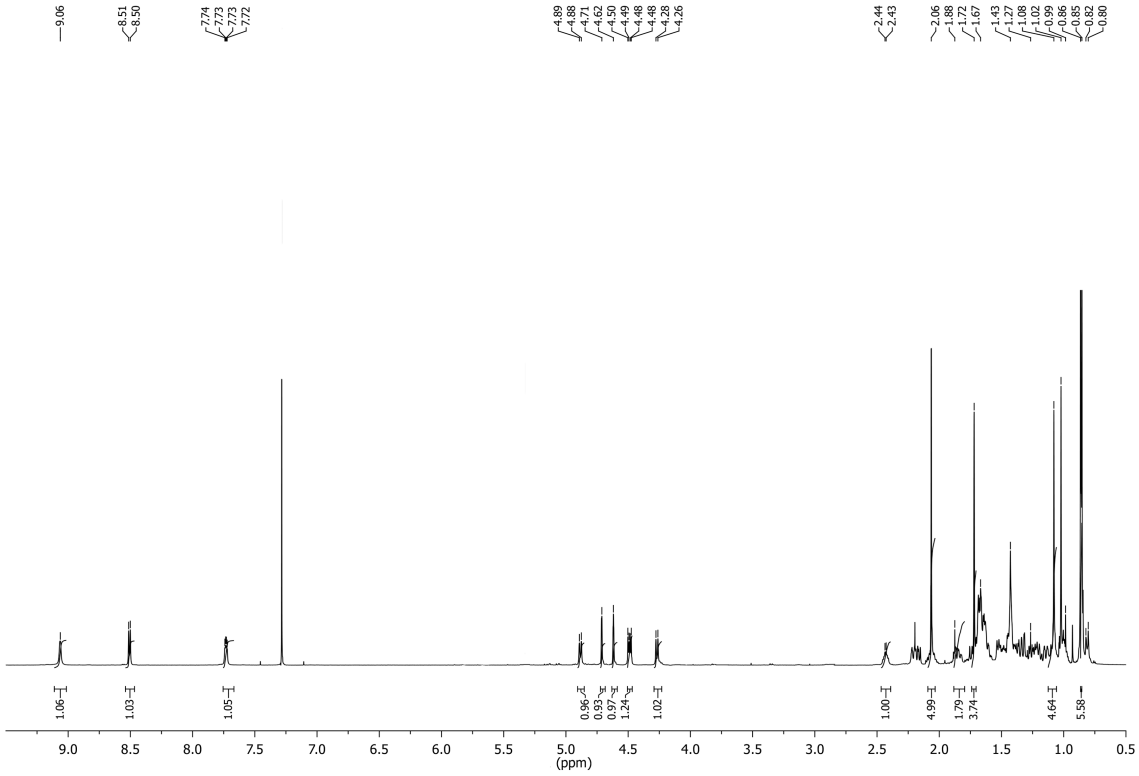


Fig. S3. The experimental (a.) and calculated (b) ^{1}H NMR chemical shifts of hybrid **2**.

a.



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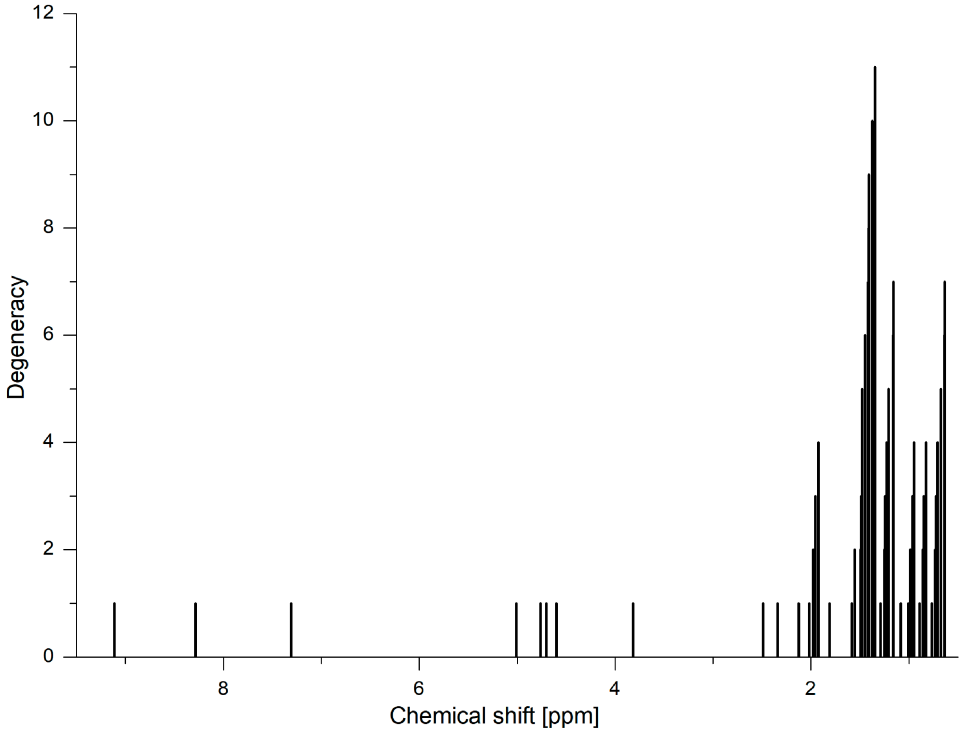
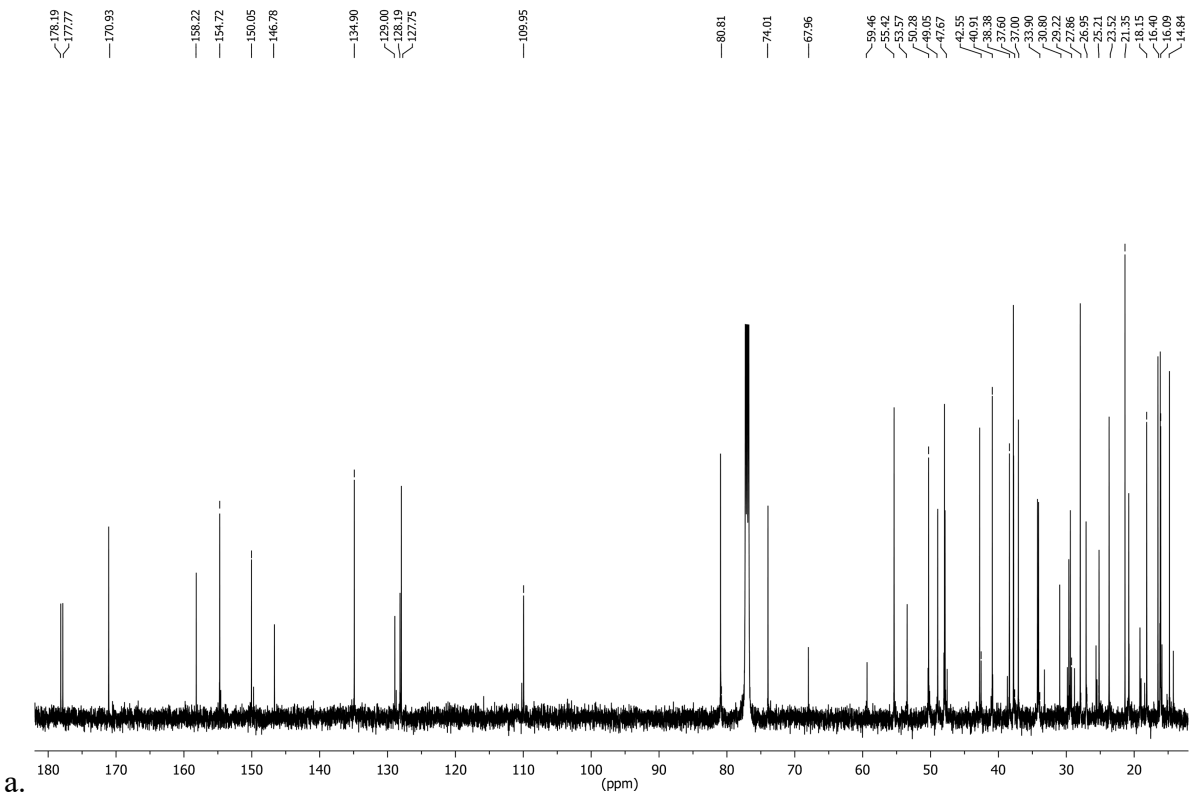
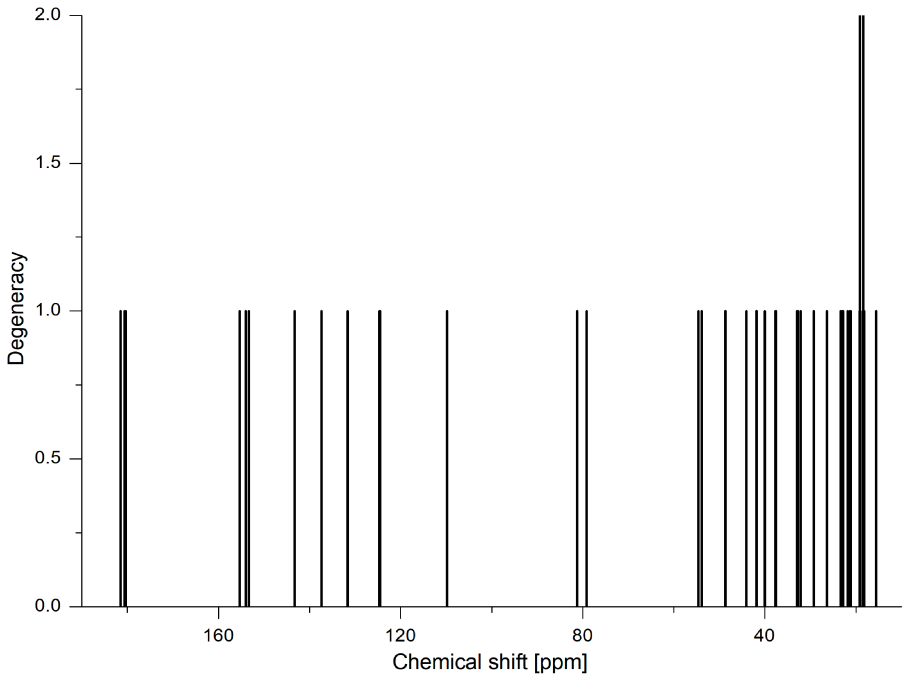


Fig. S4. The experimental (a.) and calculated (b) ^{13}C NMR chemical shifts of hybrid **2**.



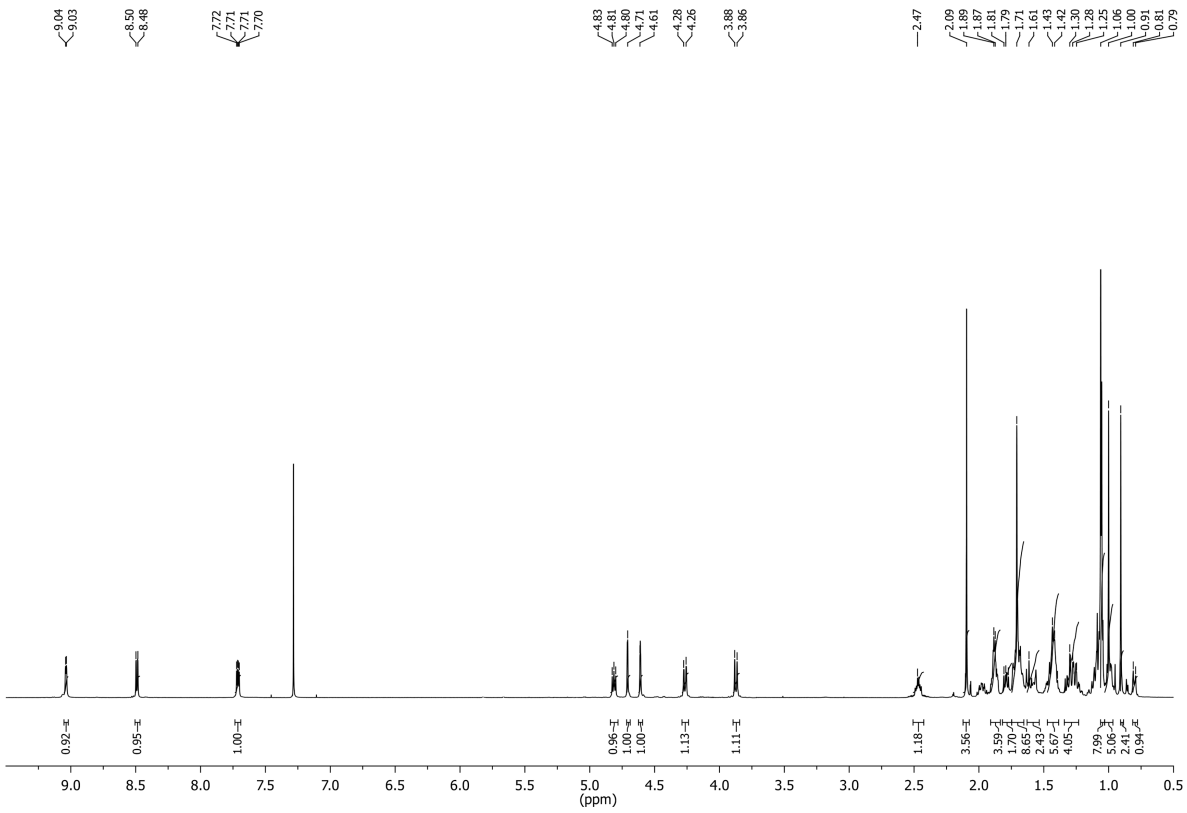
a.



b.

Fig. S5. The experimental (a.) and calculated (b) ^{1}H NMR chemical shifts of hybrid **3**.

a.



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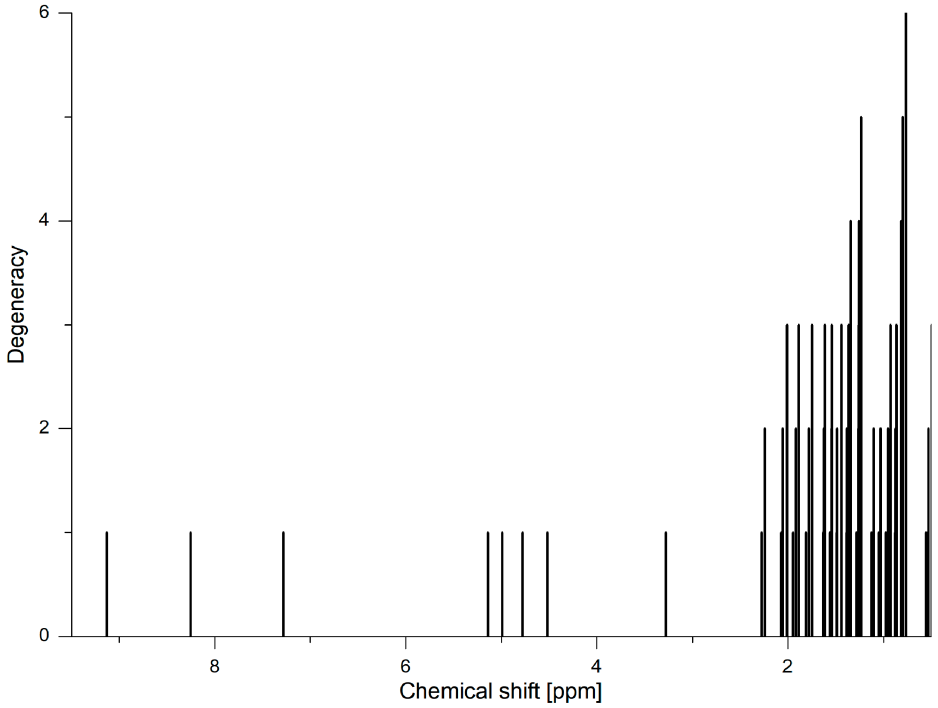
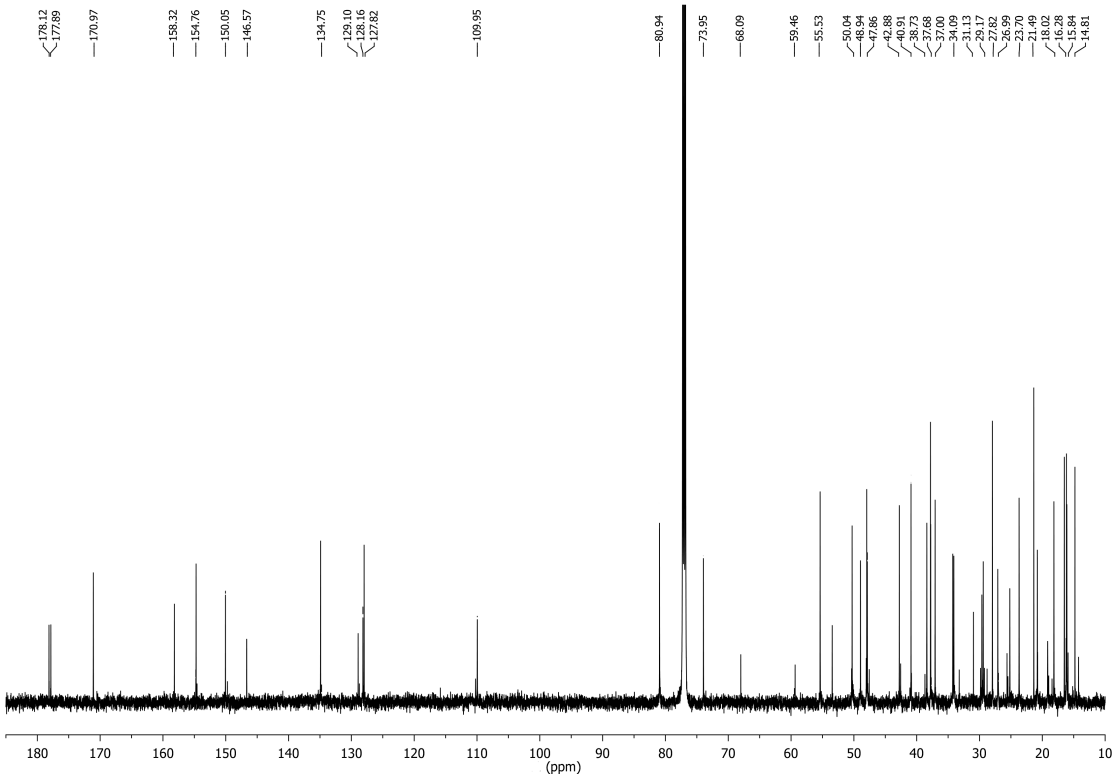


Fig. S6. The experimental (a.) and calculated (b) ^{13}C NMR chemical shifts of hybrid **3**.

a.



