Supporting Information

Octapodal corannulene porphyrin-based assemblies: allosteric behavior in fullerene hosting

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NMR spectra

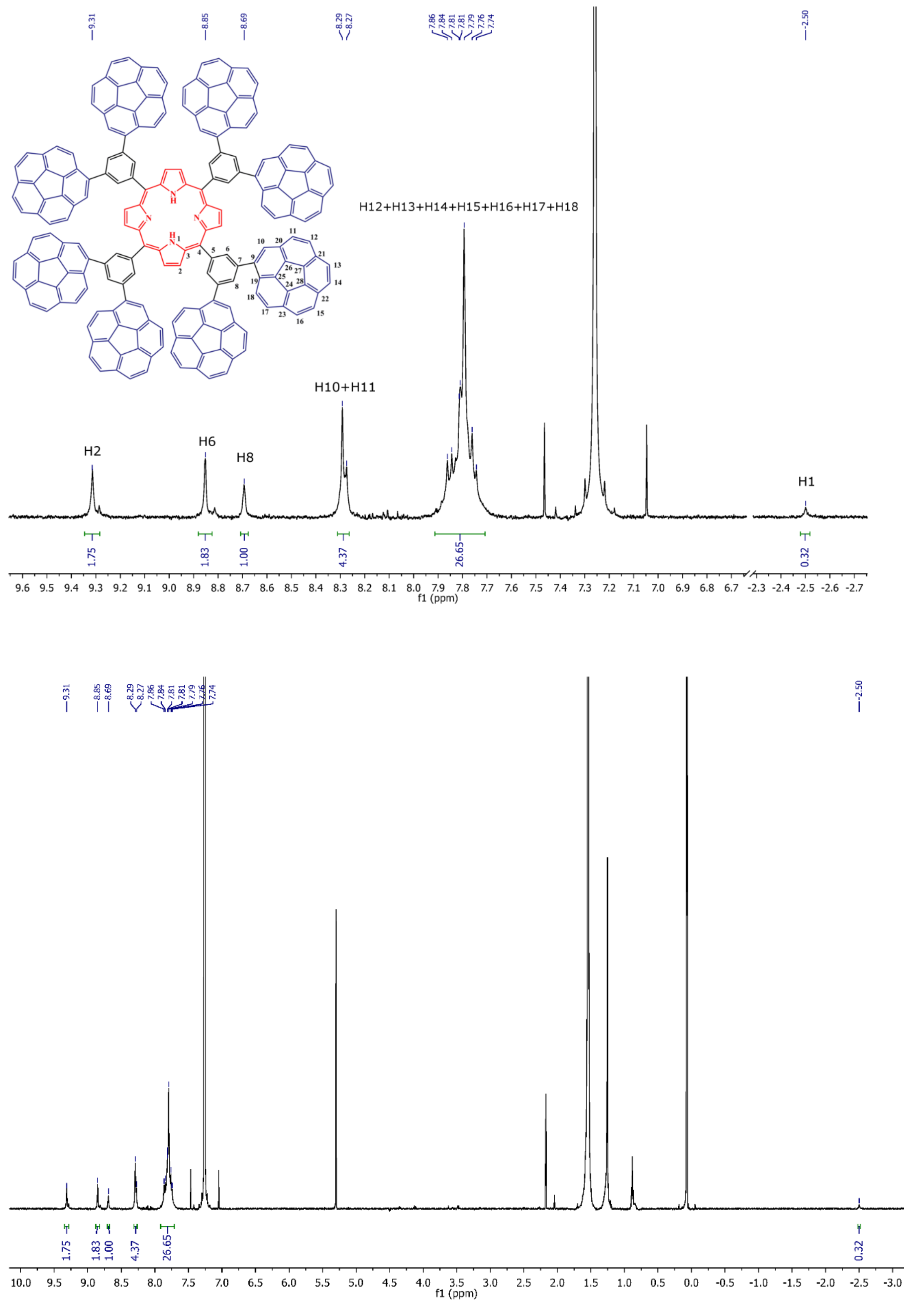


Figure S1: ^{1}H NMR (500 MHz, $CDCl_3$) of **2H-POctaCor,** selected regions (above) and full spectrum (below).

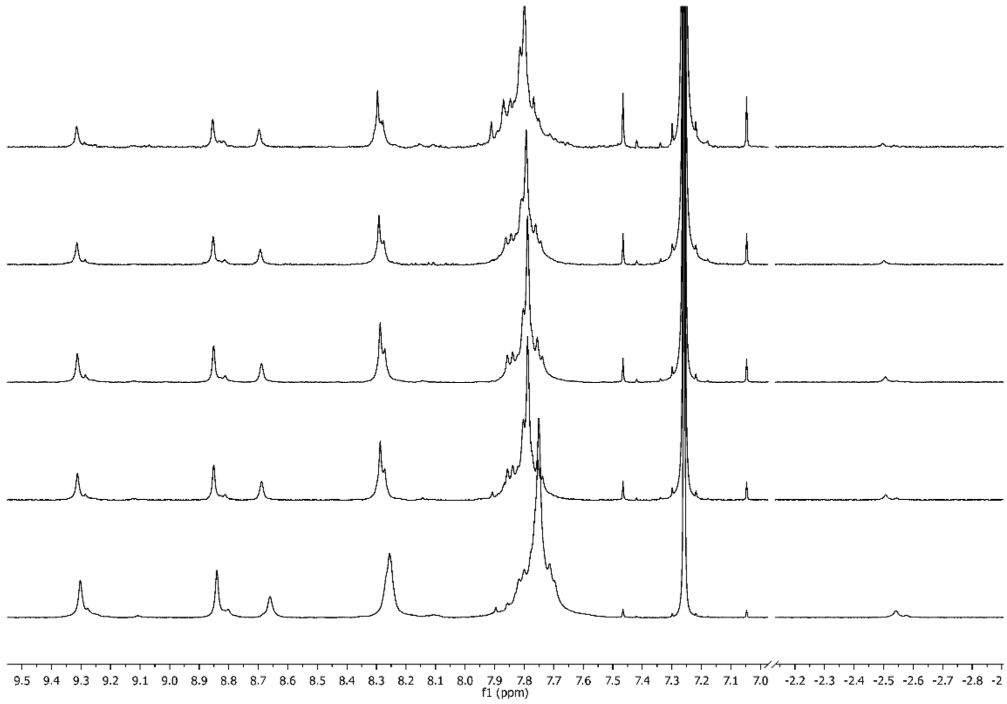


Figure S2: ^{1}H NMR (500 MHz, $CDCl_3$) of **2H-POctaCor** with aliquots of $CDCl_3$**.** Initial experiment: 10^{-4} M. Final experiment: 10^{-5} M.

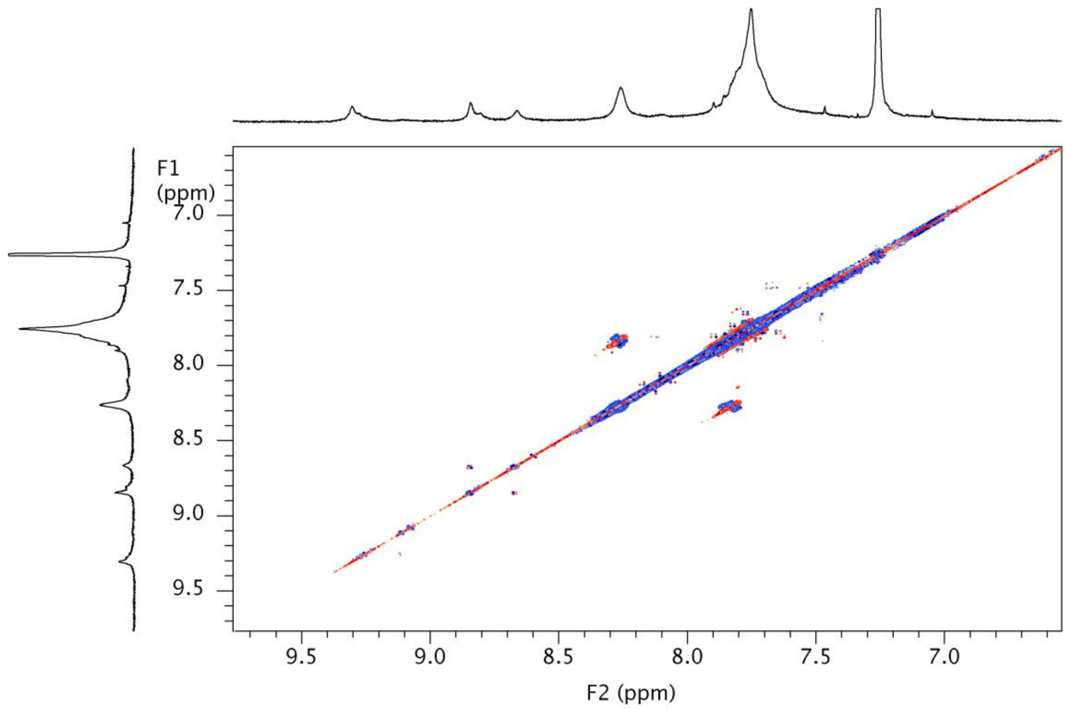


Figure S3: ^{1}H-^{1}H DQFCOSY of **2H-POctaCor**.

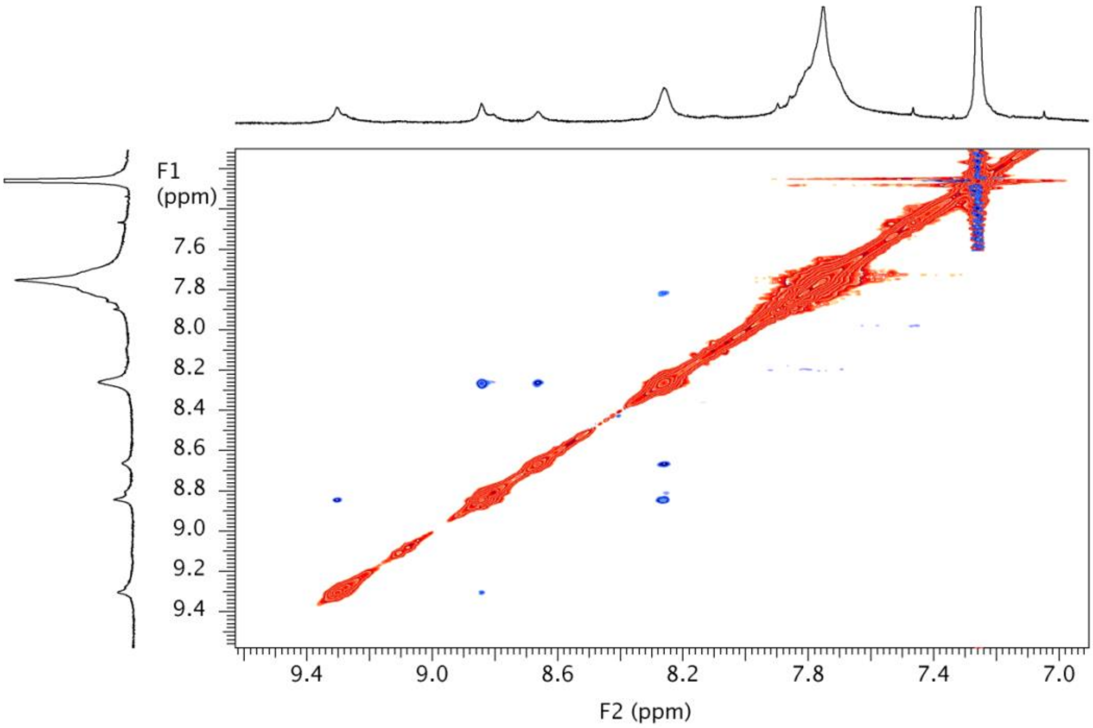


Figure S4: ^{1}H-^{1}H band selective ROESY of **2H-POctaCor**.

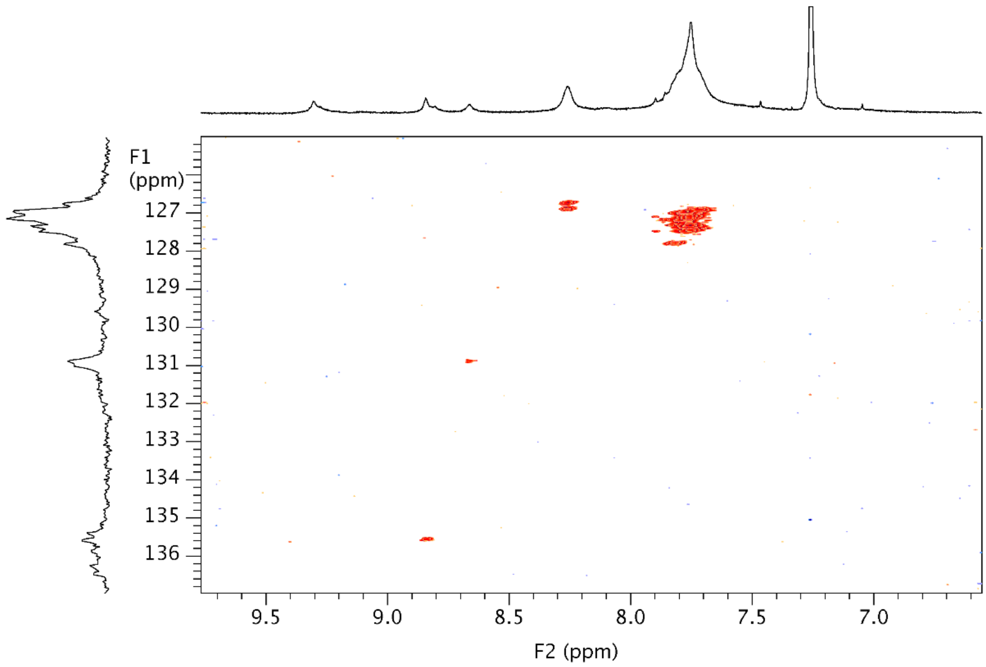


Figure S5: ^{1}H-^{13}C band selective HSQC of **2H-POctaCor**.

