Electronic Supporting Information (ESI)

A chromatography-free total synthesis of a π-conjugated ferrocene-containing dendrimer exhibiting the property to recognize 9,10-diphenylantracene

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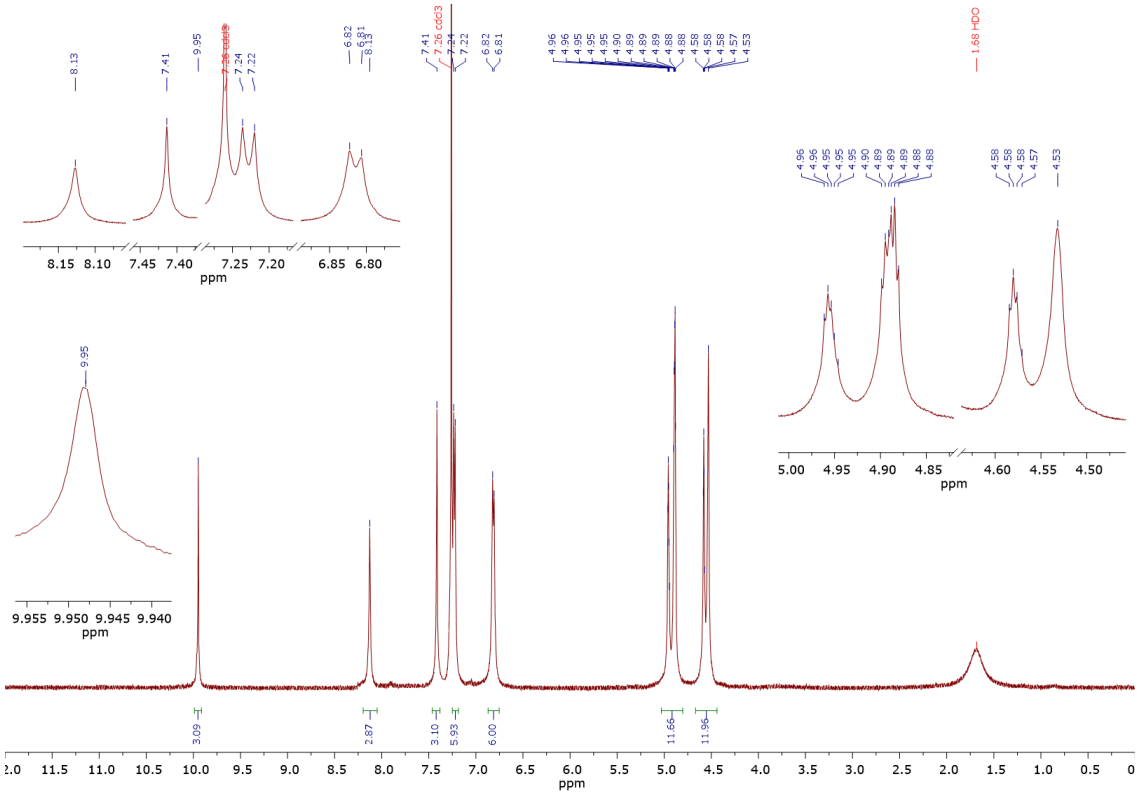

Figure S1. ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of **1**.