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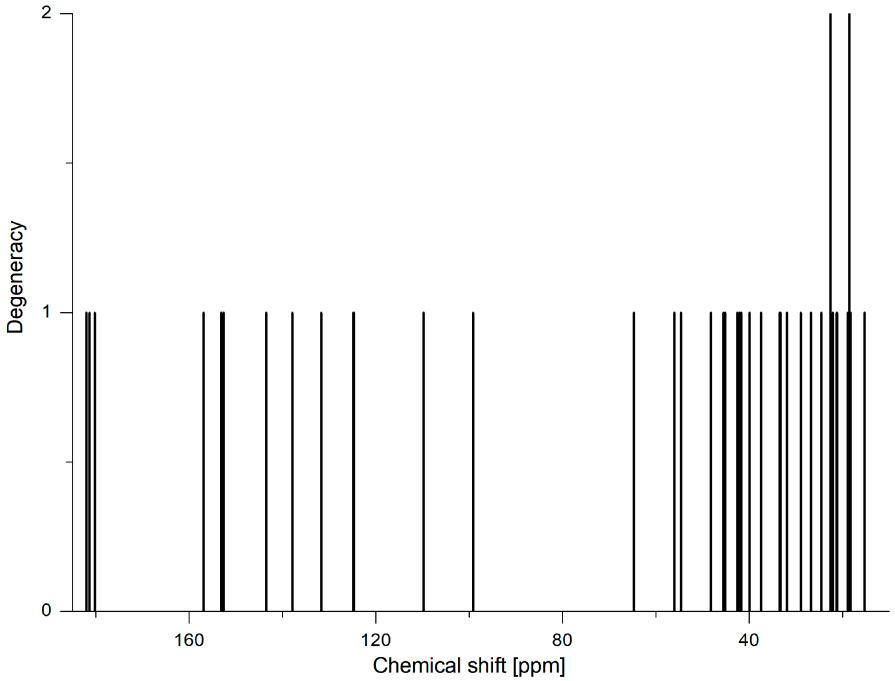
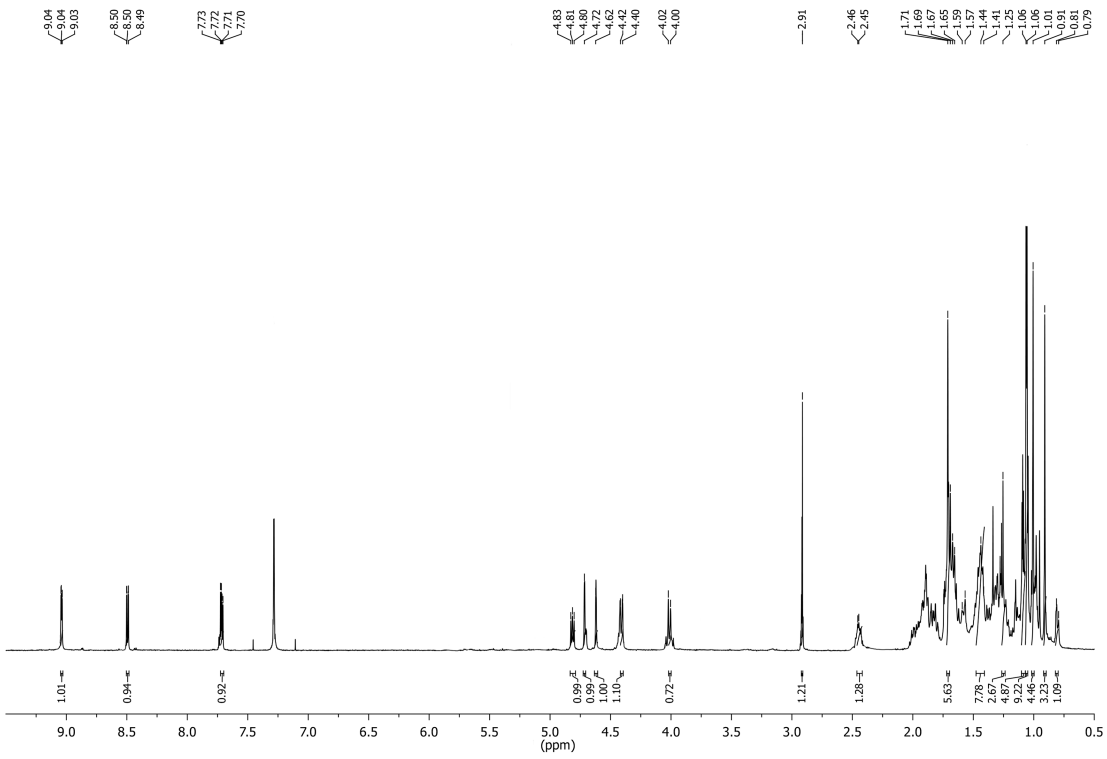


Fig. S7. The experimental (a.) and calculated (b) ^{1}H NMR chemical shifts of hybrid **4**.

a.



b.

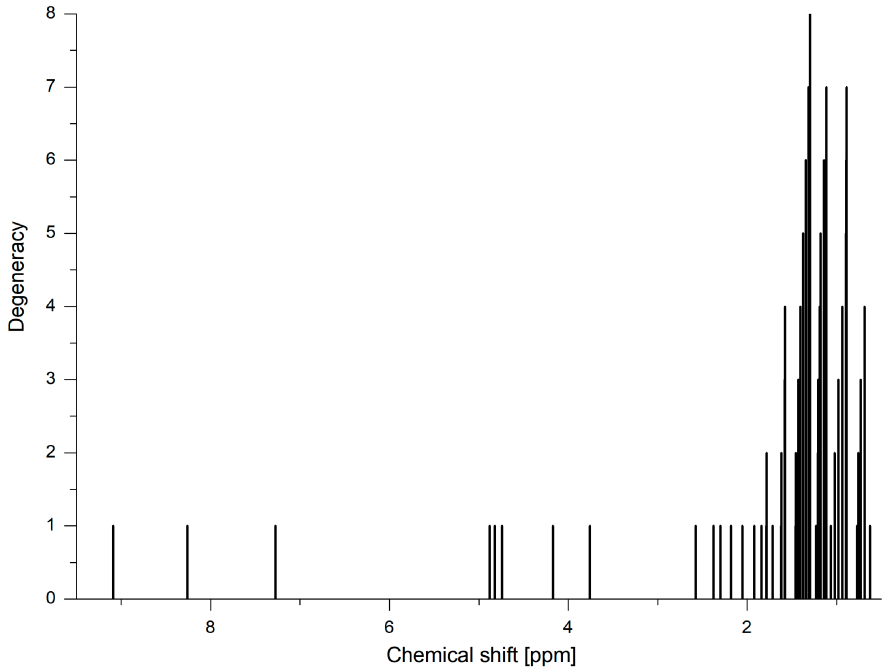
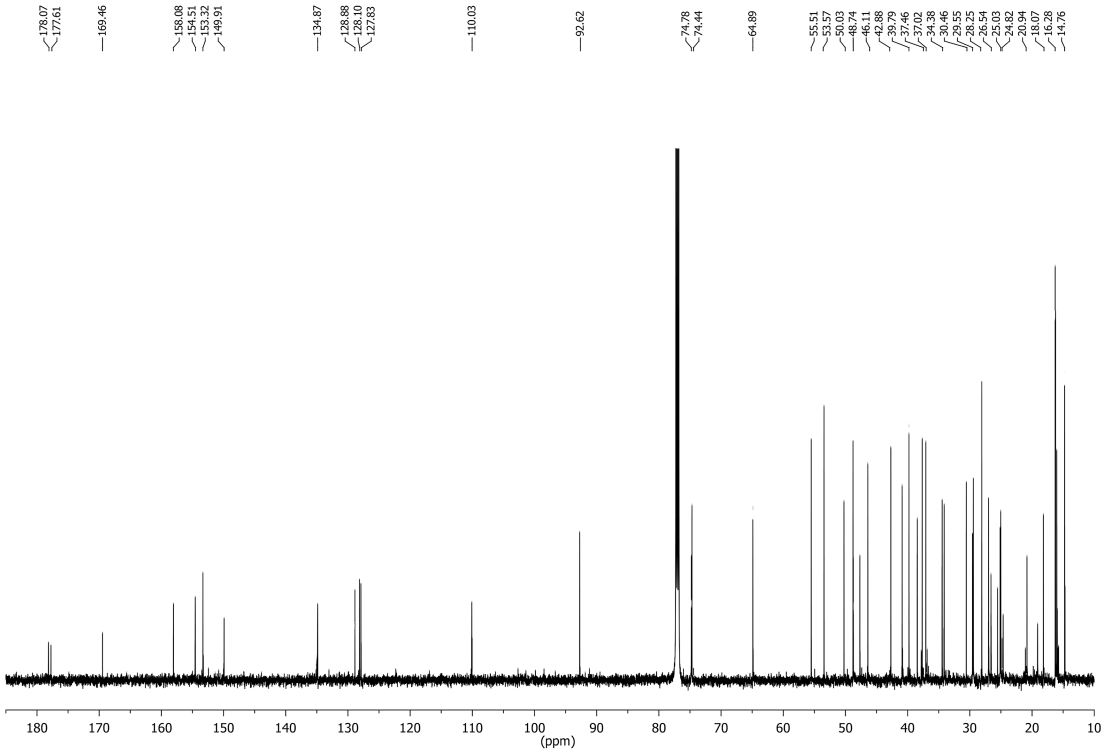
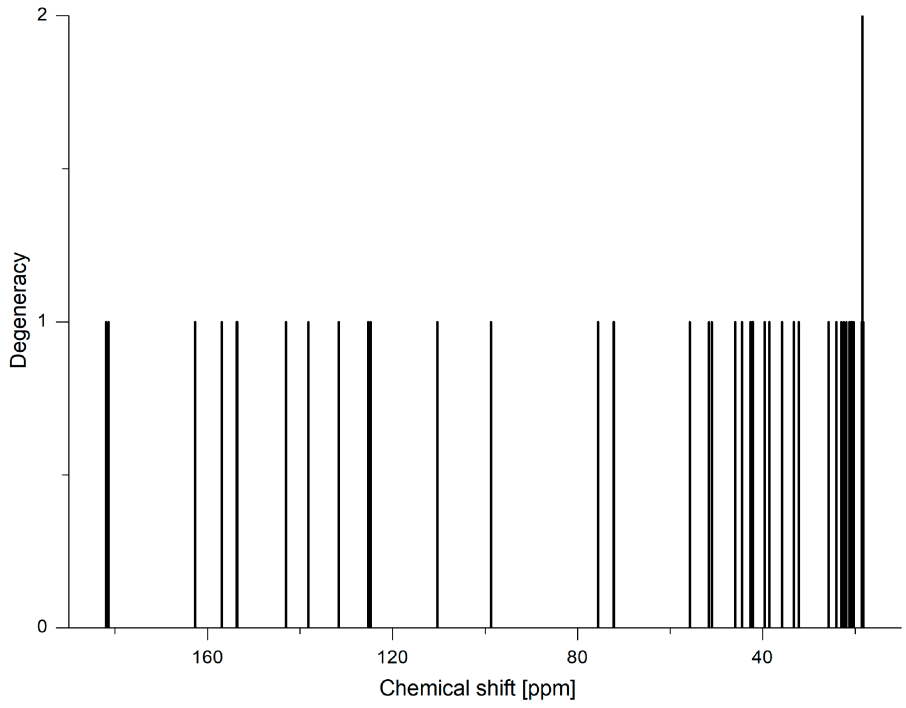


Fig. S8. The experimental (a.) and calculated (b) ^{13}C NMR chemical shifts of hybrid **4**.



a.



b.

Figure S9. Color-coded computer graphic representation of the electrostatic potentials for hybrid **1**. The positions of the potential minima (in eV) are indicated.

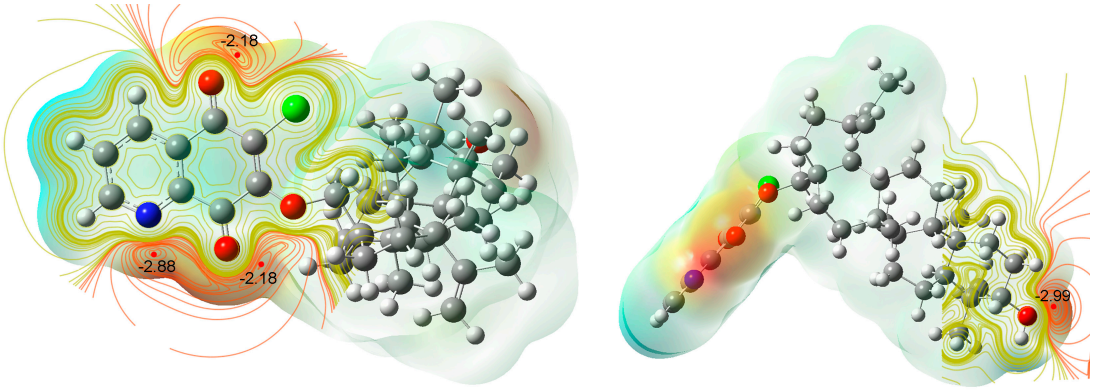


Figure S10. Color-coded computer graphic representation of the electrostatic potentials for hybrid **2**. The positions of the potential minima (in eV) are indicated.

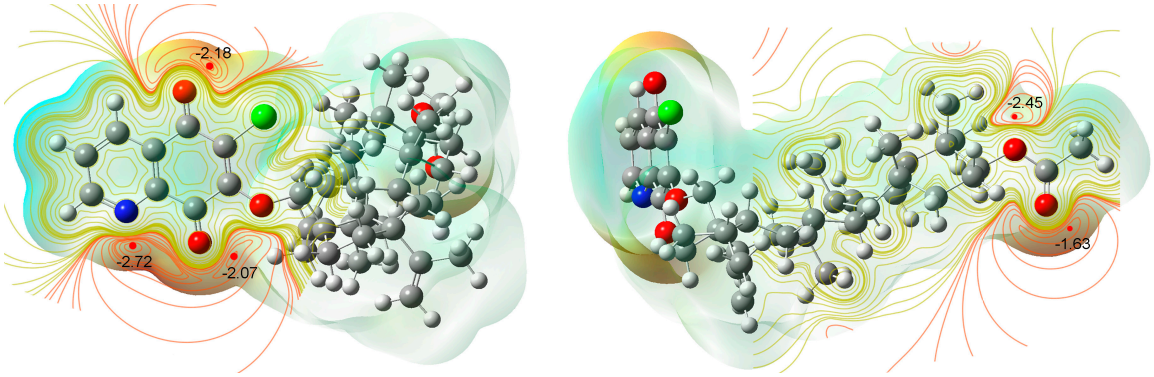


Figure S11. Color-coded computer graphic representation of the electrostatic potentials for hybrid **3**. The positions of the potential minima (in eV) are indicated.

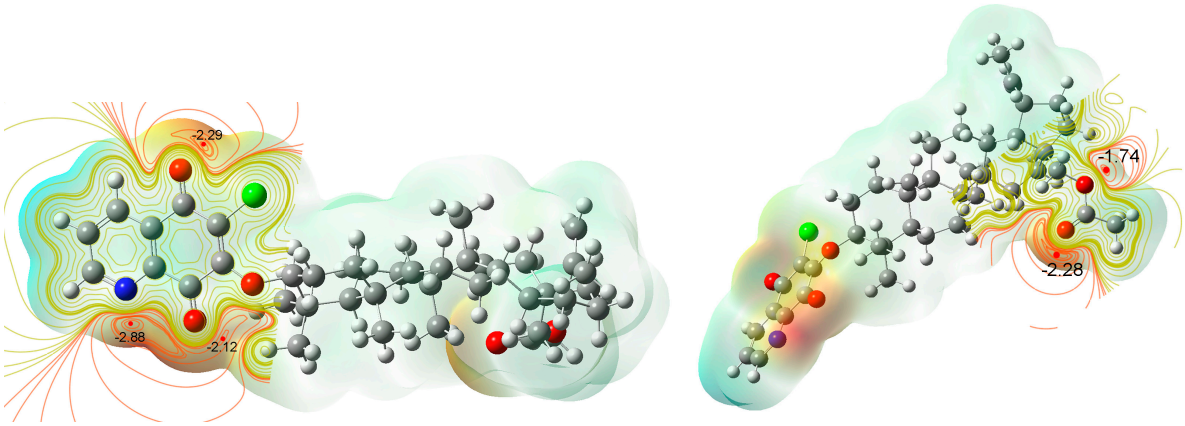


Figure S12. Color-coded computer graphic representation of the electrostatic potentials for hybrid **4**. The positions of the potential minima (in eV) are indicated.