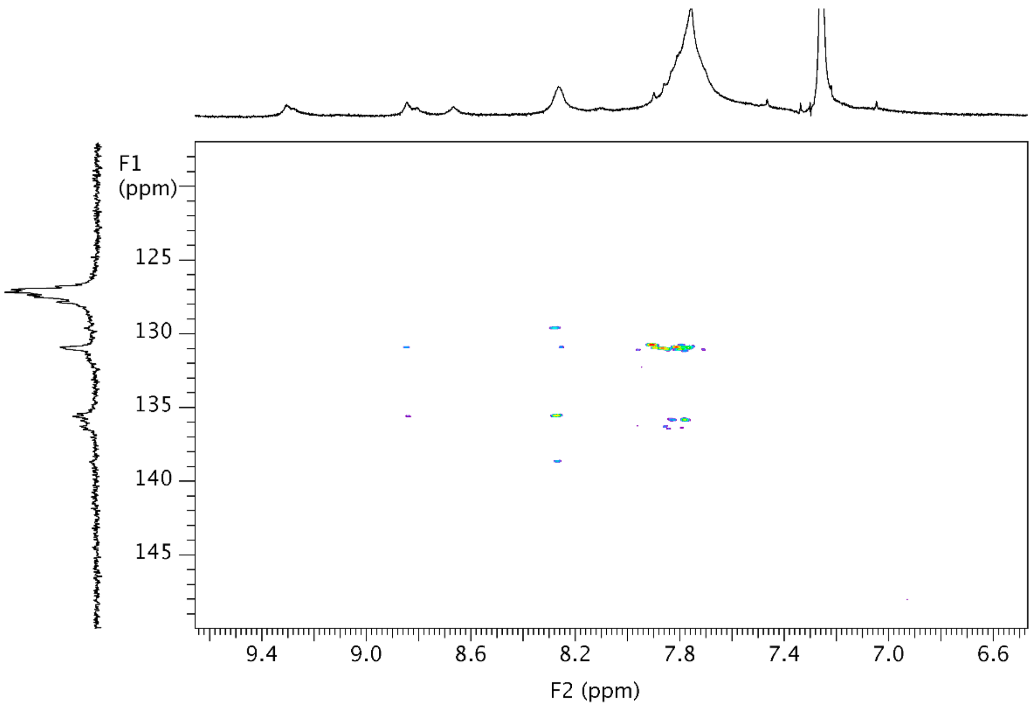


Figure S6: ^{1}H-^{13}C band selective HMBC of **2H-POctaCor.**

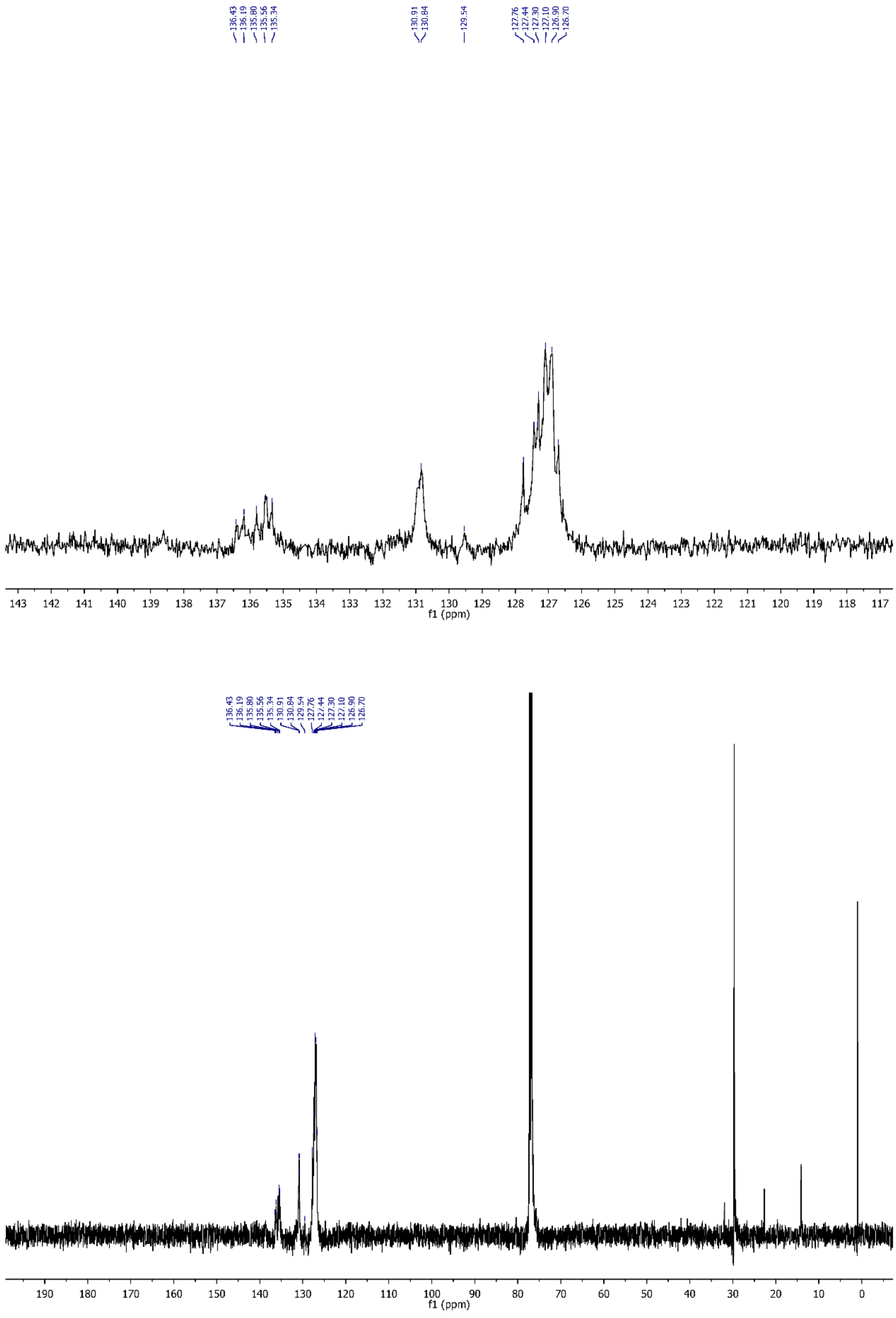
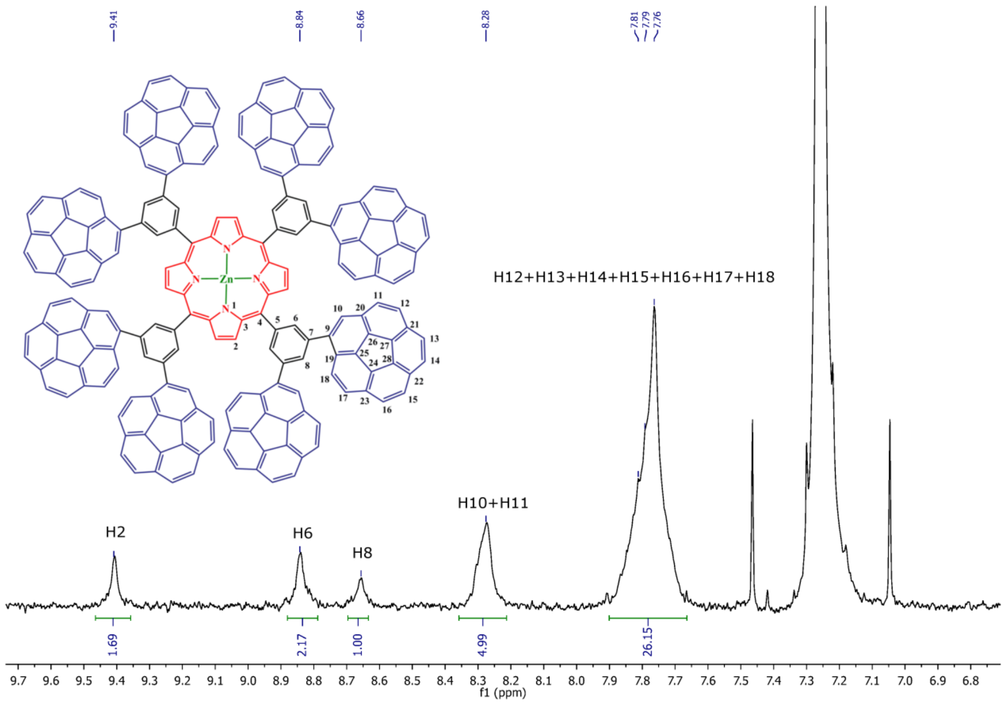


Figure S7: $^{13}C\ \{^{1}H\}$ NMR (126 MHz, $CDCl_3$) of **2H-POctaCor**, selected regions (above) and full spectrum (below).



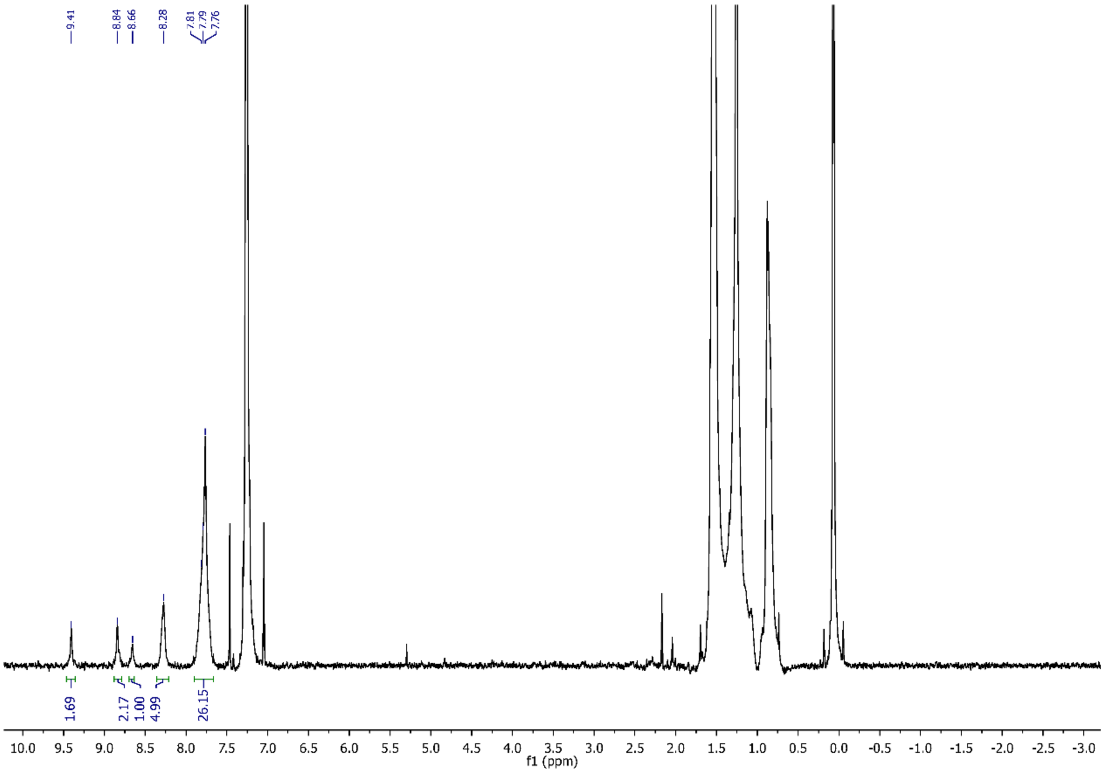
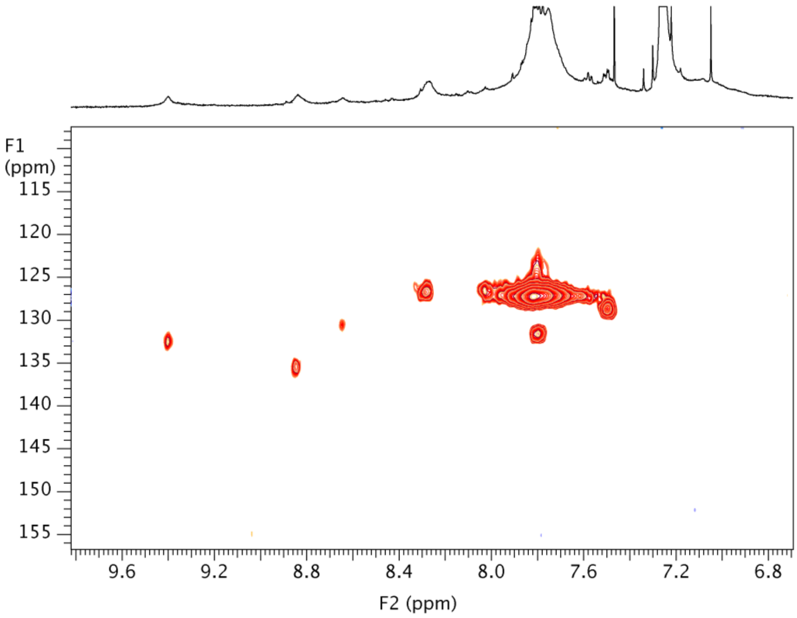


Figure S8: ^{1}H NMR (500 MHz, $CDCl_3$) of **Zn-POctaCor**, selected regions (above) and full spectrum (below).



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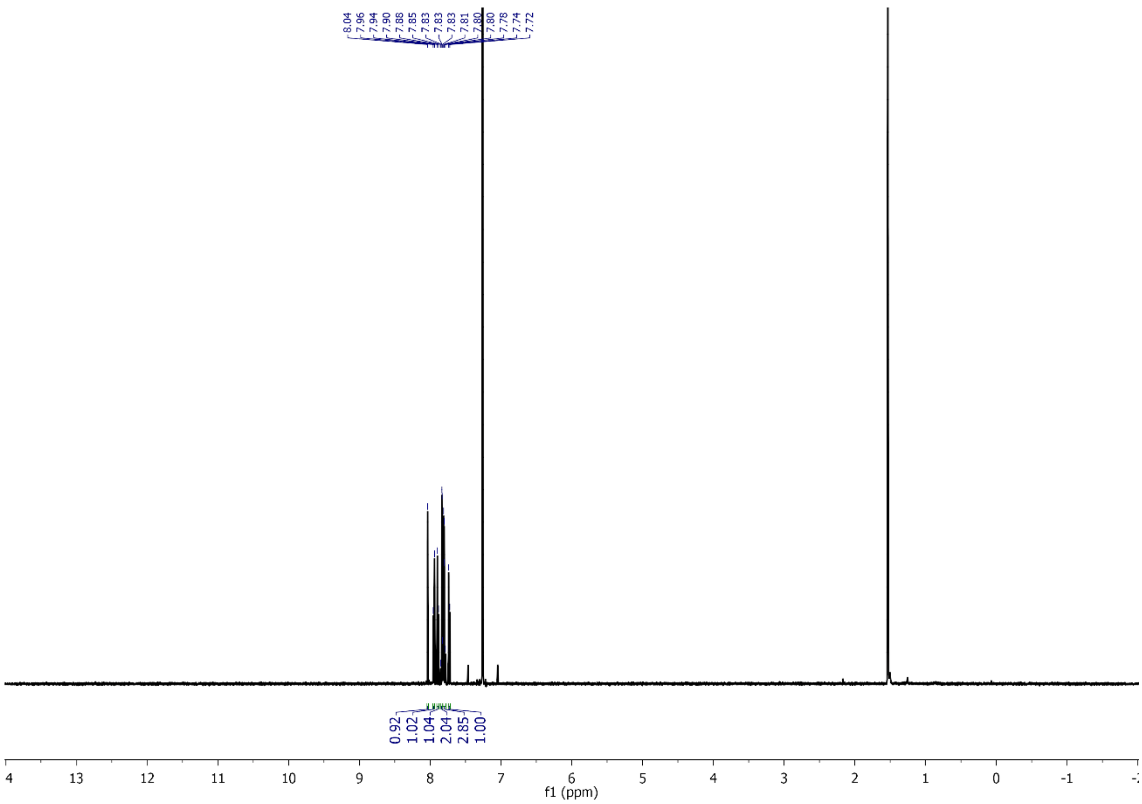


Figure S10: Full ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **Br-Cor**.

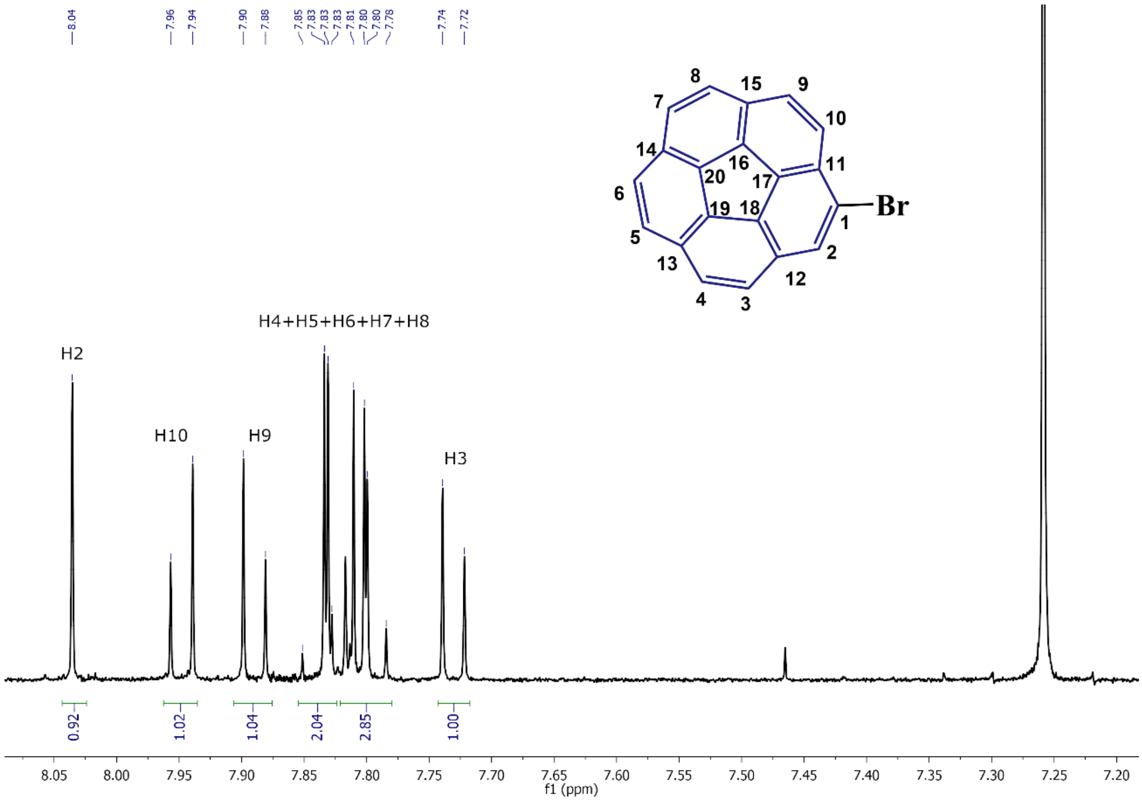


Figure S11: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **Br-Cor** selected regions.

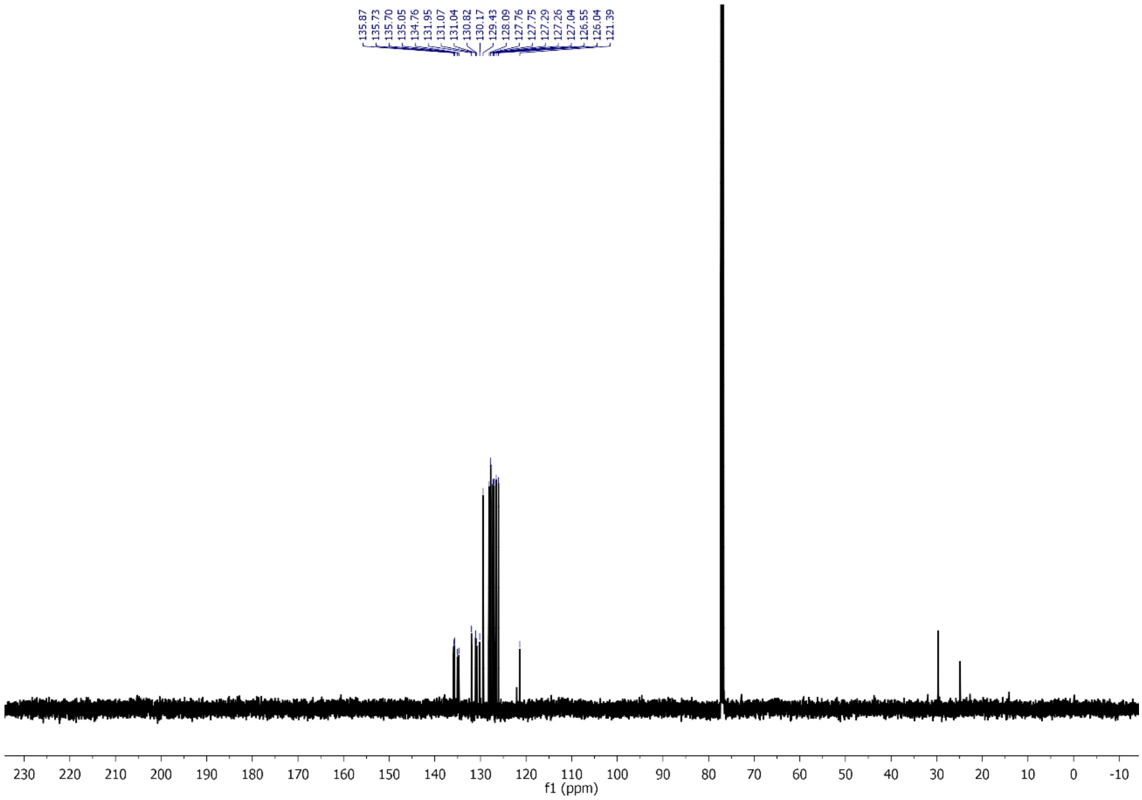


Figure S12: Full ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) spectrum of **Br-Cor**.

