

Supramolecular self-sorting predicted by a simple harmonic oscillator model

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Experimental Procedures

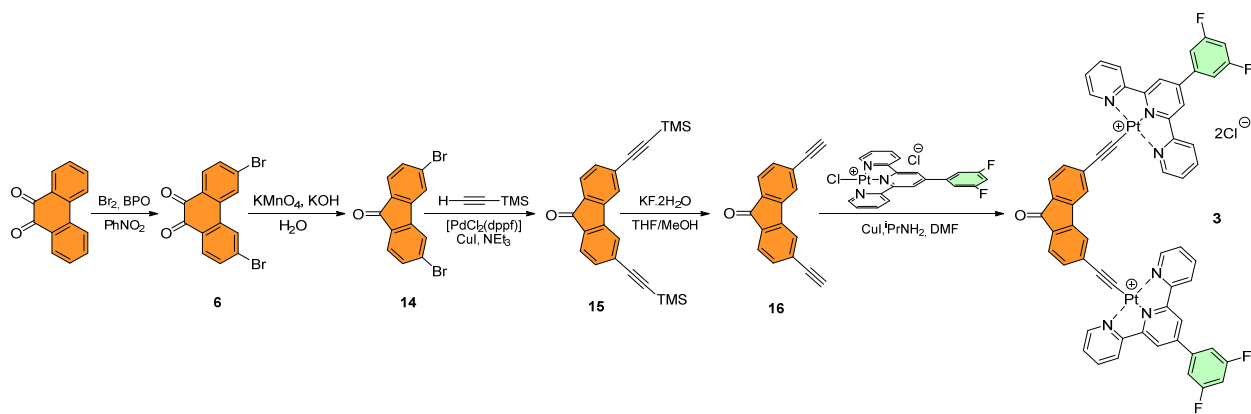
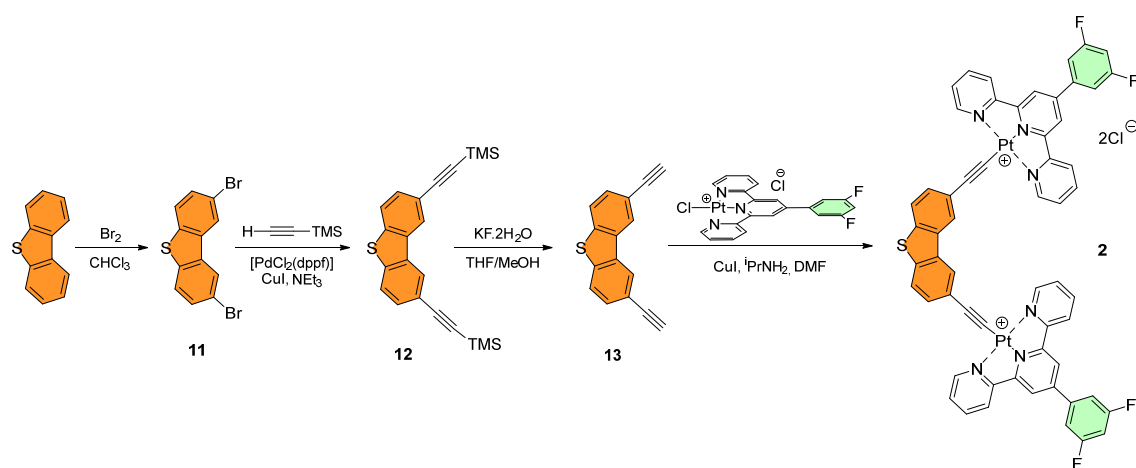
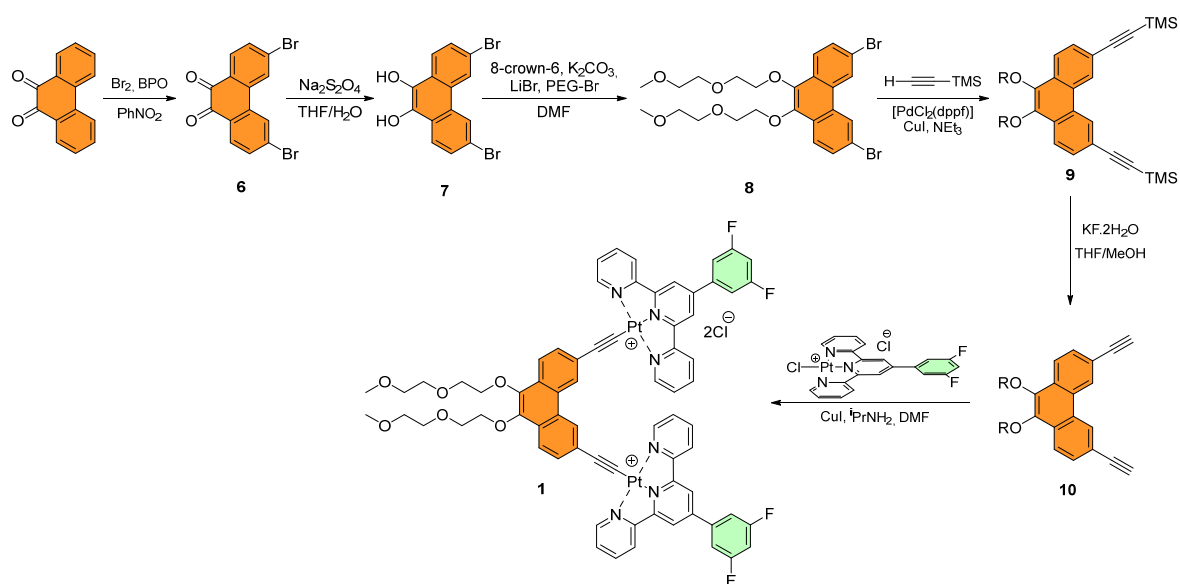
General methods

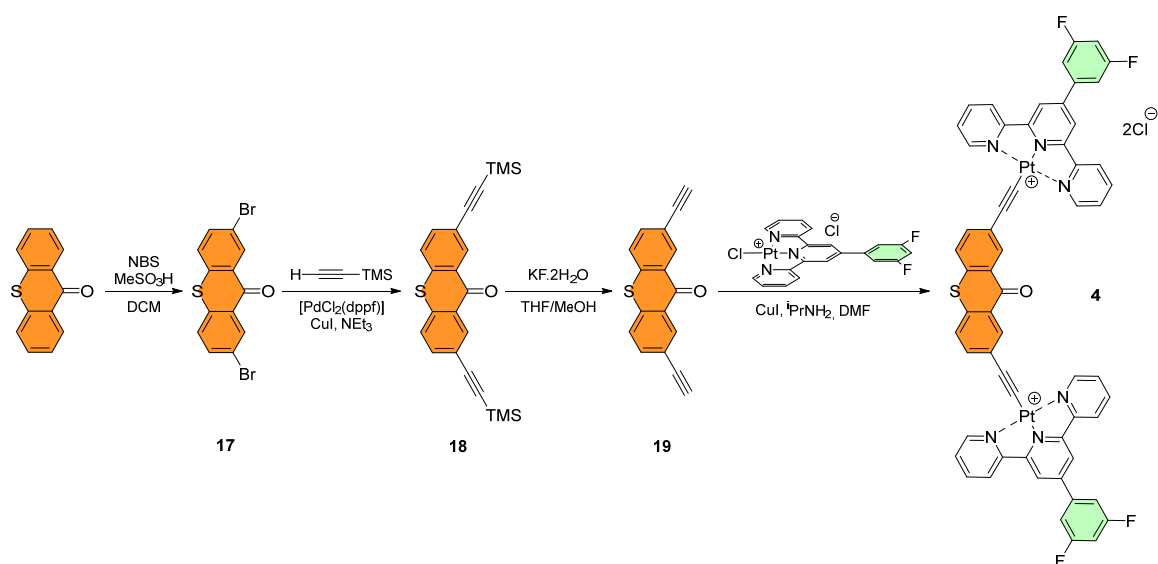
Reagents were purchased from regular suppliers (BLDpharm and Fisher Scientific, mainly) and used without further purification. They were either used as purchased or dried according to procedures described elsewhere.¹ 3,6-dibromophenanthrene-9,10-dione (**6**),² 3,6-dibromophenanthrene-9,10-diol (**7**),² 2,8-dibromodibenzo[b,d]thiophene (**11**),³ 3,6-dibromo-9H-fluoren-9-one (**14**),⁴ chloro-[4'-(3,5-difluorophenyl)-2,2':6',2''-terpyridine]platinum(II) chloride⁵ and complex **5**⁶ were prepared according to previously reported methods.

Microwave reactions were carried out with an Anton Paar Monowave 300 Reactor using tightly capped flasks G30 (for volumes up to 30 mL) especially designed for the apparatus. All reactions under inert atmosphere (when needed) were performed with standard Schlenk techniques. Column chromatography separations were carried out by using Silica gel 60 (particle size 0.040-0.063 mm; 230-400 mesh; Merck, Germany) as the stationary phase and TLCs were performed on precoated silica gel plates (0.25 mm thick, 60 F254, Merck, Germany) and observed under UV light. Purifications by centrifugation were performed in a Nahita 2600 centrifuge.

NMR spectra were recorded on Agilent DD2 500, Bruker AVANCE NEO 500 and Agilent MR 400 instruments. ¹H, ¹⁹F and ¹³C NMR chemical shifts are reported in parts per million (ppm) and are referenced to TMS, using residual solvent peak as an internal reference. Coupling constants (*J*) are reported in hertz (Hz). Standard abbreviations used to indicate multiplicity: s = singlet, d = doublet, m = multiplet, t = triplet dd = doublet of doublets. ¹H assignments were performed by utilizing 2D NMR methods (gCOSY, ROESY, gHSQCAD, gHMBCAD). NMR spectra were analysed using MNova v14.2.1. High resolution mass spectra were recorded at mass spectrometry service of the Laboratory of Instrumental Techniques of the University of Valladolid (L.T.I., www.laboratoriotecnicasinstrumentales.es). Direct injection and an UPLC-MS system (UPLC: Waters ACQUITY H-class UPLC; MS: Bruker Maxis Impact) by electrospray ionization (ESI positive) was utilized as well. HRMS spectra were analysed using Bruker DataAnalysis 4.1© (www.bruker.com) and mMass v5.5.0 (with a previous conversion with MSConvert v3.0).

Synthesis overview of Pt(II) Complexes

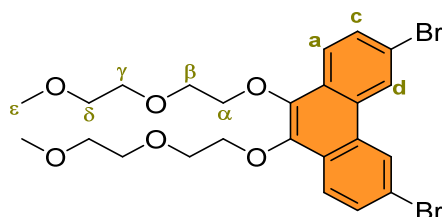




Scheme S 4. Synthetic scheme for complex **4**.

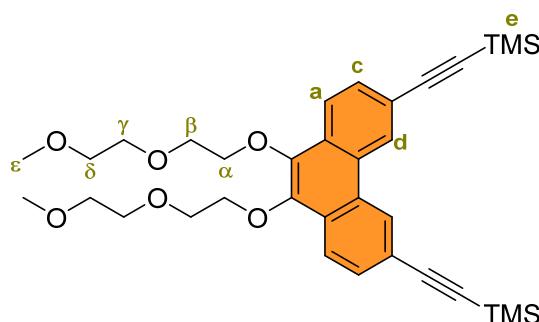
Synthetic protocols and characterization

3,6-Dibromo-9,10-bis(2-(2-methoxyethoxy)ethoxy)phenanthrene (**8**)

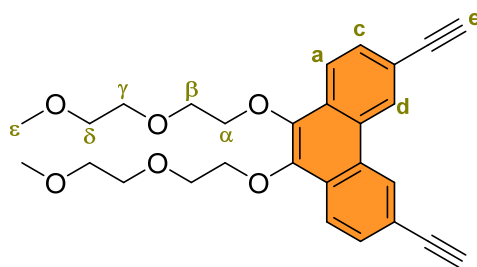


3,6-Dibromophenanthrene-9,10-diol (**7**)² (0.99 g, 2.7 mmol), 18-crown-6 (0.10 g, 0.38 mmol), potassium carbonate (1.5 g, 11 mmol) and lithium bromide (33 mg, 0.38 mmol) were suspended under an inert atmosphere in dry DMF (4 mL). 1-Bromo-2-(2-methoxyethoxy)ethane (1.5 mL, 11 mmol) was then added and the mixture was stirred and heated at 80 °C for 20 h. After this time, the solution was cooled down to room temperature and poured over water (20 mL). The reaction mixture was extracted with AcOEt (50 mL) and washed with water (3 × 20 mL), dried with MgSO₄, filtered and concentrated under vacuum before subjecting the resulting crude to purification by column chromatography on silica gel (7:1 DCM/AcOEt) to furnish the pure title compound as an off-white solid (0.90 g, 58% yield). Spectral data were in agreement with those previously reported.⁷ ¹H NMR (500 MHz, CDCl₃) δ 8.62 (d, *J* = 1.9 Hz, 2H, H^d), 8.23 (d, *J* = 8.8 Hz, 2H, H^a), 7.68 (dd, *J* = 8.8, 1.9 Hz, 2H, H^c), 4.44 – 4.34 (m, 4H, H^α), 3.87 – 3.79 (m, 4H, H^β), 3.72 – 3.64 (m, 4H, H^γ), 3.62 – 3.52 (m, 4H, H^δ), 3.39 (s, 6H, H^ε). ¹³C NMR (126 MHz, CDCl₃) δ 143.0, 130.6, 129.0, 128.6, 125.3, 124.8, 120.7, 72.5, 72.1, 70.6, 70.5, 59.2. HRMS (ESI-TOF-pos): *m/z* = 593.0143 [M+Na]⁺ (calc. 593.0145 for C₂₄H₂₈Br₂NaO₆).

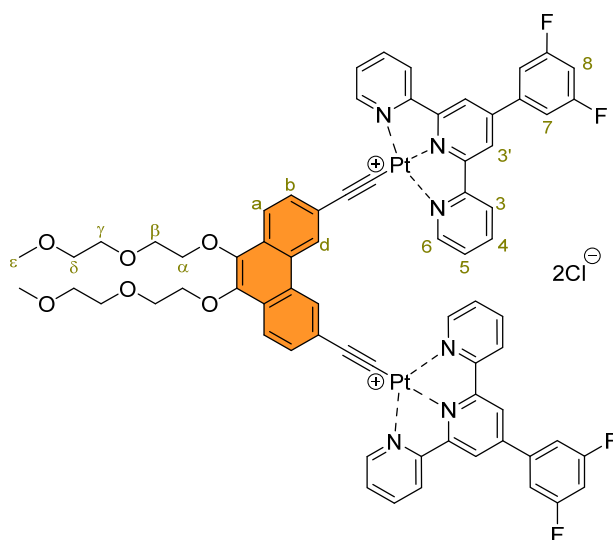
3,6-bis((Trimethylsilyl)ethynyl)-9,10-bis(2-(2-methoxyethoxy)ethoxy)phenanthrene (**9**)



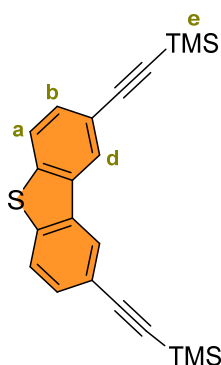
3,6-Dibromo-9,10-bis(2-(2-methoxyethoxy)ethoxy)phenanthrene (**8**) (0.32 g, 0.56 mmol), copper iodide (32 mg, 0.17 mmol) and [PdCl₂(dppf)] (62 mg, 0.080 mmol) were mixed in a microwave flask under inert atmosphere. Dry NEt₃ (5 mL) and (trimethylsilyl)acetylene (0.31 mL, 2.3 mmol) were subsequently added and the mixture was degassed. It was then irradiated in a microwave reactor at 150 °C for 30 min with stirring at 600 rpm, reaching a pressure of 1.5 bar. The solvent was removed and the crude reaction was dissolved in DCM (20 mL), filtered through a silica gel pad and concentrated under vacuum before subjecting the resulting crude to purification by column chromatography on silica gel (10:1 DCM/AcOEt) to furnish the pure title compound as an off-white solid (0.23 g, 67% yield). ¹H NMR (500 MHz, CDCl₃) δ 8.72 (d, *J* = 1.5 Hz, 2H, H^d), 8.27 (dd, *J* = 8.5, 0.5 Hz, 2H, H^d), 7.66 (dd, *J* = 8.5, 1.5 Hz, 2H), 4.46 – 4.37 (m, 4H, H^α), 3.89 – 3.82 (m, 4H, H^β), 3.73 – 3.64 (m, 4H, H^γ), 3.63 – 3.53 (m, 4H, H^δ), 3.40 (s, 6H, H^ε), 0.32 (s, 18H, H^e). ¹³C NMR (126 MHz, CDCl₃) δ 143.7, 130.2, 129.6, 127.9, 126.7, 122.9, 120.8, 105.7, 95.1, 72.5, 72.2, 70.7, 70.6, 59.3, 0.2. HRMS (ESI-TOF-pos): *m/z* = 629.2749 [M+Na]⁺ (calc. 629.2725 for C₃₄H₄₆NaO₆Si₂).

3,6-Diethynyl-9,10-bis(2-(2-methoxyethoxy)ethoxy)phenanthrene (**10**)

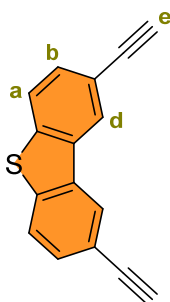
3,6-bis((Trimethylsilyl)ethynyl)-9,10-bis(2-(2-methoxyethoxy)ethoxy)phenanthrene (**9**) (0.19 g, 0.31 mmol) and $\text{KF}\cdot\text{H}_2\text{O}$ (0.18 g, 1.9 mmol) were mixed in a microwave flask. THF (3 mL) and MeOH (3 mL) were added and then, the mixture was irradiated in a microwave reactor at 50 °C for 45 min with stirring at 600 rpm, reaching a pressure of 1.0 bar. The solvent was removed and the crude reaction was dissolved in DCM (50 mL), washed with water (3 x 50 mL), dried with MgSO_4 , filtered and concentrated under vacuum. The pure title compound was obtained as a yellow solid (0.12 g, 85% yield) without further purification. Spectral data were in agreement with those previously reported.⁷ ^1H NMR (500 MHz, CDCl_3) δ 8.74 (d, J = 1.5 Hz, 2H, H^d), 8.31 (d J = 8.5 Hz, 2H, H^a), 7.69 (dd, J = 8.4, 1.5 Hz, 2H, H^c), 4.47 – 4.33 (m, 4H, H^α), 3.90 – 3.81 (m, 4H, H^β), 3.74 – 3.64 (m, 4H, H^γ), 3.62 – 3.51 (m, 4H, H^δ), 3.40 (s, 6H, H^ϵ), 3.21 (s, 2H, H^ϵ). ^{13}C NMR (126 MHz, CDCl_3) δ 143.8, 130.3, 129.8, 127.8, 126.9, 123.1, 119.8, 84.3, 78.0, 72.6, 72.2, 70.7, 70.6, 59.3. HRMS (ESI-TOF-pos): m/z = 485.1922 $[\text{M}+\text{Na}]^+$ (calc. 485.1935 for $\text{C}_{28}\text{H}_{30}\text{NaO}_6$).

Complex **1**

3,6-Diethynyl-9,10-bis(2-(2-methoxyethoxy)ethoxy)phenanthrene (**10**) (20 mg, 43 μmol) was dissolved in a mixture of $i\text{PrNH}_2$ (2 mL) and DMF (2 mL) under inert atmosphere. Copper iodide (1.6 mg, 8.6 μmol) and chloro-[4'-(3,5-difluorophenyl)-2,2':6',2''-terpyridine]platinum(II) chloride⁵ (55 mg, 90 μmol) were subsequently added and the mixture was stirred overnight at 25 °C. After this time, the obtained suspension was centrifuged and the solid was washed with MeOH (2 x 10 mL), followed by CHCl_3 (3 x 10 mL) and Et_2O (1 x 10 mL) before being dried under vacuum. The pure title compound was obtained as a dark red solid (61 mg, 88% yield). ^1H NMR (500 MHz, $\text{DMSO}-d_6$) δ 9.33 (d, J = 5.2 Hz, 4H, H^6), 9.07 (s, 4H, H^3), 8.89 (s, 2H, H^d), 8.83 (d, J = 8.0 Hz, 4H, H^3), 8.54 (t, J = 7.8 Hz, 4H, H^5), 8.22 (d, J = 8.4 Hz, 2H, H^a), 8.04 (d, J = 9.0 Hz, 4H, H^7), 7.98 (t, J = 6.6 Hz, 4H, H^4), 7.79 (d, J = 8.4 Hz, 2H, H^b), 7.62 (t, J = 9.0 Hz, 4H, H^8), 4.34 (t, J = 4.9 Hz, 4H, H^α), 3.85 (t, J = 4.6 Hz, 4H, H^β), 3.67 (t, J = 4.5 Hz, 4H, H^γ), 3.54 (d, J = 4.8 Hz, 4H, H^δ). ^{19}F NMR (470 MHz, $\text{DMSO}-d_6$) δ -108.10 (t, J = 9.0 Hz). Complex **1** was poorly soluble in any solvent and, therefore, a 1D $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum could not be recorded. However, the following list containing indirect carbon chemical shifts, obtained with HSQC and HMBC experiments, is reported. ^{13}C NMR δ 164.5, 162.6, 158.6, 155.2, 151.9, 144.6, 143.0, 138.5, 130.0, 126.6, 122.1, 111.7, 72.9, 71.8, 70.3, 70.2, 58.5. HRMS (ESI-TOF-pos): m/z = 770.1657 $[\text{M}]^{2+}$ (calc. 770.1662 for $\text{C}_{70}\text{H}_{54}\text{F}_4\text{N}_6\text{O}_6\text{Pt}_2$).

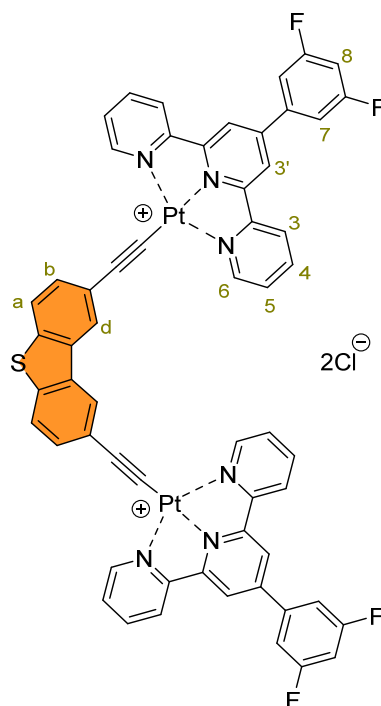
2,8-bis((Trimethylsilyl)ethynyl)dibenzo[*b,d*]thiophene (**12**)

2,8-Dibromodibenzo[*b,d*]thiophene (**11**)³ (0.26 g, 0.75 mmol), copper iodide (43 mg, 0.23 mmol) and [PdCl₂(dppf)] (82 mg, 0.11 mmol) were mixed in a round bottom flask under inert atmosphere. Dry NEt₃ (6 mL) and (trimethylsilyl)acetylene (0.42 mL, 3.0 mmol) were subsequently added and the mixture was degassed. It was then stirred and heated at 120 °C for 24 h. The solvent was removed and the crude reaction was dissolved in DCM (20 mL), filtered through a silica gel pad and concentrated under vacuum before subjecting the resulting crude to purification by column chromatography on silica gel (15:1 *n*-hexane/DCM) to furnish the pure title compound as a pale yellow solid (0.21 g, 74% yield). Spectral data were in agreement with those previously reported.⁸ ¹H NMR (500 MHz, CDCl₃) δ 8.25 (d, *J* = 1.6 Hz, 2H, H^d), 7.74 (d, *J* = 8.3 Hz, 2H, H^a), 7.54 (dd, *J* = 8.3, 1.6 Hz, 2H, H^b), 0.31 (s, 18H, H^e). ¹³C NMR (126 MHz, CDCl₃) δ 140.0, 135.0, 130.5, 125.5, 122.7, 119.7, 105.1, 94.5, 0.2. HRMS (ESI-TOF-pos): *m/z* = 377.1209 [M+H]⁺ (calc. 377.1210 for C₂₂H₂₅SSi₂).

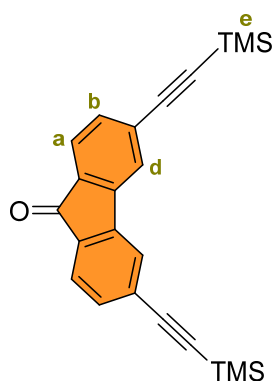
2,8-Diethynyldibenzo[*b,d*]thiophene (**13**)

2,8-bis((Trimethylsilyl)ethynyl)dibenzo[*b,d*]thiophene (**12**) (0.10 g, 0.27 mmol) and KF·H₂O (0.15 g, 1.6 mmol) were mixed in a microwave flask. THF (3 mL) and methanol (3 mL) were added and, then, the mixture was irradiated in a microwave reactor at 50 °C for 45 min with stirring at 600 rpm, reaching a pressure of 1.0 bar. The solvent was removed and the resulting material was dissolved in DCM (50 mL), washed with water (3 × 50 mL), dried with MgSO₄, filtered and concentrated under vacuum. The pure title compound was obtained as a light brown solid (65 mg, 99% yield) without further purification. Spectral data were in agreement with those previously reported.⁸ ¹H NMR (500 MHz, CDCl₃) δ 8.27 (d, *J* = 1.7 Hz, 2H, H^d), 7.79 (d, *J* = 8.3 Hz, 2H, H^a), 7.58 (dd, *J* = 8.3, 1.7 Hz, 2H, H^b), 3.16 (s, 2H, H^e). ¹³C NMR (126 MHz, CDCl₃) δ 140.4, 135.0, 130.7, 125.7, 123.0, 118.7, 83.7, 77.6.

Complex 2



2,8-Diethynyldibenzo[*b,d*]thiophene (**13**) (10 mg, 43 μ mol) was dissolved in a mixture of i PrNH₂ (2 mL) and DMF (2 mL) under inert atmosphere. Copper iodide (1.6 mg, 8.6 μ mol) and chloro-[4'-(3,5-difluorophenyl)-2,2':6',2''-terpyridine]platinum(II) chloride⁵ (55 mg, 90 μ mol) were subsequently added and the mixture was stirred overnight at 25 °C. After this time, the obtained suspension was centrifuged and the solid was washed with MeOH (2 x 10 mL), CHCl₃ (3 x 10 mL) and Et₂O (1 x 10 mL) before being dried under vacuum. The pure title compound was obtained as a dark red solid (57 mg, 95% yield). ¹H NMR (500 MHz, DMSO-*d*₆) δ 9.06 (s, 2H, H³), 8.99 (d, *J* = 5.4 Hz, 1H, H^a), 8.86 (d, *J* = 8.0 Hz, 2H, H⁶), 8.69 – 8.52 (m, 3H, H⁵ + H^d), 8.07 (d, *J* = 6.7 Hz, 2H, H³), 8.00 (t, *J* = 6.6 Hz, 2H, H⁴), 7.95 (br, 2H, H⁷), 7.73 – 7.55 (m, 2H, H^b + H⁸). ¹⁹F NMR (470 MHz, DMSO-*d*₆) δ -108.12 (t, *J* = 7.5 Hz). Complex **2** was poorly soluble in any solvent and, therefore, a 1D ¹³C{¹H}-NMR spectrum could not be recorded. However, the following list containing indirect carbon chemical shifts, obtained with HSQC and HMBC experiments, is reported. ¹³C NMR δ 158.6, 151.9, 143.2, 129.9, 126.5, 122.0, 111.8. HRMS (ESI-TOF-pos): *m/z* = 655.0804 [*M*]²⁺ (calc. 655.0813 for C₅₈H₃₂F₄N₆Pt₂S).

3,6-bis((Trimethylsilyl)ethynyl)-9*H*-fluoren-9-one (**15**)

Two procedures can be followed to prepare the title compound:

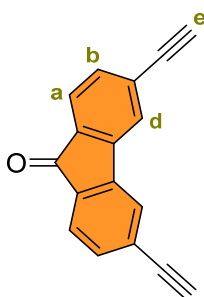
Procedure A: 3,6-Dibromo-9*H*-fluoren-9-one (**14**)⁴ (0.25 g, 0.74 mmol), copper iodide (42 mg, 0.22 mmol) and [PdCl₂(dppf)] (81 g, 0.11 mmol) were mixed in a microwave flask under inert atmosphere. Dry NEt₃ (6 mL) and (trimethylsilyl)acetylene (0.41 mL, 3.0 mmol) were subsequently added and the mixture was degassed. It was then irradiated in a microwave reactor at 150 °C for 30 min with stirring at 600 rpm, reaching a pressure of 1.5 bar. The solvent was removed and the crude reaction was dissolved in DCM (20 mL), filtered through a silica gel pad and concentrated

under vacuum before subjecting the resulting crude to purification by column chromatography on silica gel (3:1 *n*-hexane/DCM) to furnish the pure title compound as a yellow solid (0.22 g, 80% yield). Spectral data were in agreement with those previously reported.⁹

Procedure B: 3,6-Dibromo-9*H*-fluoren-9-one (**15**)⁴ (0.20 g, 0.60 mmol), copper iodide (34 mg, 0.18 mmol) and [PdCl₂(dppf)] (66 mg, 0.090 mmol) were mixed in a round bottom flask under inert atmosphere. Dry NEt₃ (5 mL) and (trimethylsilyl)acetylene (0.33 mL, 2.4 mmol) were subsequently added and the mixture was degassed. It was then heated at 120 °C for 24 h. The solvent was removed and the crude reaction was dissolved in DCM (20 mL), filtered through a silica gel pad and concentrated under vacuum before subjecting the resulting crude to purification by column chromatography on silica gel (3:1 *n*-hexane/ DCM) to furnish the pure title compound as a yellow solid (0.17 g, 76% yield). Spectral data were in agreement with those previously reported⁹.

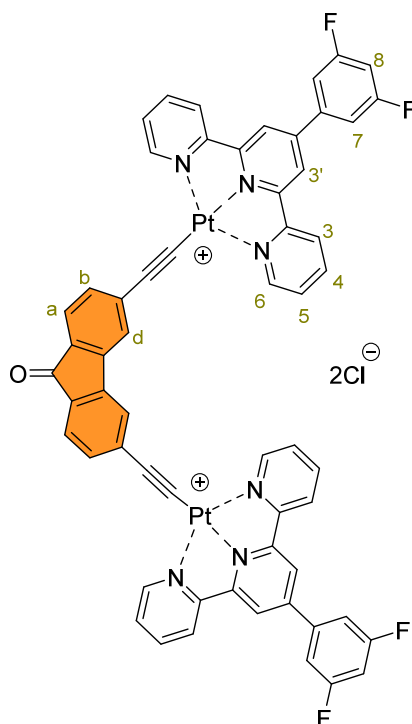
¹H NMR (500 MHz, CDCl₃) δ 7.59 - 7.56 (m, 2H, H^a, H^d), 7.38 (dd, *J* = 7.8, 1.2 Hz, 2H, H^b), 0.28 (s, 18H, H^e). ¹³C NMR (126 MHz, CDCl₃) δ 192.0, 143.7, 133.9, 133.1, 129.7, 124.3, 123.9, 104.3, 98.8, -0.1. HRMS (ESI-TOF-pos): *m/z* = 373.1444 [M+H]⁺ (calc. 373.1438 for C₂₃H₂₅OSi₂).

3,6-Diethynyl-9*H*-fluoren-9-one (**16**)

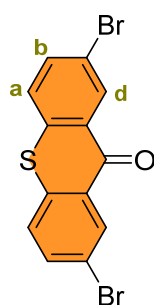


3,6-bis((Trimethylsilyl)ethynyl)-9*H*-fluoren-9-one (**15**) (0.10 g, 0.27 mmol) and KF·H₂O (0.15 g, 1.6 mmol) were mixed in a microwave flask. THF (3 mL) and MeOH (3 mL) were added and then, the mixture was irradiated in a microwave reactor at 50 °C for 45 min with stirring at 600 rpm, reaching a pressure of 1.0 bar. The solvent was removed and the crude reaction was dissolved in DCM (50 mL), washed with water (3 × 50 mL), dried with MgSO₄, filtered and concentrated under vacuum. The pure title compound was obtained as a yellow solid (41 g, 67% yield) without further purification. Spectral data were in agreement with those previously reported.⁹ ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.05 (dd, *J* = 1.4, 0.7 Hz, 2H, H^d), 7.64 (dd, *J* = 7.6, 0.7 Hz, 2H, H^a), 7.51 (dd, *J* = 7.6, 1.4 Hz, 2H, H^b), 4.58 (s, 2H, H^e). ¹³C NMR (126 MHz, DMSO-*d*₆) δ 192.0, 143.7, 134.2, 133.6, 128.8, 124.5, 124.1, 83.0, 81.0.

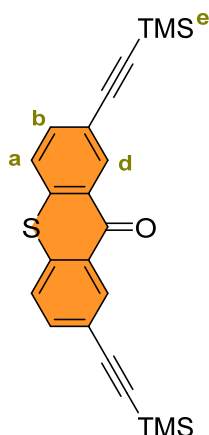
Complex 3



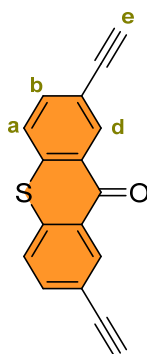
3,6-Diethynyl-9*H*-fluoren-9-one (**16**) (10 mg, 44 μ mol) was dissolved in a mixture of i PrNH₂ (2 mL) and DMF (2 mL) under inert atmosphere. Copper iodide (1.7 mg, 8.8 μ mol) and chloro-[4'-(3,5-difluorophenyl)-2,2':6',2''-terpyridine]platinum(II) chloride⁵ (56 mg, 92 μ mol) were subsequently added and the mixture was stirred overnight at 25 °C. After this time, the obtained suspension was centrifuged and the solid was washed with MeOH (2 x 10 mL), CHCl₃ (3 x 10 mL) and Et₂O (1 x 10 mL) before being dried under vacuum. The pure title compound was obtained as a red solid (59 mg, 97% yield). Complex **3** was practically insoluble in any solvent or solvent mixture (including TFA-*d*) and at any temperature to record a reasonable ¹H-NMR spectrum. However, its existence is corroborated by the MS data (Figure S 63) and the spectral data for assembly **3**₂·CB[8]₂ (Figure S 103 -Figure S 108). HRMS (ESI-TOF-pos): m/z = 653.0936 [M]²⁺ (calc. 653.0928 for C₅₉H₃₂F₄N₆O₂Pt₂).

2,7-Dibromo-9*H*-thioxanthen-9-one (**17**)

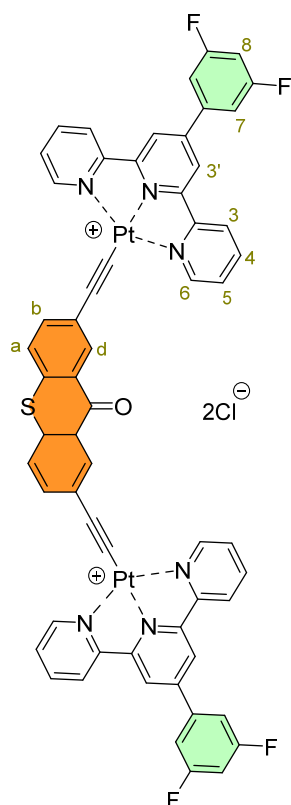
9*H*-Thioxanthen-9-one (2.0 g, 9.4 mmol) and *N*-bromosuccinimide (3.7 g, 21 mmol) were suspended in DCM (30 mL). Methanesulfonic acid (1.4 mL, 21 mmol) was added and the mixture was stirred at room temperature for 18 h. After this time, water was added (30 mL) and the reaction mixture was extracted with DCM (3 x 50 mL) and washed with water (2 x 25 mL) followed by brine (2 x 25 mL), dried with MgSO₄, filtered and concentrated under vacuum. Pure compound was obtained by recrystallization from hot toluene as a yellow solid (2.9 g, 83% yield). Spectral data were in agreement with those previously reported.¹⁰ ¹H NMR (500 MHz, CDCl₃) δ 8.74 (d, J = 2.2 Hz, 2H, H^d), 7.74 (dd, J = 8.6, 2.2 Hz, 2H, H^a), 7.47 (d, J = 8.6 Hz, 2H, H^b). ¹³C NMR (101 MHz, CDCl₃) δ 177.8, 135.8, 132.7, 130.2, 127.8, 120.8. HRMS (ESI-TOF-pos): m/z = 392.8382 [M +Na]⁺ (calc. 392.8378 for C₁₃H₆Br₂NaOS).

2,7-bis((Trimethylsilyl)ethynyl)-9*H*-thioxanthen-9-one (**18**)

2,7-Dibromo-9*H*-thioxanthen-9-one (**17**) (0.30 g, 0.81 mmol), copper iodide (46 mg, 0.30 mmol) and [PdCl₂(dppf)] (89 mg, 0.15 mmol) were mixed in a round bottom flask under inert atmosphere. Dry NEt₃ (7 mL) and (trimethylsilyl)acetylene (0.45 mL, 3.2 mmol) were subsequently added and the mixture was degassed. It was then heated at 120 °C for 24 h. The solvent was removed, and the crude reaction was dissolved in DCM (20 mL), filtered through a silica gel pad and concentrated under vacuum before subjecting the resulting crude to purification by column chromatography on silica gel (5:1 *n*-hexane/ DCM) to furnish the pure title compound as a pale yellow solid (0.20 g, 60% yield). ¹H NMR (500 MHz, CDCl₃) δ 8.71 (d, *J* = 1.9 Hz, 2H, H^d), 7.67 (dd, *J* = 8.3, 1.9 Hz, 2H, H^a), 7.52 (d, *J* = 8.3 Hz, 2H, H^b), 0.29 (s, 18H, H^e). ¹³C NMR (126 MHz, CDCl₃) δ 178.6, 136.9, 135.2, 133.7, 129.0, 126.2, 121.9, 103.7, 96.4, 0.0. HRMS (ESI-TOF-pos): *m/z* = 405.1175 [M+H]⁺ (calc. 405.1159 for C₂₃H₂₅OSSi₂).

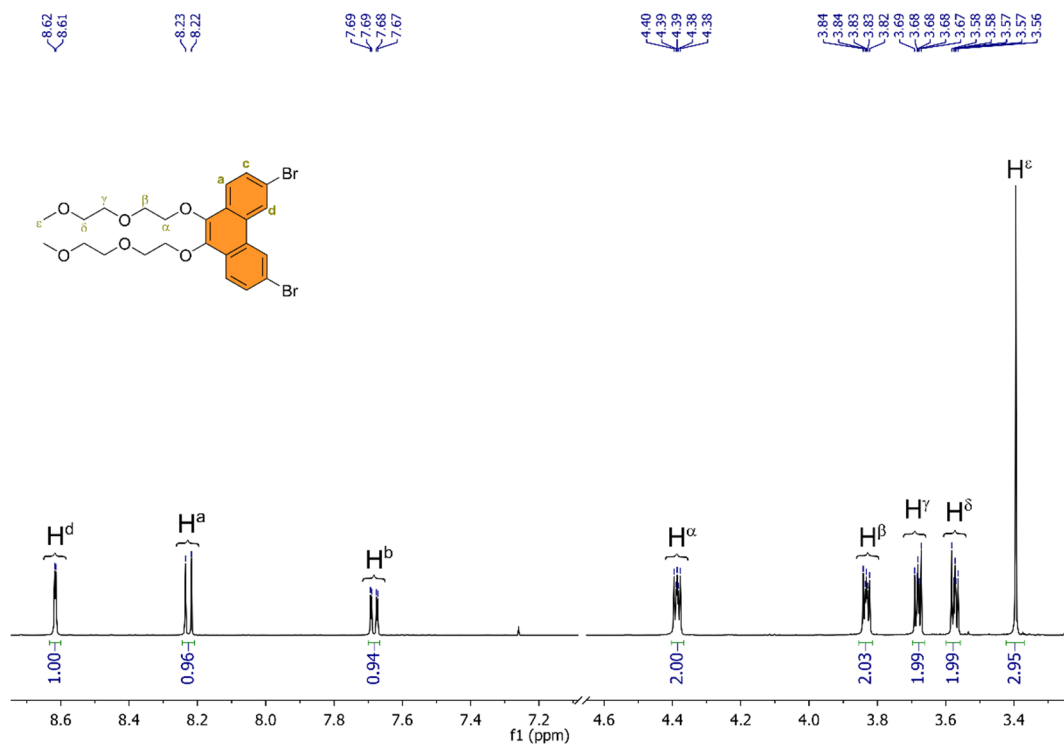
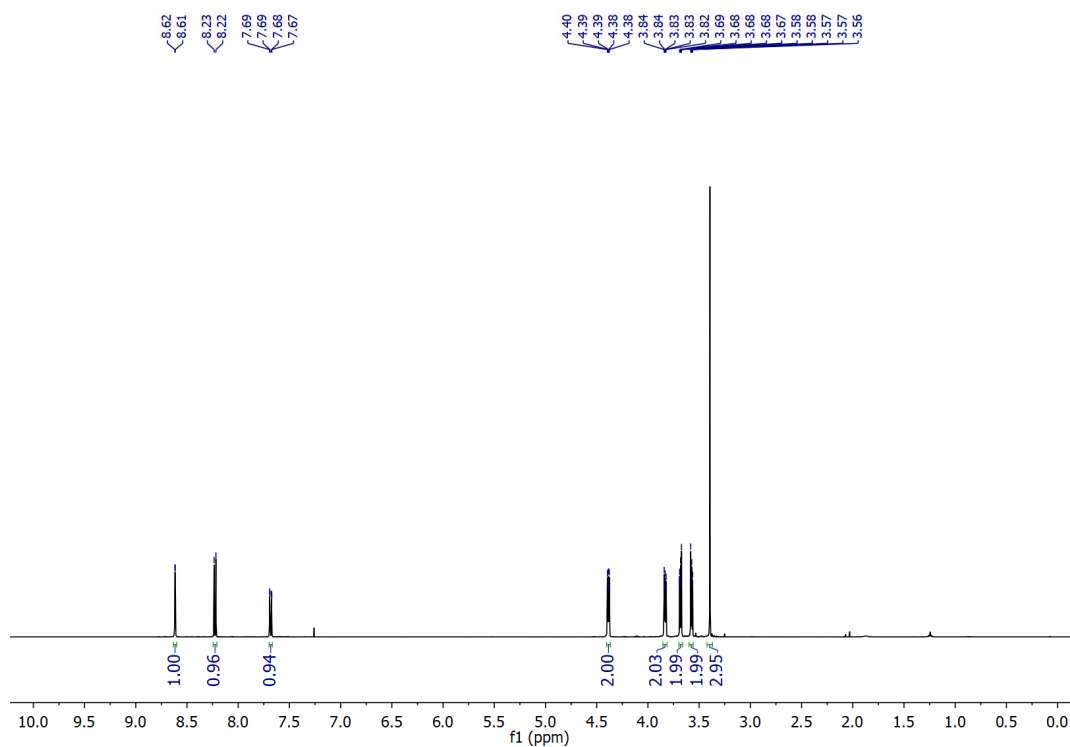
2,7-Diethynyl-9*H*-thioxanthen-9-one (**19**)

2,7-bis((Trimethylsilyl)ethynyl)-9*H*-thioxanthen-9-one (**18**) (0.10 g, 0.25 mmol) and KF·H₂O (0.14 g, 1.5 mmol) were mixed in a microwave flask. THF (3 mL) and MeOH (3 mL) were added and, then, the mixture was irradiated in a microwave reactor at 50 °C for 45 min with stirring at 600 rpm, reaching a pressure of 1.0 bar. The solvent was removed and the resulting material was dissolved in DCM (50 mL), washed with water (3 × 50 mL), dried with MgSO₄, filtered and concentrated under vacuum. The pure title compound was obtained as an off-white solid (64 mg, 98% yield) without further purification. ¹H NMR (400 MHz, CDCl₃) δ 8.72 (dt, *J* = 1.9, 0.5 Hz, 2H, H^d), 7.69 (dd, *J* = 8.3, 1.9 Hz, 2H, H^a), 7.53 (dt, *J* = 8.3, 0.9 Hz, 2H, H^b), 3.19 (s, 2H, H^e). ¹³C NMR (101 MHz, CDCl₃) δ 178.5, 137.3, 135.4, 133.9, 129.1, 126.4, 120.9, 82.4, 79.0. HRMS (ESI-TOF-pos): *m/z* = 283.0187 [M+Na]⁺ (calc. 283.0188 for C₁₇H₈BNaOS).

Complex **4**

2,7-Diethynyl-9*H*-thioxanthen-9-one (**19**) (13 mg, 50 μmol) was dissolved in a mixture of $i\text{PrNH}_2$ (2 mL) and DMF (2 mL) under inert atmosphere. Copper iodide (1.9 mg, 10 μmol) and chloro-[4'-(3,5-difluorophenyl)-2,2':6',2''-terpyridine]platinum(II) chloride⁵ (64 mg, 0.11 mmol) were subsequently added and the mixture was stirred overnight at 25 °C. After this time, the obtained suspension was centrifuged and the solid was washed with MeOH (2 x 10 mL), CHCl_3 (3 x 10 mL) and Et_2O (1 x 10 mL) before being dried under vacuum. The pure title compound was obtained as a dark red solid (65 mg, 92% yield). ^1H NMR (500 MHz, DMSO-d_6) δ 9.07 (s, 2H, H^3), 9.00 (d, $J = 6.5$ Hz, 1H, H^b), 8.82 (br, 2H, H^6), 8.65 (br, 2H, H^5), 8.41 (br, 2H, H^3), 8.07 (d, $J = 6.5$ Hz, 1H, H^a), 7.89 (br, 2H, H^4), 7.81 (br, 2H, H^7), 7.55 (br, 1H, H^8), 7.40 (br, 1H, H^d). ^{19}F NMR (470 MHz, DMSO-d_6) δ -108.12 (t, $J = 7.3$ Hz). Complex **4** was poorly soluble in any solvent and, therefore, a 1D $^{13}\text{C}\{^1\text{H}\}$ -NMR spectrum could not be recorded. However, the following list containing indirect carbon chemical shifts, obtained with HSQC experiment, is reported. ^{13}C NMR δ 142.4, 130.4, 126.7, 111.4, 107.3. HRMS (ESI-TOF-pos): $m/z = 669.0746$ [M] $^{2+}$ (calc. 669.0788 for $\text{C}_{59}\text{H}_{32}\text{F}_4\text{N}_6\text{O}_2\text{Pt}_2\text{S}_2$).

NMR and HRMS spectra of Pt(II) Complexes and precursors

Compound **8**Figure S 1. ¹H-NMR (500 MHz, CDCl₃) spectrum of relevant signals of compound **8**.Figure S 2. Full ¹H-NMR (500 MHz, CDCl₃) spectrum of compound **8**.

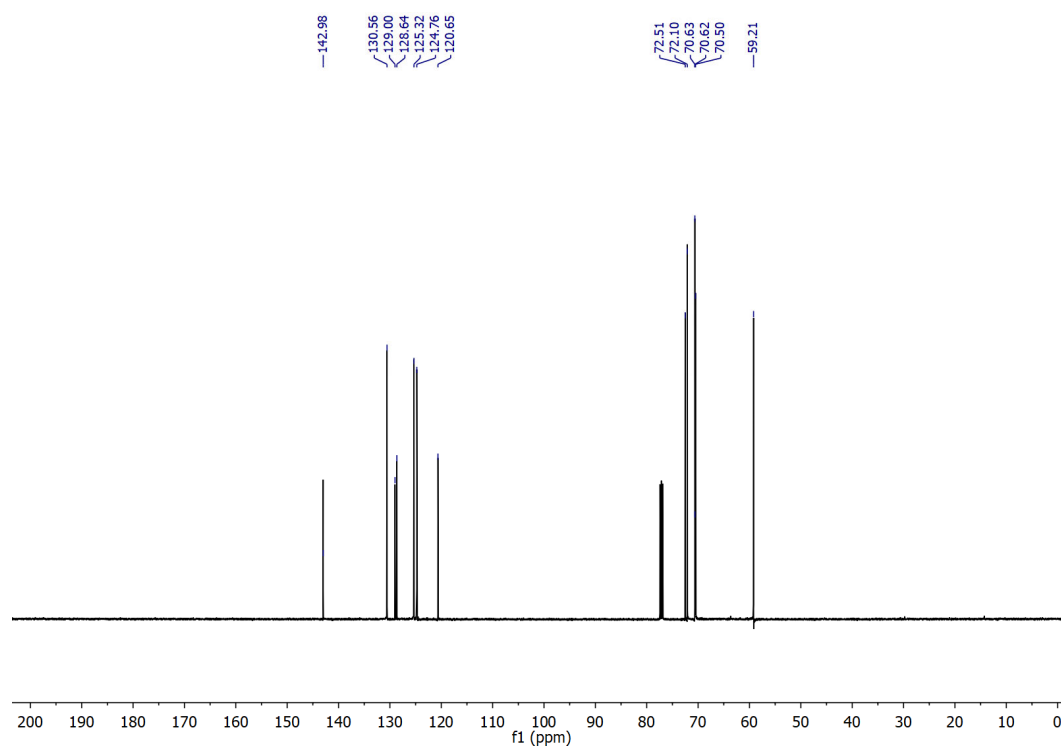


Figure S 3. $^{13}\text{C}\{^1\text{H}\}$ -NMR (126 MHz, CDCl_3) spectrum of compound **8**.

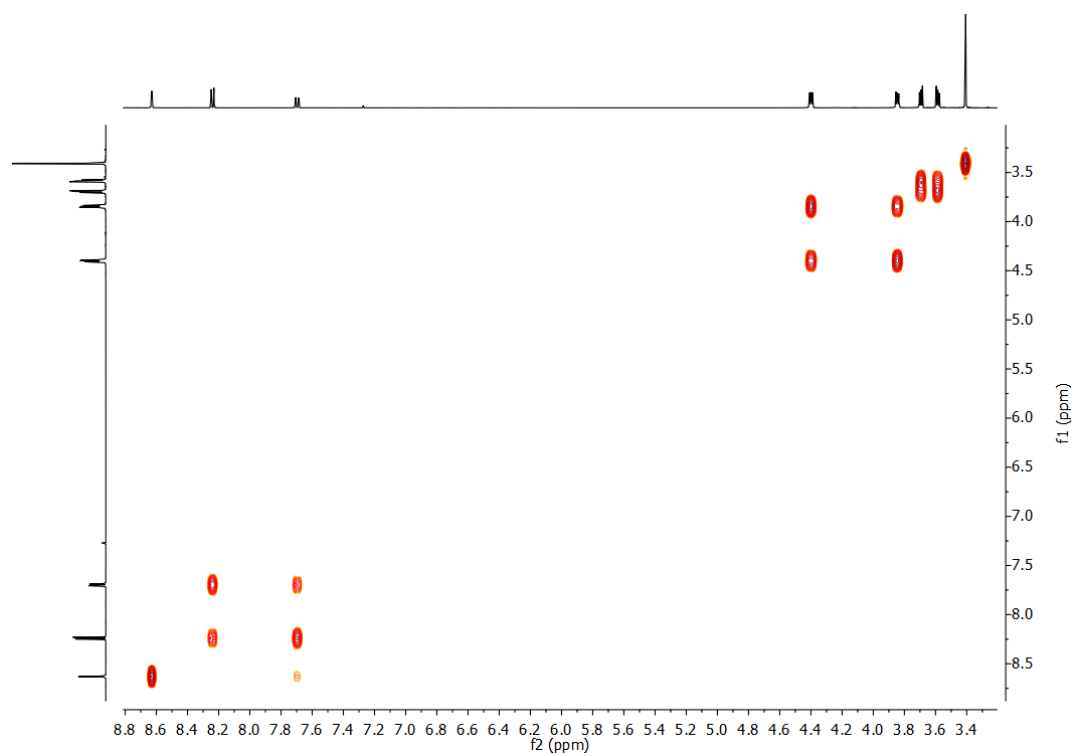


Figure S 4. ^1H - ^1H gCOSY (500 MHz, CDCl_3) spectrum of compound **8**.

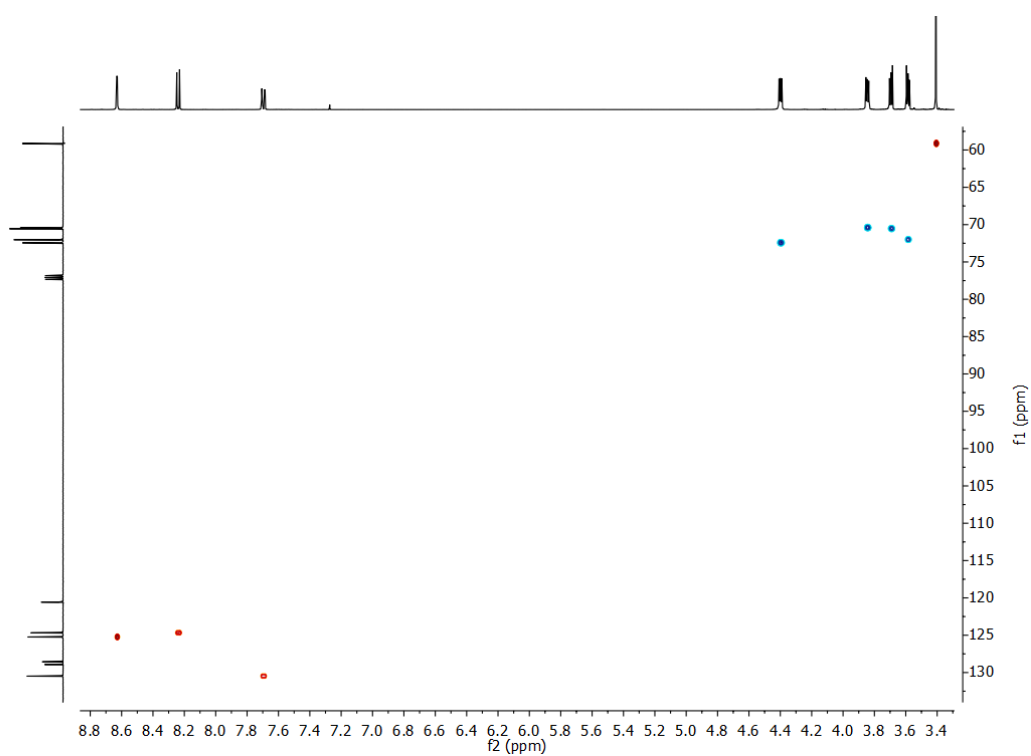


Figure S 5. ^1H - ^{13}C gHSQCAD (500 MHz, CDCl_3) spectrum of compound **8**.

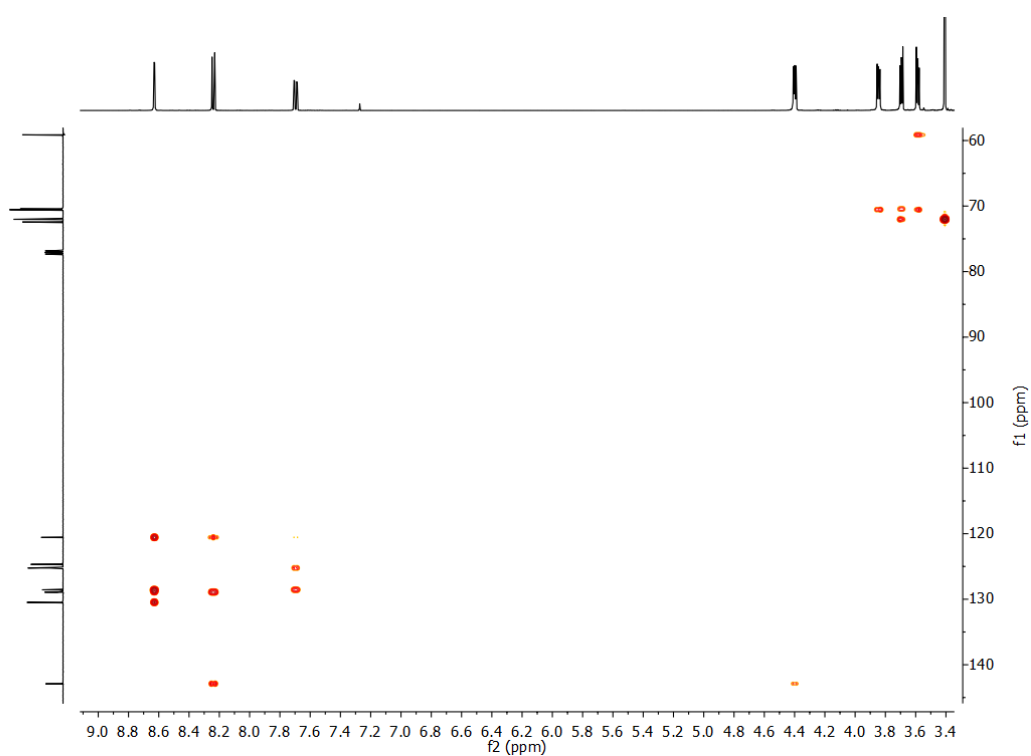


Figure S 6. ^1H - ^{13}C gHMBCAD (500 MHz, CDCl_3) spectrum of compound **8**.

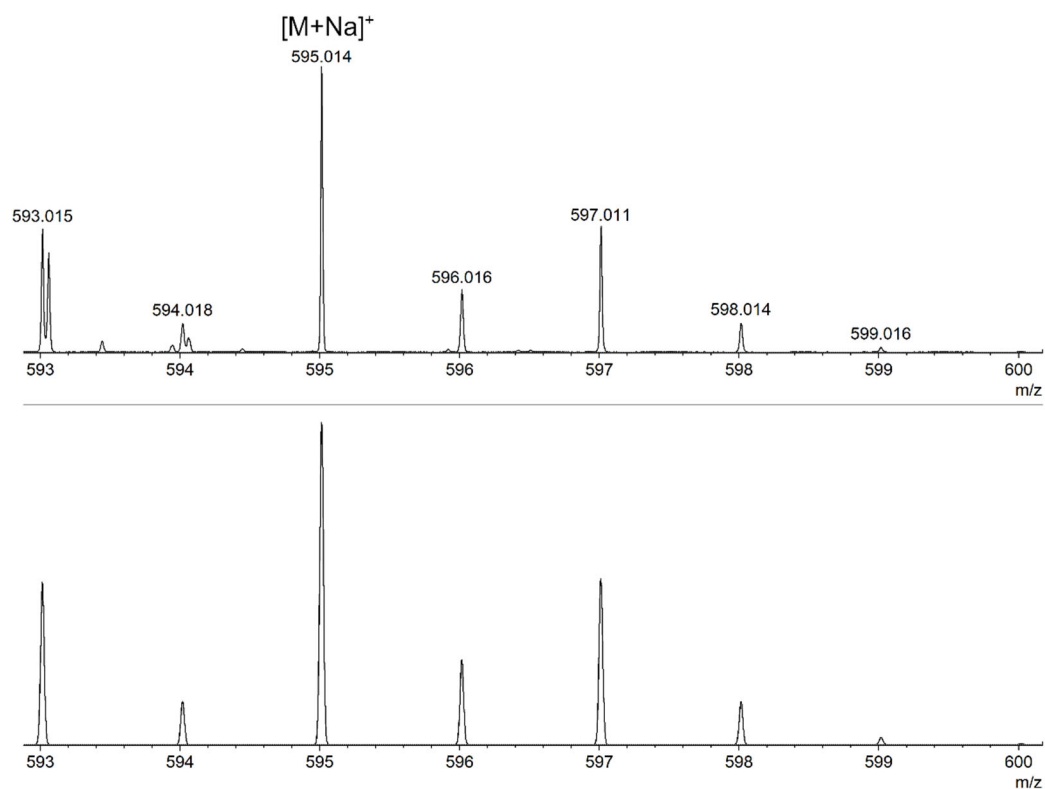
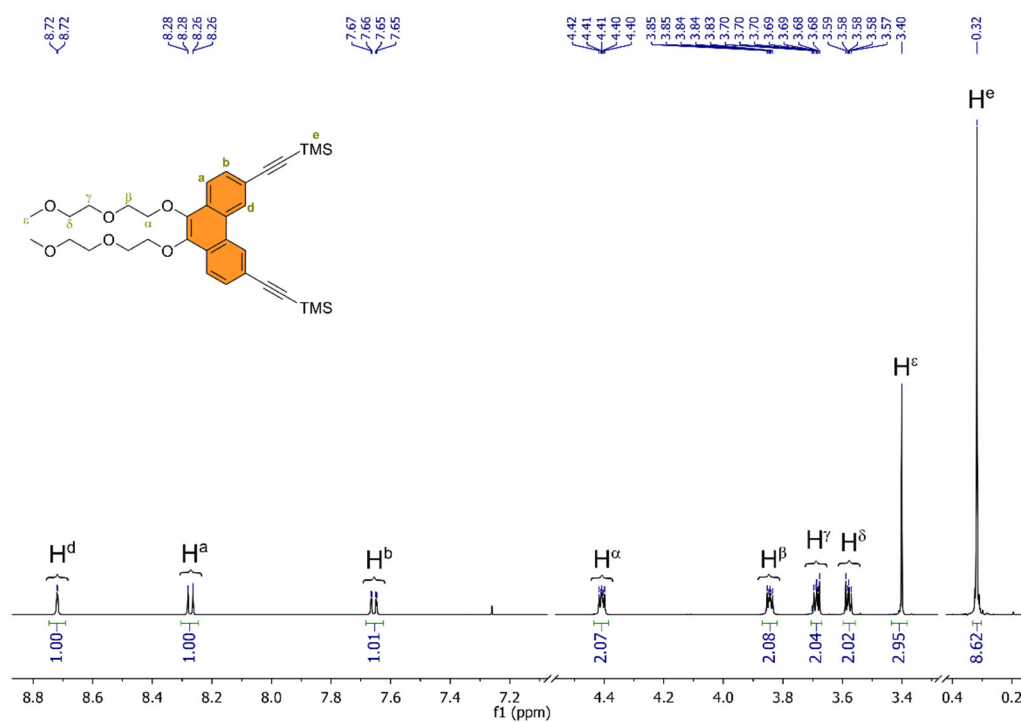
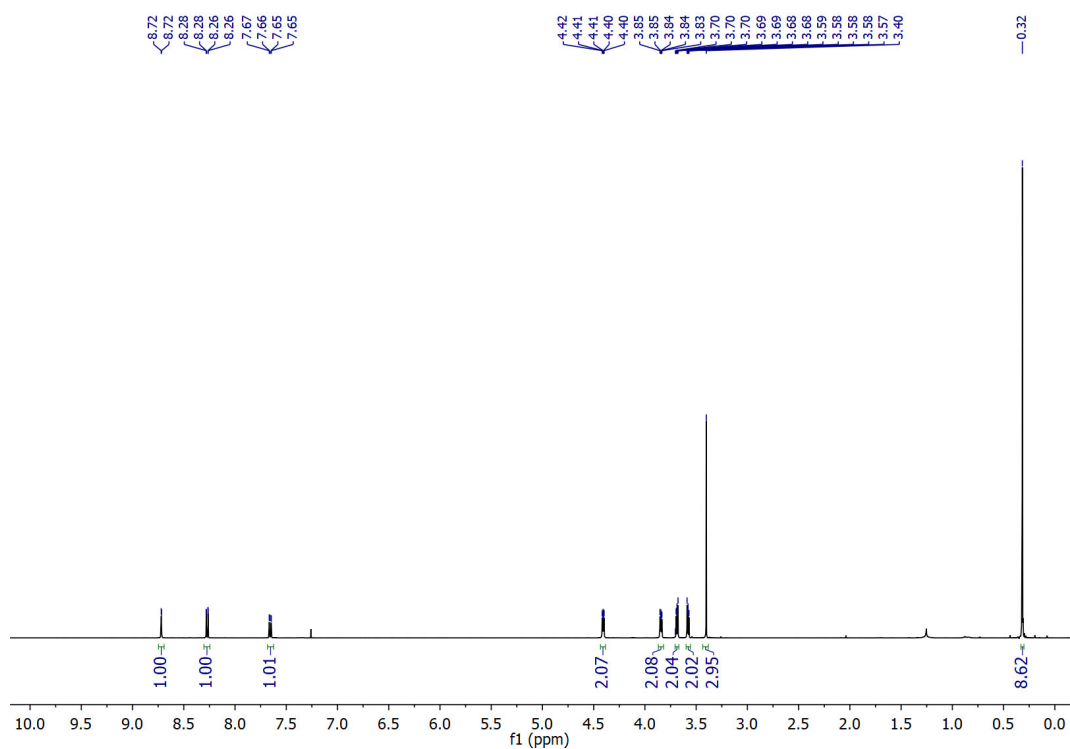


Figure S 7. HRMS (ESI-TOF-pos) of compound **8**, $[M+Na]^+$. Calculated (bottom), measured (top).