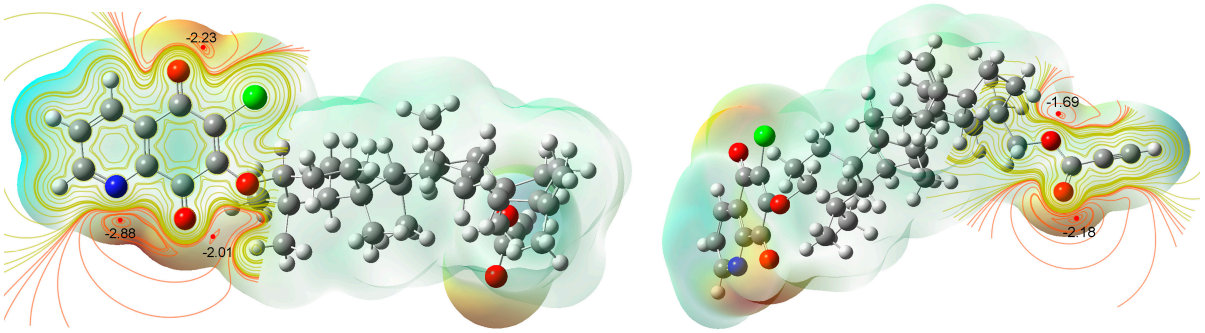


Table S1. Geometric parameters (bond length and angles) for hybrid **1** (Å, º).

Bond length, bond angles [Å, °]		Bond angles [Å, °]		Bond angles [Å, °]	
C10-C5	1.5506	C19-C21-C22	106.2605	C26-C8-C7-H7A	-113.1906
C10-C1	1.5335	C19-C21-H21A	110.4322	C26-C8-C7-H7B	5.795
C10-C9	1.5522	C19-C21-H21B	110.438	C9-C8-C14-C13	63.0032
C10-C25	1.533	C22-C21-H21A	110.0839	C9-C8-C14-C15	-176.3416
C5-C4	1.5619	C22-C21-H21B	110.0868	C9-C8-C14-C27	-56.5801
C5-C6	1.5371	H21A-C21-H21B	109.4991	C7-C8-C14-C13	-176.6657
C5-H5	1.111	C17-C22-C21	103.1024	C7-C8-C14-C15	-56.0106
C1-C2	1.5298	C17-C22-H22A	110.9213	C7-C8-C14-C27	63.751
C1-H1A	1.111	C17-C22-H22B	110.9197	C26-C8-C14-C13	-57.2045
C1-H1B	1.1109	C21-C22-H22A	111.1381	C26-C8-C14-C15	63.4506
C4-C3	1.5426	C21-C22-H22B	111.1454	C26-C8-C14-C27	-176.7878
C4-C24	1.5284	H22A-C22-H22B	109.5001	C9-C8-C26-H26A	-90.6319
C4-C23	1.5332	C19-C20-C29	121.3242	C9-C8-C26-H26B	29.3352
C2-C3	1.5294	C19-C20-C30	119.0927	C9-C8-C26-H26C	149.4132
C2-H2A	1.111	C29-C20-C30	119.5664	C7-C8-C26-H26A	149.0346
C2-H2B	1.111	C14-C27-H27A	109.4513	C7-C8-C26-H26B	-90.9984
C3-O3	1.4205	C14-C27-H27B	109.4523	C7-C8-C26-H26C	29.0797
C3-H3	1.1126	C14-C27-H27C	109.4499	C14-C8-C26-H26A	28.8574
C9-C8	1.5496	H27A-C27-H27B	109.4627	C14-C8-C26-H26B	148.8244
C9-C11	1.5416	H27A-C27-H27C	109.4623	C14-C8-C26-H26C	-91.0975
C9-H9	1.111	H27B-C27-H27C	109.5489	C5-C6-C7-C8	-57.8581
C8-C7	1.5489	C4-C24-H24A	109.4525	C5-C6-C7-H7A	-178.5499
C8-C14	1.5582	C4-C24-H24B	109.451	C5-C6-C7-H7B	62.8329
C8-C26	1.5415	C4-C24-H24C	109.4517	H6A-C6-C7-C8	-177.6143
C6-C7	1.5376	H24A-C24-H24B	109.4628	H6A-C6-C7-H7A	61.6939
C6-H6A	1.111	H24A-C24-H24C	109.4609	H6A-C6-C7-H7B	-56.9232
C6-H6B	1.111	H24B-C24-H24C	109.5483	H6B-C6-C7-C8	61.9028
C7-H7A	1.111	C4-C23-H23A	109.4476	H6B-C6-C7-H7A	-58.7891
C7-H7B	1.111	C4-C23-H23B	109.448	H6B-C6-C7-H7B	-177.4062
C11-C12	1.5387	C4-C23-H23C	109.4518	C9-C11-C12-C13	54.9295
C11-H11A	1.1111	H23A-C23-H23B	109.4622	C9-C11-C12-H12A	175.6238
C11-H11B	1.111	H23A-C23-H23C	109.4623	C9-C11-C12-H12B	-65.757
C12-C13	1.5506	H23B-C23-H23C	109.5553	H11A-C11-C12-C13	-65.3504
C12-H12A	1.111	C3-O3-H3	120.0037	H11A-C11-C12-H12A	55.344
C12-H12B	1.111	C10-C25-H25A	109.4518	H11A-C11-C12-H12B	173.9631
C14-C13	1.5759	C10-C25-H25B	109.451	H11B-C11-C12-C13	175.2101
C14-C15	1.5396	C10-C25-H25C	109.4497	H11B-C11-C12-H12A	-64.0955
C14-C27	1.5354	H25A-C25-H25B	109.4638	H11B-C11-C12-H12B	54.5237
C13-C18	1.5667	H25A-C25-H25C	109.4596	C11-C12-C13-C14	-41.5207
C13-H13	1.111	H25B-C25-H25C	109.5514	C11-C12-C13-C18	-168.6644
C15-C16	1.5246	C8-C26-H26A	109.4513	C11-C12-C13-H13	74.5303
C15-H15A	1.111	C8-C26-H26B	109.4514	H12A-C12-C13-C14	-162.0168
C15-H15B	1.111	C8-C26-H26C	109.4471	H12A-C12-C13-C18	70.8395
C16-C17	1.5345	H26A-C26-H26B	109.4642	H12A-C12-C13-H13	-45.9658
C16-H16A	1.111	H26A-C26-H26C	109.4564	H12B-C12-C13-C14	78.969
C16-H16B	1.1111	H26B-C26-H26C	109.5569	H12B-C12-C13-C18	-48.1747

C18-C17	1.5456	C17-C28-O28	108.89	H12B-C12-C13-H13	-164.98
C18-C19	1.5622	C17-C28-H28A	111.0385	C8-C14-C13-C12	-17.16
C18-H18	1.111	C17-C28-H28B	111.0331	C8-C14-C13-C18	108.6781
C17-C22	1.5202	O28-C28-H28A	108.1447	C8-C14-C13-H13	-133.9117
C17-C28	1.5322	O28-C28-H28B	108.1406	C15-C14-C13-C12	-137.2752
C19-C21	1.5442	H28A-C28-H28B	109.5007	C15-C14-C13-C18	-11.4371
C19-C20	1.5202	C20-C29-H29A	119.9996	C15-C14-C13-H13	105.973
C19-H19	1.1146	C20-C29-H29B	119.9994	C27-C14-C13-C12	102.8631
C21-C22	1.5295	H29A-C29-H29B	120.0009	C27-C14-C13-C18	-131.2989
C21-H21A	1.111	C20-C30-H30A	109.4432	C27-C14-C13-H13	-13.8887
C21-H21B	1.111	C20-C30-H30B	109.4415	C8-C14-C15-C16	-169.8046
C22-H22A	1.111	C20-C30-H30C	109.4491	C8-C14-C15-H15A	-50.1734
C22-H22B	1.111	H30A-C30-H30B	109.4685	C8-C14-C15-H15B	70.5581
C20-C29	1.3423	H30A-C30-H30C	109.467	C13-C14-C15-C16	-48.9335
C20-C30	1.511	H30B-C30-H30C	109.5579	C13-C14-C15-H15A	70.6976
C27-H27A	1.1111	C28-O28-C7q	124.7183	C13-C14-C15-H15B	-168.5708
C27-H27B	1.1112	O28-C7q-C8q	118.7246	C27-C14-C15-C16	70.4595
C27-H27C	1.1112	O28-C7q-C6q	121.2405	C27-C14-C15-H15A	-169.9093
C24-H24A	1.1111	C8q-C7q-C6q	120.0344	C27-C14-C15-H15B	-49.1778
C24-H24B	1.1112	C4Aq-C8Aq-C8q	119.7272	C8-C14-C27-H27A	159.6478
C24-H24C	1.1111	C4Aq-C8Aq-N1q	119.7597	C8-C14-C27-H27B	-80.3865
C23-H23A	1.1111	C8q-C8Aq-N1q	120.5119	C8-C14-C27-H27C	39.684
C23-H23B	1.1111	C8Aq-C4Aq-C5q	119.4359	C13-C14-C27-H27A	39.1602
C23-H23C	1.1112	C8Aq-C4Aq-C4q	119.7142	C13-C14-C27-H27B	159.1259
O3-H3	1.012	C5q-C4Aq-C4q	120.8494	C13-C14-C27-H27C	-80.8036
C25-H25A	1.111	C7q-C8q-C8Aq	120.1208	C15-C14-C27-H27A	-80.9231
C25-H25B	1.1111	C7q-C8q-O8q	119.8972	C15-C14-C27-H27B	39.0426
C25-H25C	1.1112	C8Aq-C8q-O8q	119.9705	C15-C14-C27-H27C	159.1131
C26-H26A	1.1111	C4Aq-C5q-C6q	119.9126	C12-C13-C18-C17	179.8865
C26-H26B	1.1111	C4Aq-C5q-O5q	120.1173	C12-C13-C18-C19	-63.6215
C26-H26C	1.1111	C6q-C5q-O5q	119.9622	C12-C13-C18-H18	56.7
C28-O28	1.4248	C7q-C6q-C5q	120.5224	C14-C13-C18-C17	53.0753
C28-H28A	1.111	C7q-C6q-Clq	119.7672	C14-C13-C18-C19	169.5673
C28-H28B	1.111	C5q-C6q-Clq	119.7089	C14-C13-C18-H18	-70.1112
C29-H29A	1.111	C8Aq-N1q-C2q	120.6157	H13-C13-C18-C17	-63.4809
C29-H29B	1.111	N1q-C2q-C3q	119.6526	H13-C13-C18-C19	53.0111
C30-H30A	1.1111	N1q-C2q-H2q	120.2036	H13-C13-C18-H18	173.3326
C30-H30B	1.1112	C3q-C2q-H2q	120.1438	C14-C15-C16-C17	74.9028
C30-H30C	1.1111	C4Aq-C4q-C3q	120.5806	C14-C15-C16-H16A	-164.941
O28-C7q	1.3656	C4Aq-C4q-H4q	119.6618	C14-C15-C16-H16B	-45.2477
C7q-C8q	1.4779	C3q-C4q-H4q	119.7576	H15A-C15-C16-C17	-44.9698
C7q-C6q	1.346	C2q-C3q-C4q	119.6762	H15A-C15-C16-H16A	75.1864
C8Aq-C4Aq	1.382	C2q-C3q-H3q	120.111	H15A-C15-C16-H16B	-165.1202
C8Aq-C8q	1.4742	C4q-C3q-H3q	120.2128	H15B-C15-C16-C17	-165.2265
C8Aq-N1q	1.3831	C1-C10-C5-C4	-33.9738	H15B-C15-C16-H16A	-45.0703
C4Aq-C5q	1.4741	C1-C10-C5-C6	113.5342	H15B-C15-C16-H16B	74.6231
C4Aq-C4q	1.3836	C1-C10-C5-H5	-136.8474	C15-C16-C17-C18	-31.7789
C8q-O8q	1.2092	C9-C10-C5-C4	-153.8875	C15-C16-C17-C22	-150.9323

C5q-C6q	1.4803	C9-C10-C5-C6	-6.3795	C15-C16-C17-C28	88.6005
C5q-O5q	1.209	C9-C10-C5-H5	103.2389	H16A-C16-C17-C18	-151.7708
C6q-Clq	1.717	C25-C10-C5-C4	85.8821	H16A-C16-C17-C22	89.0758
N1q-C2q	1.3844	C25-C10-C5-C6	-126.61	H16A-C16-C17-C28	-31.3914
C2q-C3q	1.3836	C25-C10-C5-H5	-16.9916	H16B-C16-C17-C18	88.2058
C2q-H2q	1.111	C5-C10-C1-C2	54.565	H16B-C16-C17-C22	-30.9476
C4q-C3q	1.3852	C5-C10-C1-H1A	174.5398	H16B-C16-C17-C28	-151.4148
C4q-H4q	1.111	C5-C10-C1-H1B	-65.4152	C13-C18-C17-C16	-29.45
C3q-H3q	1.111	C9-C10-C1-C2	174.4251	C13-C18-C17-C22	90.7301
C5-C10-C1	109.899	C9-C10-C1-H1A	-65.6001	C13-C18-C17-C28	-149.2043
C5-C10-C9	109.2236	C9-C10-C1-H1B	54.4448	C19-C18-C17-C16	-156.6315
C5-C10-C25	109.3154	C25-C10-C1-C2	-65.3499	C19-C18-C17-C22	-36.4514
C1-C10-C9	109.3117	C25-C10-C1-H1A	54.6249	C19-C18-C17-C28	83.6142
C1-C10-C25	109.2183	C25-C10-C1-H1B	174.6698	H18-C18-C17-C16	82.8338
C9-C10-C25	109.861	C5-C10-C9-C8	-48.8711	H18-C18-C17-C22	-156.9861
C10-C5-C4	119.9373	C5-C10-C9-C11	172.1728	H18-C18-C17-C28	-36.9205
C10-C5-C6	114.2933	C5-C10-C9-H9	62.9341	C13-C18-C19-C21	-101.9355
C10-C5-H5	100.1825	C1-C10-C9-C8	-169.1457	C13-C18-C19-C20	18.2526
C4-C5-C6	117.4444	C1-C10-C9-C11	51.8982	C13-C18-C19-H19	138.219
C4-C5-H5	95.8433	C1-C10-C9-H9	-57.3406	C17-C18-C19-C21	21.8871
C6-C5-H5	103.2072	C25-C10-C9-C8	71.024	C17-C18-C19-C20	142.0751
C10-C1-C2	109.6099	C25-C10-C9-C11	-67.9322	C17-C18-C19-H19	-97.9585
C10-C1-H1A	109.4741	C25-C10-C9-H9	-177.1709	H18-C18-C19-C21	145.4628
C10-C1-H1B	109.4789	C5-C10-C25-H25A	-163.8292	H18-C18-C19-C20	-94.3491
C2-C1-H1A	109.3798	C5-C10-C25-H25B	-43.8626	H18-C18-C19-H19	25.6173
C2-C1-H1B	109.3819	C5-C10-C25-H25C	76.21	C16-C17-C22-C21	158.3594
H1A-C1-H1B	109.5027	C1-C10-C25-H25A	-43.5556	C16-C17-C22-H22A	-82.604
C5-C4-C3	114.3928	C1-C10-C25-H25B	76.4111	C16-C17-C22-H22B	39.3151
C5-C4-C24	108.6049	C1-C10-C25-H25C	-163.5163	C18-C17-C22-C21	37.3796
C5-C4-C23	109.979	C9-C10-C25-H25A	76.3317	C18-C17-C22-H22A	156.4162
C3-C4-C24	109.1587	C9-C10-C25-H25B	-163.7017	C18-C17-C22-H22B	-81.6647
C3-C4-C23	106.1326	C9-C10-C25-H25C	-43.6291	C28-C17-C22-C21	-82.2431
C24-C4-C23	108.4151	C10-C5-C4-C3	27.4758	C28-C17-C22-H22A	36.7934
C1-C2-C3	108.5244	C10-C5-C4-C24	-94.7241	C28-C17-C22-H22B	158.7125
C1-C2-H2A	109.7143	C10-C5-C4-C23	146.7832	C16-C17-C28-O28	105.6678
C1-C2-H2B	109.7131	C6-C5-C4-C3	-119.04	C16-C17-C28-H28A	-135.3677
C3-C2-H2A	109.6883	C6-C5-C4-C24	118.76	C16-C17-C28-H28B	-13.2884
C3-C2-H2B	109.6862	C6-C5-C4-C23	0.2673	C18-C17-C28-O28	-133.0885
H2A-C2-H2B	109.4985	H5-C5-C4-C3	132.7837	C18-C17-C28-H28A	-14.124
C4-C3-C2	110.5913	H5-C5-C4-C24	10.5838	C18-C17-C28-H28B	107.9554
C4-C3-O3	108.8618	H5-C5-C4-C23	-107.9089	C22-C17-C28-O28	-14.4379
C4-C3-H3	109.2101	C10-C5-C6-C7	58.2595	C22-C17-C28-H28A	104.5266
C2-C3-O3	109.1594	C10-C5-C6-H6A	178.0246	C22-C17-C28-H28B	-133.3941
C2-C3-H3	108.8831	C10-C5-C6-H6B	-61.51	C18-C19-C21-C22	-0.5837
O3-C3-H3	110.1283	C4-C5-C6-C7	-153.3778	C18-C19-C21-H21A	118.7818
C10-C9-C8	115.6946	C4-C5-C6-H6A	-33.6127	C18-C19-C21-H21B	-119.9558
C10-C9-C11	117.0479	C4-C5-C6-H6B	86.8527	C20-C19-C21-C22	-121.8339
C10-C9-H9	100.4727	H5-C5-C6-C7	-49.5082	C20-C19-C21-H21A	-2.4684