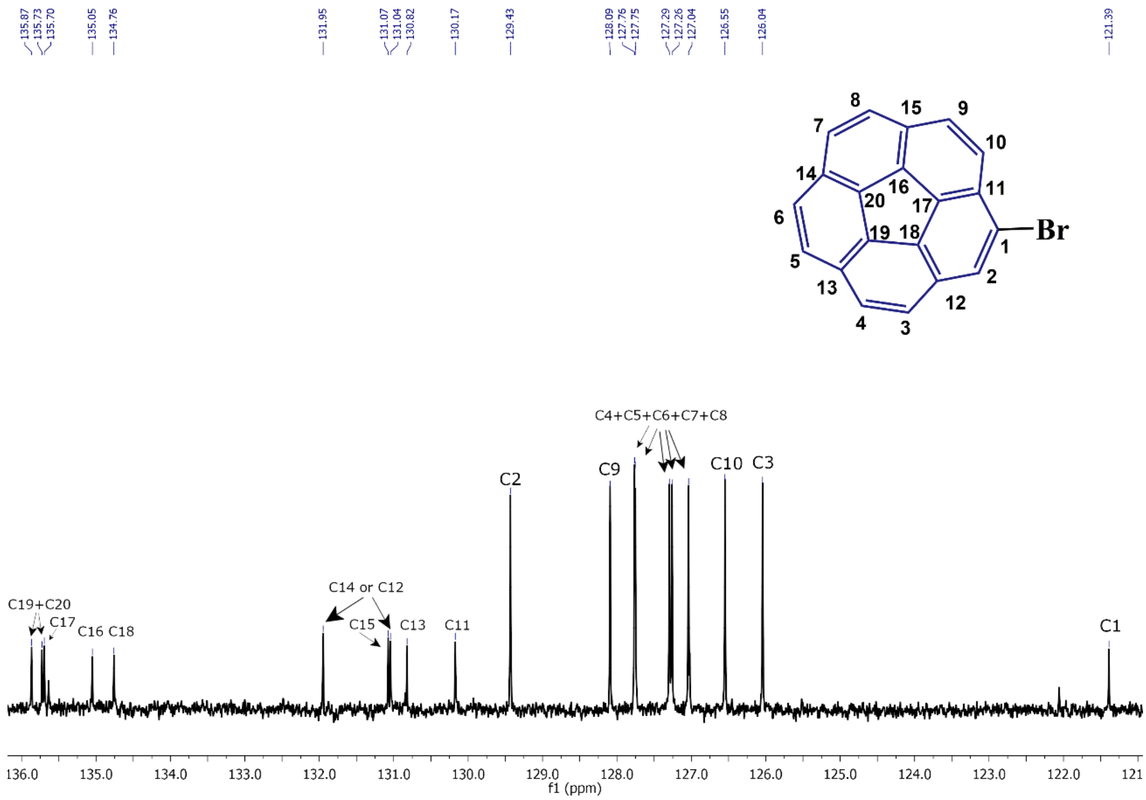


Figure S13: $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) spectrum of **Br-Cor** selected regions.

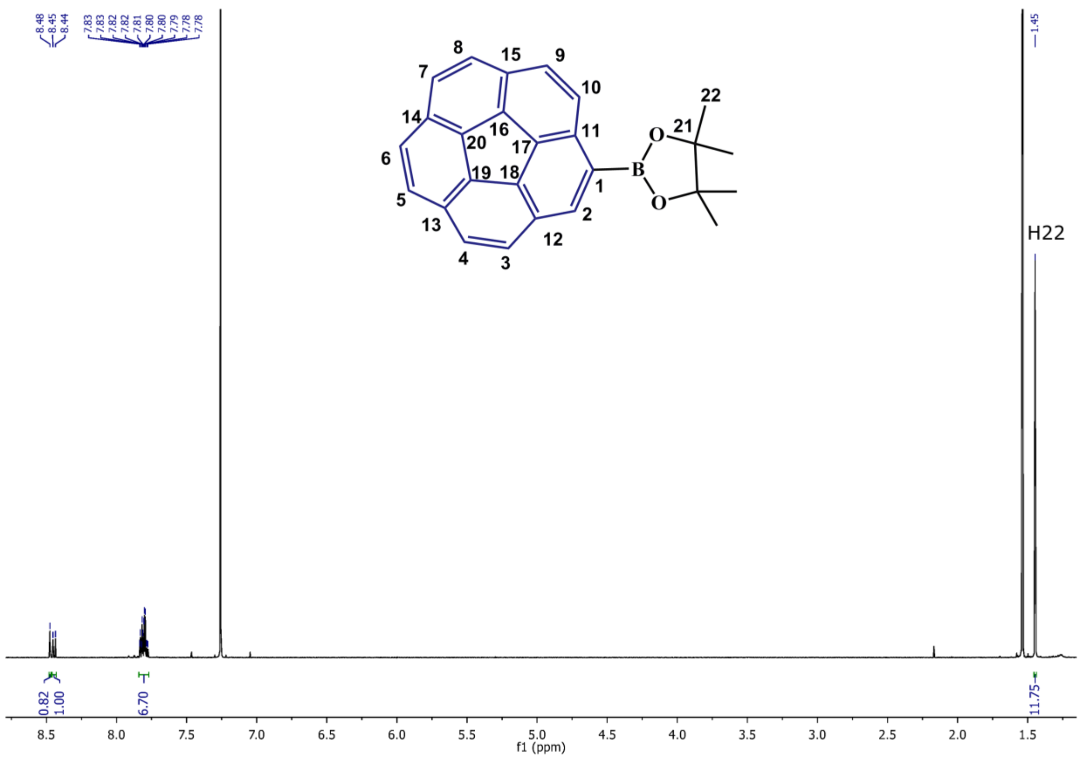


Figure S14: Full ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **Bpin-Cor**.

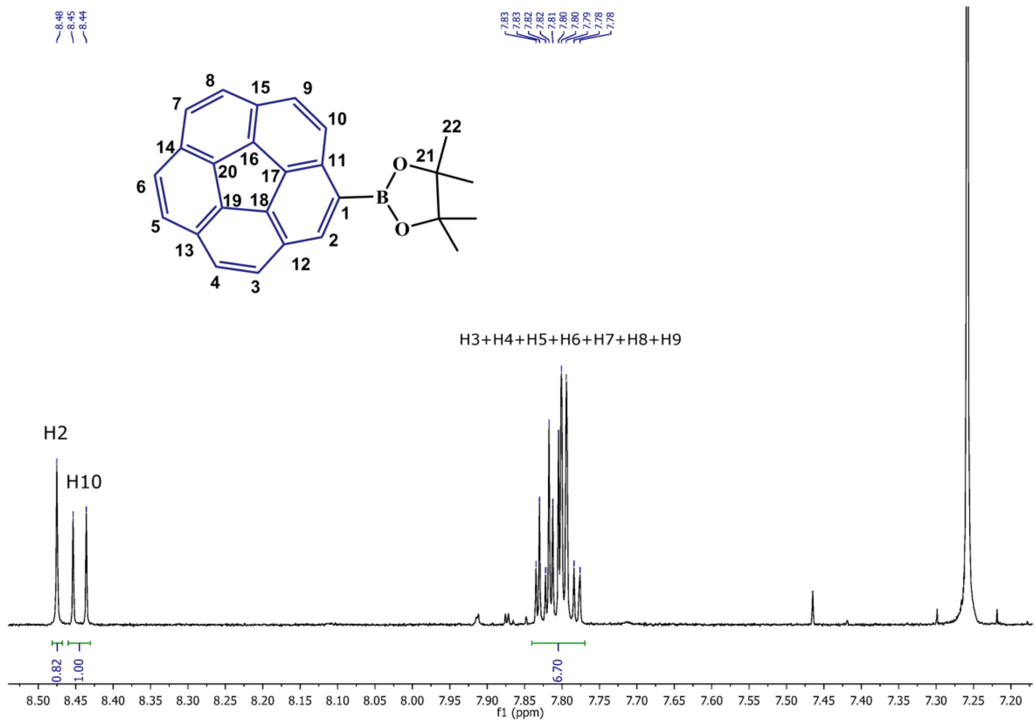


Figure S15: ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **Bpin-Cor** selected regions.

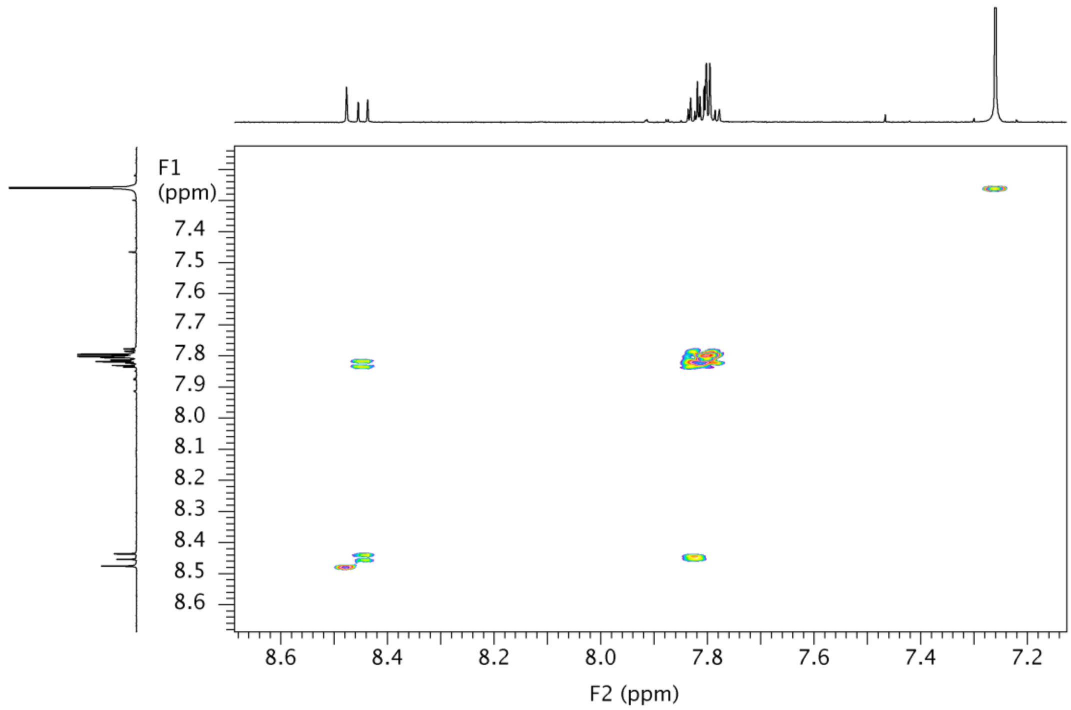


Figure S16: ^{1}H-^{1}H COSY of **Bpin-Cor**.

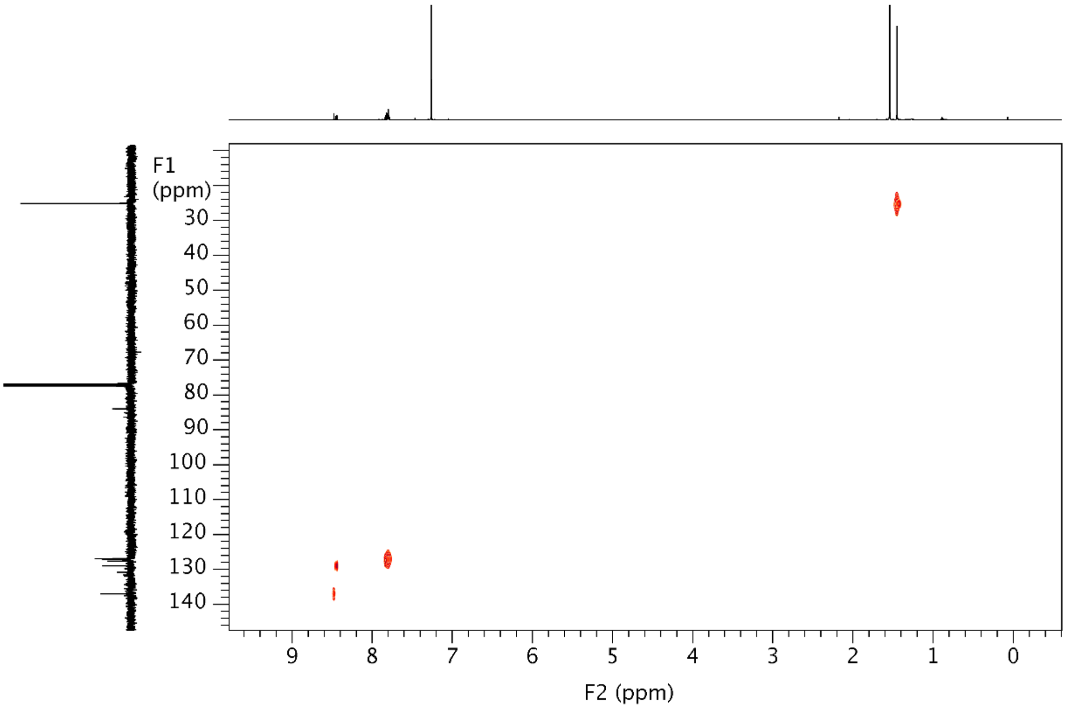


Figure S17: ^{1}H-^{13}C HSQC of **Bpin-Cor**.

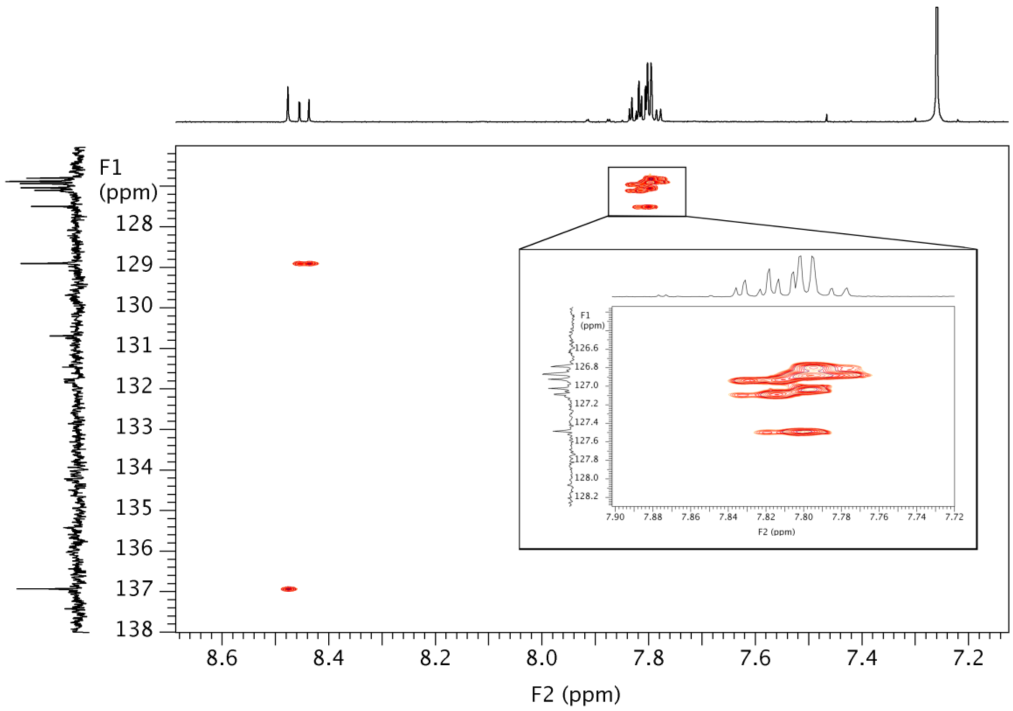


Figure S18: ^{1}H-^{13}C band selective HSQC of **Bpin-Cor**.

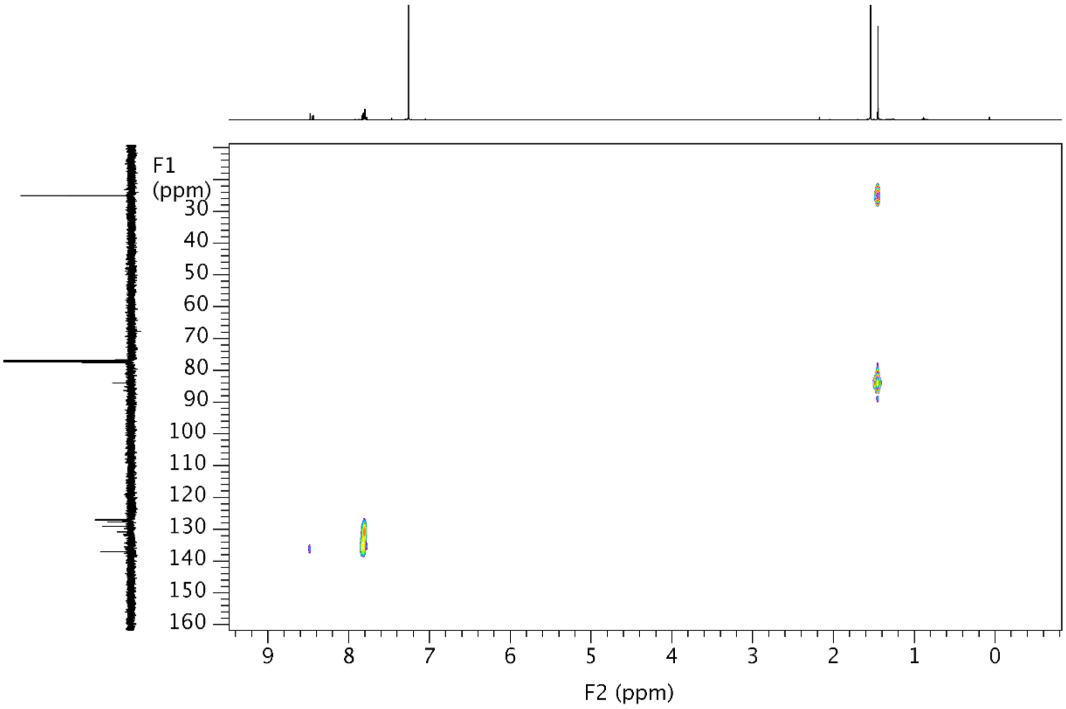


Figure S19: ^{1}H-^{13}C HMBC of **Bpin-Cor**.