Compound **9****Figure S 8.** 1H -NMR (500 MHz, $CDCl_3$) spectrum of relevant signals of compound **9**.**Figure S 9.** Full 1H -NMR (500 MHz, $CDCl_3$) spectrum of compound **9**.

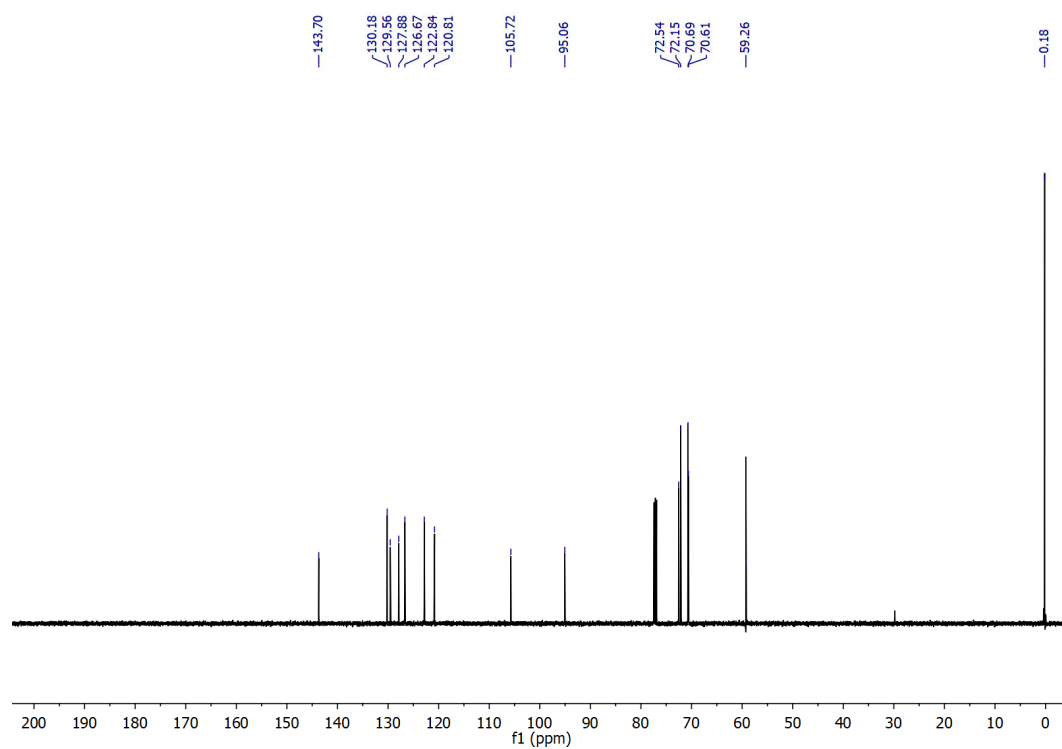


Figure S 10. $^{13}\text{C}\{^1\text{H}\}$ -NMR (126 MHz, CDCl_3) spectrum of compound **9**.

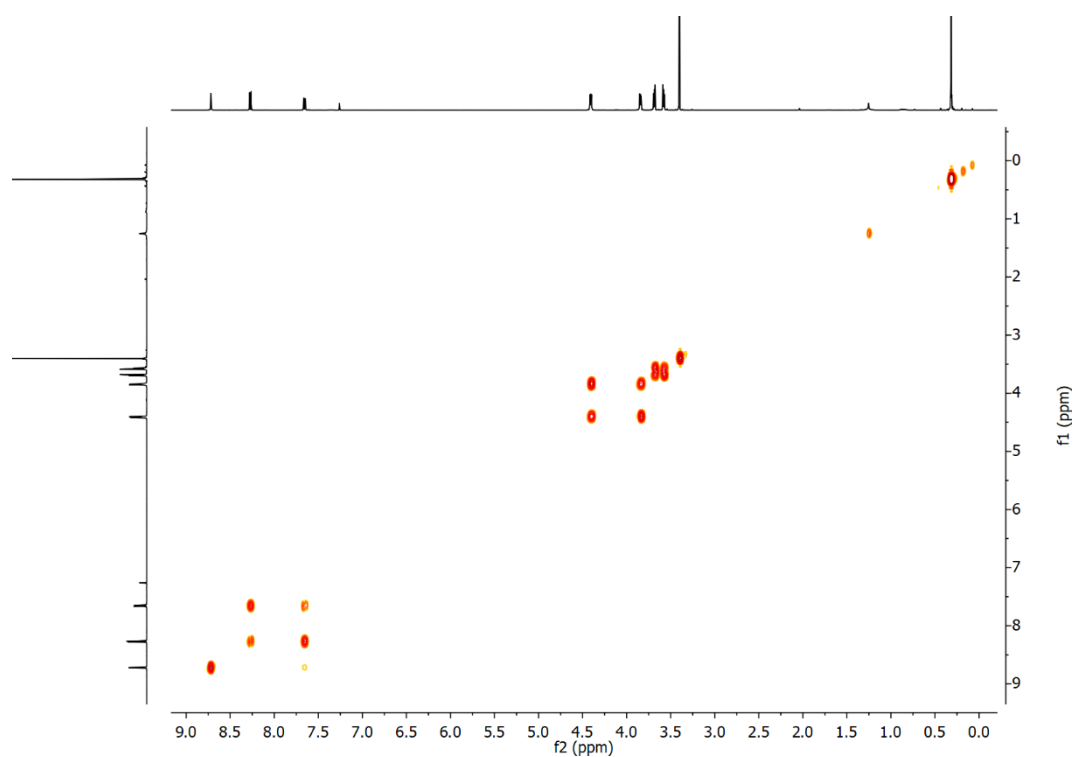


Figure S 11. ^1H - ^1H gCOSY (500 MHz, CDCl_3) spectrum of compound **9**.

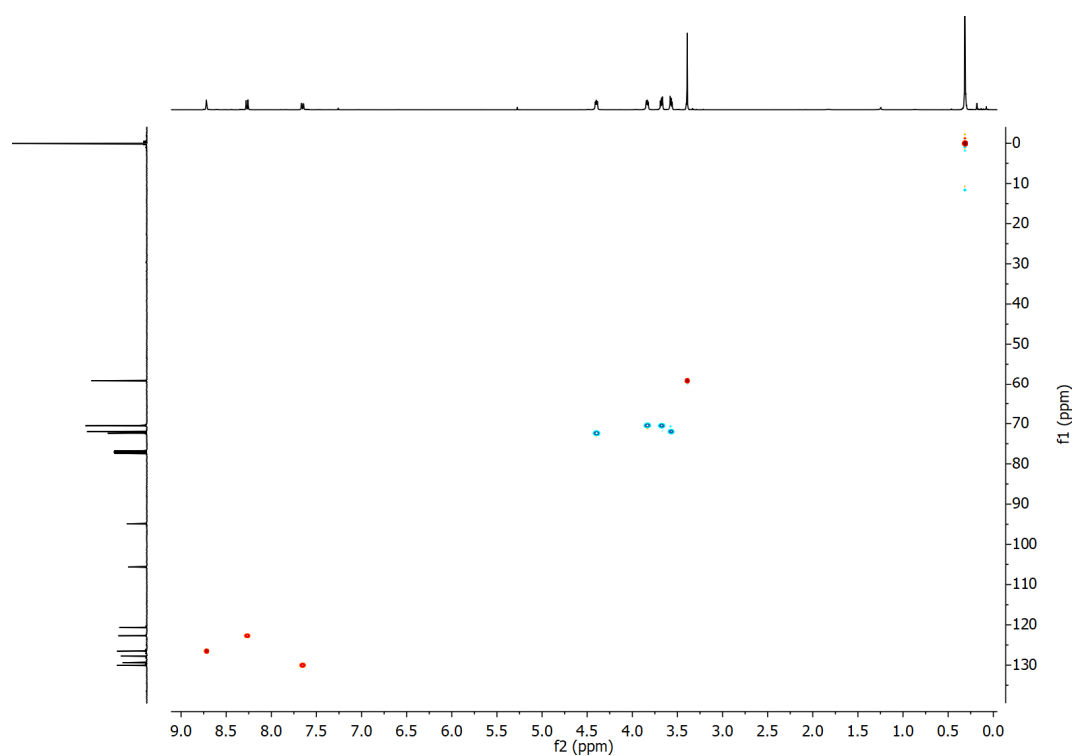


Figure S 12. ^1H - ^{13}C gHSQCAD (500 MHz, CDCl_3) spectrum of compound **9**.

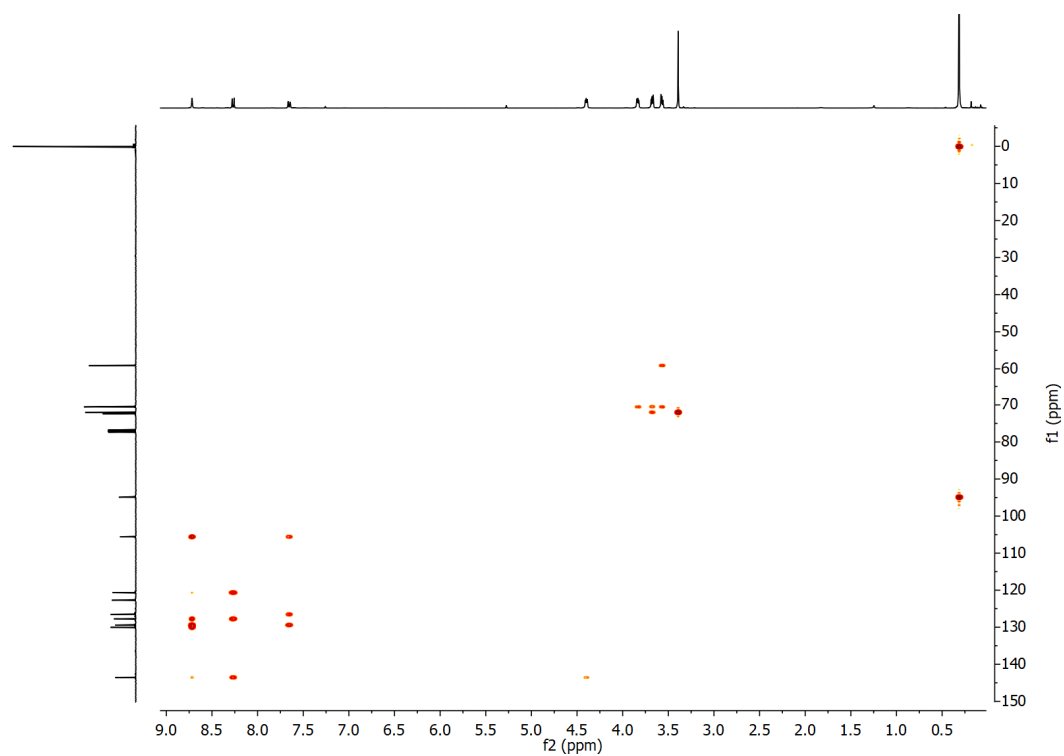


Figure S 13. ^1H - ^{13}C gHMBCAD (500 MHz, CDCl_3) spectrum of compound **9**.

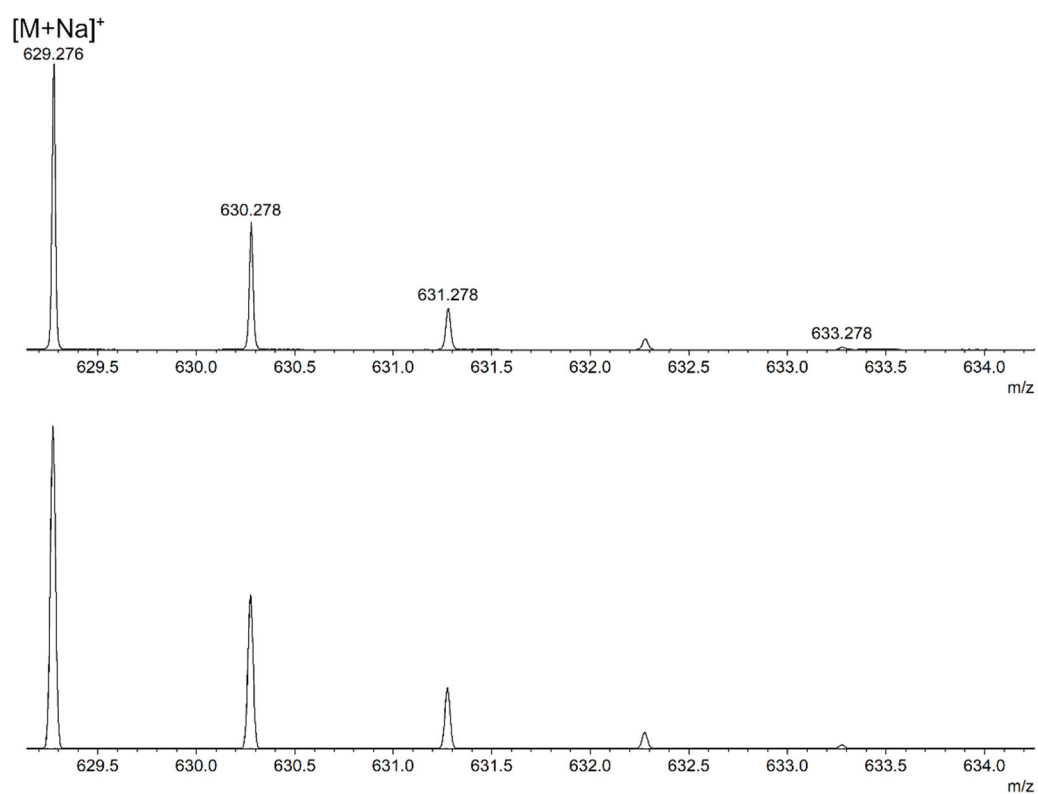
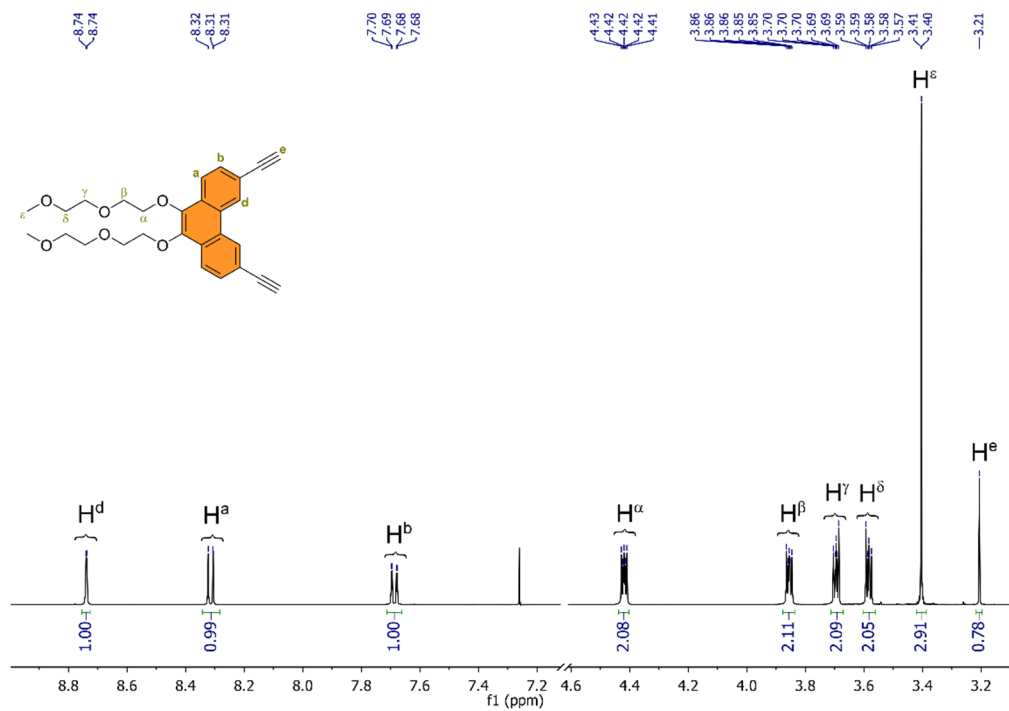
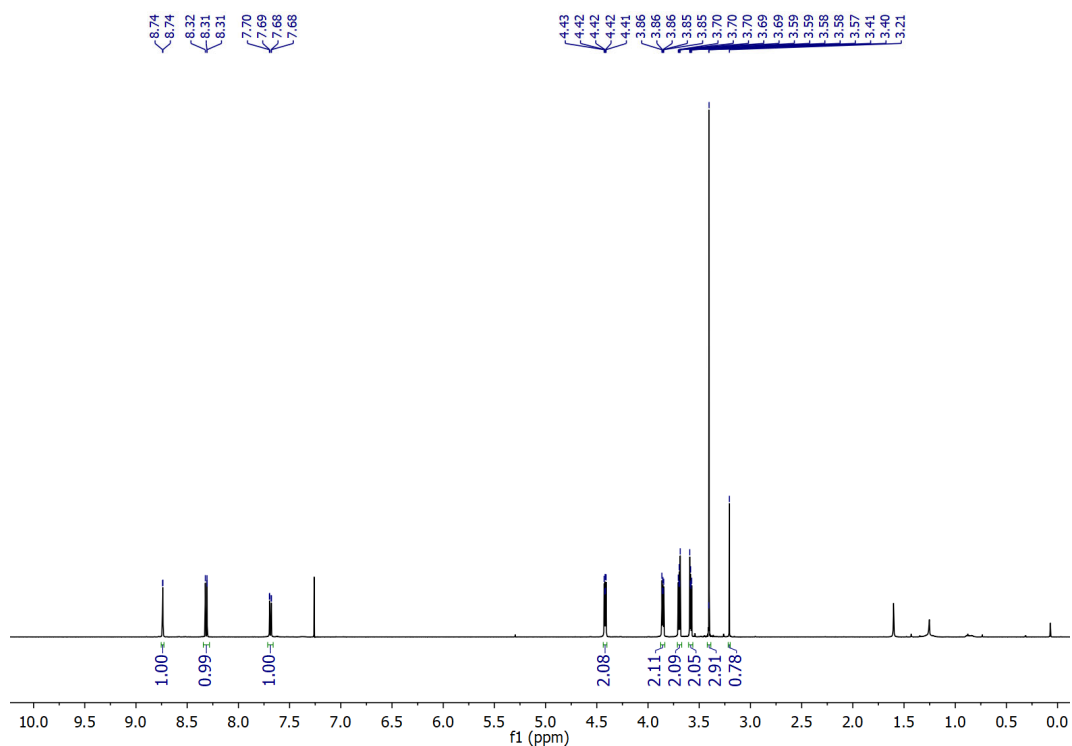


Figure S 14. HRMS (ESI-TOF-pos) of compound **9**, $[M+Na]^+$. Calculated (bottom), measured (top).

Compound **10**Figure S 15. ¹H-NMR (500 MHz, CDCl₃) spectrum of relevant signals of compound **10**.Figure S 16. Full ¹H-NMR (500 MHz, CDCl₃) spectrum of compound **10**.

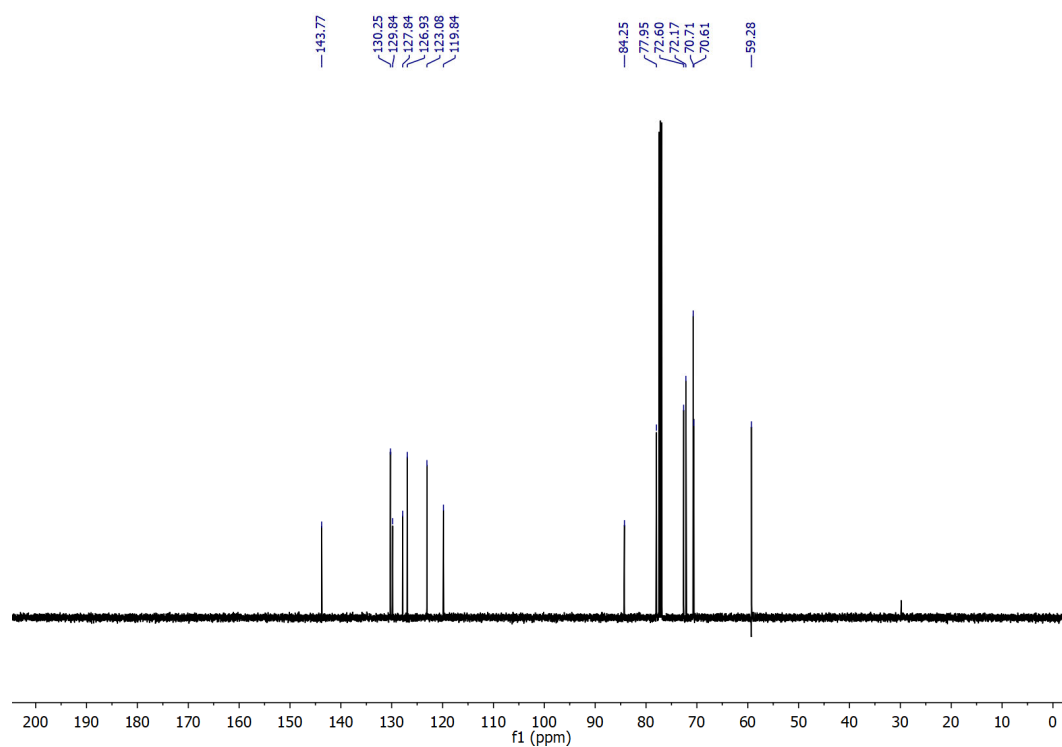


Figure S 17. $^{13}\text{C}\{^1\text{H}\}$ -NMR (126 MHz, CDCl_3) spectrum of compound **10**.

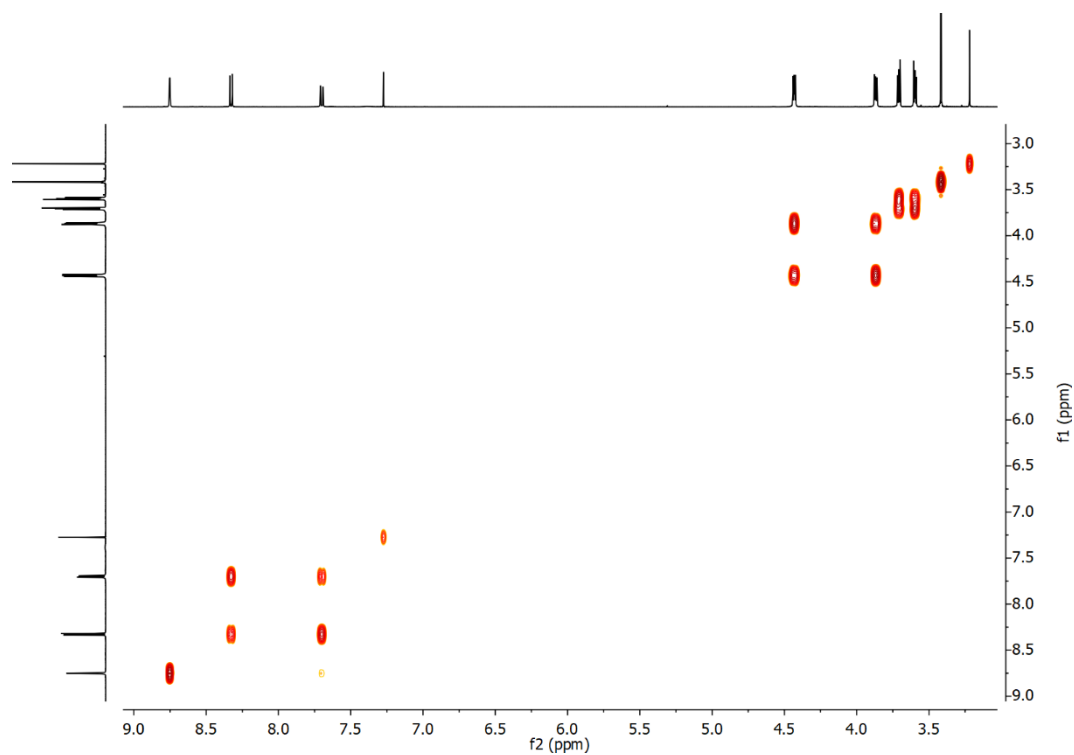


Figure S 18. ^1H - ^1H gCOSY (500 MHz, CDCl_3) spectrum of compound **10**.

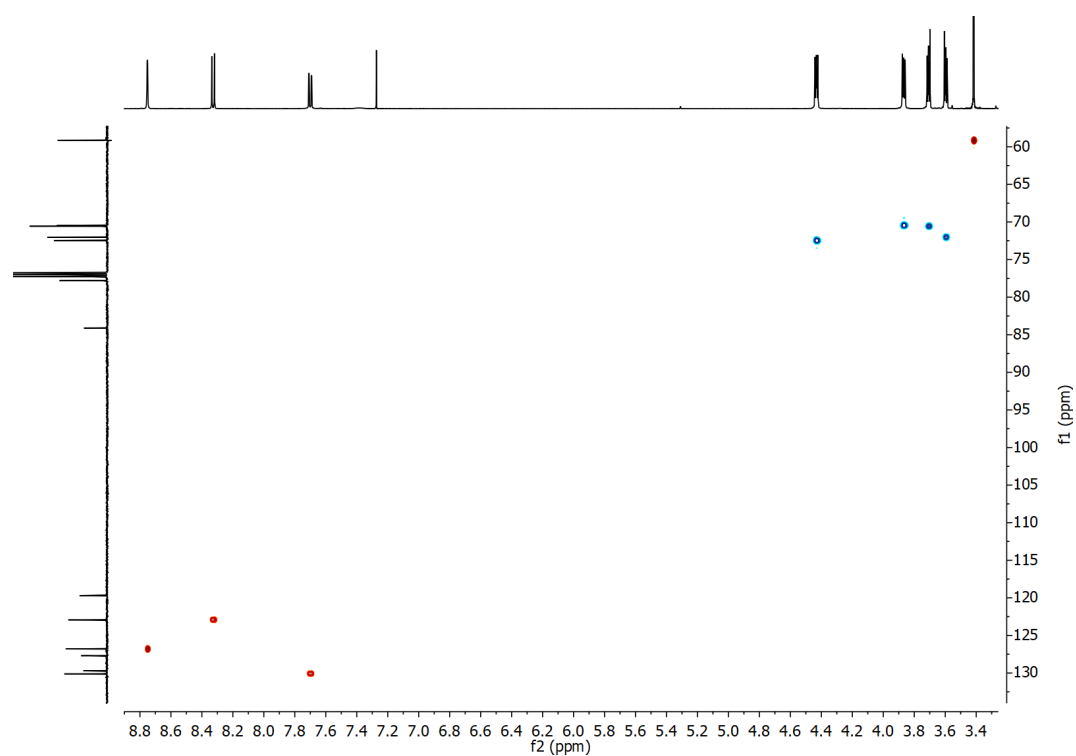


Figure S 19. ^1H - ^{13}C gHSQCAD (500 MHz, CDCl_3) spectrum of compound **10**.

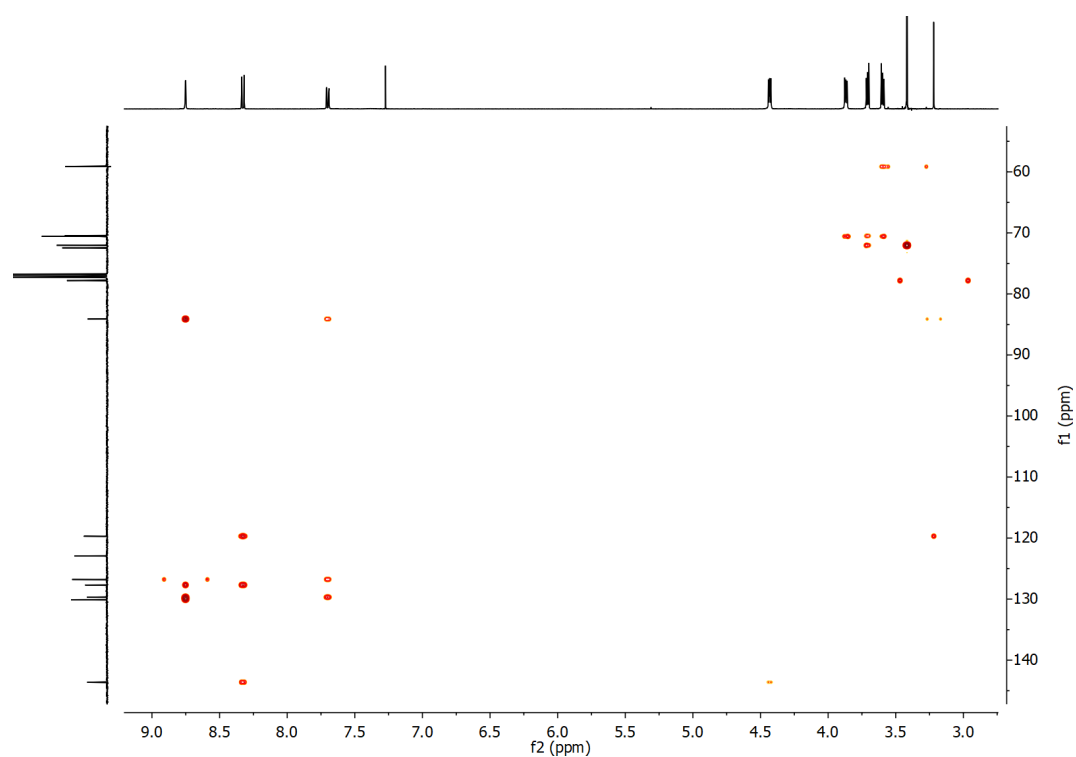


Figure S 20. ^1H - ^{13}C gHMBCAD (500 MHz, CDCl_3) spectrum of compound **10**.

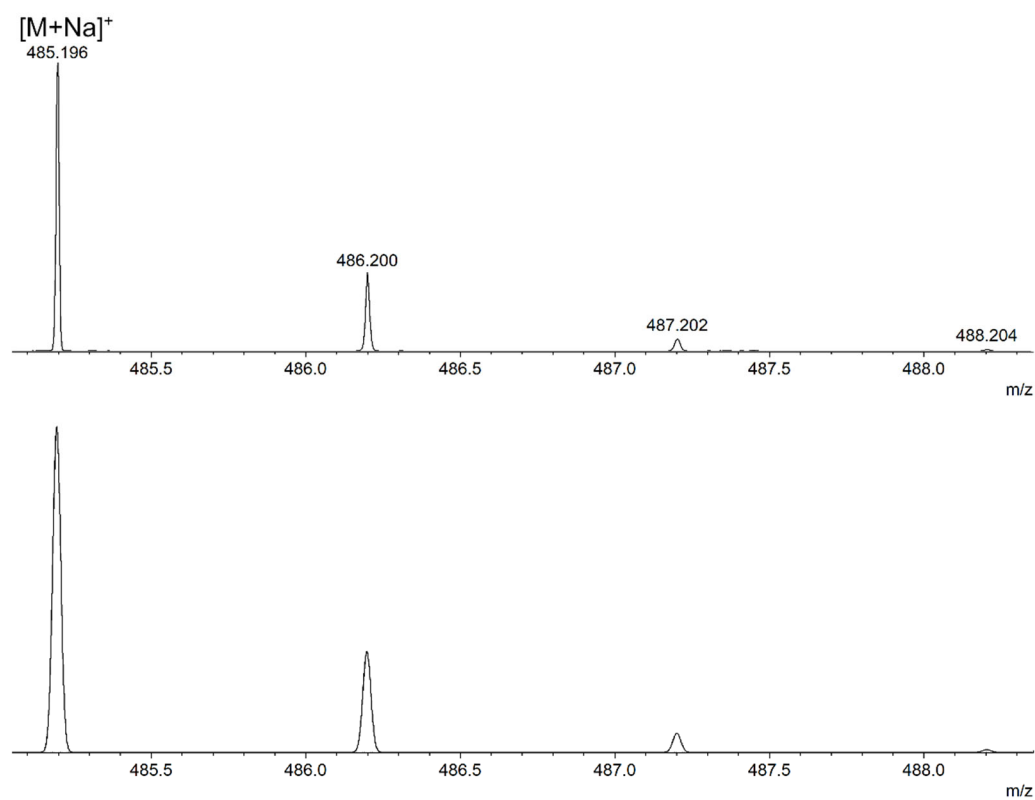
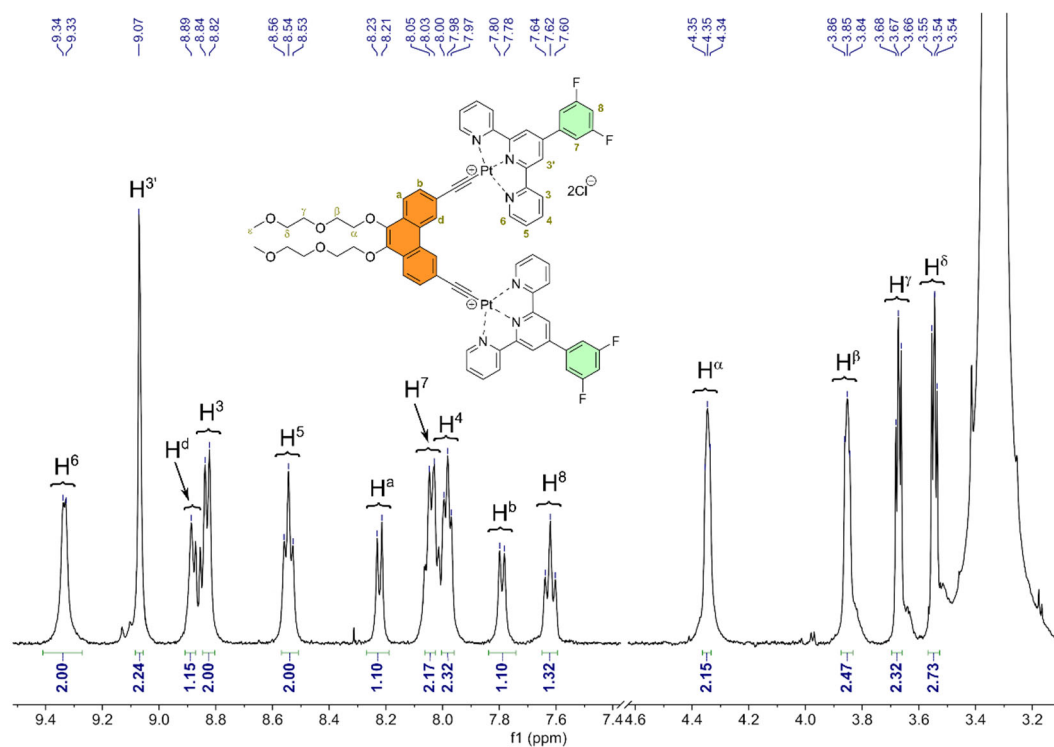
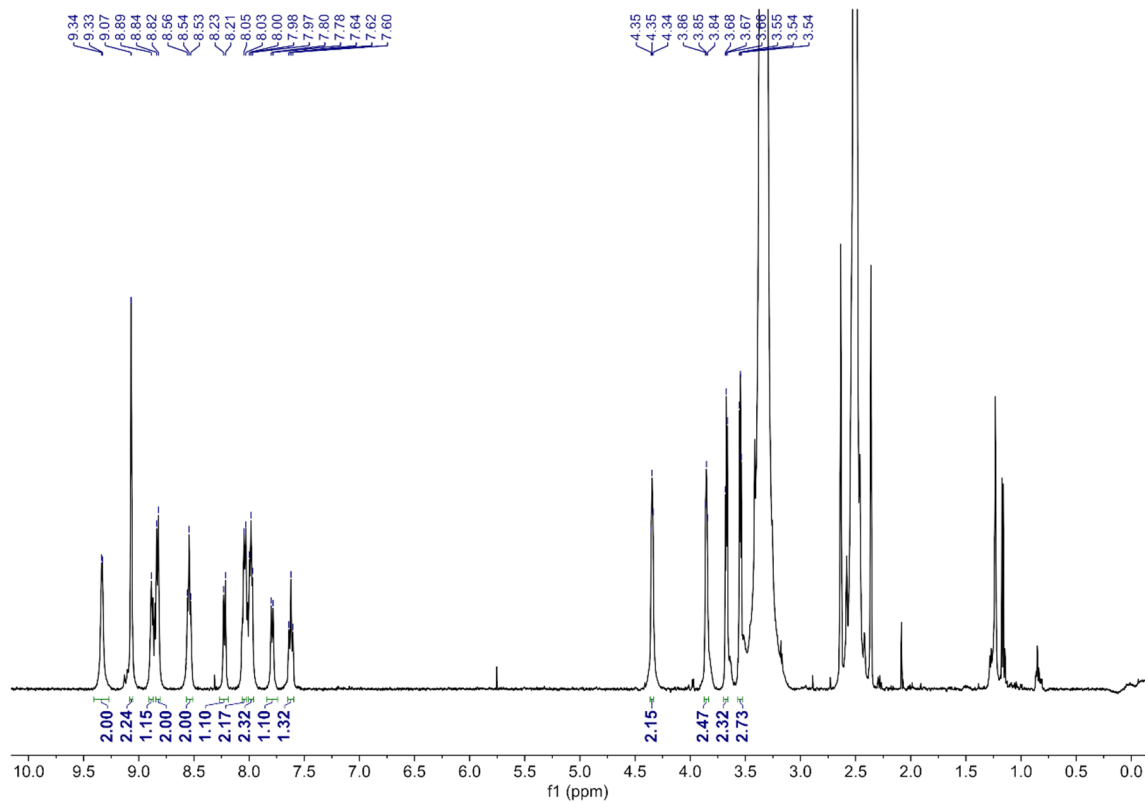


Figure S 21. HRMS (ESI-TOF-pos) of compound **10**, $[M+Na]^+$. Calculated (bottom), measured (top).

Complex 1

Figure S 22. ¹H-NMR (500 MHz, DMSO-d₆) spectrum of relevant signals of complex 1.Figure S 23. Full ¹H-NMR (500 MHz, DMSO-d₆) spectrum of complex 1.

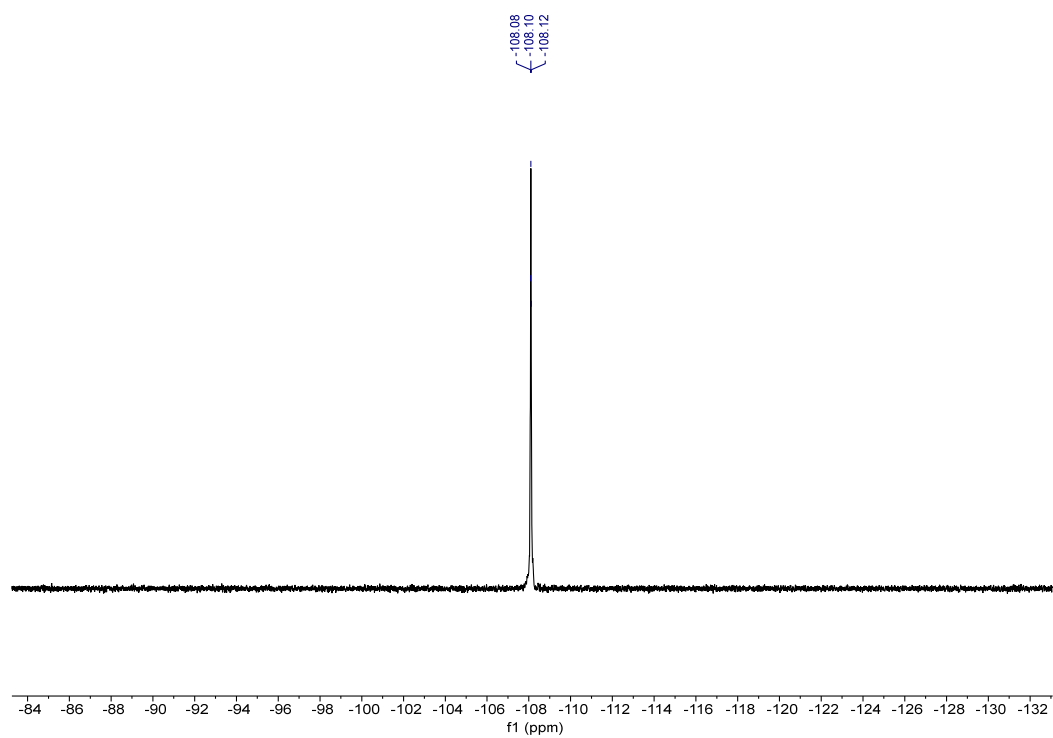


Figure S 24. ^{19}F -NMR (470 MHz, DMSO-d_6) spectrum of complex **1**.

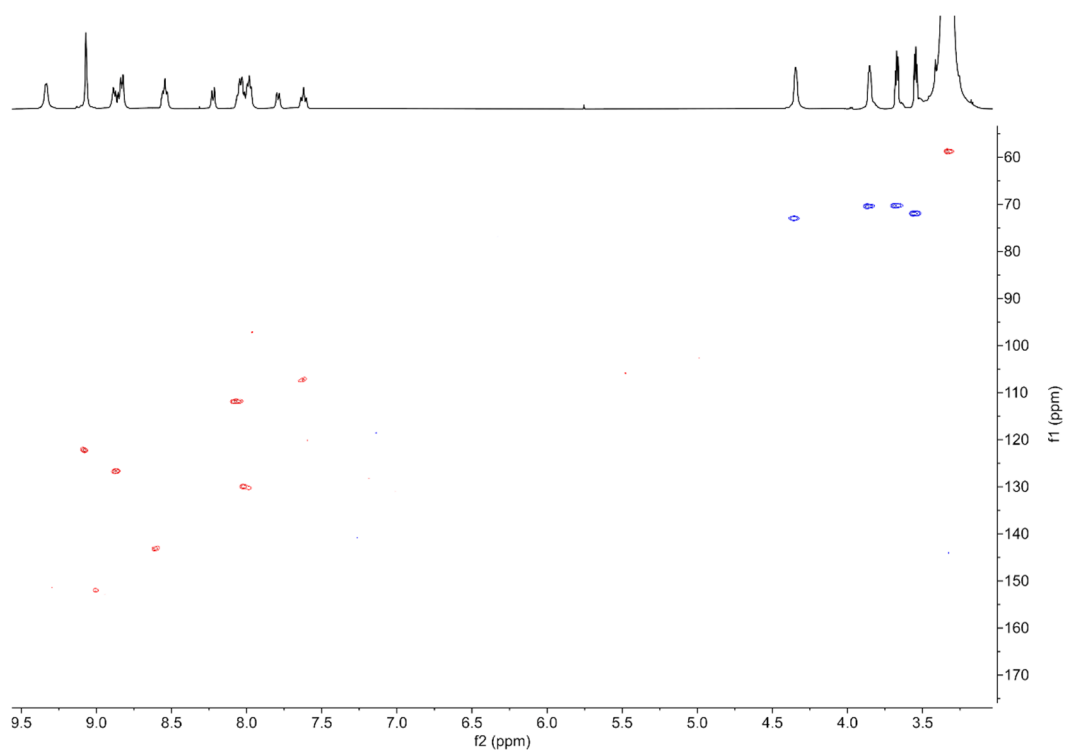


Figure S 25. ^1H - ^{13}C gHSQCAD (500 MHz, DMSO-d_6) spectrum of complex **1**.

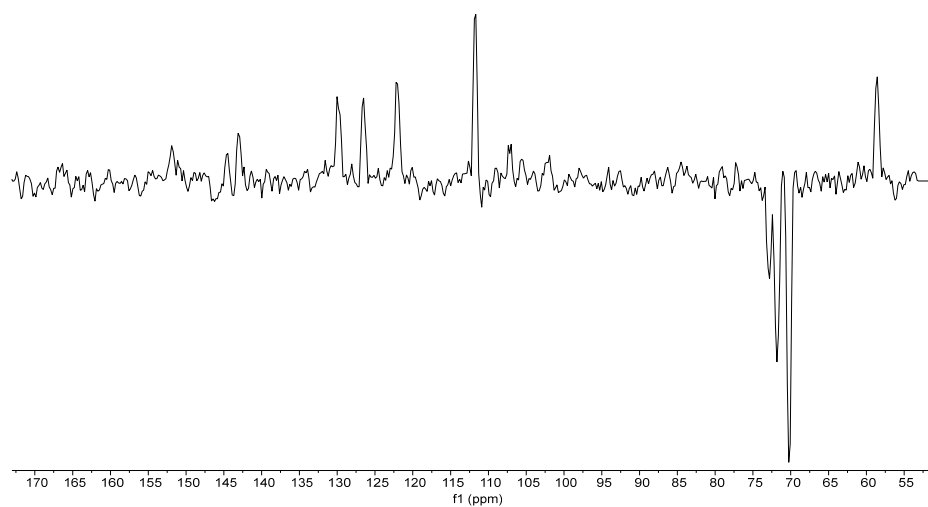


Figure S 26. Extracted vertical trace from the ^1H - ^{13}C gHSQCAD (500 MHz, DMSO-d_6) spectrum of complex **1**.

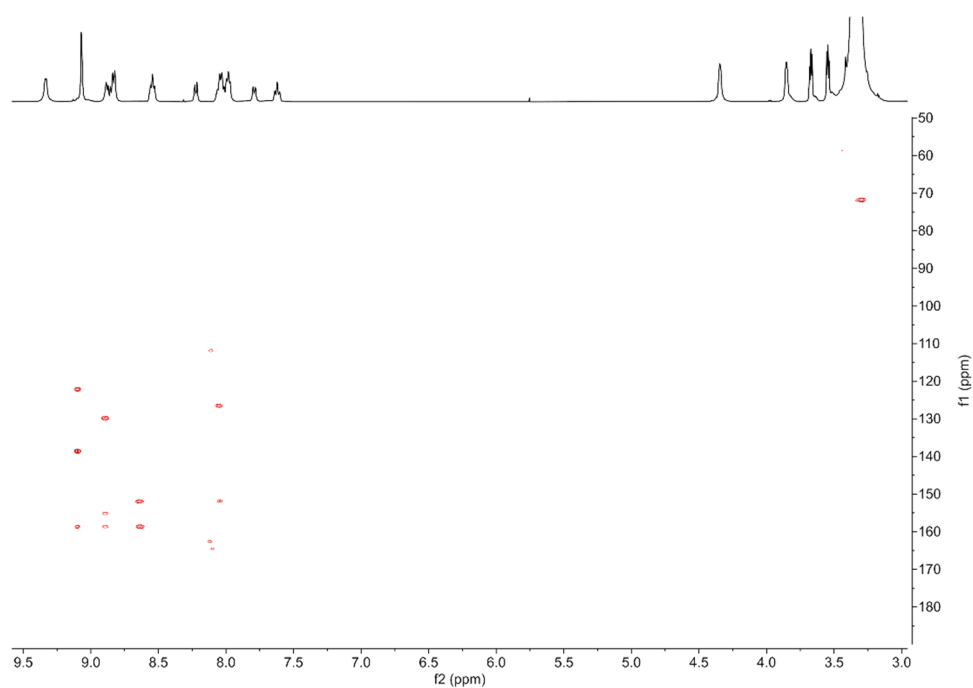


Figure S 27. ^1H - ^{13}C gHMBCAD (500 MHz, DMSO-d_6) spectrum of complex **1**.

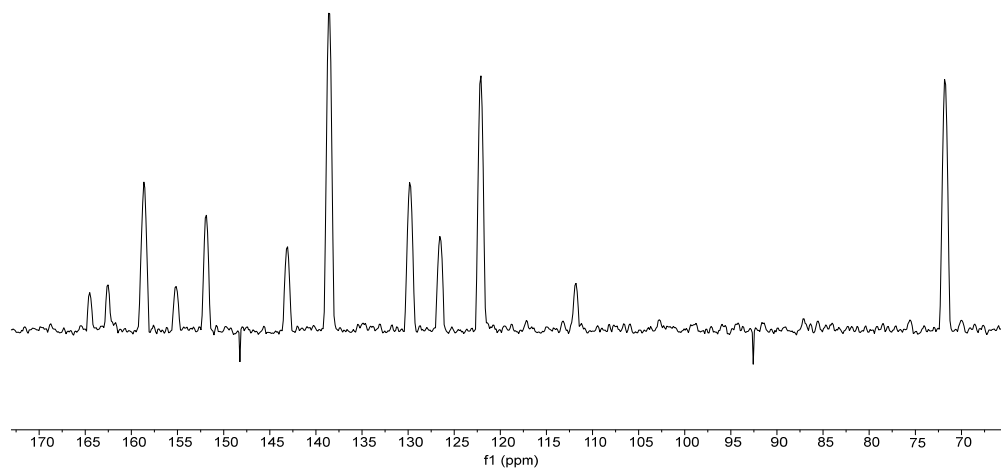


Figure S 28. Extracted vertical trace from the ^1H - ^{13}C gHMBCAD (500 MHz, DMSO-d_6) spectrum of complex **1**.

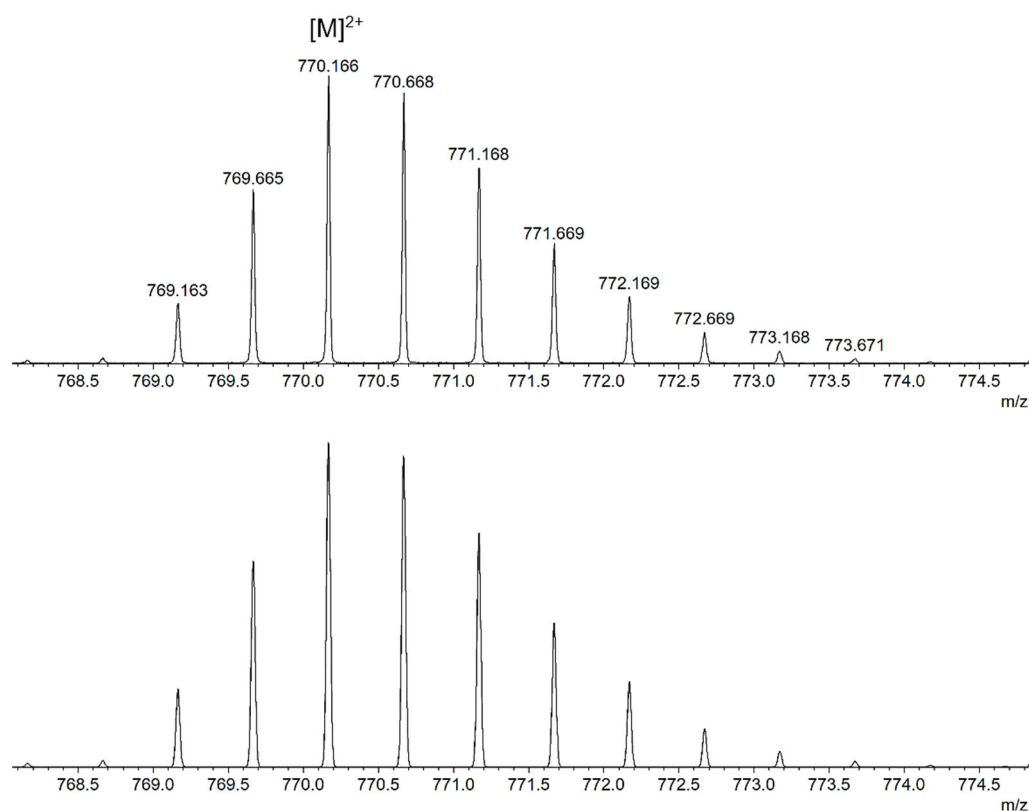
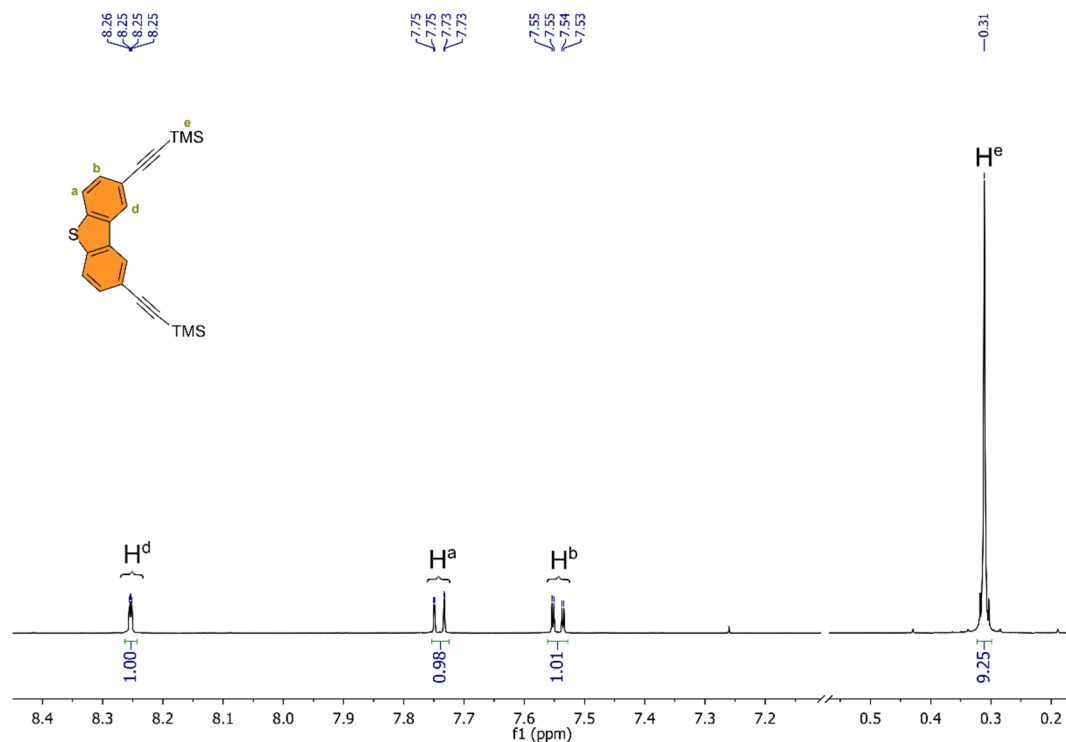
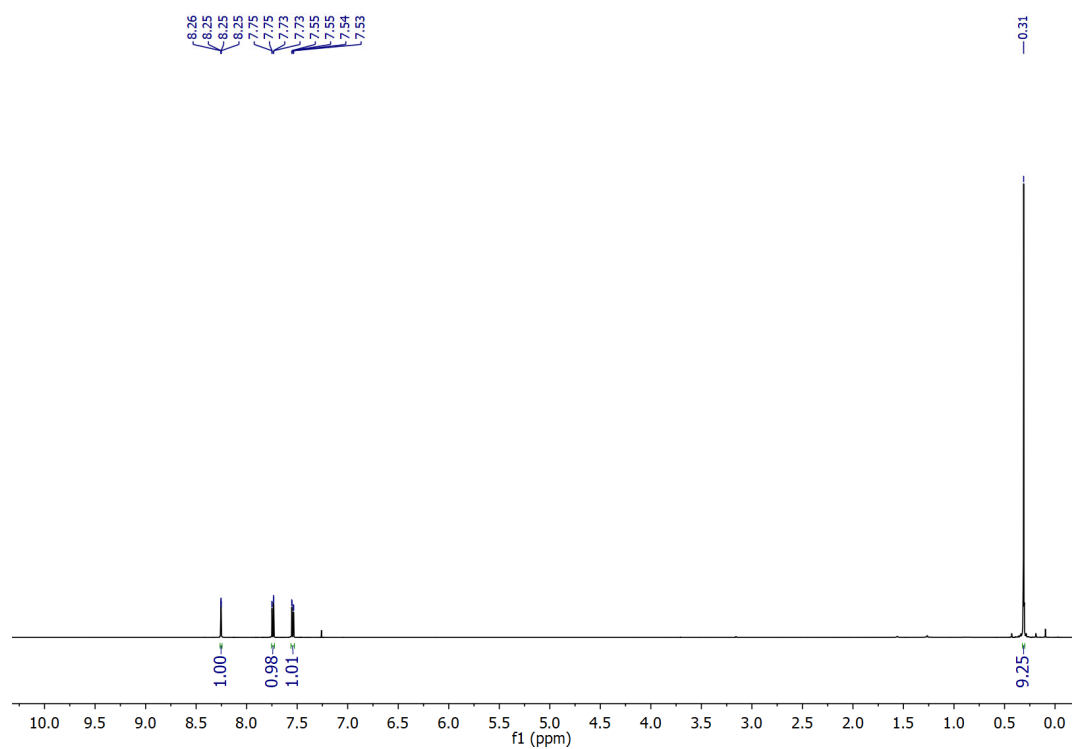


Figure S 29. HRMS (ESI-TOF-pos) of complex **1**, $[\text{M}]^{2+}$. Calculated (below), measured (top).

Compound **12****Figure S 30.** ¹H-NMR (500 MHz, CDCl₃) spectrum of relevant signals of compound **12**.**Figure S 31.** Full ¹H-NMR (500 MHz, CDCl₃) spectrum of compound **12**.

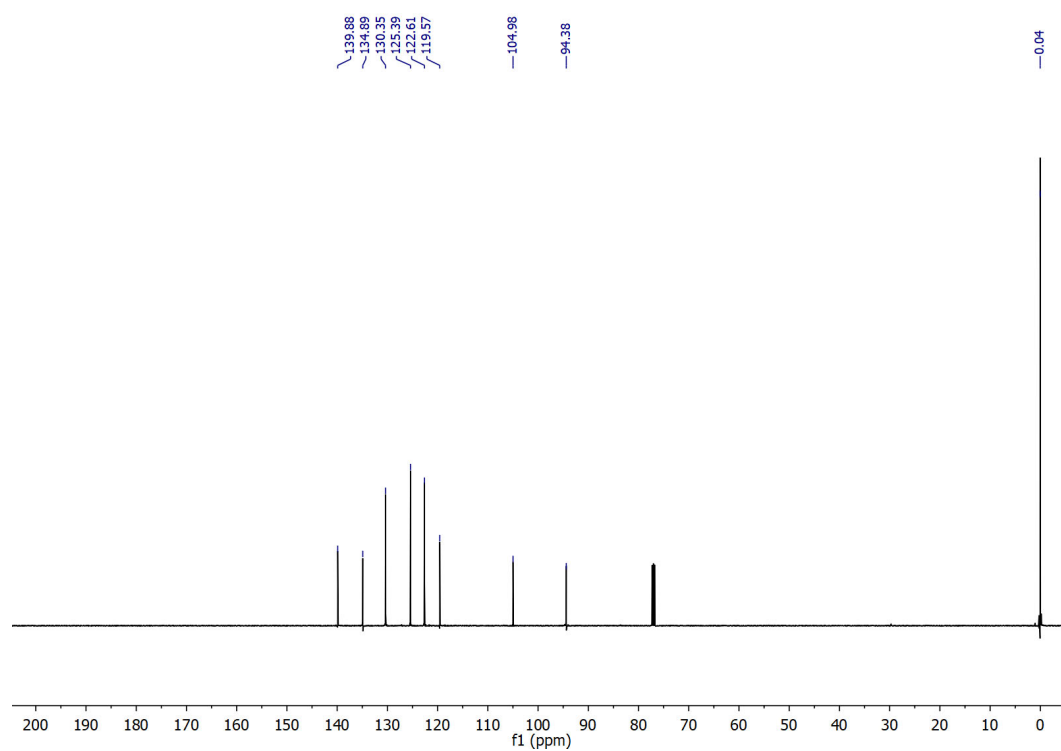


Figure S 32. $^{13}\text{C}\{^1\text{H}\}$ -NMR (126 MHz, CDCl_3) spectrum of compound **12**.

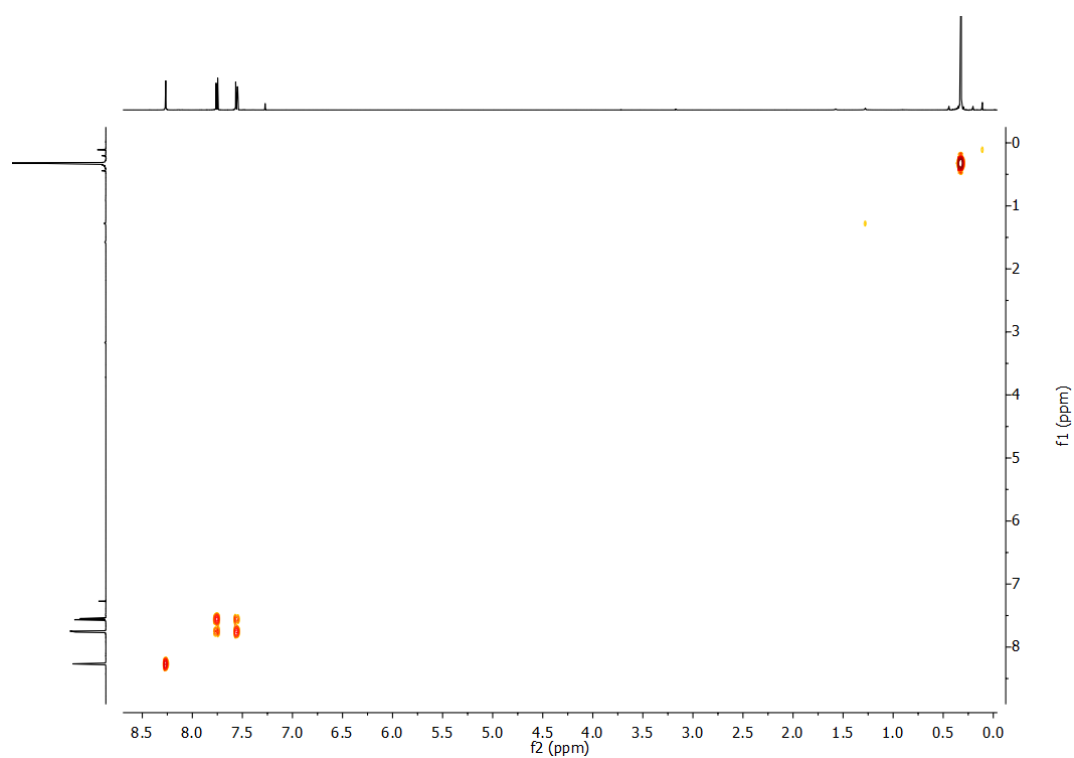


Figure S 33. ^1H - ^1H gCOSY (500 MHz, CDCl_3) spectrum of compound **12**.