C8-C9-C11	114.0877	H5-C5-C6-H6A	70.257	C20-C19-C21-H21B	118.794
C8-C9-H9	104.4974	H5-C5-C6-H6B	-169.2776	H19-C19-C21-C22	118.5835
C11-C9-H9	101.8834	C10-C1-C2-C3	-71.5608	H19-C19-C21-H21A	-122.051
C9-C8-C7	109.9832	C10-C1-C2-H2A	48.2741	H19-C19-C21-H21B	-0.7887
C9-C8-C14	108.6511	C10-C1-C2-H2B	168.6077	C18-C19-C20-C29	-90.1459
C9-C8-C26	109.8322	H1A-C1-C2-C3	168.4068	C18-C19-C20-C30	91.3456
C7-C8-C14	109.8141	H1A-C1-C2-H2A	-71.7583	C21-C19-C20-C29	29.8977
C7-C8-C26	108.6374	H1A-C1-C2-H2B	48.5753	C21-C19-C20-C30	-148.6107
C14-C8-C26	109.9157	H1B-C1-C2-C3	48.4787	H19-C19-C20-C29	150.0184
C5-C6-C7	108.0276	H1B-C1-C2-H2A	168.3136	H19-C19-C20-C30	-28.49
C5-C6-H6A	109.815	H1B-C1-C2-H2B	-71.3528	C19-C21-C22-C17	-21.6386
C5-C6-H6B	109.8177	C5-C4-C3-C2	-40.2984	C19-C21-C22-H22A	-140.5246
C7-C6-H6A	109.8292	C5-C4-C3-O3	-160.2218	C19-C21-C22-H22B	97.2489
C7-C6-H6B	109.8314	C5-C4-C3-H3	79.5045	H21A-C21-C22-C17	-141.2315
H6A-C6-H6B	109.501	C24-C4-C3-C2	81.599	H21A-C21-C22-H22A	99.8825
C8-C7-C6	113.6351	C24-C4-C3-O3	-38.3244	H21A-C21-C22-H22B	-22.3439
C8-C7-H7A	108.5752	C24-C4-C3-H3	-158.5981	H21B-C21-C22-C17	97.9628
C8-C7-H7B	108.5751	C23-C4-C3-C2	-161.7454	H21B-C21-C22-H22A	-20.9232
C6-C7-H7A	108.2484	C23-C4-C3-O3	78.3311	H21B-C21-C22-H22B	-143.1496
C6-C7-H7B	108.2472	C23-C4-C3-H3	-41.9425	C19-C20-C29-H29A	-178.5073
H7A-C7-H7B	109.5084	C5-C4-C24-H24A	-158.9459	C19-C20-C29-H29B	1.4942
C9-C11-C12	111.2811	C5-C4-C24-H24B	-38.98	C30-C20-C29-H29A	-0.0058
C9-C11-H11A	109.0455	C5-C4-C24-H24C	81.0901	C30-C20-C29-H29B	179.9957
C9-C11-H11B	109.0432	C3-C4-C24-H24A	75.7251	C19-C20-C30-H30A	-172.4011
C12-C11-H11A	108.9726	C3-C4-C24-H24B	-164.3089	C19-C20-C30-H30B	-52.4397
C12-C11-H11B	108.9781	C3-C4-C24-H24C	-44.2388	C19-C20-C30-H30C	67.6347
H11A-C11-H11B	109.5	C23-C4-C24-H24A	-39.4702	C29-C20-C30-H30A	9.0638
C11-C12-C13	113.5552	C23-C4-C24-H24B	80.4957	C29-C20-C30-H30B	129.0252
C11-C12-H12A	108.2597	C23-C4-C24-H24C	-159.4342	C29-C20-C30-H30C	-110.9004
C11-C12-H12B	108.2574	C5-C4-C23-H23A	-78.3132	C17-C28-O28-C7q	-116.2425
C13-C12-H12A	108.6115	C5-C4-C23-H23B	41.6471	H28A-C28-O28-C7q	122.9988
C13-C12-H12B	108.6065	C5-C4-C23-H23C	161.724	H28B-C28-O28-C7q	4.5071
H12A-C12-H12B	109.5	C3-C4-C23-H23A	45.9233	C28-O28-C7q-C8q	-167.825
C8-C14-C13	110.2277	C3-C4-C23-H23B	165.8836	C28-O28-C7q-C6q	11.9053
C8-C14-C15	108.978	C3-C4-C23-H23C	-74.0395	O28-C7q-C8q-C8Aq	176.3343
C8-C14-C27	109.4772	C24-C4-C23-H23A	163.0773	O28-C7q-C8q-O8q	-2.4343
C13-C14-C15	109.8756	C24-C4-C23-H23B	-76.9624	C6q-C7q-C8q-C8Aq	-3.3994
C13-C14-C27	108.7504	C24-C4-C23-H23C	43.1145	C6q-C7q-C8q-O8q	177.832
C15-C14-C27	109.5186	C1-C2-C3-C4	62.656	O28-C7q-C6q-C5q	179.8325
C12-C13-C14	112.3422	C1-C2-C3-O3	-177.5994	O28-C7q-C6q-Clq	0.2784
C12-C13-C18	110.5195	C1-C2-C3-H3	-57.3432	C8q-C7q-C6q-C5q	-0.4407
C12-C13-H13	107.1779	H2A-C2-C3-C4	-57.1951	C8q-C7q-C6q-Clq	-179.9948
C14-C13-C18	112.9423	H2A-C2-C3-O3	62.5495	C8q-C8Aq-C4Aq-C5q	1.0113
C14-C13-H13	106.0105	H2A-C2-C3-H3	-177.1943	C8q-C8Aq-C4Aq-C4q	-179.2326
C18-C13-H13	107.4566	H2B-C2-C3-C4	-177.4956	N1q-C8Aq-C4Aq-C5q	-179.3816
C14-C15-C16	107.9632	H2B-C2-C3-O3	-57.751	N1q-C8Aq-C4Aq-C4q	0.3745
C14-C15-H15A	110.03	H2B-C2-C3-H3	62.5052	C4Aq-C8Aq-C8q-C7q	3.0849
C14-C15-H15B	110.025	C4-C3-O3-H3	-119.708	C4Aq-C8Aq-C8q-O8q	-178.1473

C16-C15-H15A	109.6476	C2-C3-O3-H3	119.4851	N1q-C8Aq-C8q-C7q	-176.5192
C16-C15-H15B	109.6551	H3-C3-O3-H3	-0.003	N1q-C8Aq-C8q-O8q	2.2486
H15A-C15-H15B	109.4992	C10-C9-C8-C7	49.2109	C4Aq-C8Aq-N1q-C2q	-0.2429
C15-C16-C17	110.0266	C10-C9-C8-C14	169.4371	C8q-C8Aq-N1q-C2q	179.361
C15-C16-H16A	109.1909	C10-C9-C8-C26	-70.3034	C8Aq-C4Aq-C5q-C6q	-4.8145
C15-C16-H16B	109.1862	C11-C9-C8-C7	-170.6258	C8Aq-C4Aq-C5q-O5q	174.1653
C17-C16-H16A	109.4621	C11-C9-C8-C14	-50.3995	C4q-C4Aq-C5q-C6q	175.4323
C17-C16-H16B	109.4598	C11-C9-C8-C26	69.86	C4q-C4Aq-C5q-O5q	-5.588
H16A-C16-H16B	109.5006	H9-C9-C8-C7	-60.2254	C8Aq-C4Aq-C4q-C3q	-0.2361
C13-C18-C17	113.7374	H9-C9-C8-C14	60.0009	C8Aq-C4Aq-C4q-H4q	179.7602
C13-C18-C19	118.6109	H9-C9-C8-C26	-179.7396	C5q-C4Aq-C4q-C3q	179.5164
C13-C18-H18	97.6295	C10-C9-C11-C12	132.3034	C5q-C4Aq-C4q-H4q	-0.4873
C17-C18-C19	99.5386	C10-C9-C11-H11A	-107.4598	C4Aq-C5q-C6q-C7q	4.5608
C17-C18-H18	116.3068	C10-C9-C11-H11B	12.0611	C4Aq-C5q-C6q-Clq	-175.8848
C19-C18-H18	112.0679	C8-C9-C11-C12	-7.2946	O5q-C5q-C6q-C7q	-174.4205
C16-C17-C18	110.9423	C8-C9-C11-H11A	112.9422	O5q-C5q-C6q-Clq	5.1339
C16-C17-C22	109.6651	C8-C9-C11-H11B	-127.5369	C8Aq-N1q-C2q-C3q	-0.0313
C16-C17-C28	108.4948	H9-C9-C11-C12	-119.2754	C8Aq-N1q-C2q-H2q	179.9686
C18-C17-C22	107.9478	H9-C9-C11-H11A	0.9614	N1q-C2q-C3q-C4q	0.1712
C18-C17-C28	109.5446	H9-C9-C11-H11B	120.4824	N1q-C2q-C3q-H3q	-179.8319
C22-C17-C28	110.2466	C9-C8-C7-C6	6.0615	H2q-C2q-C3q-C4q	-179.8288
C18-C19-C21	108.9355	C9-C8-C7-H7A	126.5694	H2q-C2q-C3q-H3q	0.1681
C18-C19-C20	110.908	C9-C8-C7-H7B	-114.4449	C4Aq-C4q-C3q-C2q	-0.038
C18-C19-H19	108.8328	C14-C8-C7-C6	-113.4583	C4Aq-C4q-C3q-H3q	179.9651
C21-C19-C20	109.1781	C14-C8-C7-H7A	7.0496	H4q-C4q-C3q-C2q	179.9657
C21-C19-H19	109.9243	C14-C8-C7-H7B	126.0352	H4q-C4q-C3q-H3q	-0.0312
C20-C19-H19	109.0518	C26-C8-C7-C6	126.3015		

Table S2. Geometric parameters (bond length and angles) for hybrid **2** (Å, º).

Bond length, bond angles [Å, °]		Bond length, bond angles [Å, °]		Bond length, bond angles [Å, °]	
C10-C5	1.5504	C19-C21-H21B	110.4362	C26-C8-C7-H7A	-111.0373
C10-C1	1.5328	C22-C21-H21A	110.0769	C26-C8-C7-H7B	7.9406
C10-C9	1.5525	C22-C21-H21B	110.0797	C9-C8-C14-C13	63.1951
C10-C25	1.5332	H21A-C21-H21B	109.4991	C9-C8-C14-C15	-176.2786
C5-C4	1.562	C17-C22-C21	102.3904	C9-C8-C14-C27	-56.4292
C5-C6	1.5375	C17-C22-H22A	111.0785	C7-C8-C14-C13	-176.4879
C5-H5	1.111	C17-C22-H22B	111.0787	C7-C8-C14-C15	-55.9616
C1-C2	1.5334	C21-C22-H22A	111.3276	C7-C8-C14-C27	63.8878
C1-H1A	1.1111	C21-C22-H22B	111.3306	C26-C8-C14-C13	-57.0509
C1-H1B	1.111	H22A-C22-H22B	109.4976	C26-C8-C14-C15	63.4754
C4-C3	1.5448	C19-C20-C29	121.3746	C26-C8-C14-C27	-176.6752
C4-C24	1.529	C19-C20-C30	119.2614	C9-C8-C26-H26A	-89.8172
C4-C23	1.5344	C29-C20-C30	119.3528	C9-C8-C26-H26B	30.1532
C2-C3	1.5361	C14-C27-H27A	109.453	C9-C8-C26-H26C	150.2205
C2-H2A	1.111	C14-C27-H27B	109.4459	C7-C8-C26-H26A	149.8677
C2-H2B	1.1109	C14-C27-H27C	109.4488	C7-C8-C26-H26B	-90.1619
C3-O3	1.4248	H27A-C27-H27B	109.4641	C7-C8-C26-H26C	29.9054

C3-H3	1.1142	H27A-C27-H27C	109.4672	C14-C8-C26-H26A	29.7685
C9-C8	1.5514	H27B-C27-H27C	109.5483	C14-C8-C26-H26B	149.7389
C9-C11	1.5406	C4-C24-H24A	109.4457	C14-C8-C26-H26C	-90.1939
C9-H9	1.111	C4-C24-H24B	109.448	C5-C6-C7-C8	-58.7489
C8-C7	1.5495	C4-C24-H24C	109.4507	C5-C6-C7-H7A	-179.4434
C8-C14	1.5574	H24A-C24-H24B	109.4601	C5-C6-C7-H7B	61.9456
C8-C26	1.5414	H24A-C24-H24C	109.4687	H6A-C6-C7-C8	-178.5148
C6-C7	1.5385	H24B-C24-H24C	109.554	H6A-C6-C7-H7A	60.7907
C6-H6A	1.111	C4-C23-H23A	109.45	H6A-C6-C7-H7B	-57.8203
C6-H6B	1.111	C4-C23-H23B	109.4473	H6B-C6-C7-C8	61.0168
C7-H7A	1.111	C4-C23-H23C	109.4473	H6B-C6-C7-H7A	-59.6777
C7-H7B	1.111	H23A-C23-H23B	109.4652	H6B-C6-C7-H7B	-178.2887
C11-C12	1.5421	H23A-C23-H23C	109.465	C9-C11-C12-C13	53.9335
C11-H11A	1.111	H23B-C23-H23C	109.5526	C9-C11-C12-H12A	174.6736
C11-H11B	1.111	C3-O3-H3	123.841	C9-C11-C12-H12B	-66.8106
C12-C13	1.5528	C10-C25-H25A	109.4518	H11A-C11-C12-C13	-66.3303
C12-H12A	1.1111	C10-C25-H25B	109.4504	H11A-C11-C12-H12A	54.4098
C12-H12B	1.111	C10-C25-H25C	109.448	H11A-C11-C12-H12B	172.9256
C14-C13	1.5787	H25A-C25-H25B	109.4649	H11B-C11-C12-C13	174.1888
C14-C15	1.5372	H25A-C25-H25C	109.4609	H11B-C11-C12-H12A	-65.0711
C14-C27	1.5367	H25B-C25-H25C	109.5513	H11B-C11-C12-H12B	53.4447
C13-C18	1.5724	C8-C26-H26A	109.4523	C11-C12-C13-C14	-41.6574
C13-H13	1.111	C8-C26-H26B	109.4503	C11-C12-C13-C18	-168.4878
C15-C16	1.5229	C8-C26-H26C	109.4515	C11-C12-C13-H13	74.5777
C15-H15A	1.111	H26A-C26-H26B	109.4669	H12A-C12-C13-C14	-162.2291
C15-H15B	1.1111	H26A-C26-H26C	109.4598	H12A-C12-C13-C18	70.9405
C16-C17	1.5358	H26B-C26-H26C	109.5465	H12A-C12-C13-H13	-45.994
C16-H16A	1.111	C17-C28-O28	109.0134	H12B-C12-C13-C14	78.9192
C16-H16B	1.111	C17-C28-H28A	111.0202	H12B-C12-C13-C18	-47.9112
C18-C17	1.5469	C17-C28-H28B	111.0201	H12B-C12-C13-H13	-164.8457
C18-C19	1.564	O28-C28-H28A	108.0976	C8-C14-C13-C12	-16.6121
C18-H18	1.111	O28-C28-H28B	108.0997	C8-C14-C13-C18	109.0249
C17-C22	1.5217	H28A-C28-H28B	109.4956	C8-C14-C13-H13	-133.3824
C17-C28	1.5327	C20-C29-H29A	120.0031	C15-C14-C13-C12	-136.6087
C19-C21	1.5472	C20-C29-H29B	119.9996	C15-C14-C13-C18	-10.9716
C19-C20	1.5242	H29A-C29-H29B	119.9973	C15-C14-C13-H13	106.6211
C19-H19	1.1164	C20-C30-H30A	109.4518	C27-C14-C13-C12	103.4279
C21-C22	1.5327	C20-C30-H30B	109.4459	C27-C14-C13-C18	-130.9351
C21-H21A	1.111	C20-C30-H30C	109.4491	C27-C14-C13-H13	-13.3424
C21-H21B	1.111	H30A-C30-H30B	109.466	C8-C14-C15-C16	-170.0734
C22-H22A	1.111	H30A-C30-H30C	109.4605	C8-C14-C15-H15A	-50.3959
C22-H22B	1.111	H30B-C30-H30C	109.554	C8-C14-C15-H15B	70.2542
C20-C29	1.3434	C28-O28-C7q	124.2026	C13-C14-C15-C16	-49.3119
C20-C30	1.5093	O28-C7q-C8q	118.7773	C13-C14-C15-H15A	70.3656
C27-H27A	1.1111	O28-C7q-C6q	121.0776	C13-C14-C15-H15B	-168.9843
C27-H27B	1.1111	C8q-C7q-C6q	120.1438	C27-C14-C15-C16	70.1554
C27-H27C	1.1111	C4Aq-C8Aq-C8q	119.6648	C27-C14-C15-H15A	-170.1671
C24-H24A	1.1111	C4Aq-C8Aq-N1q	119.7173	C27-C14-C15-H15B	-49.517