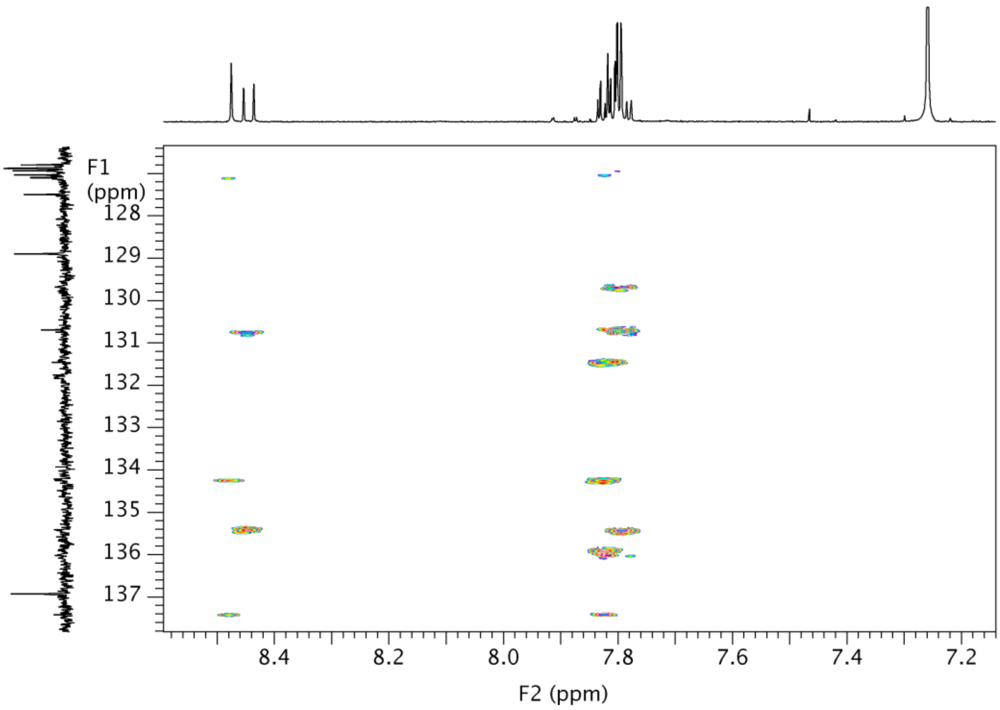


Figure S20: ^{1}H-^{13}C band selective HMBC of **Bpin-Cor**.

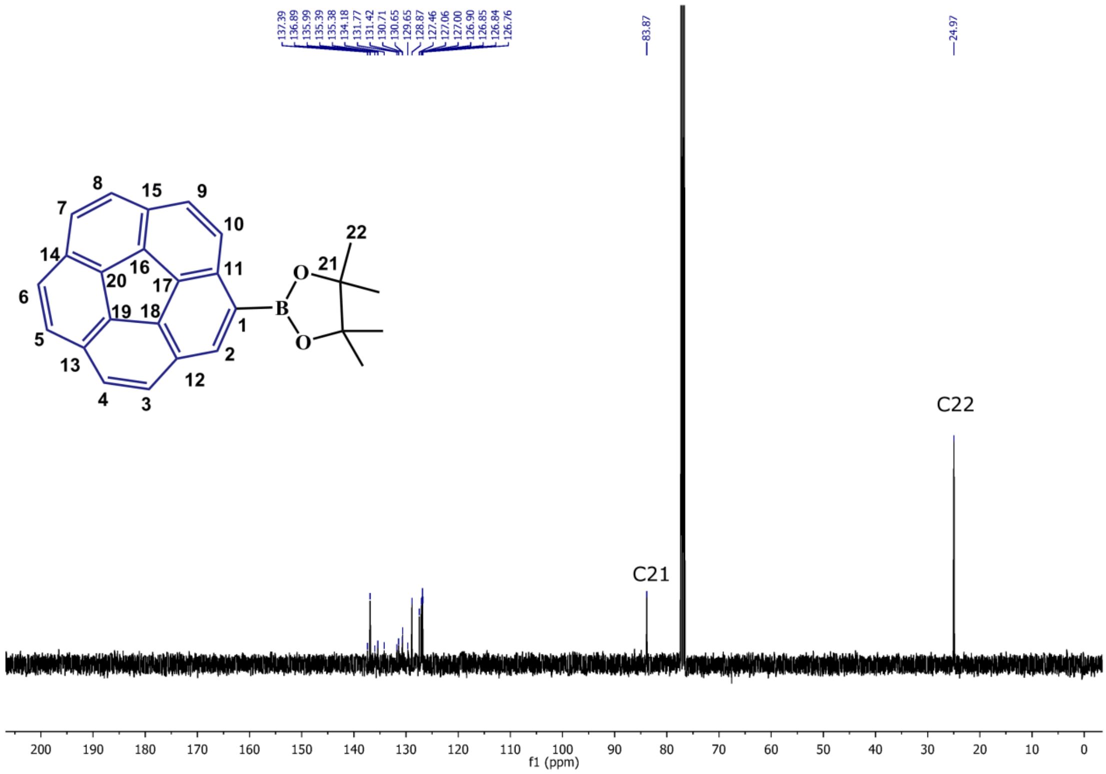


Figure S21: Full $^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **Bpin-Cor**.

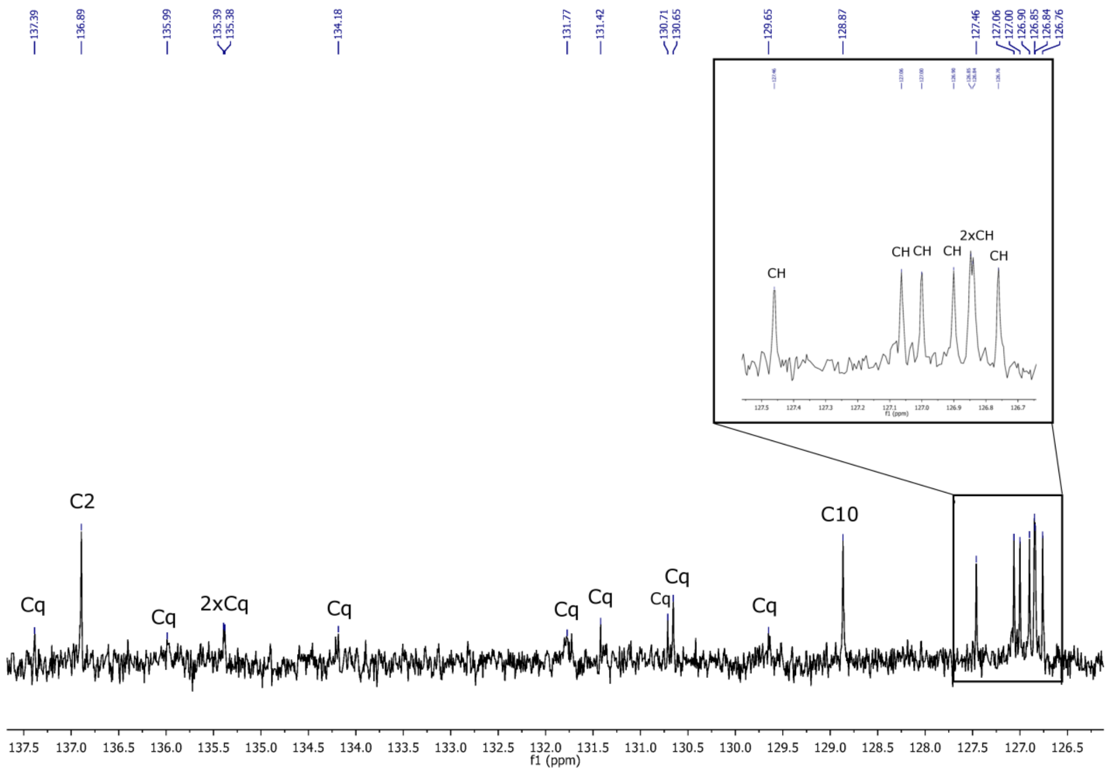


Figure S22: $^{13}C\ \{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **Bpin-Cor** selected regions.

UV/Vis spectra for compounds 2H-POctaCor and Zn-POctaCor

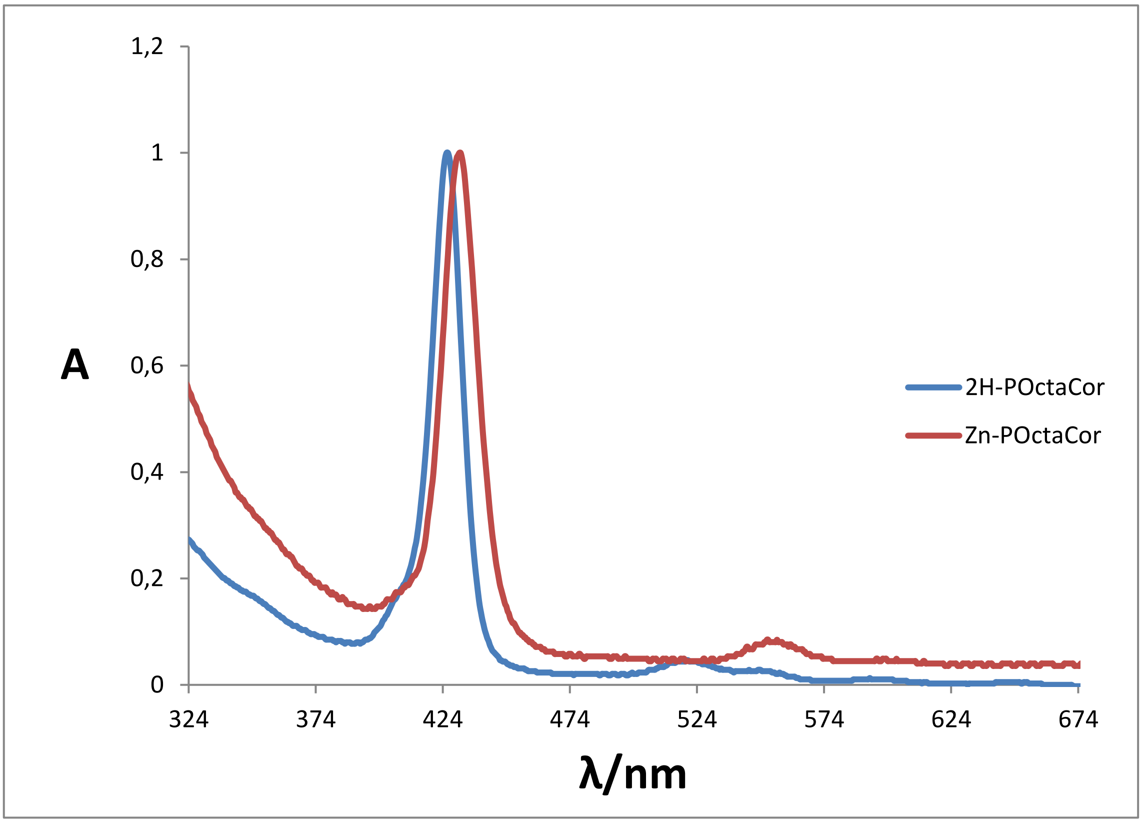


Figure S23: Normalized UV-Vis absorption spectra of **2H-POctaCor** and **Zn-POctaCor** in toluene.

MS spectra for compounds 2H-POctaCor and Zn-POctaCor

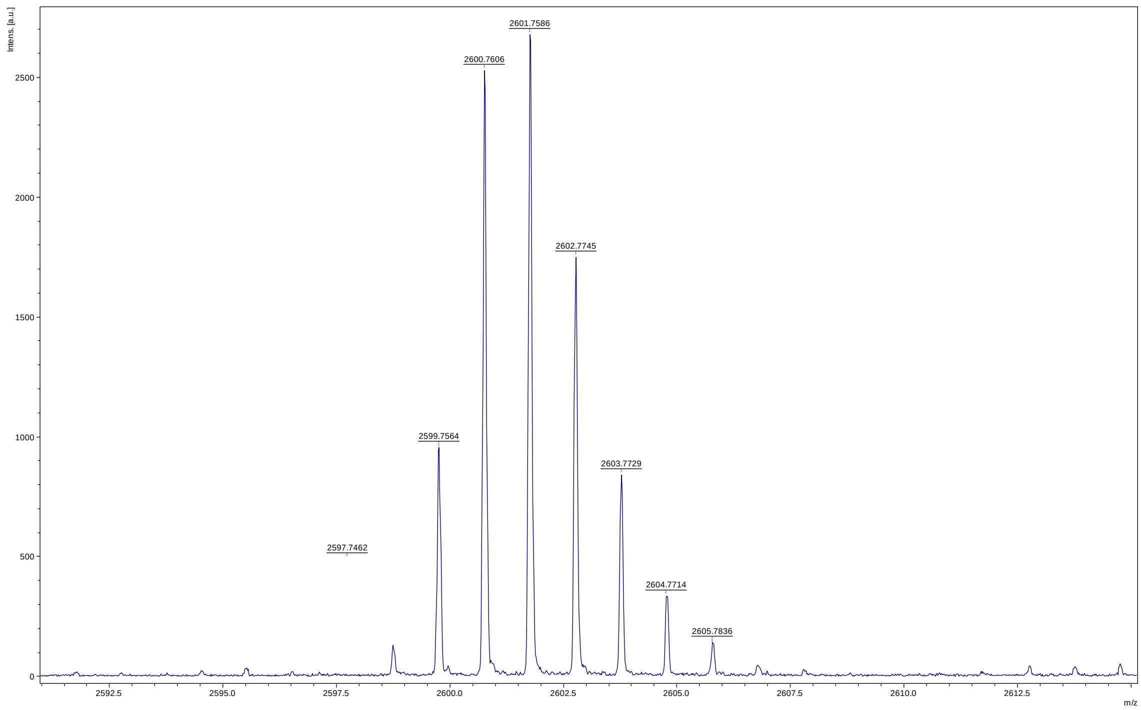


Figure S24: MS (MALDI-TOF) in dithranol of **2H-POctaCor** $[M+H]^+$.

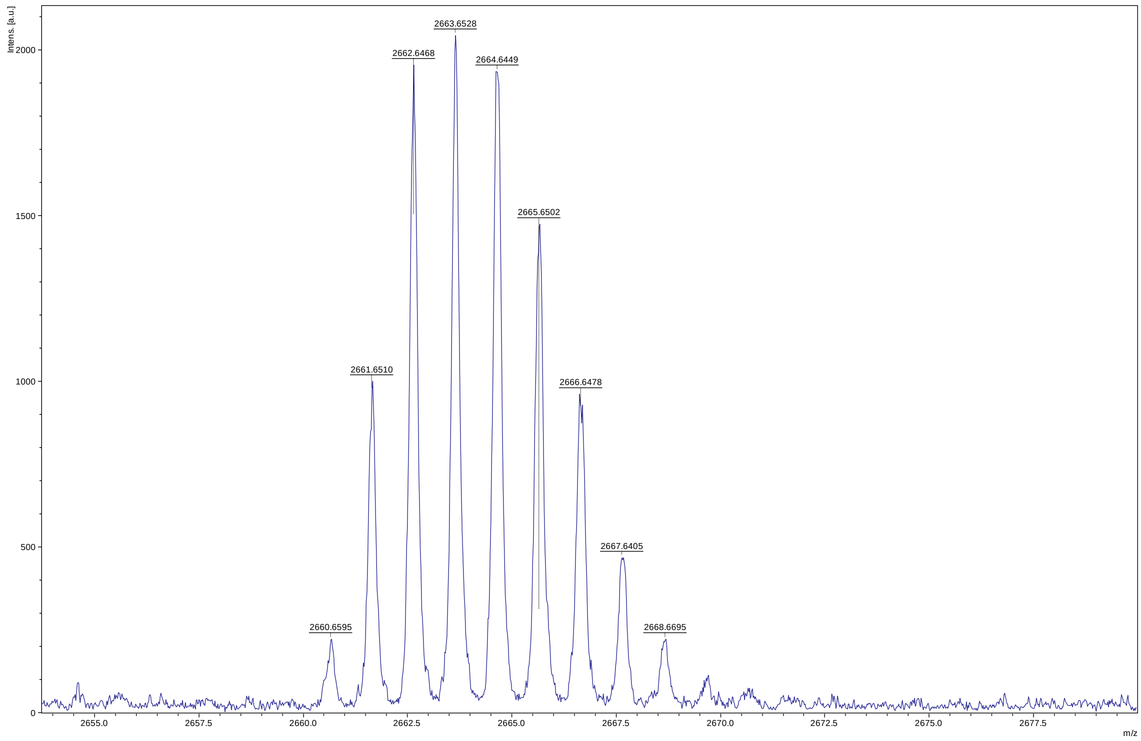


Figure S25: MS (MALDI-TOF) in DCTB of **Zn-POctaCor** $[M]^+$.

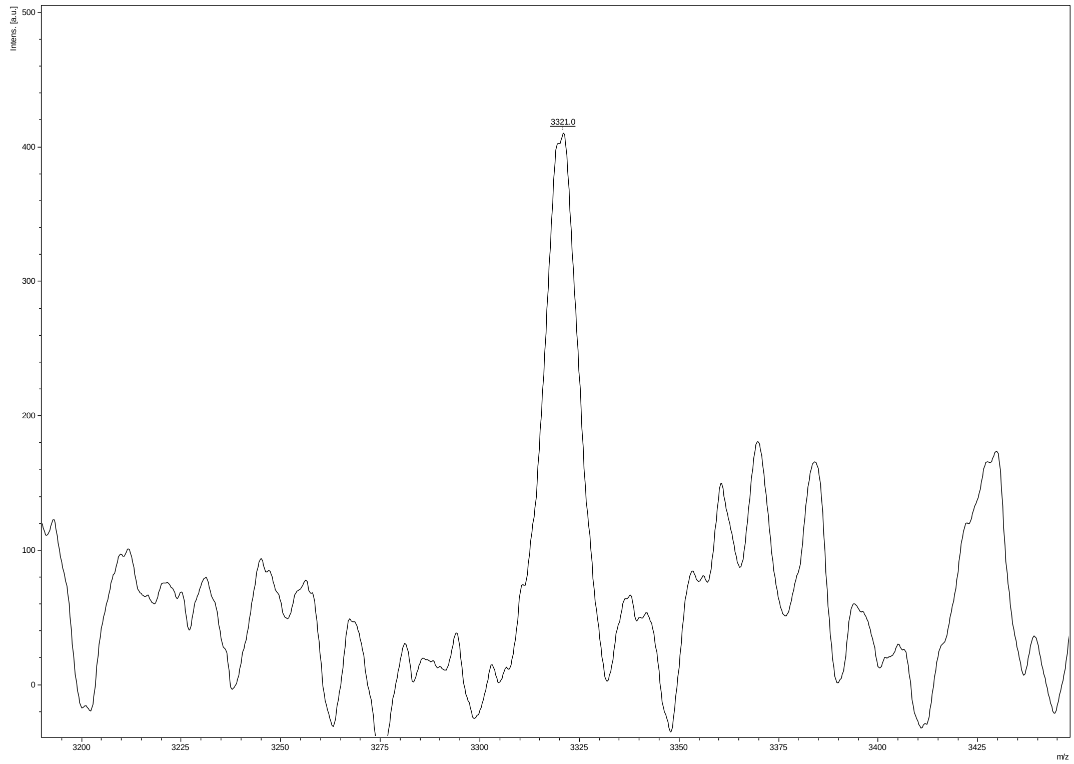


Figure S26: MS (MALDI-TOF) in DCTB of **C_{60}@2H-POctaCor** $[M]^+$ (Linear mode).