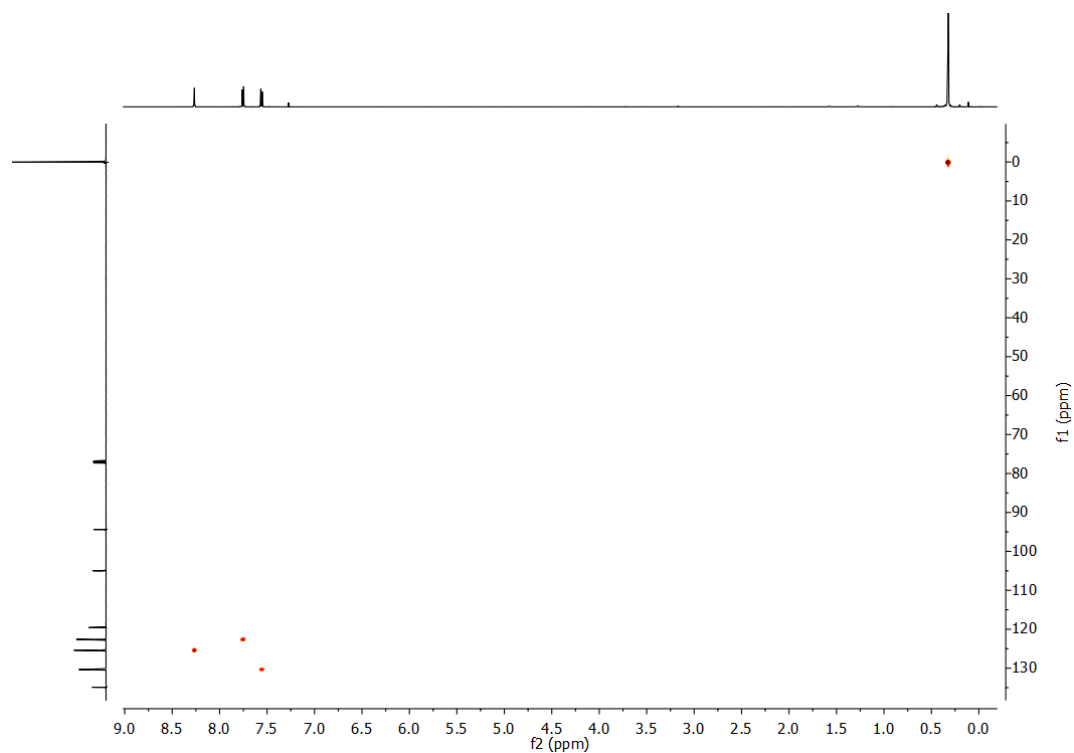


Figure S 34. ^1H - ^{13}C gHSQCAD (500 MHz, CDCl_3) spectrum of compound 12.

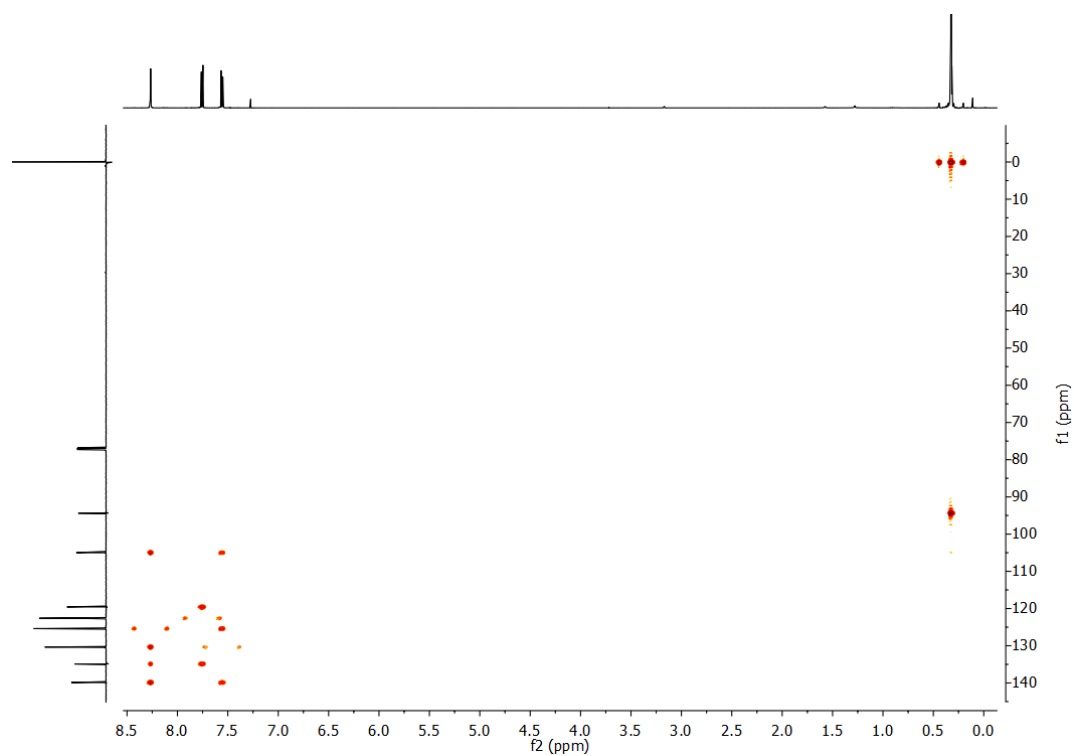


Figure S 35. ^1H - ^{13}C gHMBCAD (500 MHz, CDCl_3) spectrum of compound 12.

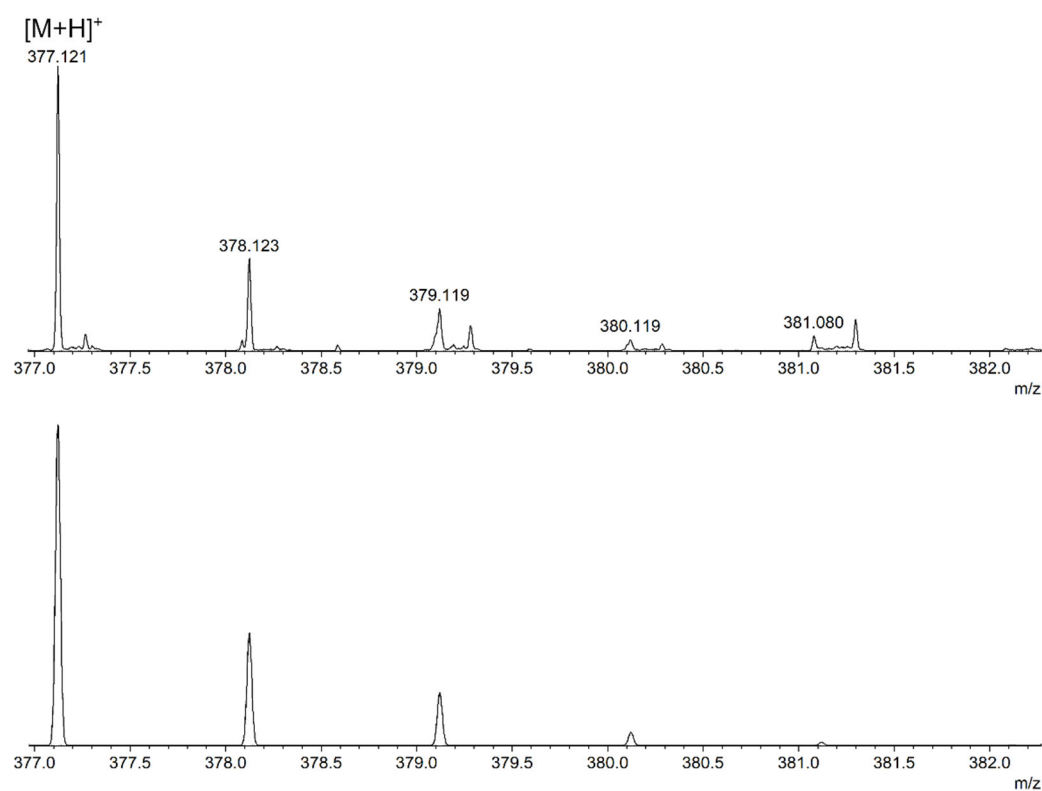
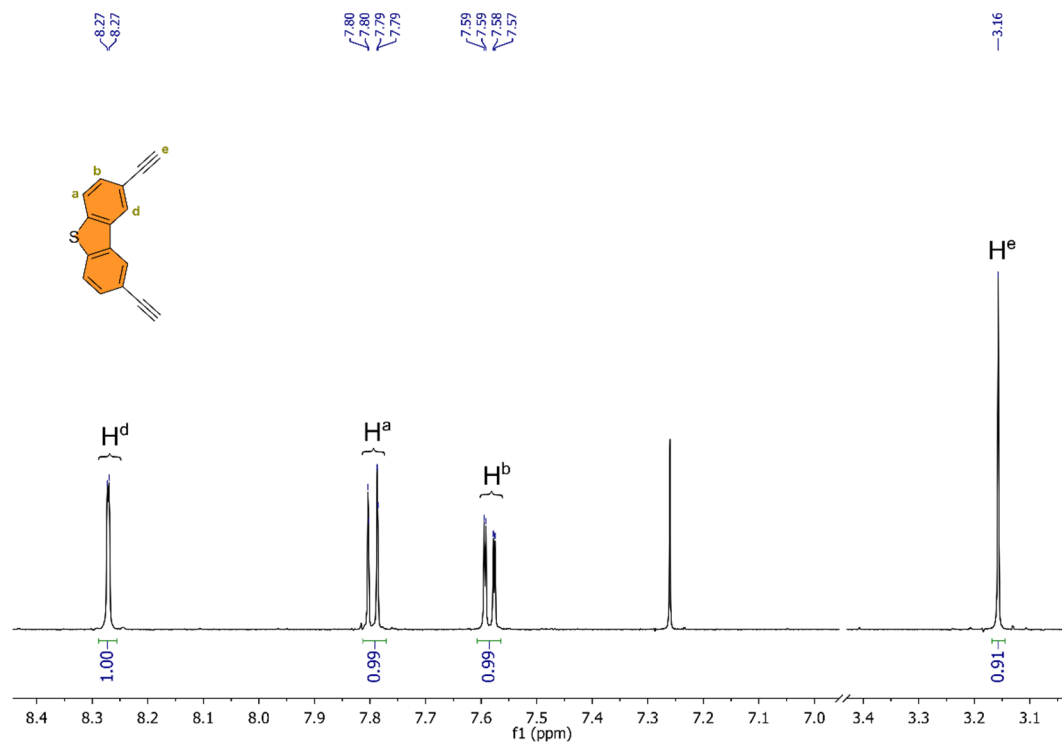
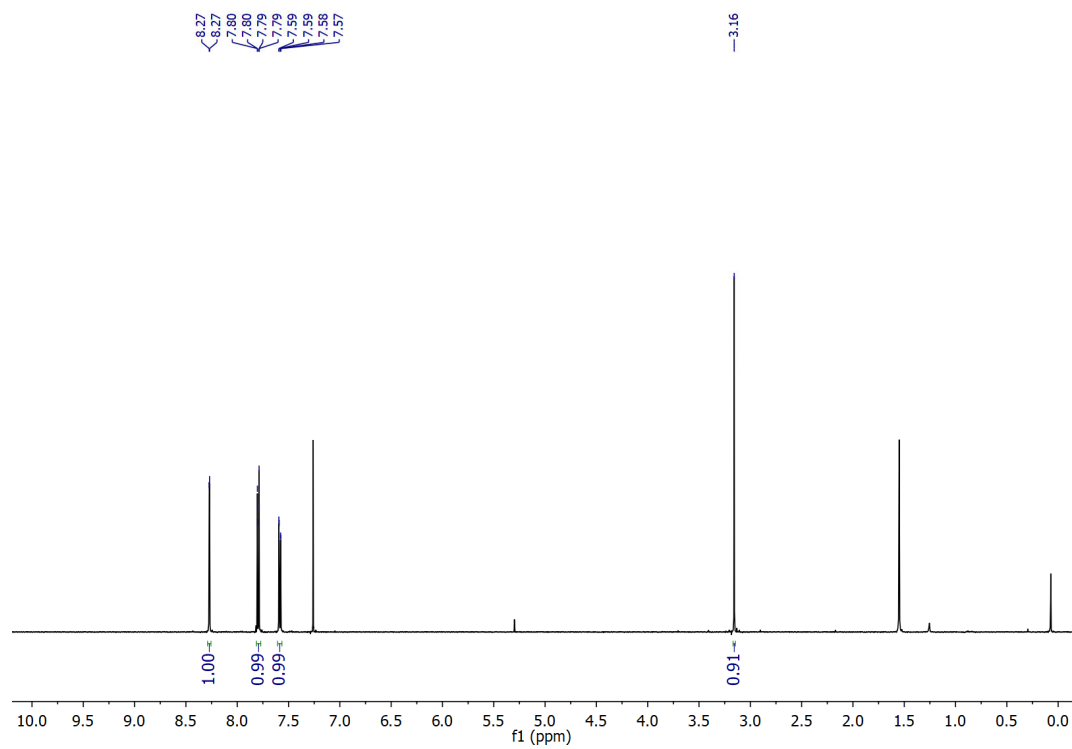


Figure S 36. HRMS (ESI-TOF-pos) of compound **12**, $[M+H]^+$. Calculated (below), measured (top).

Compound **13**Figure S 37. ^1H -NMR (500 MHz, CDCl_3) spectrum of relevant signals of compound **13**.Figure S 38. Full ^1H -NMR (500 MHz, CDCl_3) spectrum of compound **13**.

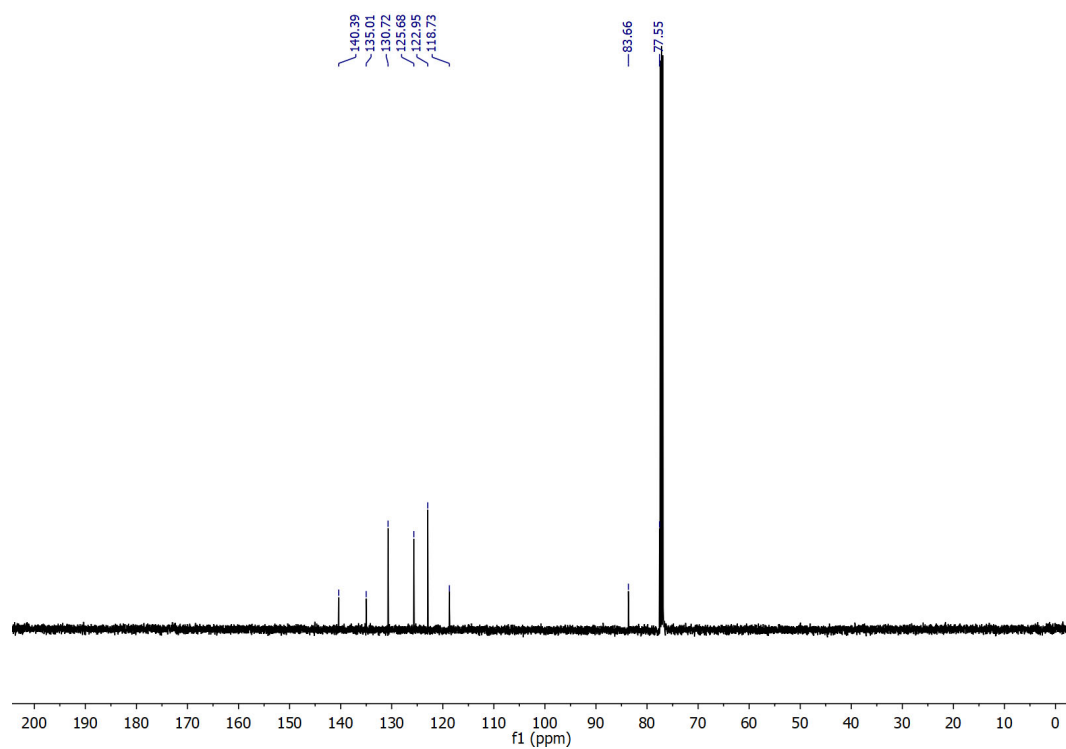


Figure S 39. $^{13}\text{C}\{^1\text{H}\}$ -NMR (126 MHz, CDCl_3) spectrum of compound **13**.

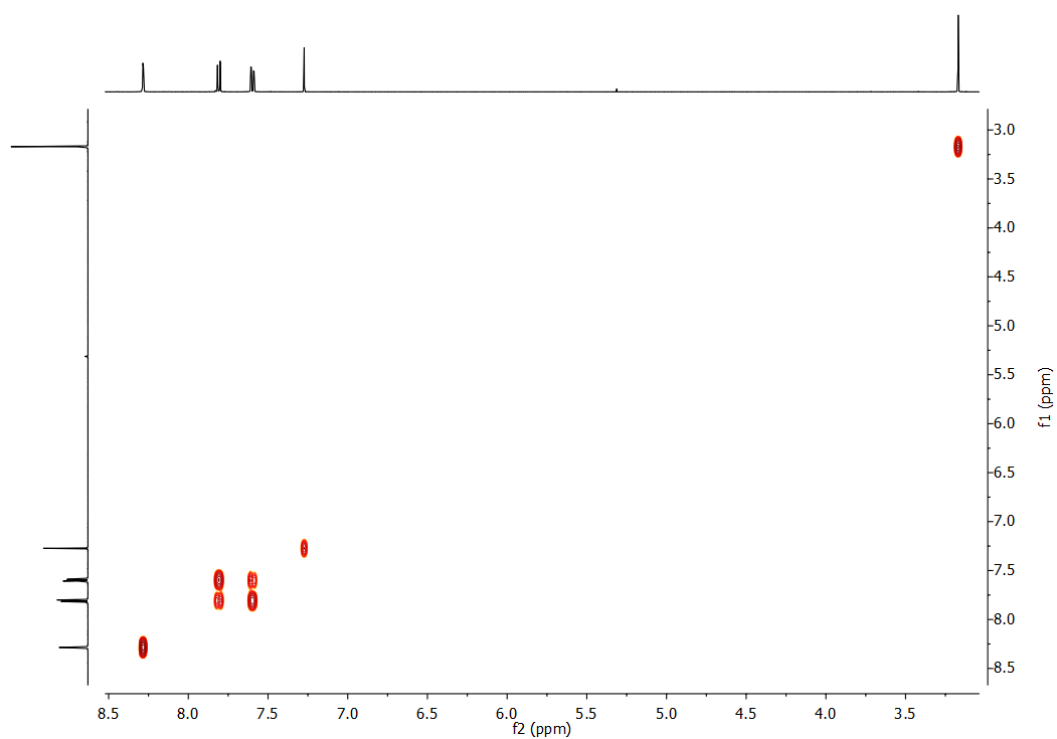


Figure S 40. ^1H - ^1H gCOSY (500 MHz, CDCl_3) spectrum of compound **13**.

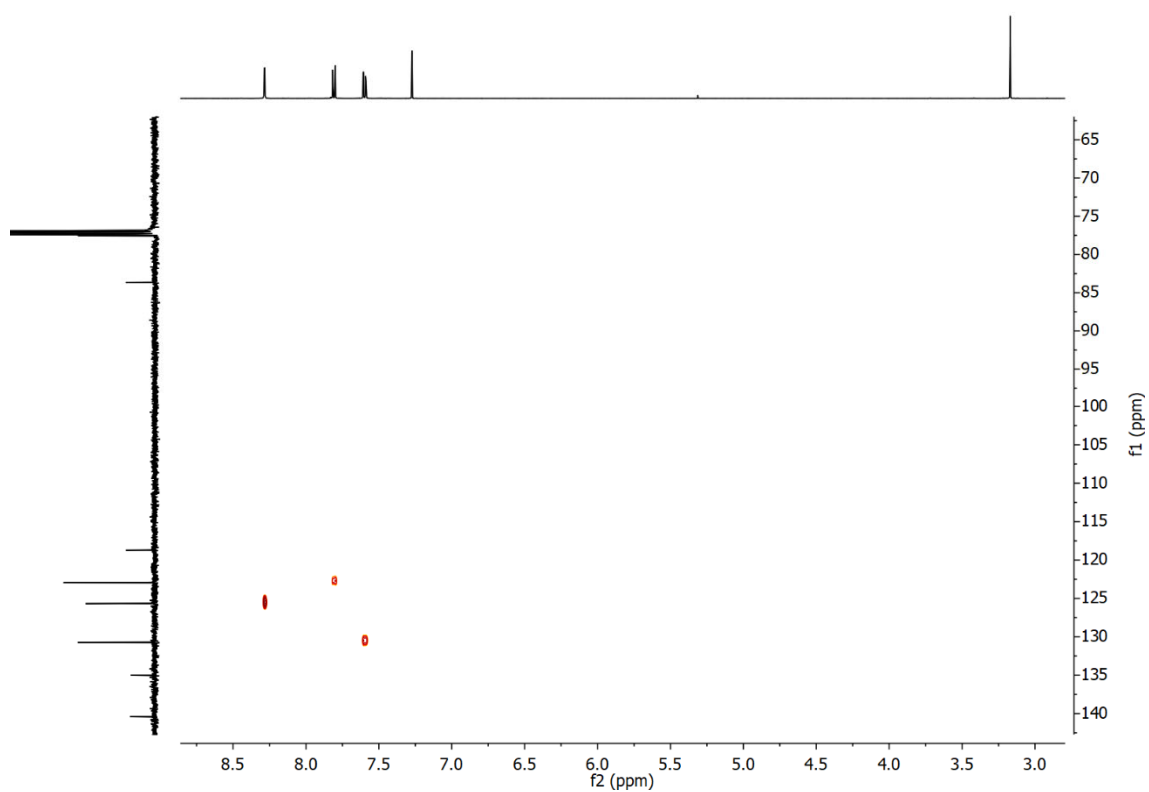


Figure S 41. ^1H - ^{13}C gHSQCAD (500 MHz, CDCl_3) spectrum of compound **13**.

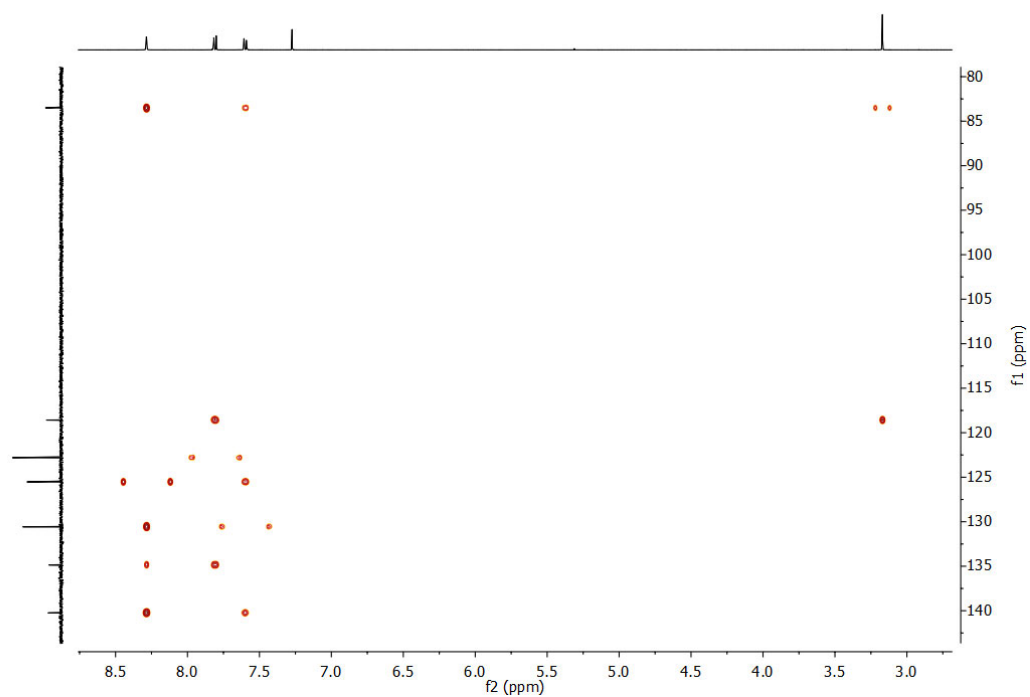


Figure S 42. ^1H - ^{13}C gHMBCAD (500 MHz, CDCl_3) spectrum of compound **13**.

Complex 2

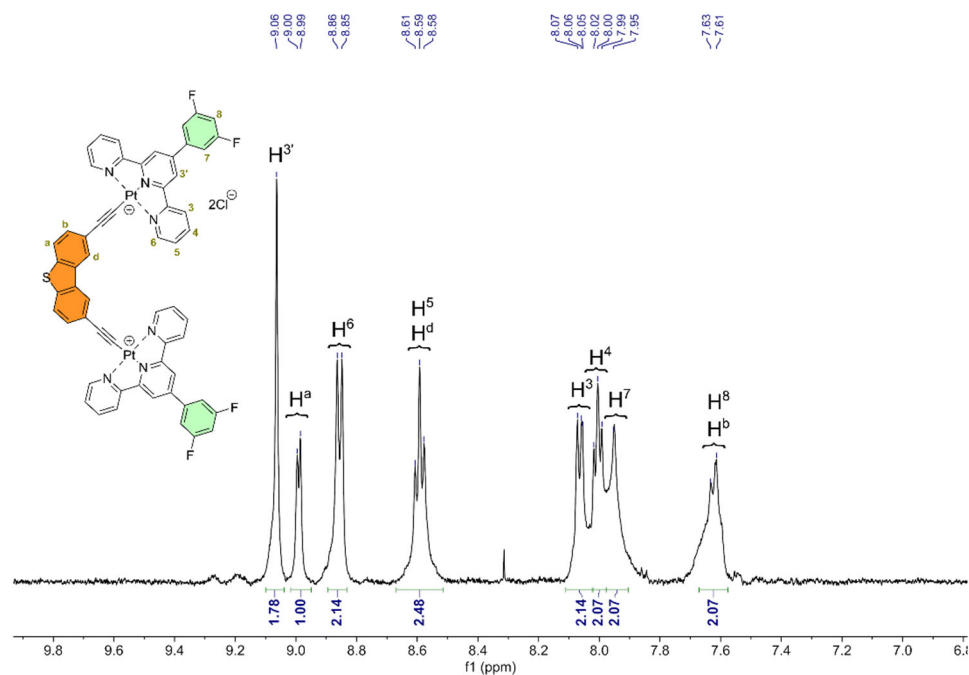


Figure S 43. 1H -NMR (500 MHz, DMSO- d_6) spectrum of relevant signals of complex 2.

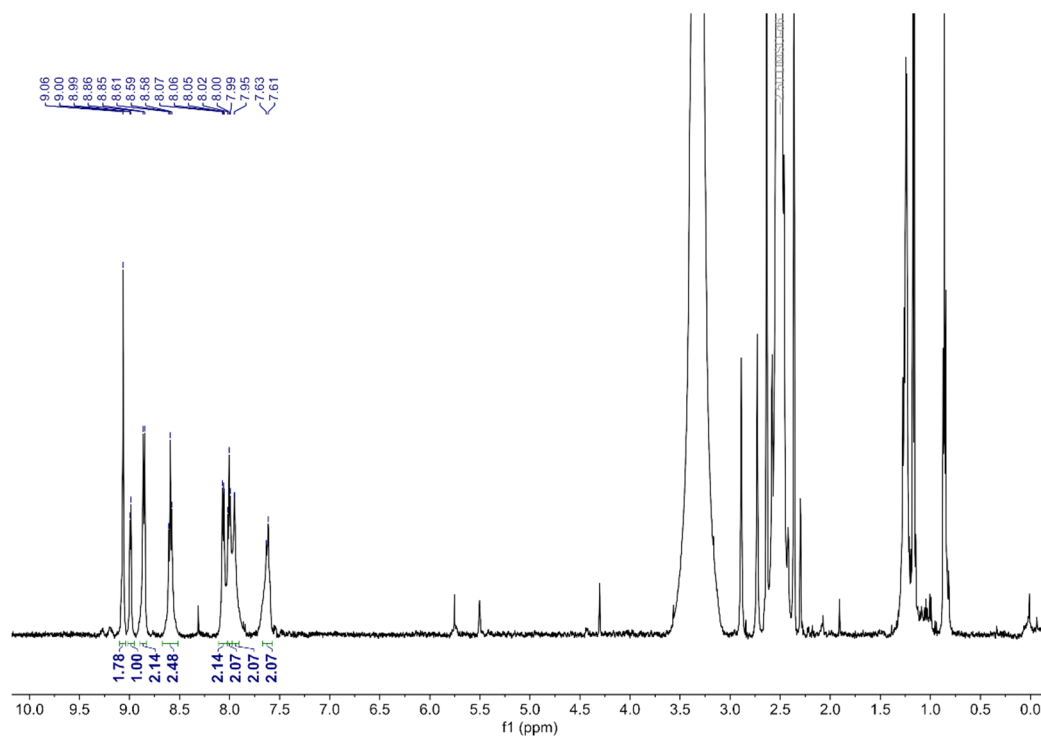


Figure S 44. Full 1H -NMR (500 MHz, DMSO- d_6) spectrum of complex 2.

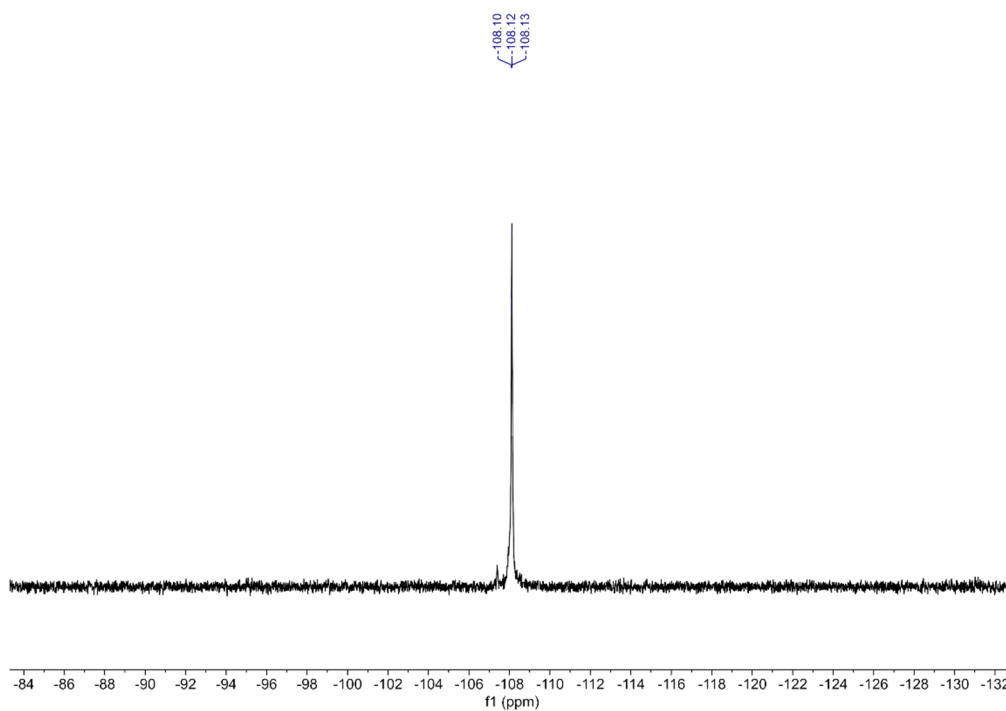


Figure S 45. ^{19}F -NMR (470 MHz, DMSO-d_6) spectrum of complex 2.

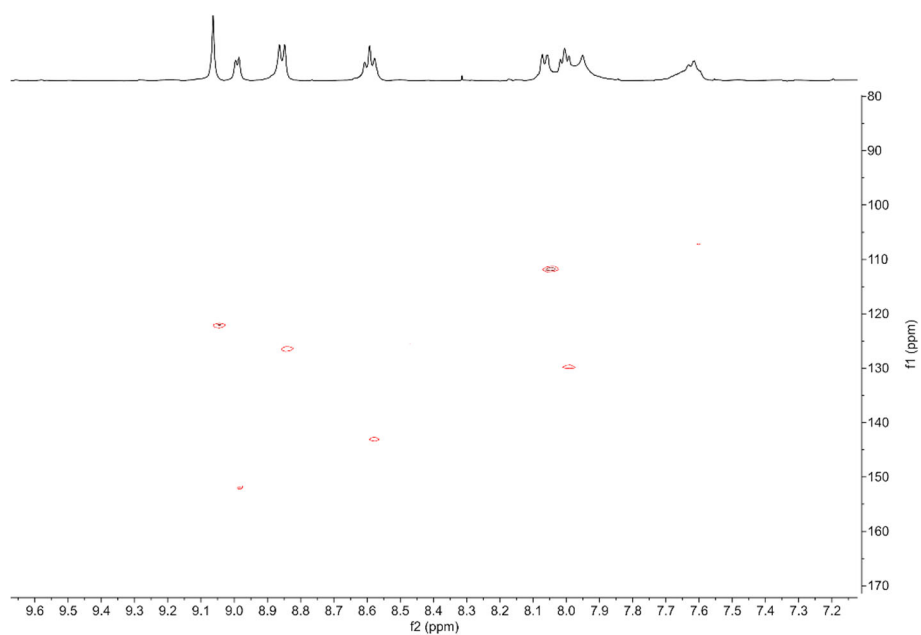


Figure S 46. ^1H - ^{13}C gHSQCAD (500 MHz, DMSO-d_6) spectrum of complex 2.

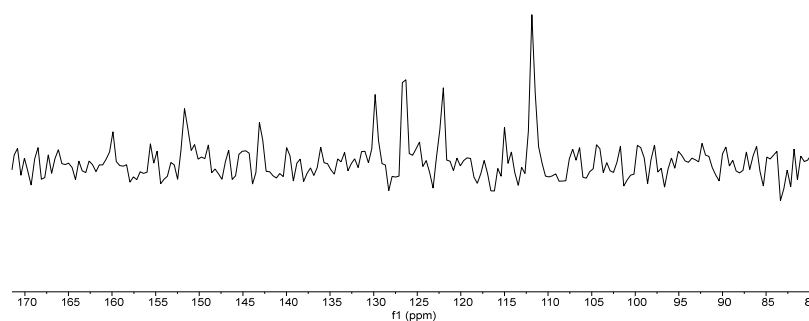


Figure S 47. Extracted vertical trace from the ^1H - ^{13}C gHSQCAD (500 MHz, DMSO-d_6) spectrum of complex **2**.

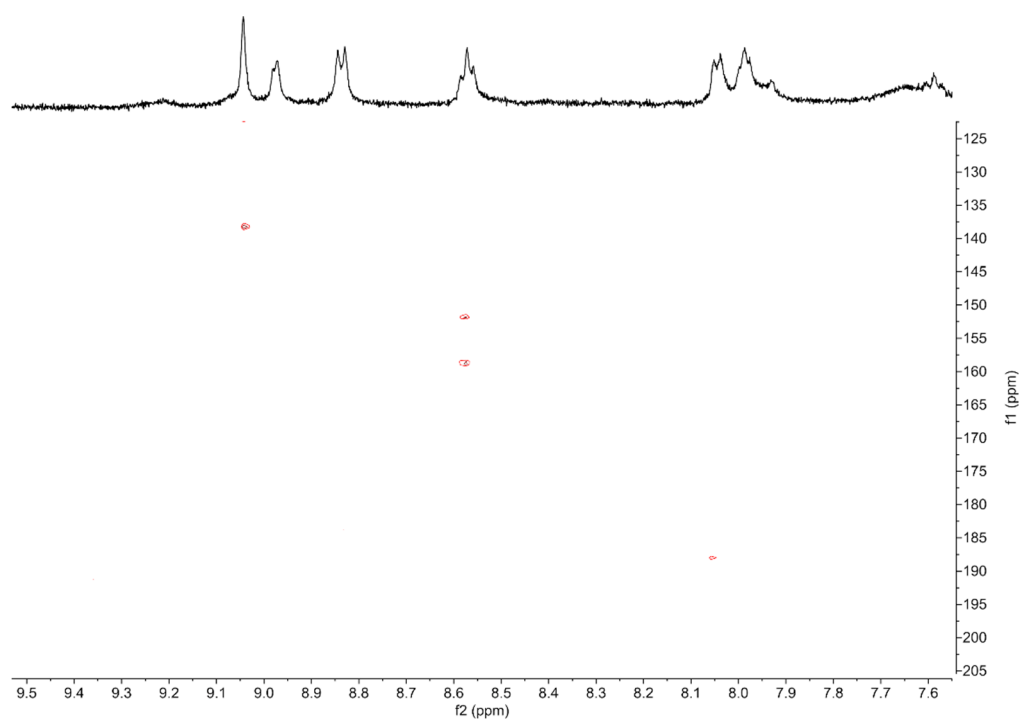


Figure S 48. ^1H - ^{13}C gHMBCAD (500 MHz, $\text{DMSO-d}_6/\text{TFA-d}$, 95:5) spectrum of complex **2**.

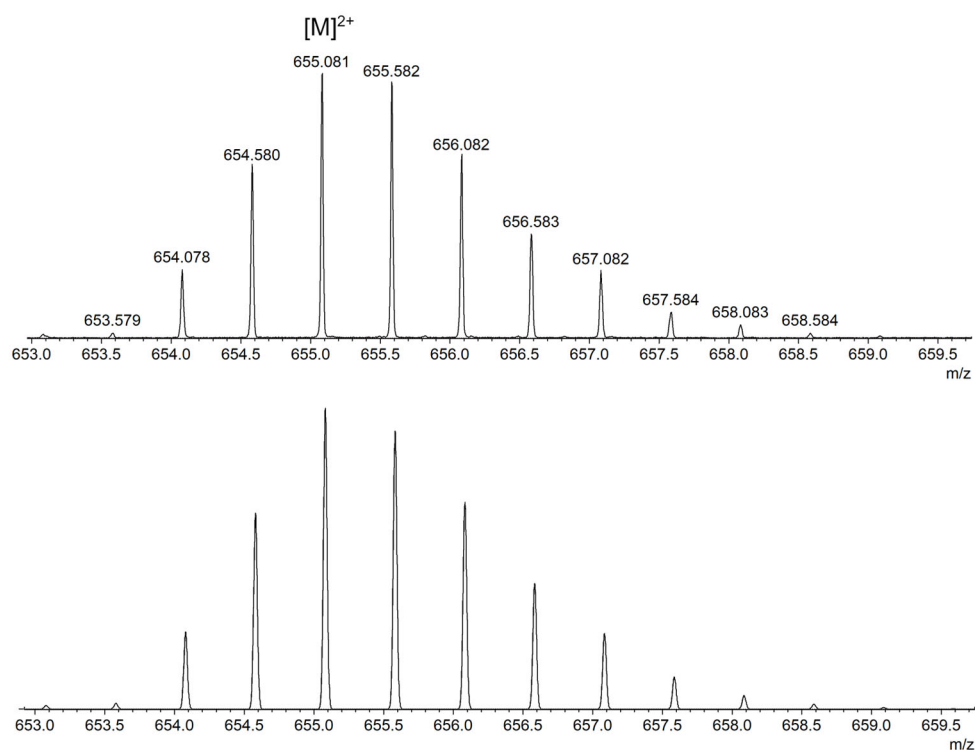
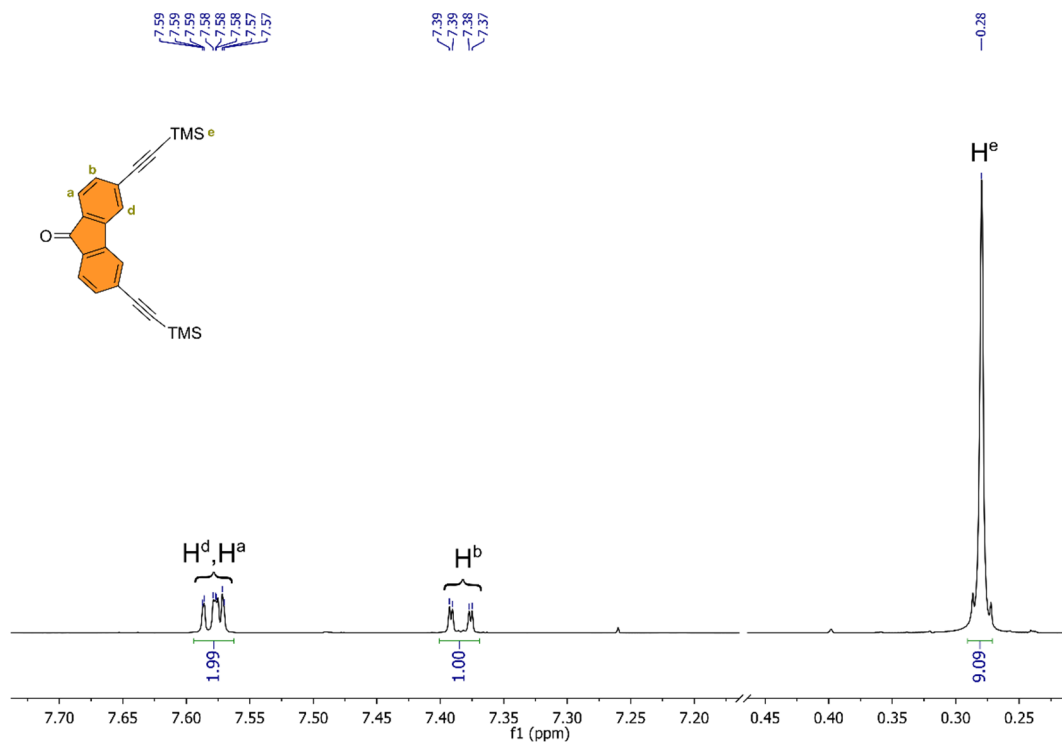
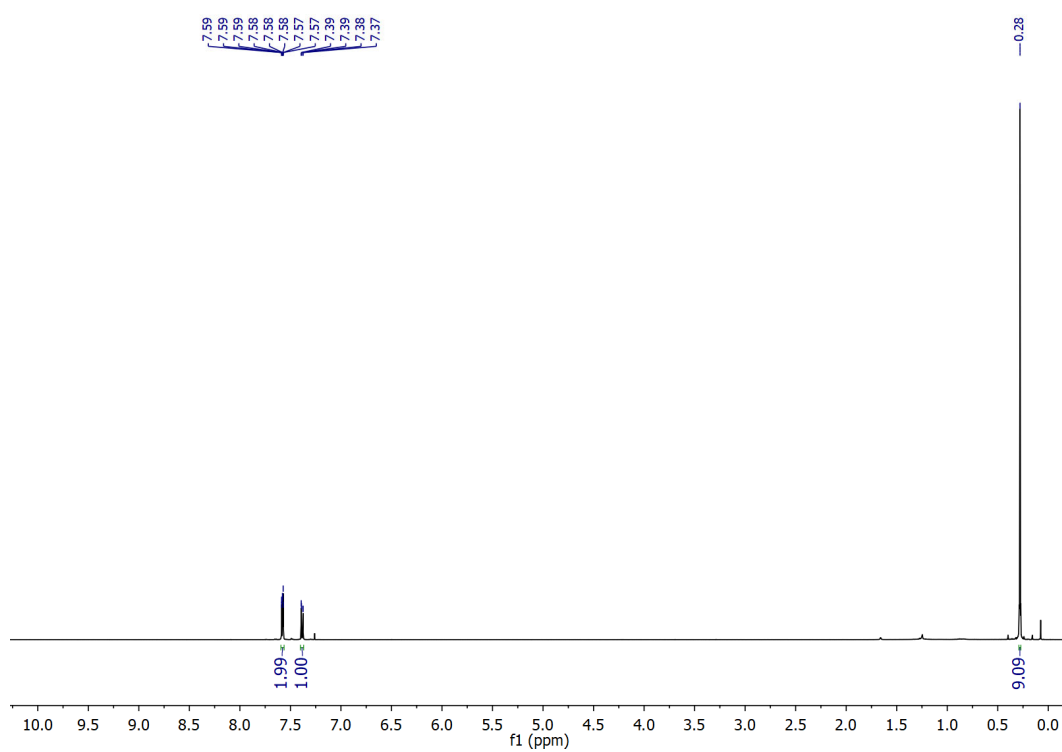


Figure S 49. HRMS (ESI-TOF-pos) of complex 2, $[M]^{2+}$. Calculated (below), measured (top).

Compound **15****Figure S 50.** ¹H-NMR (500 MHz, CDCl₃) spectrum of relevant signals of compound **15**.**Figure S 51.** Full ¹H-NMR (500 MHz, CDCl₃) spectrum of compound **15**.

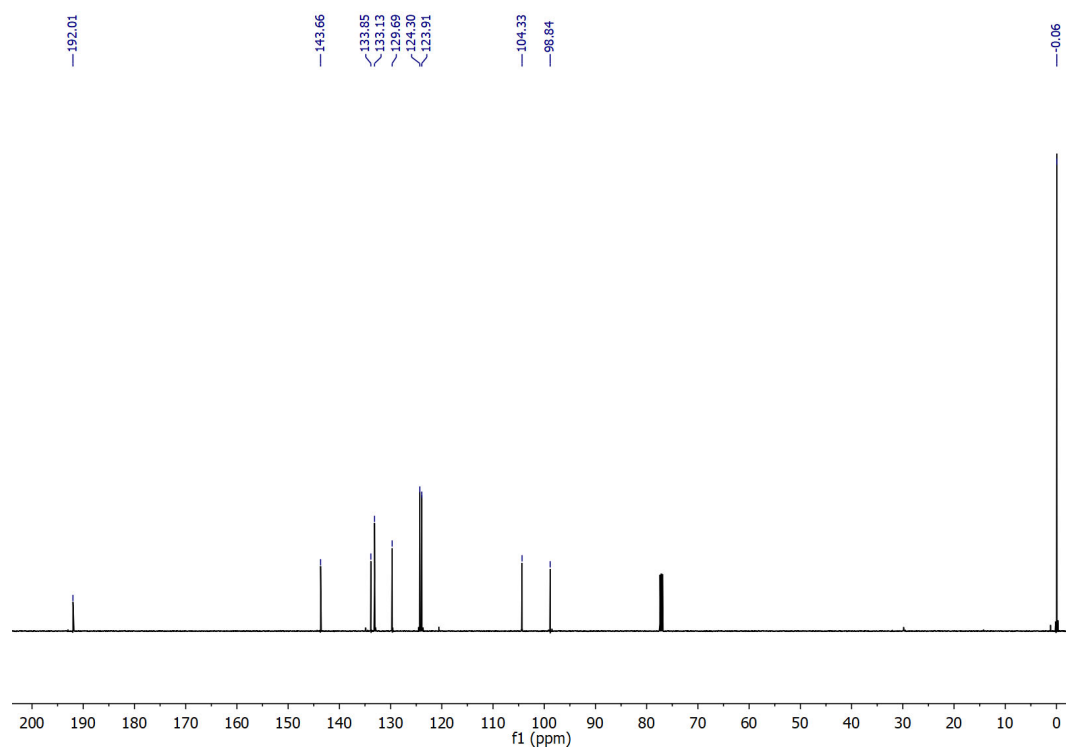


Figure S 52. $^{13}\text{C}\{^1\text{H}\}$ -NMR (126 MHz, CDCl_3) spectrum of compound **15**.

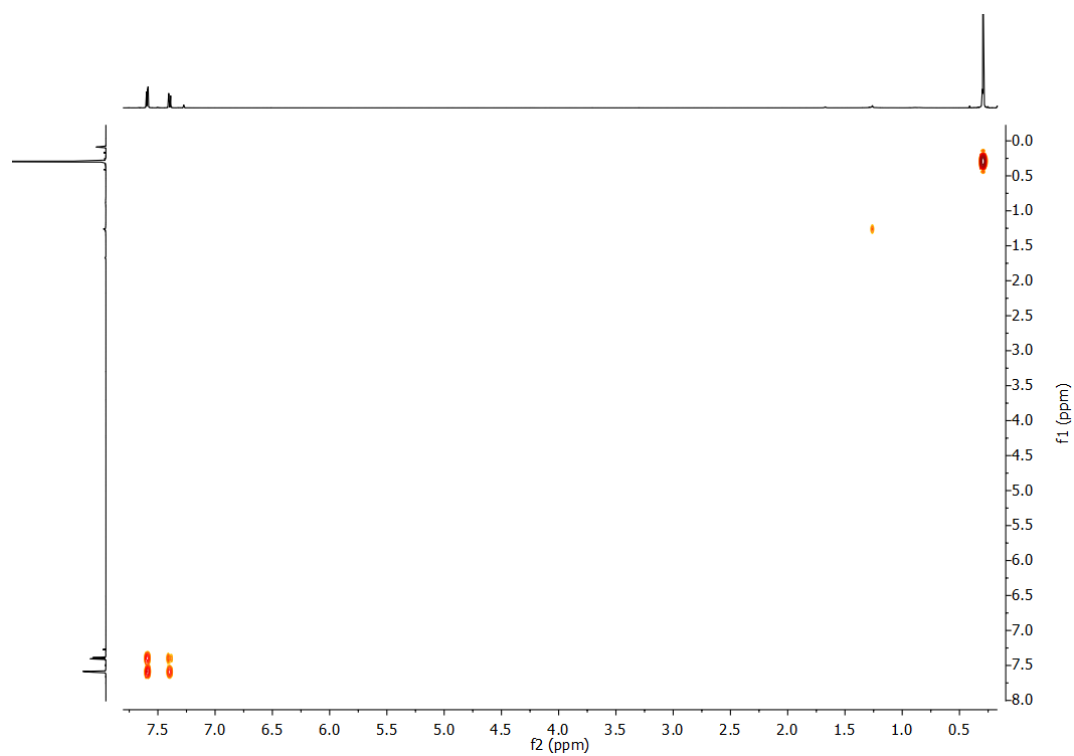


Figure S 53. ^1H - ^1H gCOSY (500 MHz, CDCl_3) spectrum of compound **15**.

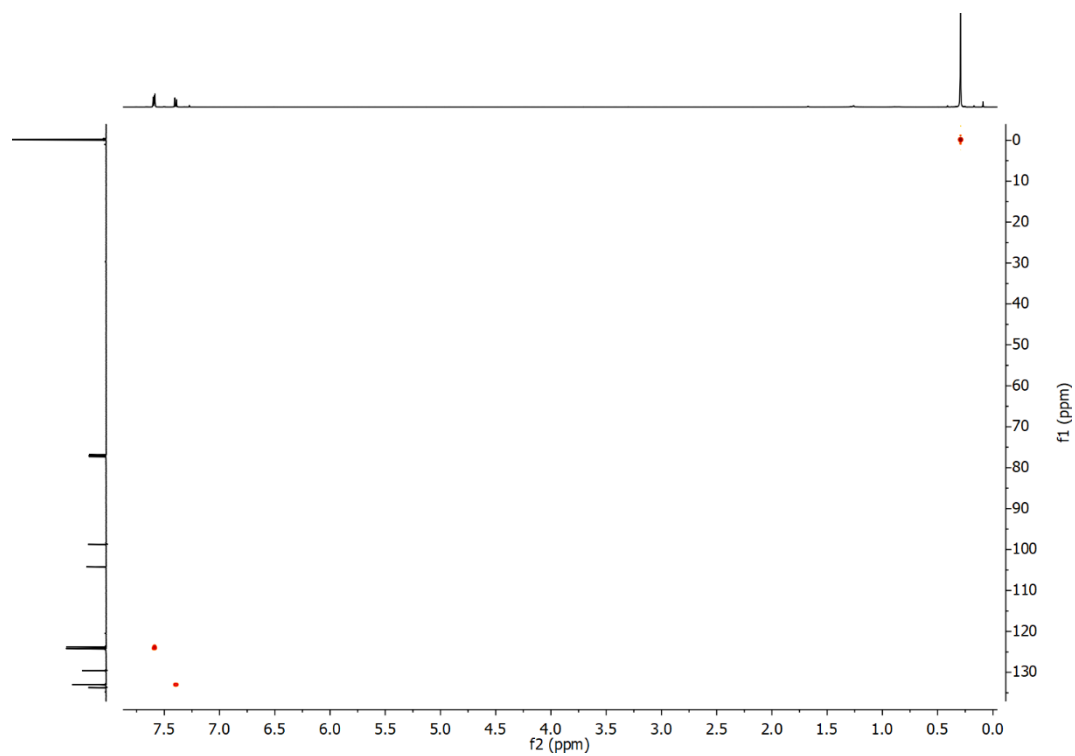


Figure S 54. ^1H - ^{13}C gHSQCAD (500 MHz, CDCl_3) spectrum of compound **15**.

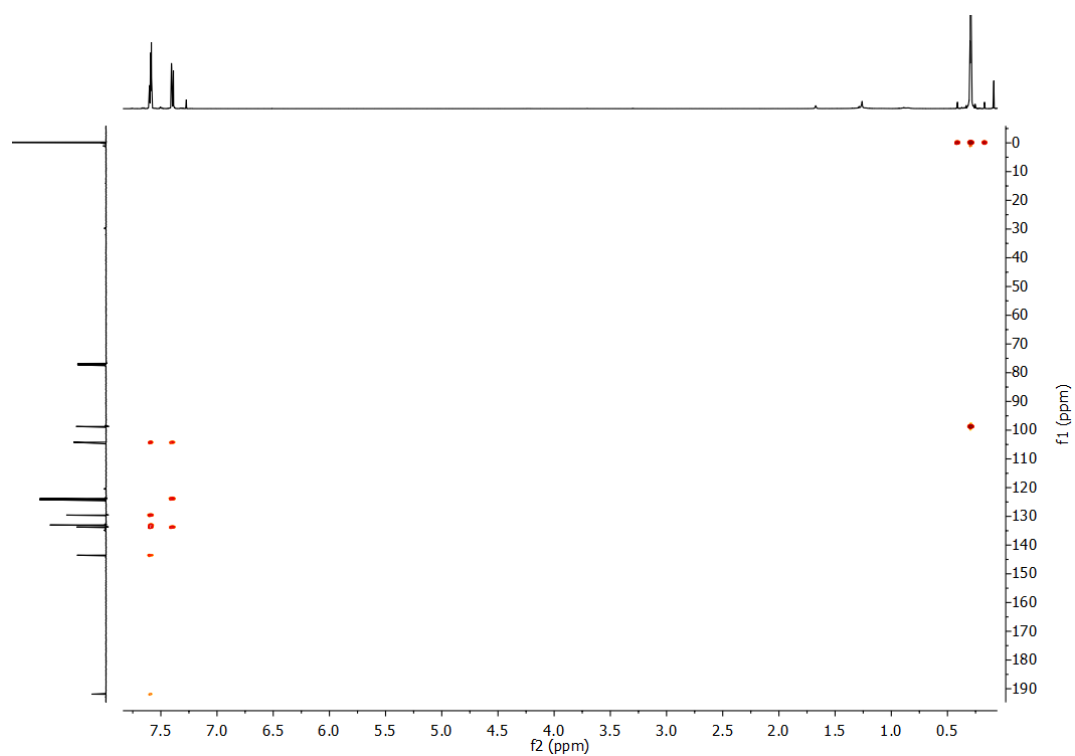


Figure S 55. ^1H - ^{13}C gHMBCAD (500 MHz, CDCl_3) spectrum of compound **15**.

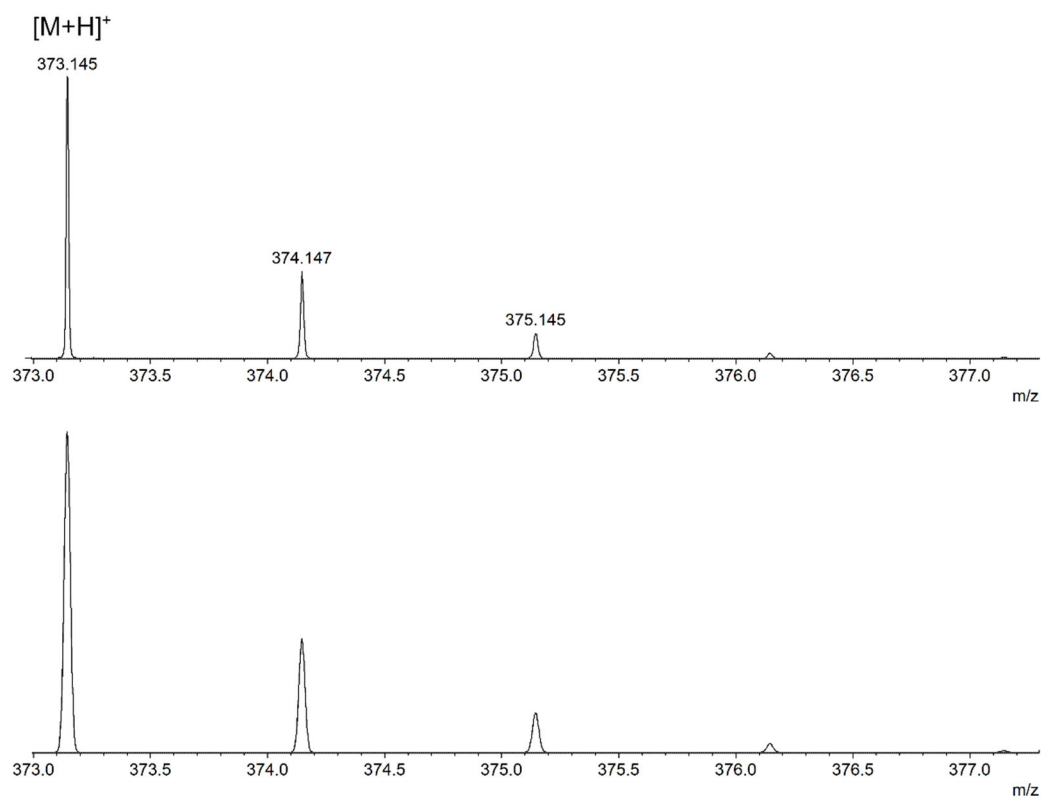
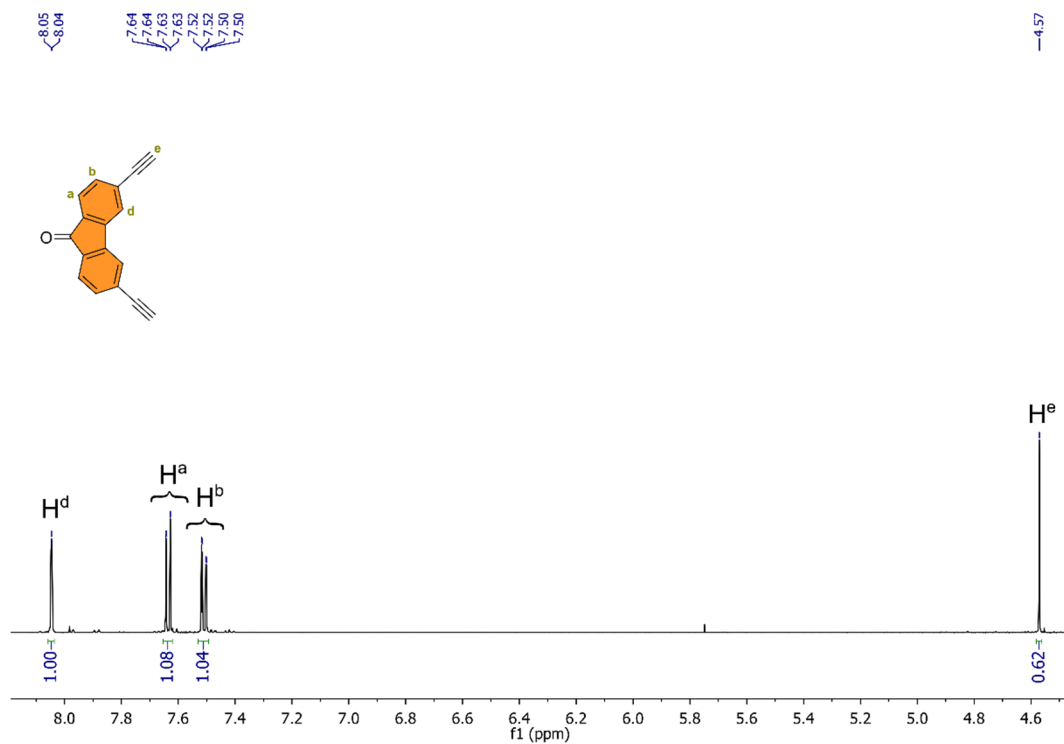
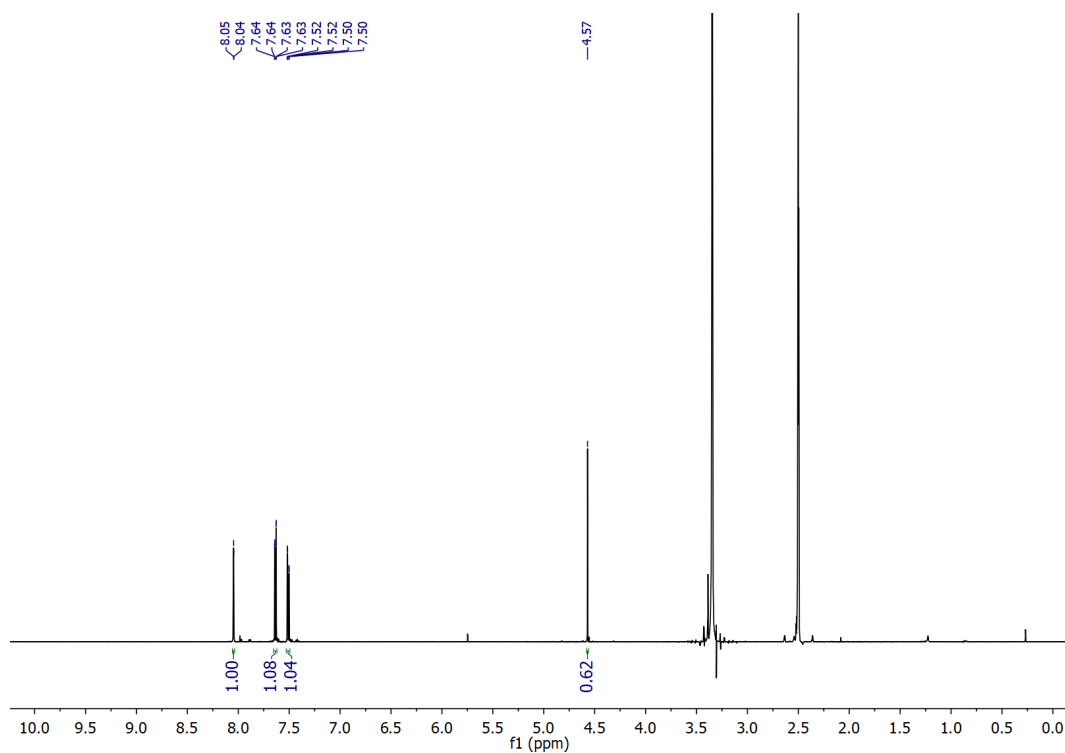


Figure S 56. HRMS (ESI-TOF-pos) of compound **15**, $[M+H]^+$. Calculated (below), measured (top).