C24-H24B	1.1111	C8q-C8Aq-N1q	120.6165	C8-C14-C27-H27A	158.3914
C24-H24C	1.1111	C8Aq-C4Aq-C5q	119.6036	C8-C14-C27-H27B	-81.644
C23-H23A	1.1111	C8Aq-C4Aq-C4q	119.6526	C8-C14-C27-H27C	38.4211
C23-H23B	1.1112	C5q-C4Aq-C4q	120.7431	C13-C14-C27-H27A	37.9122
C23-H23C	1.1112	C7q-C8q-C8Aq	120.0518	C13-C14-C27-H27B	157.8768
O3-C31	1.3616	C7q-C8q-O8q	119.9468	C13-C14-C27-H27C	-82.058
C25-H25A	1.1111	C8Aq-C8q-O8q	119.9919	C15-C14-C27-H27A	-82.1758
C25-H25B	1.1112	C4Aq-C5q-C6q	119.8771	C15-C14-C27-H27B	37.7888
C25-H25C	1.1112	C4Aq-C5q-O5q	120.0265	C15-C14-C27-H27C	157.8539
C26-H26A	1.111	C6q-C5q-O5q	120.0901	C12-C13-C18-C17	178.7069
C26-H26B	1.1111	C7q-C6q-C5q	120.4287	C12-C13-C18-C19	-64.1561
C26-H26C	1.1112	C7q-C6q-Clq	119.7898	C12-C13-C18-H18	55.9471
C28-O28	1.4247	C5q-C6q-Clq	119.781	C14-C13-C18-C17	52.2796
C28-H28A	1.1111	C8Aq-N1q-C2q	120.6413	C14-C13-C18-C19	169.4165
C28-H28B	1.111	N1q-C2q-C3q	119.6493	C14-C13-C18-H18	-70.4803
C29-H29A	1.111	N1q-C2q-H2q	120.209	H13-C13-C18-C17	-64.5784
C29-H29B	1.111	C3q-C2q-H2q	120.1417	H13-C13-C18-C19	52.5586
C30-H30A	1.111	C4Aq-C4q-C3q	120.6533	H13-C13-C18-H18	172.6617
C30-H30B	1.1111	C4Aq-C4q-H4q	119.6373	C14-C15-C16-C17	75.4921
C30-H30C	1.1111	C3q-C4q-H4q	119.7094	C14-C15-C16-H16A	-164.3674
O28-C7q	1.3654	C2q-C3q-C4q	119.6853	C14-C15-C16-H16B	-44.6513
C7q-C8q	1.4808	C2q-C3q-H3q	120.109	H15A-C15-C16-C17	-44.4185
C7q-C6q	1.3472	C4q-C3q-H3q	120.2057	H15A-C15-C16-H16A	75.722
C8Aq-C4Aq	1.3832	O3-C31-O31	120.0635	H15A-C15-C16-H16B	-164.5619
C8Aq-C8q	1.4752	O3-C31-C32	119.85	H15B-C15-C16-C17	-164.6027
C8Aq-N1q	1.3844	O31-C31-C32	120.0856	H15B-C15-C16-H16A	-44.4622
C4Aq-C5q	1.4743	C31-C32-H32A	109.4459	H15B-C15-C16-H16B	75.254
C4Aq-C4q	1.3841	C31-C32-H32B	109.4473	C15-C16-C17-C18	-32.3918
C8q-O8q	1.2097	C31-C32-H32C	109.4503	C15-C16-C17-C22	-151.639
C5q-C6q	1.4827	H32A-C32-H32B	109.4638	C15-C16-C17-C28	87.9144
C5q-O5q	1.2097	H32A-C32-H32C	109.4626	H16A-C16-C17-C18	-152.3236
C6q-Clq	1.7202	H32B-C32-H32C	109.5573	H16A-C16-C17-C22	88.4292
N1q-C2q	1.3845	C1-C10-C5-C4	-33.1763	H16A-C16-C17-C28	-32.0174
C2q-C3q	1.3835	C1-C10-C5-C6	116.7327	H16B-C16-C17-C18	87.5393
C2q-H2q	1.111	C1-C10-C5-H5	-134.1582	H16B-C16-C17-C22	-31.7079
C4q-C3q	1.3849	C9-C10-C5-C4	-153.2807	H16B-C16-C17-C28	-152.1546
C4q-H4q	1.111	C9-C10-C5-C6	-3.3717	C13-C18-C17-C16	-28.6017
C3q-H3q	1.111	C9-C10-C5-H5	105.7374	C13-C18-C17-C22	91.6307
C31-O31	1.2088	C25-C10-C5-C4	86.6137	C13-C18-C17-C28	-148.3086
C31-C32	1.5121	C25-C10-C5-C6	-123.4773	C19-C18-C17-C16	-156.1943
C32-H32A	1.111	C25-C10-C5-H5	-14.3682	C19-C18-C17-C22	-35.9619
C32-H32B	1.1111	C5-C10-C1-C2	55.1146	C19-C18-C17-C28	84.0988
C32-H32C	1.1111	C5-C10-C1-H1A	175.0261	H18-C18-C17-C16	83.4538
C5-C10-C1	109.7	C5-C10-C1-H1B	-64.8039	H18-C18-C17-C22	-156.3138
C5-C10-C9	109.1295	C9-C10-C1-C2	174.9236	H18-C18-C17-C28	-36.253
C5-C10-C25	109.5443	C9-C10-C1-H1A	-65.1648	C13-C18-C19-C21	-105.1587
C1-C10-C9	109.6136	C9-C10-C1-H1B	55.0051	C13-C18-C19-C20	15.1025
C1-C10-C25	109.1488	C25-C10-C1-C2	-64.9168	C13-C18-C19-H19	135.0158

C9-C10-C25	109.6921	C25-C10-C1-H1A	54.9948	C17-C18-C19-C21	19.35
C10-C5-C4	120.5959	C25-C10-C1-H1B	175.1647	C17-C18-C19-C20	139.6111
C10-C5-C6	114.6781	C5-C10-C9-C8	-50.627	C17-C18-C19-H19	-100.4755
C10-C5-H5	99.0413	C5-C10-C9-C11	170.9374	H18-C18-C19-C21	142.508
C4-C5-C6	117.6611	C5-C10-C9-H9	61.7216	H18-C18-C19-C20	-97.2308
C4-C5-H5	94.701	C1-C10-C9-C8	-170.7845	H18-C18-C19-H19	22.6826
C6-C5-H5	103.1888	C1-C10-C9-C11	50.7799	C16-C17-C22-C21	159.8063
C10-C1-C2	108.9617	C1-C10-C9-H9	-58.436	C16-C17-C22-H22A	-81.263
C10-C1-H1A	109.5822	C25-C10-C9-C8	69.3876	C16-C17-C22-H22B	40.872
C10-C1-H1B	109.5864	C25-C10-C9-C11	-69.0479	C18-C17-C22-C21	38.8618
C2-C1-H1A	109.5982	C25-C10-C9-H9	-178.2638	C18-C17-C22-H22A	157.7926
C2-C1-H1B	109.6018	C5-C10-C25-H25A	-164.8311	C18-C17-C22-H22B	-80.0725
H1A-C1-H1B	109.4963	C5-C10-C25-H25B	-44.8636	C28-C17-C22-C21	-80.7727
C5-C4-C3	114.8625	C5-C10-C25-H25C	75.2075	C28-C17-C22-H22A	38.158
C5-C4-C24	108.2633	C1-C10-C25-H25A	-44.7039	C28-C17-C22-H22B	160.293
C5-C4-C23	109.9429	C1-C10-C25-H25B	75.2636	C16-C17-C28-O28	108.323
C3-C4-C24	108.8856	C1-C10-C25-H25C	-164.6652	C16-C17-C28-H28A	-132.7038
C3-C4-C23	106.1254	C9-C10-C25-H25A	75.4075	C16-C17-C28-H28B	-10.6527
C24-C4-C23	108.6068	C9-C10-C25-H25B	-164.625	C18-C17-C28-O28	-130.5551
C1-C2-C3	109.0171	C9-C10-C25-H25C	-44.5539	C18-C17-C28-H28A	-11.5819
C1-C2-H2A	109.5361	C10-C5-C4-C3	24.8889	C18-C17-C28-H28B	110.4693
C1-C2-H2B	109.5434	C10-C5-C4-C24	-97.0212	C22-C17-C28-O28	-11.8141
C3-C2-H2A	109.6122	C10-C5-C4-C23	144.4779	C22-C17-C28-H28A	107.1591
C3-C2-H2B	109.6139	C6-C5-C4-C3	-124.1556	C22-C17-C28-H28B	-130.7898
H2A-C2-H2B	109.5039	C6-C5-C4-C24	113.9343	C18-C19-C21-C22	2.992
C4-C3-C2	110.4221	C6-C5-C4-C23	-4.5666	C18-C19-C21-H21A	122.3585
C4-C3-O3	108.5282	H5-C5-C4-C3	128.2922	C18-C19-C21-H21B	-116.3789
C4-C3-H3	109.4912	H5-C5-C4-C24	6.3821	C20-C19-C21-C22	-118.093
C2-C3-O3	109.6419	H5-C5-C4-C23	-112.1188	C20-C19-C21-H21A	1.2736
C2-C3-H3	108.6007	C10-C5-C6-C7	56.1943	C20-C19-C21-H21B	122.5361
O3-C3-H3	110.1519	C10-C5-C6-H6A	175.98	H19-C19-C21-C22	122.3018
C10-C9-C8	115.5572	C10-C5-C6-H6B	-63.5934	H19-C19-C21-H21A	-118.3316
C10-C9-C11	117.1588	C4-C5-C6-C7	-152.9666	H19-C19-C21-H21B	2.9309
C10-C9-H9	100.3838	C4-C5-C6-H6A	-33.1809	C18-C19-C20-C29	-90.546
C8-C9-C11	113.8071	C4-C5-C6-H6B	87.2458	C18-C19-C20-C30	90.6731
C8-C9-H9	105.0499	H5-C5-C6-C7	-50.3828	C21-C19-C20-C29	29.4056
C11-C9-H9	101.8746	H5-C5-C6-H6A	69.403	C21-C19-C20-C30	-149.3754
C9-C8-C7	109.9329	H5-C5-C6-H6B	-170.1704	H19-C19-C20-C29	149.5304
C9-C8-C14	108.7683	C10-C1-C2-C3	-72.5033	H19-C19-C20-C30	-29.2505
C9-C8-C26	109.8526	C10-C1-C2-H2A	47.4312	C19-C21-C22-C17	-24.6084
C7-C8-C14	109.7731	C10-C1-C2-H2B	167.5555	C19-C21-C22-H22A	-143.3637
C7-C8-C26	108.6873	H1A-C1-C2-C3	167.595	C19-C21-C22-H22B	94.1484
C14-C8-C26	109.818	H1A-C1-C2-H2A	-72.4704	H21A-C21-C22-C17	-144.2083
C5-C6-C7	108.1162	H1A-C1-C2-H2B	47.6538	H21A-C21-C22-H22A	97.0364
C5-C6-H6A	109.785	H1B-C1-C2-C3	47.4056	H21A-C21-C22-H22B	-25.4514
C5-C6-H6B	109.7838	H1B-C1-C2-H2A	167.3402	H21B-C21-C22-C17	94.9951
C7-C6-H6A	109.8165	H1B-C1-C2-H2B	-72.5356	H21B-C21-C22-H22A	-23.7602
C7-C6-H6B	109.8187	C5-C4-C3-C2	-37.4027	H21B-C21-C22-H22B	-146.2481

H6A-C6-H6B	109.5022	C5-C4-C3-O3	-157.6066	C19-C20-C29-H29A	-178.7741
C8-C7-C6	113.633	C5-C4-C3-H3	82.1248	C19-C20-C29-H29B	1.2202
C8-C7-H7A	108.5784	C24-C4-C3-C2	84.1693	C30-C20-C29-H29A	0.0057
C8-C7-H7B	108.5754	C24-C4-C3-O3	-36.0346	C30-C20-C29-H29B	-180.0
C6-C7-H7A	108.2483	C24-C4-C3-H3	-156.3031	C19-C20-C30-H30A	-171.6509
C6-C7-H7B	108.2536	C23-C4-C3-C2	-159.0907	C19-C20-C30-H30B	-51.6846
H7A-C7-H7B	109.5002	C23-C4-C3-O3	80.7054	C19-C20-C30-H30C	68.3877
C9-C11-C12	111.373	C23-C4-C3-H3	-39.5632	C29-C20-C30-H30A	9.5432
C9-C11-H11A	108.9637	C5-C4-C24-H24A	-151.1767	C29-C20-C30-H30B	129.5095
C9-C11-H11B	108.9619	C5-C4-C24-H24B	-31.2201	C29-C20-C30-H30C	-110.4182
C12-C11-H11A	109.0154	C5-C4-C24-H24C	88.8545	C17-C28-O28-C7q	-7.8684
C12-C11-H11B	109.0059	C3-C4-C24-H24A	83.3144	H28A-C28-O28-C7q	172.472
H11A-C11-H11B	109.4999	C3-C4-C24-H24B	-156.729	H28B-C28-O28-C7q	-115.2393
C11-C12-C13	114.0212	C3-C4-C24-H24C	-36.6544	C28-O28-C7q-C8q	123.9799
C11-C12-H12A	108.163	C23-C4-C24-H24A	-31.8303	C28-O28-C7q-C6q	5.5426
C11-C12-H12B	108.1662	C23-C4-C24-H24B	88.1263	O28-C7q-C8q-C8Aq	-169.4111
C13-C12-H12A	108.4646	C23-C4-C24-H24C	-151.7991	O28-C7q-C8q-O8q	10.1616
C13-C12-H12B	108.466	C5-C4-C23-H23A	-77.6473	C6q-C7q-C8q-C8Aq	176.1105
H12A-C12-H12B	109.5007	C5-C4-C23-H23B	42.3177	C6q-C7q-C8q-O8q	-2.7684
C8-C14-C13	110.1941	C5-C4-C23-H23C	162.388	O28-C7q-C6q-C5q	-3.4663
C8-C14-C15	108.9322	C3-C4-C23-H23A	47.1367	O28-C7q-C6q-Clq	177.6548
C8-C14-C27	109.484	C3-C4-C23-H23B	167.1017	C8q-C7q-C6q-C5q	-179.7255
C13-C14-C15	109.8112	C3-C4-C23-H23C	-72.828	C8q-C7q-C6q-Clq	0.5362
C13-C14-C27	108.7971	C24-C4-C23-H23A	164.0637	C8q-C8Aq-C4Aq-C5q	-0.1586
C15-C14-C27	109.6102	C24-C4-C23-H23B	-75.9713	C8q-C8Aq-C4Aq-C4q	-179.8969
C12-C13-C14	112.0806	C24-C4-C23-H23C	44.099	N1q-C8Aq-C4Aq-C5q	1.0657
C12-C13-C18	110.6096	C1-C2-C3-C4	61.6512	N1q-C8Aq-C4Aq-C4q	-179.2412
C12-C13-H13	107.1715	C1-C2-C3-O3	-178.8158	C4Aq-C8Aq-C8q-C7q	-179.3519
C14-C13-C18	112.806	C1-C2-C3-H3	-58.4132	C4Aq-C8Aq-C8q-O8q	0.3413
C14-C13-H13	106.2836	H2A-C2-C3-C4	-58.2363	N1q-C8Aq-C8q-C7q	2.9772
C18-C13-H13	107.5274	H2A-C2-C3-O3	61.2966	N1q-C8Aq-C8q-O8q	-178.1445
C14-C15-C16	108.1969	H2A-C2-C3-H3	-178.3007	C4Aq-C8Aq-N1q-C2q	-176.6015
C14-C15-H15A	109.9695	H2B-C2-C3-C4	-178.4512	C8q-C8Aq-N1q-C2q	2.2769
C14-C15-H15B	109.9663	H2B-C2-C3-O3	-58.9182	C8Aq-C4Aq-C5q-C6q	-0.221
C16-C15-H15A	109.5984	H2B-C2-C3-H3	61.4844	C8Aq-C4Aq-C5q-O5q	179.3574
C16-C15-H15B	109.5957	C4-C3-O3-H3	166.6709	C4q-C4Aq-C5q-C6q	-4.6607
H15A-C15-H15B	109.495	C2-C3-O3-H3	45.983	C4q-C4Aq-C5q-O5q	174.4261
C15-C16-C17	109.81	H3-C3-O3-H3	-73.472	C8Aq-C4Aq-C4q-C3q	175.6495
C15-C16-H16A	109.2065	C10-C9-C8-C7	48.2043	C8Aq-C4Aq-C4q-H4q	-5.2636
C15-C16-H16B	109.2041	C10-C9-C8-C14	168.4225	C5q-C4Aq-C4q-C3q	-0.2169
C17-C16-H16A	109.5496	C10-C9-C8-C26	-71.3529	C5q-C4Aq-C4q-H4q	179.7888
C17-C16-H16B	109.5532	C11-C9-C8-C7	-171.9773	C4Aq-C5q-C6q-C7q	179.4726
H16A-C16-H16B	109.5027	C11-C9-C8-C14	-51.7592	C4Aq-C5q-C6q-Clq	-0.5216
C13-C18-C17	114.1308	C11-C9-C8-C26	68.4654	O5q-C5q-C6q-C7q	4.2231
C13-C18-C19	118.6533	H9-C9-C8-C7	-61.3966	O5q-C5q-C6q-Clq	-176.0386
C13-C18-H18	97.4595	H9-C9-C8-C14	58.8216	C8Aq-N1q-C2q-C3q	-174.8631
C17-C18-C19	99.7443	H9-C9-C8-C26	179.0462	C8Aq-N1q-C2q-H2q	4.8752
C17-C18-H18	115.8857	C10-C9-C11-C12	133.5388	N1q-C2q-C3q-C4q	-0.0281

C19-C18-H18	111.9724	C10-C9-C11-H11A	-106.1669	N1q-C2q-C3q-H3q	179.9786
C16-C17-C18	110.8412	C10-C9-C11-H11B	13.2576	H2q-C2q-C3q-C4q	0.1541
C16-C17-C22	109.7015	C8-C9-C11-C12	-5.6012	H2q-C2q-C3q-H3q	-179.8485
C16-C17-C28	108.5189	C8-C9-C11-H11A	114.693	C4Aq-C4q-C3q-C2q	-179.8526
C18-C17-C22	108.0557	C8-C9-C11-H11B	-125.8824	C4Aq-C4q-C3q-H3q	0.1448
C18-C17-C28	109.5227	H9-C9-C11-C12	-118.1076	H4q-C4q-C3q-C2q	-0.032
C22-C17-C28	110.1997	H9-C9-C11-H11A	2.1867	H4q-C4q-C3q-H3q	179.9707
C18-C19-C21	108.8569	H9-C9-C11-H11B	121.6112	H4q-C4q-C3q-C2q	179.9622
C18-C19-C20	110.7141	C9-C8-C7-C6	8.1886	H4q-C4q-C3q-H2q-	-0.0351
C18-C19-H19	109.0239	C9-C8-C7-H7A	128.6973	O3-C31-C32-H32A	-100.5288
C21-C19-C20	109.3748	C9-C8-C7-H7B	-112.3248	O3-C31-C32-H32B	19.432
C21-C19-H19	109.8529	C14-C8-C7-C6	-111.4189	O3-C31-C32-H32C	139.51
C20-C19-H19	109.0069	C14-C8-C7-H7A	9.0898	O31-C31-C32-H32A	79.8117
C19-C21-C22	106.2744	C14-C8-C7-H7B	128.0677	O31-C31-C32-H32B	-160.2275
C19-C21-H21A	110.4344	C26-C8-C7-C6	128.454	O31-C31-C32-H32C	-40.1495

Table S3. Geometric parameters (bond length and angles) for hybrid **3** (Å, º).