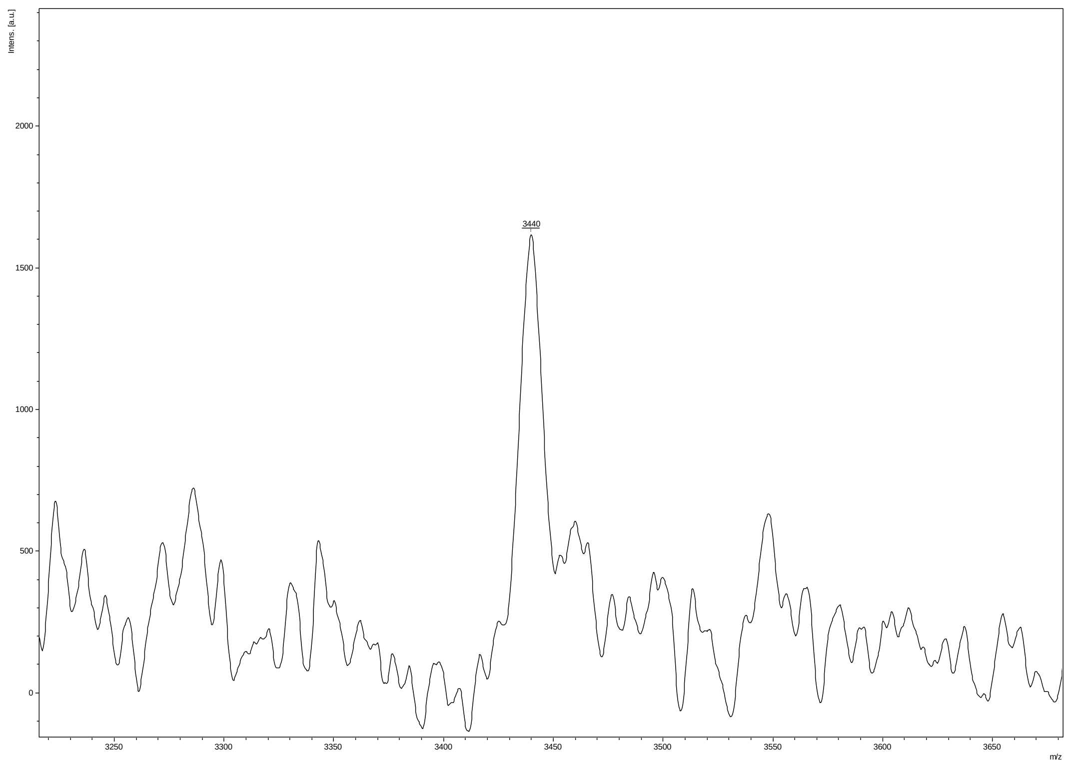


Figure S27: MS (MALDI-TOF) in DCTB of **C_{70}@2H-POctaCor** $[M]^+$ (Linear mode).

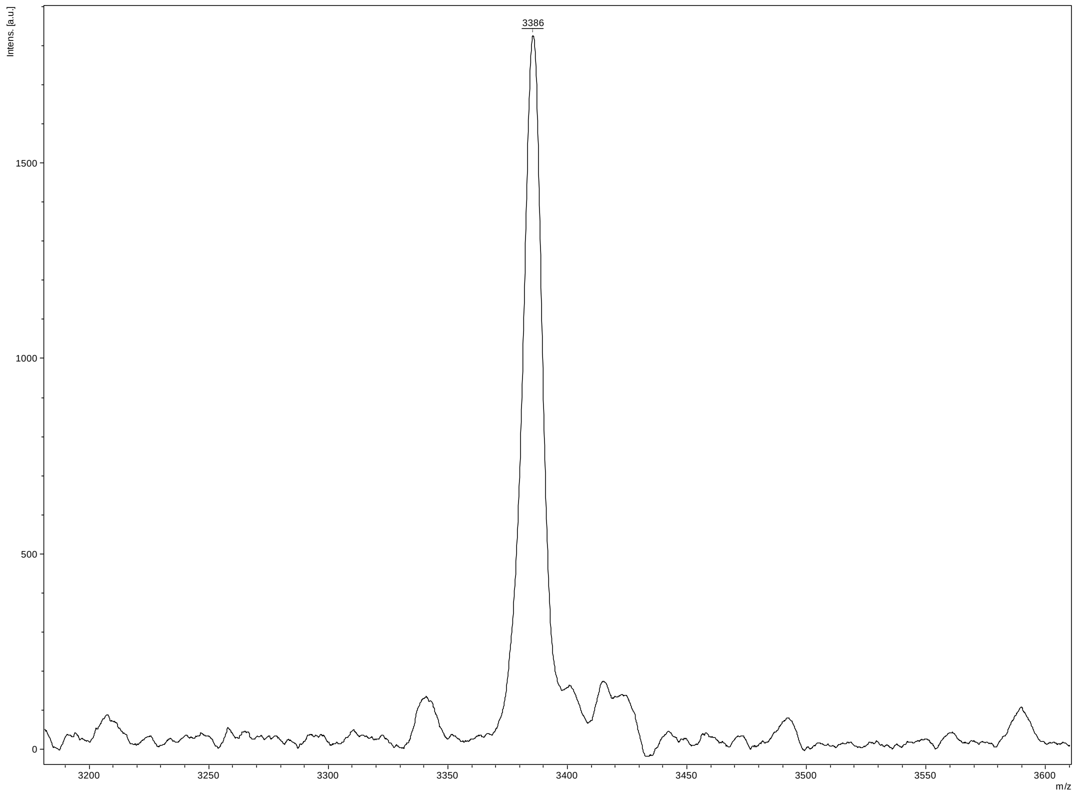


Figure S28: MS (MALDI-TOF) in DCTB of **C_{60}@ Zn-POctaCor** $[M]^+$ (Linear mode).

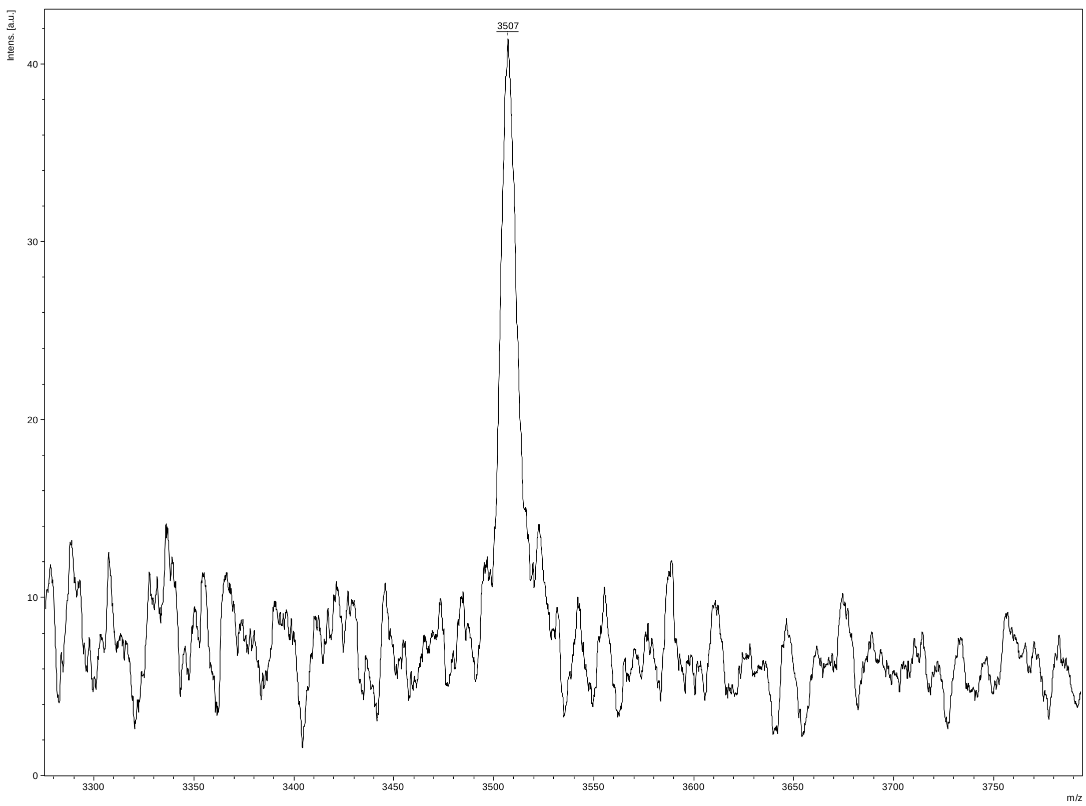


Figure S29: MS (MALDI-TOF) in DCTB of **C_{70}@ Zn-POctaCor** $[M]^+$ (Linear mode).

Complexation measurements

In order to estimate the association constants (K_a) of the compounds **2H-POctaCor** and **Zn-POctaCor** with fullerenes, the dilution method was applied. A 10^{-5} M solution of each compound in deuterated toluene was prepared, and a known volume was transferred to an NMR tube (500 µL). The titration was carried out by adding known portions of a stock solution of C_{60} or C_{70} (10^{-4} M) in deuterated toluene to cover a wide range of equivalents. In the case of the **C_{70}@Zn-POctaCor** adduct, a 10^{-3} M stock solution of C_{70} was used. A ^{1}H NMR spectrum was recorded at room temperature after each addition. Once all data had been obtained, the changes in the chemical shifts (Δδ) of selected protons were plotted as a function of the molar fraction of the guest, and the resulting curve was fitted by a nonlinear method using the global analysis approach according to the following equations, depending of the type of equilibrium:[1]

<u>1:1 Equilibrium</u>

General expression for the equilibrium constant:

$$K_a = \frac{[HG]}{[H][G]} \quad \text{eq.1}$$

Changes upon NMR titration:

$$\Delta\delta = \Delta\delta_{\Delta HG}\left(\frac{[HG]}{[H]_0}\right) \quad \text{eq.2}$$

Where:

[HG] is the concentration of the guest of the complex, and is calculated using the following equation:

$$[HG] = \frac{1}{2}\left([G_0] + [H_0] + \frac{1}{K_a}\right) - \sqrt{\left([\mathrm{G}_0] + [\mathrm{H}_0] + \frac{1}{\mathrm{K_a}}\right)^2 + 4[\mathrm{G}_0][\mathrm{H}_0]} \quad \text{eq.3}$$

Where:

$[G_0]$ is the total concentration of the guest

$[H_0]$ is the total concentration of the host

$\Delta\delta_{\Delta HG}$ is Δδ at maximum complexation (100% supramolecular complex formation)

K_a is the estimated association constant for a 1:1 equilibrium

$\Delta\delta_{\Delta HG}$ and K_a for a 1:1 equilibrium were extracted using the non-linear curve fitting tool at the open access web portal *http://supramolecular.org* (accessed since 2016). Links to all the fittings of the data are provided below for every case.

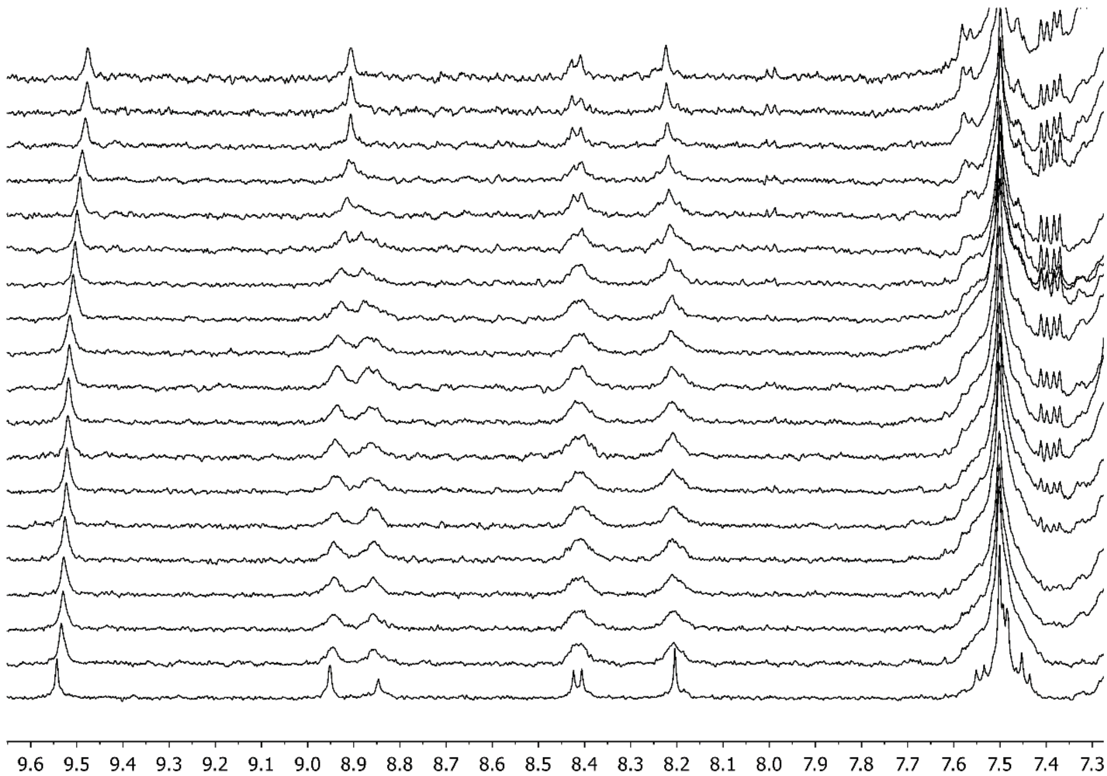


Figure S30: ^{1}H-NMR spectra of the titration of **2H-POctaCor** (10^{-5}M) with variable concentrations of C_{60} (10^{-4} M) in toluene-d_8.

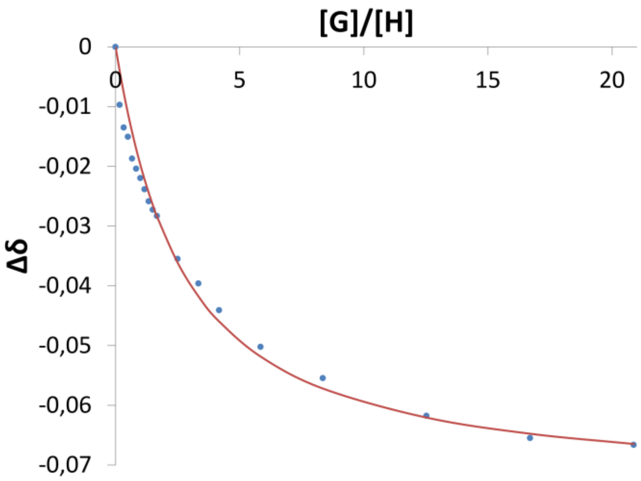


Figure S31: Nonlinear regression for the results of the titration of **2H-POctaCor** with C_{60} for the selected proton (β-pyrrole proton (H_2), 1:1 binding model).

For additional information see:

http://app.supramolecular.org/bindfit/view/f09b4585-d534-402c-a7fd-39218aaee0bf

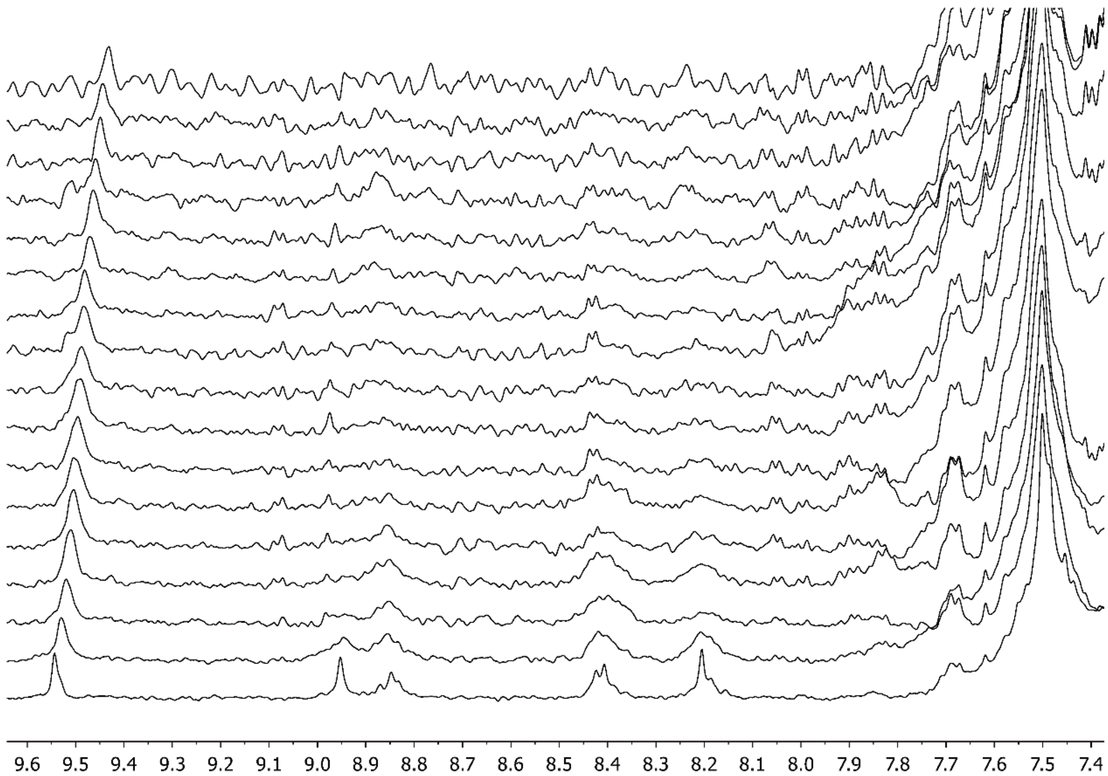


Figure S32: [1]H-NMR spectra of the titration of **2H-POctaCor** (10^{-5}M) with variable concentrations of C_{70} (10^{-4} M) in toluene-d_8.

