Supplementary Information

Self-assembled rosette nanotubes from tetra guanine-cytosine modules

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Self-assembly

Stock solution of **4a** was prepared in water at a concentration of 0.25 mg/mL and was aged for 1 day. For self-assembly study in methanol, **4a** was prepared in methanol at a concentration of 0.1 mg/mL and was aged for 14 days. At these concentrations, the compound was not fully dissolved in both solvents and existed as suspensions though sonication and heating were used to aid the solubility. Aliquots of the supernatant of these stock solutions were used for microscopy.

Scanning electron microscopy (SEM) imaging

The SEM samples were prepared by floating a carbon-coated 400-mesh copper grid (Electron Microscopy Sciences) on a droplet of the **4a** solution for 10 s. The grid was blotted using filter paper. The RNT-coated grid was then air-dried and heated on a hotplate (100 °C) for 15 min before imaging to remove any residual solvents. All SEM images were obtained without negative staining (unless indicated otherwise), at accelerating voltage of 30 kV and a working distance of 7.0 mm on a high-resolution Hitachi S-4800 cold field emission SEM. SEM was used to image the **4a** and But-TBL modules on the same carbon-coated TEM grid. This was done by first casting a diluted But-TBL RNT solution (0.0125 mg/mL). The excess solution was blotted and an aliquot of the **4a** solution in water was then deposited on the dried grid. The excess solution was then blotted and dried prior to SEM imaging.

Transmission electron microscopy (TEM) imaging

TEM imaging was performed on a JEOL 2200 FS TEM – 200kV Schottky field emission instrument equipped with an in-column omega filter. An aliquot (0.02 mL) of **4a** stock solution in water was deposited on a 400-mesh carbon coated grid (Electron Microscopy Sciences), then blotted after 10 s using filter paper. The samples were negatively stained with either 2% uranyl acetate. Uranyl acetate solutions were prepared by dissolving uranyl acetate crystals in MeOH or in dH_2O by sonicating for 10 min. The stains were then filtered through a 0.25 μm Whatmann filter membrane and stored in the dark at room temperature for subsequent uses. The TEM grid was air-dried before imaging and heated on a hotplate (100 °C) for 15 min prior to imaging to remove any residual solvents.