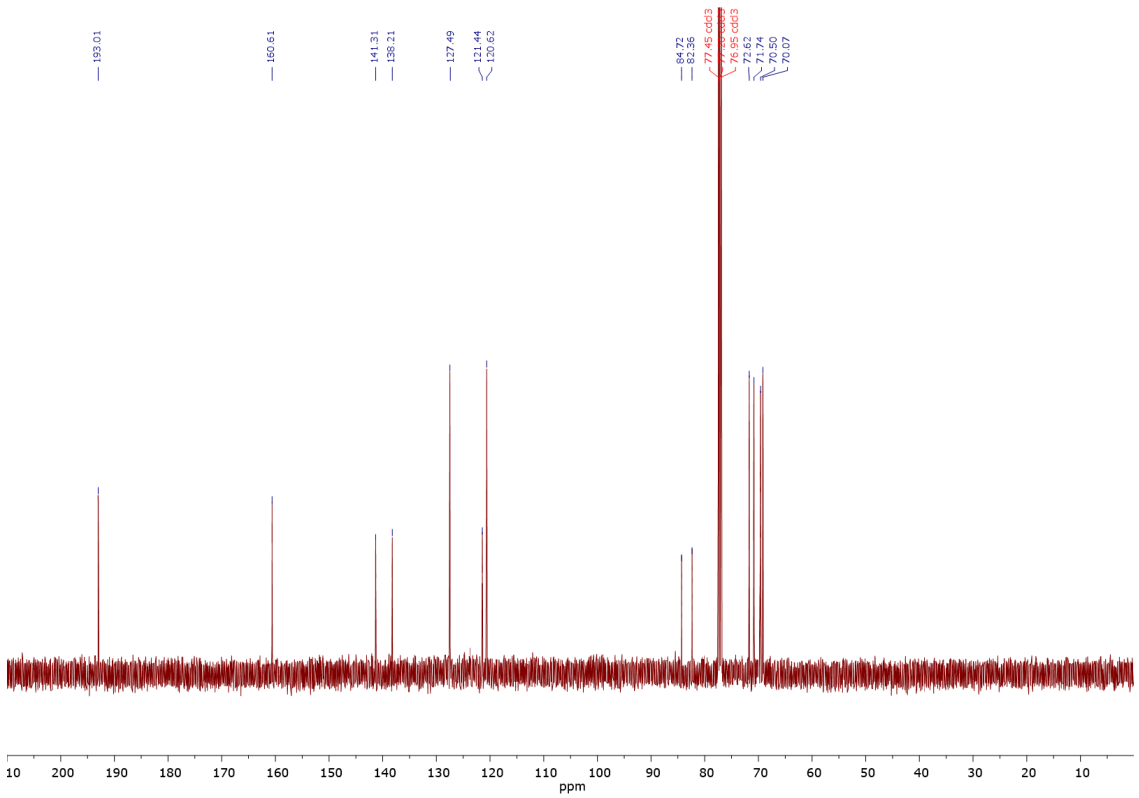

Figure S2. ^{13}C NMR ($CDCl_3$, 125 MHz) spectrum of **1**.