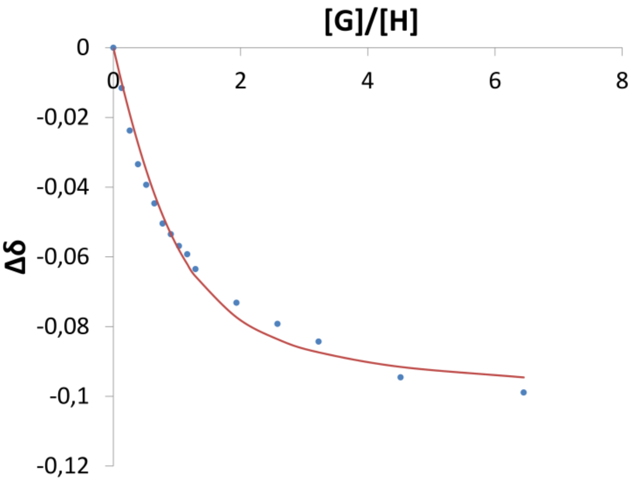


Figure S33: Nonlinear regression for the results of the titration of **2H-POctaCor** with C_{70} for the selected proton (β-pyrrole proton (H_2), 1:1 binding model).

For additional information see:

http://app.supramolecular.org/bindfit/view/a865a6fe-7c2a-4fb2-8be1-938088d7126d

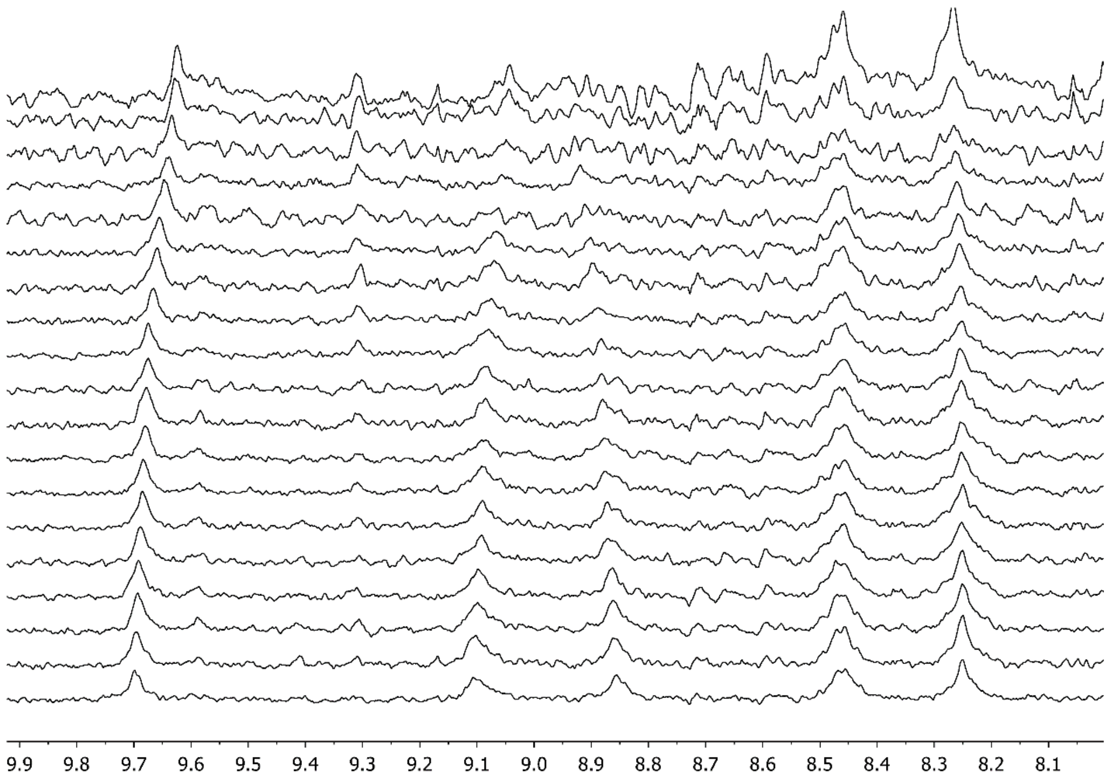


Figure S34: ^{1}H-NMR spectra of the titration of **Zn-POctaCor** (10^{-5}M) with variable concentrations of C_{60} (10^{-4} M) in toluene-d_8.

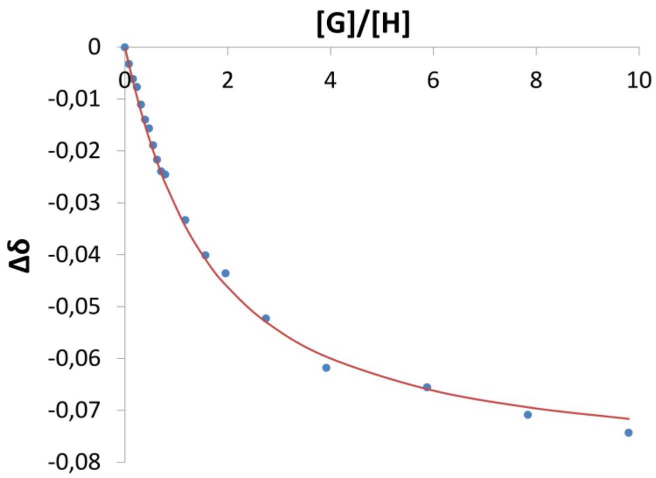


Figure S35: Nonlinear regression for the results of the titration of **Zn-POctaCor** with C_{60} for the selected proton (β-pyrrole proton (H_2), 1:1 binding model).

For additional information see:

http://app.supramolecular.org/bindfit/view/8033f78b-9ab6-4d8f-bab8-ac50044d314f

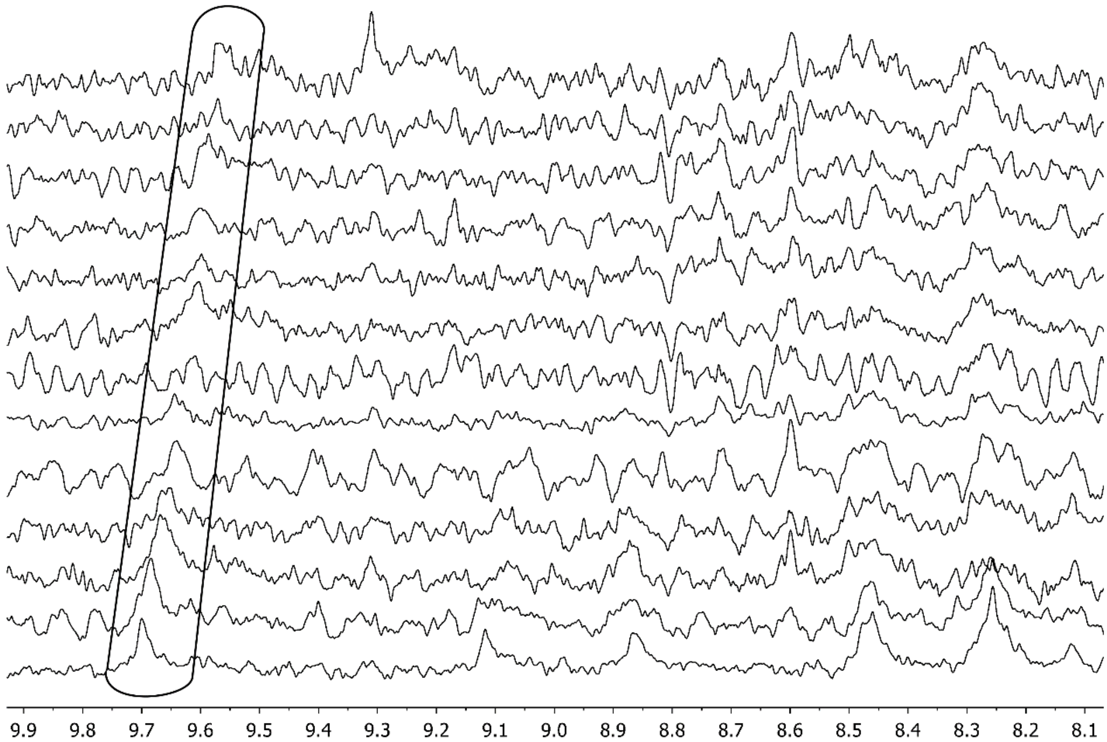


Figure S36: ^{1}H-NMR spectra of the titration of **Zn-POctaCor** (10^{-5}M) with variable concentrations of C_{70} (10^{-3} M) in toluene-d_8. (See Figure S33 for line fitting.)

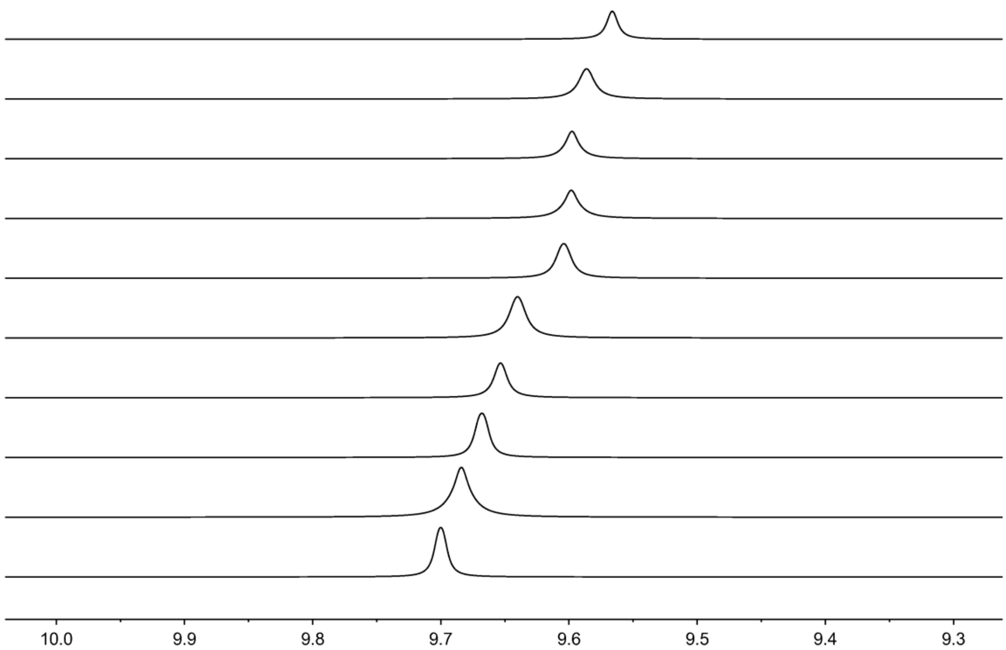


Figure S37: ^{1}H-NMR spectra of the titration of **Zn-POctaCor** (10^{-5}M) with variable concentrations of C_{70} (10^{-3} M) in toluene-d_8 for the selected proton signal H_2 of Figure S32 using line fitting of MNova Software.

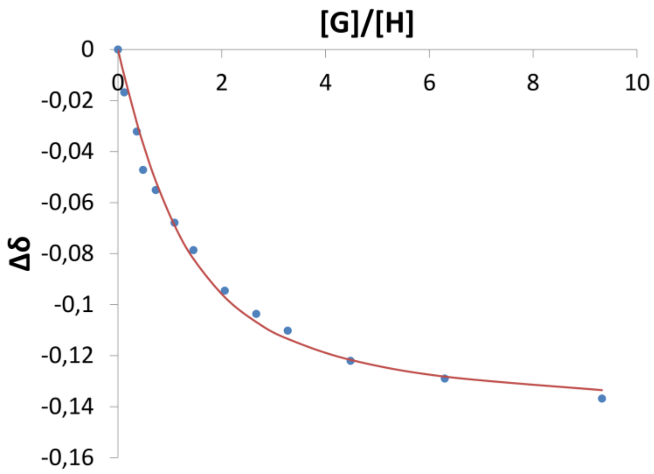


Figure S38: Nonlinear regression for the results of the titration of **Zn-POctaCor** with C_{70} for the selected proton (β-pyrrole proton (H_2), 1:1 binding model).

For additional information see:

http://app.supramolecular.org/bindfit/view/f4a435b0-772a-497d-8633-5f6ae4f04cd7

Computational methods

Compound **2H-POctaCor** was first subjected to a conformational search based on molecular mechanics in a non-periodic system with toluene described as the implicit solvent by running a series of dynamics at 500 K, 1000 K and 2000 K using the Langevin dynamics model and generalized Amber force field (GAFF) in the Amber package.[2] The results were subjected to clustering analysis, and the most populated cluster was further optimized by DFT methods in the Gaussian 16 package[3] with Grimme's B97D3 functional containing the Becke-Johnson damping empirical dispersion correction.[4] Pople and collaborators' split valence basis set 6-31G(d,p) was chosen.[5] For supramolecular assemblies C_{60}@**2H-POctaCor** and $(C_{60})_2$@**2H-POctaCor**, the strategy consisted of carrying out several optimization runs with the semi-empirical PM6 Hamiltonian[6] by placing a C_{60} molecule over the porphyrin core and modifying the orientations of the corannulene substituents. The most stable minimum with chemical significance was further subjected to DFT optimization using the protocol described above. All minima were confirmed by vibrational analysis to have zero imaginary frequencies in all cases. Interaction energies were calculated on the optimized geometries by using a more extended 6-31+G(d,p) basis set that includes diffuse functions[7] and taking into account basis set superposition error (BSSE) with the Boys–Bernardi functional counterpoise scheme[8] as follows:

$$E_{int}(AB) = E_{AB}^{\alpha\beta}(AB) - E_{AB}^{\alpha\beta}(A) - E_{AB}^{\alpha\beta}(B)$$

Where the subscripts denote the geometry used (inclusion complex in all cases) and the superscripts refer to the basis set (the one from the supramolecular assembly in all cases); A and B correspond to the molecular entities interaction to furnish the AB adduct. It is worth noting that all the quantum mechanics calculations were performed in the gas phase. Applying an implicit solvent model (toluene in this case) would have increased the accuracy, but remarkably increased the time needed to reach convergence in the first attempts we performed due to the significant size of the system (over 400 atoms). Since all the molecules are neutral and the solvent is not very polar, we assume the stabilization energy provided by solvation would not substantially modify the results presented in this work.

Non-covalent interactions were obtained by location critical points where the reduced density gradient decreases at low electronic density values according to Yang and collaborators' scheme with the help of the NCIPlot package.[9] Calculations were performed with promolecular densities and gradient isosurfaces were plotted with an isovalue of 0.3 a.u. and colored on a blue-green-red scale according to values of the sign of λ_2 (second eigenvalue of the electron-density Hessian). Red indicates repulsion, green means weak attraction, and blue represents strong attraction. Graphics were visualized in Chimera[10] with the help of Tangram NCIPlot GUI built by Insilichem Group.[11]

Discussion for $(C_{60})_2$@2H-POctaCor

The structure of the inclusion complex $(C_{60})_2$@**2H-POctaCor** is shown in Figure S39. The presence of the first molecule of fullerene on the porphyrin hampers the efficient association of the second molecule that approaches from the other face. The approximation of C_{60} is not hindered, but the arrangement of the corannulene arms is highly obstructed owing to an important loss of interaction with the previous fullerene due to the rotation of the phenylene substituents. In order to minimize this loss, one of the corannulene substituents has moved away from the optimum distance as a result of phenylene rotation (with a torsional angle of 94°), allowing at least two other corannulene units to form a tweezer-like conformation in order to bind the second fullerene molecule. The porphyrin core is substantially deformed to accommodate the double partial association, adopting a ruffled conformation. This particular structure rearrangement shows that there is indeed a negative allosteric induction due to the fact that the receptor must adopt a sub-optimal conformation in order to maintain an efficient interaction with the previously associated C_{60} in the inclusion complex.

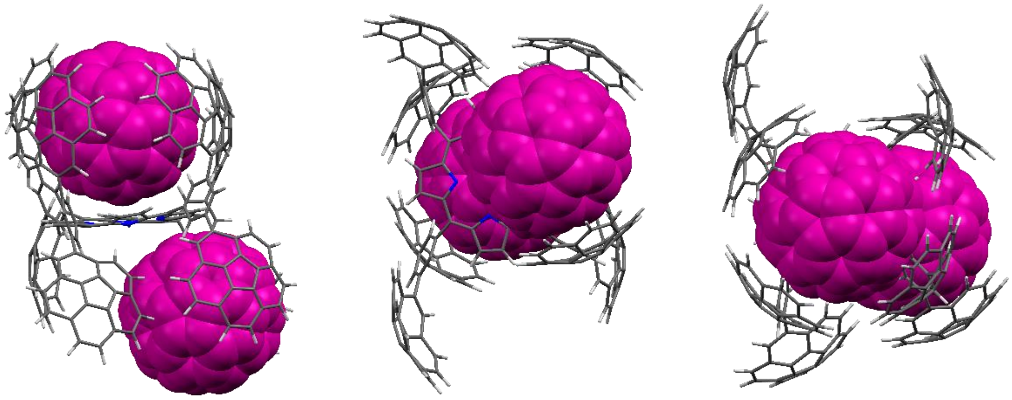


Figure S39. Side (a), top (b), and bottom (c) views of the optimized structure of $(C_{60})_2$@**2H-POctaCor.**

Figure S39 reveals that the first fullerene molecule lost one corannulene interaction. One very powerful method to visualize this effect is the depiction of supramolecular interactions on the basis of critical points observed for reduced density gradient at low values of electron density allowed by NCIPlot code.[10-11] In the optimized structure of $(C_{60})_2$@**2H-POctaCor**, only four surfaces are observed in one fullerene molecule, whereas the second fullerene species is partially covered by two corannulene substituents and less than half of the porphyrin core in a pincer-like arrangement as shown in Figure S40. This figure shows that the second fullerene displays only two interactions with the molecular clip. This is in contrast to (C_{60})@**2H-POctaCor**, which exhibits five bowl-shaped strongly attractive interactions within the distance between the fullerene and molecular clip **2H-POctaCor**, four from the four corannulene moieties and one with the porphyrin core, demonstrating the excellent complementarity between both species, as almost all the C_{60} is covered (Figs 4c and 4d in the main text). This analysis can also support the observed lower Gibbs energy for the binding of one fullerene compared to the association of two, which agrees well with the experimental data, which shows a 1:1 rather than 1:2 binding stoichiometry.