Compound **16****Figure S 57.** ¹H-NMR (400 MHz, DMSO-*d*₆) spectrum of relevant signals of compound **16**.**Figure S 58.** Full ¹H-NMR (400 MHz, DMSO-*d*₆) spectrum of compound **16**.

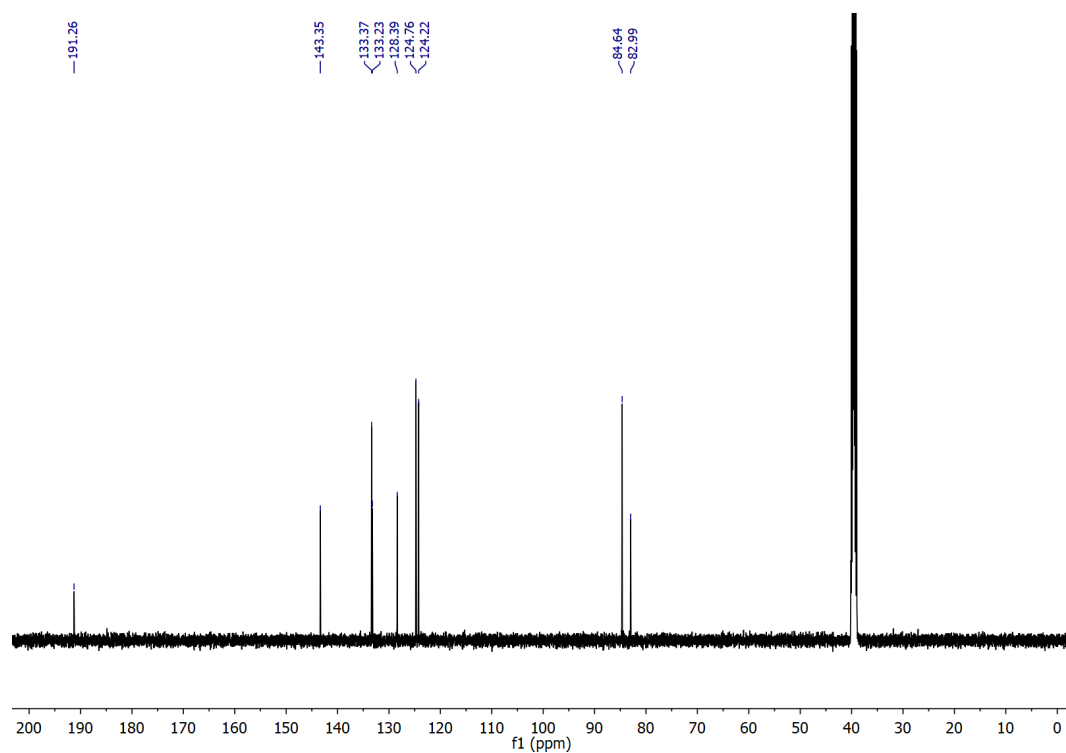


Figure S 59. $^{13}\text{C}\{^1\text{H}\}$ -NMR (126 MHz, $\text{DMSO}-d_6$) spectrum of compound **16**.

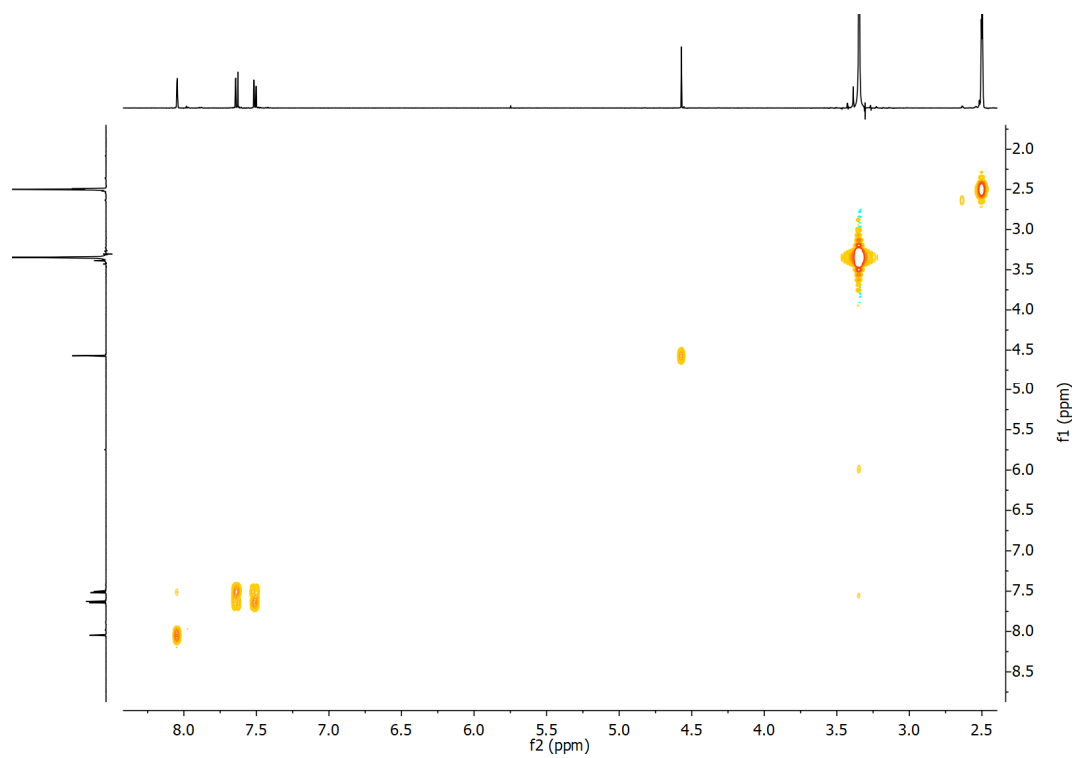


Figure S 60. $^1\text{H}-^{13}\text{C}$ gCOSY (400 MHz, $\text{DMSO}-d_6$) spectrum of compound **16**.

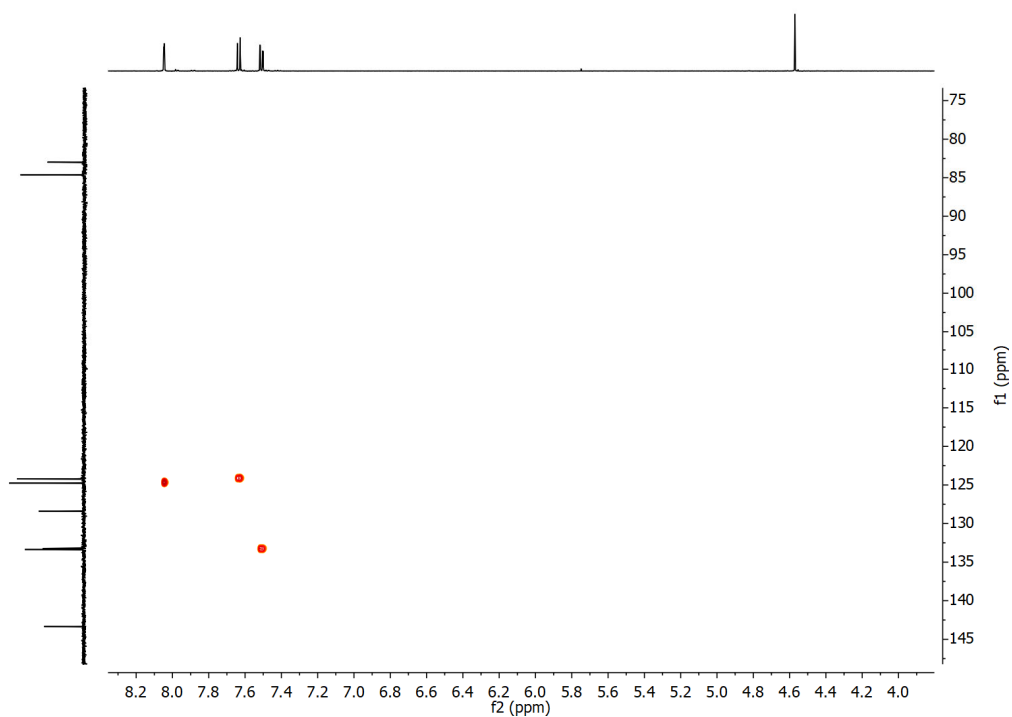


Figure S 61. ^1H - ^{13}C gHSQCAD (400 MHz, $\text{DMSO}-d_6$) spectrum of compound **16**.

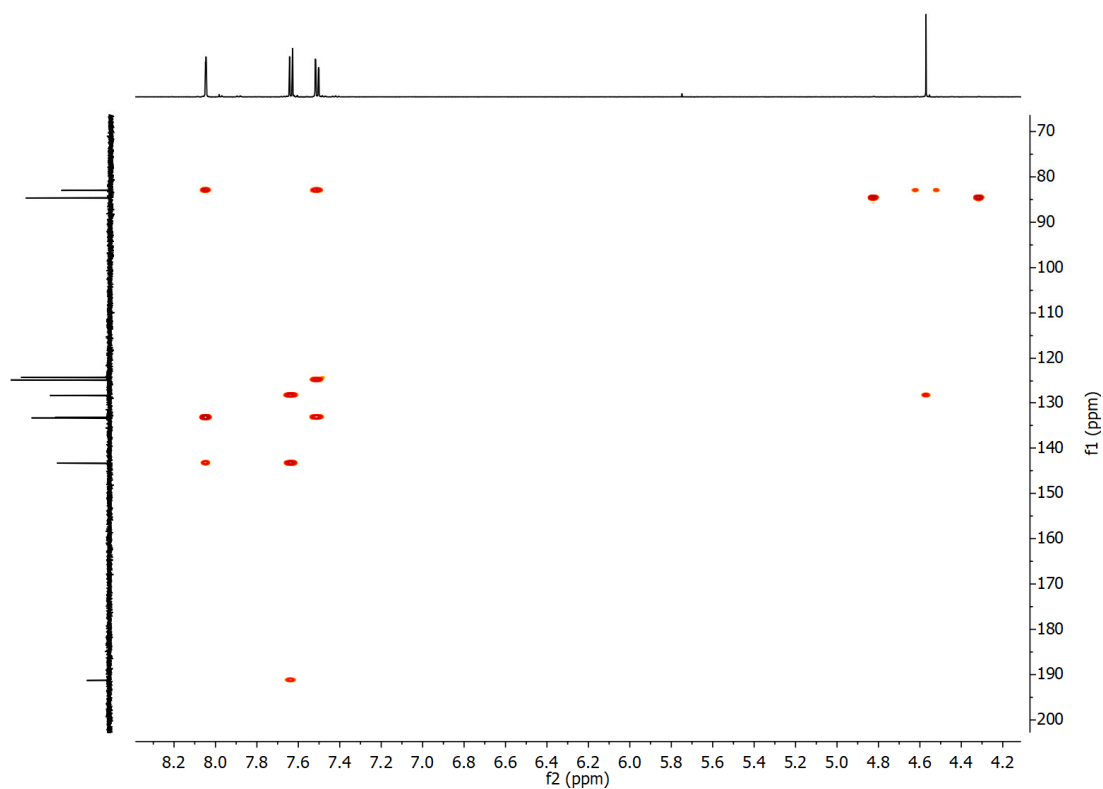


Figure S 62. ^1H - ^{13}C gHMBCAD (400 MHz, $\text{DMSO}-d_6$) spectrum of compound **16**.

Complex 3

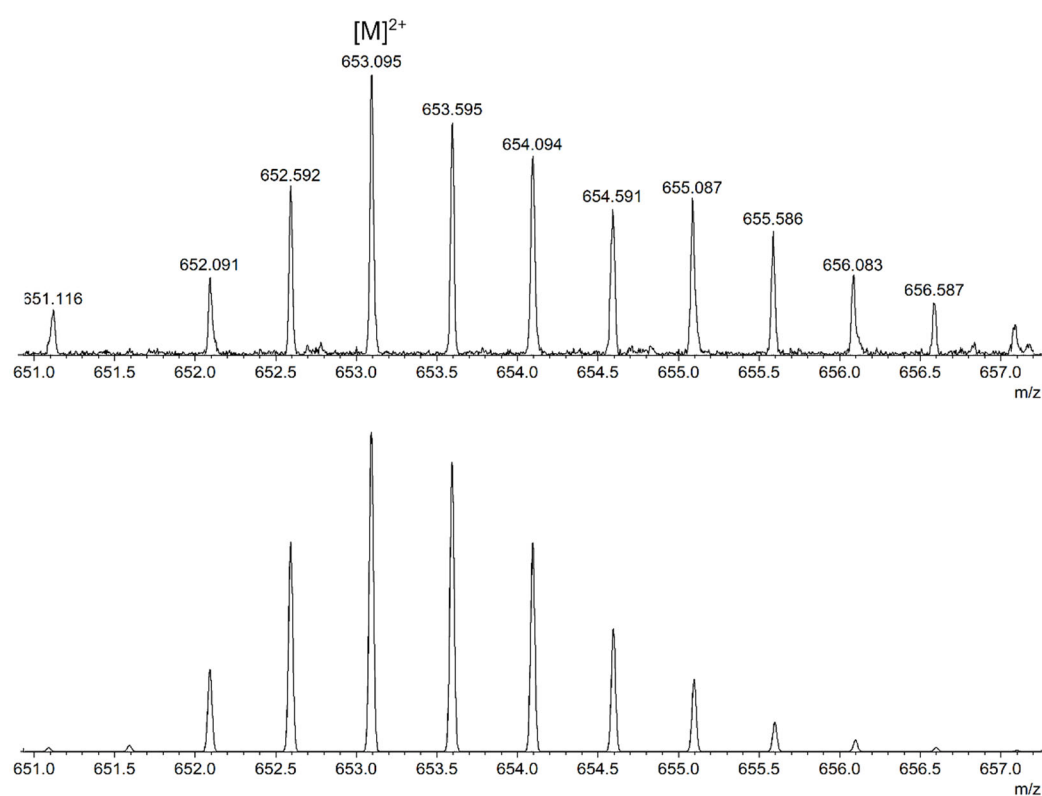
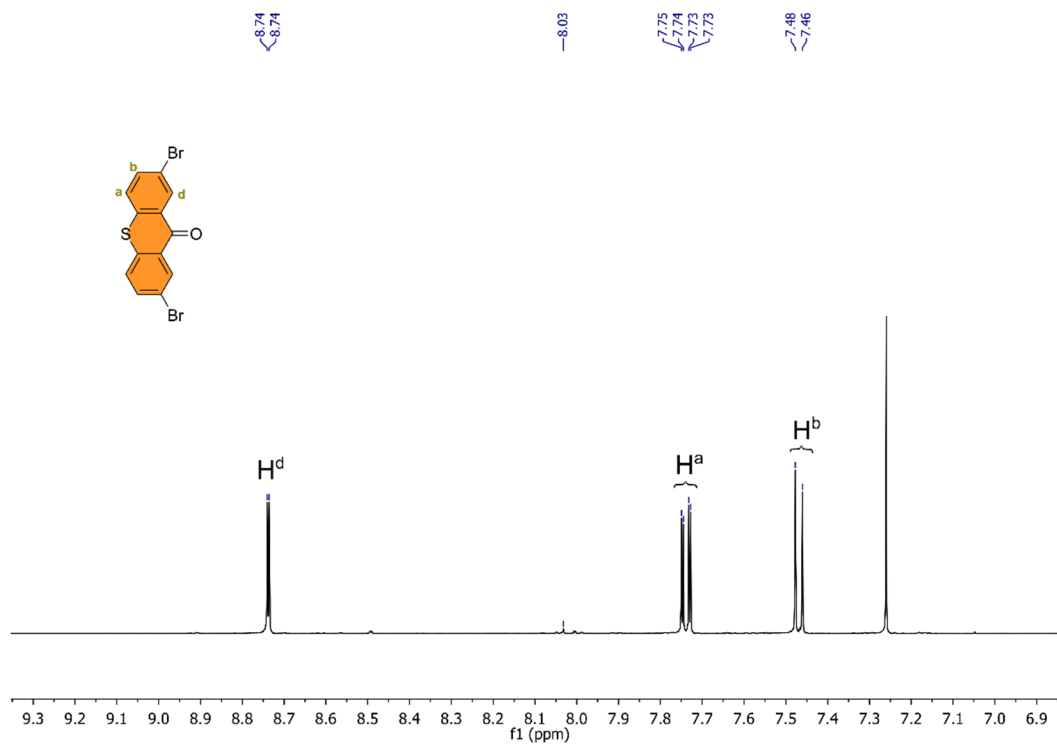
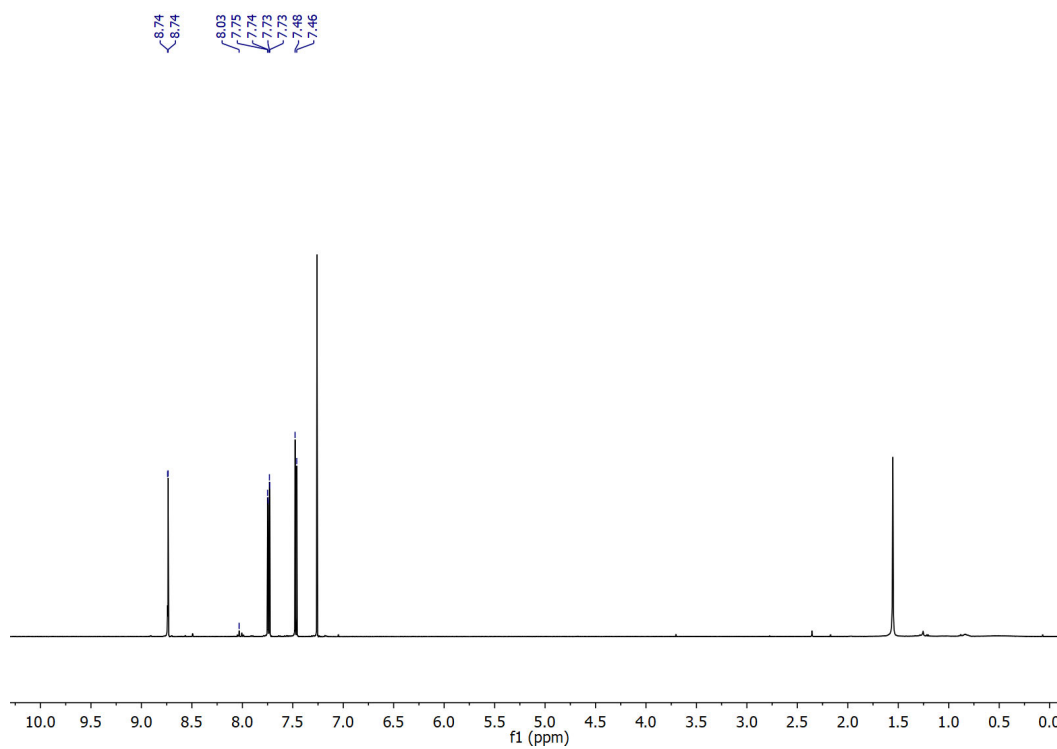


Figure S 63. HRMS (ESI-TOF-pos) of complex 3, $[M]^{2+}$. Calculated (below), measured (top).

Compound 17

**Figure S 64.** ¹H-NMR (500 MHz, CDCl₃) spectrum of relevant signals of compound 17.**Figure S 65.** Full ¹H-NMR (500 MHz, CDCl₃) spectrum of compound 17.

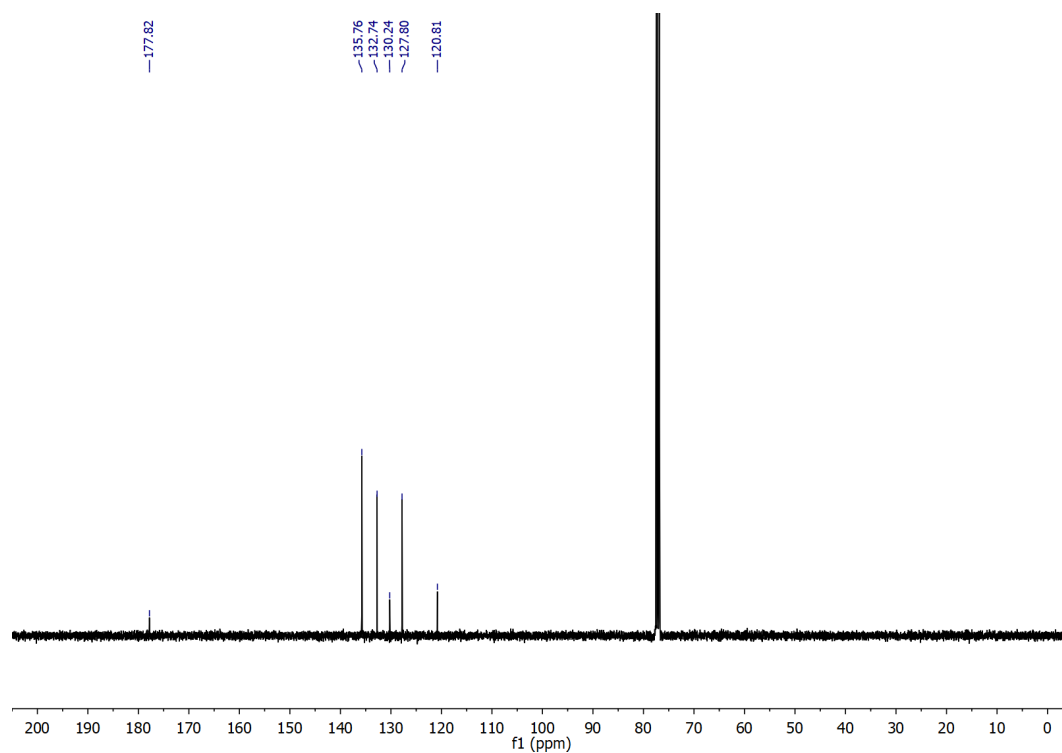


Figure S 66. $^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3) spectrum of compound 17.

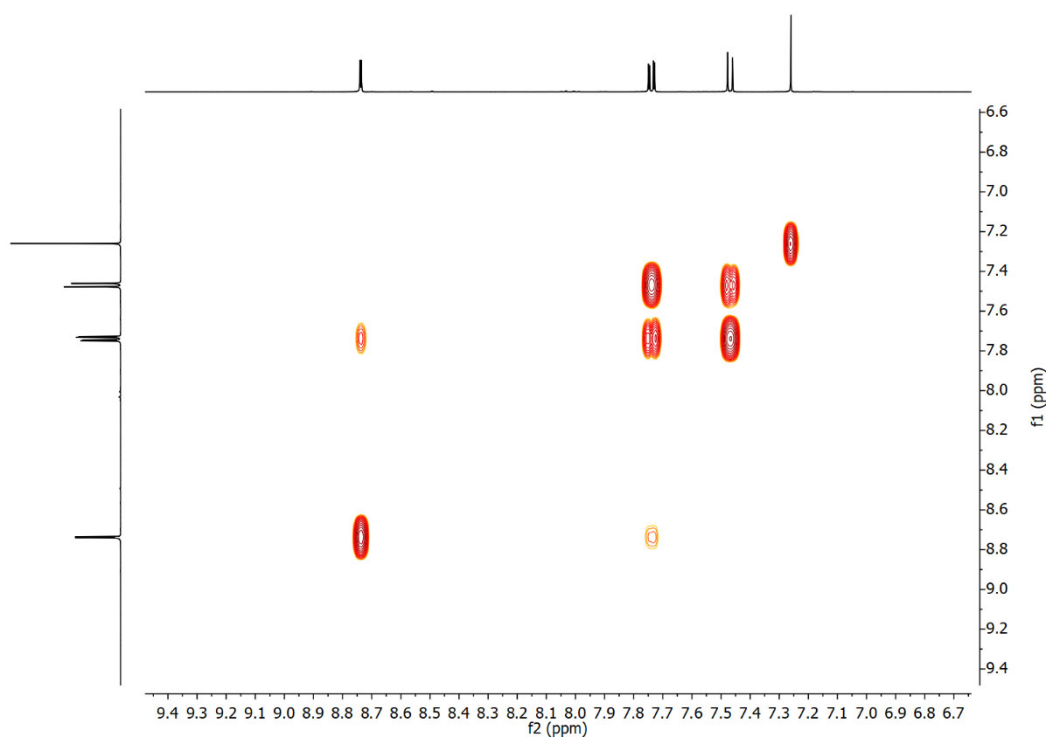


Figure S 67. ^1H - ^1H gCOSY (500 MHz, CDCl_3) spectrum of compound 17.

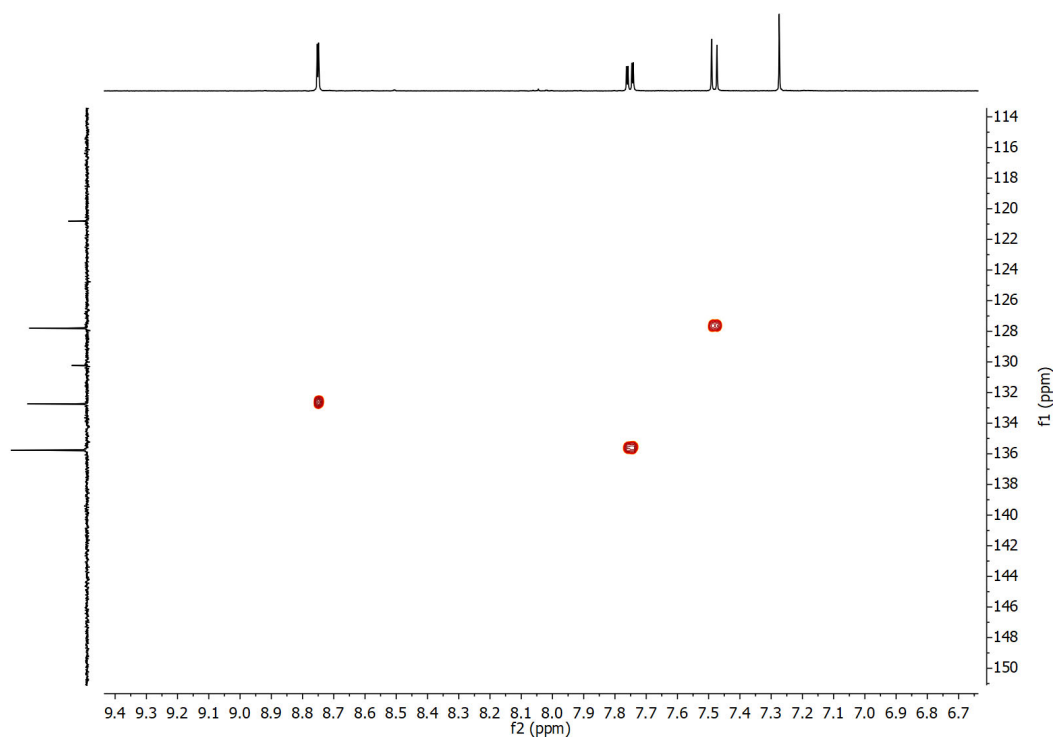


Figure S 68. ^1H - ^{13}C gHSQCAD (500 MHz, CDCl_3) spectrum of compound 17.

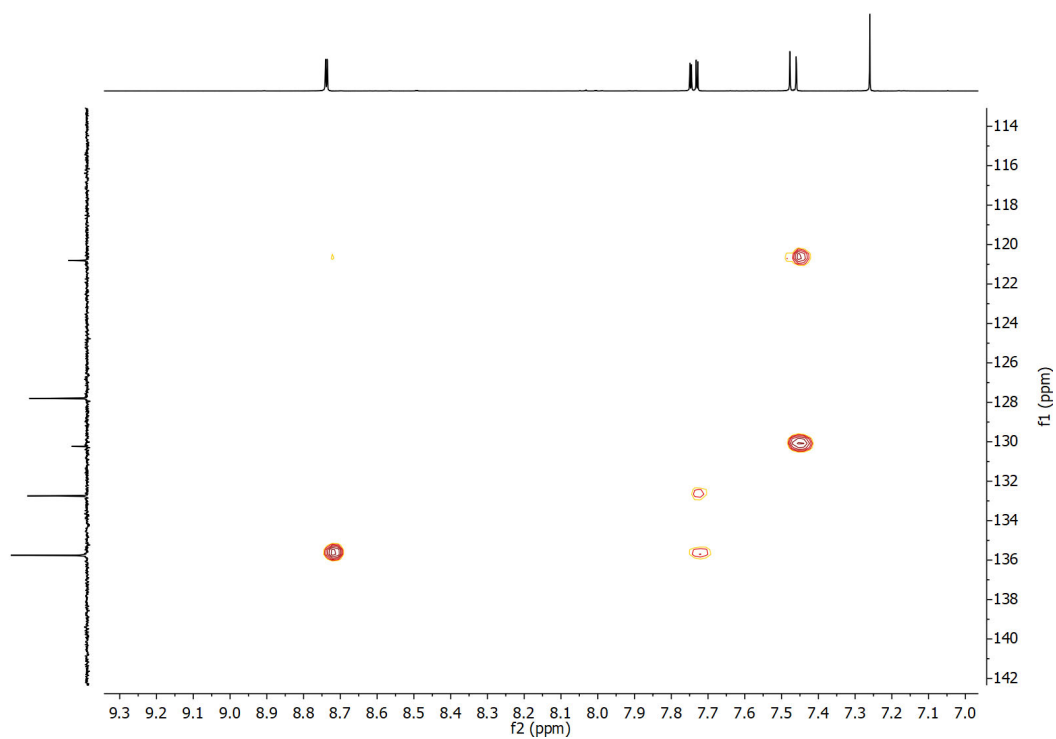


Figure S 69. ^1H - ^{13}C gHMBCAD (500 MHz, CDCl_3) spectrum of compound 17.

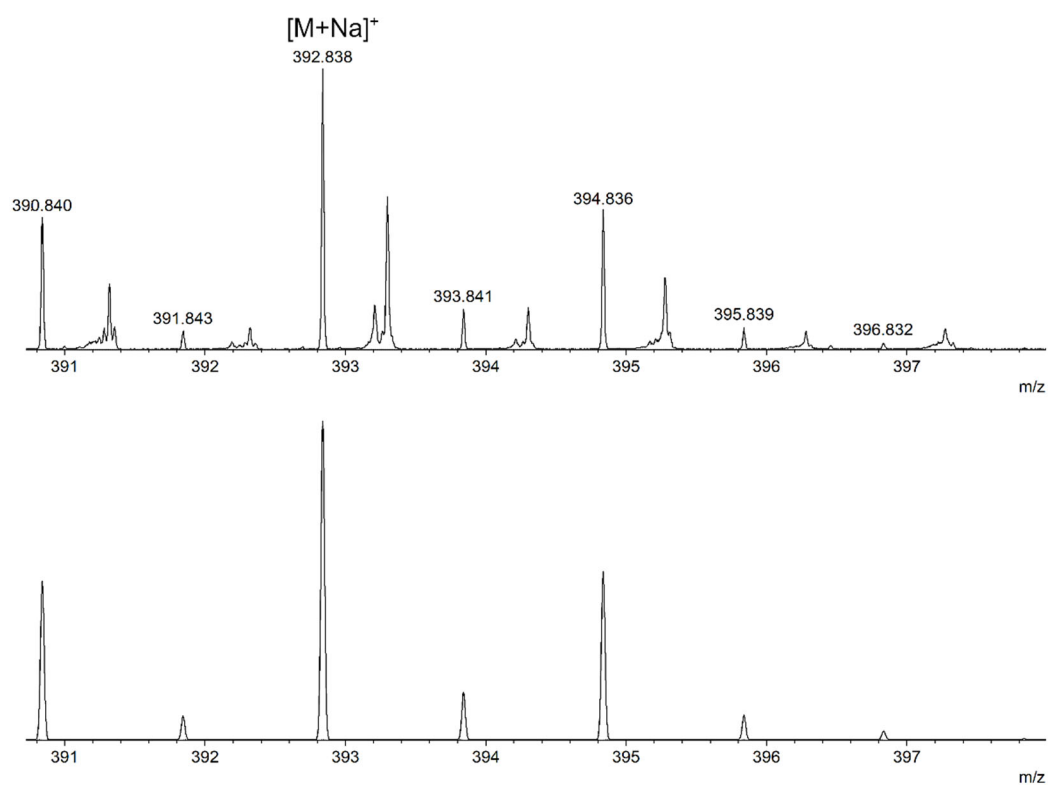
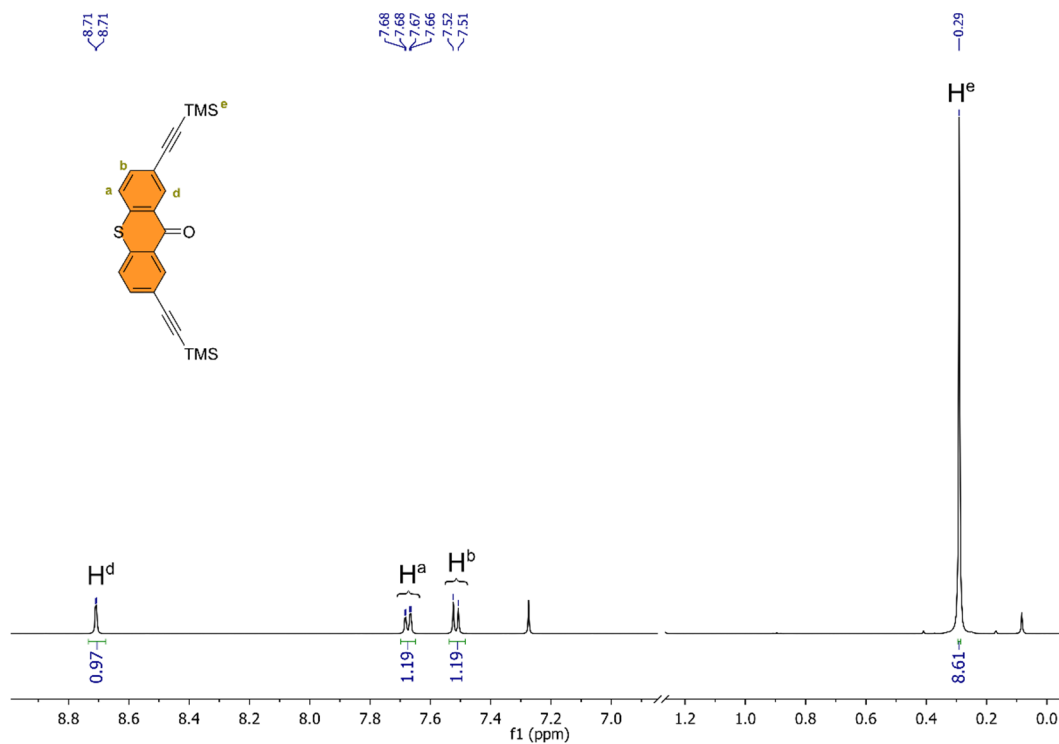
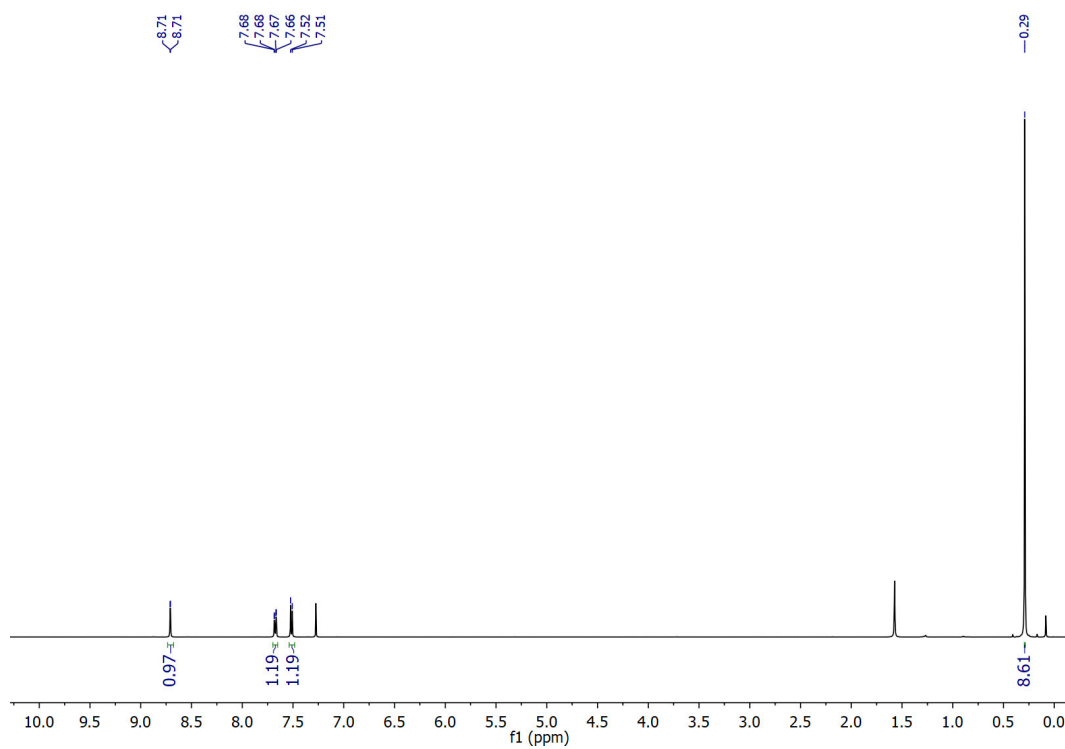


Figure S 70. HRMS (ESI-TOF-pos) of compound 17, $[M+Na]^+$. Calculated (below), measured (top).

Compound **18****Figure S 71.** ^1H -NMR (500 MHz, CDCl_3) spectrum of relevant signals of compound **18**.**Figure S 72.** Full ^1H -NMR (500 MHz, CDCl_3) spectrum of compound **18**.

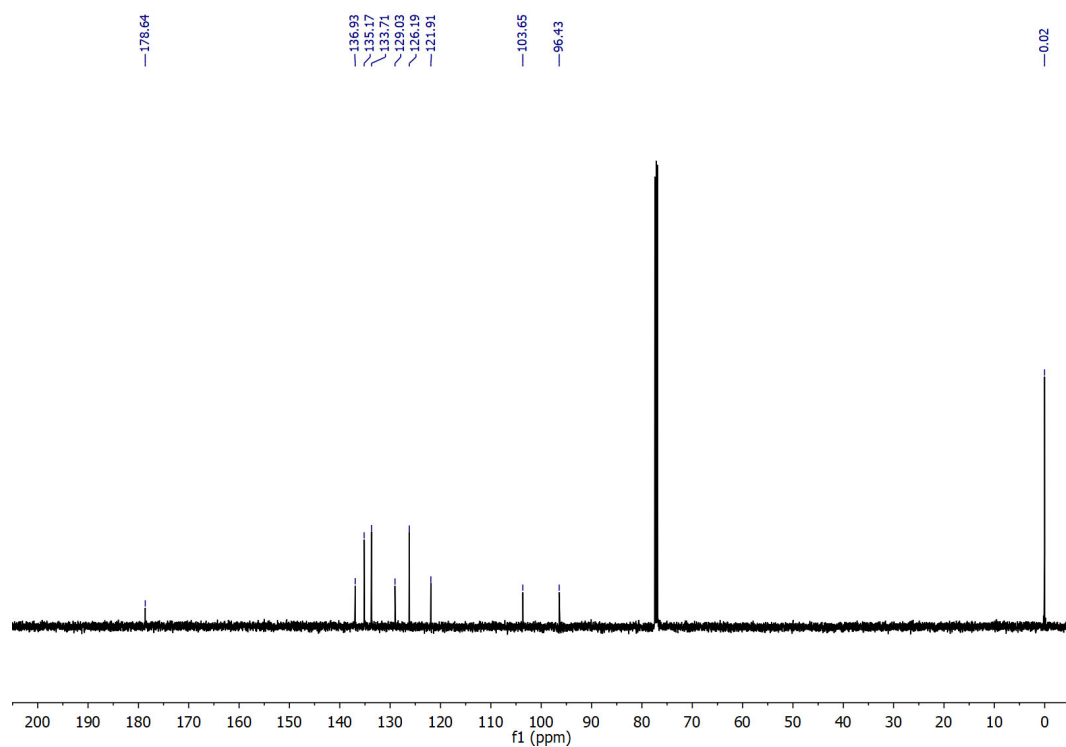


Figure S 73. $^{13}\text{C}\{^1\text{H}\}$ -NMR (126 MHz, CDCl_3) spectrum of compound **18**.

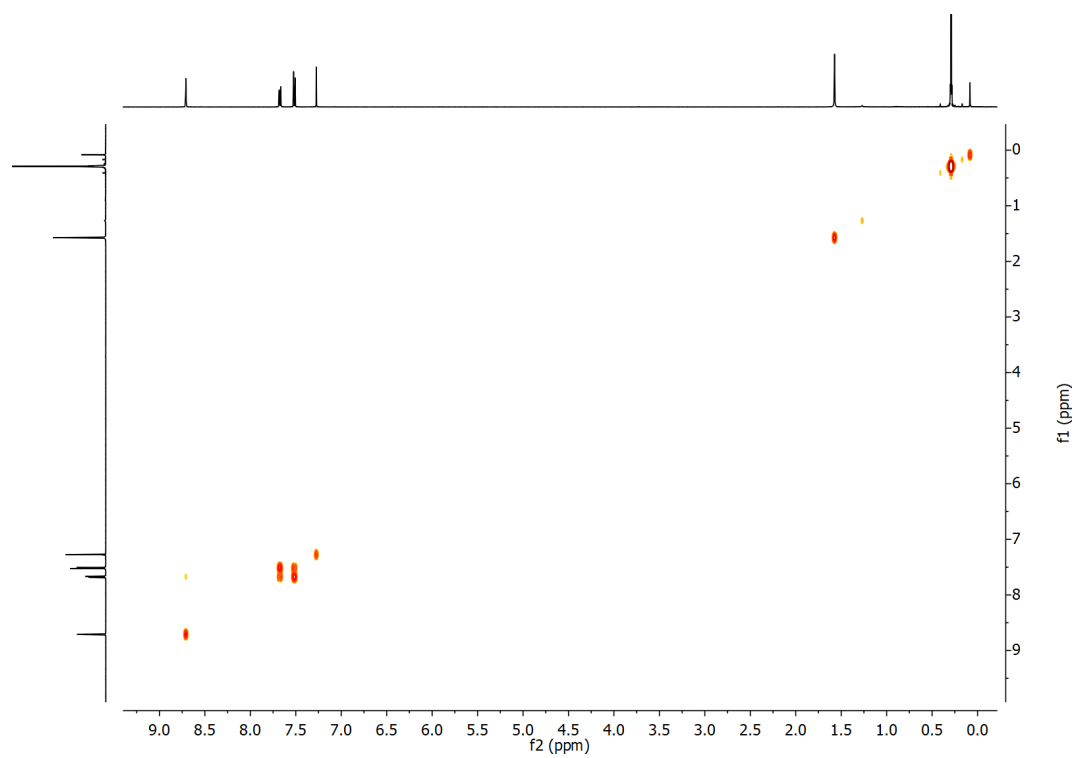


Figure S 74. ^1H - ^{13}C gCOSY (500 MHz, CDCl_3) spectrum of compound **18**.

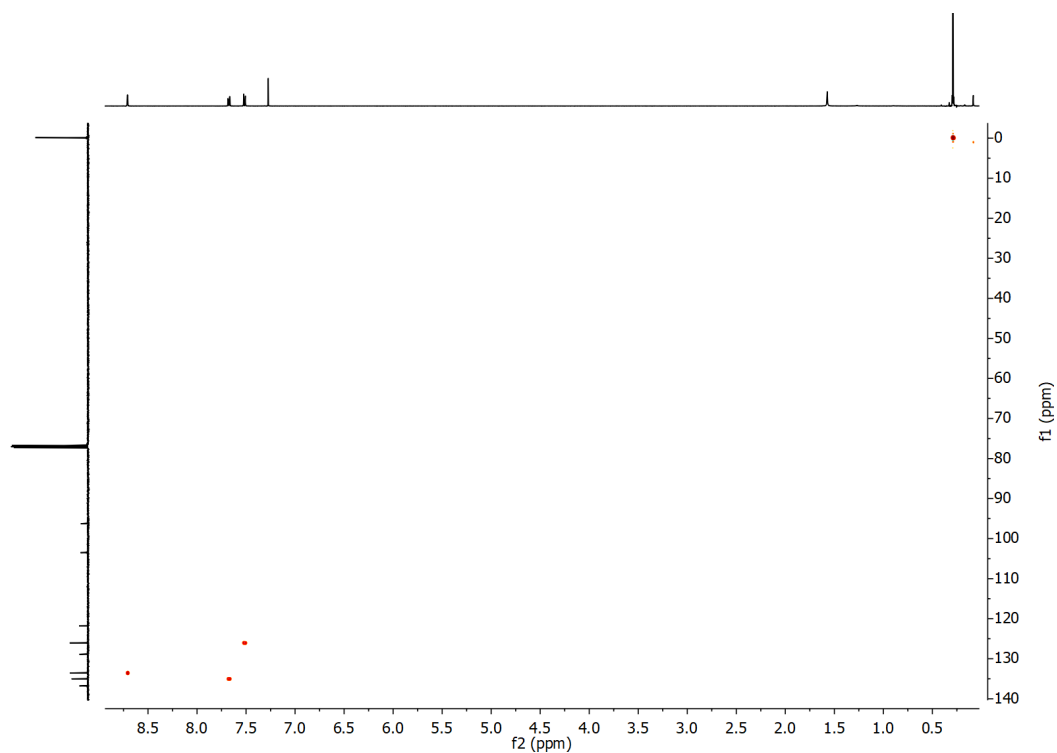


Figure S 75. ^1H - ^{13}C gHSQCAD (500 MHz, CDCl_3) spectrum of compound **18**.

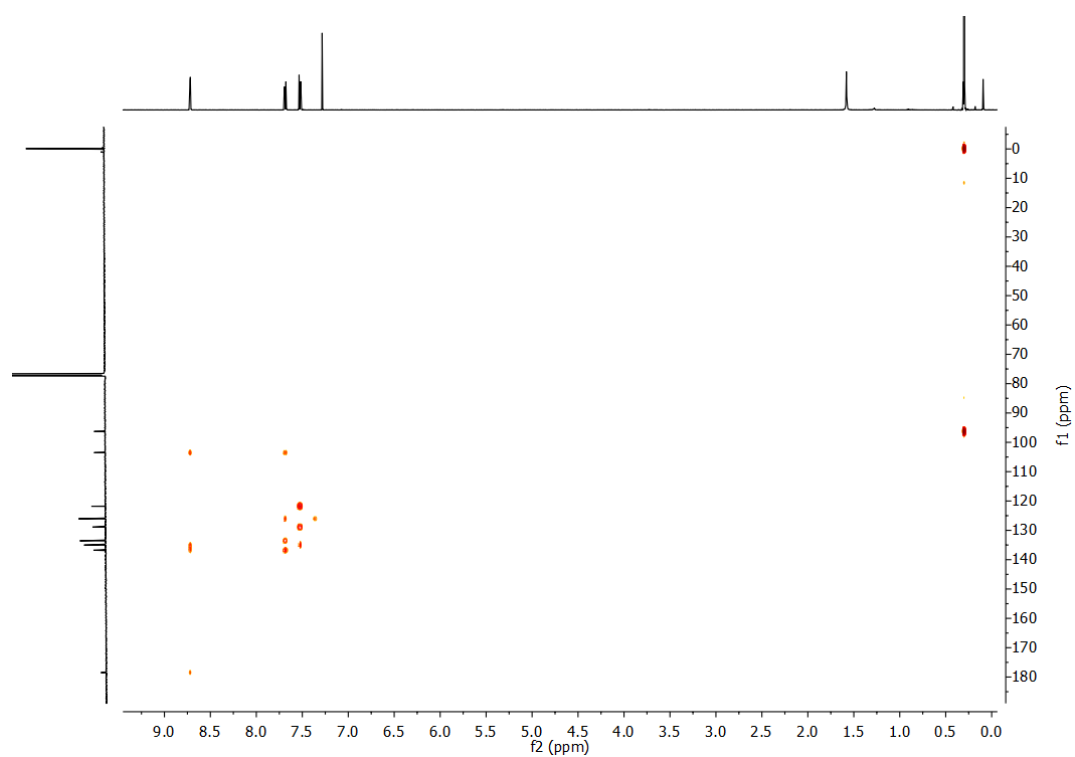


Figure S 76. ^1H - ^{13}C gHMBC (500 MHz, CDCl_3) spectrum of compound **18**.

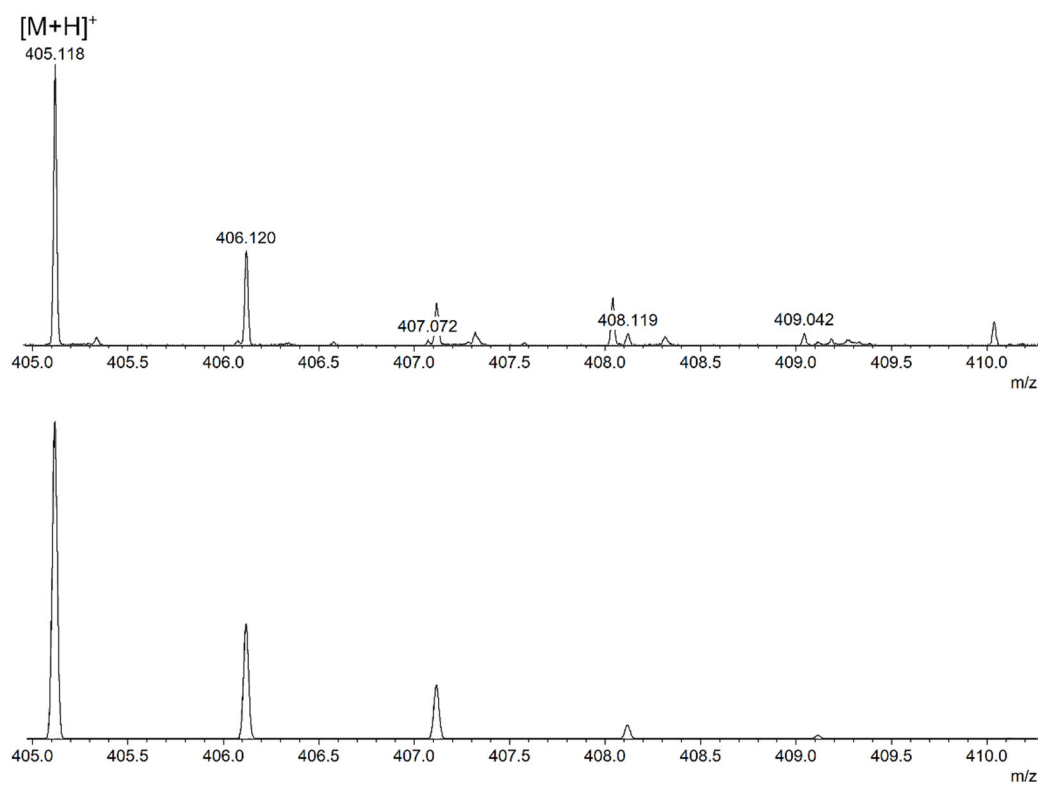
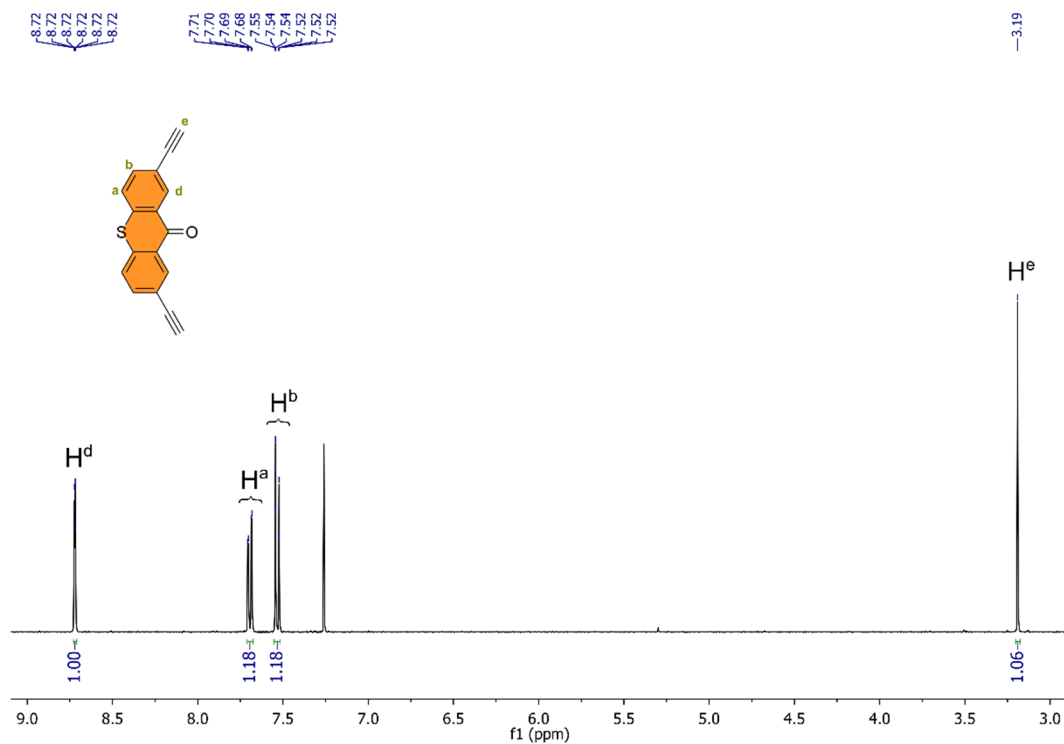
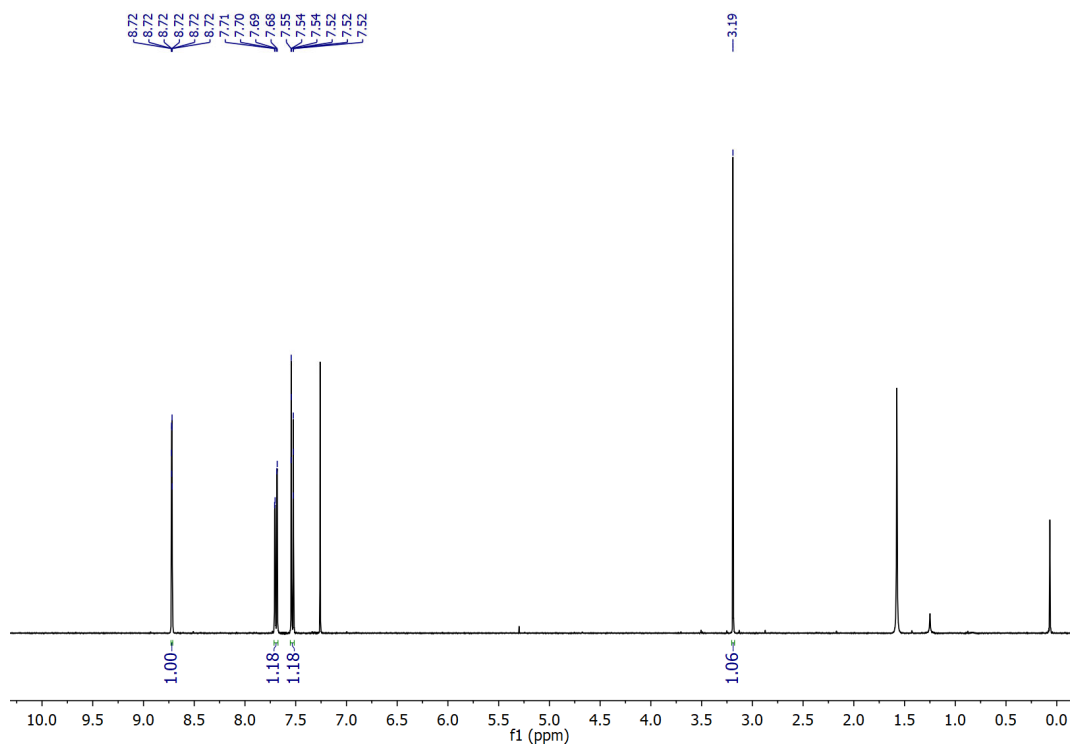


Figure S 77. HRMS (ESI-TOF-pos) of compound **18**, $[M+H]^+$. Calculated (below), measured (top).

Compound **19****Figure S 78.** ¹H-NMR (400 MHz, CDCl₃) spectrum of relevant signals of compound **19**.**Figure S 79.** Full ¹H-NMR (400 MHz, CDCl₃) spectrum of compound **19**.

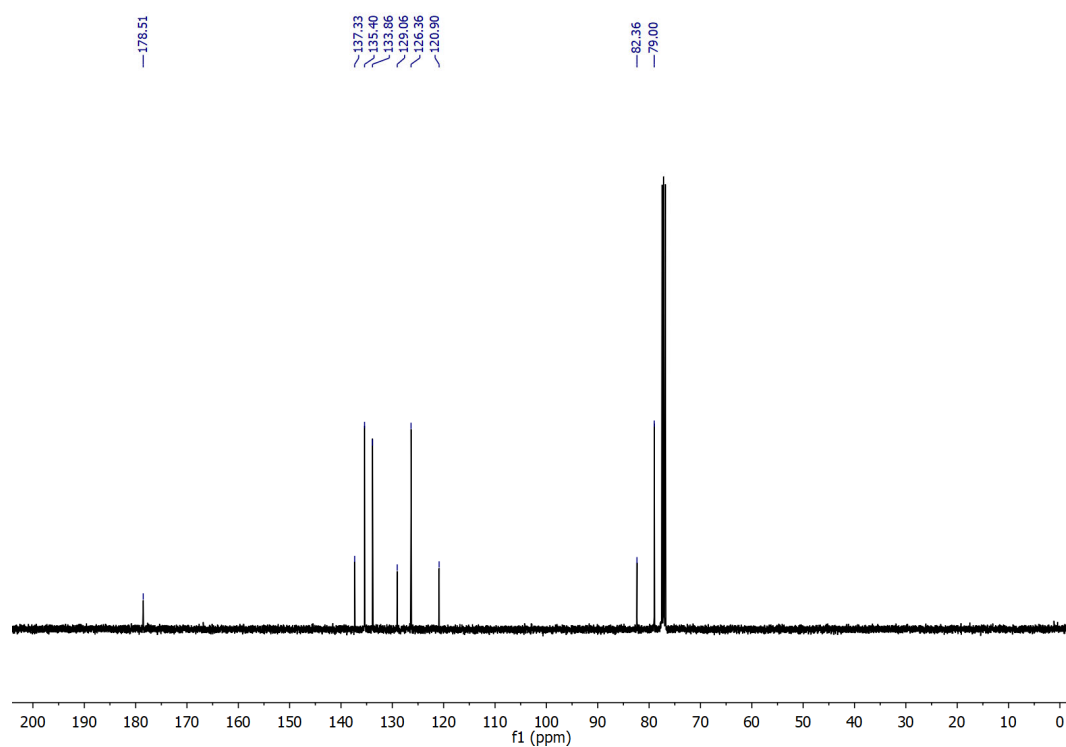


Figure S 80. $^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3) spectrum of compound **19**.

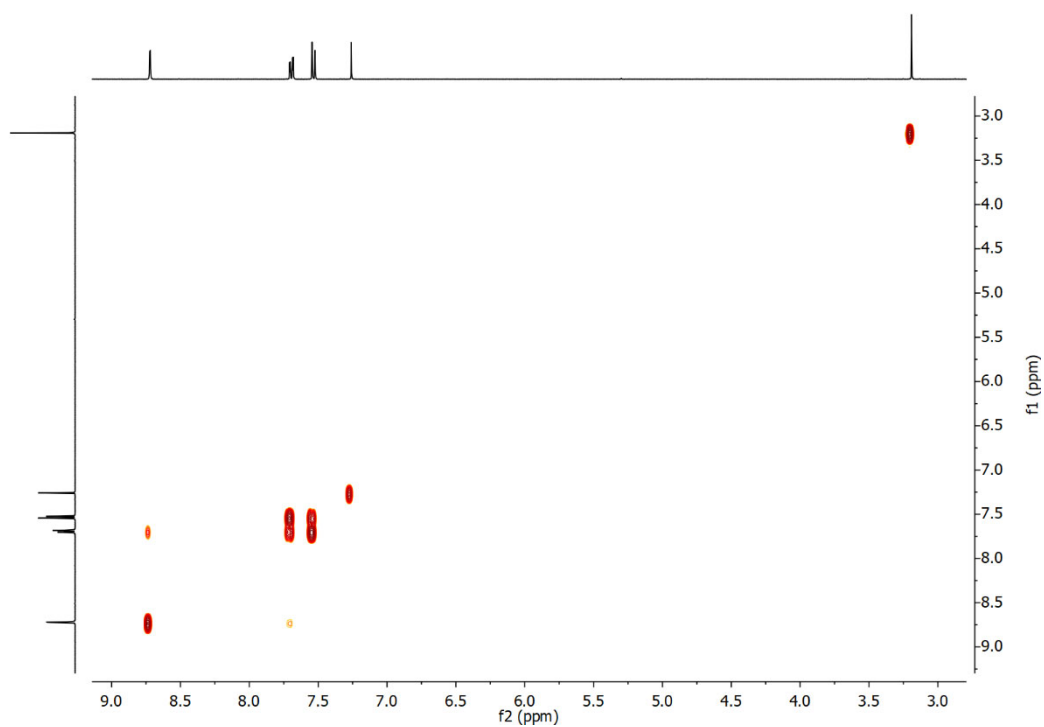


Figure S 81. ^1H - ^1H gCOSY (400 MHz, CDCl_3) spectrum of compound **19**.

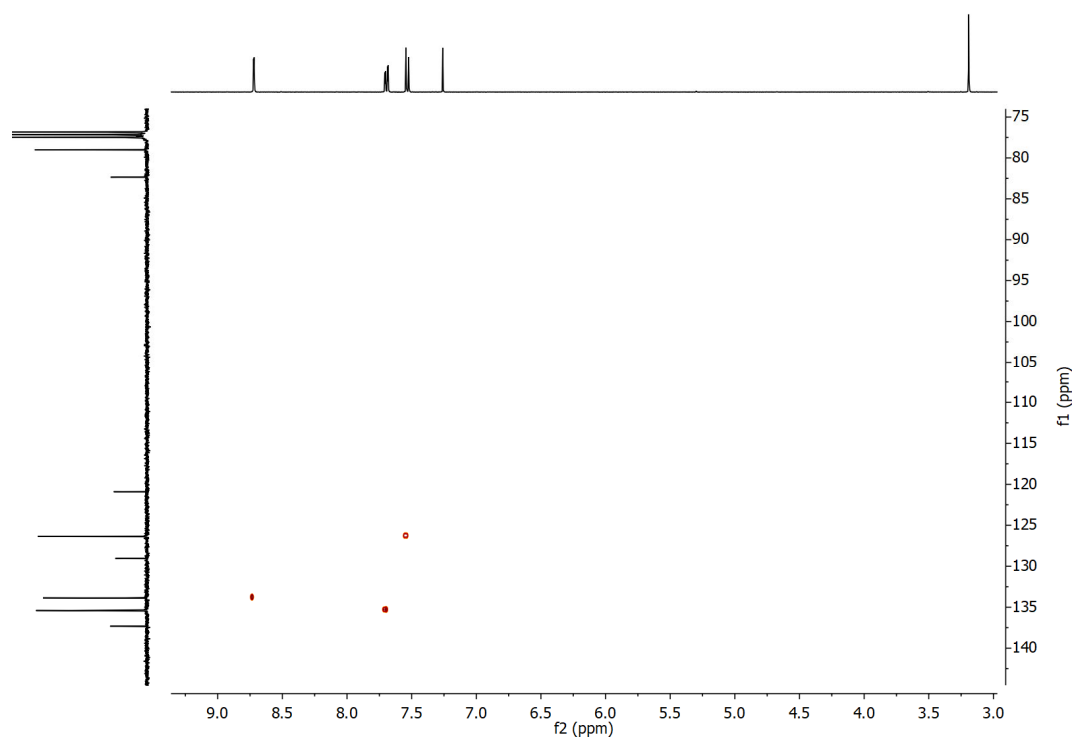


Figure S 82. ^1H - ^{13}C gHSQCAD (400 MHz, CDCl_3) spectrum of compound **19**.