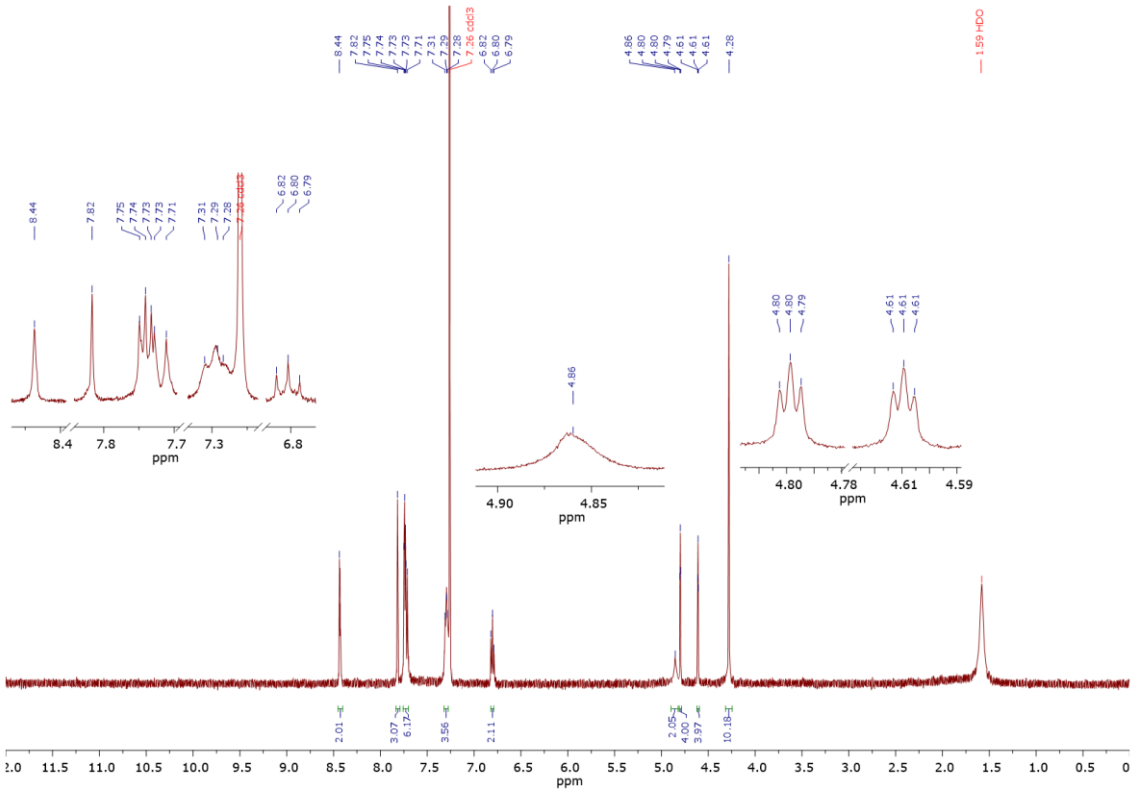

Figure S3. ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of **2**.