Bond length, bond angles [Å, °]		Bond length, bond angles [Å, °]		Bond length, bond angles [Å, °]	
C10-C5	1.5524	C19-C21-H21B	110.3946	C26-C8-C7-H7A	-116.6282
C10-C1	1.5274	C22-C21-H21A	110.0689	C26-C8-C7-H7B	2.1915
C10-C9	1.5483	C22-C21-H21B	110.0747	C9-C8-C14-C13	60.4388
C10-C25	1.535	H21A-C21-H21B	109.5015	C9-C8-C14-C15	-179.0178
C5-C4	1.5692	C17-C22-C21	103.6366	C9-C8-C14-C27	-59.135
C5-C6	1.5418	C17-C22-H22A	110.8106	C7-C8-C14-C13	-179.4935
C5-H5	1.111	C17-C22-H22B	110.817	C7-C8-C14-C15	-58.95
C1-C2	1.5215	C21-C22-H22A	110.9902	C7-C8-C14-C27	60.9328
C1-H1A	1.1109	C21-C22-H22B	110.9899	C26-C8-C14-C13	-59.9722
C1-H1B	1.1109	H22A-C22-H22B	109.4992	C26-C8-C14-C15	60.5712
C4-C3	1.5498	C19-C20-C29	121.4052	C26-C8-C14-C27	-179.546
C4-24	1.5303	C19-C20-C30	119.3669	C9-C8-C26-H26A	-80.3602
C4-C23	1.5338	C29-C20-C30	119.2182	C9-C8-C26-H26B	39.5956
C2-C3	1.5276	C14-C27-H27A	109.449	C9-C8-C26-H26C	159.6726
C2-H2A	1.111	C14-C27-H27B	109.4465	C7-C8-C26-H26A	159.6613
C2-H2B	1.111	C14-C27-H27C	109.4464	C7-C8-C26-H26B	-80.3829
C3-O3	1.4337	H27A-C27-H27B	109.4679	C7-C8-C26-H26C	39.6941
C3-H3	1.1157	H27A-C27-H27C	109.4614	C14-C8-C26-H26A	39.47
C9-C8	1.5518	H27B-C27-H27C	109.5561	C14-C8-C26-H26B	159.4258
C9-C11	1.5398	C4-C24-H24A	109.4474	C14-C8-C26-H26C	-80.4972
C9-H9	1.1111	C4-C24-H24B	109.4466	C5-C6-C7-C8	-54.3525
C8-C7	1.5535	C4-C24-H24C	109.4521	C5-C6-C7-H7A	-175.07
C8-C14	1.5611	H24A-C24-H24B	109.4617	C5-C6-C7-H7B	66.3614
C8-C26	1.5402	H24A-C24-H24C	109.4651	H6A-C6-C7-C8	-174.3093
C6-C7	1.5457	H24B-C24-H24C	109.5543	H6A-C6-C7-H7A	64.9733
C6-H6A	1.111	C4-C23-H23A	109.4512	H6A-C6-C7-H7B	-53.5953
C6-H6B	1.111	C4-C23-H23B	109.453	H6B-C6-C7-C8	65.5984
C7-H7A	1.111	C4-C23-H23C	109.4511	H6B-C6-C7-H7A	-55.1191
C7-H7B	1.1109	H23A-C23-H23B	109.4651	H6B-C6-C7-H7B	-173.6876

C11-C12	1.5315	H23A-C23-H23C	109.4567	C9-C11-C12-C13	57.1663
C11-H11A	1.111	H23B-C23-H23C	109.5502	C9-C11-C12-H12A	177.8134
C11-H11B	1.111	C3-O3-C7q	128.2738	C9-C11-C12-H12B	-63.4741
C12-C13	1.5501	C10-C25-H25A	109.4503	H11A-C11-C12-C13	-63.0458
C12-H12A	1.1109	C10-C25-H25B	109.4539	H11A-C11-C12-H12A	57.6013
C12-H12B	1.111	C10-C25-H25C	109.4505	H11A-C11-C12-H12B	176.3138
C14-C13	1.5806	H25A-C25-H25B	109.4631	H11B-C11-C12-C13	177.3823
C14-C15	1.5409	H25A-C25-H25C	109.4586	H11B-C11-C12-H12A	-61.9707
C14-C27	1.5365	H25B-C25-H25C	109.551	H11B-C11-C12-H12B	56.7419
C13-C18	1.5649	C8-C26-H26A	109.4488	C11-C12-C13-C14	-44.7036
C13-H13	1.111	C8-C26-H26B	109.4453	C11-C12-C13-C18	-171.3776
C15-C16	1.525	C8-C26-H26C	109.4517	C11-C12-C13-H13	71.2042
C15-H15A	1.111	H26A-C26-H26B	109.4592	H12A-C12-C13-C14	-165.0404
C15-H15B	1.111	H26A-C26-H26C	109.4654	H12A-C12-C13-C18	68.2856
C16-C17	1.5359	H26B-C26-H26C	109.5568	H12A-C12-C13-H13	-49.1326
C16-H16A	1.111	C17-C28-O28	110.3667	H12B-C12-C13-C14	75.6318
C16-H16B	1.111	C17-C28-H28A	110.8352	H12B-C12-C13-C18	-51.0421
C18-C17	1.5428	C17-C28-H28B	110.8359	H12B-C12-C13-H13	-168.4603
C18-C19	1.5639	O28-C28-H28A	107.5972	C8-C14-C13-C12	-14.2985
C18-H18	1.1109	O28-C28-H28B	107.5964	C8-C14-C13-C18	109.942
C17-C22	1.5223	H28A-C28-H28B	109.4994	C8-C14-C13-H13	-132.0456
C17-C28	1.537	C20-C29-H29A	119.9992	C15-C14-C13-C12	-134.2647
C19-C21	1.5432	C20-C29-H29B	120.0051	C15-C14-C13-C18	-10.0242
C19-C20	1.5228	H29A-C29-H29B	119.9956	C15-C14-C13-H13	107.9881
C19-H19	1.1148	C20-C30-H30A	109.4457	C27-C14-C13-C12	105.8083
C21-C22	1.53	C20-C30-H30B	109.4456	C27-C14-C13-C18	-129.9512
C21-H21A	1.111	C20-C30-H30C	109.448	C27-C14-C13-H13	-11.9389
C21-H21B	1.111	H30A-C30-H30B	109.4645	C8-C14-C15-C16	-169.4006
C22-H22A	1.1111	H30A-C30-H30C	109.4657	C8-C14-C15-H15A	-49.6397
C22-H22B	1.1109	H30B-C30-H30C	109.5579	C8-C14-C15-H15B	70.8434
C20-C29	1.3426	C29-O28-C31	121.7688	C13-C14-C15-C16	-48.6437
C20-C30	1.5096	O28-C31-O31	120.0674	C13-C14-C15-H15A	71.1172
C27-H27A	1.1111	O28-C31-C32	119.8239	C13-C14-C15-H15B	-168.3997
C27-H27B	1.1111	O31-C31-C32	120.1086	C27-C14-C15-C16	70.7313
C27-H27C	1.1111	O3-C7q-C6q	121.5493	C27-C14-C15-H15A	-169.5078
C24-H24A	1.1111	O3-C7q-C8q	118.8866	C27-C14-C15-H15B	-49.0247
C24-H24B	1.1112	C6q-C7q-C8q	119.5583	C8-C14-C27-H27A	141.3334
C24-H24C	1.1111	C31-C32-H32A	109.4504	C8-C14-C27-H27B	-98.6995
C23-H23A	1.1111	C31-C32-H32B	109.4443	C8-C14-C27-H27C	21.3741
C23-H23B	1.1111	C31-C32-H32C	109.4505	C13-C14-C27-H27A	20.8495
C23-H23C	1.1112	H32A-C32-H32B	109.4563	C13-C14-C27-H27B	140.8167
O3-C7q	1.3749	H32A-C32-H32C	109.4644	C13-C14-C27-H27C	-99.1097
C25-H25A	1.1111	H32B-C32-H32C	109.5614	C15-C14-C27-H27A	-99.2252
C25-H25B	1.1112	C7q-C6q-C5q	121.0563	C15-C14-C27-H27B	20.742
C25-H25C	1.1111	C7q-C6q-Clq	157.3586	C15-C14-C27-H27C	140.8155
C26-H26A	1.1111	C5q-C6q-Clq	81.562	C12-C13-C18-C17	177.2032
C26-H26B	1.1112	C6q-C5q-C4Aq	119.8883	C12-C13-C18-C19	-65.5179
C26-H26C	1.1111	C6q-C5q-O5q	119.9036	C12-C13-C18-H18	54.8502

C28-O28	1.4211	C4Aq-C5q-O5q	120.2002	C14-C13-C18-C17	51.062
C28-H28A	1.111	C7q-C8q-C8Aq	120.0687	C14-C13-C18-C19	168.3409
C28-H28B	1.1109	C7q-C8q-O8q	119.9598	C14-C13-C18-H18	-71.2909
C29-H29A	1.111	C8Aq-C8q-O8q	119.9594	H13-C13-C18-C17	-65.2589
C29-H29B	1.111	C5q-C4Aq-C8Aq	119.7194	H13-C13-C18-C19	52.02
C30-H30A	1.1111	C5q-C4Aq-C4q	120.4114	H13-C13-C18-H18	172.3881
C30-H30B	1.1111	C8Aq-C4Aq-C4q	119.8668	C14-C15-C16-C17	73.4651
C30-H30C	1.1111	C8q-C8Aq-C4Aq	119.6924	C14-C15-C16-H16A	-166.2782
O28-C31	1.3591	C8q-C8Aq-N1q	120.7768	C14-C15-C16-H16B	-46.8035
C31-O31	1.2089	C4Aq-C8Aq-N1q	119.5301	H15A-C15-C16-C17	-46.5518
C31-C32	1.5087	C4Aq-C4q-C3q	120.6613	H15A-C15-C16-H16A	73.7049
C7q-C6q	1.3482	C4Aq-C4q-H4q	119.6614	H15A-C15-C16-H16B	-166.8204
C7q-C8q	1.4851	C3q-C4q-H4q	119.6772	H15B-C15-C16-C17	-166.5257
C32-H32A	1.1111	C4q-C3q-C2q	119.5359	H15B-C15-C16-H16A	-46.2689
C32-H32B	1.1112	C4q-C3q-H3q	120.2482	H15B-C15-C16-H16B	73.2058
C32-H32C	1.1111	C2q-C3q-H3q	120.2159	C15-C16-C17-C18	-30.9863
C6q-C5q	1.477	C8Aq-N1q-C2q	120.6474	C15-C16-C17-C22	-150.2563
C6q-Clq	1.54	C3q-C2q-N1q	119.7578	C15-C16-C17-C28	89.1507
C5q-C4Aq	1.4707	C3q-C2q-H2q	120.0669	H16A-C16-C17-C18	-151.0645
C5q-O5q	1.2085	N1q-C2q-H2q	120.1753	H16A-C16-C17-C22	89.6655
C8q-C8Aq	1.478	C1-C10-C5-C4	-32.4846	H16A-C16-C17-C28	-30.9275
C8q-O8q	1.2089	C1-C10-C5-C6	116.9137	H16B-C16-C17-C18	89.1085
C4Aq-C8Aq	1.3816	C1-C10-C5-H5	-134.215	H16B-C16-C17-C22	-30.1615
C4Aq-C4q	1.3837	C9-C10-C5-C4	-152.4294	H16B-C16-C17-C28	-150.7545
C8Aq-N1q	1.3845	C9-C10-C5-C6	-3.0311	C13-C18-C17-C16	-28.676
C4q-C3q	1.3838	C9-C10-C5-H5	105.8403	C13-C18-C17-C22	91.2801
C4q-H4q	1.111	C25-C10-C5-C4	87.3287	C13-C18-C17-C28	-148.616
C3q-C2q	1.3835	C25-C10-C5-C6	-123.273	C19-C18-C17-C16	-156.5023
C3q-H3q	1.1109	C25-C10-C5-H5	-14.4016	C19-C18-C17-C22	-36.5462
N1q-C2q	1.385	C5-C10-C1-C2	56.3543	C19-C18-C17-C28	83.5577
C2q-H2q	1.111	C5-C10-C1-H1A	176.0684	H18-C18-C17-C16	82.5851
C5-C10-C1	109.8304	C5-C10-C1-H1B	-63.364	H18-C18-C17-C22	-157.4588
C5-C10-C9	109.2515	C9-C10-C1-C2	176.2348	H18-C18-C17-C28	-37.3549
C5-C10-C25	109.3901	C9-C10-C1-H1A	-64.0511	C13-C18-C19-C21	-100.7722
C1-C10-C9	109.3572	C9-C10-C1-H1B	56.5165	C13-C18-C19-C20	19.5511
C1-C10-C25	109.1802	C25-C10-C1-C2	-63.5869	C13-C18-C19-H19	139.4232
C9-C10-C25	109.8192	C25-C10-C1-H1A	56.1272	C17-C18-C19-C21	24.3722
C10-C5-C4	120.1455	C25-C10-C1-H1B	176.6949	C17-C18-C19-C20	144.6955
C10-C5-C6	114.3992	C5-C10-C9-C8	-52.3664	C17-C18-C19-H19	-95.4324
C10-C5-H5	99.9054	C5-C10-C9-C11	170.1395	H18-C18-C19-C21	147.5077
C4-C5-C6	118.0594	C5-C10-C9-H9	60.0833	H18-C18-C19-C20	-92.169
C4-C5-H5	94.9795	C1-C10-C9-C8	-172.6019	H18-C18-C19-H19	27.7031
C6-C5-H5	102.6565	C1-C10-C9-C11	49.904	C16-C17-C22-C21	156.1961
C10-C1-C2	108.0225	C1-C10-C9-H9	-60.1523	C16-C17-C22-H22A	-84.691
C10-C1-H1A	109.8945	C25-C10-C9-C8	67.6119	C16-C17-C22-H22B	37.0805
C10-C1-H1B	109.8946	C25-C10-C9-C11	-69.8821	C18-C17-C22-C21	35.1956
C2-C1-H1A	109.7514	C25-C10-C9-H9	-179.9384	C18-C17-C22-H22A	154.3085
C2-C1-H1B	109.7548	C5-C10-C25-H25A	-165.4694	C18-C17-C22-H22B	-83.92

H1A-C1-H1B	109.5038	C5-C10-C25-H25B	-45.5028	C28-C17-C22-C21	-84.1517
C5-C4-C3	114.6032	C5-C10-C25-H25C	74.5716	C28-C17-C22-H22A	34.9611
C5-C4-C24	108.2685	C1-C10-C25-H25A	-45.2573	C28-C17-C22-H22B	156.7327
C5-C4-C23	109.8621	C1-C10-C25-H25B	74.7093	C16-C17-C28-O28	99.3163
C3-C4-C24	108.7408	C1-C10-C25-H25C	-165.2164	C16-C17-C28-H28A	-141.5842
C3-C4-C23	106.3784	C9-C10-C25-H25A	74.6367	C16-C17-C28-H28B	-19.7825
C24-C4-C23	108.8624	C9-C10-C25-H25B	-165.3967	C18-C17-C28-O28	-139.405
C1-C2-C3	108.6041	C9-C10-C25-H25C	-45.3224	C18-C17-C28-H28A	-20.3055
C1-C2-H2A	109.6053	C10-C5-C4-C3	23.0673	C18-C17-C28-H28B	101.4962
C1-C2-H2B	109.6021	C10-C5-C4-C24	-98.4854	C22-C17-C28-O28	-20.6454
C3-C2-H2A	109.7598	C10-C5-C4-C23	142.7482	C22-C17-C28-H28A	98.454
C3-C2-H2B	109.7554	C6-C5-C4-C3	-125.2407	C22-C17-C28-H28B	-139.7443
H2A-C2-H2B	109.4983	C6-C5-C4-C24	113.2066	C18-C19-C21-C22	-4.5021
C4-C3-C2	110.1538	C6-C5-C4-C23	-5.5599	C18-C19-C21H21A	114.8883
C4-C3-O3	108.7773	H5-C5-C4-C3	127.5613	C18-C19-C21-H21B	-123.8968
C4-C3-C7q	109.4373	H5-C5-C4-C24	6.0086	C20-C19-C21-C22	-125.6818
C2-C3-O3	109.6102	H5-C5-C4-C23	-112.7578	C20-C19-C21-H21A	-6.2914
C2-C3-C7q	108.873	C10-C5-C6-C7	54.8171	C20-C19-C21-H21B	114.9235
O3-C3-C7q	109.98	C10-C5-C6-H6A	174.8338	H19-C19-C21-C22	114.7878
C10-C9-C8	114.827	C10-C5-C6-H6B	-65.1977	H19-C19-C21-H21A	-125.8219
C10-C9-C11	115.8286	C4-C5-C6-C7	-155.107	H19-C19-C21-H21B	-4.607
C10-C9-H9	102.5677	C4-C5-C6-H6A	-35.0903	C18-C19-C20-C29	-90.8522
C8-C9-C11	114.7904	C4-C5-C6-H6B	84.8782	C18-C19-C20-C30	90.2889
C8-C9-H9	104.2948	H5-C5-C6-C7	-52.3679	C21-C19-C20-C29	29.1597
C11-C9-H9	101.9165	H5-C5-C6-H6A	67.6488	C21-C19-C20-C30	-149.6992
C9-C8-C7	109.5112	H5-C5-C6-H6B	-172.3827	H19-C19-C20-C29	149.2378
C9-C8-C14	109.0493	C10-C1-C2-C3	-74.9536	H19-C19-C20-C30	-29.6212
C9-C8-C26	109.9994	C10-C1-C2-H2A	44.9518	C19-C21-C22-C17	-17.959
C7-C8-C14	109.9272	C10-C1-C2-H2B	165.1481	C19-C21-C22-H22A	-136.9484
C7-C8-C26	108.834	H1A-C1-C2-C3	165.2421	C19-C21-C22-H22B	101.0377
C14-C8-C26	109.5091	H1A-C1-C2-H2A	-74.8525	H21A-C21-C22-C17	-137.5646
C5-C6-C7	109.4637	H1A-C1-C2-H2B	45.3439	H21A-C21-C22-H22A	103.4461
C5-C6-H6A	109.4176	H1B-C1-C2-C3	44.8527	H21A-C21-C22-H22B	-18.5679
C5-C6-H6B	109.4123	H1B-C1-C2-H2A	164.7581	H21B-C21-C22-C17	101.6442
C7-C6-H6A	109.5154	H1B-C1-C2-H2B	-75.0455	H21B-C21-C22-H22A	-17.3452
C7-C6-H6B	109.5166	C5-C4-C3-C2	-36.6564	H21B-C21-C22-H22B	-139.3591
H6A-C6-H6B	109.5017	C5-C4-C3-O3	-156.8144	C19-C20-C29-H29A	-178.8625
C8-C7-C6	113.9925	C5-C4-C3-C7q	83.0074	C19-C20-C29-H29B	1.134
C8-C7-H7A	108.4355	C24-C4-C3-C2	84.6376	C30-C20-C29-H29A	-0.0019
C8-C7-H7B	108.4327	C24-C4-C3-O3	-35.5204	C30-C20-C29-H29B	179.9946
C6-C7-H7A	108.2093	C24-C4-C3-C7q	-155.6986	C19-C20-C30-H30A	-173.8931
C6-C7-H7B	108.2094	C23-C4-C3-C2	-158.2619	C19-C20-C30-H30B	-53.9327
H7A-C7-H7B	109.5034	C23-C4-C3-O3	81.58	C19-C20-C30-H30C	66.1435
C9-C11-C12	110.5418	C23-C4-C3-C7q	-38.5982	C29-C20-C30-H30A	7.2228
C9-C11-H11A	109.3054	C5-C4-C24-H24A	-153.6322	C29-C20-C30-H30B	127.1832
C9-C11-H11B	109.3078	C5-C4-C24-H24B	-33.6735	C29-C20-C30-H30C	-112.7406
C12-C11-H11A	109.0818	C5-C4-C24-H24C	86.4015	C3-O3-C7q-C6q	-24.2669
C12-C11-H11B	109.083	C3-C4-C24-H24A	81.27	C3-O3-C7q-C8q	156.6128