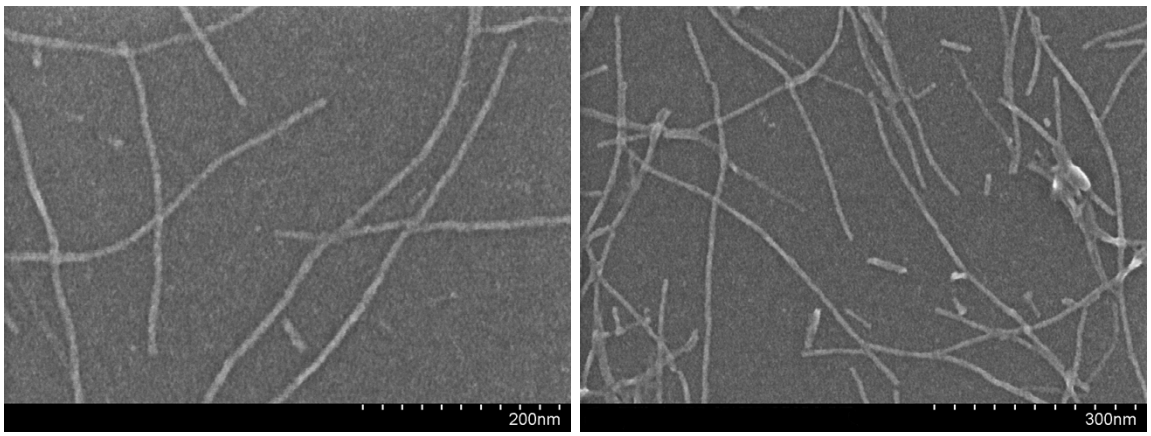

Figure S1: SEM images of **4a** in water

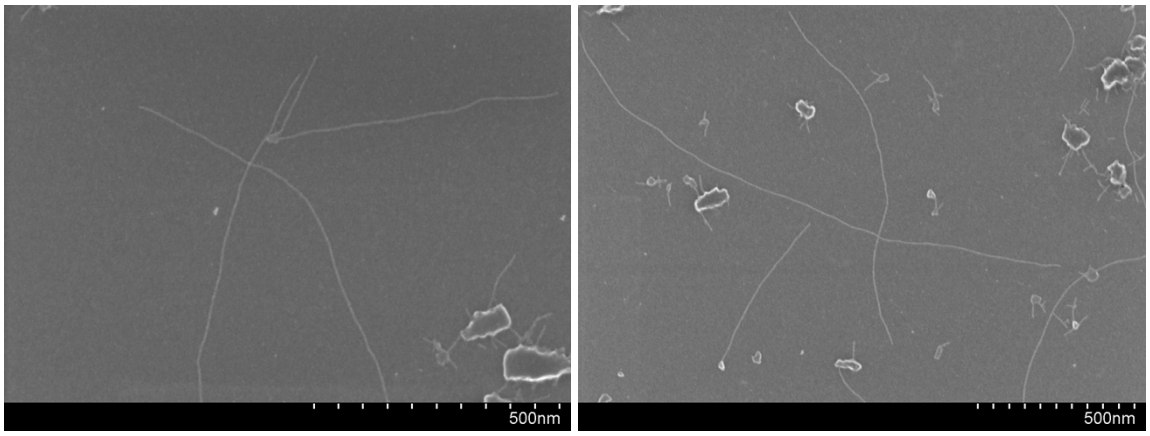

Figure S2: SEM images of **4a** in MeOH

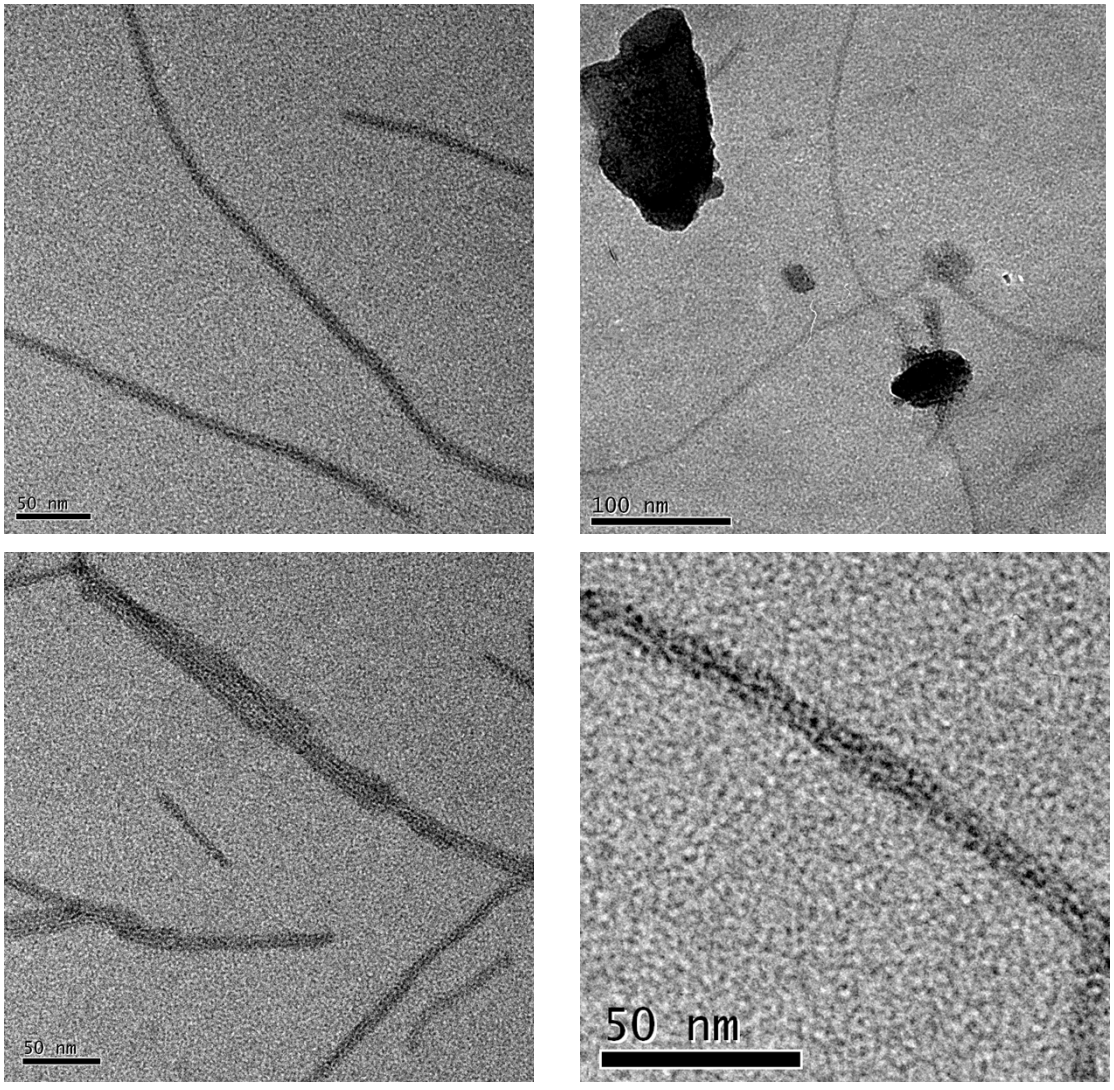

Figure S3: TEM images of **4a** in water

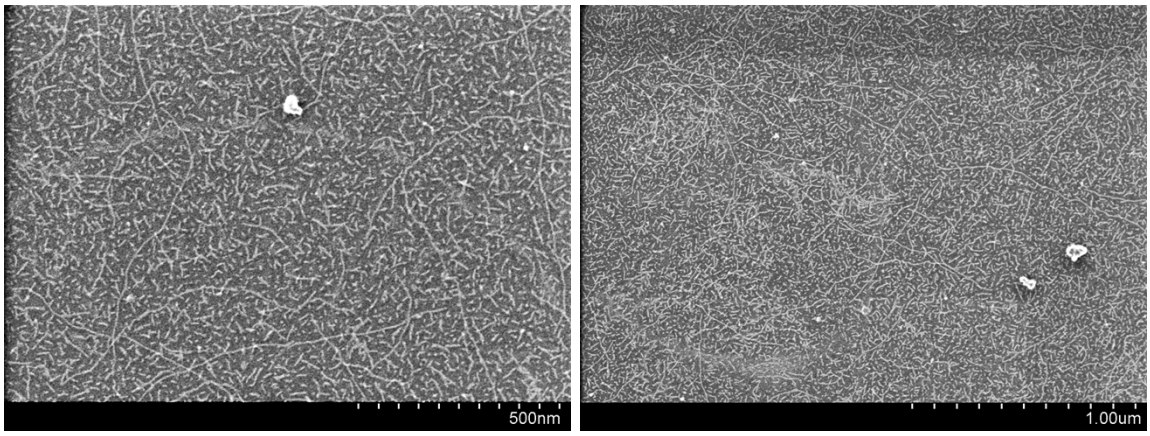

Figure S4: SEM images of **4b** in water

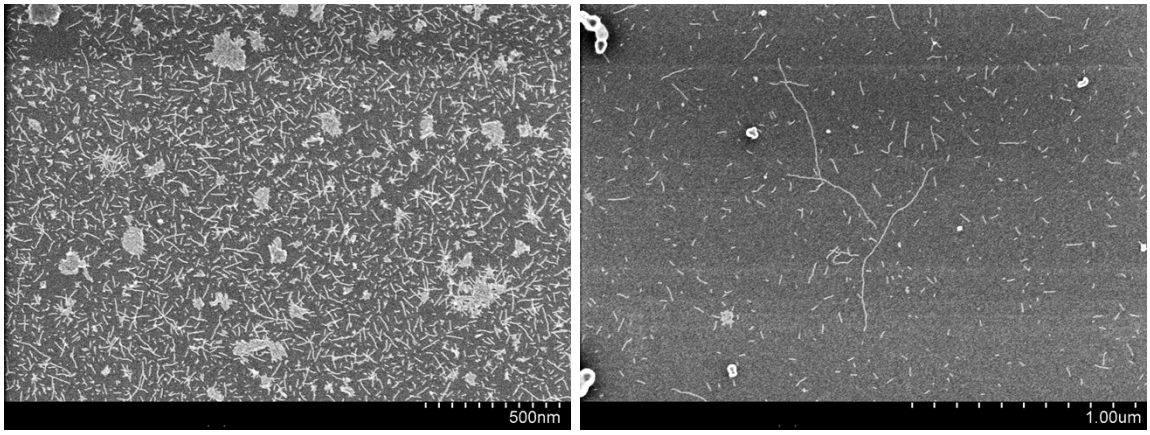

Figure S5: SEM images of **4c** in water

Molecular modeling study

The module conformations were generated by using Macromodel 8.6.[S1] The geometries were optimized in GB/SA water model with OPLS2001 force field parameters. [S1, S2] Based on the experimental observations suggesting that **4a** forms the self-assembled nanotube with the diameter of 3.2 ± 0.1 nm (TEM measurements), we explored the possible supramolecular structures of **4a** based on the molecular modeling studies. During the geometry optimization, the G∧C units for all conformations were kept fixed to be planar and all G∧C units were kept fixed such that they have either the syn-syn-syn (SSS) or the syn-anti-syn (SAS) intramolecular π-π stackings, respectively. The conformational restraint of G∧C units in the present modeling study is based on the assumption that the **4a** module will have the favorable intramolecular π-π interaction as we have seen in the twin G∧C system. [S3] The outer diameters (including van der Waals size of each atom taken from the OPLS2001 force field parameters) of the models were measured to be 3.1 nm. The conformations (SSS and SAS) can have complete complementary hydrogen bond network, favorable intermolecular π- π stacking, and the diameters were consistent with the TEM measurements. RNTs composed of 1-7 quad-rosette rings were built based on the SSS and SAS conformations, as shown in Figure S6. The stacking distance and staggered angle between rosette rings were adopted from the previous modeling study for the twin G^C system. [S3] The free energy *F* of self-assembly module or RNT can be defined as the sum of its internal energy and solvation free energy. The association free energy Δ*F(N)* of the RNT composed of N quad-rosette rings is the difference between the free energy of the RNT composed of N quad-rosette rings and the free energy of isolated self-assembly module multiplied by 6N. We obtained the internal energy based on the Molecular

Mechanics calculations using Macromodel 8.6 with the OPLS2001 force field parameters, and determined the solvation free energy in aqueous environment using the statistical mechanical theory of molecular liquid (3D-RISM theory). [S4, S5] In the 3D-RISM calculation, the self-assembling module and the RNT were modeled by the OPLS2001 force field to be consistent with the internal energy calculation, and the solvent environment was described by SPC/E water model[S6] and the chloride counter ion.[S7] As a result, we obtained the association free energies, which clearly showed that the self-assembly processes of SSS and SAS conformations in the aqueous environment are thermodynamically favorable. The present modeling procedure has been used in previous studies for the self-assembly process of organic nanotubes (S3, S8 and S9).

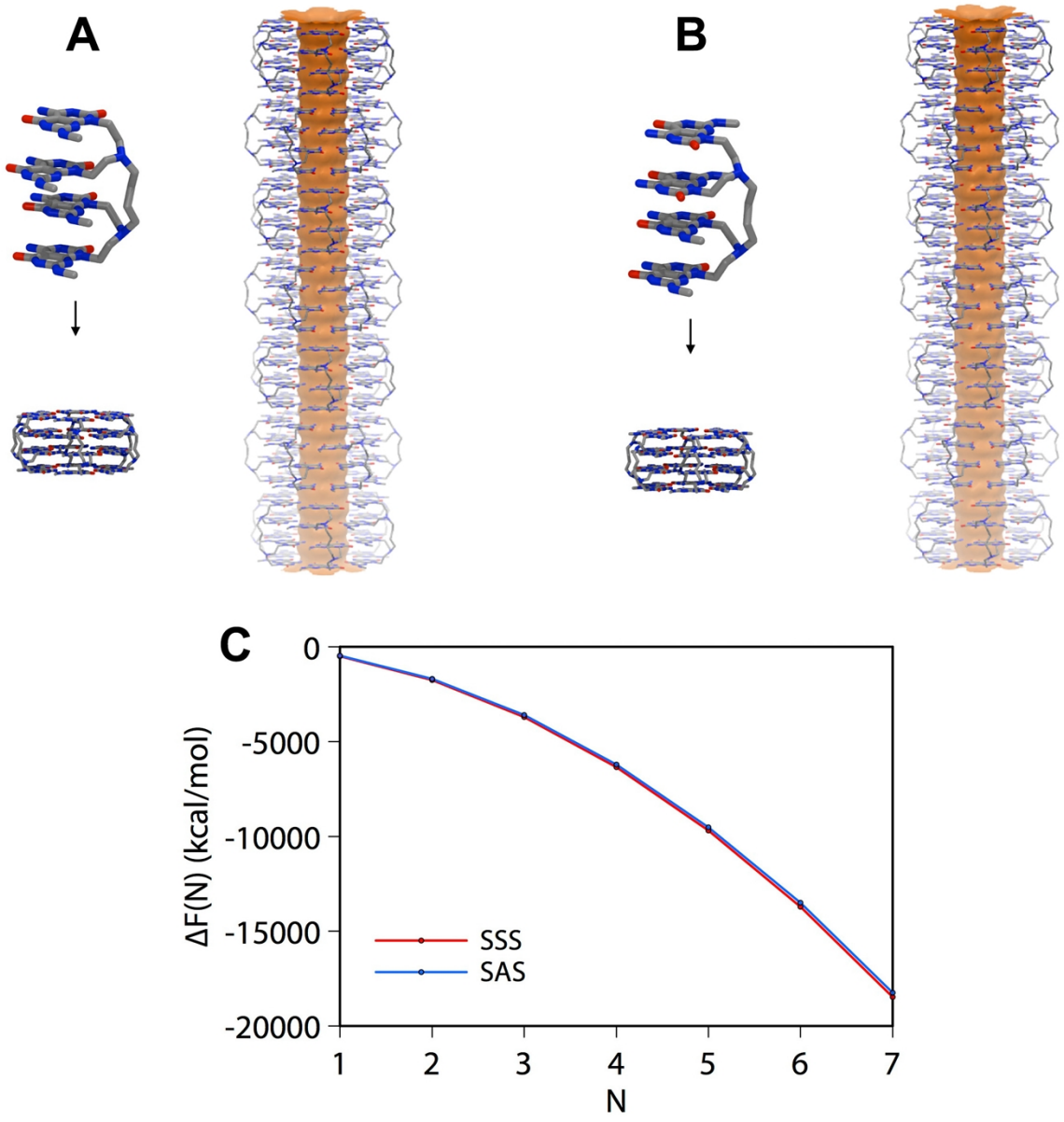

Figure S6: SSS (A) and SAS (B)conformations and resulting RNTs and association free energy as a function of number of quad rosette rings (C)