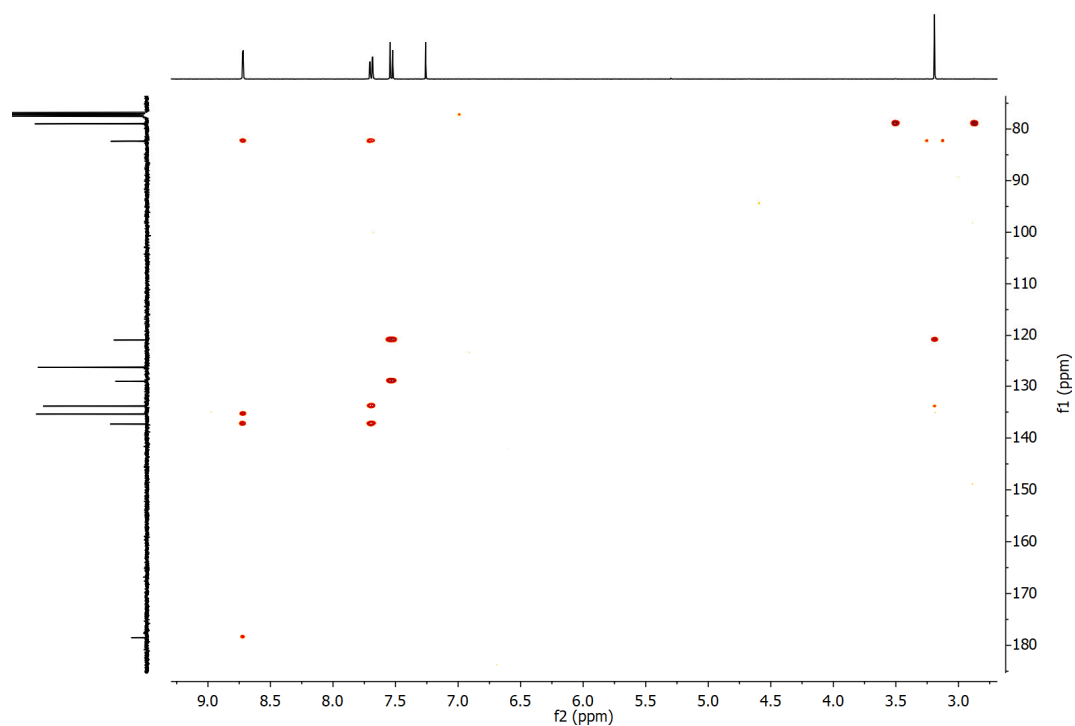


Figure S 83. ^1H - ^{13}C gHMBCAD (400 MHz, CDCl_3) spectrum of compound **19**.

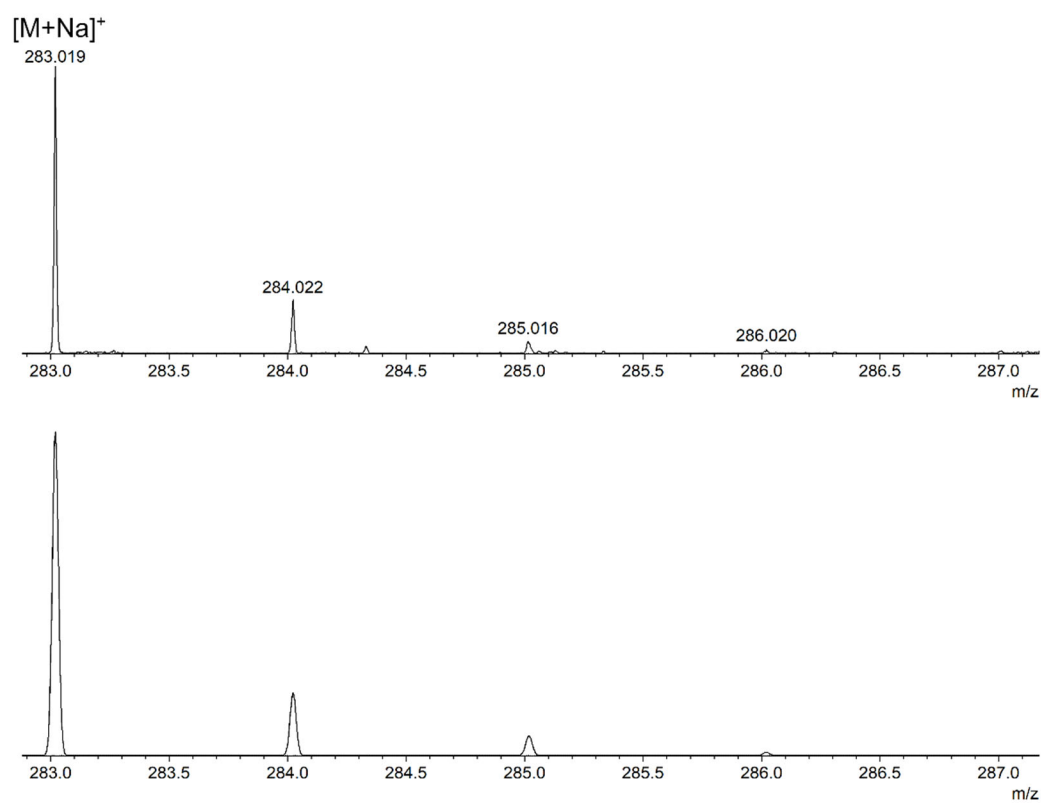
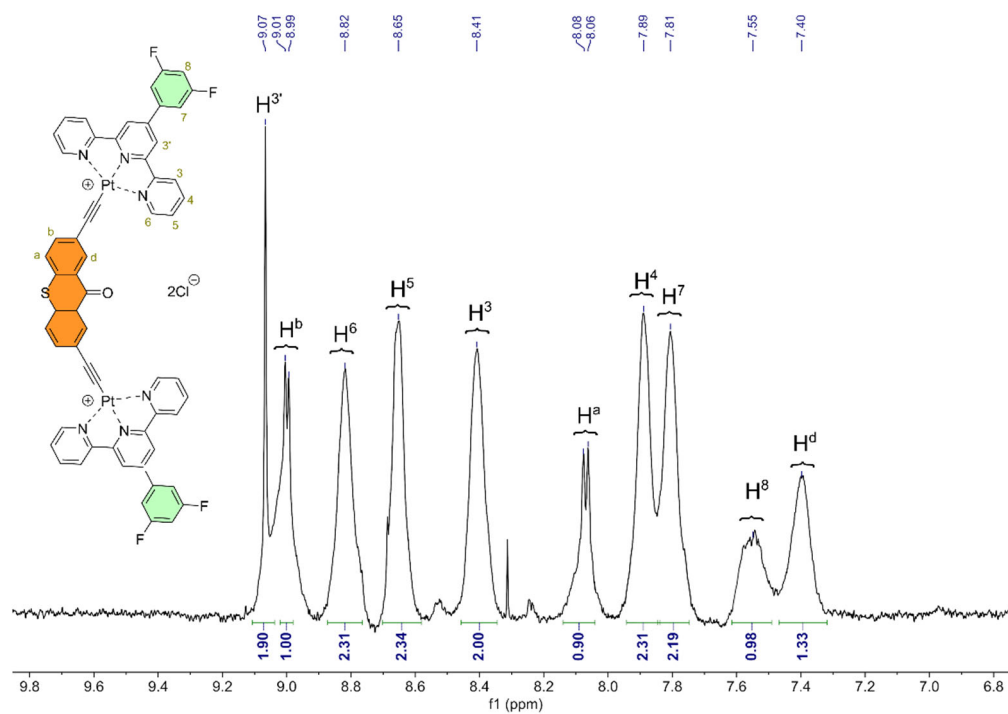
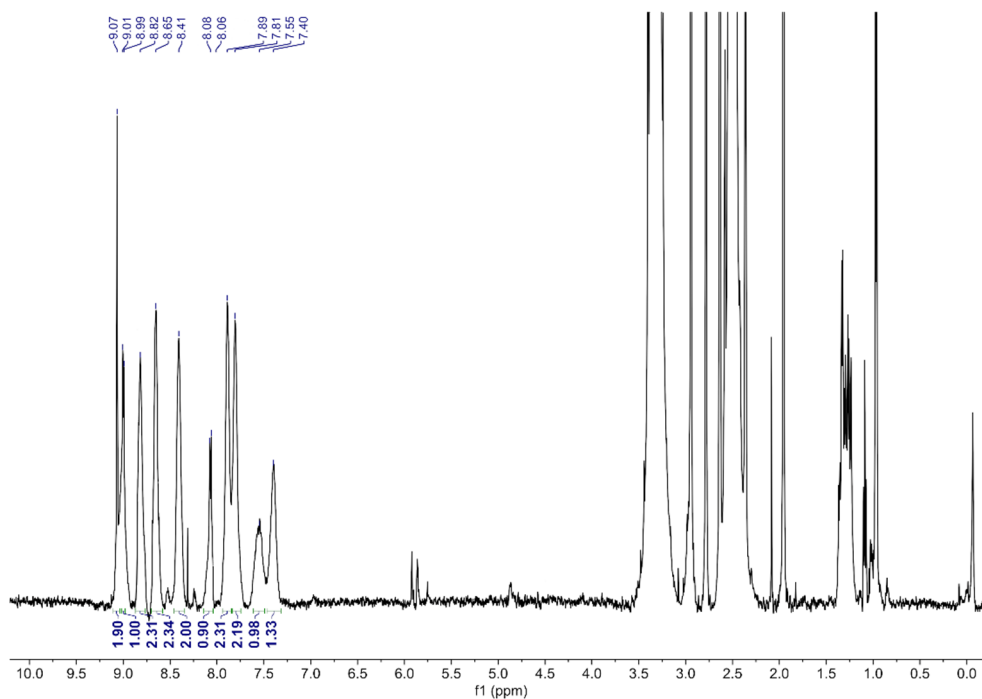


Figure S 84. HRMS (ESI-TOF-pos) of compound **19**, $[M+Na]^+$. Calculated (below), measured (top).

Complex 4

Figure S 85. ¹H-NMR (500 MHz, DMSO-d₆) spectrum of relevant signals of complex 4.Figure S 86. Full ¹H-NMR (500 MHz, DMSO-d₆) spectrum of complex 4.

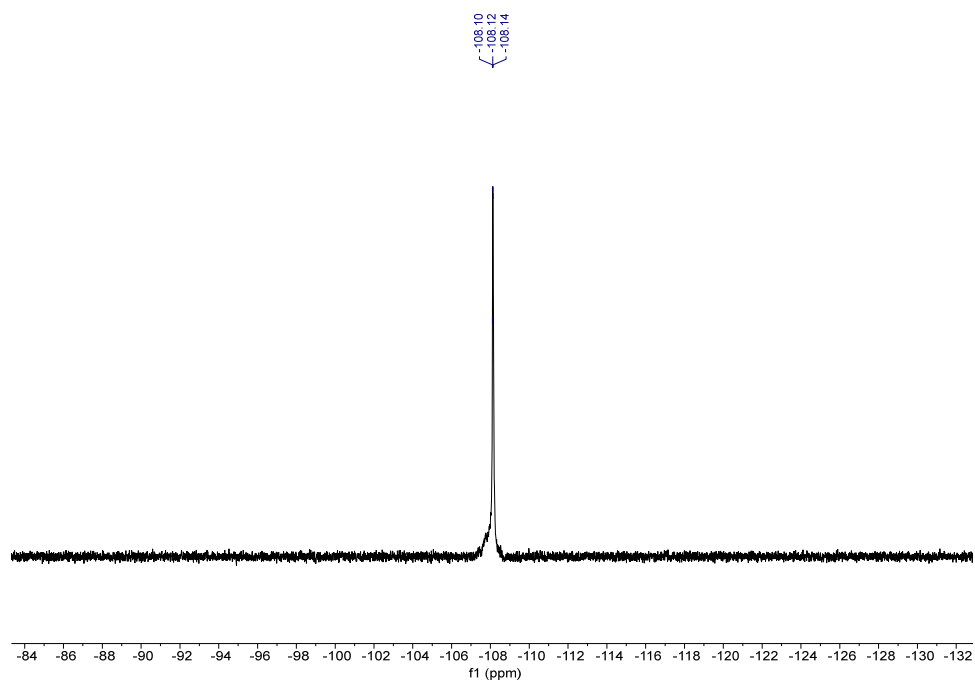


Figure S 87. ^{19}F -NMR (470 MHz, DMSO-d_6) spectrum of complex **4**.

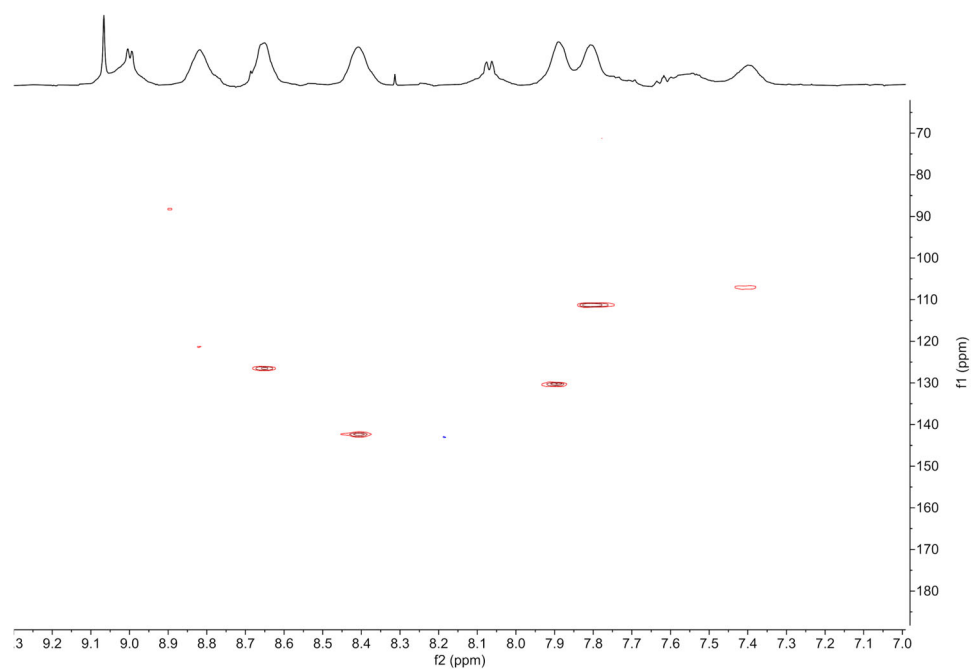


Figure S 88. ^1H - ^{13}C gHSQCAD (500 MHz, DMSO-d_6) spectrum of complex **4**.

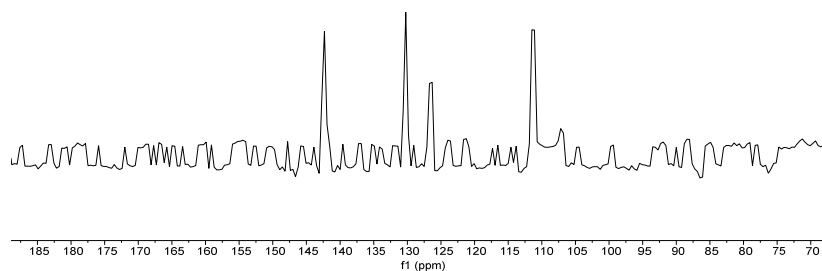


Figure S 89. Extracted vertical trace from the ^1H - ^{13}C gHSQCAD (500 MHz, DMSO-d_6) spectrum of complex **4**.

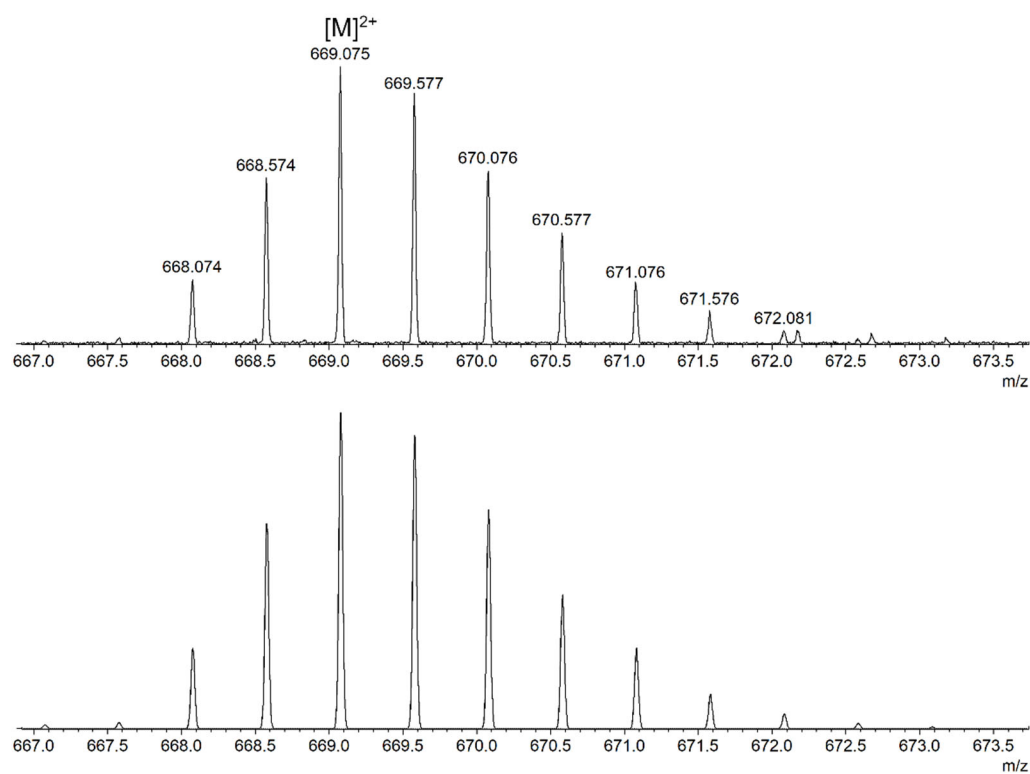
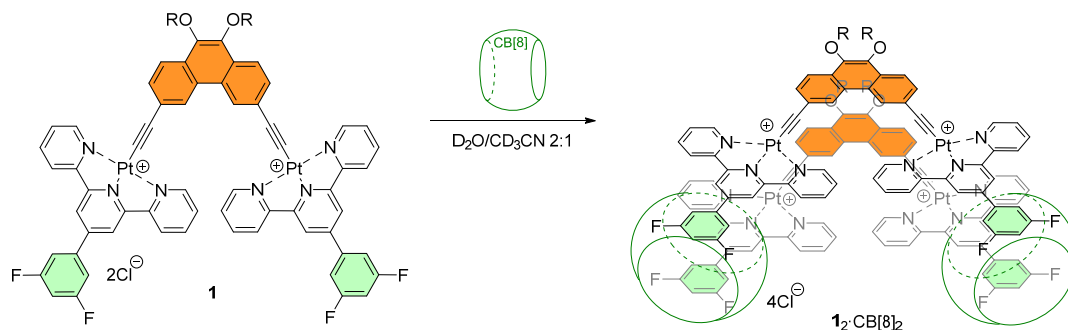


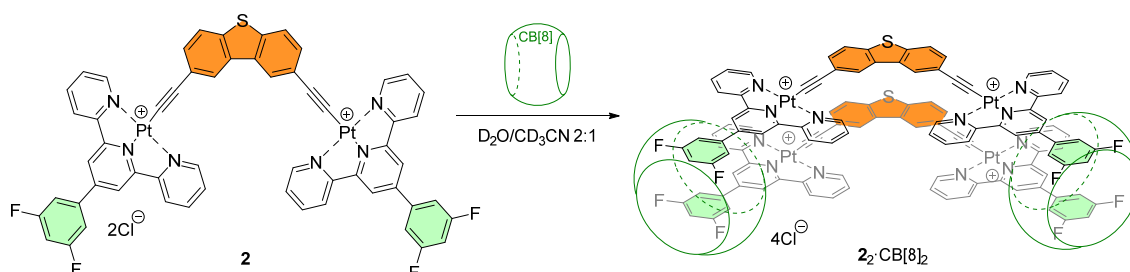
Figure S 90. HRMS (ESI-TOF-pos) of complex **4**, $[\text{M}]^{2+}$. Calculated (below), measured (top).

General preparation of homoquaternary assemblies

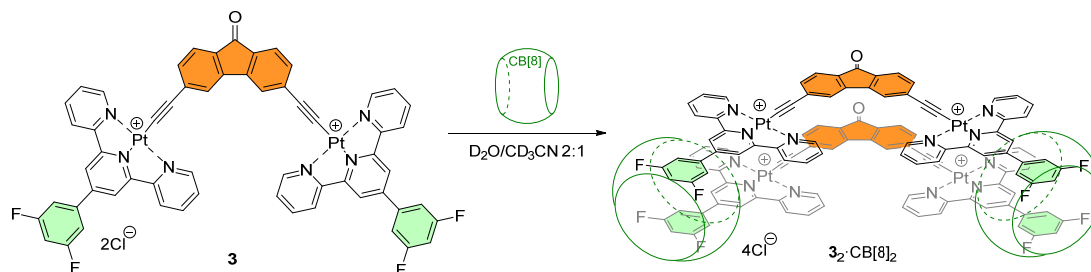
Pt complex **1 – 5** (1.0 μmol) was suspended in a 2:1 mixture of D_2O and CD_3CN (1.0 mL) in a suitable Eppendorf tube and sonicated for 20 min. CB[8] (1.3 mg, 1.0 μmol) was subsequently added and the mixture was thoroughly sonicated for 40 min before being transferred to an NMR tube (0.6 mL). The mixture was then heated at 40 $^\circ\text{C}$ for 20 min and sonicated for additional 10 min.



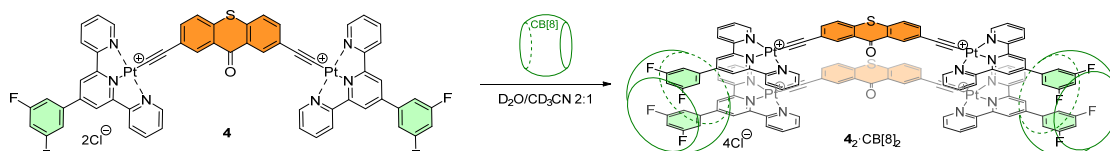
Scheme S 5. Preparation of assembly **1₂·CB[8]₂**.



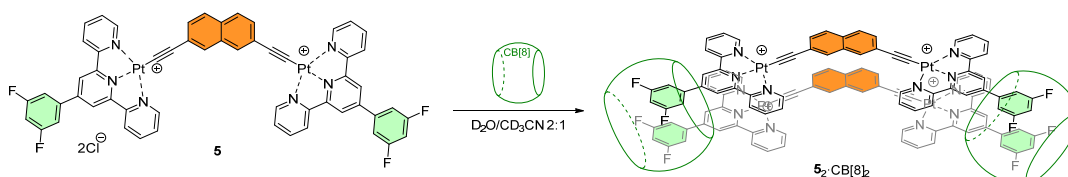
Scheme S 6. Preparation of assembly **2₂·CB[8]₂**.



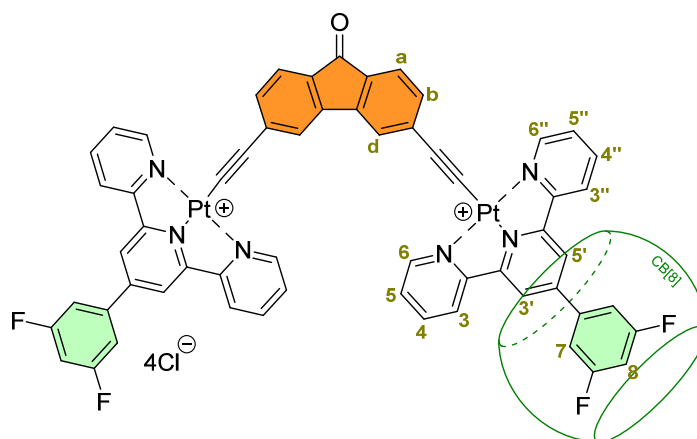
Scheme S 7. Preparation of assembly **3₂·CB[8]₂**.



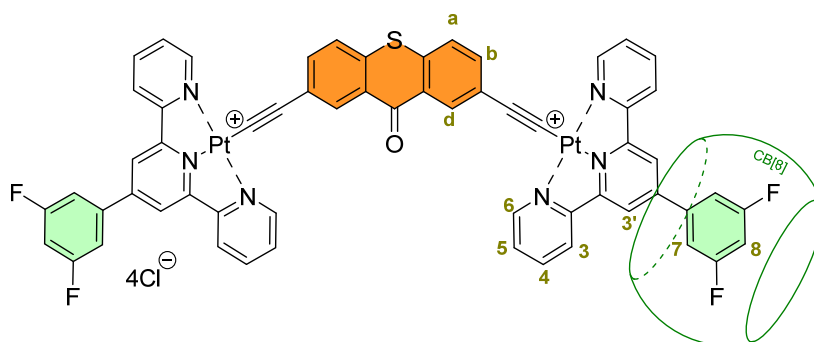
Scheme S 8. Preparation of assembly **4₂·CB[8]₂**.



Scheme S 9. Preparation of assembly **5₂·CB[8]₂**.

Assembly **3**₂·CB[8]₂

¹H NMR (500 MHz, D₂O:CD₃CN, 2:1) δ 9.30 (d, *J* = 5.5 Hz, 4H, H^b), 9.21 (d, *J* = 5.5 Hz, 4H, H^{6''}), 8.68 (d, *J* = 8.0 Hz, 8H, H³, H^{3''}), 8.27 (d, *J* = 4.3 Hz, 8H, H^{3'}, H^{5'}), 8.20 (q, *J* = 8.0 Hz, 8H, H⁴, H^{4''}), 7.68 (t, *J* = 6.7 Hz, 4H, H⁵), 7.64 (t, *J* = 6.7 Hz, 4H, H^{5''}), 7.58 (s, 4H, H^d), 7.33 (d, *J* = 7.6 Hz, 4H, H^b), 7.25 (d, *J* = 7.6 Hz, 4H, H^a), 6.58 (m, 8H, H⁷), 6.48 (t, *J* = 8.6 Hz, 4H, H⁸), 5.76 (d, *J* = 15.4 Hz, 8H, H^{CB8ax}), 5.63 (d, *J* = 15.4 Hz, 8H, H^{CB8ax'}), 5.31 (s, 32H, H^{CB8eq}), 4.03 (t, *J* = 14.8 Hz, 16H, H^{CB8ax}). ¹³C NMR (126 MHz, D₂O:CD₃CN, 2:1) δ 194.53, 164.88, 164.77, 162.88, 162.77, 158.99, 158.84, 157.51, 157.29, 155.53, 154.09, 153.98, 152.13, 144.65, 143.11, 137.92, 134.96, 133.90, 132.33, 130.29, 130.20, 127.12, 124.82, 124.72, 122.64, 122.55, 110.11, 109.92, 106.95, 106.79, 72.63, 54.30, 54.24. ¹⁹F NMR (470 MHz, D₂O:CD₃CN, 2:1) δ -103.89. HRMS (ESI-TOF-pos): *m/z* = 1319.0411 [M]⁴⁺ (calc. 1318.0405 for C₂₁₄H₁₆₀F₈N₇₆O₃₄Pt₄).

Assembly **4**₂·CB[8]₂

¹H NMR (500 MHz, D₂O:CD₃CN, 2:1) δ 9.64 (s, 4H, H^b), 9.54 (s, 4H, H^b), 8.97 (d, *J* = 8.0 Hz, 8H, H³), 8.62 (s, 4H, H^d), 8.56 (s, 8H, H^{3'}), 8.51 (s, 8H, H⁴), 8.02 (s, 8H, H⁵), 7.95 – 7.88 (m, 4H, H^b), 7.68 (d, *J* = 8.2 Hz, 4H, H^a), 6.89 (d, *J* = 6.8 Hz, 8H, H⁷), 6.77 (t, *J* = 8.6 Hz, 4H, H⁸), 6.06 (d, *J* = 15.2 Hz, 8H, H^{CB8ax}), 5.94 (d, *J* = 15.3 Hz, 8H, H^{CB8ax'}), 5.61 (s, 32H, H^{CB8eq}), 4.33 (dd, *J* = 17.1, 12.0 Hz, 16H, H^{CB8ax}). ¹³C NMR (126 MHz, D₂O:CD₃CN, 2:1) δ 179.55, 164.20, 162.27, 162.18, 158.30, 156.90, 156.70, 155.05, 153.44, 151.34, 142.39, 137.37, 136.28, 135.37, 132.09, 129.68, 127.77, 126.47, 126.34, 125.54, 121.96, 109.49, 109.32, 106.44, 104.76, 101.64, 72.04, 53.68. ¹⁹F NMR (470 MHz, D₂O:CD₃CN, 2:1) δ -106.57. HRMS (ESI-TOF-pos): *m/z* = 1334.0264 [M]⁴⁺ (calc. 1334.0264 for C₂₁₄H₁₆₀F₈N₇₆O₃₄Pt₄S₂).

NMR and HRMS spectra of homoquatary assemblies

Assembly $1_2 \cdot \text{CB}[8]_2$

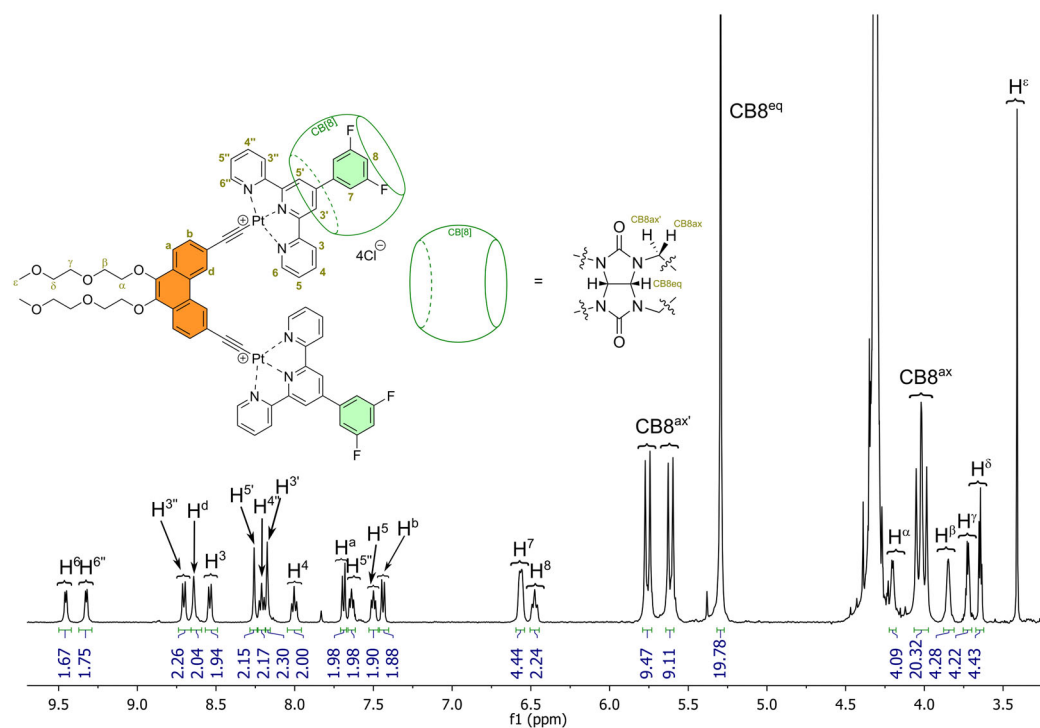


Figure S 91. ^1H -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectrum of relevant signals of assembly $1_2 \cdot \text{CB}[8]_2$.

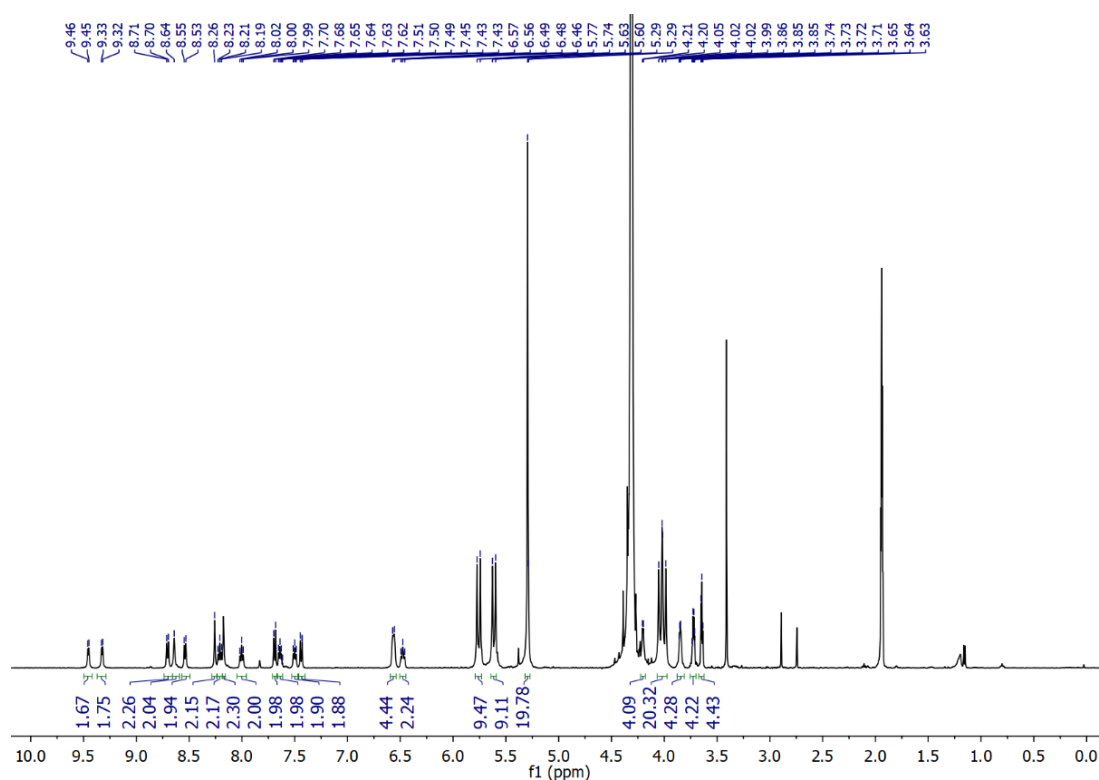


Figure S 92. ^1H -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectrum of relevant signals of assembly $1_2 \cdot \text{CB}[8]_2$.

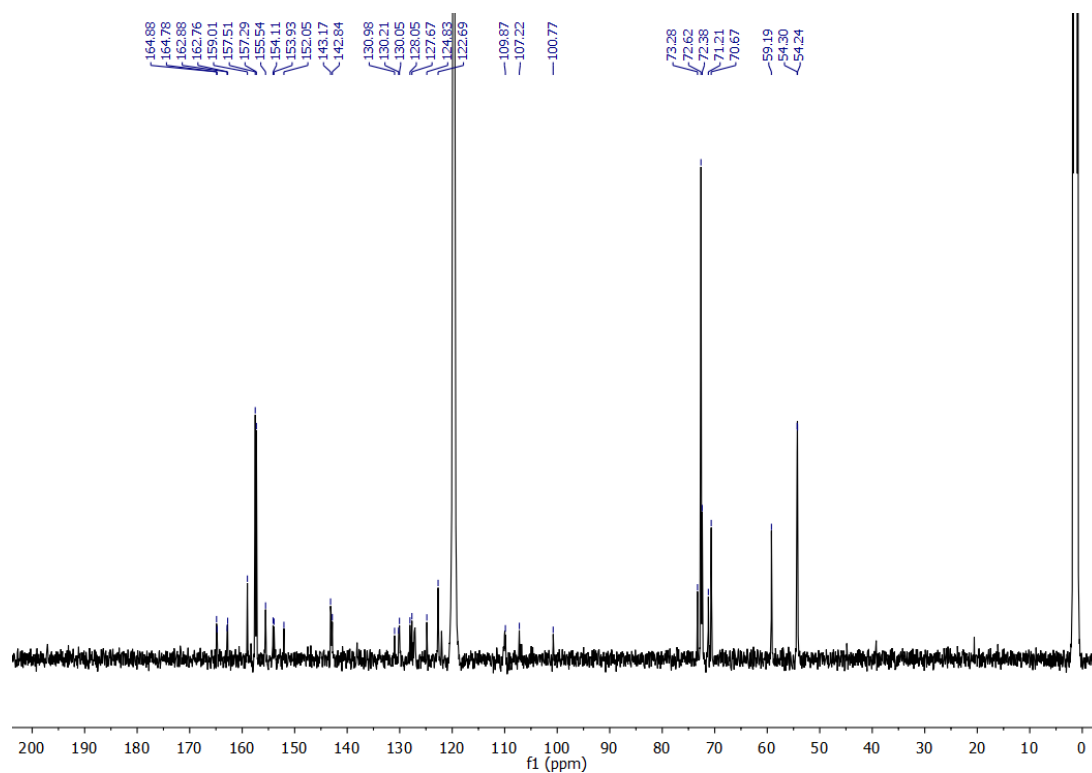


Figure S 93. $^{13}\text{C}\{^1\text{H}\}$ -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectrum of assembly $1_2\cdot\text{CB}[8]_2$.

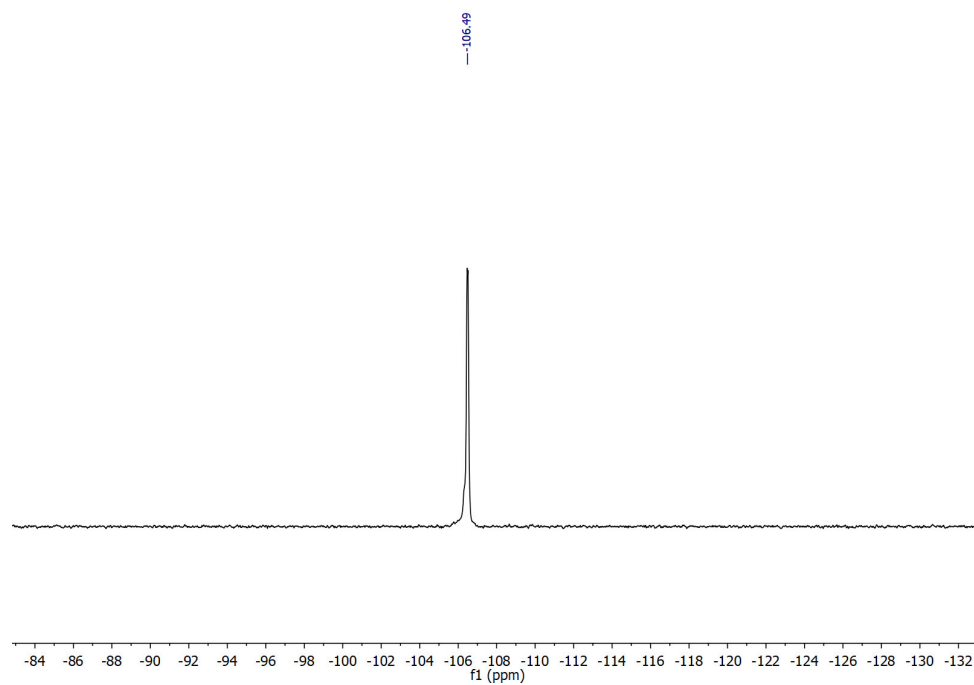


Figure S 94. ^{19}F -NMR (470 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectrum of assembly $1_2\cdot(\text{CB}[8])_2$.

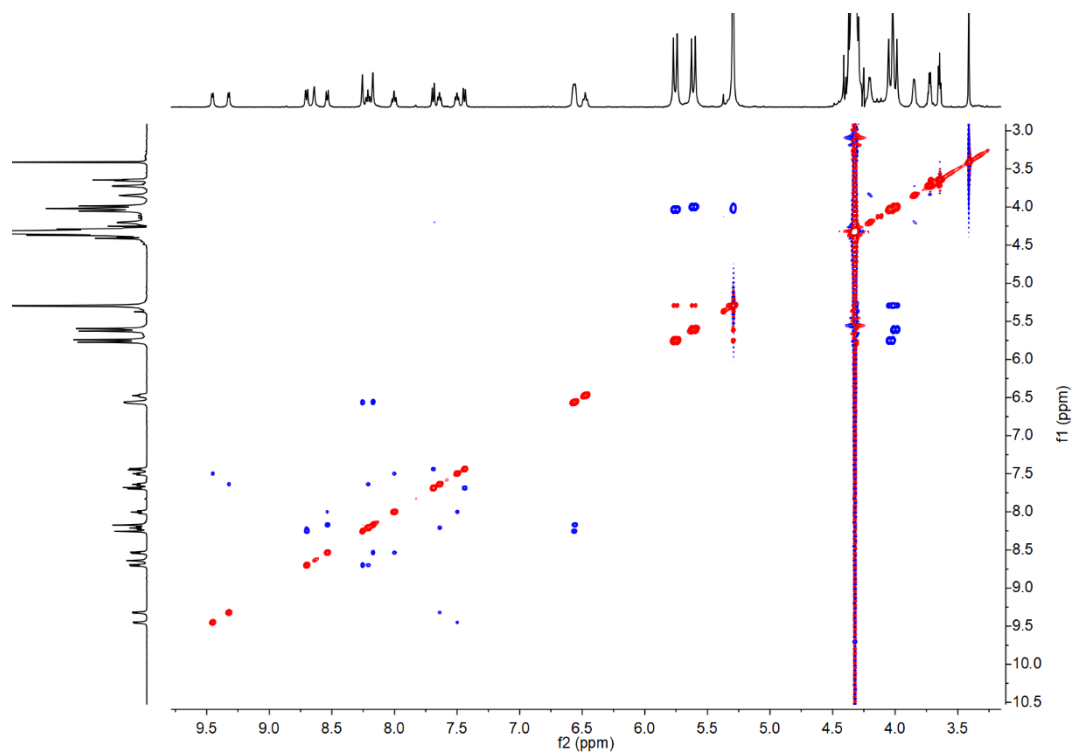


Figure S 95. ^1H - ^1H ROESY (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectrum of assembly $1_2\cdot\text{CB}[8]_2$.

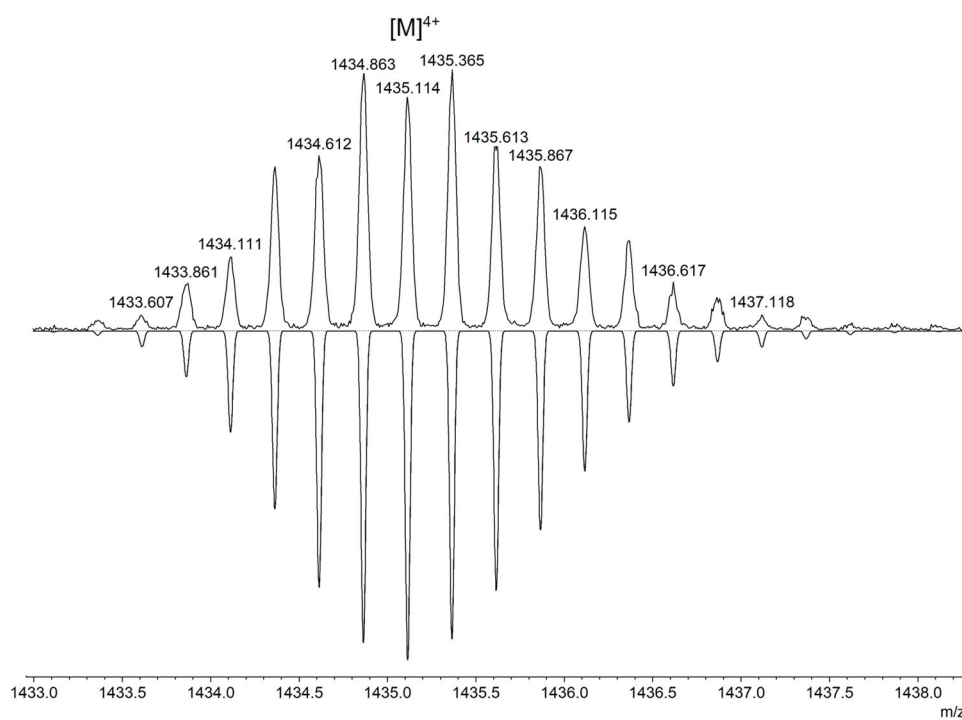


Figure S 96. HRMS (ESI-TOF-pos) of assembly $1_2\cdot\text{CB}[8]_2$, $[\text{M}]^{4+}$. Calculated (below), measured (top).

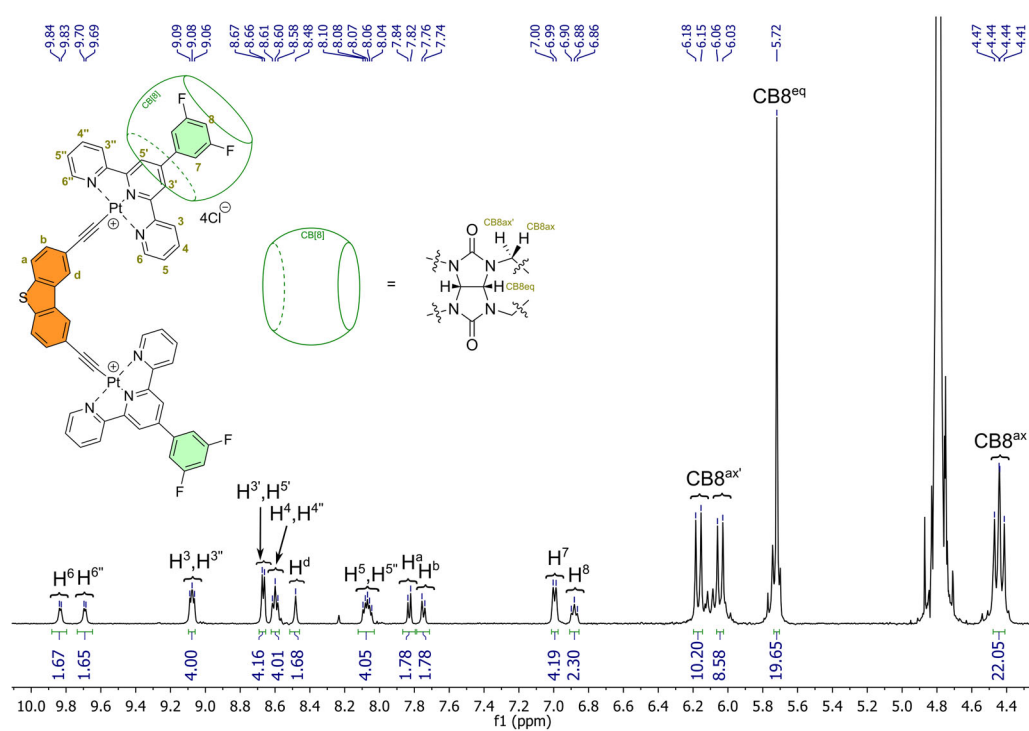
Assembly $2_2 \cdot \text{CB}[8]_2$ 

Figure S 97. ^1H -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectrum of relevant signals of assembly $2_2 \cdot \text{CB}[8]_2$.

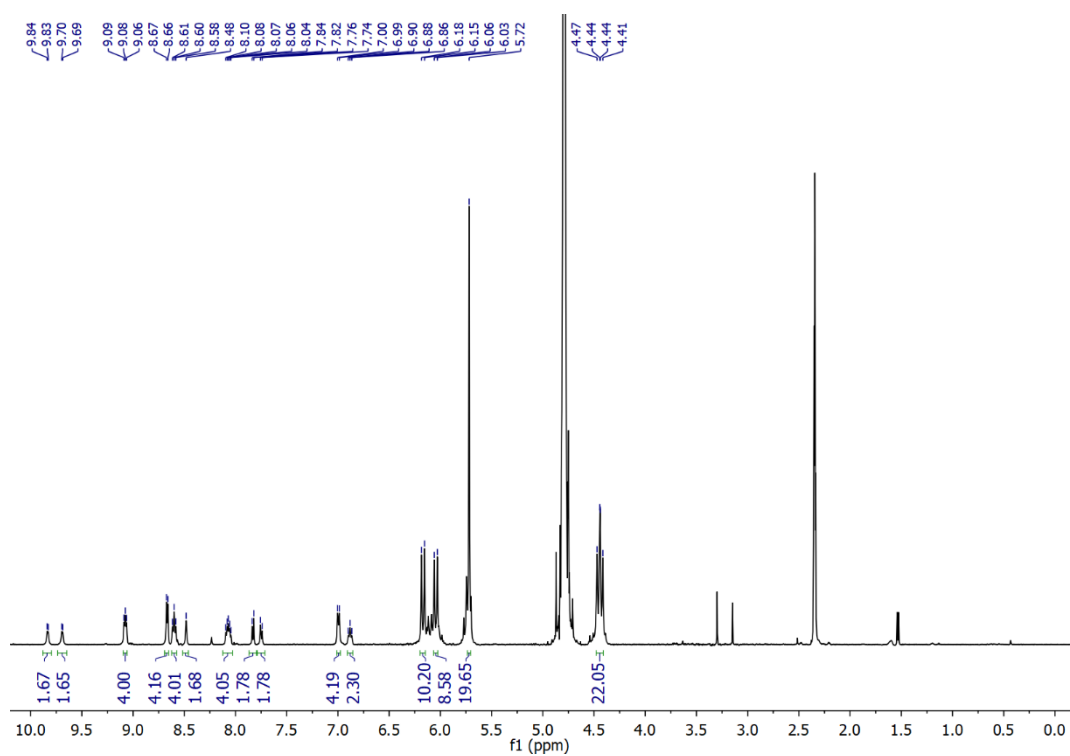


Figure S 98. Full ^1H -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectrum of assembly $2_2 \cdot \text{CB}[8]_2$.

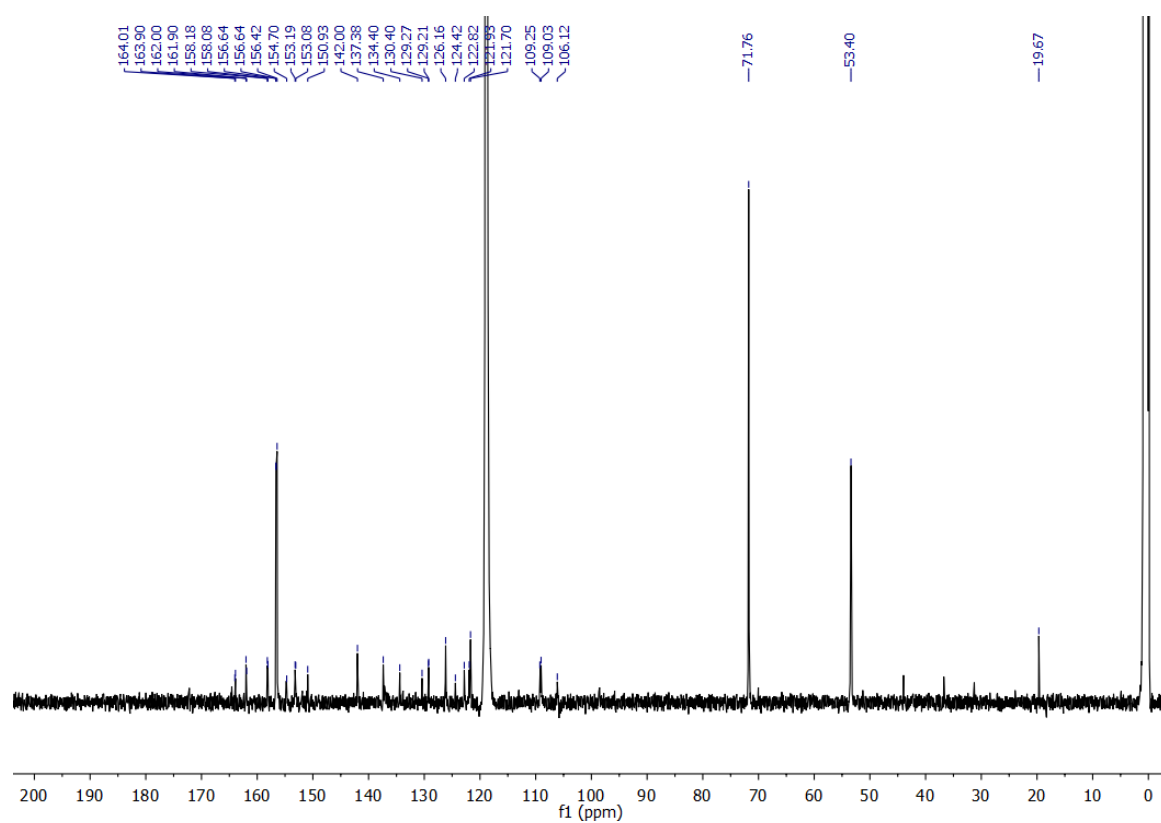


Figure S 99. $^{13}\text{C}\{^1\text{H}\}$ -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectrum of assembly $\mathbf{2}_2 \cdot \text{CB}[8]_2$.

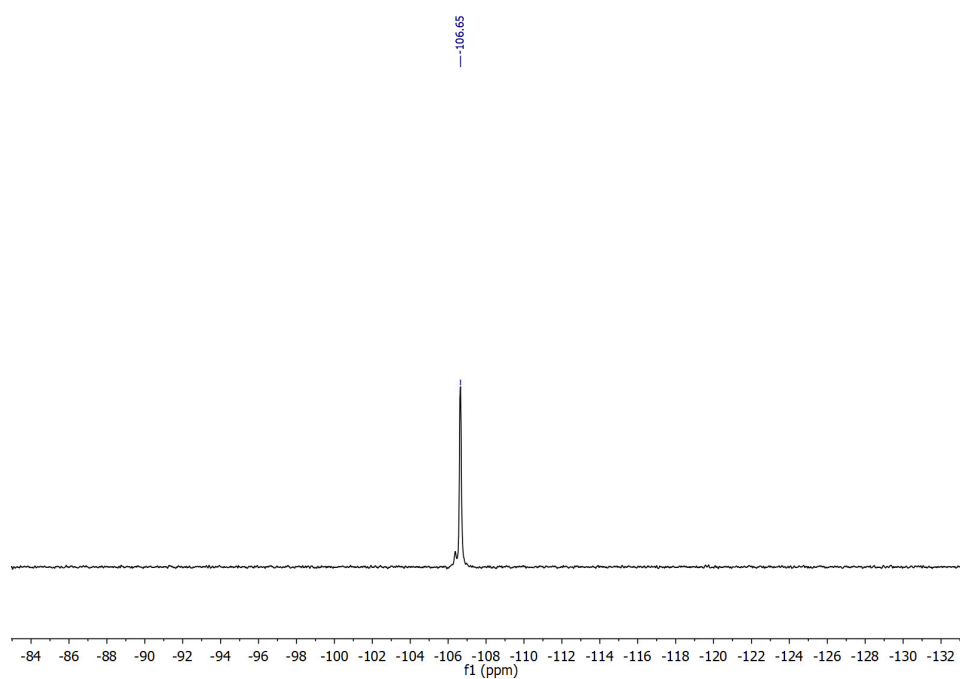


Figure S 100. ^{19}F -NMR (470 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectrum of assembly $\mathbf{2}_2 \cdot (\text{CB}[8])_2$.

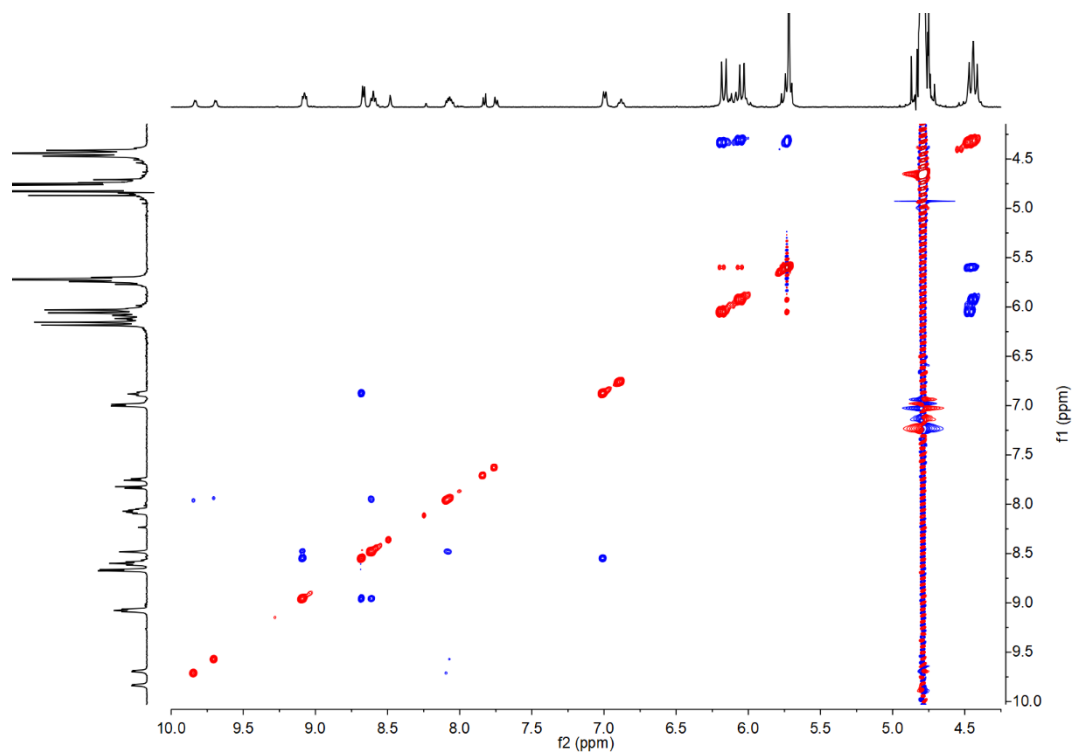


Figure S 101. ^1H - ^1H ROESY (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectrum of assembly $2_2\cdot\text{CB}[8]_2$.

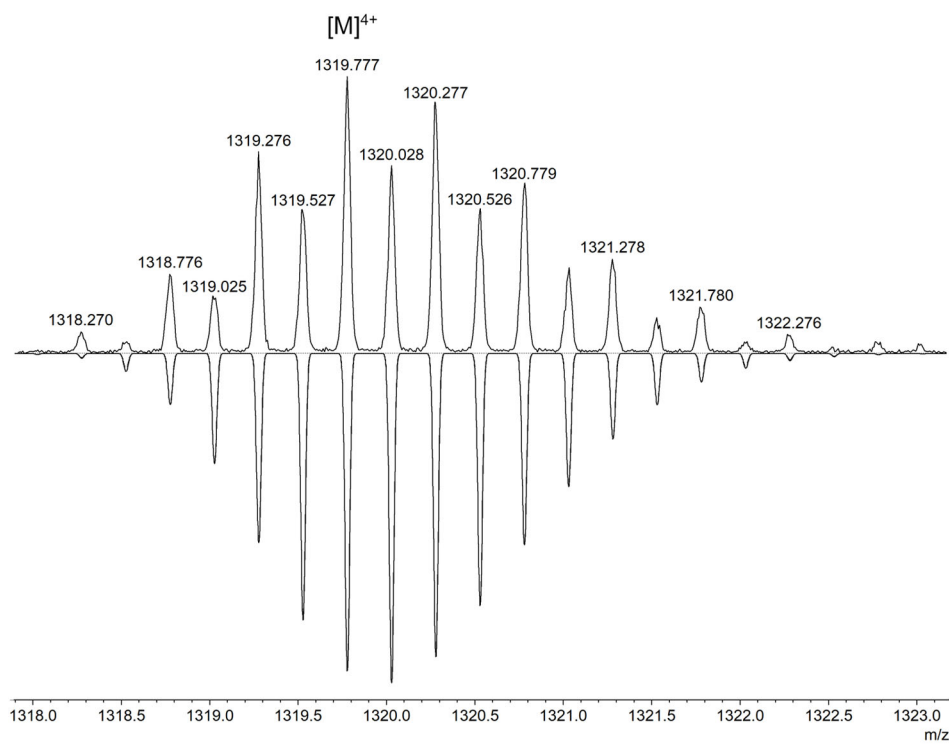


Figure S 102. HRMS (ESI-TOF-pos) of assembly $2_2\cdot\text{CB}[8]_2$, $[\text{M}]^{4+}$. Calculated (below), measured (top).

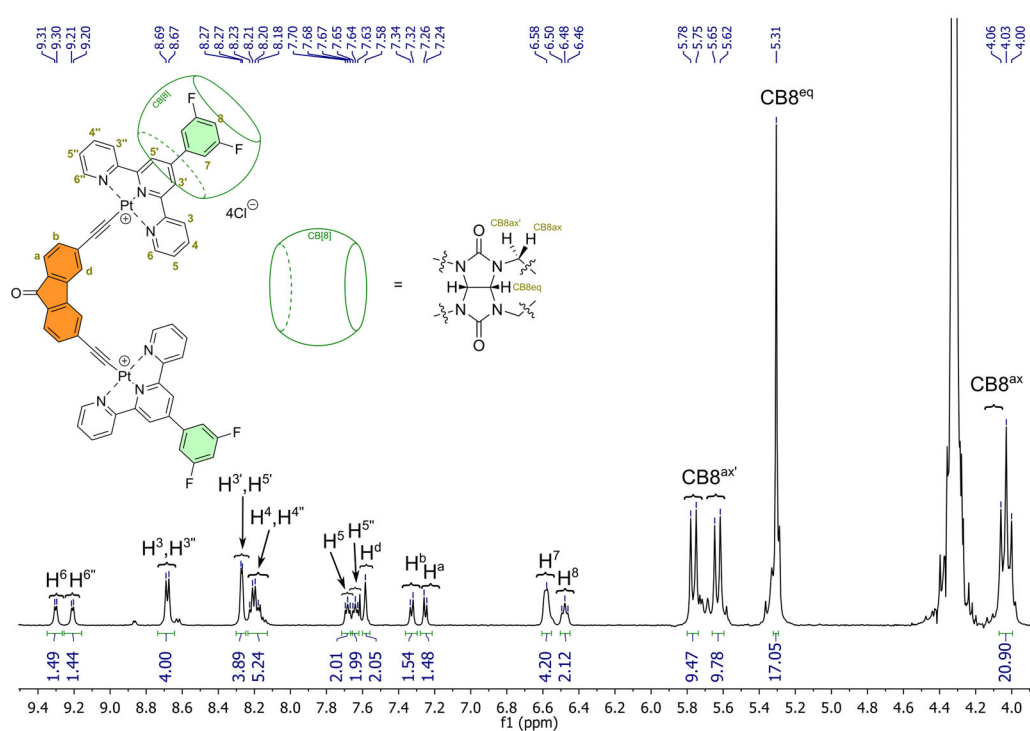
Assembly $3_2 \cdot \text{CB}[8]_2$ 

Figure S 103. ^1H -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectrum of relevant signals of assembly $3_2 \cdot \text{CB}[8]_2$.