H11A-C11-H11B	109.5049	C3-C4-C24-H24B	-158.7713	C17-C28-O28-C31	-85.9536
C11-C12-C13	112.8457	C3-C4-C24-H24C	-38.6963	H28A-C28-O28-C31	152.9976
C11-C12-H12A	108.3442	C23-C4-C24-H24A	-34.2342	H28B-C28-O28-C31	35.0955
C11-C12-H12B	108.3468	C23-C4-C24-H24B	85.7246	C28-O28-C31-O31	-1.5846
C13-C12-H12A	108.8866	C23-C4-C24-H24C	-154.2004	C28-O28-C31-C32	178.5288
C13-C12-H12B	108.8799	C5-C4-C23-H23A	-77.8291	O28-C31-C32-H32A	-106.8738
H12A-C12-H12B	109.497	C5-C4-C23-H23B	42.14	O28-C31-C32-H32B	13.0787
C8-C14-C13	110.1942	C5-C4-C23-H23C	162.2132	O28-C31-C32-H32C	133.16
C8-C14-C15	108.8893	C3-C4-C23-H23A	46.7512	O31-C31-C32-H32A	73.2396
C8-C14-C27	109.5853	C3-C4-C23-H23B	166.7203	O31-C31-C32-H32B	-166.8079
C13-C14-C15	109.847	C3-C4-C23-H23C	-73.2065	O31-C31-C32-H32C	-46.7267
C13-C14-C27	108.7046	C24-C4-C23-H23A	163.7706	O3-C7q-C6q-C5q	-179.6512
C15-C14-C27	109.6091	C24-C4-C23-H23B	-76.2603	O3-C7q-C6q-Clq	-2.4686
C12-C13-C14	112.4984	C24-C4-C23-H23C	43.8129	C8q-C7q-C6q-C5q	-0.5367
C12-C13-C18	108.9574	C1-C2-C3-C4	63.1524	C8q-C7q-C6q-Clq	176.6459
C12-C13-H13	108.3252	C1-C2-C3-O3	-177.1937	O3-C7q-C8q-C8Aq	-179.5907
C14-C13-C18	113.4258	C1-C2-C3-C7q	-56.8532	O3-C7q-C8q-O8q	1.6726
C14-C13-H13	105.2414	H2A-C2-C3-C4	-56.6567	C6q-C7q-C8q-C8Aq	1.2711
C18-C13-H13	108.1363	H2A-C2-C3-O3	62.9972	C6q-C7q-C8q-O8q	-177.4656
C14-C15-C16	108.8321	H2A-C2-C3-C7q	-176.6623	C7q-C6q-C5q-C4Aq	0.0839
C14-C15-H15A	109.8301	H2B-C2-C3-C4	-177.0449	C7q-C6q-C5q-O5q	-178.8952
C14-C15-H15B	109.8244	H2B-C2-C3-O3	-57.391	Clq-C6q-C5q-C4Aq	-178.82
C16-C15-H15A	109.4175	H2B-C2-C3-C7q	62.9495	Clq-C6q-C5q-O5q	2.2009
C16-C15-H15B	109.4163	C4-C3-O3-C7q	165.9041	C6q-C5q-C4Aq-C8Aq	-0.3792
H15A-C15-H15B	109.5041	C2-C3-O3-C7q	45.41	C6q-C5q-C4Aq-C4q	-179.8049
C15-C16-C17	110.7122	C7q-C3-O3-C7q	-74.2543	O5q-C5q-C4Aq-C8Aq	178.5969
C15-C16-H16A	108.9997	C10-C9-C8-C7	52.7028	O5q-C5q-C4Aq-C4q	-0.8289
C15-C16-H16B	109.0112	C10-C9-C8-C14	173.0267	C7q-C8q-C8Aq-C4Aq	-1.5673
C17-C16-H16A	109.2985	C10-C9-C8-C26	-66.8641	C7q-C8q-C8AqN1q	178.73
C17-C16-H16B	109.3021	C11-C9-C8-C7	-169.3567	O8q-C8q-C8Aq-C4Aq	177.1694
H16A-C16-H16B	109.4998	C11-C9-C8-C14	-49.0328	O8q-C8q-C8Aq-N1q	-2.5333
C13-C18-C17	114.8087	C11-C9-C8-C26	71.0764	C5q-C4Aq-C8Aq-C8q	1.1102
C13-C18-C19	118.7389	H9-C9-C8-C7	-58.7228	C5q-C4Aq-C8Aq-N1q	-179.1835
C13-C18-H18	96.5463	H9-C9-C8-C14	61.6011	C4q-C4Aq-C8Aq-C8q	-179.461
C17-C18-C19	99.383	H9-C9-C8-C26	-178.2897	C4q-C4Aq-C8Aq-N1q	0.2454
C17-C18-H18	115.7691	C10-C9-C11-C12	128.6872	C5q-C4Aq-C4q-C3q	179.3845
C19-C18-H18	112.6794	C10-C9-C11-H11A	-111.2348	C5q-C4Aq-C4q-H4q	-0.6105
C16-C17-C18	111.0046	C10-C9-C11-H11B	8.606	C8Aq-C4Aq-C4q-C3q	-0.0404
C16-C17-C22	109.3311	C8-C9-C11-C12	-8.8224	C8Aq-C4Aq-C4q-H4q	179.9646
C16-C17-C28	108.8183	C8-C9-C11-H11A	111.2557	C8q-C8Aq-N1q-C2q	179.4654
C18-C17-C22	108.1828	C8-C9-C11-H11B	-128.9035	C4Aq-C8Aq-N1q-C2q	-0.2377
C18-C17-C28	109.1494	H9-C9-C11-C12	-120.8735	C4Aq-C4q-C3q-C2q	-0.1752
C22-C17-C28	110.3524	H9-C9-C11-H11A	-0.7954	C4Aq-C4q-C3q-H3q	179.8187
C18-C19-C21	108.8655	H9-C9-C11-H11B	119.0454	H4q-C4q-C3q-C2q	179.8199
C18-C19-C20	110.7809	C9-C8-C7-C6	2.5001	H4q-C4q-C3q-H3q	-0.1862
C18-C19-H19	109.0105	C9-C8-C7-H7A	123.0912	C4q-C3q-C2q-N1q	0.1831
C21-C19-C20	109.3874	C9-C8-C7-H7B	-118.0891	C4q-C3q-C2q-H2q	-179.8086
C21-C19-H19	109.838	C14-C8-C7-C6	-117.287	H3q-C3q-C2q-N1q	-179.8108

C20-C19-H19	108.9471	C14-C8-C7-H7A	3.3041	H3q-C3q-C2q-H2q	0.1975
C19-C21-C22	106.3633	C14-C8-C7-H7B	122.1239	C8Aq-N1q-C2q-C3q	0.0225
C19-C21-H21A	110.3992	C26-C8-C7-C6	122.7807	C8Aq-N1q-C2q-H2q	-179.9857

Table S4. Geometric parameters (bond length and angles) for hybrid **4** (Å, º).

Bond length, bond angles [Å, °]		Bond length, bond angles [Å, °]		Bond length, bond angles [Å, °]	
C10-C5	1.5519	C19-C21-C22	105.4848	C26-C8-C7-C6	124.043
C10-C1	1.5267	C19-C21-H21A	110.5377	C26-C8-C7-H7A	-115.3574
C10-C9	1.5518	C19-C21-H21B	110.5309	C26-C8-C7-H7B	3.4397
C10-C25	1.5343	C22-C21-H21A	110.3689	C9-C8-C14-C13	61.1186
C5-C4	1.5701	C22-C21-H21B	110.3682	C9-C8-C14-C15	-178.3907
C5-C6	1.5409	H21A-C21-H21B	109.4975	C9-C8-C14-C27	-58.5227
C5-H5	1.111	C17-C22-C21	105.1384	C7-C8-C14-C13	-178.8385
C1-C2	1.5221	C17-C22-H22A	110.544	C7-C8-C14--C15	-58.3478
C1-H1A	1.1111	C17-C22-H22B	110.5433	C7-C8-C14-C27	61.5202
C1-H1B	1.111	C21-C22-H22A	110.5312	C26-C8-C14-C13	-59.2217
C4-C3	1.5489	C21-C22-H22B	110.5261	C26-C8-C14-C15	61.2689
C4-C24	1.5274	H22A-C22-H22B	109.4982	C26-C8-C14-C27	-178.8631
C4-C23	1.5338	C19-C20-C29	121.5637	C9-C8-C26-H26A	-78.1371
C2-C3	1.5272	C19-C20-C30	119.7714	C9-C8-C26-H26B	41.8261
C2-H2A	1.111	C29-C20-C30	118.6535	C9-C8-C26-H26C	161.903
C2-H2B	1.111	C14-C27-H27A	109.4517	C7-C8-C26-H26A	161.8886
C3-O3	1.4318	C14-C27-H27B	109.4468	C7-C8-C26-H26B	-78.1482
C3-C7q	1.114	C14-C27-H27C	109.4521	C7-C8-C26-H26C	41.9287
C9-C8	1.5499	H27A-C27-H27B	109.4619	C14-C8-C26-H26A	41.6578
C9-C11	1.5396	H27A-C27-H27C	109.4594	C14-C8-C26-H26B	161.621
C9-H9	1.1109	H27B-C27-H27C	109.5554	C14-C8-C26-H26C	-78.3021
C8-C7	1.5548	C4-C24-H24A	109.4472	C5-C6-C7-C8	-54.9636
C8-C14	1.5618	C4-C24-H24B	109.4499	C5-C6-C7-H7A	-175.7018
C8-C26	1.5409	C4-C24-H24C	109.4476	C5-C6-C7-H7B	65.7822
C6-C7	1.5461	H24A-C24-H24B	109.4658	H6A-C6-C7-C8	-174.9064
C6-H6A	1.111	H24A-C24-H24C	109.4603	H6A-C6-C7-H7A	64.3554
C6-H6B	1.111	H24B-C24-H24C	109.5565	H6A-C6-C7-H7B	-54.1605
C7-H7A	1.1111	C4-C23-H23A	109.4478	H6B-C6-C7-C8	64.9792
C7-H7B	1.1109	C4-C23-H23B	109.4515	H6B-C6-C7-H7A	-55.759
C11-C12	1.5325	C4-C23-H23C	109.4468	H6B-C6-C7-H7B	-174.275
C11-H11A	1.111	H23A-C23-H23B	109.4663	C9-C11-C12-C13	56.0412
C11-H11B	1.1111	H23A-C23-H23C	109.4622	C9-C11-C12-H12A	176.7675
C12-C13	1.5485	H23B-C23-H23C	109.5527	C9-C11-C12-H12B	-64.6973
C12-H12A	1.111	C3-O3-C7q	127.9637	H11A-C11-C12-C13	-64.2217
C12-H12B	1.1109	C10-C25-H25A	109.4546	H11A-C11-C12-H12A	56.5046
C14-C13	1.5836	C10-C25-H25B	109.4509	H11A-C11-C12-H12B	175.0398
C14-C15	1.5412	C10-C25-H25C	109.4475	H11B-C11-C12-C13	176.2963
C14-C27	1.5373	H25A-C25-H25B	109.4672	H11B-C11-C12-H12A	-62.9774
C13-C18	1.5692	H25A-C25-H25C	109.4613	H11B-C11-C12-H12B	55.5578
C13-H13	1.111	H25B-C25-H25C	109.5457	C11-C12-C13-C14	-42.8308
C15-C16	1.5216	C8-C26-H26A	109.4474	C11-C12-C13-C18	-169.4812

C15-H15A	1.111
C15-H15B	1.111
C16-C17	1.5348
C16-H16A	1.111
C16-H16B	1.111
C18-C17	1.5519
C18-C19	1.5594
C18-H18	1.111
C17-C22	1.5288
C17-C28	1.5354
C19-C21	1.535
C19-C20	1.526
C19-H19	1.1147
C21-C22	1.5284
C21-H21A	1.1109
C21-H21B	1.111
C22-H22A	1.111
C22-H22B	1.111
C20-C29	1.3427
C20-C30	1.5065
C27-H27A	1.1111
C27-H27B	1.1111
C27-H27C	1.1111
C24-H24A	1.111
C24-H24B	1.1111
C24-H24C	1.1111
C23-H23A	1.1111
C23-H23B	1.1112
C23-H23C	1.1111
O3-C7q	1.3746
C25-H25A	1.111
C25-H25B	1.1111
C25-H25C	1.1112
C26-H26A	1.1111
C26-H26B	1.1111
C26-H26C	1.1111
C28-O28	1.4214
C28-H28A	1.111
C28-H28B	1.111
C29-H29A	1.111
C29-H29B	1.111
C30-H30A	1.1112
C30-H30B	1.1111
C30-H30C	1.1111
O28-C31	1.3586
C31-O31	1.2097
C31-C32	1.4283
C7q-C6q	1.3483

C8-C26-H26B	109.4535
C8-C26-H26C	109.4487
H26A-C26-H26B	109.462
H26A-C26-H26C	109.4616
H26B-C26-H26C	109.5541
C17-C28-O28	110.2464
C17-C28-H28A	110.8373
C17-C28-H28B	110.8366
O28-C28-H28A	107.6546
O28-C28-H28B	107.6625
H28A-C28-H28B	109.497
C20-C29-H29A	119.9998
C20-C29-H29B	120.0028
H29A-C29-H29B	119.9974
C20-C30-H30A	109.4514
C20-C30-H30B	109.4487
C20-C30-H30C	109.4475
H30A-C30-H30B	109.4622
H30A-C30-H30C	109.4626
H30B-C30-H30C	109.555
C28-O28-C31	121.5659
O28-C31-O31	120.0206
O28-C31-C32	119.7969
O31-C31-C32	120.1819
O3-C7q-C6q	121.5067
O3-C7q-C8q	119.0523
C6q-C7q-C8q	119.4355
C7q-C6q-C5q	121.1505
C7q-C6q-Clq	119.9703
C5q-C6q-Clq	118.879
C6q-C5q-C4Aq	120.0311
C6q-C5q-O5q	119.9092
C4Aq-C5q-O5q	120.0536
C7q-C8q-C8Aq	120.0403
C7q-C8q-O8q	120.1525
C8Aq-C8q-O8q	119.7958
C5q-C4Aq-C8Aq	119.5462
C5q-C4Aq-C4q	120.5314
C8Aq-C4Aq-C4q	119.9211
C8q-C8Aq-C4Aq	119.7861
C8q-C8Aq-N1q	120.8066
C4Aq-C8Aq-N1q	119.4071
C4Aq-C4q-C3q	120.6648
C4Aq-C4q-H4q	119.647
C3q-C4q-H4q	119.6882
C4q-C3q-C2q	119.5227
C4q-C3q-H3q	120.2488
C2q-C3q-H3q	120.2285