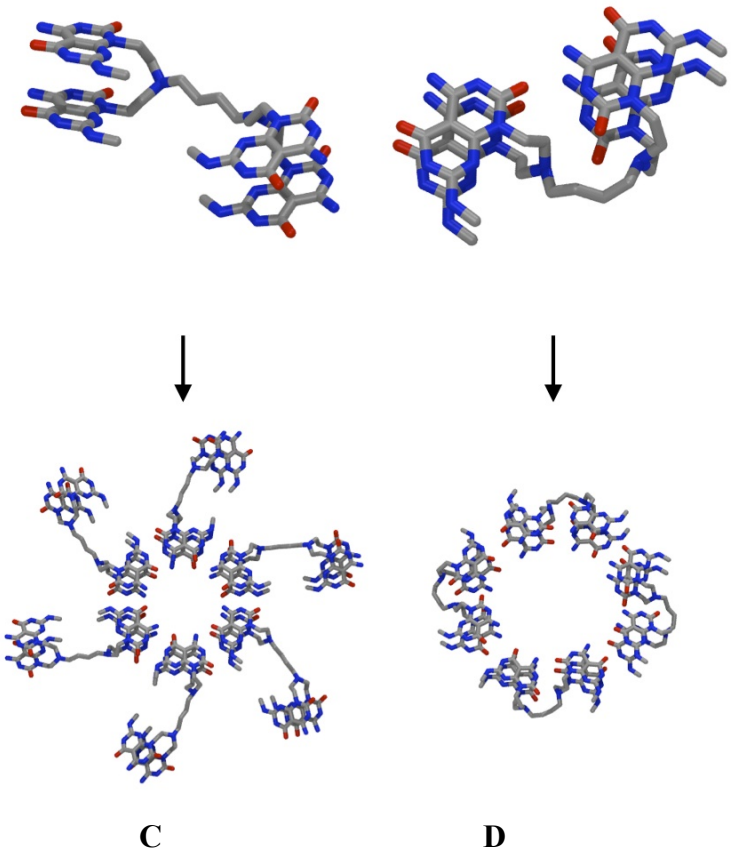

Figure S7: Two additional conformations (C and D) examined using Macromodel 8.6

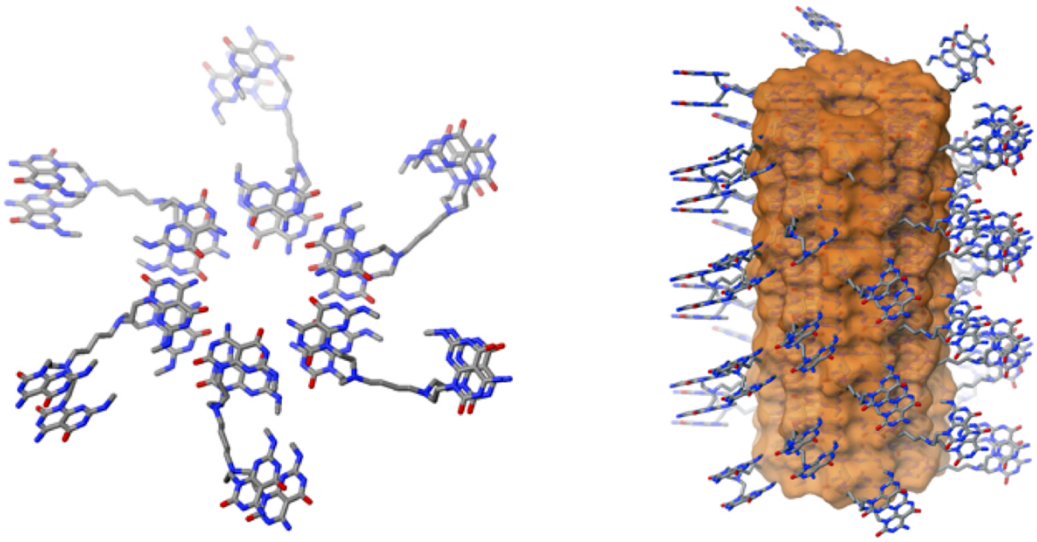

Figure S8: Rosette and nanotube of 5.1 nm constructed using conformation C

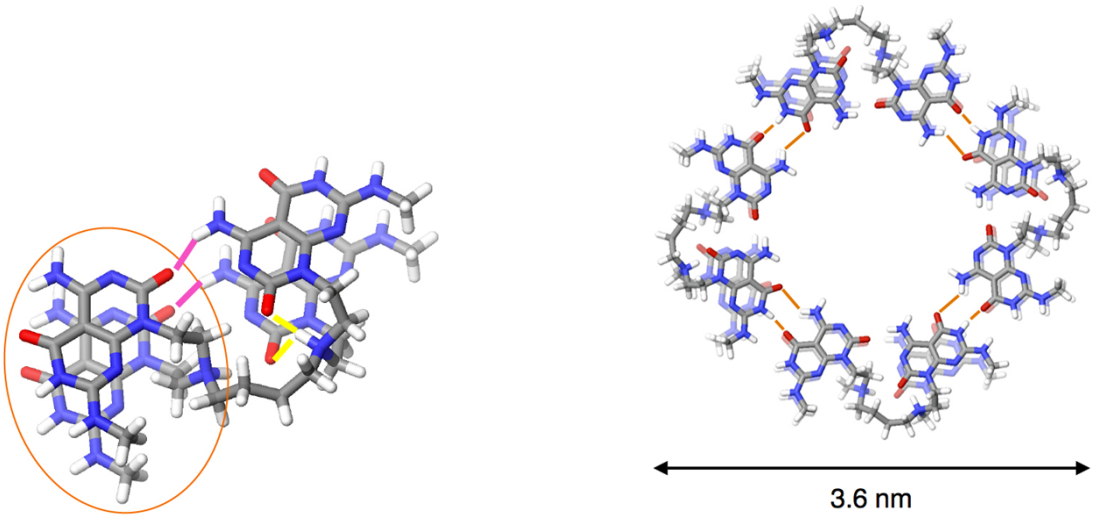

Figure S9: H-bonding interactions for single molecule and rosette constructed using conformation D

XYZ coordinates of SSS and SAS and their rosette rings

SSS

O	3.43690	-9.41710	7.00000
O	-1.43710	-5.33110	7.00000
N	1.13190	-9.43310	7.00000
N	2.40490	-7.42210	7.00000
N	-2.46710	-7.42210	7.00000
N	-3.51610	-9.48410	7.00000
N	1.46790	-5.36410	7.00000
N	-1.18310	-9.34610	7.00000
C	-2.31910	-8.78810	7.00000
C	-1.29710	-6.56110	7.00000
C	-0.04510	-7.33710	7.00000
C	-0.06510	-8.71210	7.00000
C	2.38090	-8.78410	7.00000
C	1.27090	-6.69510	7.00000
C	-3.66410	-10.93110	7.00000
H	-3.38110	-6.99310	7.00000
H	-4.38310	-8.95710	7.00000
H	2.40390	-4.97910	7.00000
H	0.67390	-4.73110	7.00000
H	-4.71610	-11.21710	7.00000
H	-3.19110	-11.36410	6.11800
H	-3.19110	-11.36410	7.88200
H	0.50920	-11.22250	6.20500
C	1.16490	-10.93110	7.00000
H	2.17510	-11.30920	6.93090
O	3.43690	-9.41710	11.00000
O	-1.43710	-5.33110	11.00000
N	1.13190	-9.43310	11.00000
N	2.40490	-7.42210	11.00000
N	-2.46710	-7.42210	11.00000
N	-3.51610	-9.48410	11.00000
N	1.46790	-5.36410	11.00000
N	-1.18310	-9.34610	11.00000
C	-2.31910	-8.78810	11.00000
C	-1.29710	-6.56110	11.00000
C	-0.04510	-7.33710	11.00000

C	-0.06510	-8.71210	11.00000
C	2.38090	-8.78410	11.00000
C	1.27090	-6.69510	11.00000
C	-3.66410	-10.93110	11.00000
H	-3.38110	-6.99310	11.00000
H	-4.38310	-8.95710	11.00000
H	2.40390	-4.97910	11.00000
H	0.67390	-4.73110	11.00000
H	-4.71610	-11.21710	11.00000
H	-3.19110	-11.36410	10.11800
H	-3.19110	-11.36410	11.88200
H	1.67490	-11.18140	11.93320
H	0.18270	-11.37680	11.14690
C	1.16490	-10.93110	11.00000
C	1.96620	-11.75700	9.80330
H	2.67690	-11.10440	9.29300
N	1.14050	-12.53650	8.75110
H	2.59560	-12.49560	10.30160
C	0.31970	-11.55810	8.08840
H	-0.08190	-10.82620	8.78760
H	-0.55390	-12.06950	7.67770
H	0.51240	-13.05270	9.35120
O	3.46800	-9.46400	0.00000
O	-1.40600	-5.37800	0.00000
N	1.16300	-9.48000	0.00000
N	2.43600	-7.46900	0.00000
N	-2.43600	-7.46900	0.00000
N	-3.48500	-9.53100	0.00000
N	1.49900	-5.41100	0.00000
N	-1.15200	-9.39300	0.00000
C	-2.28800	-8.83500	0.00000
C	-1.26600	-6.60800	0.00000
C	-0.01400	-7.38400	0.00000
C	-0.03400	-8.75900	0.00000
C	2.41200	-8.83100	0.00000
C	1.30200	-6.74200	0.00000
C	-3.63300	-10.97800	0.00000
H	-3.35000	-7.04000	0.00000
H	-4.35200	-9.00400	0.00000
H	2.43500	-5.02600	0.00000

H	0.70500	-4.77800	0.00000
H	-4.68500	-11.26400	0.00000
H	-3.16000	-11.41100	-0.88200
H	-3.16000	-11.41100	0.88200
H	0.62950	-11.22890	-0.89850
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H	2.17440	-11.39480	-0.24200
O	3.46800	-9.46400	4.00000
O	-1.40600	-5.37800	4.00000
N	1.16300	-9.48000	4.00000
N	2.43600	-7.46900	4.00000
N	-2.43600	-7.46900	4.00000
N	-3.48500	-9.53100	4.00000
N	1.49900	-5.41100	4.00000
N	-1.15200	-9.39300	4.00000
C	-2.28800	-8.83500	4.00000
C	-1.26600	-6.60800	4.00000
C	-0.01400	-7.38400	4.00000
C	-0.03400	-8.75900	4.00000
C	2.41200	-8.83100	4.00000
C	1.30200	-6.74200	4.00000
C	-3.63300	-10.97800	4.00000
H	-3.35000	-7.04000	4.00000
H	-4.35200	-9.00400	4.00000
H	2.43500	-5.02600	4.00000
H	0.70500	-4.77800	4.00000
H	-4.68500	-11.26400	4.00000
H	-3.16000	-11.41100	3.11800
H	-3.16000	-11.41100	4.88200
H	1.82750	-11.27470	4.80790
H	0.19690	-11.39620	4.00670
C	1.19600	-10.97800	4.00000
C	2.13910	-11.53210	2.92970
H	2.48350	-10.79440	2.20540
N	1.44690	-12.58200	2.25820
H	3.05540	-11.94340	3.36350
C	0.52880	-11.88700	1.21580
H	-0.24870	-11.31050	1.71790
H	-0.00970	-12.69860	0.72520
H	2.15890	-12.99960	1.67040

C	1.03540	-13.73890	3.24440
H	0.13800	-14.17850	2.80620
H	1.79860	-14.50410	3.09150
C	1.70250	-13.64690	7.78370
H	1.07840	-14.51980	7.98030
H	2.66970	-13.92100	8.20980
C	1.91820	-13.61470	6.11100
H	2.46120	-14.54760	5.94760
H	2.70960	-12.91980	5.83790
C	0.78900	-13.68560	4.91310
H	0.33700	-14.66130	5.10020
H	-0.05490	-13.04980	5.16480

SSS rosette ring

O	3.43690	-9.16738	7.00000
O	-1.43710	-5.08138	7.00000
N	1.13190	-9.18338	7.00000
N	2.40490	-7.17238	7.00000
N	-2.46710	-7.17238	7.00000
N	-3.51610	-9.23438	7.00000
N	1.46790	-5.11438	7.00000
N	-1.18310	-9.09638	7.00000
C	-2.31910	-8.53838	7.00000
C	-1.29710	-6.31138	7.00000
C	-0.04510	-7.08738	7.00000
C	-0.06510	-8.46238	7.00000
C	2.38090	-8.53438	7.00000
C	1.27090	-6.44538	7.00000
C	-3.66410	-10.68138	7.00000
H	-3.38110	-6.74338	7.00000
H	-4.38310	-8.70738	7.00000
H	2.40390	-4.72938	7.00000
H	0.67390	-4.48138	7.00000
H	-4.71610	-10.96738	7.00000
H	-3.19110	-11.11438	6.11800
H	-3.19110	-11.11438	7.88200
H	0.50920	-10.97278	6.20500
C	1.16490	-10.68138	7.00000

H	2.17510	-11.05948	6.93090
O	3.43690	-9.16738	11.00000
O	-1.43710	-5.08138	11.00000
N	1.13190	-9.18338	11.00000
N	2.40490	-7.17238	11.00000
N	-2.46710	-7.17238	11.00000
N	-3.51610	-9.23438	11.00000
N	1.46790	-5.11438	11.00000
N	-1.18310	-9.09638	11.00000
C	-2.31910	-8.53838	11.00000
C	-1.29710	-6.31138	11.00000
C	-0.04510	-7.08738	11.00000
C	-0.06510	-8.46238	11.00000
C	2.38090	-8.53438	11.00000
C	1.27090	-6.44538	11.00000
C	-3.66410	-10.68138	11.00000
H	-3.38110	-6.74338	11.00000
H	-4.38310	-8.70738	11.00000
H	2.40390	-4.72938	11.00000
H	0.67390	-4.48138	11.00000
H	-4.71610	-10.96738	11.00000
H	-3.19110	-11.11438	10.11800
H	-3.19110	-11.11438	11.88200
H	1.67490	-10.93168	11.93320
H	0.18270	-11.12708	11.14690
C	1.16490	-10.68138	11.00000
C	1.96620	-11.50728	9.80330
H	2.67690	-10.85468	9.29300
N	1.14050	-12.28678	8.75110
H	2.59560	-12.24588	10.30160
C	0.31970	-11.30838	8.08840
H	-0.08190	-10.57648	8.78760
H	-0.55390	-11.81978	7.67770
H	0.51240	-12.80298	9.35120
O	3.46800	-9.21428	0.00000
O	-1.40600	-5.12828	0.00000
N	1.16300	-9.23028	0.00000
N	2.43600	-7.21928	0.00000
N	-2.43600	-7.21928	0.00000
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N	1.49900	-5.16128	0.00000
N	-1.15200	-9.14328	0.00000
C	-2.28800	-8.58528	0.00000
C	-1.26600	-6.35828	0.00000
C	-0.01400	-7.13428	0.00000
C	-0.03400	-8.50928	0.00000
C	2.41200	-8.58128	0.00000
C	1.30200	-6.49228	0.00000
C	-3.63300	-10.72828	0.00000
H	-3.35000	-6.79028	0.00000
H	-4.35200	-8.75428	0.00000
H	2.43500	-4.77628	0.00000
H	0.70500	-4.52828	0.00000
H	-4.68500	-11.01428	0.00000
H	-3.16000	-11.16128	-0.88200
H	-3.16000	-11.16128	0.88200
H	0.62950	-10.97918	-0.89850
C	1.19600	-10.72828	0.00000
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O	-1.40600	-5.12828	4.00000
N	1.16300	-9.23028	4.00000
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N	-2.43600	-7.21928	4.00000
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C	-0.01400	-7.13428	4.00000
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C	1.30200	-6.49228	4.00000
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H	-3.35000	-6.79028	4.00000
H	-4.35200	-8.75428	4.00000
H	2.43500	-4.77628	4.00000
H	0.70500	-4.52828	4.00000
H	-4.68500	-11.01428	4.00000
H	-3.16000	-11.16128	3.11800