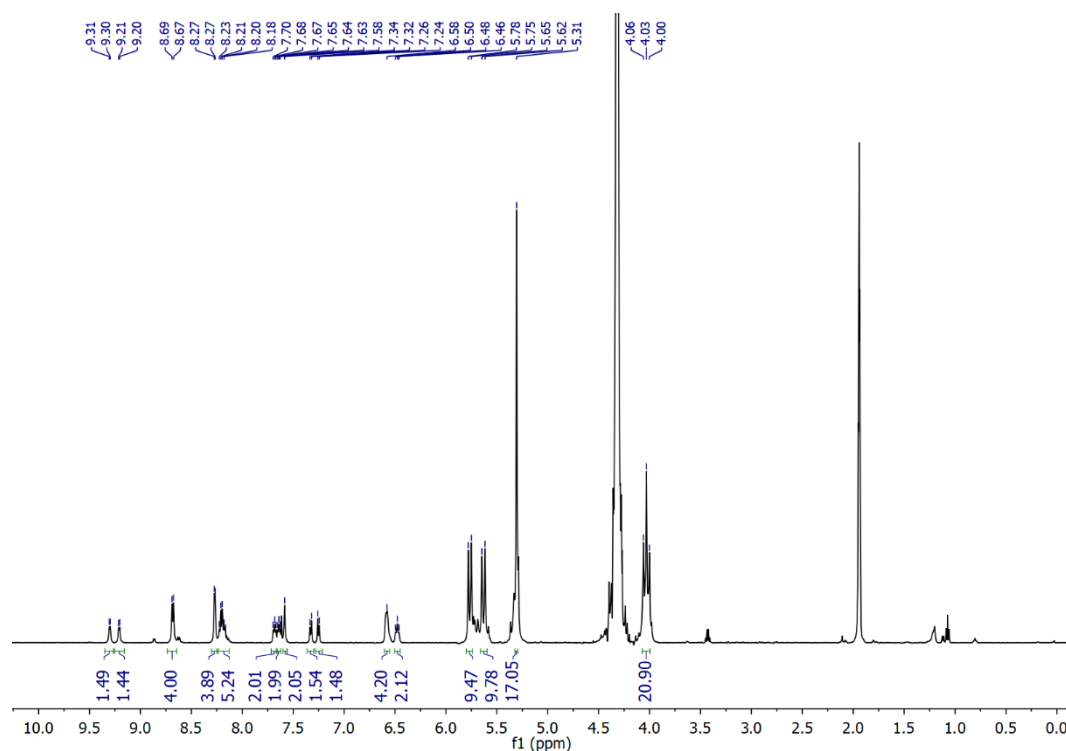


Figure S 104. Full ^1H -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectrum of assembly $3_2 \cdot \text{CB}[8]_2$.

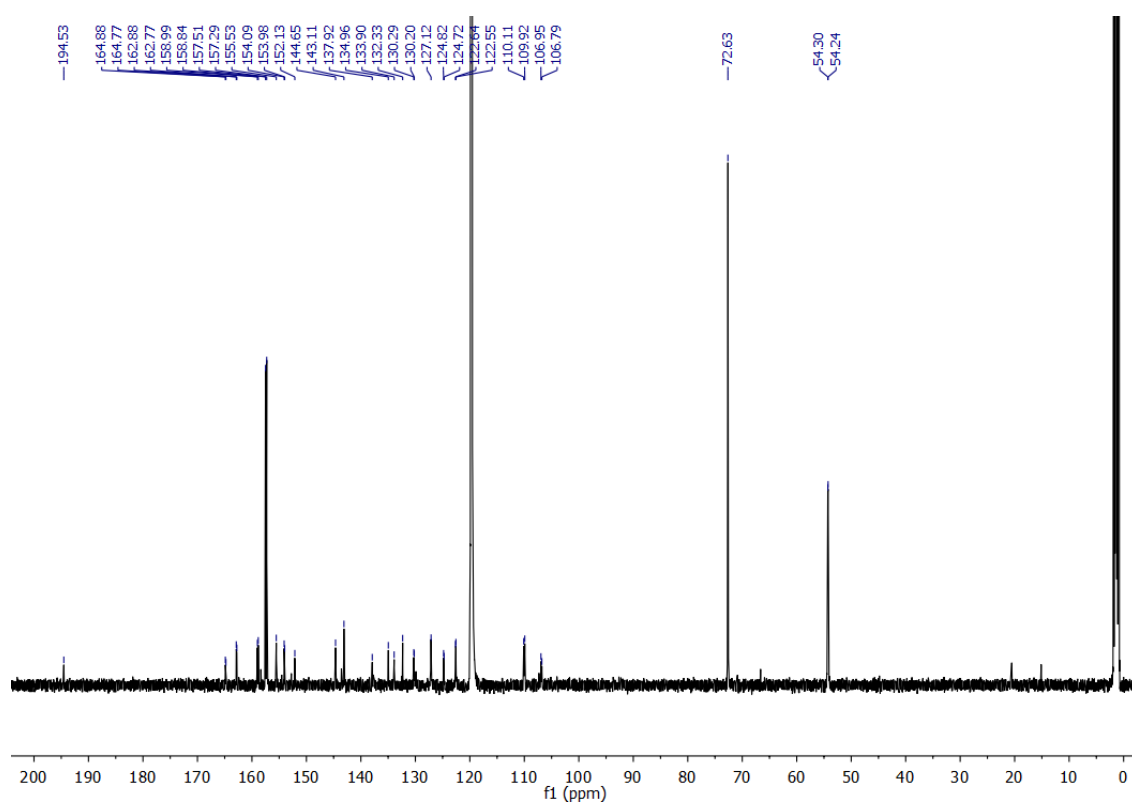


Figure S 105. $^{13}\text{C}\{^1\text{H}\}$ -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectrum of assembly $\mathbf{3}_2\text{-CB[8]}_2$.

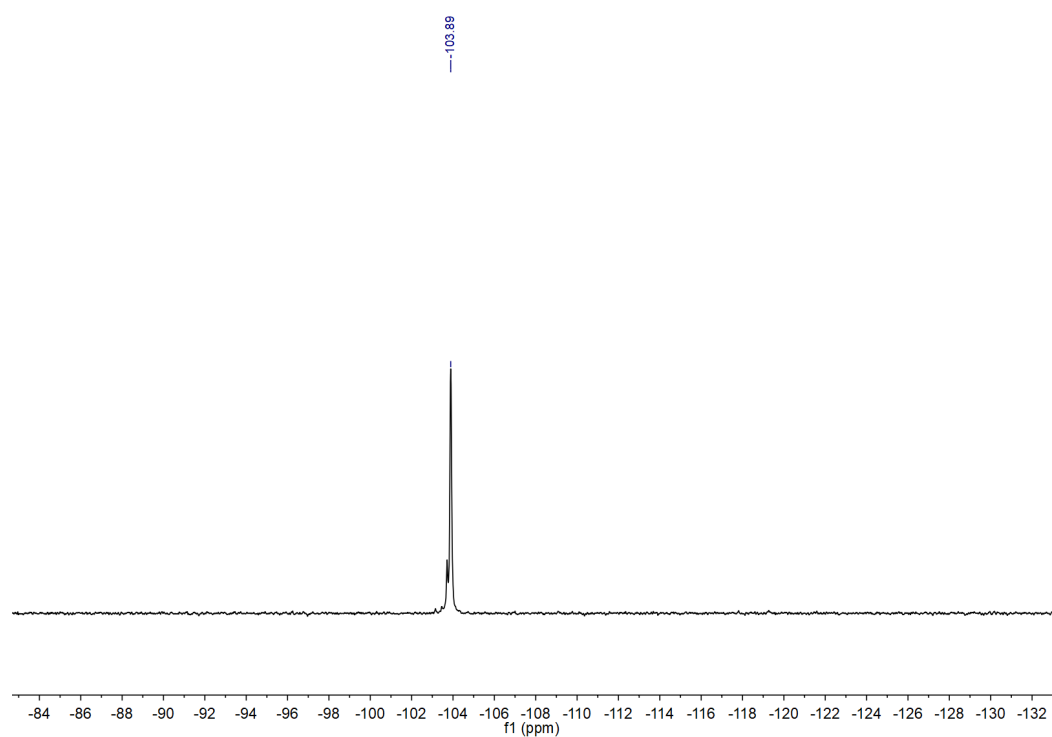


Figure S 106. ^{19}F -NMR (470 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectrum of assembly $\mathbf{3}_2\text{-CB[8]}_2$.

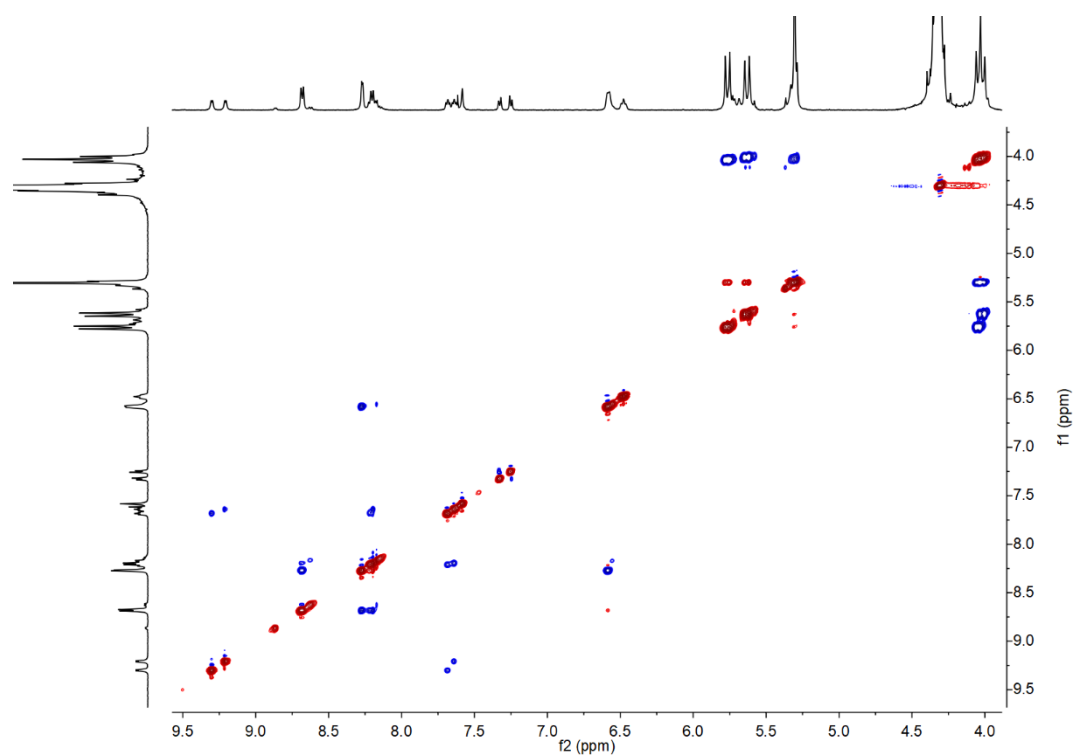


Figure S 107. ^1H - ^1H ROESY (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectrum of assembly $3_2\text{-CB}[8]_2$.

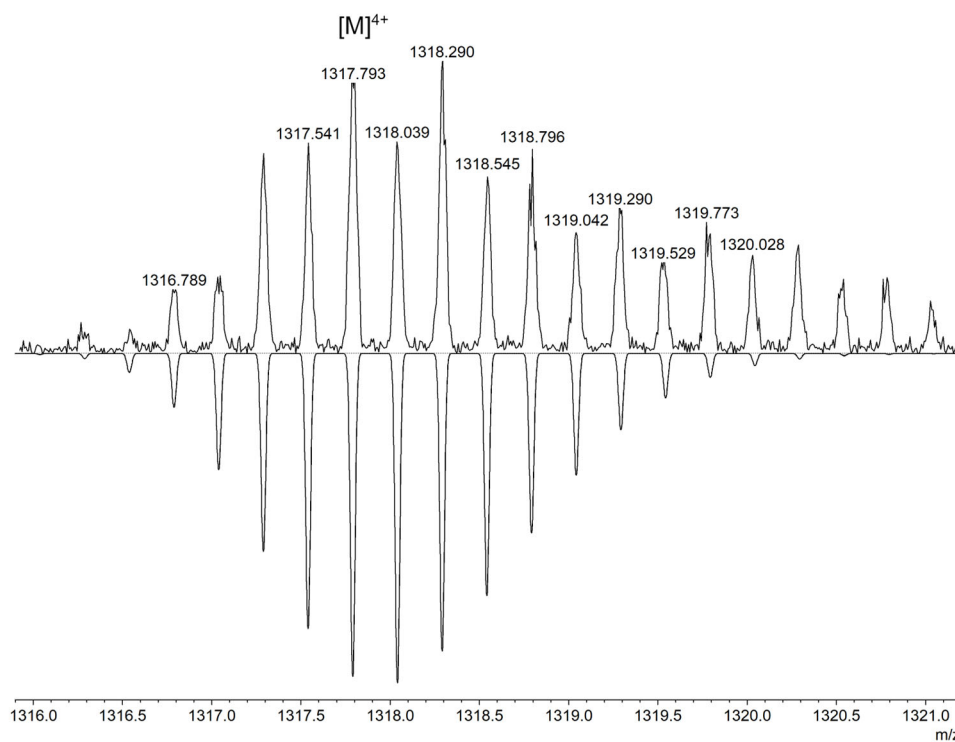


Figure S 108. HRMS (ESI-TOF-pos) of assembly $3_2\text{-CB}[8]_2$, $[\text{M}]^{4+}$. Calculated (below), measured (top).

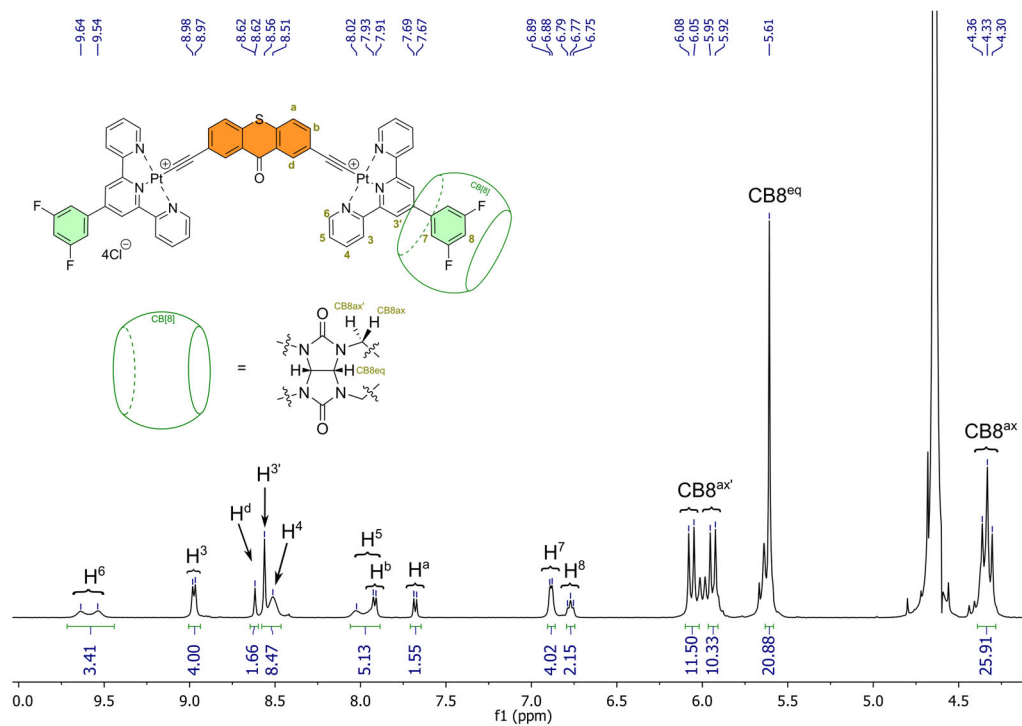


Figure S 109. ^1H -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectrum of relevant signals of assembly **4**₂-CB[8]₂.

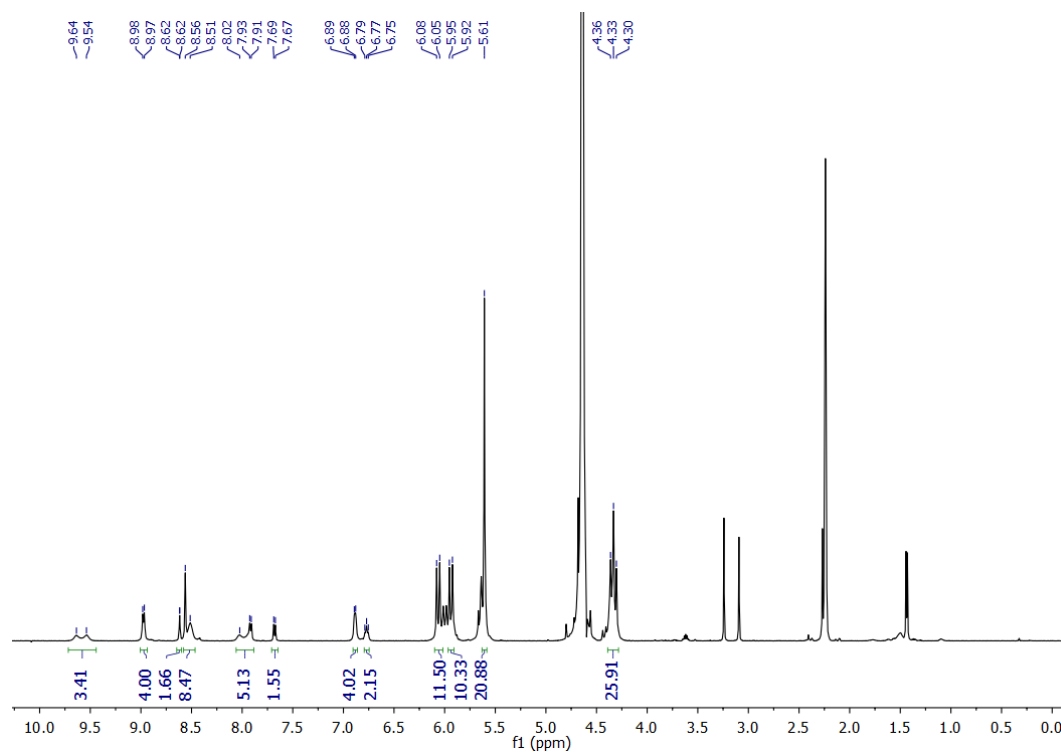


Figure S 110. Full ^1H -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectrum of assembly $4_2\cdot\text{CB}[8]_2$.

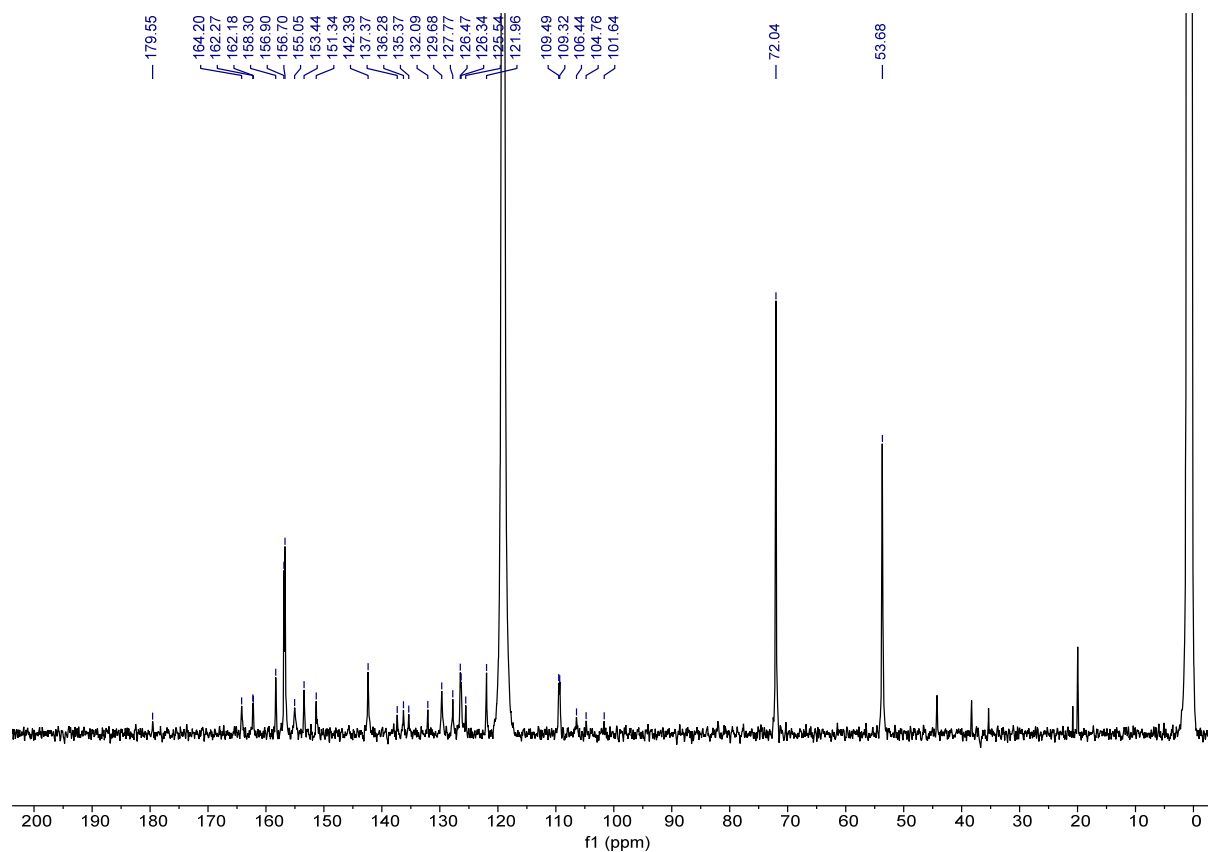


Figure S 111. $^{13}\text{C}\{^1\text{H}\}$ -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectrum of assembly $4_2\cdot\text{CB}[8]_2$ at 60 °C.

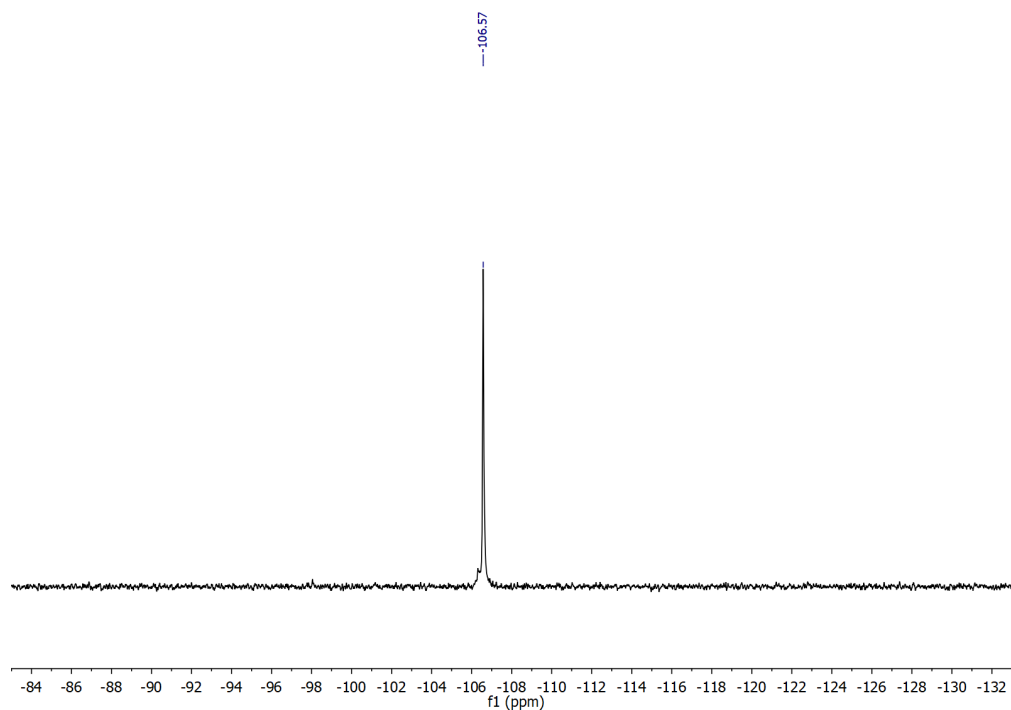


Figure S 112. ^{19}F -NMR (470 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectrum of assembly $4_2\cdot\text{CB}[8]_2$.

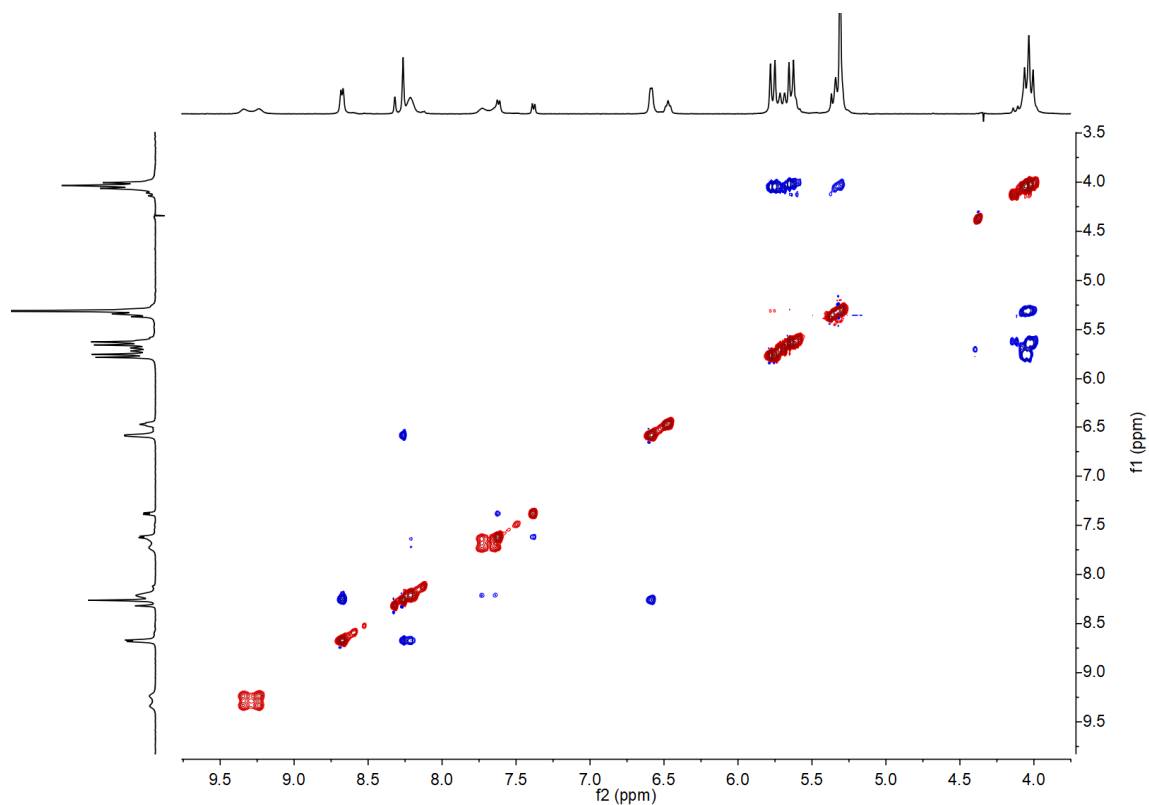


Figure S 113. ^1H - ^1H ROESY (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectrum of assembly $4_2\text{-CB}[8]_2$.

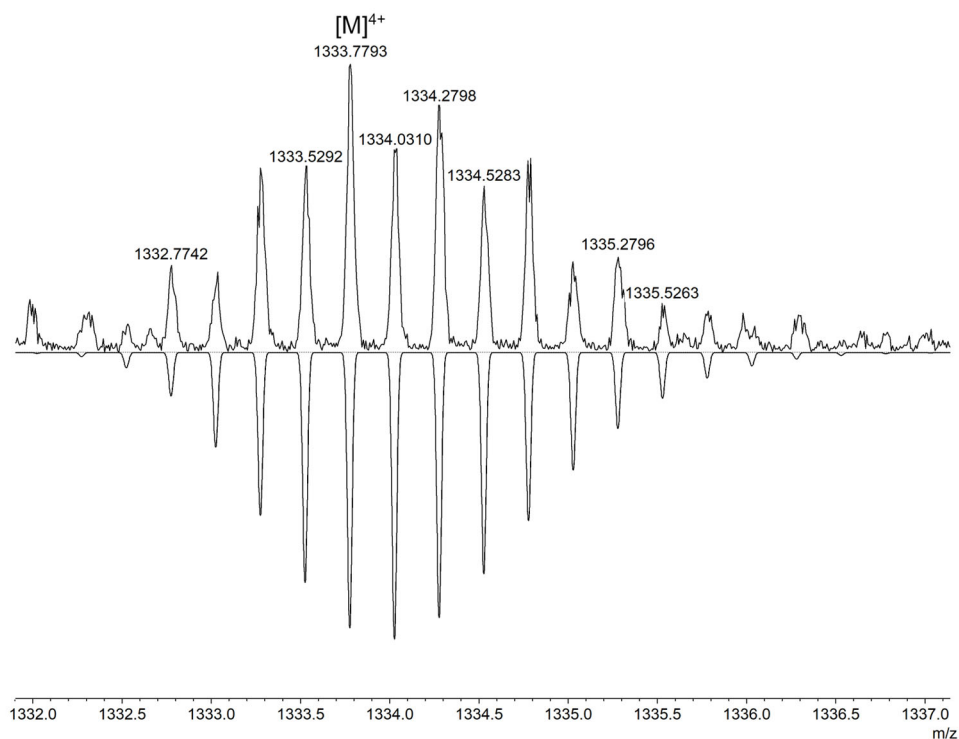


Figure S 114. HRMS (ESI-TOF-pos) of assembly $4_2\text{-CB}[8]_2$, $[\text{M}]^{4+}$. Calculated (below), measured (top).

Discussion about signal splitting in homoquaternary assemblies

^1H -NMR spectroscopy unequivocally confirms the structure of all homoquaternary assemblies due to (1) upfield chemical shifts of hydrogens H^7 and H^8 pertaining to the 3,5-difluorophenyl group encapsulated within the cavity of the macrocycle, and (2) signal splitting of both diastereotopic pseudoaxial hydrogens of the methylene bridges, indicative of the existence of two distinct portals of CB[8] (Figures S91, S92, S97, S98, S103, S104, S109, S110). A remarkable aspect of these assemblies is the pervasive splitting of all signals belonging to the tpy ligand directly connected to the Pt(II) centre (namely, H^3 to H^6 and $\text{H}^{3'}$ to $\text{H}^{6'}$) but not present in the head moiety (H^7 , H^8) or in any hydrogen of the spacer group. This effect is indicative of hindered rotation along the C(alkynyl)-Pt(II)-tpy axis. This property was not observed for free complexes **1** – **4**. Furthermore, signal splitting widens as the angle sharpens (e.g. 41 Hz and 3.5 Hz for assemblies **1**₂·CB[8]₂ and **3**₂·CB[8]₂ respectively). The trend can be fitted very precisely with an exponential decay described by $\Delta\delta \propto e^{-c(x-x_0)}$ where $\Delta\delta$ is the observed chemical shift change, x is the hinge angle or the distance between the two metal centres pertaining to the same molecule (see Computational Details), c is a constant, and x_0 is an arbitrary reference distance ($R^2 > 0.9996$; see **Figure S 115**). This effect is reminiscent of Bovey and Johnson's model that estimates the chemical shift shielding of a proton in a nearby ring current effect imposed by an aromatic π -electron density approaching perpendicularly.¹¹⁻¹³ The trend indicates that any pair of tpy protons experiencing this splitting pattern has two distinct orientations: one nucleus points toward the bulk solvent while its counterpart in the same tpy ligand points toward an aryl ring pertaining to the other tpy unit. This is a consequence of the short distance between both metal fragments stemming from the low hinge angle imposed by the bridging ligand.

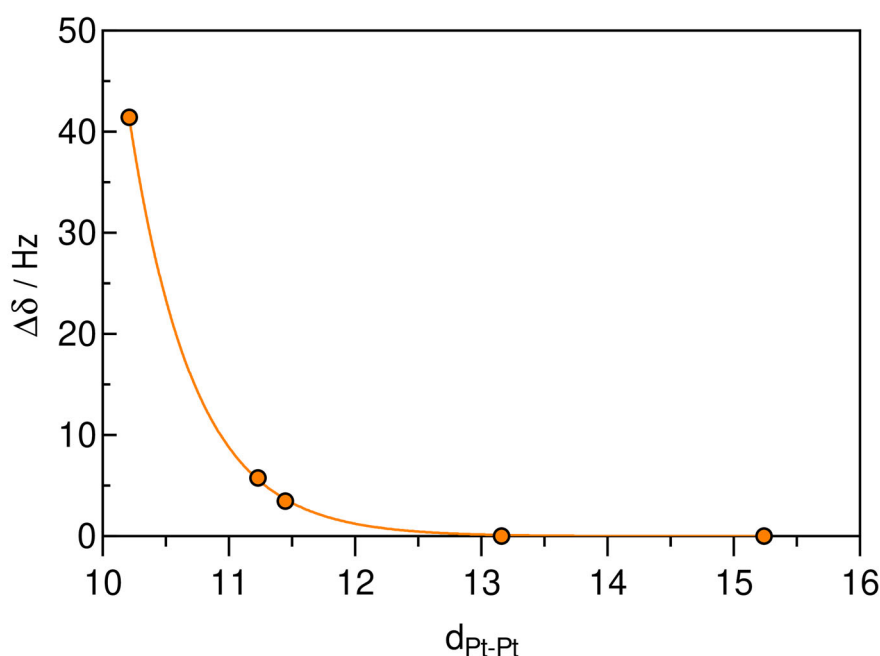


Figure S 115. Correlation between the chemical shift difference of two equal protons and the calculated intramolecular Pt-Pt distance according to an exponential decay fit of homoquaternary assemblies **1**₂·CB[8]₂ — **5**₂·CB[8]₂.

VT-NMR studies of homoquatarnary assemblies

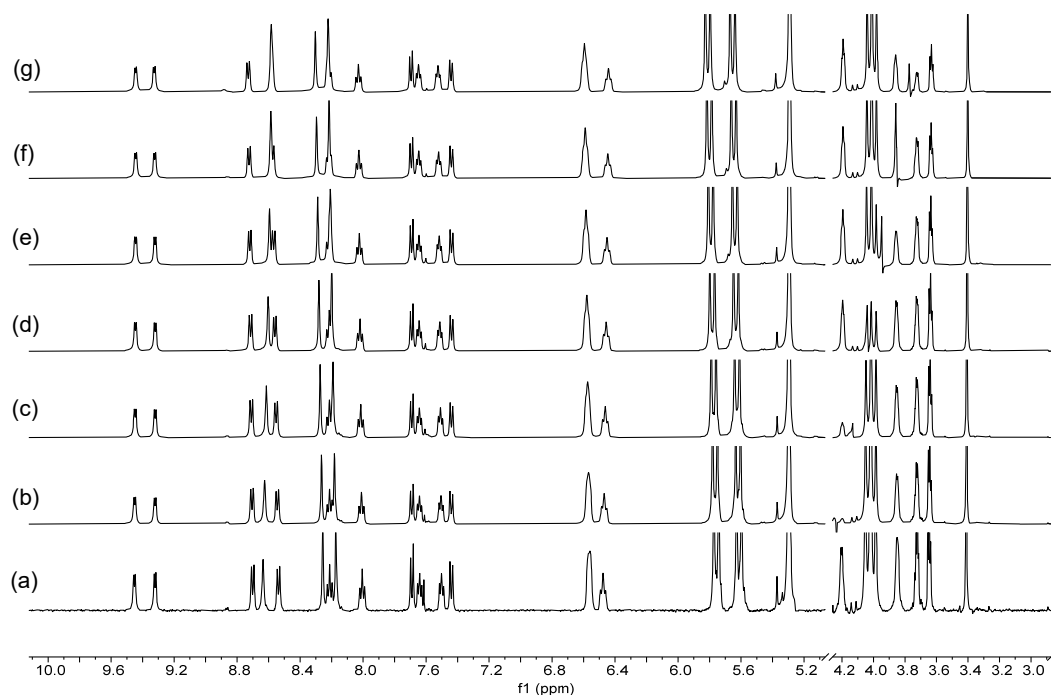


Figure S 116. Presaturated variable temperature ^1H -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectra of relevant signals of assembly 1_2-CB[8]_2 . (a) 25 °C; (b) 35 °C; (c) 45 °C; (d) 55 °C; (e) 65 °C; (f) 75 °C; (g) 85 °C.

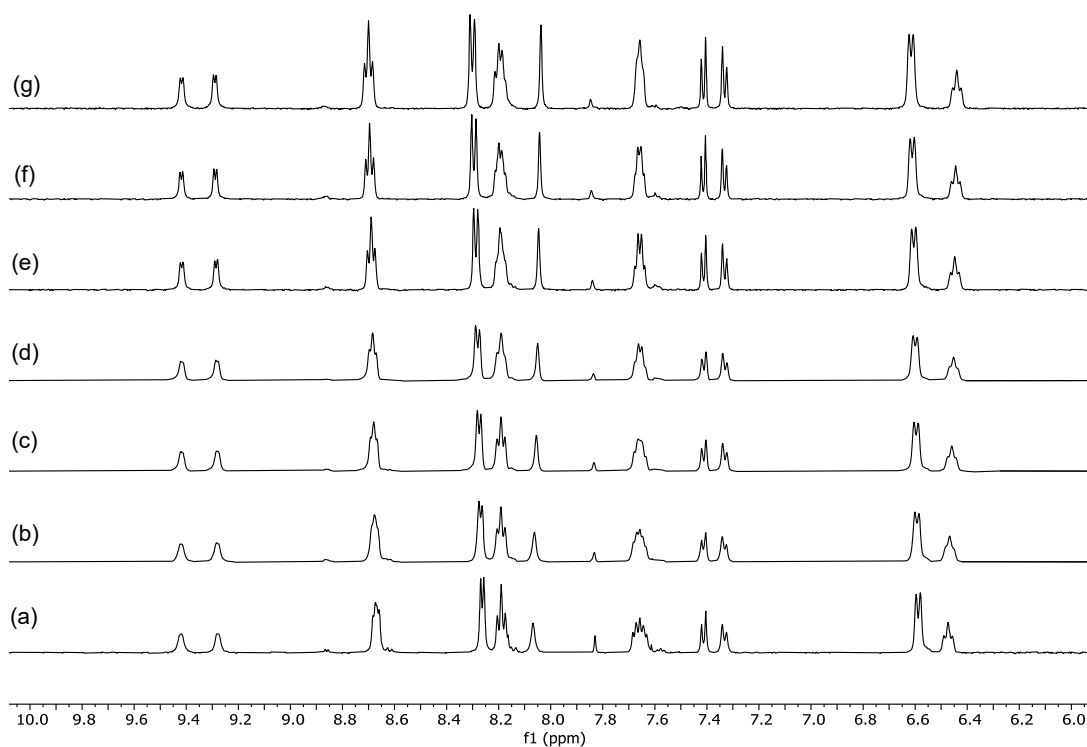


Figure S 117. Presaturated variable temperature ^1H -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectra of relevant signals of assembly 2_2-CB[8]_2 . (a) 25 °C; (b) 35 °C; (c) 45 °C; (d) 55 °C; (e) 65 °C; (f) 75 °C; (g) 85 °C.

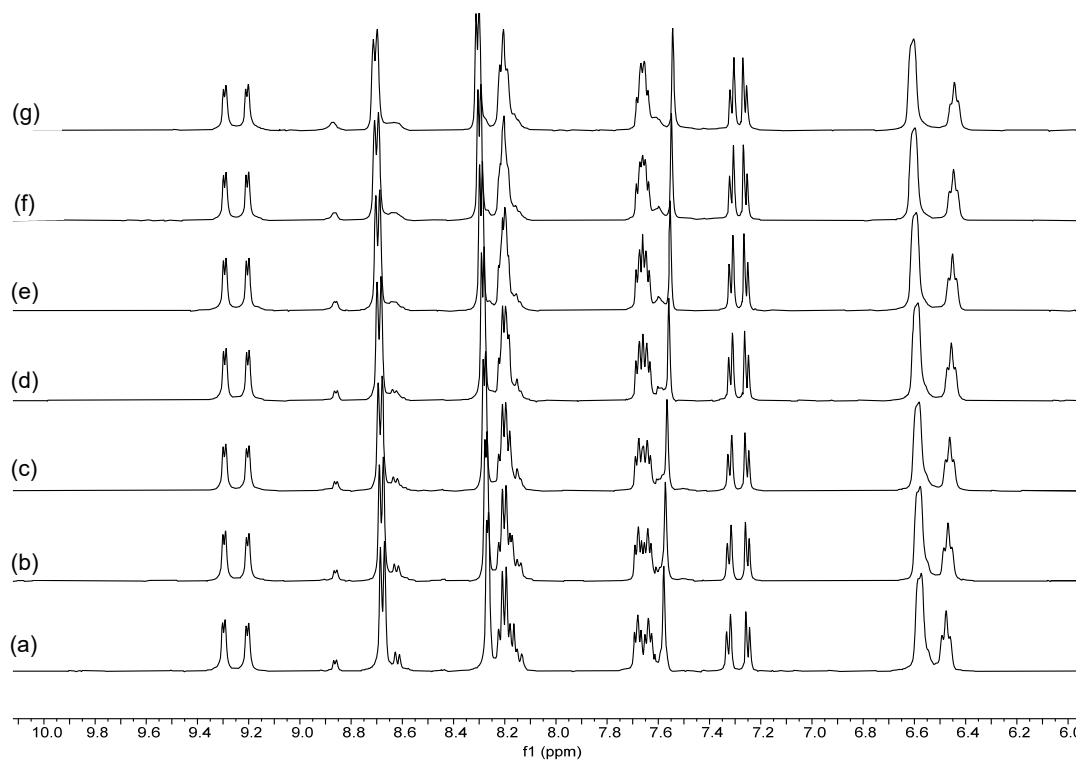


Figure S 118. Presaturated variable temperature ^1H -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectra of relevant signals of assembly $3_2\text{-CB}[8]_2$. (a) 25 °C; (b) 35 °C; (c) 45 °C; (d) 55 °C; (e) 65 °C; (f) 75 °C; (g) 85 °C.

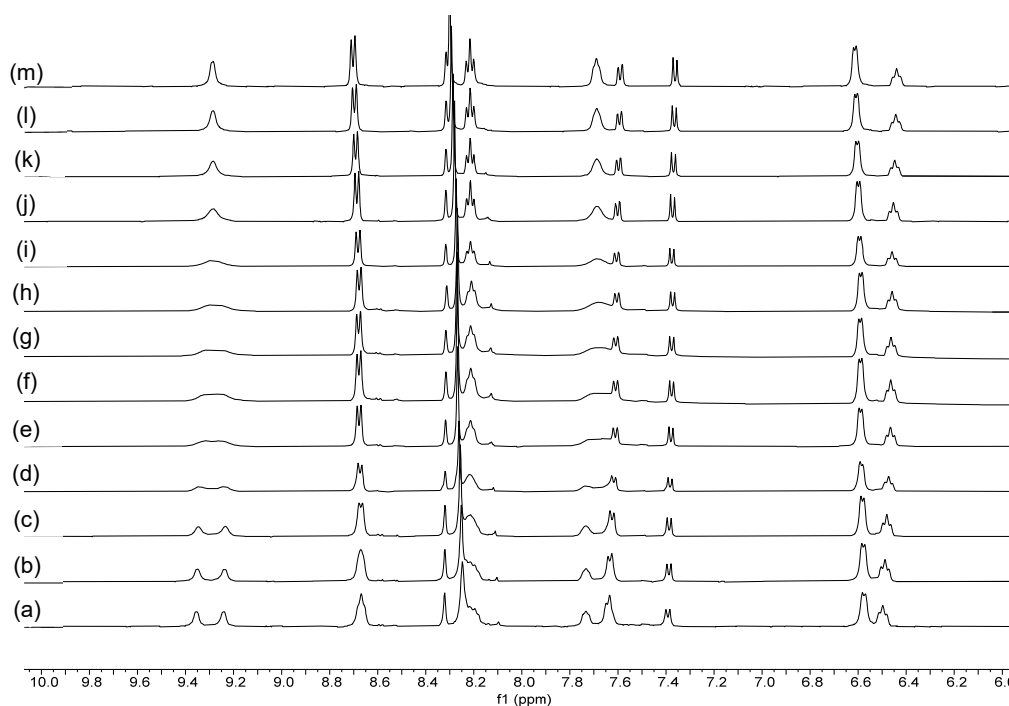


Figure S 119. Presaturated variable temperature ^1H -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectra of relevant signals of assembly $4_2\text{-CB}[8]_2$. (a) -5 °C; (b) 5 °C; (c) 15 °C; (d) 25 °C; (e) 35 °C; (f) 36 °C; (g) 38 °C; (h) 40 °C; (i) 45 °C; (j) 55 °C; (k) 65 °C; (l) 75 °C; (m) 85 °C.

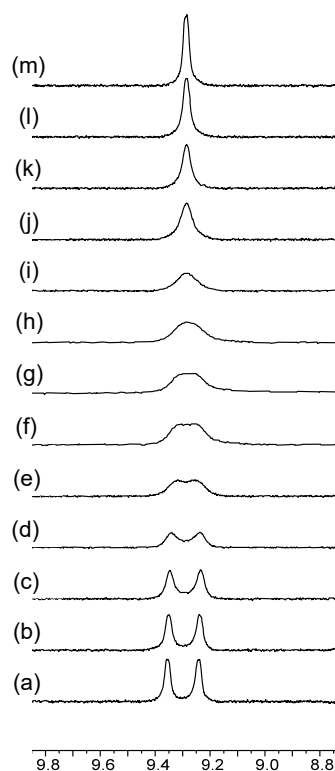


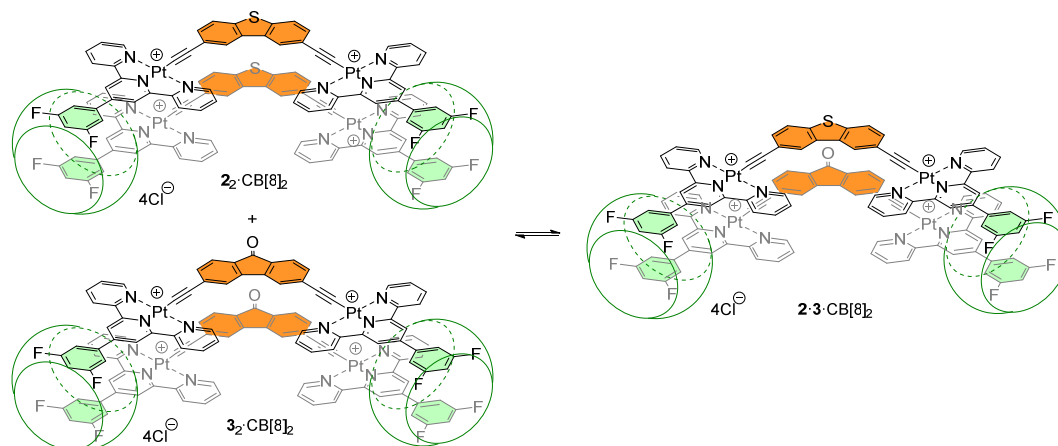
Figure S 120. Close-up of proton H⁶ from the presaturated variable temperature ¹H-NMR (500 MHz, D₂O/CD₃CN 2:1) spectra of assembly **4**₂·CB[8]₂. (a) -5 °C; (b) 5 °C; (c) 15 °C; (d) 25 °C; (e) 35 °C; (f) 36 °C; (g) 38 °C; (h) 40 °C; (i) 45 °C; (j) 55 °C; (k) 65 °C; (l) 75 °C; (m) 85 °C.

Temperature (VT) NMR experiments showed that the hindrance is strong for assemblies **1**₂·CB[8]₂ — **3**₂·CB[8]₂; the rotation barrier must be very high (> 18 kcal/mol),¹⁴ since no signal change was observed upon heating up to 85 °C (Figures S116-S118) suggesting almost negligible intracomplex motion. Conversely, assembly **4**₂·CB[8]₂, whose thioxanthone ligand has a 126° hinge angle (widest of the family), shows splitting signals that coalesce at 38 °C. The corresponding rotation barrier, obtained from the Eyring equation,¹⁵ is 15.5 kcal/mol and is attributed to hindered rotation along the C(alkynyl)-Pt(II)-tpy axis due to the presence of the carbonyl moiety (Figures S119-S120).

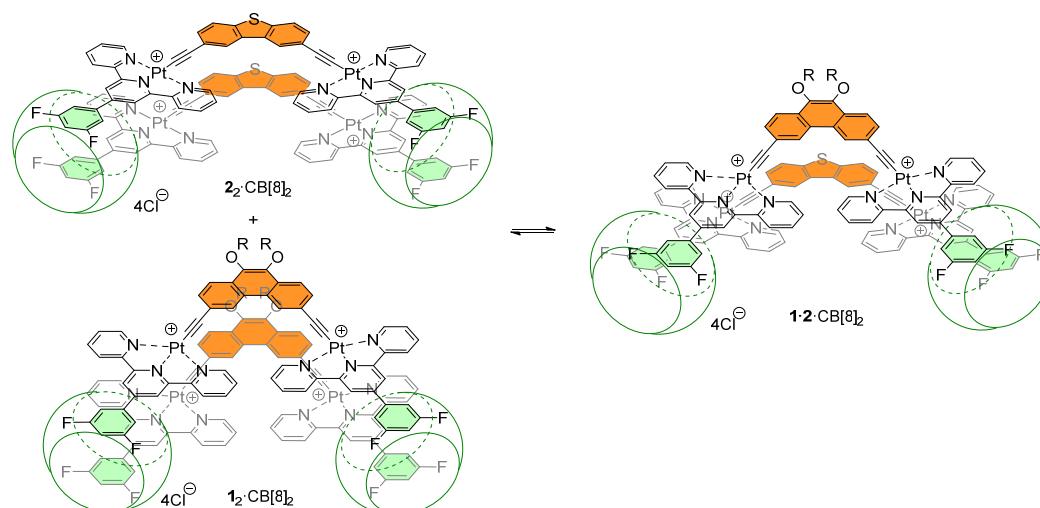
Self-sorting processes to form heteroquaternary assemblies

General method to obtain heteroquaternary assemblies mixtures

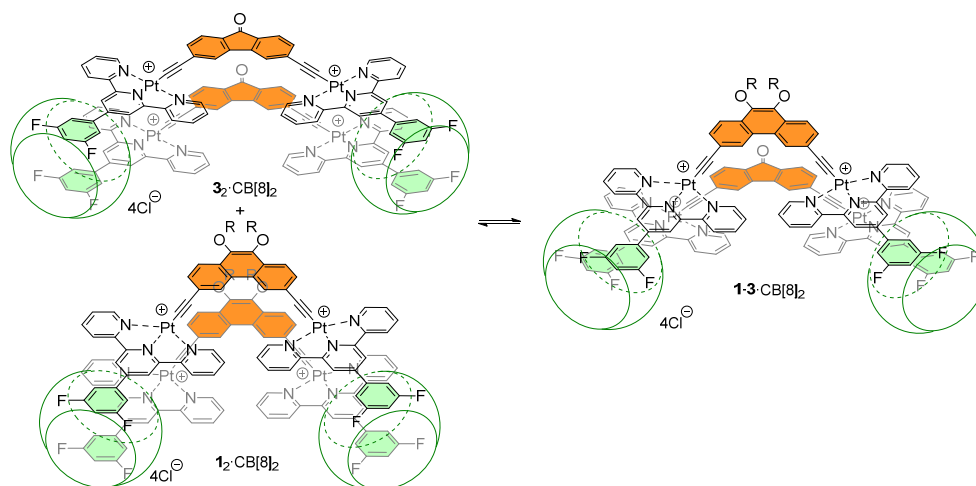
Freshly prepared homoquaternary assemblies $1_2 \cdot \text{CB}[8]_2 - 5_2 \cdot \text{CB}[8]_2$ (1.0 mM relative to Pt complex) in a 2:1 mixture of D_2O and CD_3CN were carefully combined in equal volumes (0.3 mL each, for a total of approximately 0.6 mL) in an NMR tube. The resulting solution was thoroughly shaken and sonicated for 10 minutes before being placed in a heating block set at 40 °C. The evolution of the self-sorting process was periodically checked by recording ^1H and ^{19}F -NMR spectra at intervals of 24 h. The process typically finishes after 72 h, however, all mixtures were monitored for 288 h (12 d) to make sure the system reached the thermodynamic equilibrium. No decomposition was observed within two weeks. The experiments were performed in triplicate. Peaks corresponding to heteroquaternary assemblies were assigned with the assistance of 2D NMR experiments. When needed, signal deconvolution was carried out with MNova built-in line fitting tool with default options using a generalized Lorentzian shape type.



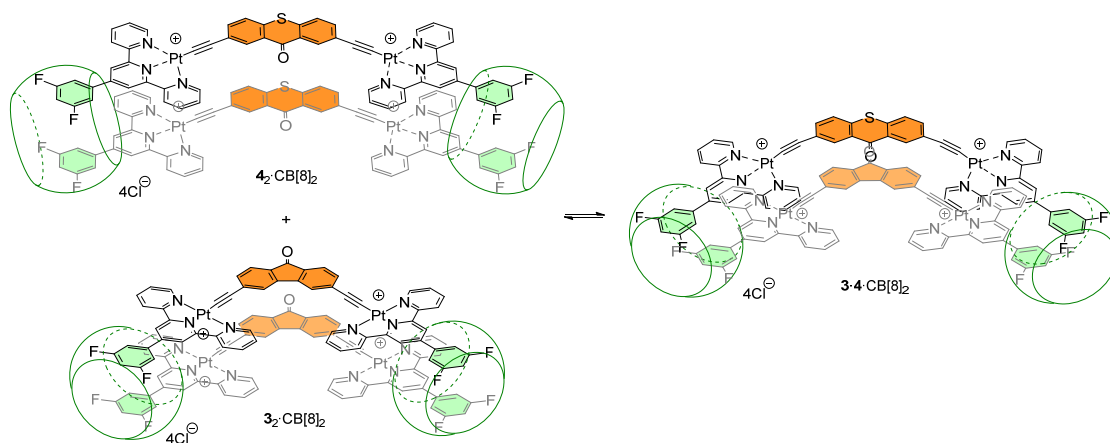
Scheme S 10. Self-sorting of assemblies $2_2 \cdot \text{CB}[8]_2$ and $3_2 \cdot \text{CB}[8]_2$ (angle mismatch of 6°; $d_{\text{Pt-Pt}}$ mismatch: 0.22 Å).



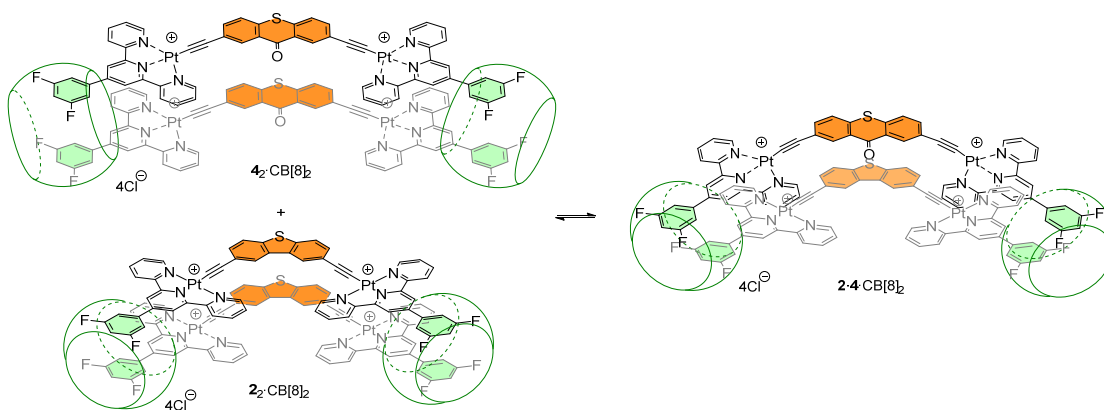
Scheme S 11. Self-sorting of assemblies $1_2 \cdot \text{CB}[8]_2$ and $2_2 \cdot \text{CB}[8]_2$ (angle mismatch of 15°; $d_{\text{Pt-Pt}}$ mismatch: 1.02 Å).



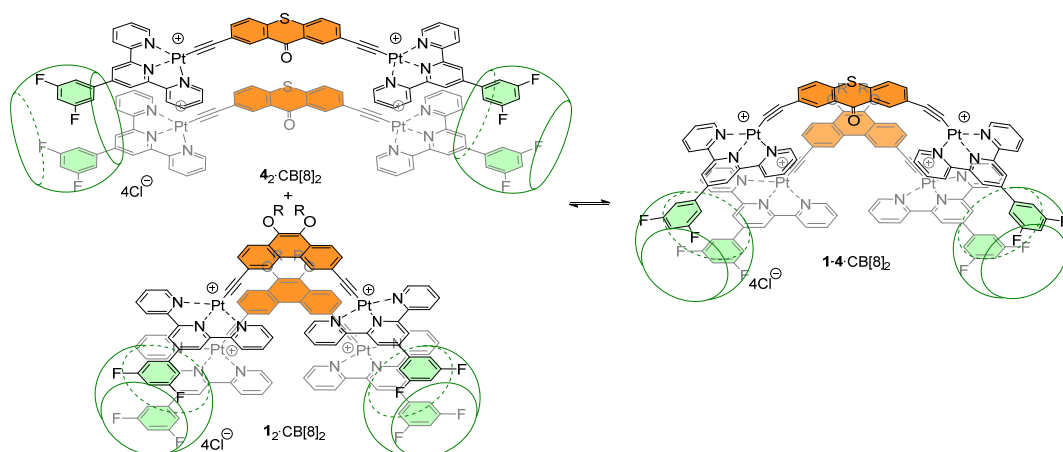
Scheme S 12. Self-sorting of assemblies $1_2 \cdot \text{CB}[8]_2$ and $3_2 \cdot \text{CB}[8]_2$ (angle mismatch of 21° ; $d_{\text{Pt-Pt}}$ mismatch: $1.24 \text{ \AA}$).



Scheme S 13. Self-sorting of assemblies $3_2 \cdot \text{CB}[8]_2$ and $4_2 \cdot \text{CB}[8]_2$ (angle mismatch of 43° ; $d_{\text{Pt-Pt}}$ mismatch: $3.79 \text{ \AA}$).



Scheme S 14. Self-sorting of assemblies $2_2 \cdot \text{CB}[8]_2$ and $4_2 \cdot \text{CB}[8]_2$ (angle mismatch of 49° ; $d_{\text{Pt-Pt}}$ mismatch: $4.01 \text{ \AA}$).



Scheme S 15. Self-sorting of assemblies $1_2\text{-CB}[8]_2$ and $4_2\text{-CB}[8]_2$ (angle mismatch of 64° ; $d_{\text{Pt-Pt}}$ mismatch: $5.03 \text{ \AA}$).

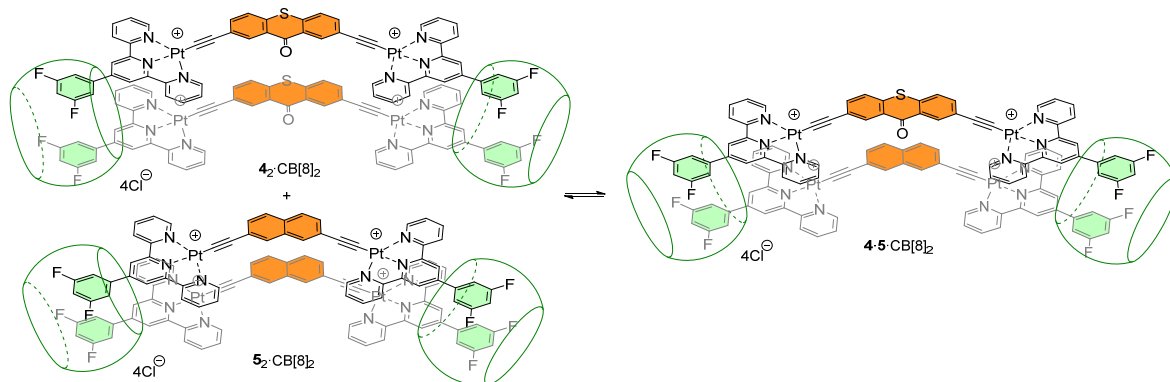


Figure S 121. Self-sorting of assemblies $4_2\text{-CB}[8]_2$ and $5_2\text{-CB}[8]_2$ (angle mismatch of 6° ; $d_{\text{Pt-Pt}}$ mismatch: $2.08 \text{ \AA}$).

NMR and HR-MS data of heteroquaternary assemblies mixtures

Mixture of assemblies $3_2 \cdot \text{CB}[8]_2$ and $2_2 \cdot \text{CB}[8]_2$ (angle mismatch of 6° ; $d_{\text{Pt-Pt}}$ mismatch: 0.22 Å).