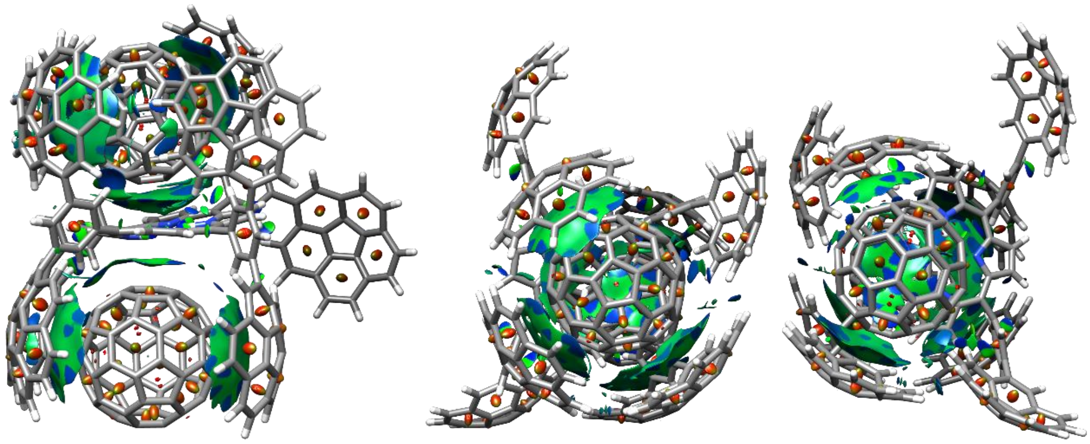
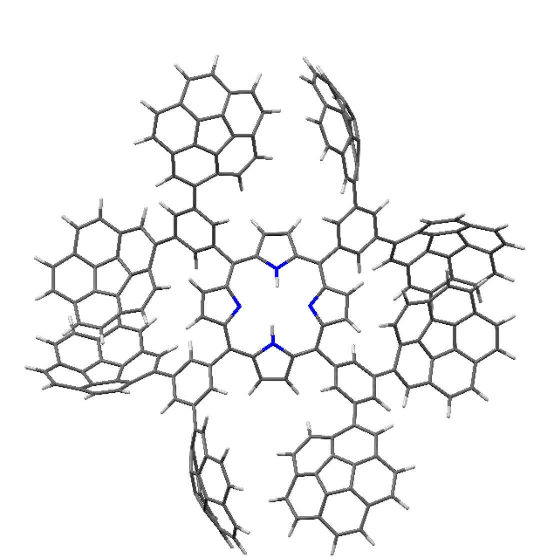
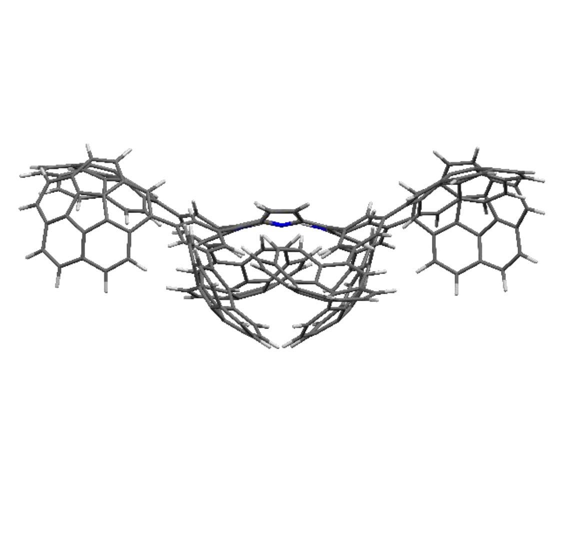


Figure S40. Side (a) top (b) and bottom (c) views of NCI plots for the optimized structure of $(C_{60})_2$@**2H-POctaCor**.

Optimized geometries

2H-POctaCor (E = -8042.223702 a.u.)





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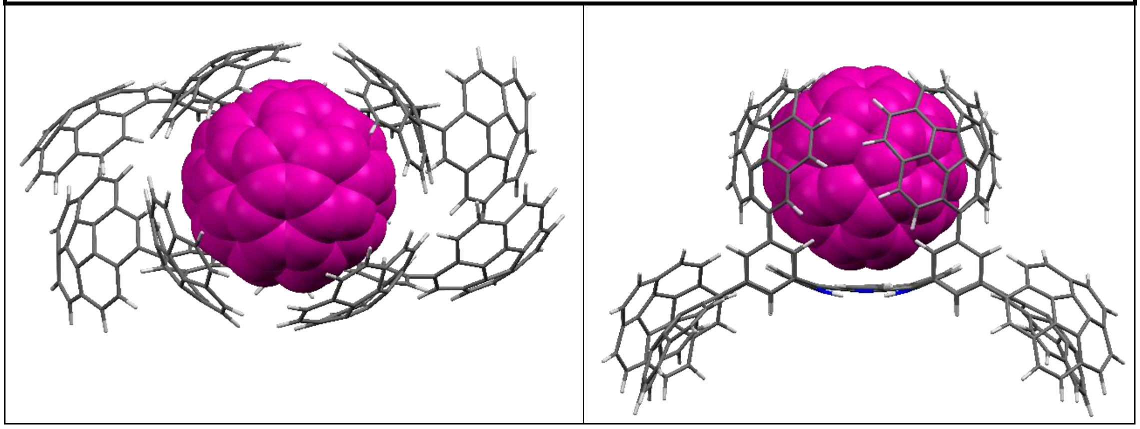

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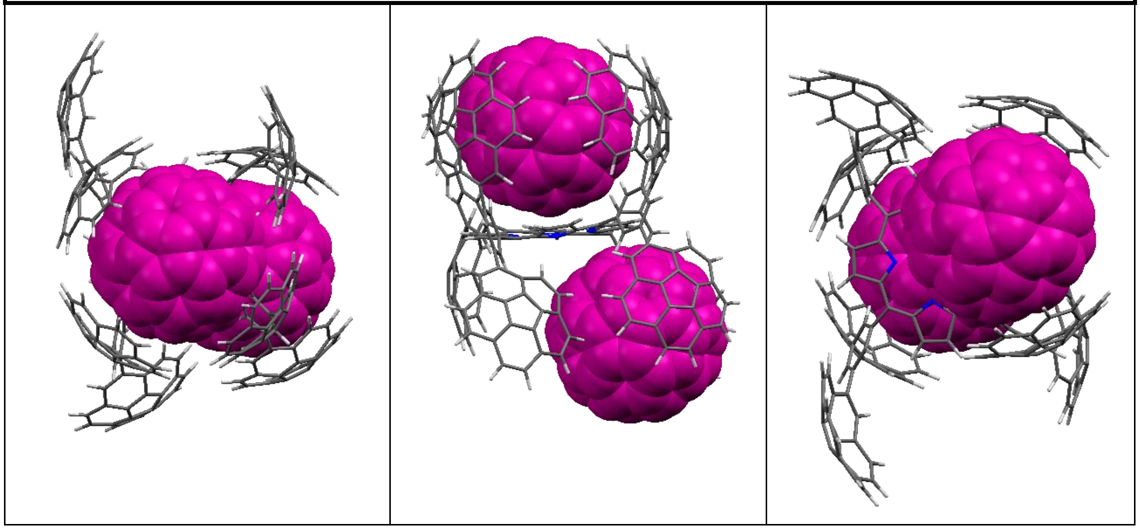

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H	-3.264178	3.399618	0.790803
C	-0.957368	4.086890	3.833863
H	0.152647	2.360233	3.174617
C	-4.235708	5.342834	2.277935
C	-2.094468	4.891850	3.613931
C	-5.298812	5.277059	3.275537
C	-4.495715	5.828130	0.985305
H	-2.290898	5.739588	4.269536
C	-5.400842	4.388740	4.417237
C	-6.492481	5.902352	2.911019
C	-5.801332	6.279941	0.566765
H	-3.700197	5.748266	0.243058
C	-6.630477	4.042371	4.976900
H	-4.502760	3.892091	4.782377
C	-7.750252	5.543690	3.483989
C	-6.738115	6.393469	1.593819
C	-6.351256	6.348534	-0.773830
C	-7.882277	4.542794	4.447112
H	-6.649133	3.285673	5.762088
C	-8.769433	5.820053	2.523453
C	-8.143012	6.342996	1.354131
C	-7.725328	6.303027	-1.006593
H	-5.678250	6.335416	-1.630589
C	-9.209808	3.970966	4.550570
C	-9.974016	5.117324	2.480460
C	-8.682185	6.182533	0.076747
H	-8.071195	6.254631	-2.039685
C	-10.207413	4.246646	3.614924
H	-9.407329	3.218870	5.315119
C	-10.645083	5.141227	1.196424
C	-10.028592	5.647272	0.051390
H	-11.148536	3.699972	3.681869
H	-11.613431	4.650850	1.092581
H	-10.537317	5.532851	-0.906342
C	0.871080	2.884519	-4.564156
C	-0.173681	3.623232	-5.140570
C	2.137518	3.468592	-4.424101
C	-0.001827	4.979727	-5.470727
H	-1.155731	3.165582	-5.237094
C	2.336228	4.824678	-4.739763
H	2.923303	2.914062	-3.919173
C	-1.173806	5.791663	-5.903676
C	1.259351	5.572727	-5.256155
C	-2.378301	5.834009	-5.065784
C	-1.146511	6.431387	-7.152217
H	1.388373	6.638432	-5.442185
C	-2.801571	4.968197	-3.977404
C	-3.371486	6.701900	-5.517735
C	-2.288140	7.133181	-7.696840
H	-0.263023	6.280270	-7.774029
C	-4.139883	4.840071	-3.602820
H	-2.078924	4.329519	-3.477795
C	-4.740857	6.574159	-5.132660
C	-3.332587	7.331698	-6.795456
C	-2.625849	7.405250	-9.080905
C	-5.194967	5.575102	-4.272176
H	-4.395395	4.100740	-2.844035
C	-5.543952	7.108425	-6.181912
C	-4.673723	7.577009	-7.209187
C	-3.941041	7.636190	-9.487441
H	-1.850032	7.330274	-9.844098
C	-6.607048	5.267116	-4.389816
C	-6.840500	6.662020	-6.438762
C	-5.048858	7.623809	-8.551614
H	-4.145799	7.732607	-10.554663
C	-7.390134	5.785255	-5.423093
H	-7.047922	4.531800	-3.718034
C	-7.309207	6.915373	-7.787344
C	-6.456173	7.372748	-8.793387
H	-8.418601	5.434073	-5.520370
H	-8.333046	6.649729	-8.054451
H	-6.844293	7.447471	-9.810219
C	2.994368	-3.787352	-3.825818
C	2.765866	-5.096968	-4.276655
C	4.313699	-3.303055	-3.772293
C	3.842175	-5.944672	-4.610218
H	1.748712	-5.481198	-4.308439
C	5.402309	-4.141137	-4.050841
H	4.496114	-2.293432	-3.422106
C	3.601774	-7.349388	-5.032913
C	5.156863	-5.465070	-4.458411
C	2.664083	-7.661977	-6.111277
C	4.207500	-8.377393	-4.289372
H	5.995360	-6.125868	-4.674121
C	1.638512	-6.838188	-6.726232
C	2.589802	-9.013738	-6.445989
C	3.934057	-9.776774	-4.518662
H	4.807922	-8.085206	-3.426599
C	0.533590	-7.393344	-7.373161
H	1.682545	-5.755864	-6.617029
C	1.462342	-9.579678	-7.113502
C	3.203553	-10.043298	-5.675445
C	4.046432	-10.896098	-3.602623
C	0.349913	-8.826434	-7.485366
H	-0.250045	-6.722554	-7.728248
C	1.372589	-10.952326	-6.740576
C	2.449242	-11.239184	-5.851807
C	3.302579	-12.064372	-3.772191
H	4.652359	-10.789457	-2.701749
C	-0.866970	-9.592426	-7.666878
C	0.161442	-11.643341	-6.703104
C	2.375692	-12.232107	-4.875089
H	3.352492	-12.830091	-2.996679
C	-0.957316	-10.933998	-7.291872
H	-1.768963	-9.086701	-8.014414
C	0.160754	-12.814450	-5.848456
C	1.215203	-13.094673	-4.977536
H	-1.927377	-11.428801	-7.357905
H	-0.728776	-13.444769	-5.808296
H	1.111386	-13.933424	-4.287676
H	0.240644	-1.788296	-1.347134
H	-0.452775	0.333657	-1.403320
C	-10.721570	-1.684401	-0.843504
C	-10.306813	-2.576015	0.235071
C	-10.143688	-2.074359	1.536756
C	-10.390994	-0.662180	1.810697
C	-10.789394	0.195271	0.772862
C	-10.958182	-0.325894	-0.579848
C	-10.008796	-2.079743	-2.055082
C	-9.153182	-3.215743	-1.724217
C	-9.334925	-3.517964	-0.308766
C	-8.239090	-3.922123	0.467519
C	-9.003969	-2.497772	2.343983
C	-9.403710	-0.213917	2.789703
C	-8.852967	1.072771	2.689540
C	-9.266464	1.962144	1.608205
C	-10.219532	1.536375	0.672058
C	-10.035554	1.843059	-0.743908
C	-10.490719	0.691596	-1.516890
C	-9.806413	0.310976	-2.682343
C	-9.560029	-1.101643	-2.955866
C	-7.881120	-3.331380	-2.307818
C	-7.414599	-2.312396	-3.243906
C	-8.237700	-1.220282	-3.562376
C	-7.666577	0.119176	-3.663348
C	-8.636514	1.065542	-3.119732

C	-8.197600	2.172112	-2.374875
C	-8.910091	2.569623	-1.163854
C	-7.923530	3.017308	-0.185306
C	-8.098621	2.721570	1.173827
C	-8.548445	-1.350429	3.121490
C	-4.837291	1.045320	1.730228
C	-5.281159	0.067379	2.635126
C	-5.037473	-1.345255	2.359264
C	-4.356838	-1.723680	1.190994
C	-3.899017	-0.708903	0.251527
C	-4.541766	1.539736	-0.561817
C	-5.509293	2.489180	-0.015898
C	-5.691743	2.183056	1.401353
C	-6.961239	2.297182	1.983690
C	-7.426616	1.279004	2.921679
C	-6.604445	0.186479	3.242015
C	-6.205876	-2.101305	2.798365
C	-6.644802	-3.208301	2.054265
C	-5.931818	-3.604955	0.842204
C	-4.809624	-2.877078	0.418867
C	-4.622836	-2.572416	-0.998930
C	-4.056049	-1.230129	-1.100052
C	-4.449106	-0.372509	-2.139728
C	-4.695294	1.041980	-1.865528
C	-6.601571	2.900999	-0.793123
C	-6.769106	2.374974	-2.144702
C	-5.836160	1.465685	-2.671003
C	-6.294160	0.315097	-3.444526
C	-5.437456	-0.820709	-3.115263
C	-5.987086	-2.109750	-3.017088
C	-5.571470	-3.003371	-1.939297
C	-6.742454	-3.757622	-1.499745
C	-6.919180	-4.048245	-0.138047
C	-7.175612	-1.154746	3.344121
C	-8.070429	-3.404217	1.819066
C	-4.132379	0.646756	0.516724
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C	2.090976	-5.180121	7.612467
C	2.303168	-2.884924	7.737099
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C	3.433955	-3.468365	8.380830
C	0.669340	-3.803588	6.123367
C	1.908133	-6.350952	6.877367
C	2.346485	-1.625626	7.138926
C	4.402252	-5.744570	8.288836
C	4.674136	-2.830691	8.443562
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C	0.531939	-2.439079	5.647668
C	0.887792	-6.272080	5.854354
C	2.952318	-7.342425	7.048905
C	1.326951	-1.400978	6.134167
C	3.552570	-0.868643	7.405460
C	4.141312	-7.052003	7.719199
C	5.671787	-5.106578	8.575919
C	4.664819	-1.445189	8.019487
C	5.801166	-3.718885	8.648832
H	-0.136932	-2.220687	4.818591
H	0.652945	-7.156815	5.260876
H	2.854755	-8.310491	6.555444
H	1.242601	-0.422201	5.661892
H	3.644796	0.140369	7.009001
H	4.931968	-7.803789	7.725883
H	6.573316	-5.717776	8.639140
H	5.584334	-0.860772	8.079747
H	6.799258	-3.294273	8.766311
C	8.851287	-3.893252	-2.560817
C	9.370721	-2.750290	-3.238564
C	9.572571	-4.044295	-1.338625
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C	10.548910	-3.006457	-1.269983
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C	8.588187	-1.966485	-4.087678
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C	7.718482	-5.246476	-0.412120
C	9.641340	-4.242703	1.048051
C	10.117265	-0.090874	-3.519278
C	11.449431	-0.374774	-1.290150
C	10.601390	-3.232461	1.113809
C	11.572783	-1.156697	-0.141653
H	6.006432	-5.508493	-1.674576
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H	8.552186	0.043243	-4.977560
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H	11.781758	0.663197	-1.251567
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C	5.995307	5.725823	-4.353444
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C	4.897662	4.992319	-4.800075
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H	4.443685	3.147126	-5.907165
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H	3.996244	7.900500	-0.793935
H	6.705159	2.251064	-5.893788
H	9.237400	2.437176	-4.668465
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H	10.484927	3.538231	-2.885351
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C	1.974009	5.901826	5.335265
C	2.345677	5.016831	6.390135
C	3.130459	6.650092	4.961862
C	3.726640	5.226996	6.677480
C	4.210955	6.239626	5.797473
C	0.943648	5.616913	4.441658
C	1.713382	3.790566	6.595899
C	3.326654	7.137748	3.669560
C	4.548684	4.228958	7.200784
C	5.544808	6.311803	5.395567
C	0.124521	4.458819	4.788236
C	1.041667	6.294956	3.163109
C	0.512949	3.586326	5.813766
C	2.498370	2.824089	7.340763
C	2.176992	7.017618	2.796297
C	4.707613	7.419472	3.331783
C	3.847540	3.034486	7.630527
C	5.965063	4.432128	6.969653
C	5.764026	7.031707	4.155347
C	6.440210	5.426632	6.112535
H	0.252349	6.150727	2.426500
H	-0.063427	2.669141	5.944703
H	2.053163	1.864297	7.605477
H	2.236998	7.409818	1.780105
H	4.937479	7.849982	2.356839
H	4.406093	2.228370	8.108288
H	6.680063	3.721557	7.385616
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H	7.507352	5.453426	5.890316
C	2.971147	2.038732	3.607570
C	2.524213	0.698643	3.228411
C	3.446833	-0.272146	3.813209
C	4.464729	0.467748	4.548606
C	4.170455	1.892925	4.424459
C	4.279934	-2.282450	0.949305
C	5.479434	-2.419792	1.770907
C	5.179015	-1.895925	3.102260
C	3.795578	-1.432521	3.103234
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C	6.886628	0.979653	4.425288
C	5.794567	0.018933	4.554585
C	6.158910	-1.184233	3.814818
C	7.354951	3.165599	3.348427
C	6.432156	4.130304	2.757826
C	5.113996	3.914424	3.347186
C	5.220310	2.812838	4.294766
C	6.604000	2.348460	4.297031
C	4.081664	4.421480	1.148478
C	3.062716	3.683875	0.405592
C	2.319994	2.864462	1.360265
C	2.871539	3.100008	2.691815
C	3.962772	4.058809	2.561117
C	2.199653	1.053012	-0.328664
C	2.484075	-0.372265	-0.200529
C	2.358975	-0.733728	1.207824
C	1.998292	0.472417	1.948864
C	1.901570	1.575255	0.998445
C	4.228243	-0.141531	-1.942730
C	5.611708	-0.605691	-1.941833
C	5.717921	-1.713509	-0.993318
C	4.398799	-1.931981	-0.406283
C	3.480972	-0.959121	-0.991204
C	6.868678	-1.849149	-0.205152
C	7.960503	-0.888078	-0.335895
C	8.509029	-0.649596	0.994230
C	7.763103	-1.466030	1.945708
C	6.747148	-2.208442	1.204184
C	8.947662	0.632465	1.357694
C	8.843878	1.734824	0.405200
C	8.477401	2.938945	1.147370
C	8.356044	2.578987	2.557020
C	8.648060	1.153876	2.687287
C	7.584736	3.863325	0.582464
C	7.029709	3.631147	-0.747329
C	5.649499	4.102968	-0.750350
C	5.348948	4.626490	0.580619
C	6.548298	4.480272	1.403787
C	4.670149	3.396476	-1.466245
C	5.037789	2.189773	-2.205599
C	3.946902	1.228388	-2.072853
C	2.908152	1.839268	-1.247467
C	3.352071	3.179810	-0.874589
C	6.369004	1.740443	-2.204377
C	7.383858	2.476986	-1.459256
C	8.308215	1.508922	-0.872205
C	7.856185	0.173125	-1.245719
C	6.660953	0.316370	-2.071795