H	-3.16000	-11.16128	4.88200
H	1.82750	-11.02498	4.80790
H	0.19690	-11.14648	4.00670
C	1.19600	-10.72828	4.00000
C	2.13910	-11.28238	2.92970
H	2.48350	-10.54468	2.20540
N	1.44690	-12.33228	2.25820
H	3.05540	-11.69368	3.36350
C	0.52880	-11.63728	1.21580
H	-0.24870	-11.06078	1.71790
H	-0.00970	-12.44888	0.72520
H	2.15890	-12.74988	1.67040
C	1.03540	-13.48918	3.24440
H	0.13800	-13.92878	2.80620
H	1.79860	-14.25438	3.09150
C	1.70250	-13.39718	7.78370
H	1.07840	-14.27008	7.98030
H	2.66970	-13.67128	8.20980
C	1.91820	-13.36498	6.11100
H	2.46120	-14.29788	5.94760
H	2.70960	-12.67008	5.83790
C	0.78900	-13.43588	4.91310
H	0.33700	-14.41158	5.10020
H	-0.05490	-12.80008	5.16480
O	-6.22073	-7.56013	7.00000
O	-5.11915	-1.29612	7.00000
N	-7.38709	-5.57194	7.00000
N	-5.00901	-5.66889	7.00000
N	-7.44501	-1.44962	7.00000
N	-9.75525	-1.57216	7.00000
N	-3.69523	-3.82843	7.00000
N	-8.46924	-3.52359	7.00000
C	-8.55400	-2.26079	7.00000
C	-6.11436	-2.03237	7.00000
C	-6.16040	-3.50463	7.00000
C	-7.36118	-4.17481	7.00000
C	-6.20054	-6.32911	7.00000
C	-4.94641	-4.32332	7.00000
C	-11.08239	-2.16748	7.00000
H	-7.53048	-0.44357	7.00000

H	-9.73236	-0.55781	7.00000
H	-2.89381	-4.44653	7.00000
H	-3.54404	-2.82430	7.00000
H	-11.85608	-1.39943	7.00000
H	-11.22088	-2.79361	6.11800
H	-11.22088	-2.79361	7.88200
H	-9.24810	-5.92737	6.20500
C	-8.66789	-6.34952	7.00000
H	-8.49024	-7.41343	6.93090
O	-6.22073	-7.56013	11.00000
O	-5.11915	-1.29612	11.00000
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C	-8.55400	-2.26079	11.00000
C	-6.11436	-2.03237	11.00000
C	-6.16040	-3.50463	11.00000
C	-7.36118	-4.17481	11.00000
C	-6.20054	-6.32911	11.00000
C	-4.94641	-4.32332	11.00000
C	-11.08239	-2.16748	11.00000
H	-7.53048	-0.44357	11.00000
H	-9.73236	-0.55781	11.00000
H	-2.89381	-4.44653	11.00000
H	-3.54404	-2.82430	11.00000
H	-11.85608	-1.39943	11.00000
H	-11.22088	-2.79361	10.11800
H	-11.22088	-2.79361	11.88200
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C	-8.98249	-7.45642	9.80330
H	-8.06197	-7.74560	9.29300
N	-10.07041	-7.13109	8.75110
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C	-9.63349	-5.93106	8.08840
H	-9.20045	-5.21731	8.78760

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H	-10.83150	-6.84524	9.35120
O	-6.24580	-7.61051	0.00000
O	-5.14422	-1.34651	0.00000
N	-7.41215	-5.62233	0.00000
N	-5.03408	-5.71928	0.00000
N	-7.47008	-1.50000	0.00000
N	-9.78032	-1.62254	0.00000
N	-3.72030	-3.87881	0.00000
N	-8.49431	-3.57398	0.00000
C	-8.57907	-2.31117	0.00000
C	-6.13943	-2.08275	0.00000
C	-6.18546	-3.55501	0.00000
C	-7.38625	-4.22519	0.00000
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C	-4.97148	-4.37370	0.00000
C	-11.10746	-2.21787	0.00000
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H	-11.88114	-1.44981	0.00000
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H	-9.19350	-6.03475	-0.89850
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H	-9.96227	-8.24460	1.67040
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H	-11.99367	-7.08390	2.80620
H	-11.44535	-8.68482	3.09150
C	-10.75104	-8.17300	7.78370
H	-11.81905	-8.06896	7.98030
H	-10.50482	-9.14767	8.20980
C	-10.61531	-8.34370	6.11100
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H	-11.90304	3.87508	10.30160
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H	-8.08595	8.31728	4.88200
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H	-9.75158	5.40272	4.00670
C	-9.88896	4.32837	4.00000
C	-10.84037	3.78867	2.92970
H	-10.37371	3.12156	2.20540
N	-11.40351	4.91309	2.25820
H	-11.65472	3.20078	3.36350
C	-10.34258	5.36068	1.21580
H	-9.45456	5.74577	1.71790
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H	-12.13167	6.84488	2.80620
H	-13.24395	5.56955	3.09150
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H	-12.89745	6.20112	7.98030
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C	2.31910	8.53838	7.00000
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H	3.19110	11.11438	7.88200
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H	3.19110	11.11438	11.88200
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C	-1.96620	11.50728	9.80330
H	-2.67690	10.85468	9.29300
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H	-2.59560	12.24588	10.30160
C	-0.31970	11.30838	8.08840
H	0.08190	10.57648	8.78760
H	0.55390	11.81978	7.67770
H	-0.51240	12.80298	9.35120
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C	1.26600	6.35828	0.00000
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C	3.63300	10.72828	0.00000
H	3.35000	6.79028	0.00000
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H	-0.70500	4.52828	0.00000
H	4.68500	11.01428	0.00000
H	3.16000	11.16128	-0.88200
H	3.16000	11.16128	0.88200

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C	-1.19600	10.72828	4.00000
C	-2.13910	11.28238	2.92970
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H	-3.05540	11.69368	3.36350
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C	-1.03540	13.48918	3.24440
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H	-1.79860	14.25438	3.09150
C	-1.70250	13.39718	7.78370

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H	-2.70960	12.67008	5.83790
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O	6.22073	7.56013	7.00000
O	5.11915	1.29612	7.00000
N	7.38709	5.57194	7.00000
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C	6.11436	2.03237	7.00000
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C	7.36118	4.17481	7.00000
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C	4.94641	4.32332	7.00000
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H	11.85608	1.39943	7.00000
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H	11.22088	2.79361	11.88200
H	8.62966	6.91634	11.93320
H	9.54498	5.72176	11.14690
C	8.66789	6.34952	11.00000
C	8.98249	7.45642	9.80330
H	8.06197	7.74560	9.29300
N	10.07041	7.13109	8.75110
H	9.30744	8.37079	10.30160
C	9.63349	5.93106	8.08840
H	9.20045	5.21731	8.78760
H	10.51318	5.43020	7.67770
H	10.83150	6.84524	9.35120
O	6.24580	7.61051	0.00000
O	5.14422	1.34651	0.00000
N	7.41215	5.62233	0.00000
N	5.03408	5.71928	0.00000
N	7.47008	1.50000	0.00000
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N	8.49431	3.57398	0.00000
C	8.57907	2.31117	0.00000
C	6.13943	2.08275	0.00000
C	6.18546	3.55501	0.00000
C	7.38625	4.22519	0.00000
C	6.22560	6.37949	0.00000
C	4.97148	4.37370	0.00000

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H	3.56910	2.87469	0.00000
H	11.88114	1.44981	0.00000
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H	8.56472	7.45562	-0.24200
O	6.24580	7.61051	4.00000
O	5.14422	1.34651	4.00000
N	7.41215	5.62233	4.00000
N	5.03408	5.71928	4.00000
N	7.47008	1.50000	4.00000
N	9.78032	1.62254	4.00000
N	3.72030	3.87881	4.00000
N	8.49431	3.57398	4.00000
C	8.57907	2.31117	4.00000
C	6.13943	2.08275	4.00000
C	6.18546	3.55501	4.00000
C	7.38625	4.22519	4.00000
C	6.22560	6.37949	4.00000
C	4.97148	4.37370	4.00000
C	11.10746	2.21787	4.00000
H	7.55555	0.49395	4.00000
H	9.75743	0.60820	4.00000
H	2.91888	4.49691	4.00000
H	3.56910	2.87469	4.00000
H	11.88114	1.44981	4.00000
H	11.24595	2.84400	3.11800
H	11.24595	2.84400	4.88200
H	8.63416	7.09515	4.80790
H	9.55468	5.74376	4.00670
C	8.69296	6.39990	4.00000
C	8.70127	7.49370	2.92970
H	7.89021	7.42311	2.20540
N	9.95661	7.41919	2.25820
H	8.59932	8.49289	3.36350

C	9.81378	6.27659	1.21580
H	9.70326	5.31501	1.71790
H	10.78589	6.21604	0.72520
H	9.96227	8.24460	1.67040
C	11.16427	7.64127	3.24440
H	11.99367	7.08390	2.80620
H	11.44535	8.68482	3.09150
C	10.75104	8.17300	7.78370
H	11.81905	8.06896	7.98030
H	10.50482	9.14767	8.20980
C	10.61531	8.34370	6.11100
H	11.15172	9.28040	5.94760
H	9.61781	8.68162	5.83790
C	11.24131	7.40123	4.91310
H	12.31229	7.49764	5.10020
H	11.11264	6.35249	5.16480
O	9.65763	-1.60725	7.00000
O	3.68205	-3.78525	7.00000
N	8.51899	-3.61143	7.00000
N	7.41391	-1.50348	7.00000
N	4.97791	-5.72276	7.00000
N	6.23915	-7.66222	7.00000
N	5.16313	-1.28595	7.00000
N	7.28614	-5.57278	7.00000
C	6.23490	-6.27759	7.00000
C	4.81726	-4.27901	7.00000
C	6.11530	-3.58275	7.00000
C	7.29608	-4.28757	7.00000
C	8.58144	-2.20527	7.00000
C	6.21731	-2.12206	7.00000
C	7.41829	-8.51389	7.00000
H	4.14938	-6.29981	7.00000
H	5.34926	-8.14956	7.00000
H	5.29771	-0.28285	7.00000
H	4.21794	-1.65707	7.00000
H	7.13998	-9.56795	7.00000
H	8.02978	-8.32076	6.11800
H	8.02978	-8.32076	7.88200
H	9.75730	-5.04541	6.20500
C	9.83279	-4.33185	7.00000