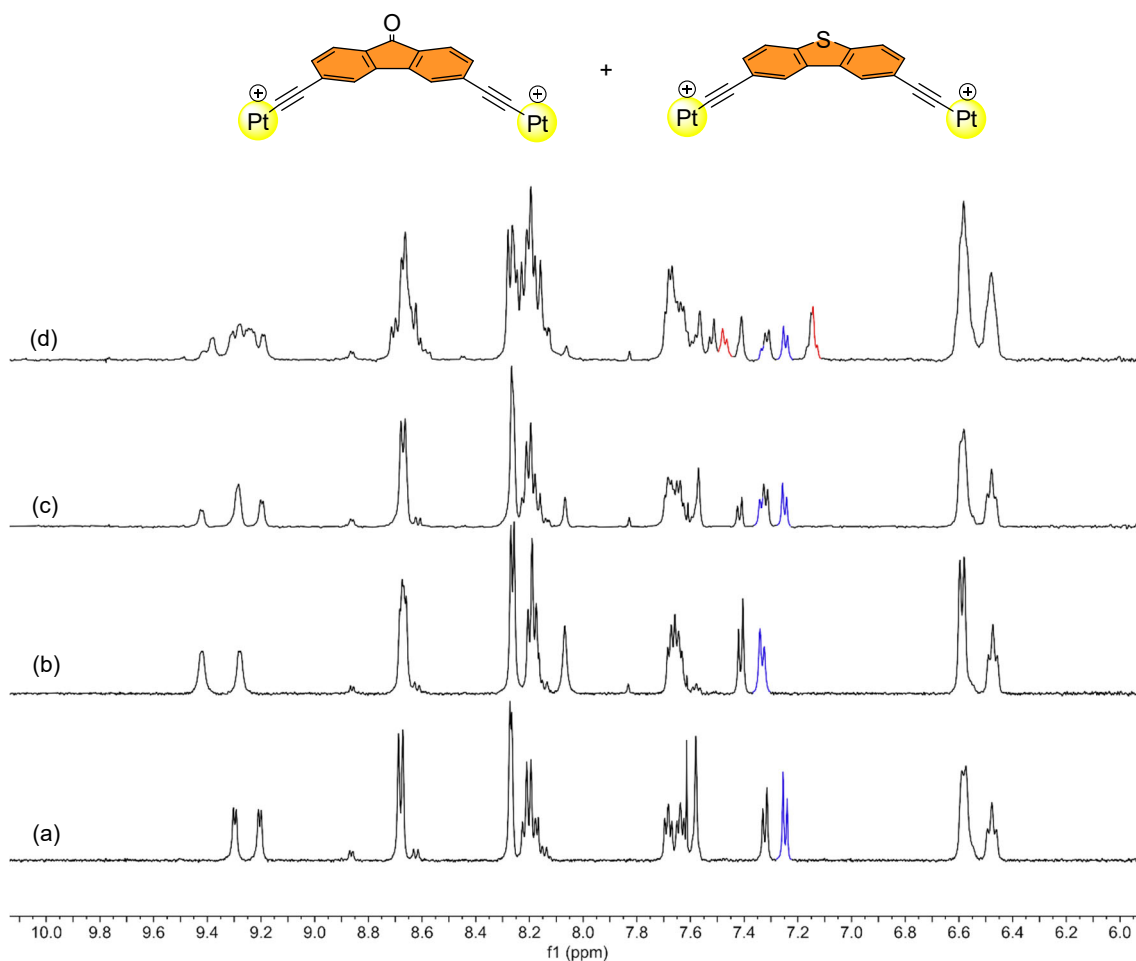


Figure S 122. Aromatic region of the ¹H-NMR (500 MHz, D₂O/CD₃CN 2:1) spectra of relevant signals of (a) assembly $3_2 \cdot \text{CB}[8]_2$, (b) assembly $2_2 \cdot \text{CB}[8]_2$, (c) their equimolar mixture at t = 0 and (d) their equimolar mixture at t = 288 h. Highlighted blue and red signals correspond to homoquaternary and heteroquaternary assemblies, respectively and were used for integration to estimate the binding free energy (see below).

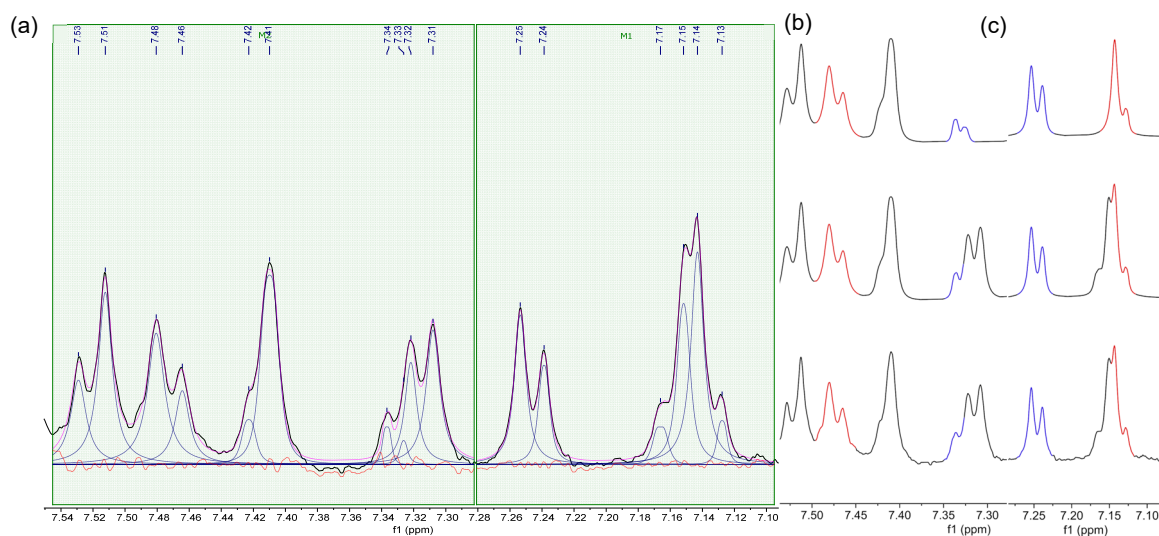


Figure S 123. (a) Deconvoluted ¹H-NMR (500 MHz, D₂O/CD₃CN 2:1) spectrum regions of the equimolar mixture of assemblies $3_2 \cdot \text{CB}[8]_2$ and $2_2 \cdot \text{CB}[8]_2$ at t = 288 h. (b and c) Comparison between the spectrum (bottom), fitted spectrum (middle) and fitted spectrum after signal subtraction (top) for integration purposes. Highlighted blue and red signals

correspond to homoquatarnary and heteroquatarnary assemblies, respectively and were used for integration to estimate the binding free energy (see below).

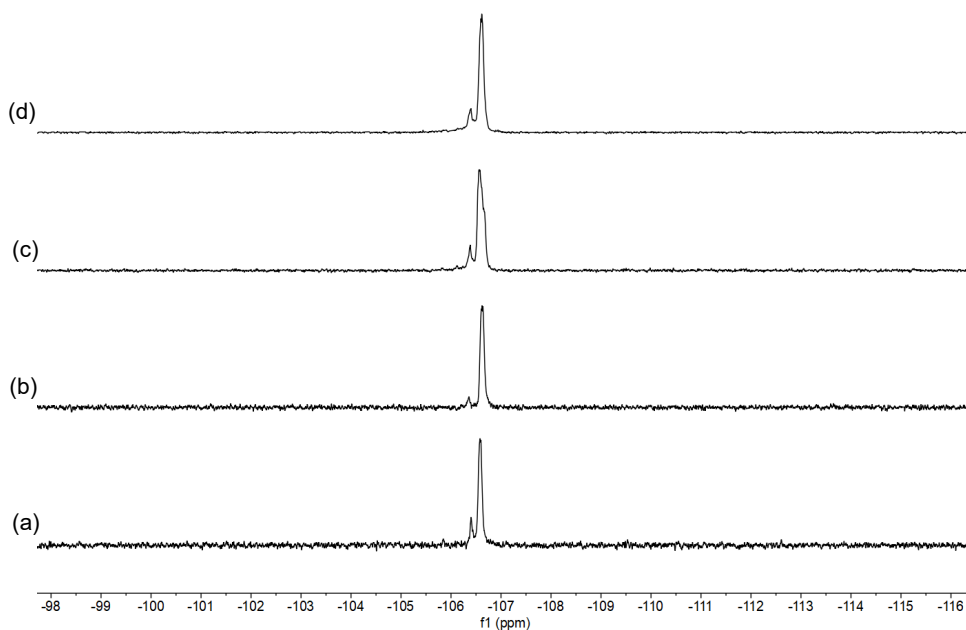


Figure S 124. ^{19}F -NMR (470 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectra of (a) assembly $3_2\cdot\text{CB}[8]_2$, (b) assembly $2_2\cdot\text{CB}[8]_2$, (c) their equimolar mixture at $t = 0$ and (d) their equimolar mixture at $t = 288$ h.

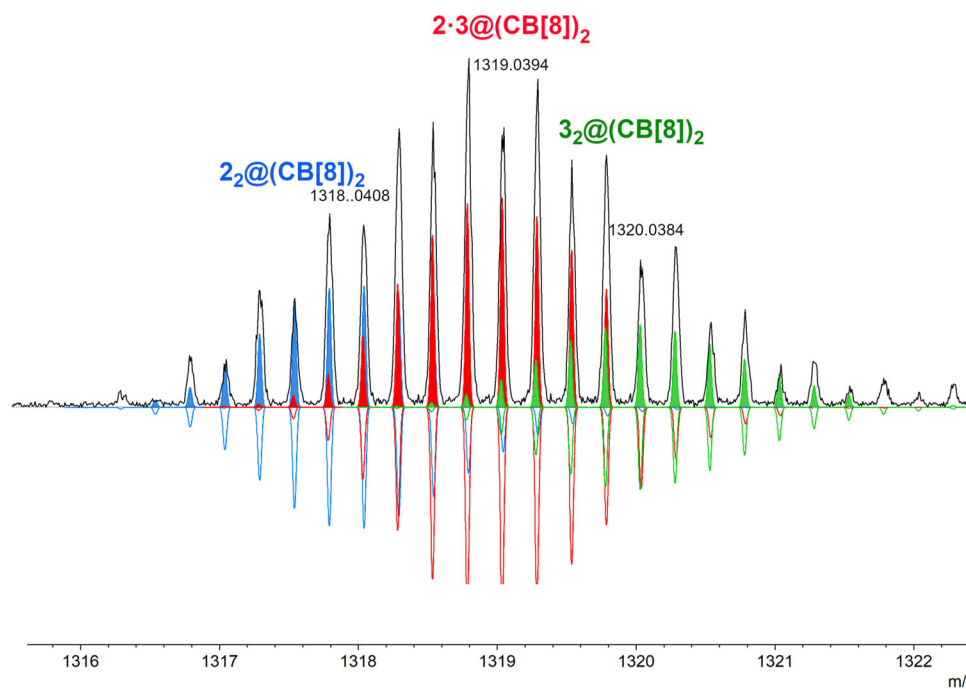


Figure S 125. HRMS (ESI-TOF-pos) of mixture of assemblies $2_2\cdot\text{CB}[8]_2$ and $3_2\cdot\text{CB}[8]_2$, $[\text{M}]^{4+}$. Calculated (below), measured (top).

HRMS hetero assembly $3_2\cdot 2_2\cdot\text{CB}[8]_2$ (ESI-TOF-pos): $m/z = 1319.0385$ $[\text{M}]^{4+}$ (calc. 1319.0347 for $\text{C}_{213}\text{H}_{160}\text{F}_8\text{N}_{76}\text{O}_{33}\text{Pt}_4\text{S}_1$).

Mixture of assemblies $2_2 \cdot \text{CB}[8]_2$ and $1_2 \cdot \text{CB}[8]_2$ (angle mismatch of 15° ; $d_{\text{Pt-Pt}}$ mismatch: 1.02 Å).

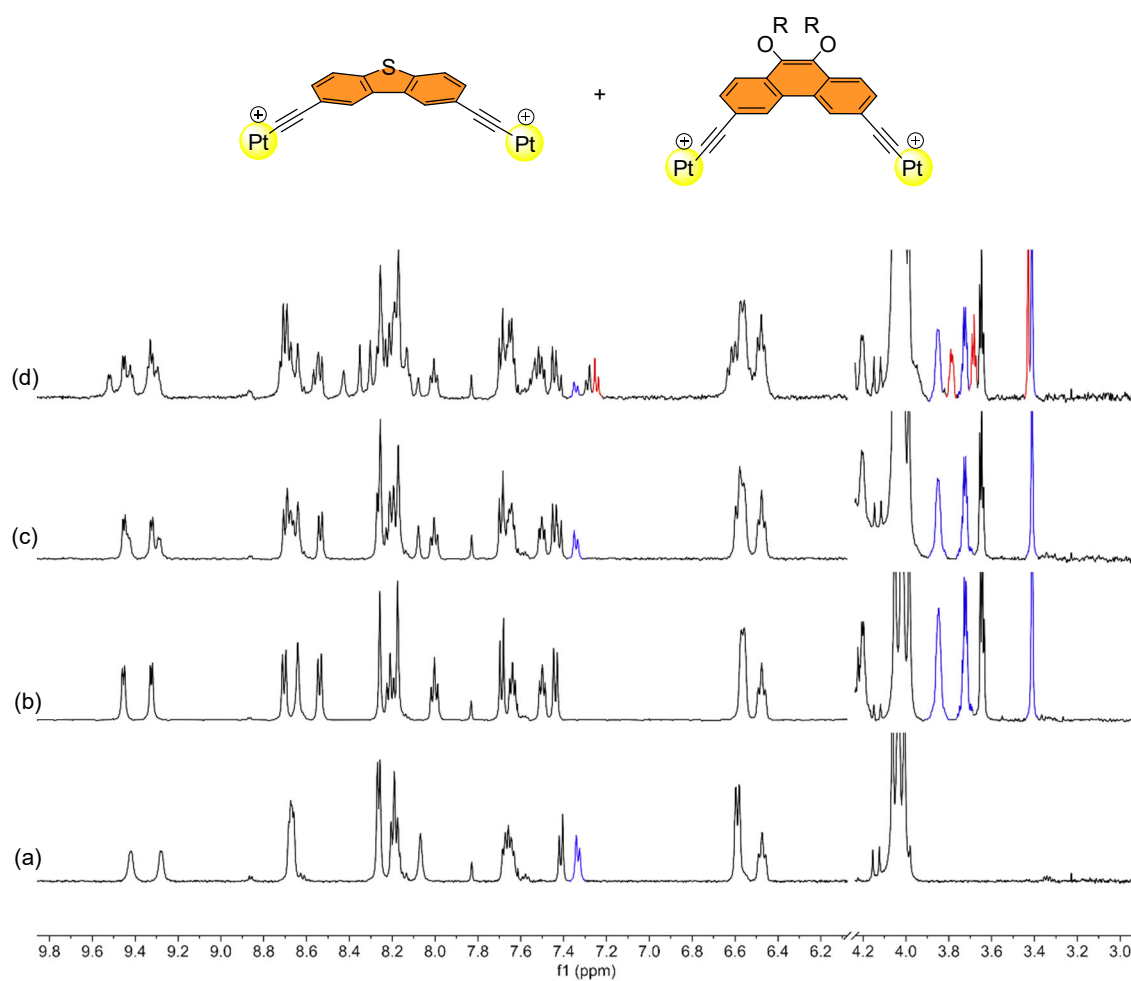


Figure S 126. ^1H -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectra of relevant signals of (a) assembly $2_2 \cdot \text{CB}[8]_2$, (b) assembly $1_2 \cdot \text{CB}[8]_2$, (c) their equimolar mixture at $t = 0$ and (d) their equimolar mixture at $t = 288$ h. Highlighted blue and red signals correspond to homoquaternary and heteroquaternary assemblies, respectively and were used for integration to estimate the binding free energy (see below).

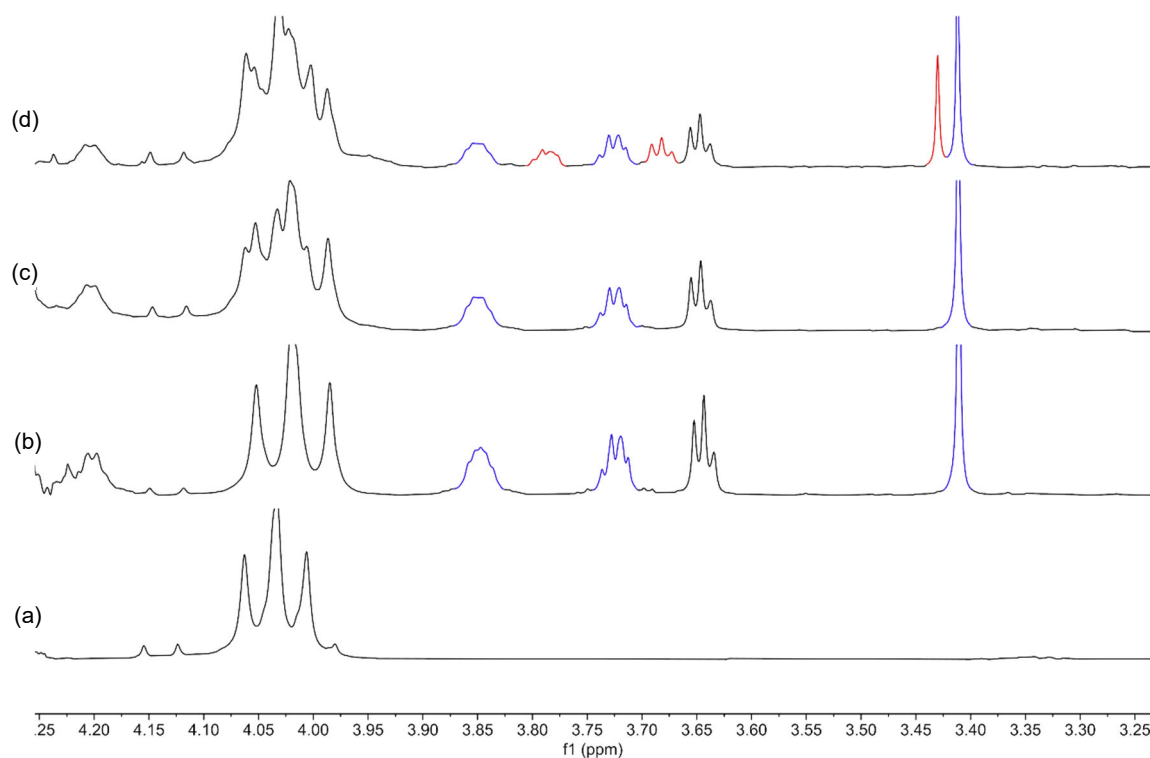


Figure S 127. Aliphatic region of ^1H -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectra of (a) assembly $2_2\cdot\text{CB}[8]_2$, (b) assembly $1_2\cdot\text{CB}[8]_2$, (c) their equimolar mixture at $t = 0$ and (d) their equimolar mixture at $t = 288$ h. Highlighted blue and red signals correspond to homoquaternary and heteroquaternary assemblies, respectively and were used for integration to estimate the binding free energy (see below).

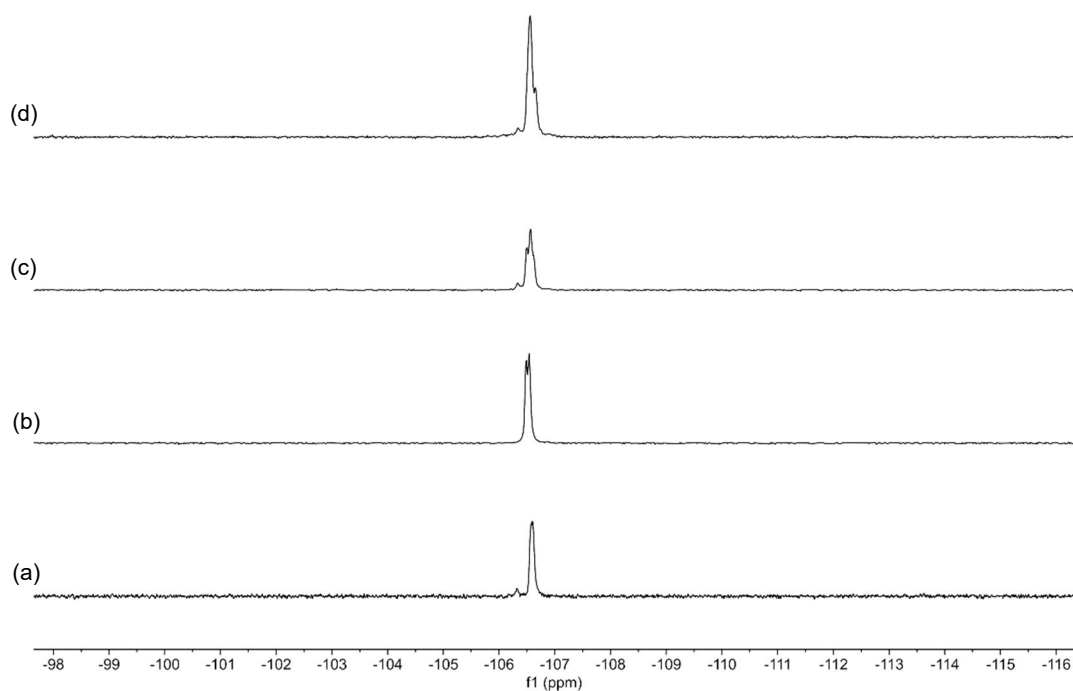


Figure S 128. ^{19}F -NMR (470 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectra of (a) assembly $2_2\cdot\text{CB}[8]_2$, (b) assembly $1_2\cdot\text{CB}[8]_2$, (c) their equimolar mixture at $t = 0$ and (d) their equimolar mixture at $t = 288$ h.

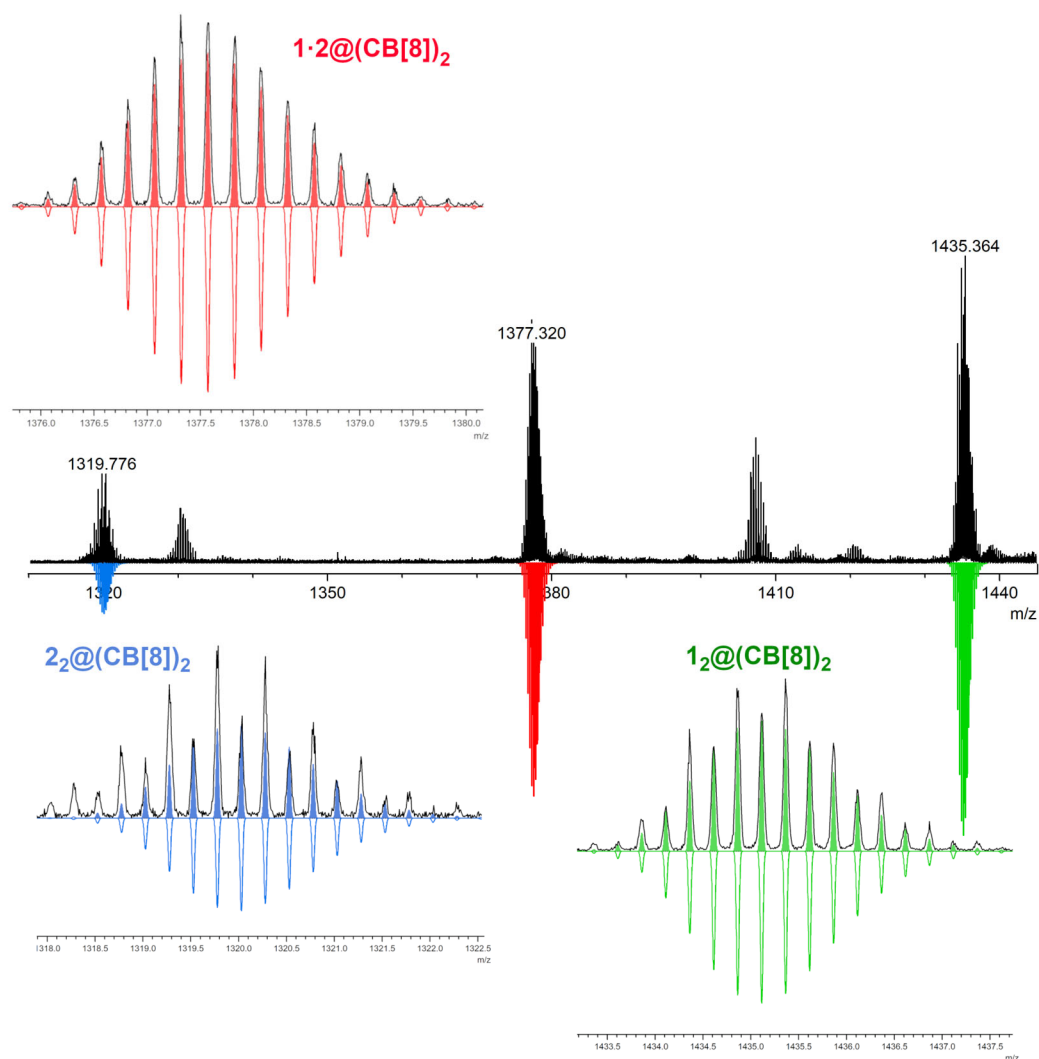


Figure S 129. HRMS (ESI-TOF-pos) of mixture of assemblies $1 \cdot \text{CB}[8]_2$ and $2 \cdot \text{CB}[8]_2$, $[\text{M}]^{4+}$. Calculated (below), measured (top).

HRMS of hetero assembly $2 \cdot 1 \cdot \text{CB}[8]_2$ (ESI-TOF-pos): $m/z = 1377.5703$ $[\text{M}]^{4+}$ (calc. 1377.5715 for $\text{C}_{224}\text{H}_{182}\text{F}_8\text{N}_{76}\text{O}_{38}\text{Pt}_4\text{S}_1$).

Mixture of assemblies $3_2 \cdot \text{CB}[8]_2$ and $1_2 \cdot \text{CB}[8]_2$ (angle mismatch of 21° ; $d_{\text{Pt-Pt}}$ mismatch: 1.24 Å).

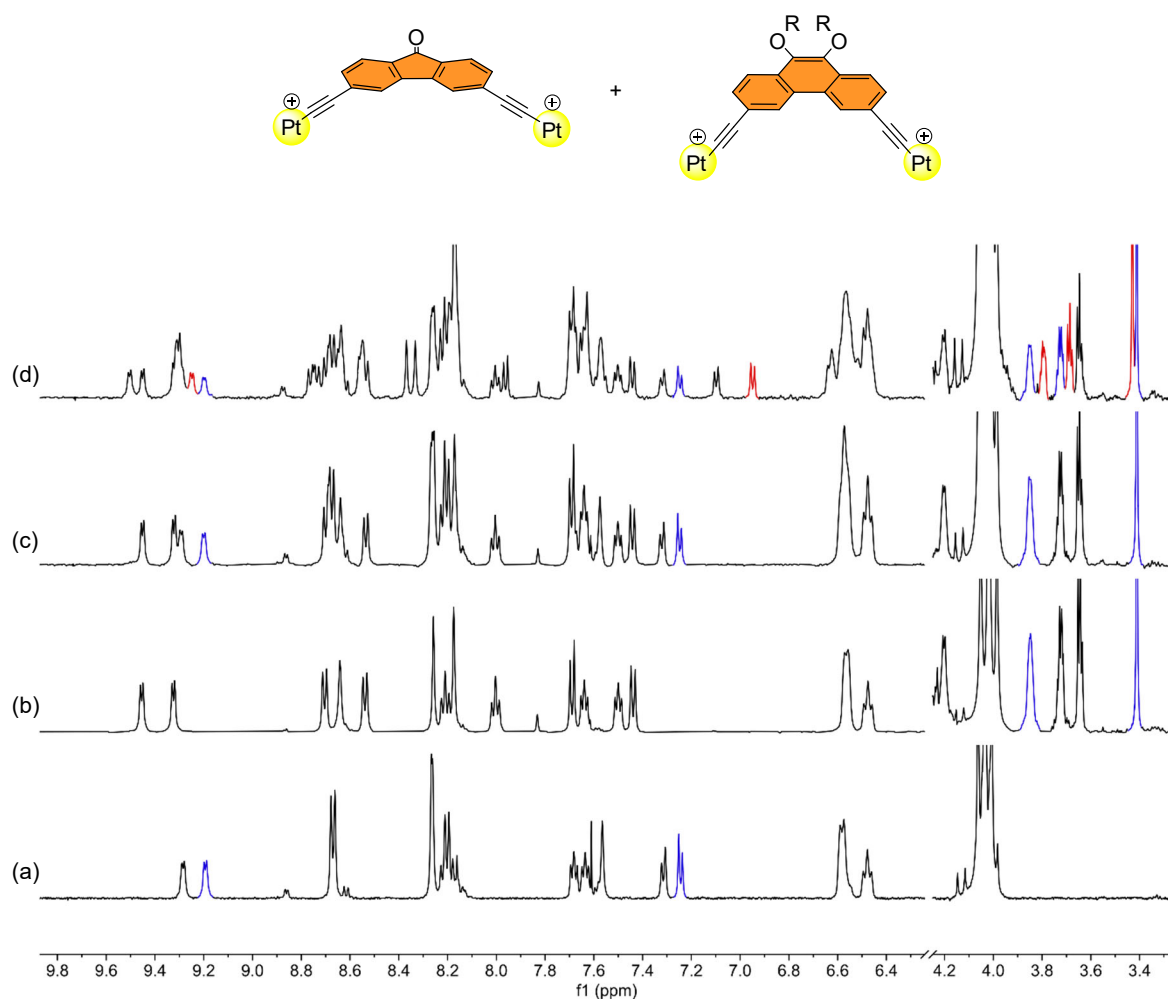


Figure S 130. ^1H -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectra of relevant signals of (a) assembly $3_2 \cdot \text{CB}[8]_2$, (b) assembly $1_2 \cdot \text{CB}[8]_2$, (c) their equimolar mixture at $t = 0$ and (d) their equimolar mixture at $t = 288$ h. Highlighted blue and red signals correspond to homoquaternary and heteroquaternary assemblies, respectively and were used for integration to estimate the binding free energy (see below).

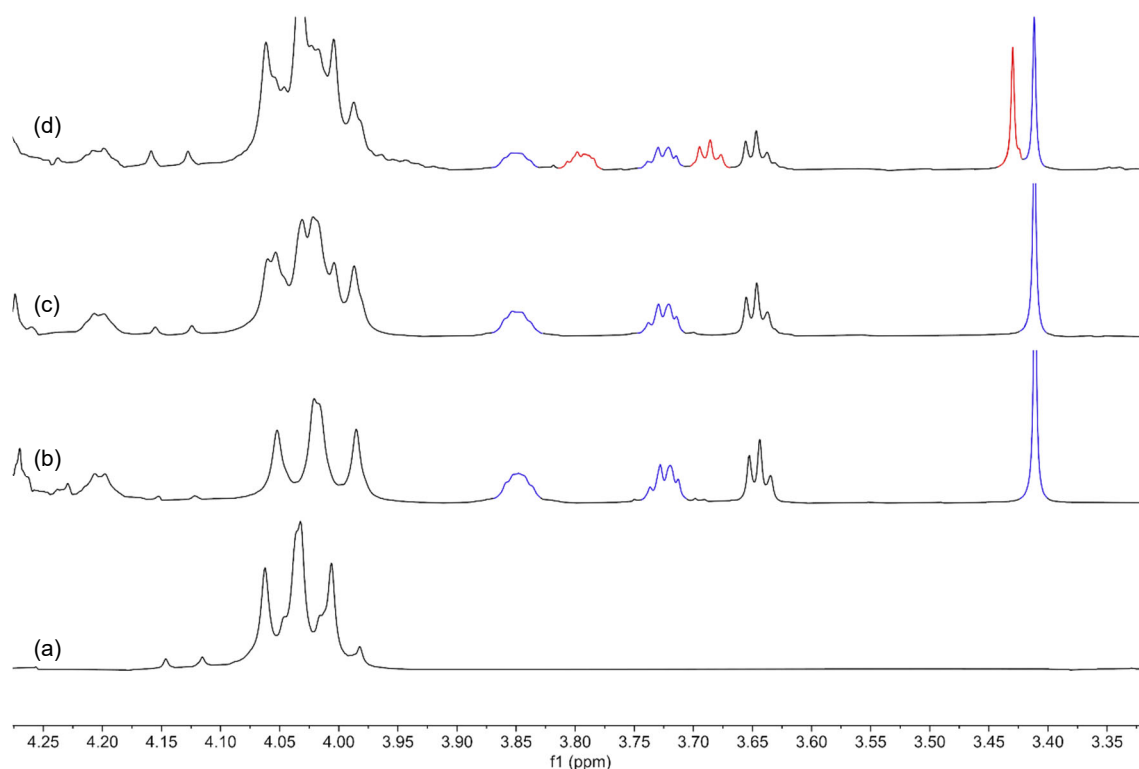


Figure S 131. Aliphatic region of ^1H -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectra of (a) assembly $3_2\cdot\text{CB}[8]_2$, (b) assembly $1_2\cdot\text{CB}[8]_2$, (c) their equimolar mixture at $t = 0$ and (d) their equimolar mixture at $t = 288$ h. Highlighted blue and red signals correspond to homoquaternary and heteroquaternary assemblies, respectively and were used for integration to estimate the binding free energy (see below).

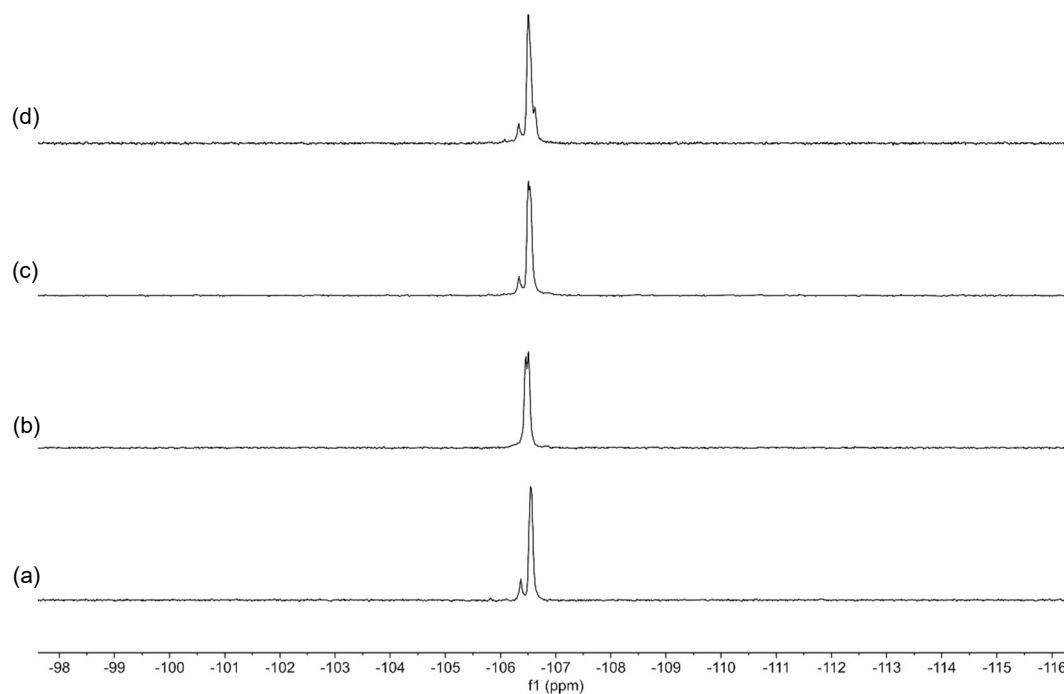


Figure S 132. ^{19}F -NMR (470 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectra of (a) assembly $3_2\cdot\text{CB}[8]_2$, (b) assembly $1_2\cdot\text{CB}[8]_2$, (c) their equimolar mixture at $t = 0$ and (d) their equimolar mixture at $t = 288$ h.

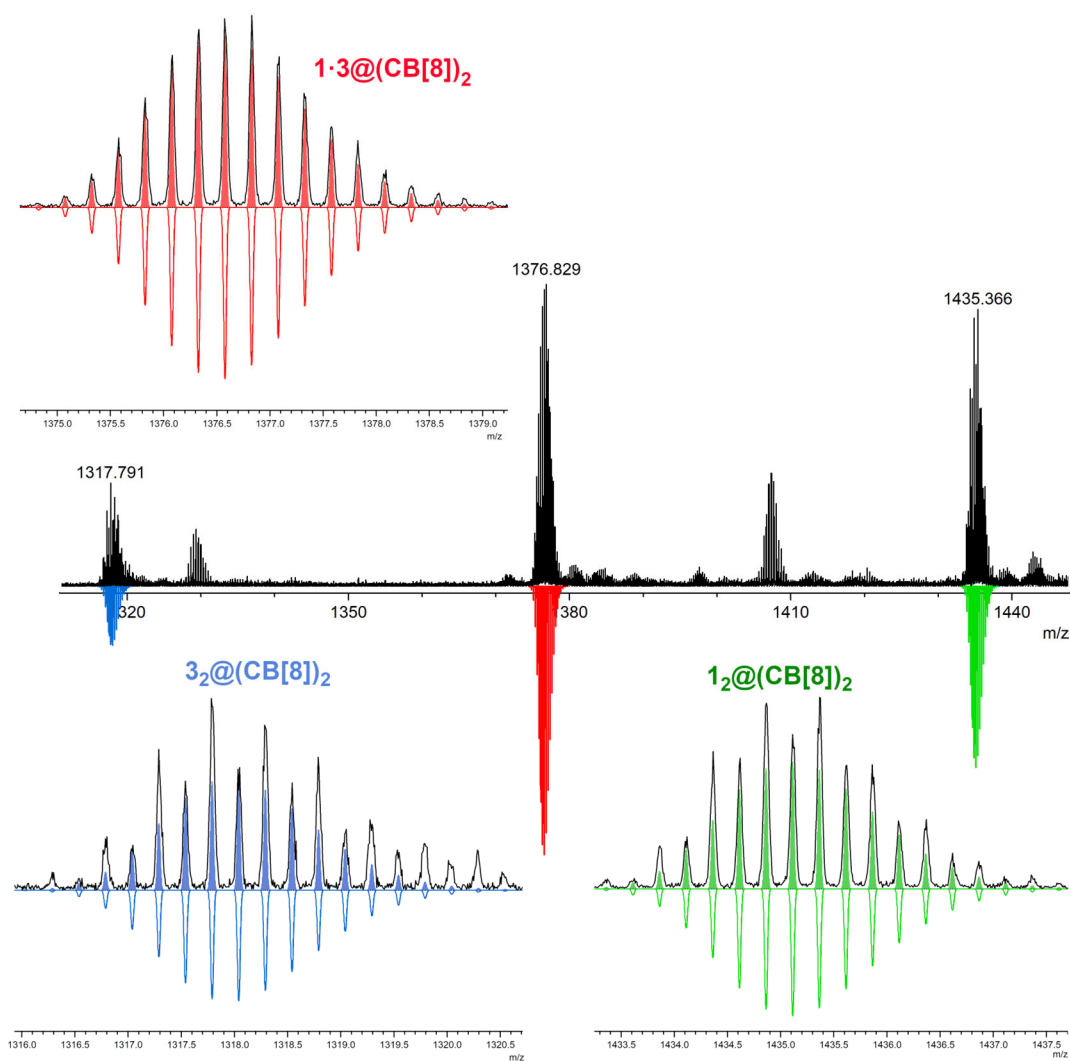


Figure S 133. HRMS (ESI-TOF-pos) of Mixture of assemblies $1_2\text{-CB}[8]_2$ and $3_2\text{-CB}[8]_2$, $[\text{M}]^{4+}$. Calculated (below), measured (top).

HRMS of hetero assembly $3_2\text{-CB}[8]_2$ (ESI-TOF-pos): $m/z = 1376.5761$ $[\text{M}]^{4+}$ (calc. 1376.5773 for $\text{C}_{225}\text{H}_{182}\text{F}_8\text{N}_{76}\text{O}_{39}\text{Pt}_4$).

Mixture of assemblies $4_2 \cdot \text{CB}[8]_2$ and $3_2 \cdot \text{CB}[8]_2$ (angle mismatch of 43° ; $d_{\text{Pt-Pt}}$ mismatch: 3.79 Å).

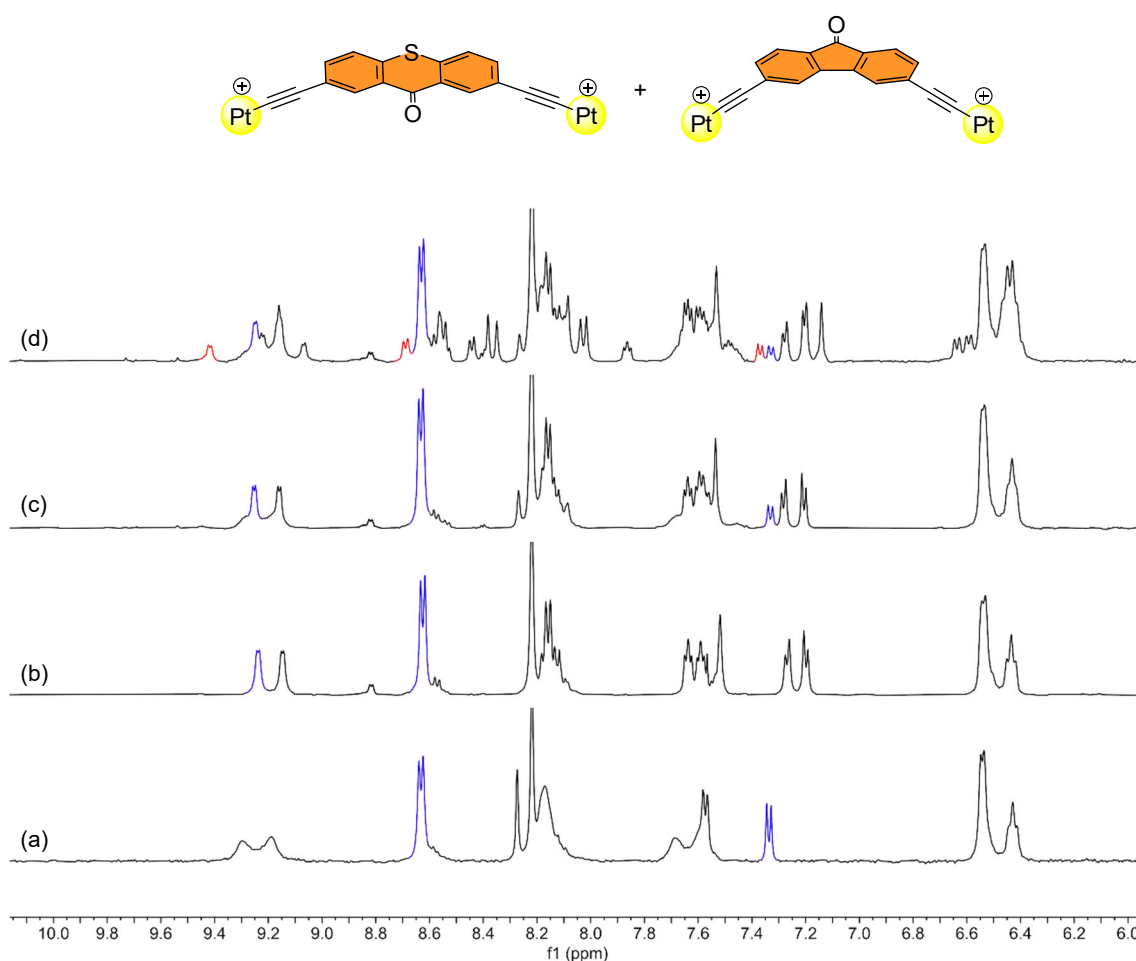


Figure S 134. ¹H-NMR (500 MHz, D₂O/CD₃CN 2:1) spectra of relevant signals of (a) assembly $4_2 \cdot \text{CB}[8]_2$, (b) assembly $3_2 \cdot \text{CB}[8]_2$, (c) their equimolar mixture at t = 0 and (d) their equimolar mixture at t = 288 h. Highlighted blue and red signals correspond to homoquaternary and heteroquaternary assemblies, respectively and were used for integration to estimate the binding free energy (see below).

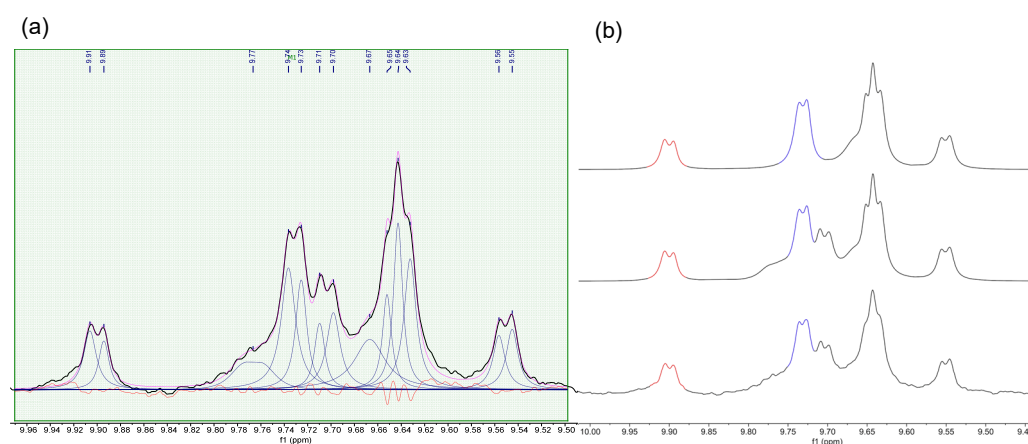


Figure S 135. (a) Deconvoluted ¹H-NMR (500 MHz, D₂O/CD₃CN 2:1) spectrum region of the equimolar mixture of assemblies $4_2 \cdot \text{CB}[8]_2$ and $3_2 \cdot \text{CB}[8]_2$ at t = 288 h. (b) Comparison between the spectrum (bottom), fitted spectrum (middle) and fitted spectrum after signal subtraction (top) for integration purposes. Highlighted blue and red signals correspond to homoquaternary and heteroquaternary assemblies, respectively and were used for integration to estimate the binding free energy (see below).

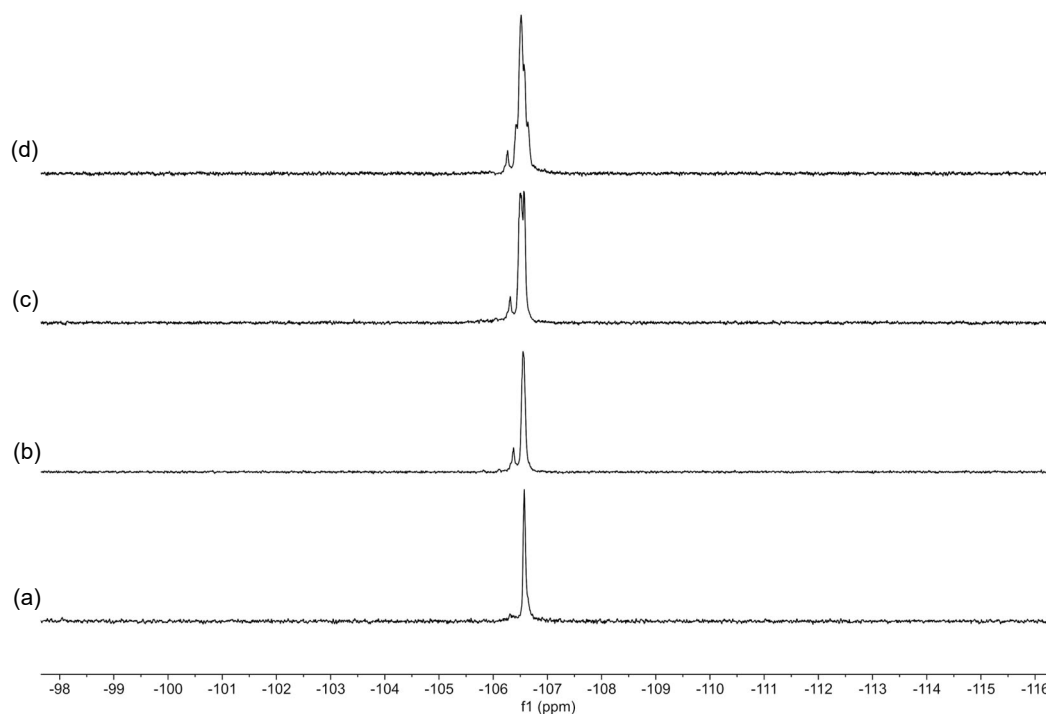


Figure S 136. ^{19}F -NMR (470 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectra of (a) assembly $4_2\text{-CB}[8]_2$, (b) assembly $3_2\text{-CB}[8]_2$, (c) their equimolar mixture at $t = 0$ and (d) their equimolar mixture at $t = 288$ h.

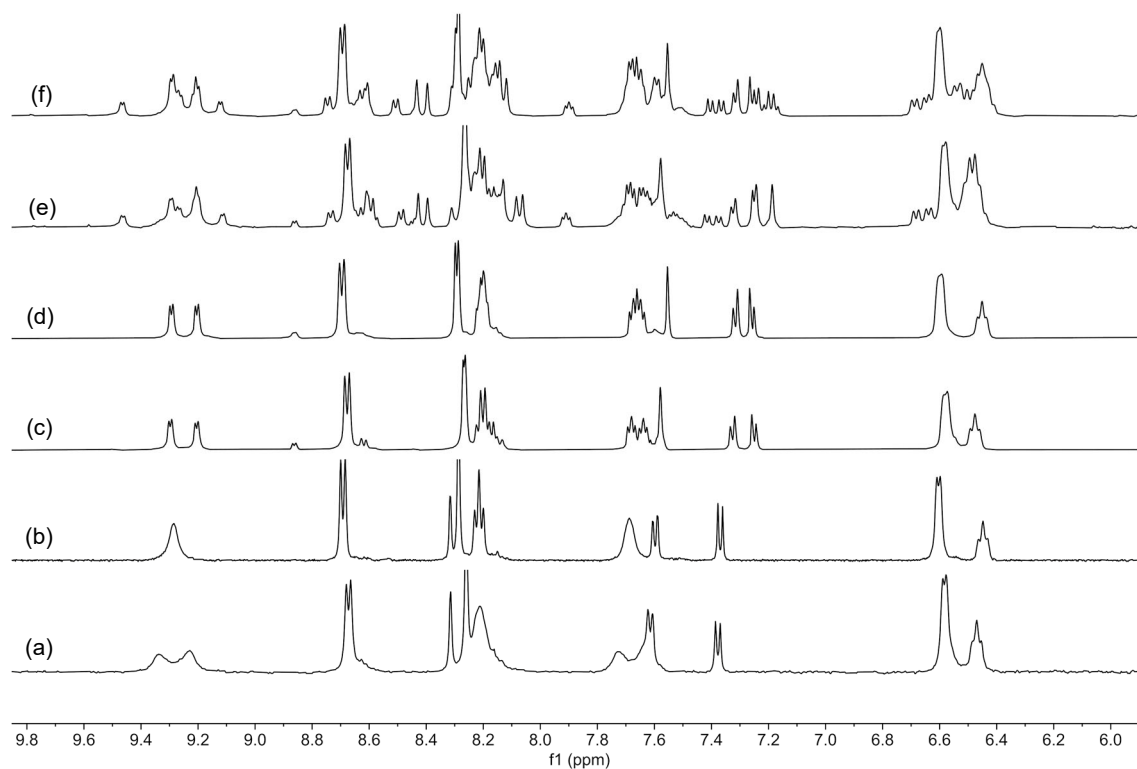


Figure S 137. ^1H -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectra of relevant signals of (a) assembly $4_2\text{-CB}[8]_2$, (b) assembly $4_2\text{-CB}[8]_2$ at 65°C , (c) assembly $3_2\text{-CB}[8]_2$, (d) assembly $3_2\text{-CB}[8]_2$ at 65°C , (e) their equimolar mixture at $t = 288$ h and (f) their equimolar mixture at $t = 288$ h and 65°C .

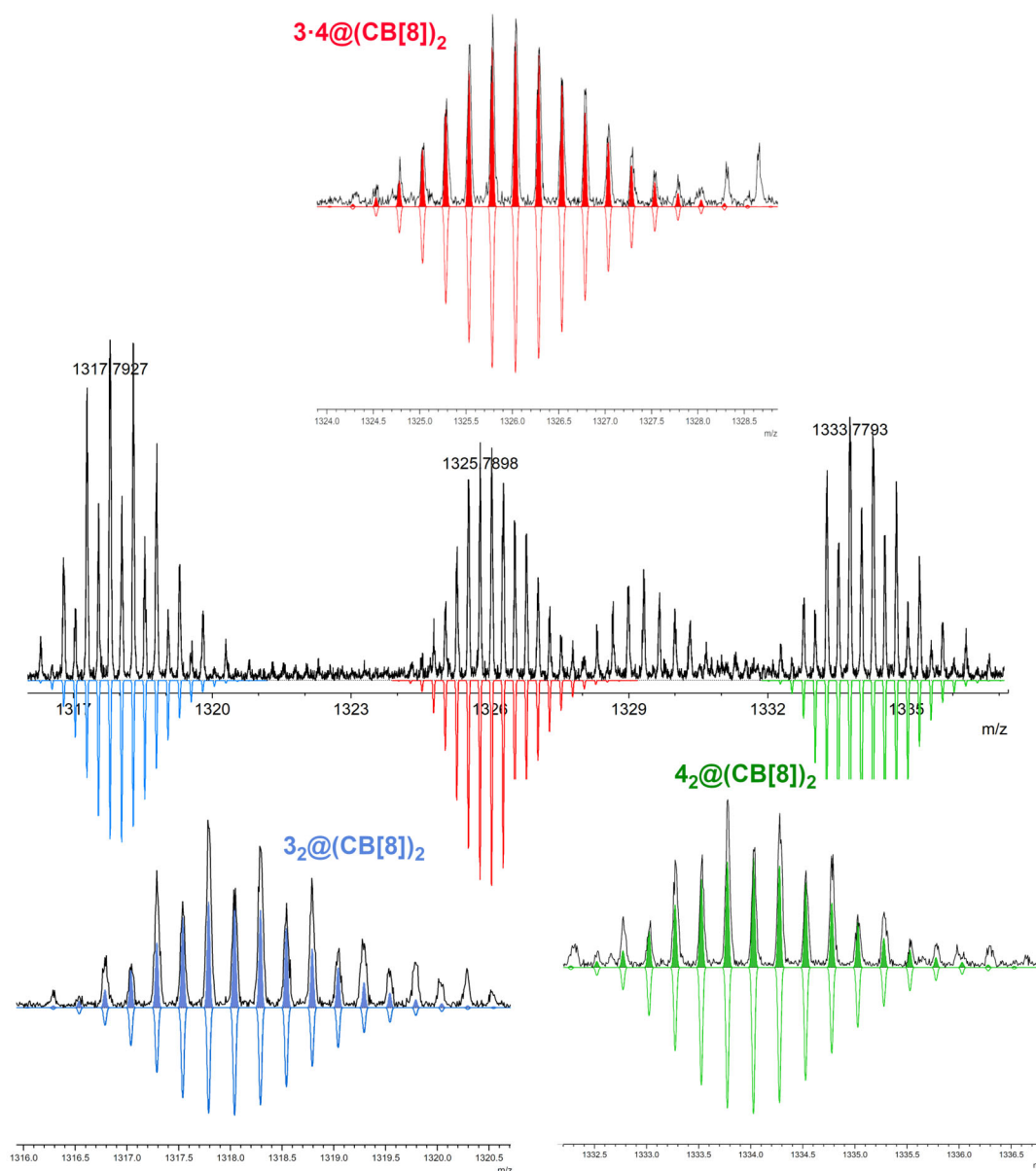


Figure S 138. HRMS (ESI-TOF-pos) of Mixture of assemblies $3_2@CB[8]_2$ and $4_2@CB[8]_2$, $[M]^{4+}$. Calculated (below), measured (top).

HRMS of hetero assembly $4 \cdot 3@CB[8]_2$ (ESI-TOF-pos): $m/z = 1326.0379$ $[M]^{4+}$ (calc. 1326.0335 for $C_{214}H_{160}F_8N_{76}O_{34}Pt_4S_1$).

Mixture of assemblies $4_2 \cdot \text{CB}[8]_2$ and $2_2 \cdot \text{CB}[8]_2$ (angle mismatch of 49° ; $d_{\text{Pt-Pt}}$ mismatch: 4.01 Å).

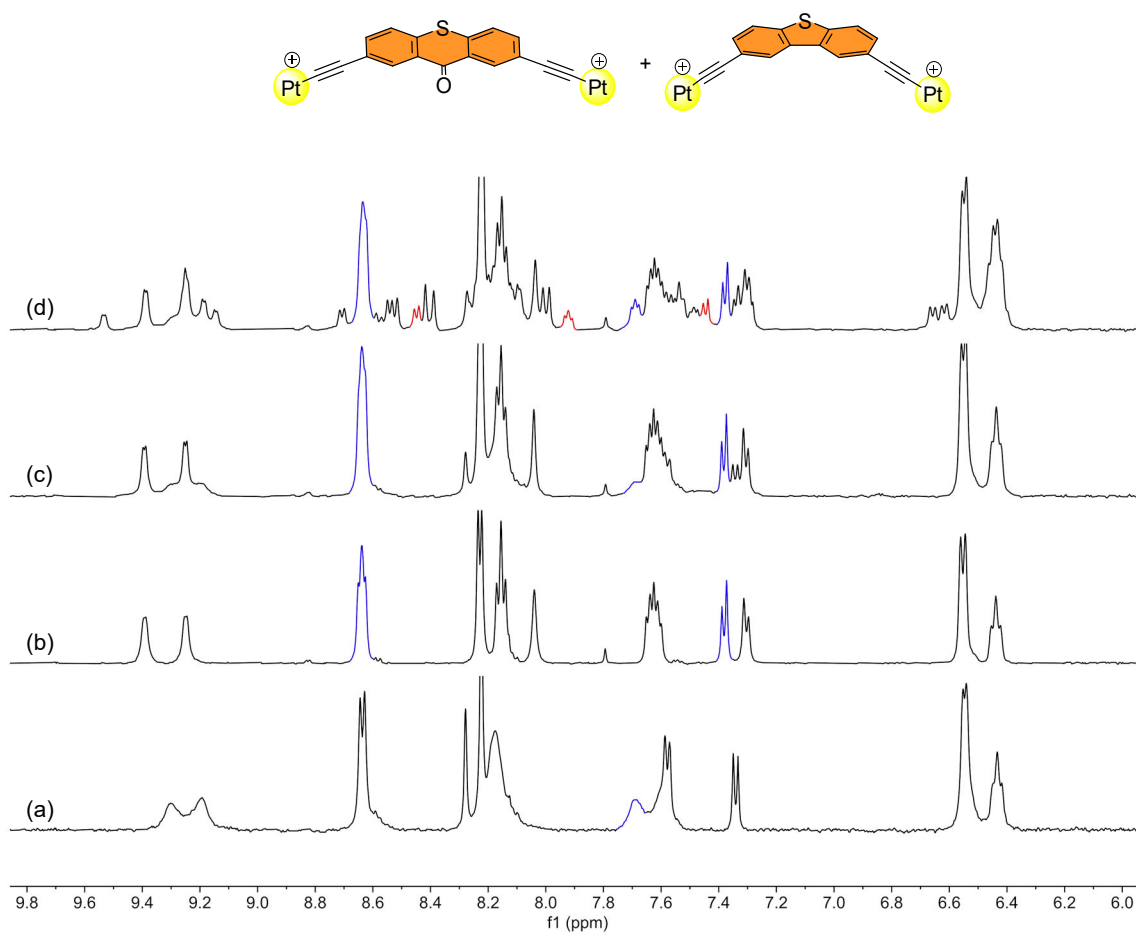


Figure S 139. ^1H -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectra of relevant signals of (a) assembly $4_2 \cdot \text{CB}[8]_2$, (b) assembly $2_2 \cdot \text{CB}[8]_2$, (c) their equimolar mixture at $t = 0$ and (d) their equimolar mixture at $t = 288$ h. Highlighted blue and red signals correspond to homoquaternary and heteroquaternary assemblies, respectively and were used for integration to estimate the binding free energy (see below).

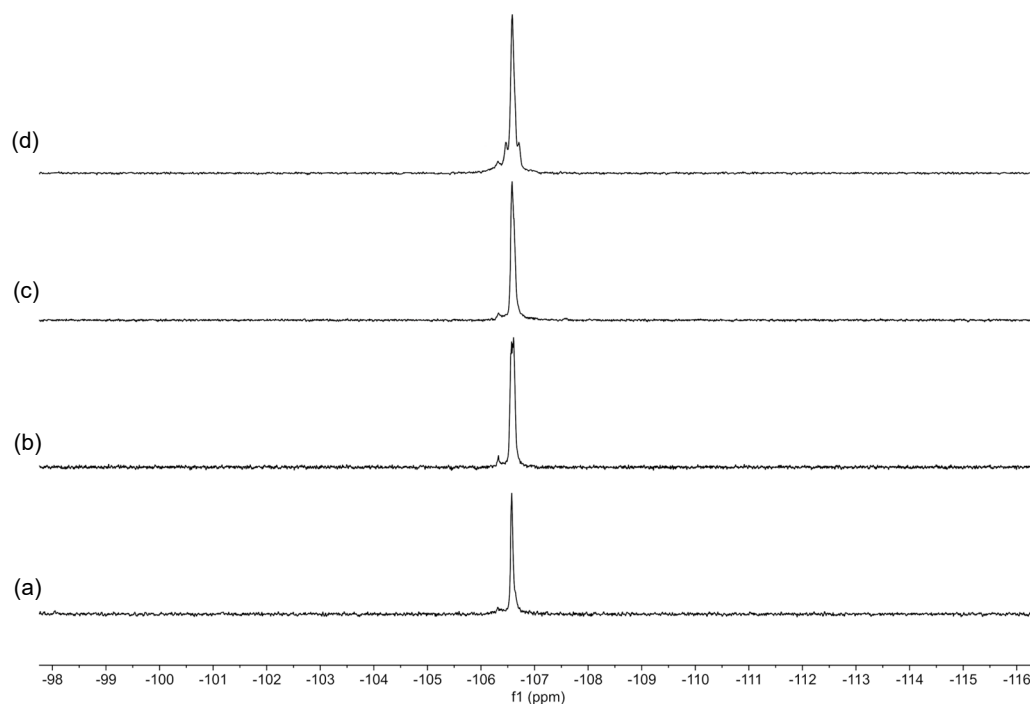


Figure S 140. ^{19}F -NMR (470 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectra of (a) assembly $4_2\cdot\text{CB}[8]_2$, (b) assembly $2_2\cdot\text{CB}[8]_2$, (c) their equimolar mixture at $t = 0$ and (d) their equimolar mixture at $t = 288$ h.

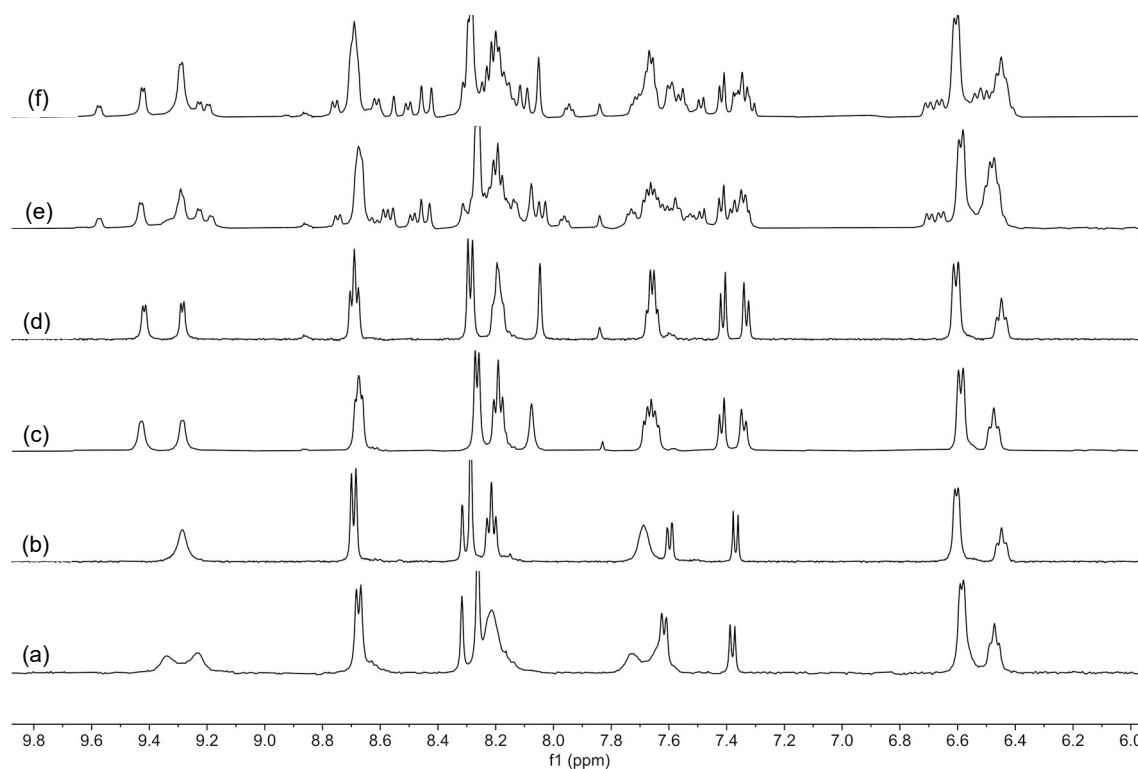


Figure S 141. ^1H -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectra of relevant signals of (a) assembly $4_2\cdot\text{CB}[8]_2$, (b) assembly $4_2\cdot\text{CB}[8]_2$ at 65°C , (c) assembly $2_2\cdot\text{CB}[8]_2$, (d) assembly $2_2\cdot\text{CB}[8]_2$ at 65°C , (e) their equimolar mixture at $t = 288$ h and (f) their equimolar mixture at $t = 288$ h and 65°C .