C11-C12-C13-H13	73.358
H12A-C12-C13-C14	-163.2953
H12A-C12-C13-C18	70.0543
H12A-C12-C13-H13	-47.1065
H12B-C12-C13-C14	77.6445
H12B-C12-C13-C18	-49.0059
H12B-C12-C13-H13	-166.1667
C8-C14-C13-C12	-15.7692
C8-C14-C13-C18	109.0137
C8-C14-C13-H13	-132.969
C15-C14-C13-C12	-135.6431
C15-C14-C13-C18	-10.8602
C15-C14-C13-H13	107.1571
C27-C14-C13-C12	104.3706
C27-C14-C13-C18	-130.8465
C27-C14-C13-H13	-12.8293
C8-C14-C15-C16	-169.4087
C8-C14-C15-H15A	-49.6866
C8-C14-C15-H15B	70.8712
C13-C14-C15-C16	-48.6088
C13-C14-C15-H15A	71.1133
C13-C14-C15-H15B	-168.3289
C27-C14-C15-C16	70.7991
C27-C14-C15-H15A	-169.4788
C27-C14-C15-H15B	-48.9211
C8-C14-C27-H27A	140.2211
C8-C14-C27-H27B	-99.8171
C8-C14-C27-H27C	20.2593
C13-C14-C27-H27A	19.6123
C13-C14-C27-H27B	139.574
C13-C14-C27-H27C	-100.3495
C15-C14-C27-H27A	-100.4575
C15-C14-C27-H27B	19.5042
C15-C14-C27-H27C	139.5807
C12-C13-C18-C17	178.5953
C12-C13-C18-C19	-66.7007
C12-C13-C18-H18	53.9723
C14-C13-C18-C17	52.3918
C14-C13-C18-C19	167.0959
C14-C13-C18-H18	-72.2312
H13-C13-C18-C17	-64.4465
H13-C13-C18-C19	50.2575
H13-C13-C18-H18	170.9304
C14-C15-C16-C17	73.6365
C14-C15-C16-H16A	-166.0561
C14-C15-C16-H16B	-46.6658
H15A-C15-C16-C17	-46.4033
H15A-C15-C16-H16A	73.904

C7q-C8q	1.4862
C32-C33	1.2094
C6q-C5q	1.4778
C6q-Clq	1.7164
C5q-C4Aq	1.4695
C5q-O5q	1.2094
C8q-C8Aq	1.4808
C8q-O8q	1.2103
C4Aq-C8Aq	1.3829
C4Aq-C4q	1.3839
C8Aq-N1q	1.3841
C4q-C3q	1.3843
C4q-H4q	1.1109
C3q-C2q	1.384
C3q-H3q	1.111
N1q-C2q	1.3856
C2q-H2q	1.1111
C33-H33	1.111
C5-C10-C1	109.8443
C5-C10-C9	109.2435
C5-C10-C25	109.3824
C1-C10-C9	109.3587
C1-C10-C25	109.1635
C9-C10-C25	109.8363
C10-C5-C4	120.3594
C10-C5-C6	114.5728
C10-C5-H5	99.3472
C4-C5-C6	117.9939
C4-C5-H5	94.9389
C6-C5-H5	102.6425
C10-C1-C2	108.0231
C10-C1-H1A	109.8827
C10-C1-H1B	109.8862
C2-C1-H1A	109.7618
C2-C1-H1B	109.7692
H1A-C1-H1B	109.4988
C5-C4-C3	114.6969
C5-C4-C24	108.3521
C5-C4-C23	109.9863
C3-C4-C24	108.7746
C3-C4-C23	106.4167
C24-C4-C23	108.4535
C1-C2-C3	108.4446
C1-C2-H2A	109.6547
C1-C2-H2B	109.6541
C3-C2-H2A	109.7861
C3-C2-H2B	109.7815
H2A-C2-H2B	109.5032

C8Aq-N1q-C2q	120.7734
C3q-C2q-N1q	119.7095
C3q-C2q-H2q	120.0894
N1q-C2q-H2q	120.2011
C31-C32-C33	179.9703
C32-C33-H33	180.002
C1-C10-C5-C4	-31.2987
C1-C10-C5-C6	118.696
C1-C10-C5-H5	-132.6914
C9-C10-C5-C4	-151.249
C9-C10-C5-C6	-1.2542
C9-C10-C5-H5	107.3584
C25-C10-C5-C4	88.4979
C25-C10-C5-C6	-121.5073
C25-C10-C5-H5	-12.8948
C5-C10-C1-C2	56.026
C5-C10-C1-H1A	175.7462
C5-C10-C1-H1B	-63.7051
C9-C10-C1-C2	175.9061
C9-C10-C1-H1A	-64.3737
C9-C10-C1-H1B	56.175
C25-C10-C1-C2	-63.9039
C25-C10-C1-H1A	55.8163
C25-C10-C1-H1B	176.3649
C5-C10-C9-C8	-53.4436
C5-C10-C9-C11	168.6302
C5-C10-C9-H9	59.1939
C1-C10-C9-C8	-173.6922
C1-C10-C9-C11	48.3816
C1-C10-C9-H9	-61.0547
C25-C10-C9-C8	66.5307
C25-C10-C9-C11	-71.3955
C25-C10-C9-H9	179.1682
C5-C10-C25-H25A	-166.3021
C5-C10-C25-H25B	-46.3297
C5-C10-C25-H25C	73.7347
C1-C10-C25-H25A	-46.0879
C1-C10-C25-H25B	73.8845
C1-C10-C25-H25C	-166.0511
C9-C10-C25-H25A	73.8081
C9-C10-C25-H25B	-166.2194
C9-C10-C25-H25C	-46.1551
C10-C5-C4-C3	21.7273
C10-C5-C4-C24	-99.994
C10-C5-C4-C23	141.6128
C6-C5-C4-C3	-127.2719
C6-C5-C4-C24	111.0068
C6-C5-C4-C23	-7.3863

H15A-C15-C16-H16B	-166.7057
H15B-C15-C16-C17	-166.3221
H15B-C15-C16-H16A	-46.0148
H15B-C15-C16-H16B	73.3755
C15-C16-C17-C18	-30.3856
C15-C16-C17-C22	-149.9764
C15-C16-C17-C28	89.5699
H16A-C16-C17-C18	-150.4839
H16A-C16-C17-C22	89.9253
H16A-C16-C17-C28	-30.5285
H16B-C16-C17-C18	89.7055
H16B-C16-C17-C22	-29.8853
H16B-C16-C17-C28	-150.3391
C13-C18-C17-C16	-29.9597
C13-C18-C17-C22	90.0144
C13-C18-C17-C28	-149.8458
C19-C18-C17-C16	-157.176
C19-C18-C17-C22	-37.2019
C19-C18-C17-C28	82.9379
H18-C18-C17-C16	82.0358
H18-C18-C17-C22	-157.9901
H18-C18-C17-C28	-37.8503
C13-C18-C19-C21	-87.9559
C13-C18-C19-C20	32.4731
C13-C18-C19-H19	152.324
C17-C18-C19-C21	35.2706
C17-C18-C19-C20	155.6996
C17-C18-C19-H19	-84.4494
H18-C18-C19-C21	160.0133
H18-C18-C19-C20	-79.5577
H18-C18-C19-H19	40.2932
C16-C17-C22-C21	147.241
C16-C17-C22-H22A	-93.4586
C16-C17-C22-H22B	27.947
C18-C17-C22-C21	26.2466
C18-C17-C22-H22A	145.547
C18-C17-C22-H22B	-93.0474
C28-C17-C22-C21	-93.1293
C28-C17-C22-H22A	26.1711
C28-C17-C22-H22B	147.5767
C16-C17-C28-O28	104.0829
C16-C17-C28-H28A	-136.8221
C16-C17-C28-H28B	-15.0215
C18-C17-C28-O28	-134.832
C18-C17-C28-H28A	-15.737
C18-C17-C28-H28B	106.0636
C22-C17-C28-O28	-15.7311
C22-C17-C28-H28A	103.3639

C4-C3-C2	110.1213	H5-C5-C4-C3	125.587	C22-C17-C28-H28B	-134.8356
C4-C3-O3	108.9214	H5-C5-C4-C24	3.8656	C18-C19-C21-C22	-21.4466
C4-C3-C7q	109.4089	H5-C5-C4-C23	-114.5275	C18-C19-C21-H21A	97.8594
C2-C3-O3	109.6204	C10-C5-C6-C7	53.5635	C18-C19-C21-H21B	-140.7483
C2-C3-C7q	108.8447	C10-C5-C6-H6A	173.5873	C20-C19-C21-C22	-142.7635
O3-C3-C7q	109.9143	C10-C5-C6-H6B	-66.4623	C20-C19-C21-H21A	-23.4574
C10-C9-C8	114.6543	C4-C5-C6-C7	-155.6904	C20-C19-C21-H21B	97.9348
C10-C9-C11	116.435	C4-C5-C6-H6A	-35.6666	H19-C19-C21-C22	97.7307
C10-C9-H9	102.4011	C4-C5-C6-H6B	84.2838	H19-C19-C21-H21A	-142.9632
C8-C9-C11	114.7319	H5-C5-C6-C7	-53.0308	H19-C19-C21-H21B	-21.571
C8-C9-H9	104.5999	H5-C5-C6-H6A	66.9929	C18-C19-C20-C29	-107.1659
C11-C9-H9	101.2686	H5-C5-C6-H6B	-173.0567	C18-C19-C20-C30	74.0814
C9-C8-C7	109.4745	C10-C1-C2-C3	-75.3589	C21-C19-C20-C29	12.7122
C9-C8-C14	109.0707	C10-C1-C2-H2A	44.5114	C21-C19-C20-C30	-166.0404
C9-C8-C26	109.9616	C10-C1-C2-H2B	164.7768	H19-C19-C20-C29	132.8679
C7-C8-C14	109.9386	H1A-C1-C2-C3	164.8447	H19-C19-C20-C30	-45.8847
C7-C8-C26	108.9372	H1A-C1-C2-H2A	-75.2851	C19-C21-C22--C17	-2.7297
C14-C8-C26	109.4474	H1A-C1-C2-H2B	44.9803	C19-C21-C22-H22A	-122.0386
C5-C6-C7	109.4453	H1B-C1-C2-C3	44.446	C19-C21-C22-H22B	116.5758
C5-C6-H6A	109.4047	H1B-C1-C2-H2A	164.3162	H21A-C21-C22-C17	-122.1476
C5-C6-H6B	109.4036	H1B-C1C2-H2B	-75.4183	H21A-C21-C22-H22A	118.5435
C7-C6-H6A	109.5368	C5-C4-C3-C2	-36.0429	H21A-C21-C22-H22B	-2.8422
C7-C6-H6B	109.5391	C5-C4-C3-O3	-156.2833	H21B-C21-C22-C17	116.6799
H6A-C6-H6B	109.4977	C5-C4-C3-C7q	83.5484	H21B-C21-C22-H22A	-2.629
C8-C7-C6	114.1072	C24-C4-C3-C2	85.4479	H21B-C21-C22-H22B	-124.0146
C8-C7-H7A	108.4166	C24-C4-C3-O3	-34.7925	C19-C20-C29-H29A	-178.7638
C8-C7-H7B	108.423	C24-C4-C3-C7q	-154.9608	C19-C20-C29-H29B	1.2288
C6-C7-H7A	108.168	C23-C4-C3-C2	-157.8925	C30-C20-C29-H29A	0.0024
C6-C7-H7B	108.1673	C23-C4-C3-O3	81.8671	C30-C20-C29-H29B	179.9949
H7A-C7-H7B	109.4979	C23-C4-C3-C7q	-38.3013	C19-C20-C30-H30A	-156.0369
C9-C11-C12	110.8928	C5-C4-C24-H24A	-152.7057	C19-C20-C30-H30B	-36.074
C9-C11-H11A	109.2058	C5-C4-C24-H24B	-32.7401	C19-C20-C30-H30C	84.0003
C9-C11-H11B	109.2015	C5-C4-C24-H24C	87.3368	C29-C20-C30-H30A	25.1742
C12-C11-H11A	109.0132	C3-C4-C24-H24A	82.0045	C29-C20-C30-H30B	145.1372
C12-C11-H11B	109.0094	C3-C4-C24-H24B	-158.0299	C29-C20-C30-H30C	-94.7886
H11A-C11-H11B	109.5001	C3-C4-C24-H24C	-37.953	C3-O3-C7q-C6q	-24.2329
C11-C12-C13	113.6199	C23-C4-C24-H24A	-33.3437	C3-O3-C7q-C8q	156.6286
C11-C12-H12A	108.182	C23-C4-C24-H24B	86.6219	C17-C28-O28-C31	-90.3419
C11-C12-H12B	108.1866	C23-C4-C24-H24C	-153.3012	H28A-C28-O28-C31	148.6424
C13-C12-H12A	108.647	C5-C4-C23-H23A	-78.3626	H28B-C28-O28-C31	30.6779
C13-C12-H12B	108.654	C5-C4-C23-H23B	41.6051	C28-O28-C31-O31	1.8067
H12A-C12-H12B	109.4986	C5-C4-C23-H23C	161.6778	C28-O28-C31-C32	-177.9194
C8-C14-C13	110.3062	C3-C4-C23-H23A	46.4328	O28-C31-O31-C32	-179.7251
C8-C14-C15	108.7796	C3-C4-C23-H23B	166.4004	O3-C7q-C6q-C5q	-179.6785
C8-C14-C27	109.5479	C3-C4-C23-H23C	-73.5268	O3-C7q-C6q-Clq	0.1636
C13-C14-C15	109.8043	C24-C4-C23-H23A	163.3068	C8q-C7q-C6q-C5q	-0.5432
C13-C14-C27	108.7223	C24-C4-C23-H23B	-76.7256	C8q-C7q-C6q-Clq	179.2989
C15-C14-C27	109.6698	C24-C4-C23-H23C	43.3472	O3-C7q-C8q-C8Aq	179.8674

C12-C13-C14	112.308	C1-C2-C3-C4	63.3206	O3-C7q-C8q-O8q	1.0999
C12-C13-C18	109.6678	C1-C2-C3-O3	-176.8618	C6q-C7q-C8q-C8Aq	0.7108
C12-C13-H13	107.6095	C1-C2-C3-C7q	-56.6128	C6q-C7q-C8q-O8q	-178.0567
C14-C13-C18	113.0964	H2A-C2-C3-C4	-56.4674	C7q-C6q-C5q-C4Aq	0.6238
C14-C13-H13	105.9222	H2A-C2-C3-O3	63.3502	C7q-C6q-C5qO5q	-178.4775
C18-C13-H13	107.9324	H2A-C2-C3-C7q	-176.4009	Clq-C6q-C5q-C4Aq	-179.22
C14-C15-C16	108.7783	H2B-C2-C3-C4	-176.8946	Clq-C6q-C5q-O5q	1.6787
C14-C15-H15A	109.8933	H2B-C2-C3-O3	-57.077	C6q-C5q-C4Aq-C8Aq	-0.875
C14-C15-H15B	109.8959	H2B-C2-C3-C7q	63.1719	C6q-C5q-C4Aq-C4q	179.5392
C16-C15-H15A	109.3816	C4-C3-O3-C7q	166.2645	O5q-C5q-C4Aq-C8Aq	178.225
C16-C15-H15B	109.3787	C2-C3-O3-C7q	45.7155	O5q-C5q-C4Aq-C4q	-1.3608
H15A-C15-H15B	109.4957	C7q-C3-O3-C7q	-73.8798	C7q-C8q-C8Aq-C4Aq	-0.9733
C15-C16-C17	110.8629	C10-C9-C8-C7	52.0317	C7q-C8q-C8Aq-N1q	179.2182
C15-C16-H16A	108.9425	C10-C9-C8-C14	172.3604	O8q-C8q-C8Aq-C4Aq	177.7986
C15-C16-H16B	108.9373	C10-C9-C8-C26	-67.6159	O8q-C8q-C8Aq-N1q	-2.0099
C17-C16-H16A	109.2935	C11-C9-C8-C7	-169.3153	C5q-C4Aq-C8Aq-C8q	1.0449
C17-C16-H16B	109.2921	C11-C9-C8-C14	-48.9866	C5q-C4Aq-C8Aq-N1q	-179.1438
H16A-C16-H16B	109.4938	C11-C9-C8-C26	71.0371	C4q-C4Aq-C8Aq-C8q	-179.3667
C13-C18-C17	114.0791	H9-C9-C8-C7	-59.298	C4q-C4Aq-C8Aq-N1q	0.4445
C13-C18-C19	119.6389	H9-C9-C8-C14	61.0306	C5q-C4Aq-C4q-C3q	179.3553
C13-C18-H18	96.2872	H9-C9-C8-C26	-178.9457	C5q-C4Aq-C4q-H4q	-0.6441
C17-C18-C19	97.4622	C10-C9-C11-C12	129.4968	C8Aq-C4Aq-C4q-C3q	-0.229
C17-C18-H18	118.0949	C10-C9-C11-H11A	-110.3549	C8Aq-C4Aq-C4q-H4q	179.7717
C19-C18-H18	112.741	C10-C9-C11-H11B	9.356	C8q-C8Aq-N1q-C2q	179.3955
C16-C17-C18	110.8614	C8-C9-C11-C12	-8.3971	C4Aq-C8Aq-N1q-C2q	-0.4137
C16-C17-C22	109.2147	C8-C9-C11-H11A	111.7511	C4Aq-C4q-C3q-C2q	-0.0251
C16-C17-C28	108.9102	C8-C9-C11-H11B	-128.5379	C4Aq-C4q-C3q-H3q	179.9826
C18-C17-C22	108.5739	H9-C9-C11-C12	-120.4065	H4q-C4q-C3q-C2q	179.9742
C18-C17-C28	109.0262	H9-C9-C11-H11A	-0.2582	H4q-C4q-C3q-H3q	-0.018
C22-C17-C28	110.25	H9-C9-C11-H11B	119.4528	C4q-C3q-C2q-N1q	0.0592
C18-C19-C21	108.5962	C9-C8-C7-C6	3.7678	C4q-C3q-C2q-H2q	-179.9438
C18-C19-C20	110.9618	C9-C8-C7-H7A	124.3674	H3q-C3q-C2q-N1q	-179.9485
C18-C19-H19	109.0252	C9-C8-C7-H7B	-116.8355	H3q-C3q-C2q-H2q	0.0485
C21-C19-C20	109.5224	C14-C8-C7-C6	-116.0298	C8Aq-N1q-C2q-C3q	0.1616
C21-C19-H19	109.8925	C14-C8-C7-H7A	4.5698	C8Aq-N1q-C2q-H2q	-179.8354
C20-C19-H19	108.832	C14-C8-C7-H7B	123.3669		