H	10.66534	-3.64605	6.93090
O	9.65763	-1.60725	11.00000
O	3.68205	-3.78525	11.00000
N	8.51899	-3.61143	11.00000
N	7.41391	-1.50348	11.00000
N	4.97791	-5.72276	11.00000
N	6.23915	-7.66222	11.00000
N	5.16313	-1.28595	11.00000
N	7.28614	-5.57278	11.00000
C	6.23490	-6.27759	11.00000
C	4.81726	-4.27901	11.00000
C	6.11530	-3.58275	11.00000
C	7.29608	-4.28757	11.00000
C	8.58144	-2.20527	11.00000
C	6.21731	-2.12206	11.00000
C	7.41829	-8.51389	11.00000
H	4.14938	-6.29981	11.00000
H	5.34926	-8.14956	11.00000
H	5.29771	-0.28285	11.00000
H	4.21794	-1.65707	11.00000
H	7.13998	-9.56795	11.00000
H	8.02978	-8.32076	10.11800
H	8.02978	-8.32076	11.88200
H	10.30456	-4.01533	11.93320
H	9.72768	-5.40532	11.14690
C	9.83279	-4.33185	11.00000
C	10.94869	-4.05086	9.80330
H	10.73887	-3.10907	9.29300
N	11.21091	-5.15569	8.75110
H	11.90304	-3.87508	10.30160
C	9.95319	-5.37732	8.08840
H	9.11855	-5.35917	8.78760
H	9.95928	-6.38958	7.67770
H	11.34390	-5.95774	9.35120
O	9.71380	-1.60376	0.00000
O	3.73822	-3.78177	0.00000
N	8.57515	-3.60795	0.00000
N	7.47008	-1.50000	0.00000
N	5.03408	-5.71928	0.00000
N	6.29532	-7.65874	0.00000

N	5.21930	-1.28247	0.00000
N	7.34231	-5.56930	0.00000
C	6.29107	-6.27410	0.00000
C	4.87343	-4.27553	0.00000
C	6.17146	-3.57926	0.00000
C	7.35225	-4.28408	0.00000
C	8.63760	-2.20178	0.00000
C	6.27348	-2.11857	0.00000
C	7.47446	-8.51041	0.00000
H	4.20555	-6.29632	0.00000
H	5.40543	-8.14608	0.00000
H	5.35388	-0.27937	0.00000
H	4.27410	-1.65359	0.00000
H	7.19614	-9.56447	0.00000
H	8.08595	-8.31728	-0.88200
H	8.08595	-8.31728	0.88200
H	9.82300	-4.94442	-0.89850
C	9.88896	-4.32837	0.00000
H	10.73912	-3.68945	-0.24200
O	9.71380	-1.60376	4.00000
O	3.73822	-3.78177	4.00000
N	8.57515	-3.60795	4.00000
N	7.47008	-1.50000	4.00000
N	5.03408	-5.71928	4.00000
N	6.29532	-7.65874	4.00000
N	5.21930	-1.28247	4.00000
N	7.34231	-5.56930	4.00000
C	6.29107	-6.27410	4.00000
C	4.87343	-4.27553	4.00000
C	6.17146	-3.57926	4.00000
C	7.35225	-4.28408	4.00000
C	8.63760	-2.20178	4.00000
C	6.27348	-2.11857	4.00000
C	7.47446	-8.51041	4.00000
H	4.20555	-6.29632	4.00000
H	5.40543	-8.14608	4.00000
H	5.35388	-0.27937	4.00000
H	4.27410	-1.65359	4.00000
H	7.19614	-9.56447	4.00000
H	8.08595	-8.31728	3.11800

H	8.08595	-8.31728	4.88200
H	10.46166	-3.92983	4.80790
H	9.75158	-5.40272	4.00670
C	9.88896	-4.32837	4.00000
C	10.84037	-3.78867	2.92970
H	10.37371	-3.12156	2.20540
N	11.40351	-4.91309	2.25820
H	11.65472	-3.20078	3.36350
C	10.34258	-5.36068	1.21580
H	9.45456	-5.74577	1.71790
H	10.77619	-6.23284	0.72520
H	12.12117	-4.50528	1.67040
C	12.19967	-5.84791	3.24440
H	12.13167	-6.84488	2.80620
H	13.24395	-5.56955	3.09150
C	12.45354	-5.22418	7.78370
H	12.89745	-6.20112	7.98030
H	13.17452	-4.52361	8.20980
C	12.53351	-5.02128	6.11100
H	13.61292	-5.01748	5.94760
H	12.32741	-3.98846	5.83790
C	12.03031	-6.03464	4.91310
H	12.64929	-6.91394	5.10020
H	11.05774	-6.44758	5.16480

SAS

O	-0.85590	-9.41710	11.00920
O	4.01810	-5.33110	11.00920
N	1.44910	-9.43310	11.00920
N	0.17610	-7.42210	11.00920
N	5.04810	-7.42210	11.00920
N	6.09710	-9.48410	11.00920
N	1.11310	-5.36410	11.00920
N	3.76410	-9.34610	11.00920
C	4.90010	-8.78810	11.00920
C	3.87810	-6.56110	11.00920
C	2.62610	-7.33710	11.00920
C	2.64610	-8.71210	11.00920

C	0.20010	-8.78410	11.00920
C	1.31010	-6.69510	11.00920
C	6.24510	-10.93110	11.00920
H	5.96210	-6.99310	11.00920
H	6.96410	-8.95710	11.00920
H	0.17710	-4.97910	11.00920
H	1.90710	-4.73110	11.00920
H	7.29710	-11.21710	11.00920
H	5.77210	-11.36410	11.89120
H	5.77210	-11.36410	10.12720
H	1.96160	-11.18190	11.92060
C	1.41610	-10.93110	11.00920
H	0.43370	-11.35360	11.22230
O	-0.85590	-9.41710	7.00920
O	4.01810	-5.33110	7.00920
N	1.44910	-9.43310	7.00920
N	0.17610	-7.42210	7.00920
N	5.04810	-7.42210	7.00920
N	6.09710	-9.48410	7.00920
N	1.11310	-5.36410	7.00920
N	3.76410	-9.34610	7.00920
C	4.90010	-8.78810	7.00920
C	3.87810	-6.56110	7.00920
C	2.62610	-7.33710	7.00920
C	2.64610	-8.71210	7.00920
C	0.20010	-8.78410	7.00920
C	1.31010	-6.69510	7.00920
C	6.24510	-10.93110	7.00920
H	5.96210	-6.99310	7.00920
H	6.96410	-8.95710	7.00920
H	0.17710	-4.97910	7.00920
H	1.90710	-4.73110	7.00920
H	7.29710	-11.21710	7.00920
H	5.77210	-11.36410	7.89120
H	5.77210	-11.36410	6.12720
H	0.72930	-11.23190	6.24840
H	2.41310	-11.34810	6.95000
C	1.41610	-10.93110	7.00920
C	0.50730	-11.49840	8.09880
H	0.15750	-10.75600	8.81490

N	1.22930	-12.53810	8.76090
H	-0.41090	-11.93340	7.69270
C	2.12440	-11.82240	9.80460
H	2.88410	-11.22520	9.29860
H	2.68650	-12.61540	10.29920
H	0.53630	-12.97940	9.35290
O	3.46800	-9.46400	0.00000
O	-1.40600	-5.37800	0.00000
N	1.16300	-9.48000	0.00000
N	2.43600	-7.46900	0.00000
N	-2.43600	-7.46900	0.00000
N	-3.48500	-9.53100	0.00000
N	1.49900	-5.41100	0.00000
N	-1.15200	-9.39300	0.00000
C	-2.28800	-8.83500	0.00000
C	-1.26600	-6.60800	0.00000
C	-0.01400	-7.38400	0.00000
C	-0.03400	-8.75900	0.00000
C	2.41200	-8.83100	0.00000
C	1.30200	-6.74200	0.00000
C	-3.63300	-10.97800	0.00000
H	-3.35000	-7.04000	0.00000
H	-4.35200	-9.00400	0.00000
H	2.43500	-5.02600	0.00000
H	0.70500	-4.77800	0.00000
H	-4.68500	-11.26400	0.00000
H	-3.16000	-11.41100	-0.88200
H	-3.16000	-11.41100	0.88200
H	0.64840	-11.22890	-0.91020
C	1.19600	-10.97800	0.00000
H	2.17800	-11.40030	-0.21540
O	3.46800	-9.46400	4.00000
O	-1.40600	-5.37800	4.00000
N	1.16300	-9.48000	4.00000
N	2.43600	-7.46900	4.00000
N	-2.43600	-7.46900	4.00000
N	-3.48500	-9.53100	4.00000
N	1.49900	-5.41100	4.00000
N	-1.15200	-9.39300	4.00000
C	-2.28800	-8.83500	4.00000

C	-1.26600	-6.60800	4.00000
C	-0.01400	-7.38400	4.00000
C	-0.03400	-8.75900	4.00000
C	2.41200	-8.83100	4.00000
C	1.30200	-6.74200	4.00000
C	-3.63300	-10.97800	4.00000
H	-3.35000	-7.04000	4.00000
H	-4.35200	-9.00400	4.00000
H	2.43500	-5.02600	4.00000
H	0.70500	-4.77800	4.00000
H	-4.68500	-11.26400	4.00000
H	-3.16000	-11.41100	3.11800
H	-3.16000	-11.41100	4.88200
H	1.87250	-11.29130	4.76420
H	0.19560	-11.38850	4.04470
C	1.19600	-10.97800	4.00000
C	2.10670	-11.54060	2.91040
H	2.45150	-10.79840	2.19190
N	1.38490	-12.58350	2.25530
H	3.02720	-11.97090	3.31630
C	0.49010	-11.87080	1.20730
H	-0.27240	-11.27470	1.71050
H	-0.06930	-12.66650	0.71370
H	2.07680	-13.03090	1.66670
C	0.93380	-13.72190	3.24960
H	-0.00290	-14.09920	2.83580
H	1.64070	-14.53310	3.06760
C	1.67850	-13.68800	7.78140
H	0.97050	-14.49620	7.97190
H	2.61430	-14.06170	8.20050
C	1.88280	-13.65660	6.10600
H	2.37730	-14.61400	5.93150
H	2.69580	-12.99530	5.81790
C	0.73210	-13.67130	4.92740
H	0.24350	-14.62920	5.11590
H	-0.08170	-13.00860	5.21120