Non-covalent interactions

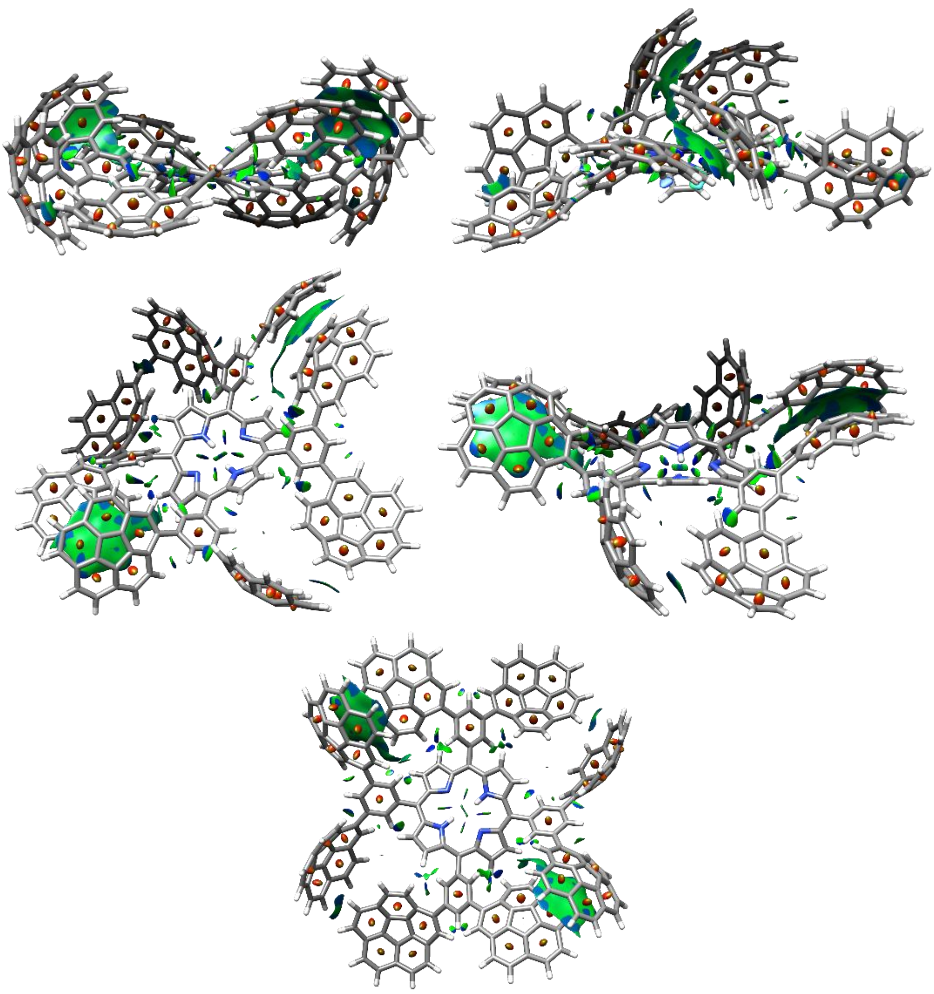

Figure S41. Non-covalent interaction isosurfaces for compound **2H-POctaCor**.

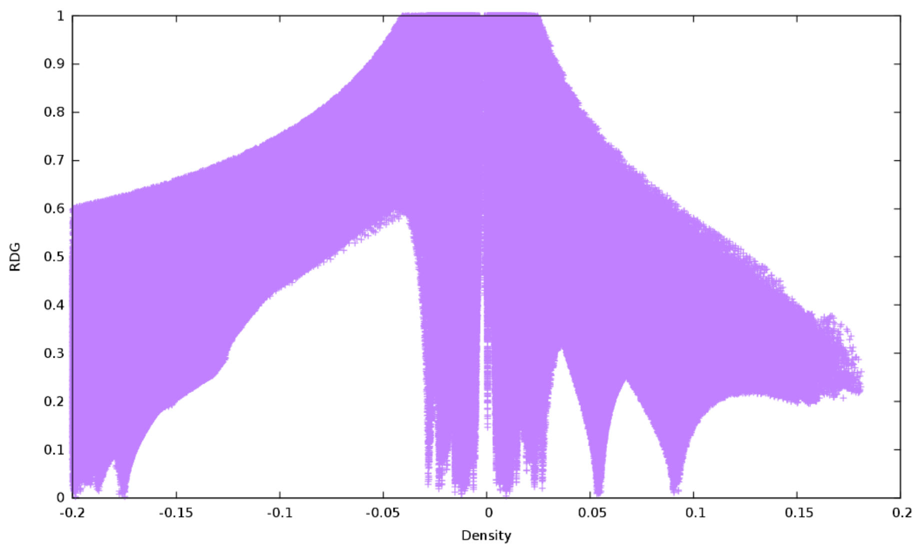

Figure S42. Plot of the reduced density gradient versus the electron density for compound **2H-POctaCor.**

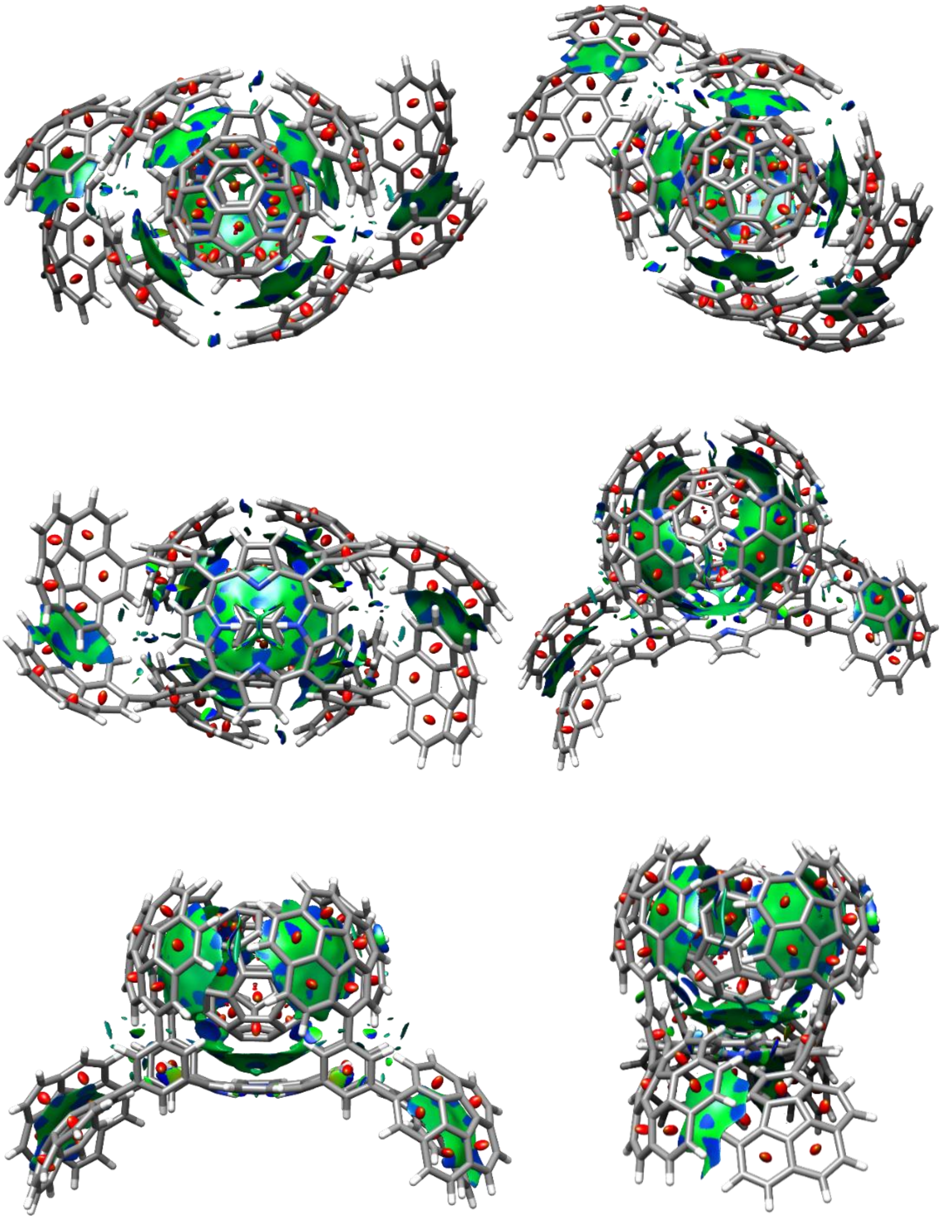

Figure S43. Non-covalent interaction isosurfaces for assembly C_{60}@**2H-POctaCor**.

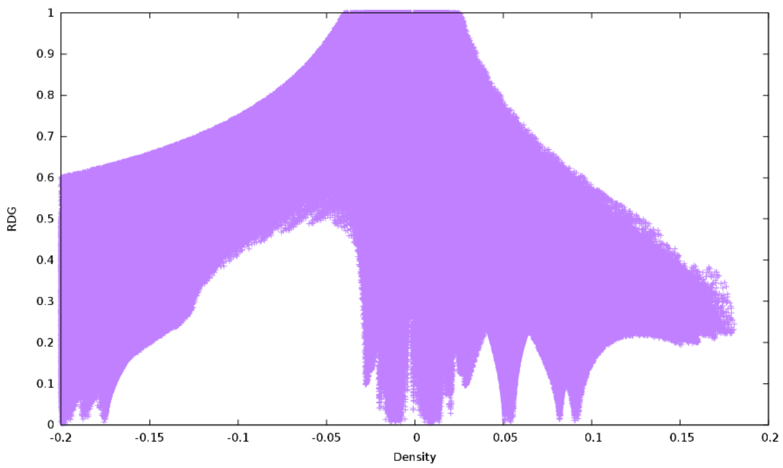

Figure S44. Plot of the reduced density gradient versus the electron density for complex C_{60}@**2H-POctaCor**.

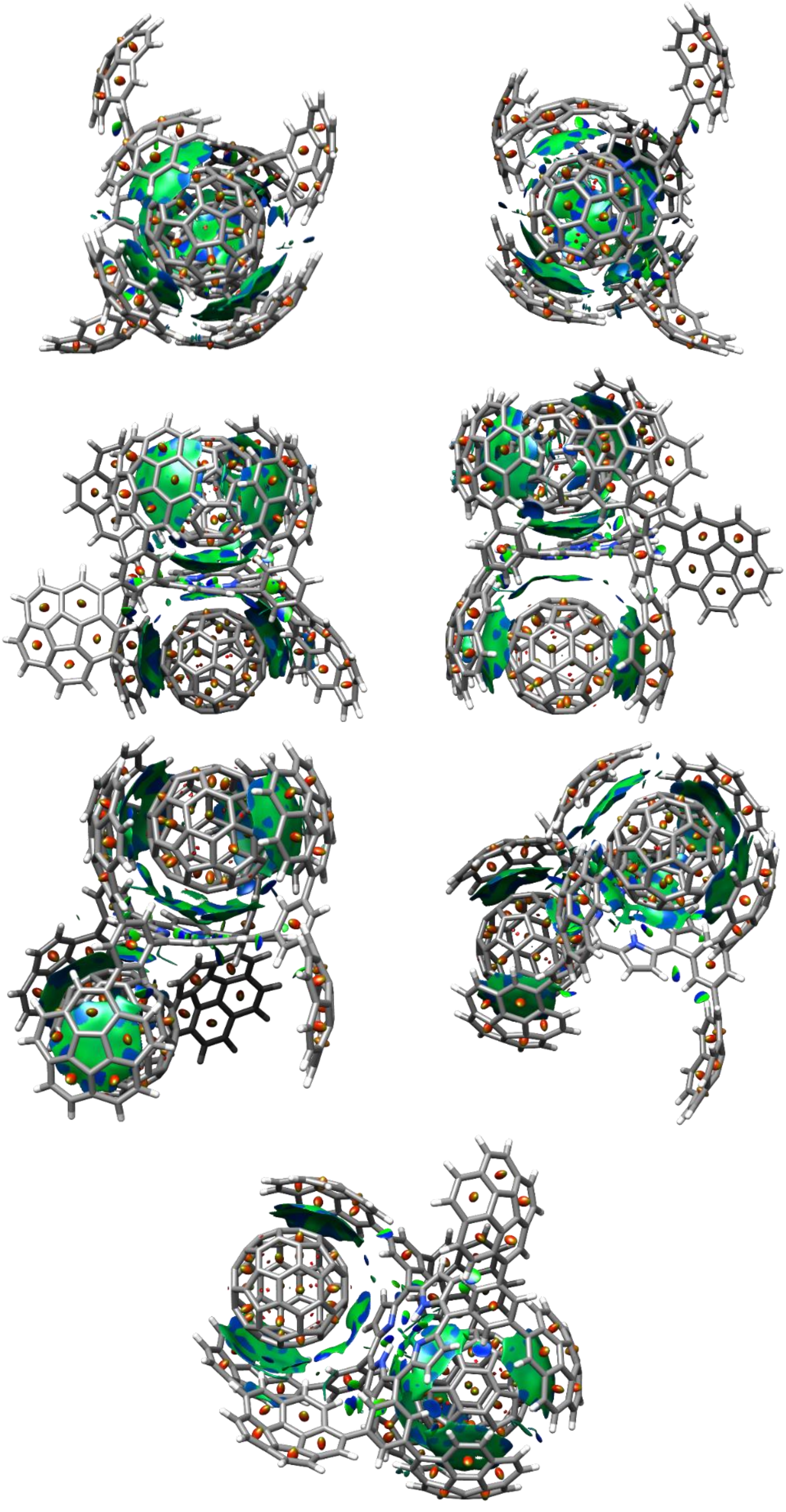

Figure S45. Non-covalent interaction isosurfaces for assembly $(C_{60})_2$@**2H-POctaCor**.

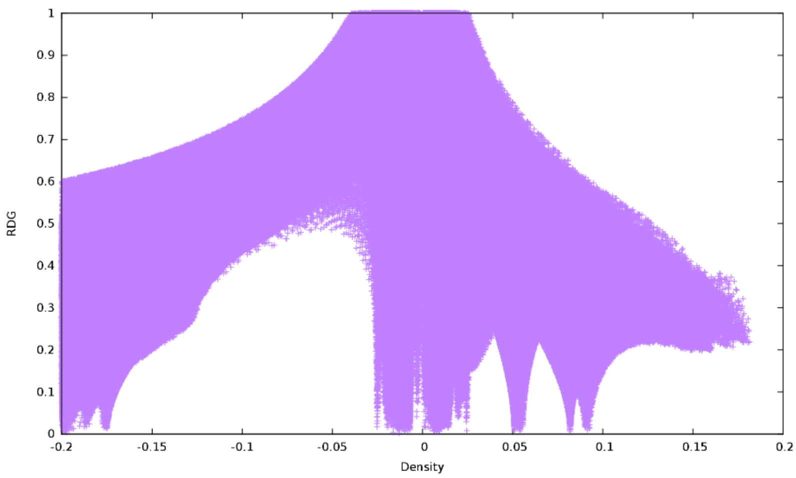

Figure S46. Plot of the reduced density gradient versus the electron density for complex $(C_{60})_2$@**2H-POctaCor**.

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