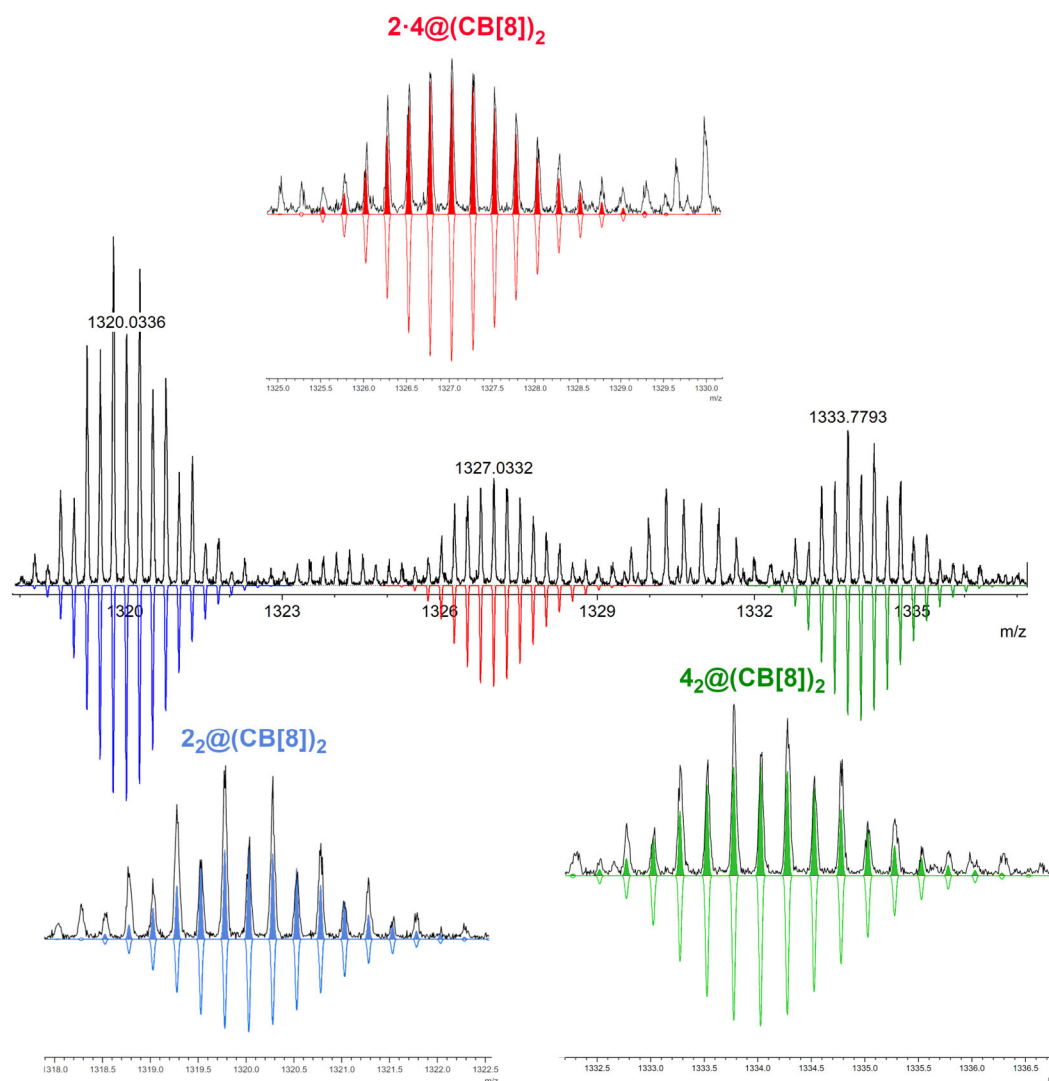


Figure S 142. HRMS (ESI-TOF-pos) of Mixture of assemblies $2 \cdot CB[8]_2$ and $4 \cdot CB[8]_2$, $[M]^{4+}$. Calculated (below), measured (top).

HRMS of hetero assembly $4 \cdot 2 \cdot CB[8]_2$ (ESI-TOF-pos): m/z = 1327.0317 $[M]^{4+}$ (calc. 1327.0277 for $C_{213}H_{160}F_8N_{76}O_{33}Pt_4S_1$).

Mixture of assemblies $4_2 \cdot \text{CB}[8]_2$ and $1_2 \cdot \text{CB}[8]_2$ (angle mismatch of 64° ; $d_{\text{Pt-Pt}}$ mismatch: 5.03 Å).

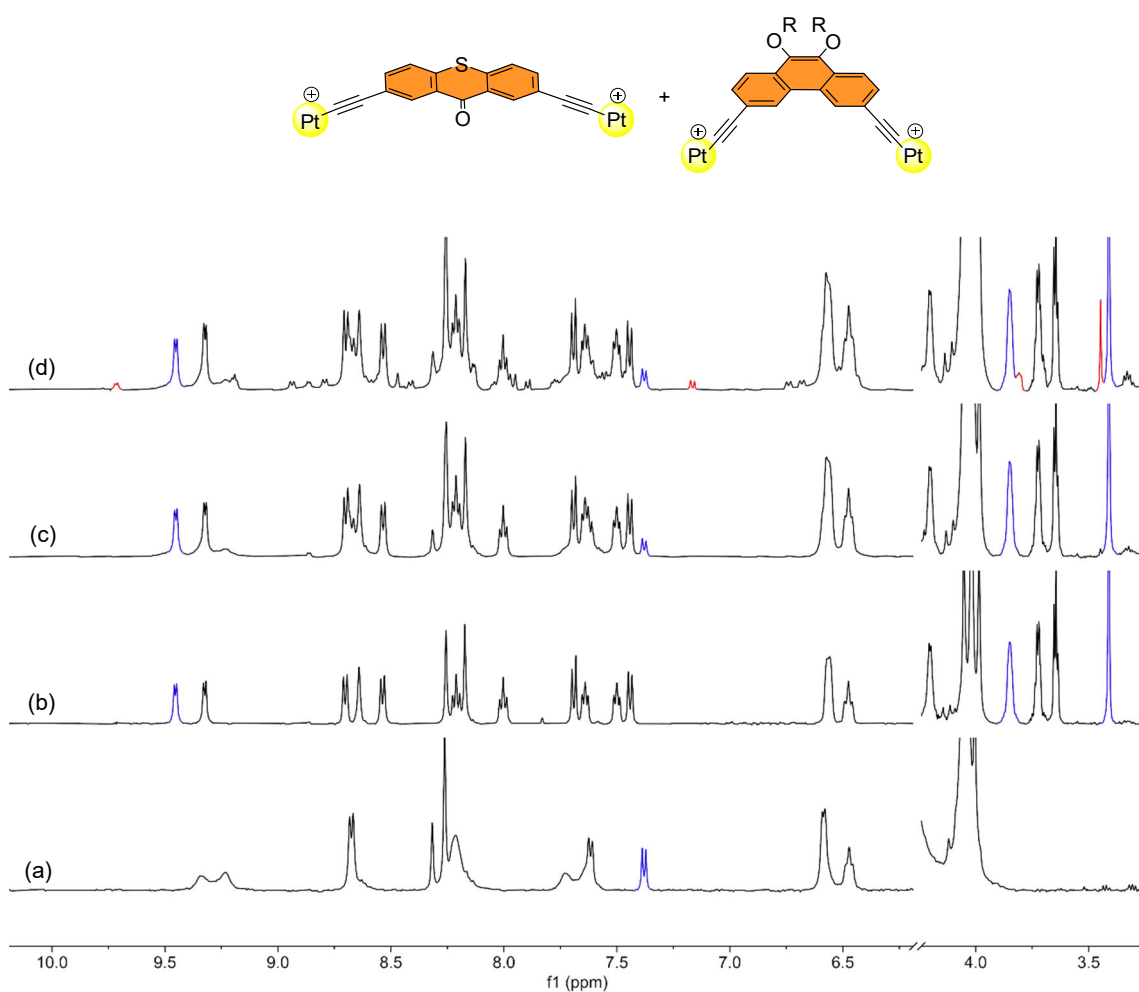


Figure S 143. ^1H -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectra of relevant signals of (a) assembly $4_2 \cdot \text{CB}[8]_2$, (b) assembly $1_2 \cdot \text{CB}[8]_2$, (c) their equimolar mixture at $t = 0$ and (d) their equimolar mixture at $t = 288$ h. Highlighted blue and red signals correspond to homoquaternary and heteroquaternary assemblies, respectively and were used for integration to estimate the binding free energy (see below).

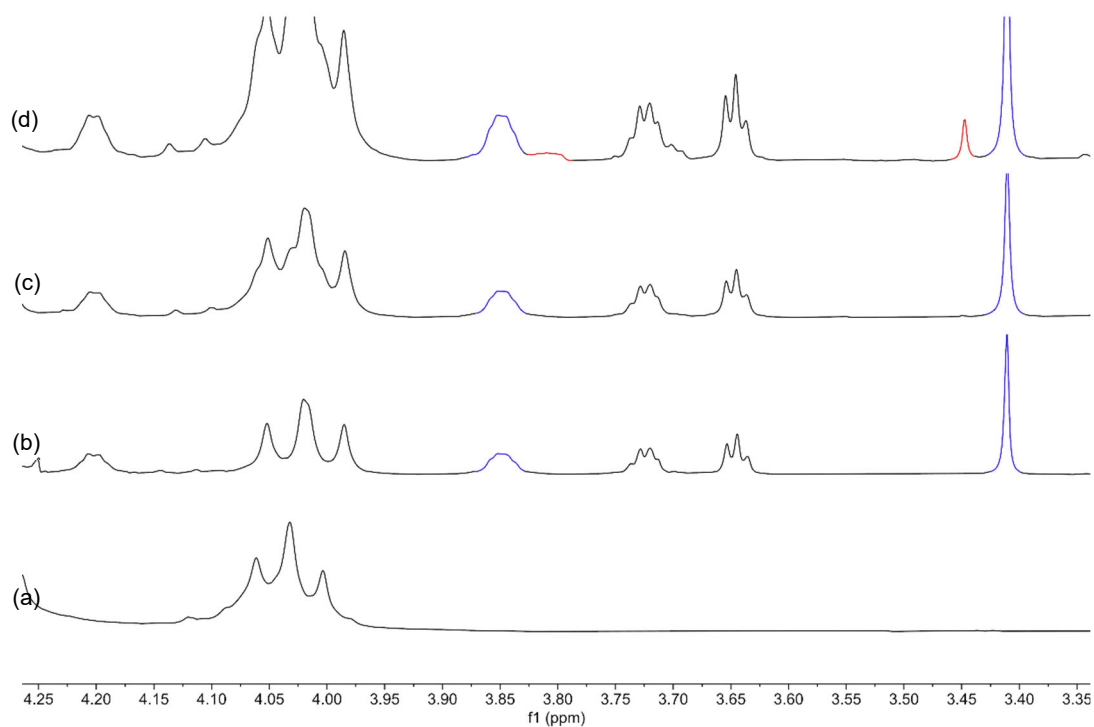


Figure S 144. Aliphatic region of ^1H -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectra of (a) assembly $4_2\cdot\text{CB}[8]_2$, (b) assembly $1_2\cdot\text{CB}[8]_2$, (c) their equimolar mixture at $t = 0$ and (d) their equimolar mixture at $t = 288$ h. Highlighted blue and red signals correspond to homoquaternary and heteroquaternary assemblies, respectively and were used for integration to estimate the binding free energy (see below).

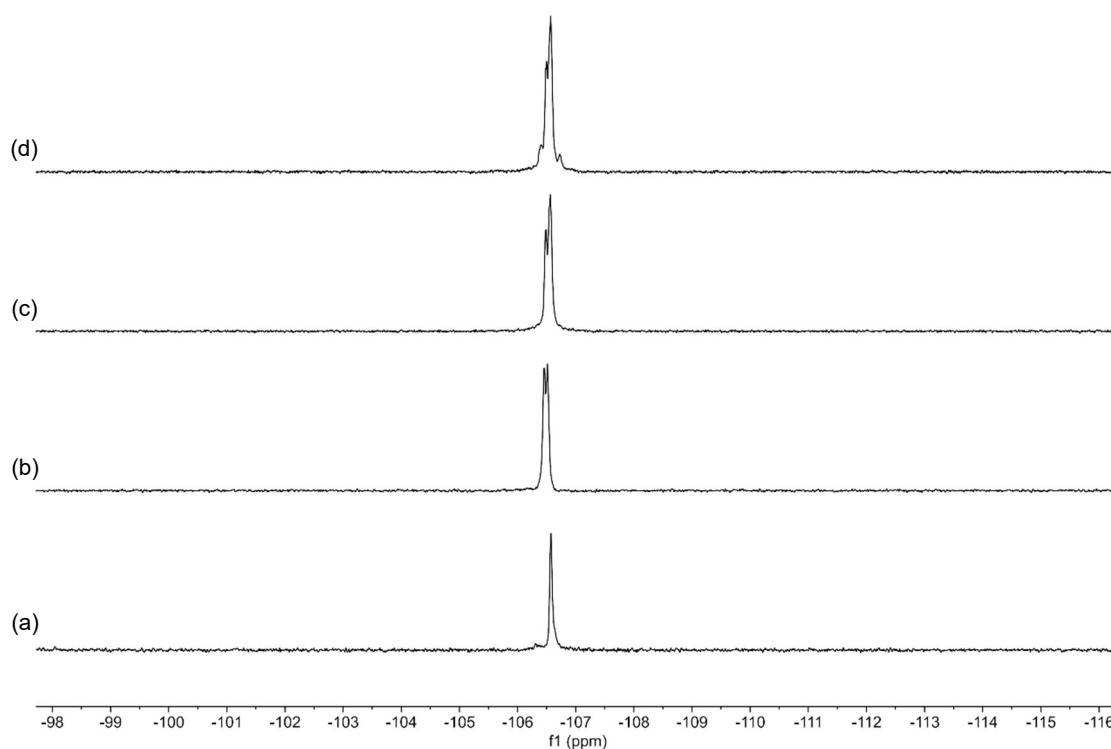


Figure S 145. ^{19}F -NMR (470 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectra of (a) assembly $4_2\cdot\text{CB}[8]_2$, (b) assembly $1_2\cdot\text{CB}[8]_2$, (c) their equimolar mixture at $t = 0$ and (d) their equimolar mixture at $t = 288$ h.

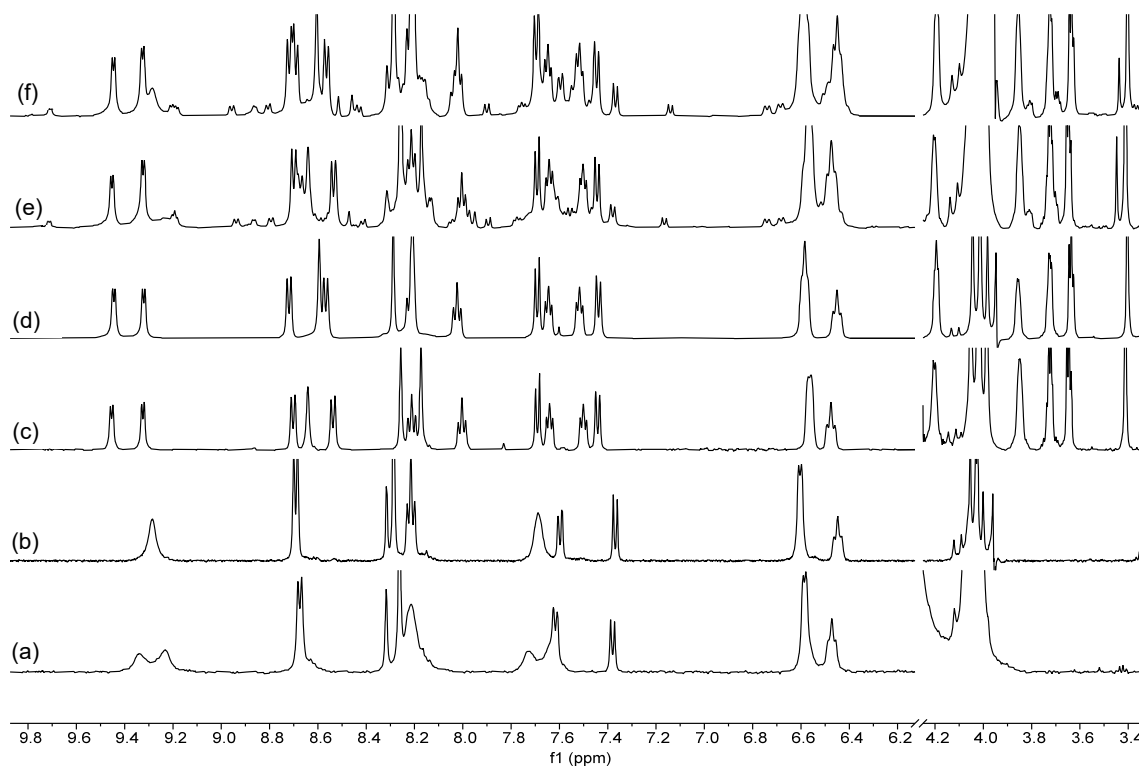


Figure S 146. ¹H-NMR (500 MHz, D₂O/CD₃CN 2:1) spectra of relevant signals of (a) assembly 4₂·CB[8]₂, (b) assembly 4₂·CB[8]₂ at 65°C, (c) assembly 1₂·CB[8]₂, (d) assembly 1₂·CB[8]₂ at 65°C, (e) their equimolar mixture at t = 288 h and (f) their equimolar mixture at t = 288 h and 65 °C.

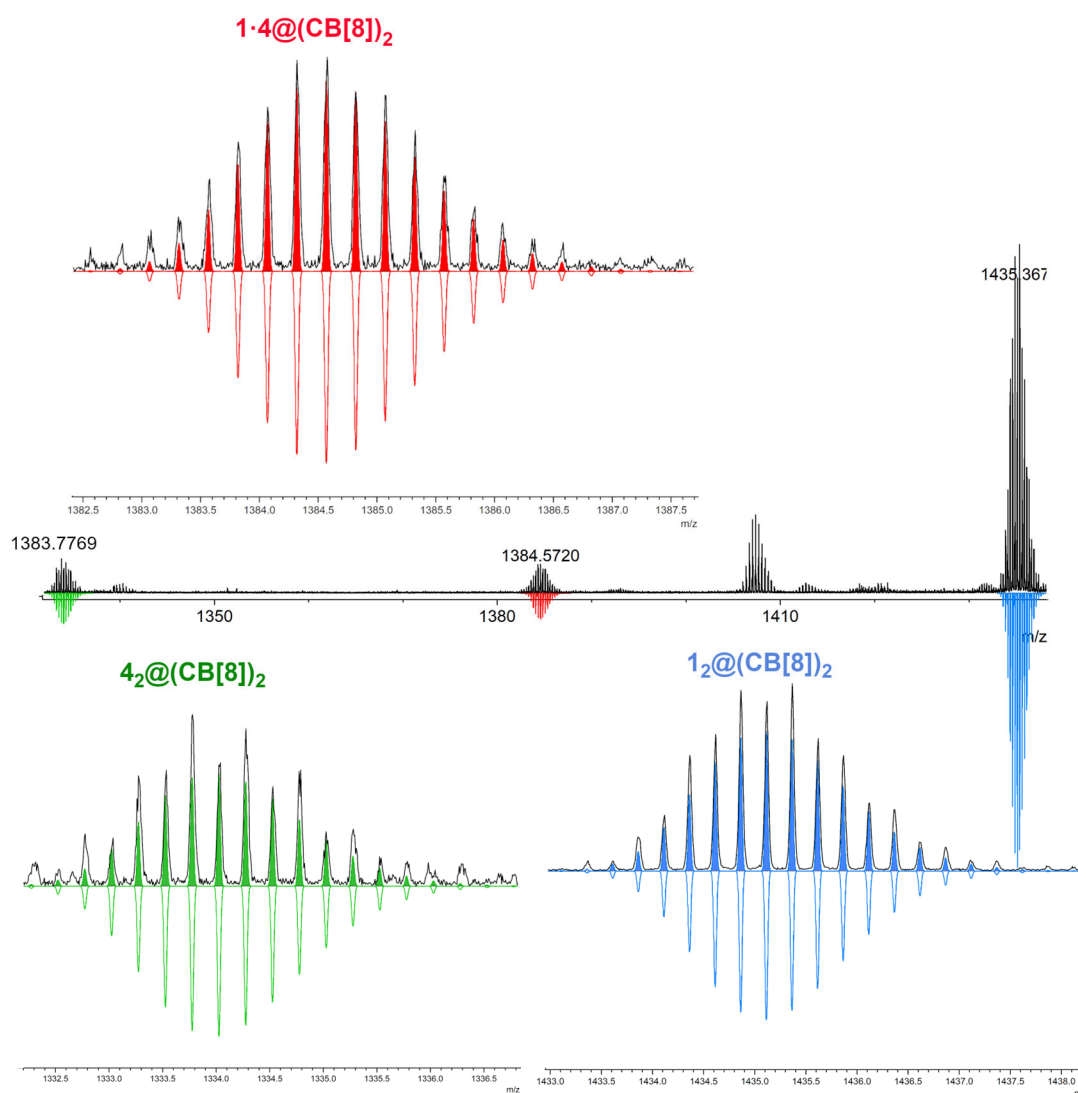


Figure S 147. HRMS (ESI-TOF-pos) of Mixture of assemblies $1_2\cdot\text{CB}[8]_2$ and $4_2\cdot\text{CB}[8]_2$, $[\text{M}]^{4+}$. Calculated (below), measured (top).

HRMS of hetero assembly $4\cdot1\cdot\text{CB}[8]_2$ (ESI-TOF-pos): m/z = 1384.5700 $[\text{M}]^{4+}$ (calc. 1384.5702 for $\text{C}_{225}\text{H}_{182}\text{F}_8\text{N}_{76}\text{O}_{39}\text{Pt}_4\text{S}_1$).

Mixture of assemblies $5_2 \cdot \text{CB}[8]_2$ and $4_2 \cdot \text{CB}[8]_2$. (angle mismatch of 6° ; $d_{\text{Pt-Pt}}$ mismatch: 2.08 Å).

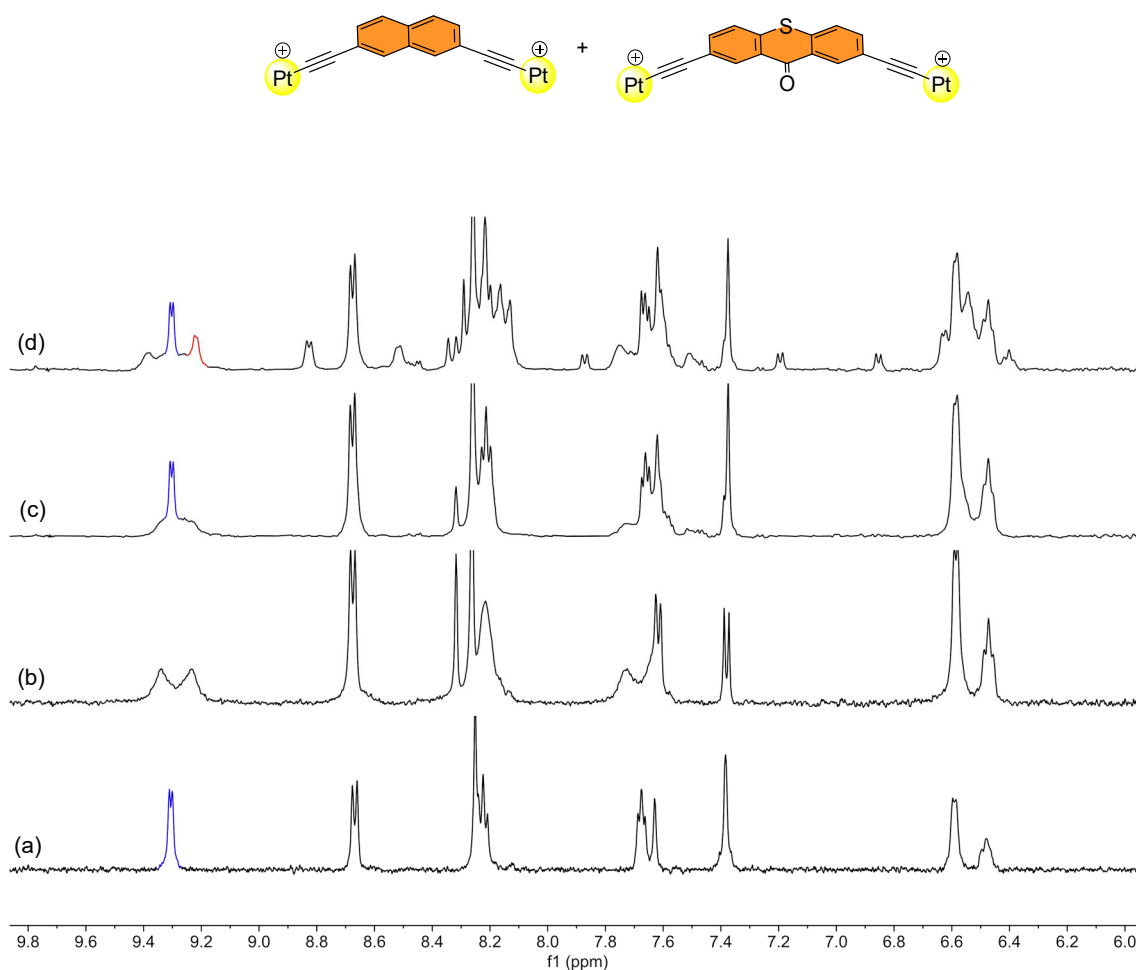


Figure S 148. ^1H -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectra of relevant signals of (a) assembly $5_2 \cdot \text{CB}[8]_2$, (b) assembly $4_2 \cdot \text{CB}[8]_2$, (c) their equimolar mixture at $t = 0$ and (d) their equimolar mixture at $t = 288$ h. Highlighted blue and red signals correspond to homoquaternary and heteroquaternary assemblies, respectively and were used for integration to estimate the binding free energy (see below).

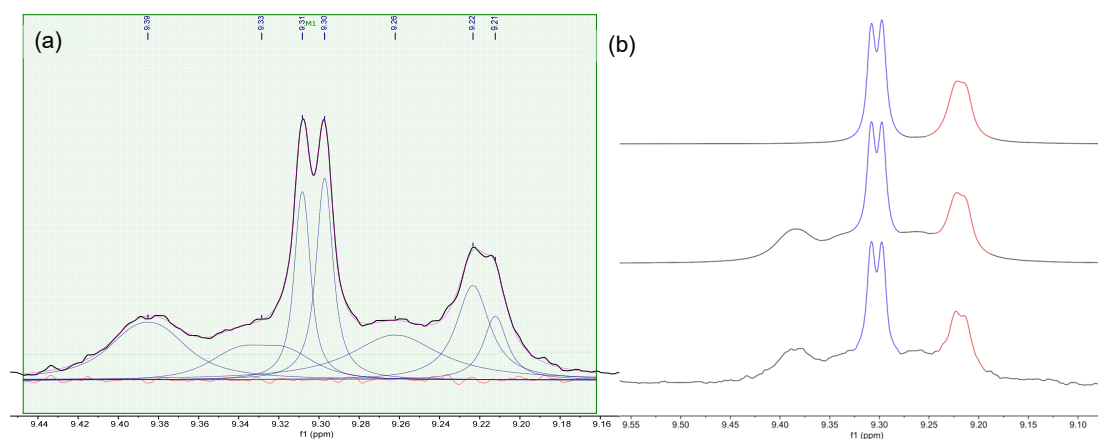


Figure S 149. (a) Deconvoluted ^1H -NMR (500 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectrum region of the equimolar mixture of assemblies $5_2 \cdot \text{CB}[8]_2$ and $4_2 \cdot \text{CB}[8]_2$ at $t = 288$ h. (b) Comparison between the spectrum (bottom), fitted spectrum (middle) and fitted spectrum after signal subtraction (top) for integration purposes. Highlighted blue and red signals correspond to homoquaternary and heteroquaternary assemblies, respectively and were used for integration to estimate the binding free energy (see below).

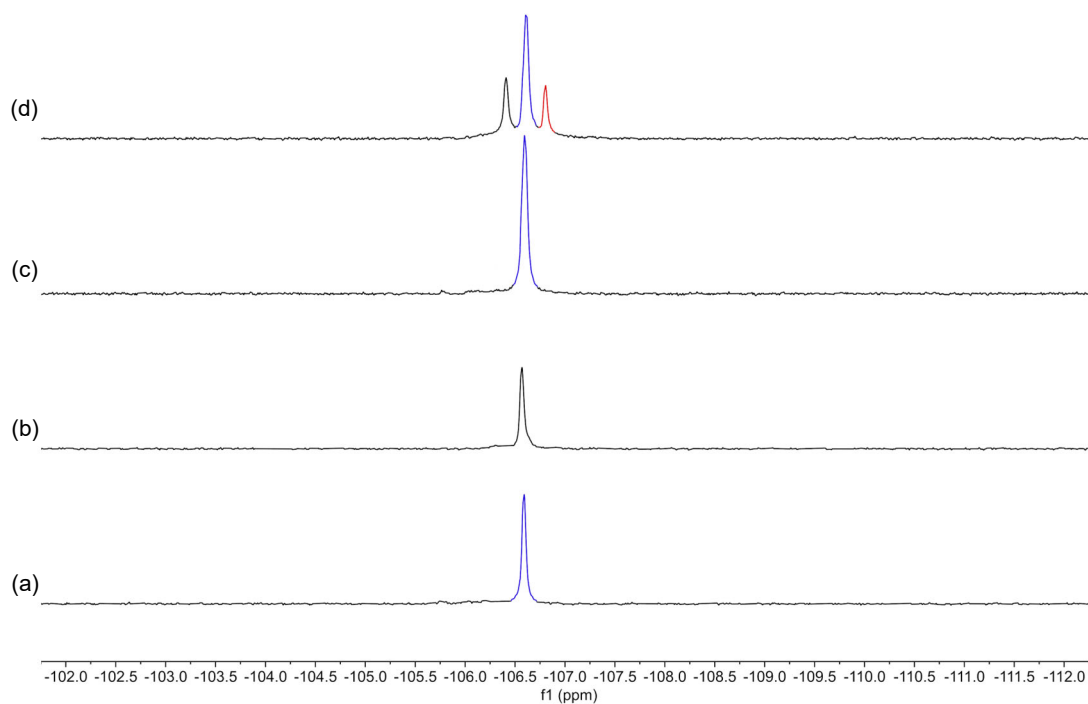


Figure S 150. ^{19}F -NMR (470 MHz, $\text{D}_2\text{O}/\text{CD}_3\text{CN}$ 2:1) spectra of (a) assembly $\mathbf{5}_2\text{-CB}[8]_2$, (b) assembly $\mathbf{4}_2\text{-CB}[8]_2$, (c) their equimolar mixture at $t = 0$ and (d) their equimolar mixture at $t = 288$ h.

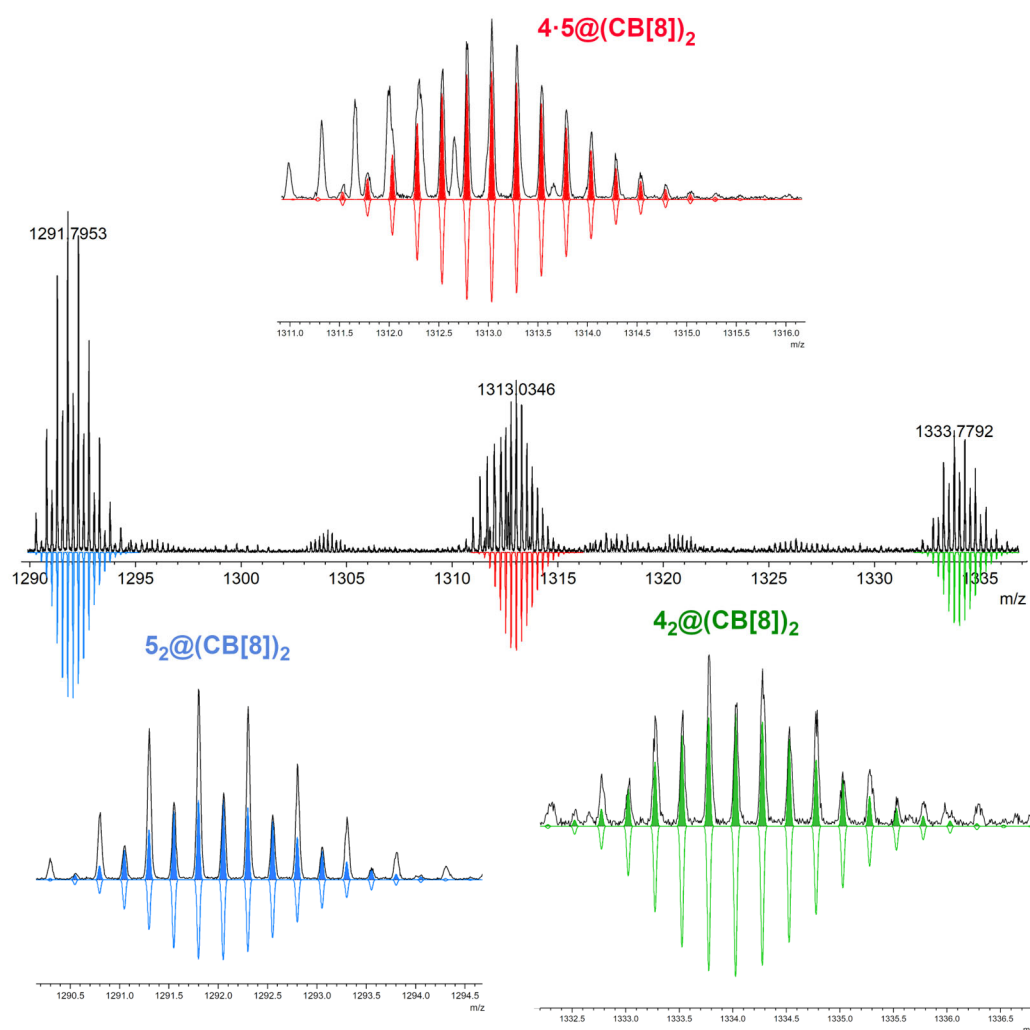
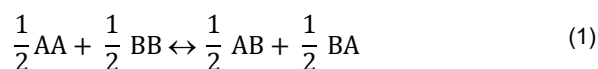


Figure S 151. HRMS (ESI-TOF-pos) of Mixture of assemblies $4_2 \cdot CB[8]_2$ and $5_2 \cdot CB[8]_2$, $[M]^{4+}$. Calculated (below), measured (top).

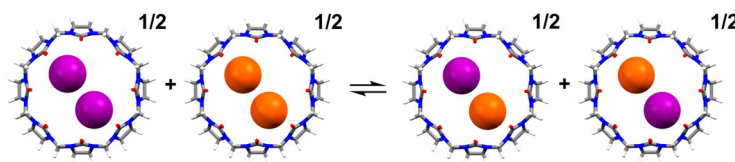
HRMS of hetero assembly $5 \cdot 4 \cdot CB[8]_2$ (ESI-TOF-pos): $m/z = 1313.0326$ $[M]^{4+}$ (calc. 1313.0347 for $C_{211}H_{160}F_8N_{76}O_{33}Pt_4S_1$).

Thermodynamics of the self-sorting processes

Considering the equilibrium, previously proposed by us (Scheme S 16),¹⁶ of a pair of homodimers (*AA* and *BB*) and their corresponding heterodimers (*AB* and *BA*):



Where *A* and *B* are different homobimetallic Pt(II)tpy complexes and their dimers (homo and hetero) are secured by two CB[8] macrocycles.



Scheme S 16. Self-sorting equilibrium depiction according to equation 1.

The equilibrium constant *K* can be written as follows:

$$K = \frac{[AB]^{1/2}[BA]^{1/2}}{[AA]^{1/2}[BB]^{1/2}} \quad (2)$$

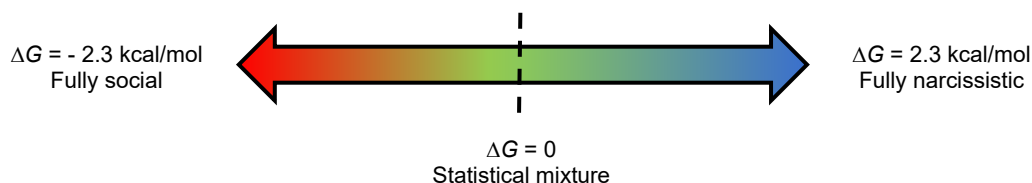
Heterodimers *AB* and *BA* are indistinguishable from one another and each account for half of the total concentration of heterodimer ($[AB] = [BA] = [AB]_{\text{tot}}/2$). Therefore, equation 2 can be rewritten as equation 3:

$$K = \frac{([AB]_{\text{tot}}/2)^{1/2}}{[AA]^{1/2}[BB]^{1/2}} = \frac{[AB]_{\text{tot}}}{2[AA]^{1/2}[BB]^{1/2}} \quad (3)$$

Above equilibrium constant is then readily converted into the relative free energy term ΔG according to:

$$\Delta G = -RT \ln K = -RT \ln \frac{[AB]_{\text{tot}}}{2[AA]^{1/2}[BB]^{1/2}} \quad (4)$$

Then, a supramolecular scale can be built based on two limiting situations that would correspond to a fully social or fully narcissistic self-sortings:



A fully social equilibrium would show a $K = 49$ and a 98% of heterodimer (1:1:98 ratio), whereas a fully narcissistic equilibrium would have a $K = 0.02$ and only 2% of heterodimer (49:49:2 ratio). On the other hand, the statistical mixture would correspond to $K = 1$ and a 50% of heterodimer (1:1:2 ratio).

Concentration estimations were carried out by NMR integration of key peaks in their ^1H -NMR (or ^{19}F) spectra of equimolar mixtures of homoquaternary assemblies after reaching thermodynamic equilibrium. Two new parameters (α and β) are introduced to relate the total concentration of heterodimer to the concentration of homodimers:

$$\alpha = \frac{[AB]_{\text{tot}}}{[AA]} \rightarrow [AA] = \frac{[AB]_{\text{tot}}}{\alpha} \quad (5)$$

$$\beta = \frac{[AB]_{\text{tot}}}{[BB]} \rightarrow [BB] = \frac{[AB]_{\text{tot}}}{\beta} \quad (6)$$

Substituting equations (5) and (6) in equation (3) returns:

$$K = \frac{[AB]_{\text{tot}}}{2 \left(\frac{[AB]_{\text{tot}}}{\alpha} \right)^{1/2} \left(\frac{[AB]_{\text{tot}}}{\beta} \right)^{1/2}} = \frac{\sqrt{\alpha\beta}}{2} \quad (7)$$

Consequently, equation (4) turns then into:

$$\Delta G = -RT \ln \frac{\sqrt{\alpha\beta}}{2} \quad (8)$$

Parameters α and β can be readily obtained from NMR integration by calculating the quotient between the absolute integral value of a peak corresponding to a specific nucleus in the heteroquaternary assembly and the absolute integral value of the peak corresponding to the same nucleus in the homoquaternary assembly. This quotient is then normalized by dividing the number of nuclei in each assembly (e.g. H⁶ in the homoquaternary assembly **3**₂·CB[8]₂ is divided by 4 whereas the same proton in any heteroquaternary assembly **3**·X·CB[8]₂ is divided by 2). Thus, both parameters can be rewritten as follows:

$$\alpha = \frac{[AB]_{\text{tot}}}{[AA]} = \frac{I_{iA}^{\text{hetero}} / n_{iA}^{\text{hetero}}}{I_{iA}^{\text{homo}} / n_{iA}^{\text{homo}}} \quad (9)$$

$$\beta = \frac{[AB]_{\text{tot}}}{[BB]} = \frac{I_{jB}^{\text{hetero}} / n_{jB}^{\text{hetero}}}{I_{jB}^{\text{homo}} / n_{jB}^{\text{homo}}} \quad (10)$$

Where:

I_{iA}^{hetero} is the absolute integral of any proton i in the heteroquaternary assembly of Pt complex A .

I_{iA}^{homo} is the absolute integral of any proton i in the heteroquaternary assembly of Pt complex A .

I_{jB}^{hetero} is the absolute integral of any proton j in the heteroquaternary assembly of Pt complex B .

I_{jB}^{homo} is the absolute integral of any proton j in the heteroquaternary assembly of Pt complex B .

This method was rigorously applied to various ¹H signals (and ¹⁹F peaks in the case of the mixture between assemblies **5**₂·CB[8]₂ and **4**₂·CB[8]₂) across multiple measurements to ensure data consistency. The experimental results are compiled in Table 1.

Table 1. Free energy term ΔG [kcal/mol] for the self-sorting of Pt complexes **1** – **5** in the presence of CB[8]. Experiments repeated in triplicate.

	1	2	3	4
2	+0.02 (± 0.01)			
3	+0.07 (± 0.01)	−0.45 (± 0.05)		
4	+0.90 (± 0.01)	+0.62 (± 0.01)	+0.56 (± 0.02)	
5				+0.16 (± 0.01)

Computational details

General methods

Pt complexes **1** – **5** and their homo- and heteroquaternary complexes with CB[8] were optimized with the semiempirical tight-binding method provided by the GFN2-xTB program,¹⁷⁻¹⁹ in conjunction with the ALPB solvation model²⁰ for water. For complex **1**, the oligoethylene chains have been simplified as methoxy groups. A simple conformational search was carried out from 3 initial structures for the quaternary complexes, bearing different Pt-Pt distances. Coordinates of the most stable assemblies, after vibrational analysis and correction for enthalpic and entropic terms, are listed in the Coordinates of optimized structures section.

Harmonic oscillator treatment

Homobimetallic complexes **1** – **5** have been modelled by simplifying them as two-point masses (m_1 and m_2) representing both Pt metals that are connected by a massless spring with force constant k (Figure S 152).

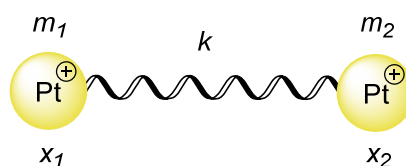


Figure S 152. Simplified model for any homobimetallic complex **1** – **5**.

Hence, the restoring force is proportional to the displacement of Pt centers with respect to the equilibrium position:

$$F = -k(x_1 + x_2) \quad (11)$$

The potential energy of the spring is obtained by integrating the negative of the force over the displacement, resulting in equation 13:

$$V(x) = \frac{1}{2} kx^2 \quad (13)$$

Subsequently, energy profiles were obtained by freezing the cartesian coordinates of the Pt centres once set at the desired distance, and by reoptimizing the structures with this constraint using GFN2-xTB and the ALPB solvation model for water. Relative energies ΔE , i.e. the electrostatic contribution to the stability at 0 K relative to the energy minimum, was then plotted as a function of the Pt-Pt distance, and fitted with quadratic function (14) that resembles equation 13, where a_0 and a are the Pt-Pt distances in the optimized relaxed and constrained structures, respectively, and k_a is the force constant (Figure S 153, Table 2).

$$\Delta E = \frac{1}{2} k_a (a_0 - a)^2 \quad (14)$$

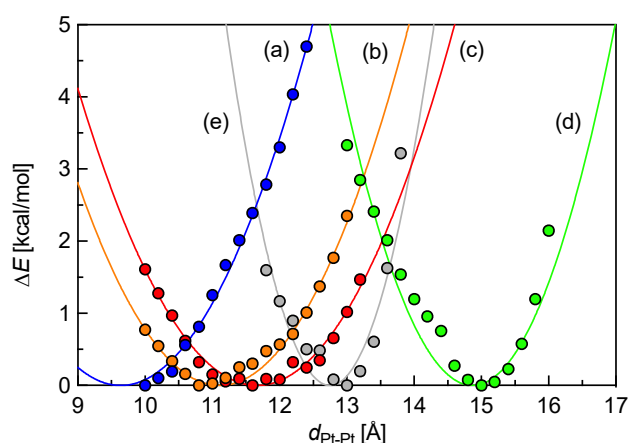


Figure S 153. Energy profiles [kcal/mol] of Pt complexes **1** (a), **2** (b), **3** (c), **4** (d) and **5** (e) as a function of Pt-Pt distance [Å] (electronic component at 0 K relative to the optimized relaxed structure).

Spring constants in mDyn/Å between two adjacent atoms (describing their local vibrational mode)²¹ are routinely calculated by common computational chemistry software from the structure's Hessian matrix obtained during vibrational

analysis (1 mDyn/Å equals 100 N/m); we did not explore that method, however, as the Pt atoms in our complexes are non-adjacent and separated by distances much longer than interatomic ones.

Table 2. Physical parameters of complexes **1** – **5** when treated as harmonic oscillators.

	1	2	3	4	5
a_0^a	10.21	11.23	11.45	15.24	13.16
k^b	1.22 ± 0.07	1.26 ± 0.05	1.16 ± 0.04	2.3 ± 0.2	4.6 ± 0.5

^a in Å. ^b force constant in kcal/mol·Å² (refer to main text for the conversion into mDyne/Å units).

Thereafter, the minimum Pt-Pt distortion required to accommodate the formation of heteroquaternary complexes was calculated as follows (Table 3): the distortion energy ΔG_{exp} is modelled as the sum of the harmonic oscillator of both Pt complexes, where k_a and k_b are the force constants, and Δa and Δb the Pt-Pt distortion in the hetero-quaternary complexes relative to the respective optimized and relaxed Pt complexes (equation 15). The difference between both distortions D (equation 16) is then minimized to extract both Δa and Δb terms (equations 19a and 19b).

$$\Delta G_{\text{exp}} = \frac{1}{2}k_a\Delta a^2 + \frac{1}{2}k_b\Delta b^2 \quad (15)$$

$$D = \Delta a - \Delta b \quad (16)$$

Equation 15 can be rearranged into equation 17 using equation 16; differential equation 18 can then be solved for Δa and Δb (see equations 19a and 19b).

$$D = \Delta a - \sqrt{\frac{\Delta G_{\text{exp}} - \frac{1}{2}k_a\Delta a^2}{\frac{1}{2}k_b}} \quad (17)$$

$$\frac{dD}{d\Delta a} = 0 = \frac{k_a\Delta a}{k_b \sqrt{\frac{\Delta G_{\text{exp}} - \frac{1}{2}k_a\Delta a^2}{\frac{1}{2}k_b}}} - 1 \quad (18)$$

$$\Delta a = \sqrt{\frac{2k_b\Delta G_{\text{exp}}}{k_a(k_a + k_b)}} \quad (19a) \quad \Delta b = \sqrt{\frac{2k_a\Delta G_{\text{exp}}}{k_b(k_a + k_b)}} \quad (19b)$$

Table 3. Proposed average Pt-Pt distortion [Å] Δa of Pt complexes **A** upon quaternary CB[8]-secured complex formation with Pt complex **B** (Δb), based on equations 15 – 19

	B	1	2	3	4	5
A						
1	0		+0.13	+0.24	+0.98	
2	−0.13		0	^a	+0.80	
3	−0.25		^a	0	+0.80	
4	−0.52		−0.43	−0.40	0	−0.30
5					+0.15	0

^a Social self-sorting observed experimentally; model not applicable.

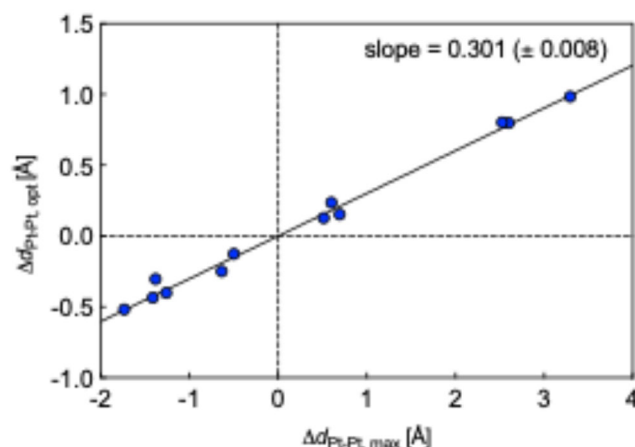


Figure S 154. Proposed average Pt-Pt distortions $\Delta d_{\text{Pt-Pt, opt}}$ [Å] of all Pt complexes upon quaternary CB[8]-secured assembly formation, based on equations 15 – 19, as a function of proposed maximal Pt-Pt distortions $\Delta d_{\text{Pt-Pt, max}}$ [Å] (see Table 3 in the main article).

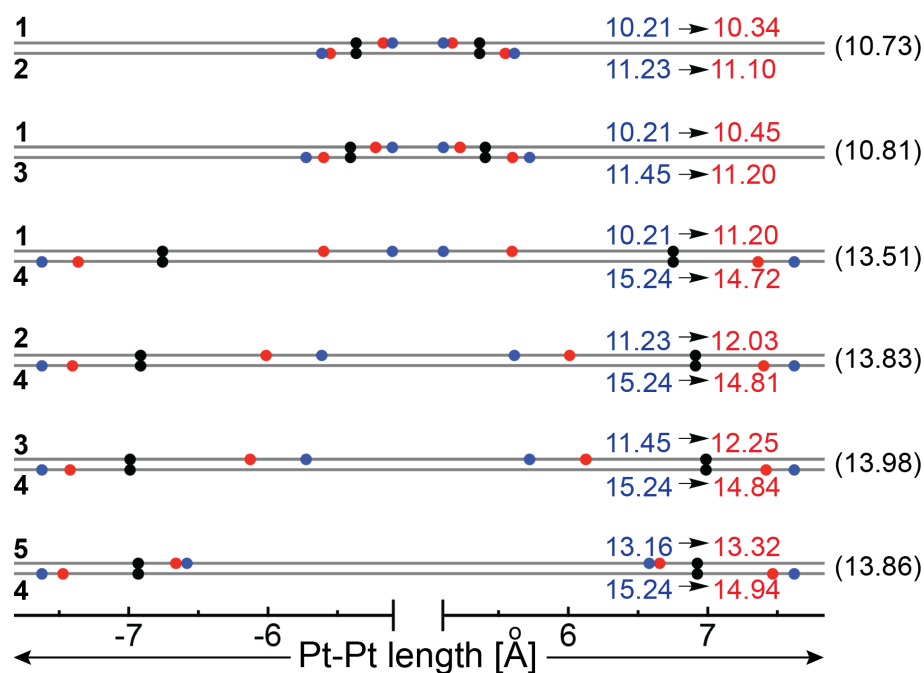
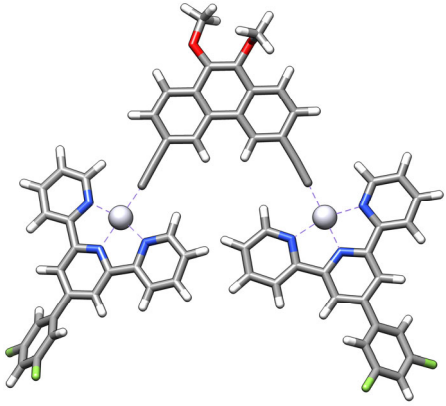
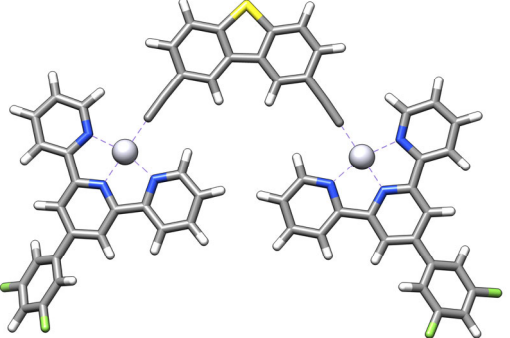


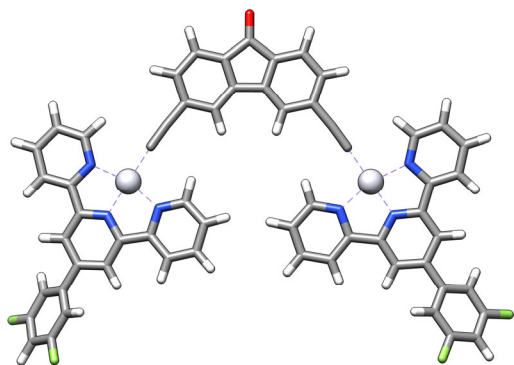
Figure S 155. Pt-Pt distances in complexes 1 – 5 (blue dots and distances), in hetero-quaternary assemblies 1·2, 1·3, 1·4, 2·4, 3·4 and 5·4 (red dots and distances) based upon equations 15 – 19, and in putative hetero-quaternary assemblies with identical Pt-Pt distances (black dots and distances in parentheses) based upon equations 5 – 7 in the main text. All distances in Å.

Coordinates of optimized structures

Structures below were prepared using the UCSF Chimera software²² from xyz output files. To provide an accurate depiction of the overlap between the central units in the CB[8]-secured quaternary complexes, orthographic projections are used, and structures are viewed along an axis perpendicular to the central units highlighted in orange.

							
Complex 1				Complex 2			
N	-45.55956894852626	-15.81858825432017	13.87450323152428	C	-27.99962134769717	-11.58596226890921	11.11128148960704
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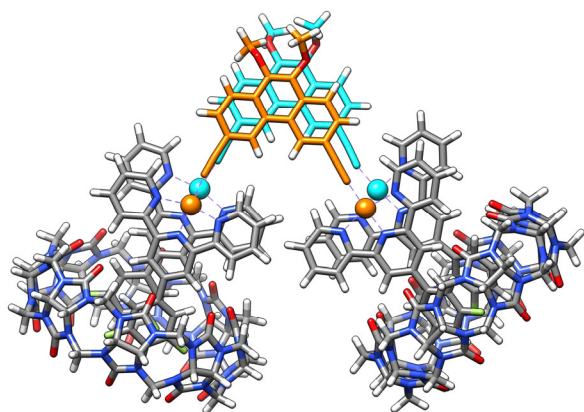
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				C	-25.88731825775899	-7.59692694555828	18.26252692024552
Pt	-25.46491552003722	-6.05208578806136	19.40651852070581	Pt	-28.88761221345163	-5.30214744655121	8.50674554088589
Pt	-28.88761221345163	-5.30214744655121	8.50674554088589	C	-28.56808018764715	-7.02272415989215	9.40645709531632



Complex 3

C	-28.12620614697875	-11.57982573547639	11.18431711599357
C	-27.73871831785225	-11.36726513425925	12.49537751673168
C	-27.55930425412481	-10.05820272698725	12.98687209827951
C	-27.77076418638147	-8.96830800162406	12.18204994945951
C	-28.16732653441629	-9.18209963651674	10.84963959660163
C	-28.33803016298761	-10.48071120856399	10.36440200612079
C	-27.45497422555851	-12.33409403423992	13.57553628061830
C	-27.08838332831177	-11.50870002430858	14.74468059590492
C	-27.14856887566065	-10.14648973893605	14.38708158169984
C	-26.72426458318769	-11.88453850695060	16.02540786768850
C	-26.41595594632196	-10.89565123085960	16.94840589361062
C	-26.46944821819681	-9.54474074922468	16.59645363046511
C	-26.84349339498260	-9.16504602643716	15.29511364802304
C	-29.13494331141717	-1.26340435135477	7.77593888296103
C	-28.81671993815787	-2.50976479495854	8.29973555138942
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C	-29.99858843905386	-3.59737291827735	6.58156176087876
C	-30.35261489814440	-2.38134775251179	6.01076034891484
C	-29.91408892772380	-1.19966589302577	6.61650320695149
C	-30.36138042927716	-4.95147340803228	6.13295895854316
C	-28.03759657616488	-2.81737268059243	9.51005328883730
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C	-29.35846085866945	-1.14621811277427	6.01849621932403
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C	-4.22489551640528	9.96513899728398	0.42377254785723	C	-2.74802553877073	5.88768326868998	-4.78616497468969
C	-5.39744382799870	8.00426468278586	1.93453570476411	C	-4.25288459004711	10.02296787452839	-4.15383556289059
C	-5.32576133836224	10.277044010139731	1.21063089262392	C	-6.03891730149017	11.37638906688489	-2.54186726823028
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C	-9.29466253212288	-2.00544974841305	3.44881535716506	H	-8.03144895573885	6.4090343728248	0.76988069306749
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C	-1.71262029819615	1.84465680769178	0.52495951614841	H	-4.98118133092822	-8.87959274320203	2.96877529455915
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S	0.09930559386904	-0.24266861434925	0.23446219591279	H	-1.99711746220077	-6.06513475096459	1.75800537291209
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Assembly 1₂-CB[8]

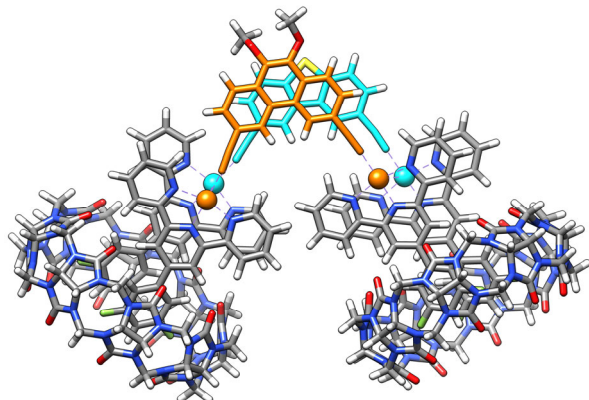
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Assembly 2·1·CB[8]

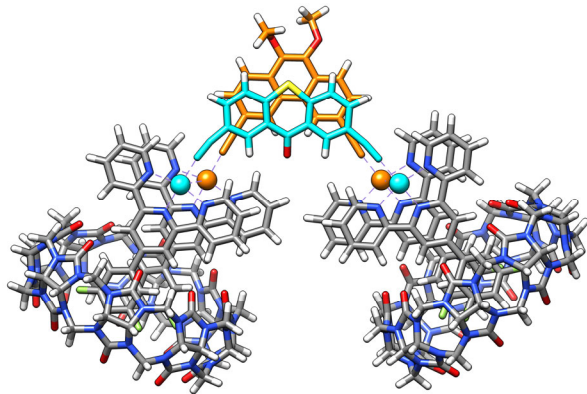
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Assembly 4-1-CB[8]

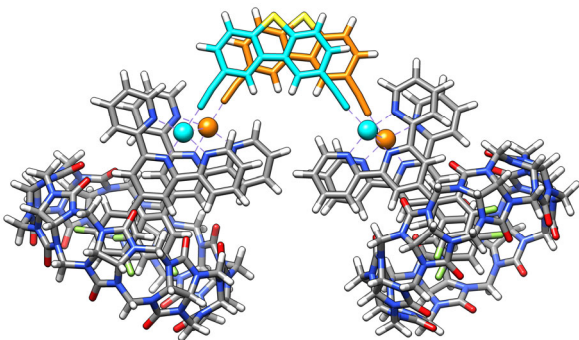
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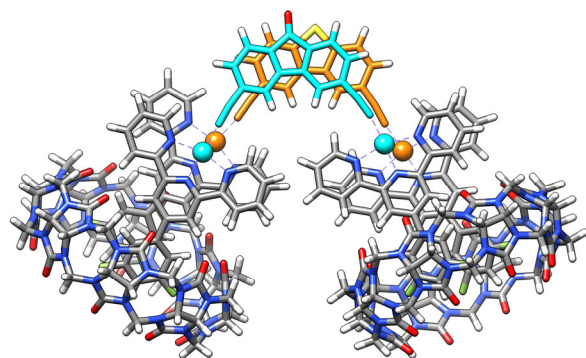
Assembly 2₂' CB[8]

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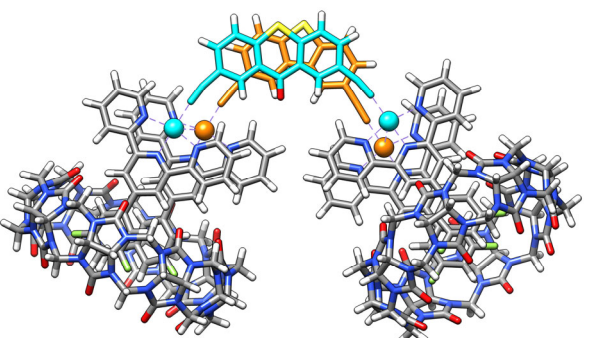
Assembly 3·2·CB[8]

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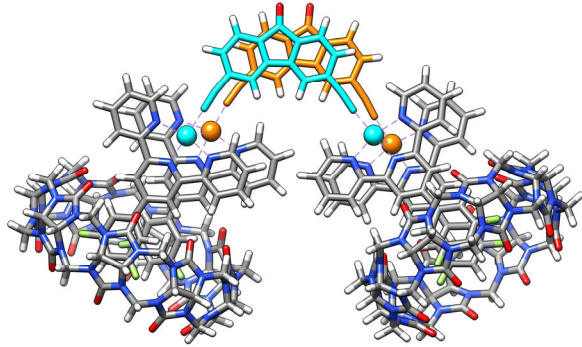
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Assembly 4·2·CB[8]							
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Assembly 3₂ CB[8]

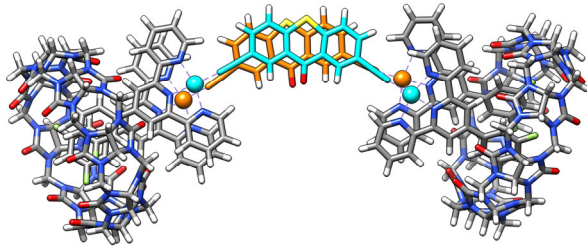
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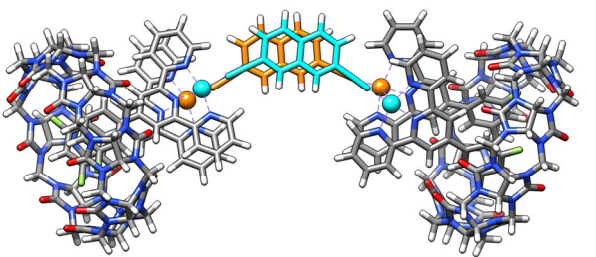
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H	-9.0531295242079						

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