SAS rosette ring

O	-0.85590	-9.16738	11.00920
O	4.01810	-5.08138	11.00920
N	1.44910	-9.18338	11.00920
N	0.17610	-7.17238	11.00920
N	5.04810	-7.17238	11.00920
N	6.09710	-9.23438	11.00920
N	1.11310	-5.11438	11.00920
N	3.76410	-9.09638	11.00920
C	4.90010	-8.53838	11.00920
C	3.87810	-6.31138	11.00920
C	2.62610	-7.08738	11.00920
C	2.64610	-8.46238	11.00920
C	0.20010	-8.53438	11.00920
C	1.31010	-6.44538	11.00920
C	6.24510	-10.68138	11.00920
H	5.96210	-6.74338	11.00920
H	6.96410	-8.70738	11.00920
H	0.17710	-4.72938	11.00920
H	1.90710	-4.48138	11.00920
H	7.29710	-10.96738	11.00920
H	5.77210	-11.11438	11.89120
H	5.77210	-11.11438	10.12720
H	1.96160	-10.93218	11.92060
C	1.41610	-10.68138	11.00920
H	0.43370	-11.10388	11.22230
O	-0.85590	-9.16738	7.00920
O	4.01810	-5.08138	7.00920
N	1.44910	-9.18338	7.00920
N	0.17610	-7.17238	7.00920
N	5.04810	-7.17238	7.00920
N	6.09710	-9.23438	7.00920
N	1.11310	-5.11438	7.00920
N	3.76410	-9.09638	7.00920
C	4.90010	-8.53838	7.00920
C	3.87810	-6.31138	7.00920
C	2.62610	-7.08738	7.00920
C	2.64610	-8.46238	7.00920
C	0.20010	-8.53438	7.00920
C	1.31010	-6.44538	7.00920
C	6.24510	-10.68138	7.00920

H	5.96210	-6.74338	7.00920
H	6.96410	-8.70738	7.00920
H	0.17710	-4.72938	7.00920
H	1.90710	-4.48138	7.00920
H	7.29710	-10.96738	7.00920
H	5.77210	-11.11438	7.89120
H	5.77210	-11.11438	6.12720
H	0.72930	-10.98218	6.24840
H	2.41310	-11.09838	6.95000
C	1.41610	-10.68138	7.00920
C	0.50730	-11.24868	8.09880
H	0.15750	-10.50628	8.81490
N	1.22930	-12.28838	8.76090
H	-0.41090	-11.68368	7.69270
C	2.12440	-11.57268	9.80460
H	2.88410	-10.97548	9.29860
H	2.68650	-12.36568	10.29920
H	0.53630	-12.72968	9.35290
O	3.46800	-9.21428	0.00000
O	-1.40600	-5.12828	0.00000
N	1.16300	-9.23028	0.00000
N	2.43600	-7.21928	0.00000
N	-2.43600	-7.21928	0.00000
N	-3.48500	-9.28128	0.00000
N	1.49900	-5.16128	0.00000
N	-1.15200	-9.14328	0.00000
C	-2.28800	-8.58528	0.00000
C	-1.26600	-6.35828	0.00000
C	-0.01400	-7.13428	0.00000
C	-0.03400	-8.50928	0.00000
C	2.41200	-8.58128	0.00000
C	1.30200	-6.49228	0.00000
C	-3.63300	-10.72828	0.00000
H	-3.35000	-6.79028	0.00000
H	-4.35200	-8.75428	0.00000
H	2.43500	-4.77628	0.00000
H	0.70500	-4.52828	0.00000
H	-4.68500	-11.01428	0.00000
H	-3.16000	-11.16128	-0.88200
H	-3.16000	-11.16128	0.88200

H	0.64840	-10.97918	-0.91020
C	1.19600	-10.72828	0.00000
H	2.17800	-11.15058	-0.21540
O	3.46800	-9.21428	4.00000
O	-1.40600	-5.12828	4.00000
N	1.16300	-9.23028	4.00000
N	2.43600	-7.21928	4.00000
N	-2.43600	-7.21928	4.00000
N	-3.48500	-9.28128	4.00000
N	1.49900	-5.16128	4.00000
N	-1.15200	-9.14328	4.00000
C	-2.28800	-8.58528	4.00000
C	-1.26600	-6.35828	4.00000
C	-0.01400	-7.13428	4.00000
C	-0.03400	-8.50928	4.00000
C	2.41200	-8.58128	4.00000
C	1.30200	-6.49228	4.00000
C	-3.63300	-10.72828	4.00000
H	-3.35000	-6.79028	4.00000
H	-4.35200	-8.75428	4.00000
H	2.43500	-4.77628	4.00000
H	0.70500	-4.52828	4.00000
H	-4.68500	-11.01428	4.00000
H	-3.16000	-11.16128	3.11800
H	-3.16000	-11.16128	4.88200
H	1.87250	-11.04158	4.76420
H	0.19560	-11.13878	4.04470
C	1.19600	-10.72828	4.00000
C	2.10670	-11.29088	2.91040
H	2.45150	-10.54868	2.19190
N	1.38490	-12.33378	2.25530
H	3.02720	-11.72118	3.31630
C	0.49010	-11.62108	1.20730
H	-0.27240	-11.02498	1.71050
H	-0.06930	-12.41678	0.71370
H	2.07680	-12.78118	1.66670
C	0.93380	-13.47218	3.24960
H	-0.00290	-13.84948	2.83580
H	1.64070	-14.28338	3.06760
C	1.67850	-13.43828	7.78140

H	0.97050	-14.24648	7.97190
H	2.61430	-13.81198	8.20050
C	1.88280	-13.40688	6.10600
H	2.37730	-14.36428	5.93150
H	2.69580	-12.74558	5.81790
C	0.73210	-13.42158	4.92740
H	0.24350	-14.37948	5.11590
H	-0.08170	-12.75888	5.21120
O	-8.36713	-3.84246	11.00920
O	-2.39155	-6.02046	11.00920
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N	-6.12341	-3.73869	11.00920
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H	6.73928	10.55597	6.12720
H	9.14619	6.12268	6.24840

H	8.40493	7.63899	6.95000
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H	9.36574	8.50942	10.29920
H	10.75607	6.82929	9.35290
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O	5.14422	1.34651	0.00000
N	7.41215	5.62233	0.00000
N	5.03408	5.71928	0.00000
N	7.47008	1.50000	0.00000
N	9.78032	1.62254	0.00000
N	3.72030	3.87881	0.00000
N	8.49431	3.57398	0.00000
C	8.57907	2.31117	0.00000
C	6.13943	2.08275	0.00000
C	6.18546	3.55501	0.00000
C	7.38625	4.22519	0.00000
C	6.22560	6.37949	0.00000
C	4.97148	4.37370	0.00000
C	11.10746	2.21787	0.00000
H	7.55555	0.49395	0.00000
H	9.75743	0.60820	0.00000
H	2.91888	4.49691	0.00000
H	3.56910	2.87469	0.00000
H	11.88114	1.44981	0.00000
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H	11.24595	2.84400	0.88200
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N	7.47008	1.50000	4.00000

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H	11.99545	6.92223	2.83580
H	11.54942	8.56258	3.06760
C	10.79864	8.17276	7.78140
H	11.85256	7.96372	7.97190
H	10.65437	9.17004	8.20050
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H	11.25118	9.24094	5.93150
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O	6.40965	0.93909	11.00920
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N	6.29951	-3.43368	11.00920
N	8.73551	0.78559	11.00920
N	11.04575	0.66306	11.00920
N	4.98573	-1.59322	11.00920
N	9.75974	-1.28838	11.00920
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C	7.40486	0.20285	11.00920
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N	7.34231	-5.56930	0.00000
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C	6.17146	-3.57926	0.00000
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C	6.27348	-2.11857	0.00000
C	7.47446	-8.51041	0.00000
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H	8.08595	-8.31728	0.88200

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H	10.36117	-3.15128	2.19190
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H	12.10722	-4.59203	1.66670
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H	13.19012	-5.72080	3.06760
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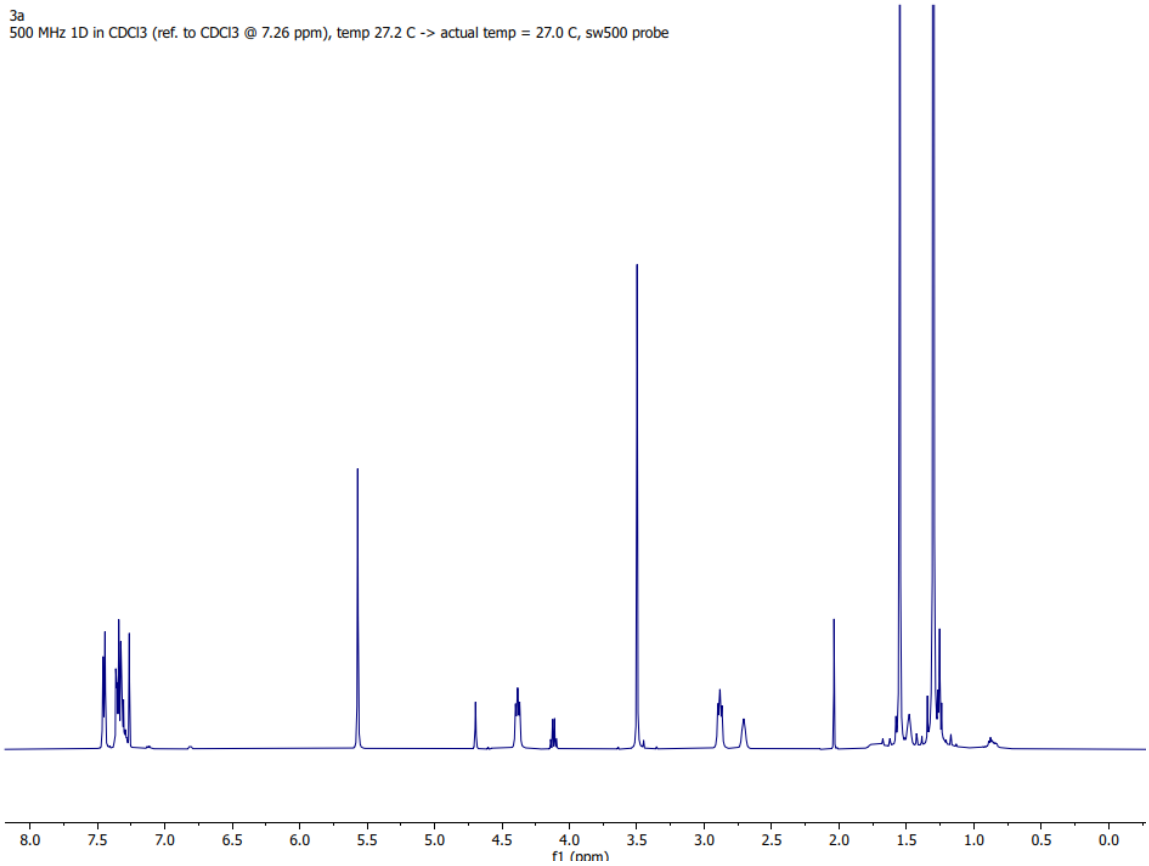
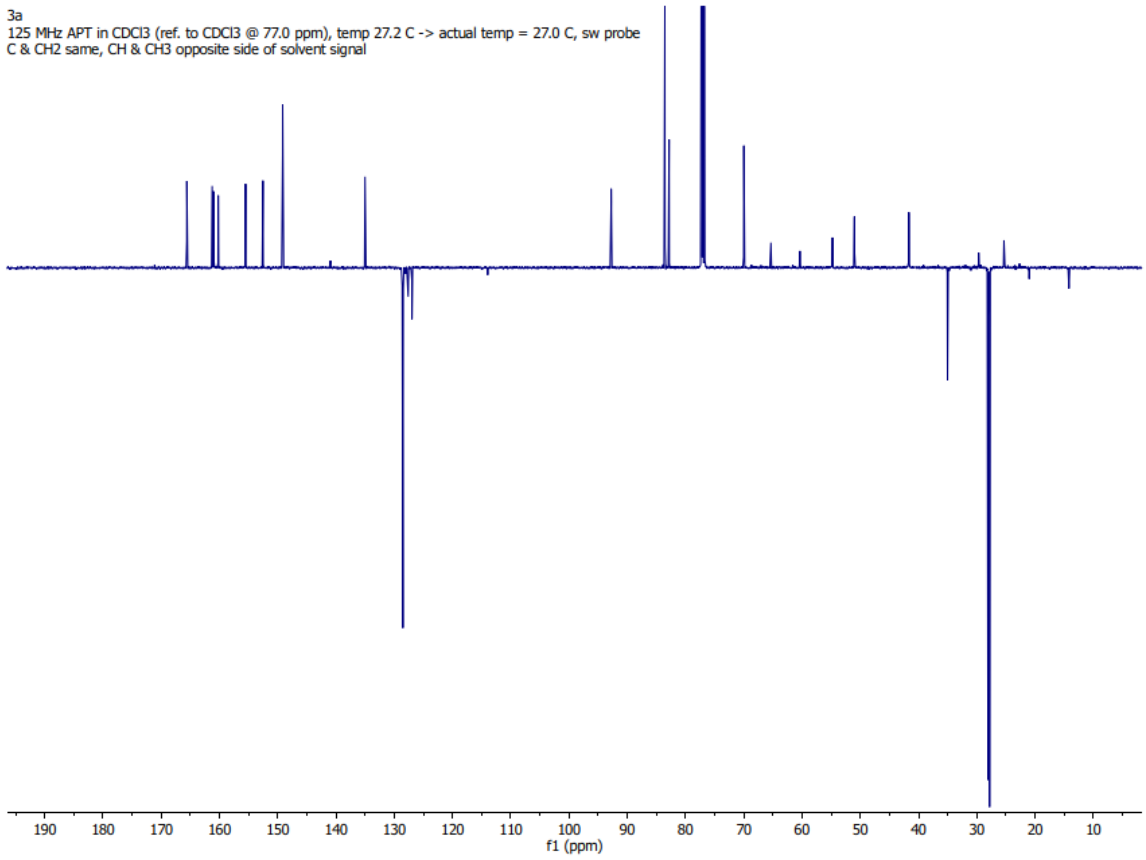
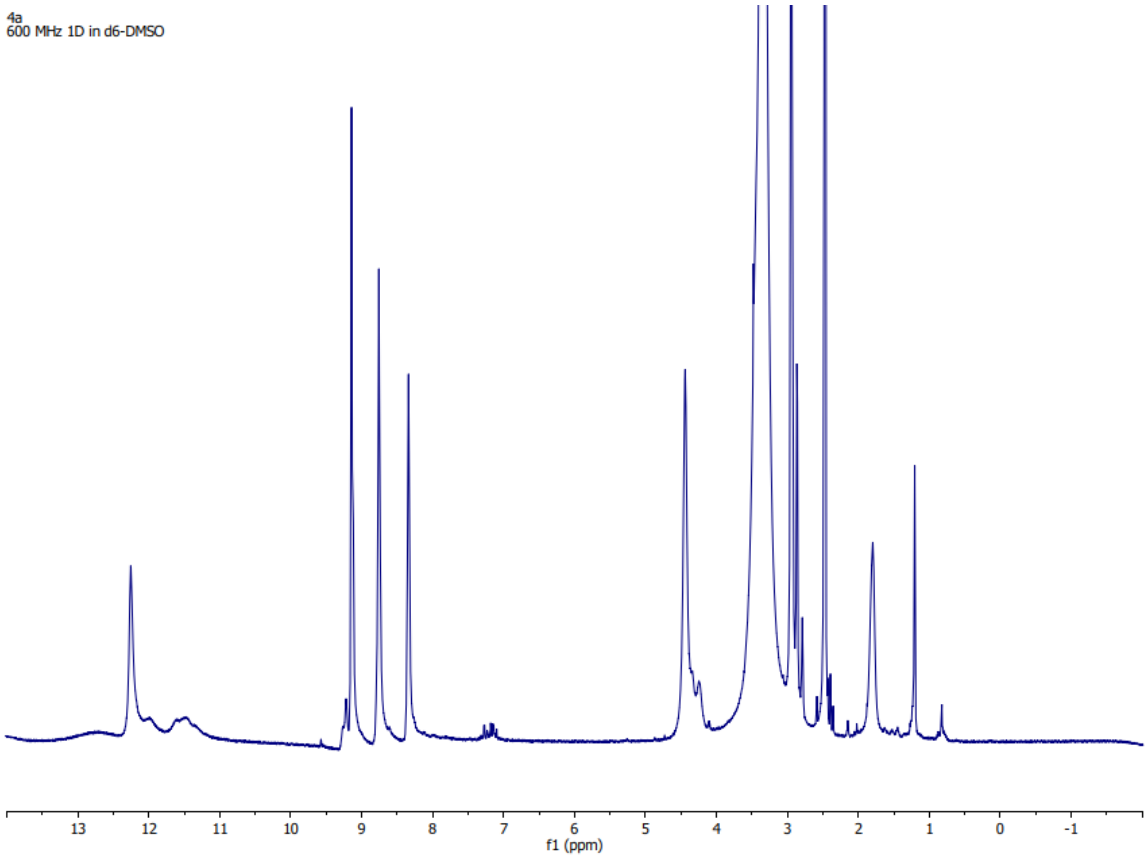
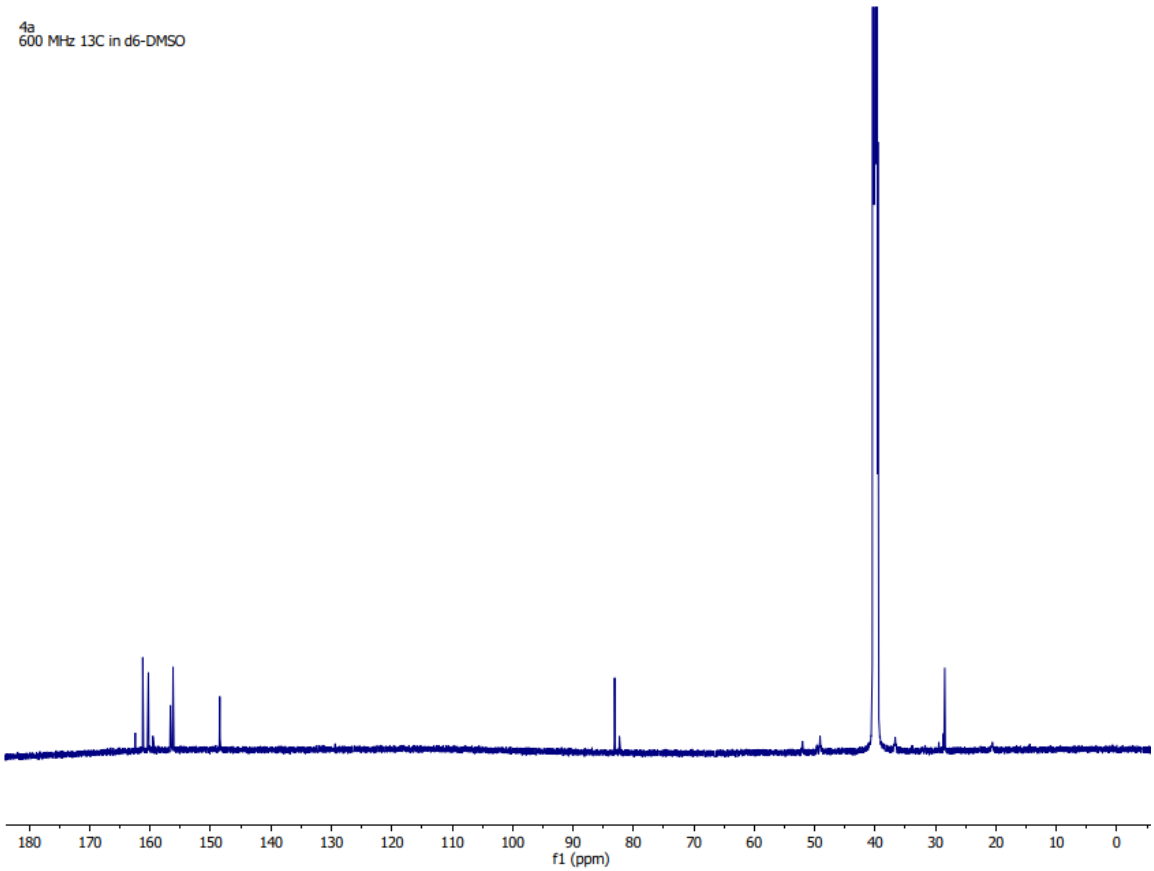
H	11.00866	-6.45019	5.21120

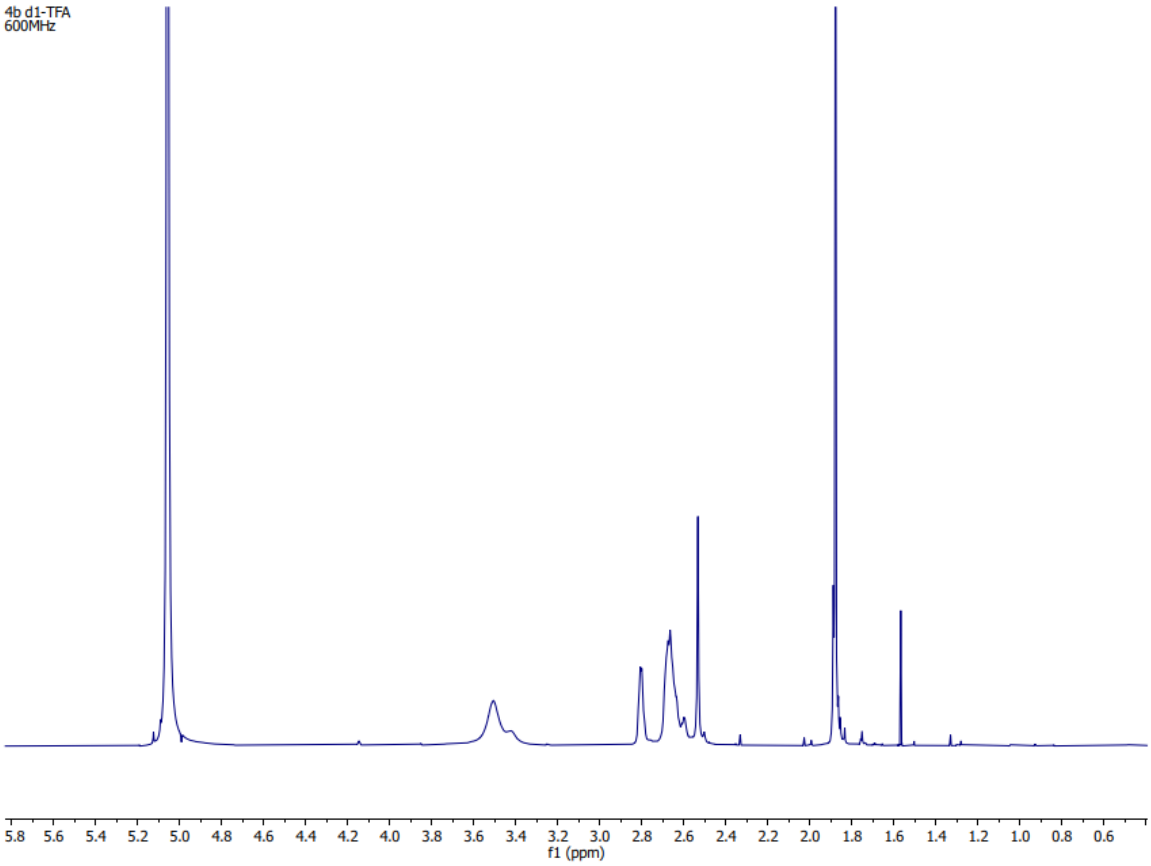
NMR spectra

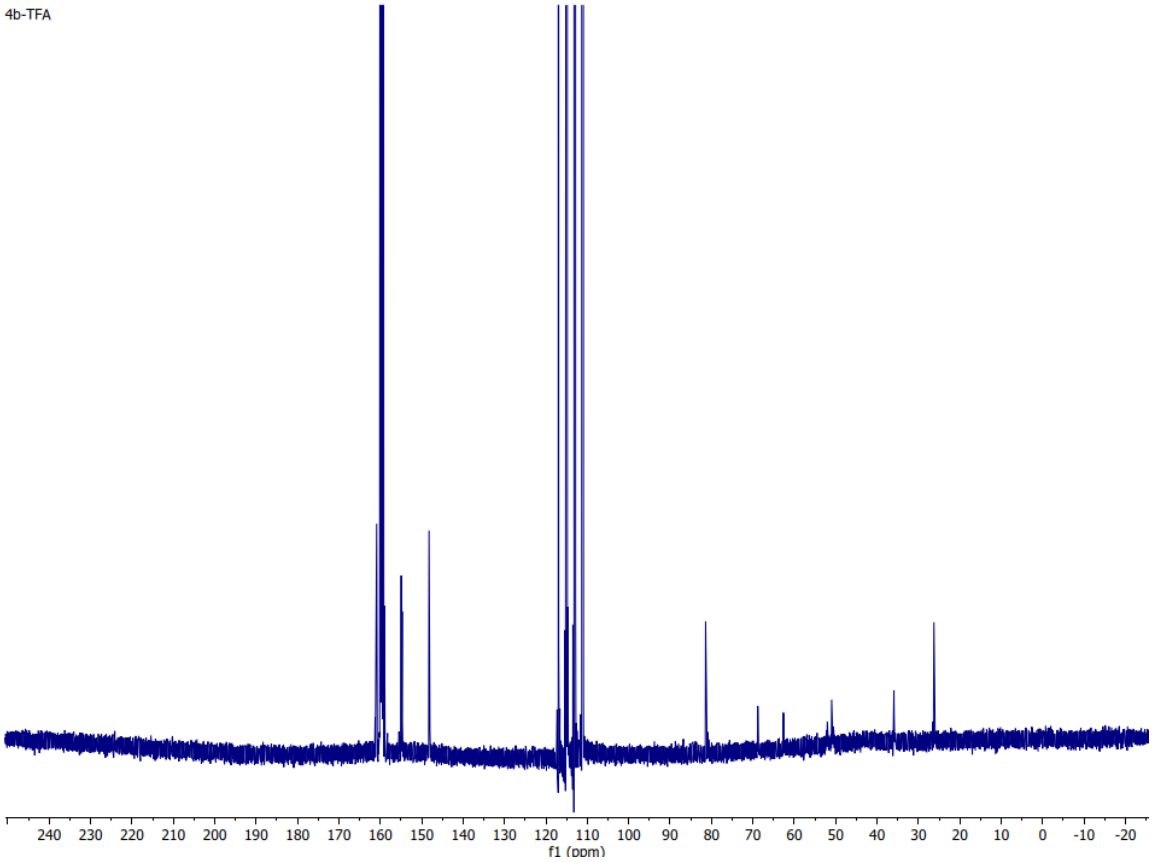

3a
500 MHz 1D in CDCl3 (ref. to CDCl3 @ 7.26 ppm), temp 27.2 C -> actual temp = 27.0 C, sw500 probe
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

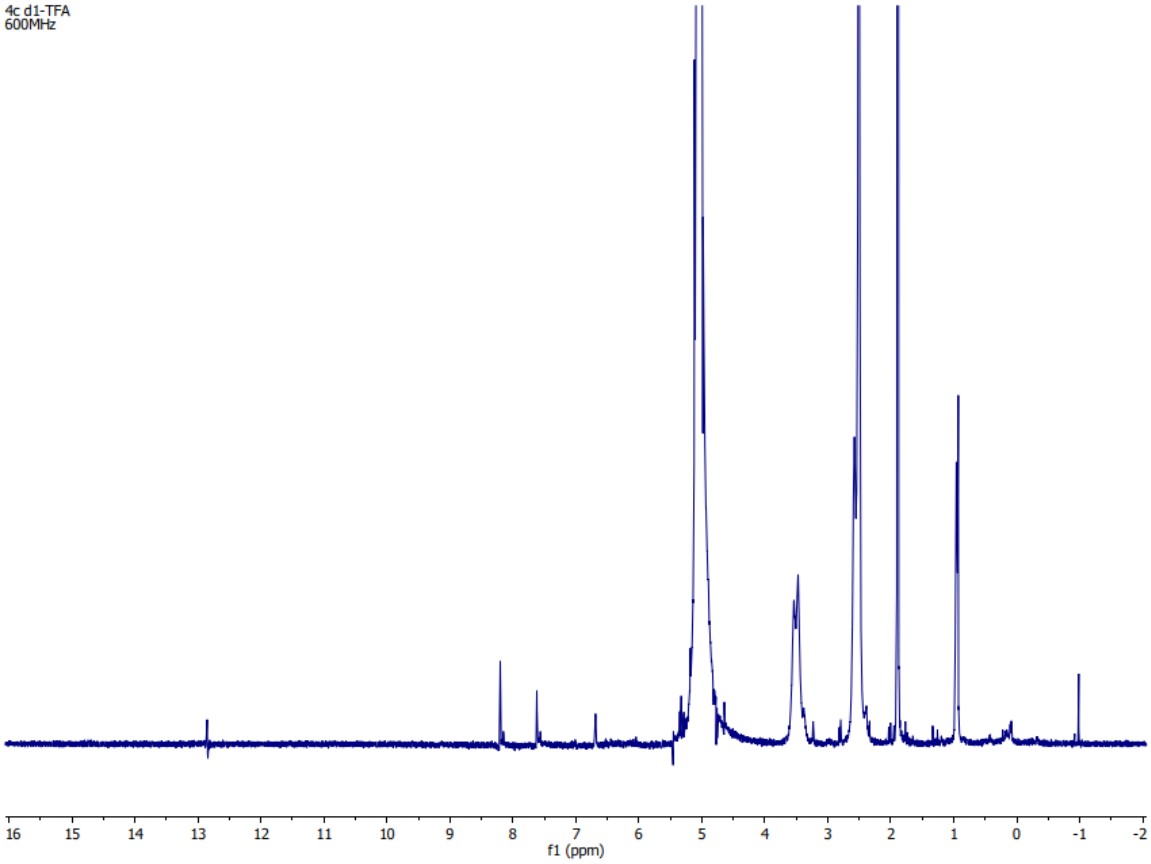

3a
125 MHz APT in CDCl3 (ref. to CDCl3 @ 77.0 ppm), temp 27.2 C -> actual temp = 27.0 C, sw probe
C & CH2 same, CH & CH3 opposite side of solvent signal
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

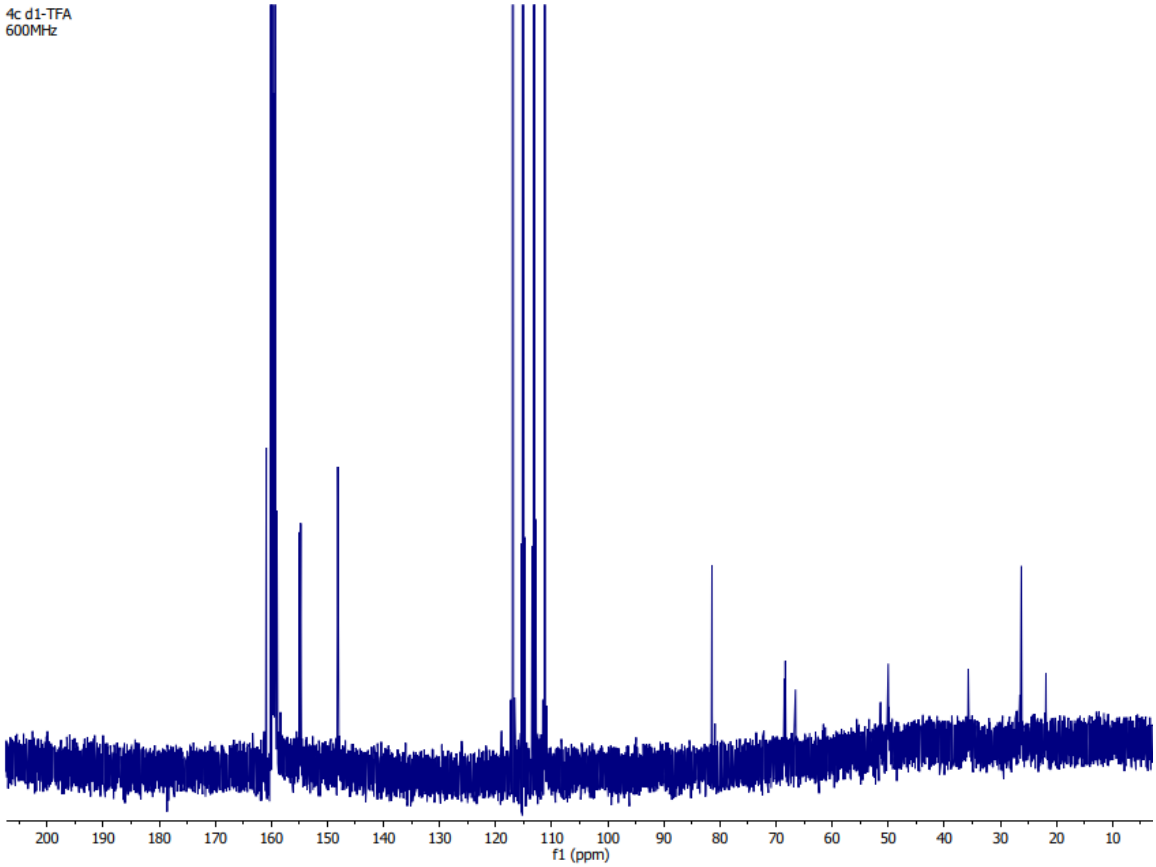

4a
600 MHz 1D in d6-DMSO
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)


4a
600 MHz 13C in d6-DMSO
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


4b d1-TFA
600MHz
5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8 0.6
f1 (ppm)


4b-TFA
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


4c d1-TFA
600MHz
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)


4c d1-TFA
600MHz
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

References:

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