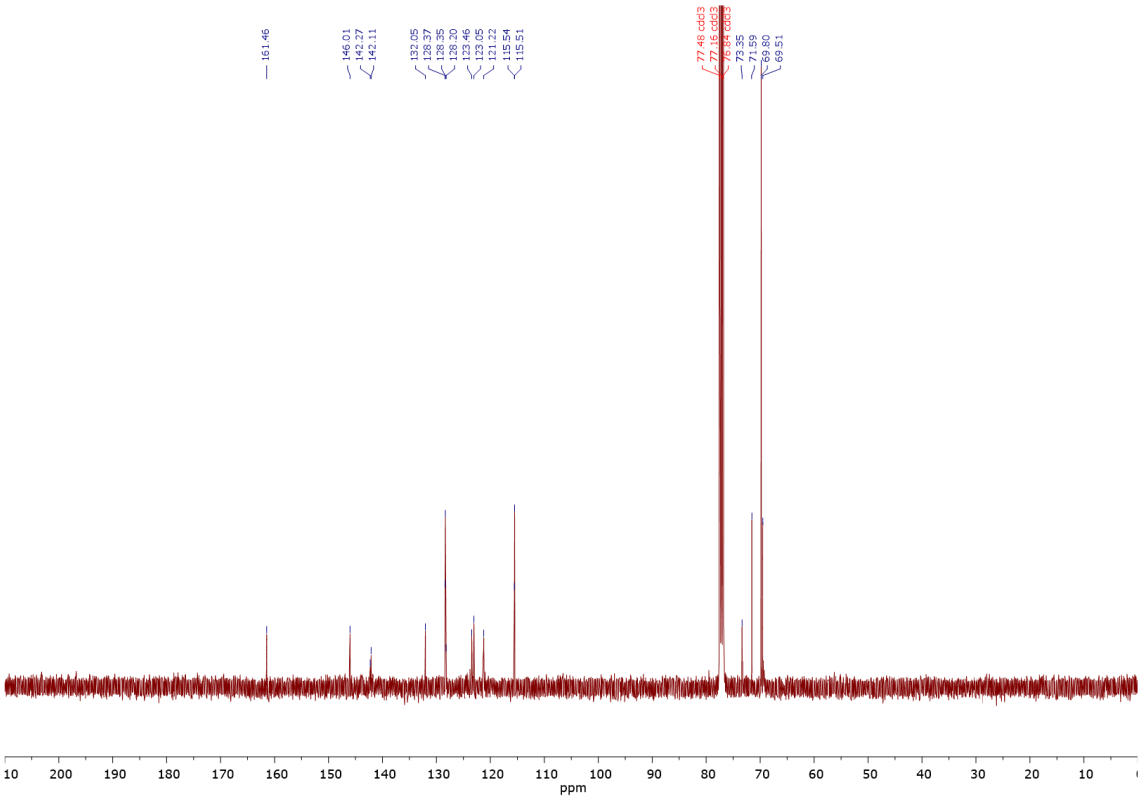

Figure S4. ^{13}C NMR ($CDCl_3$, 125 MHz) spectrum of **2**.

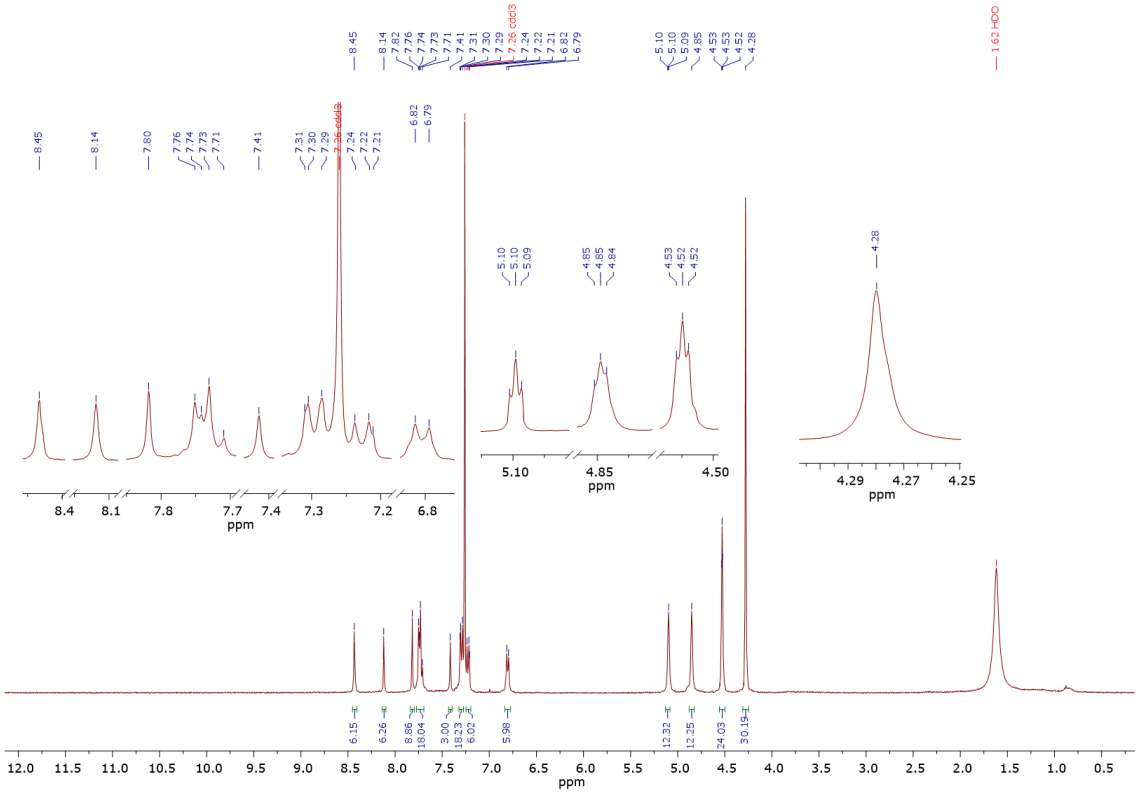

Figure S5. ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of **Fc-den**.

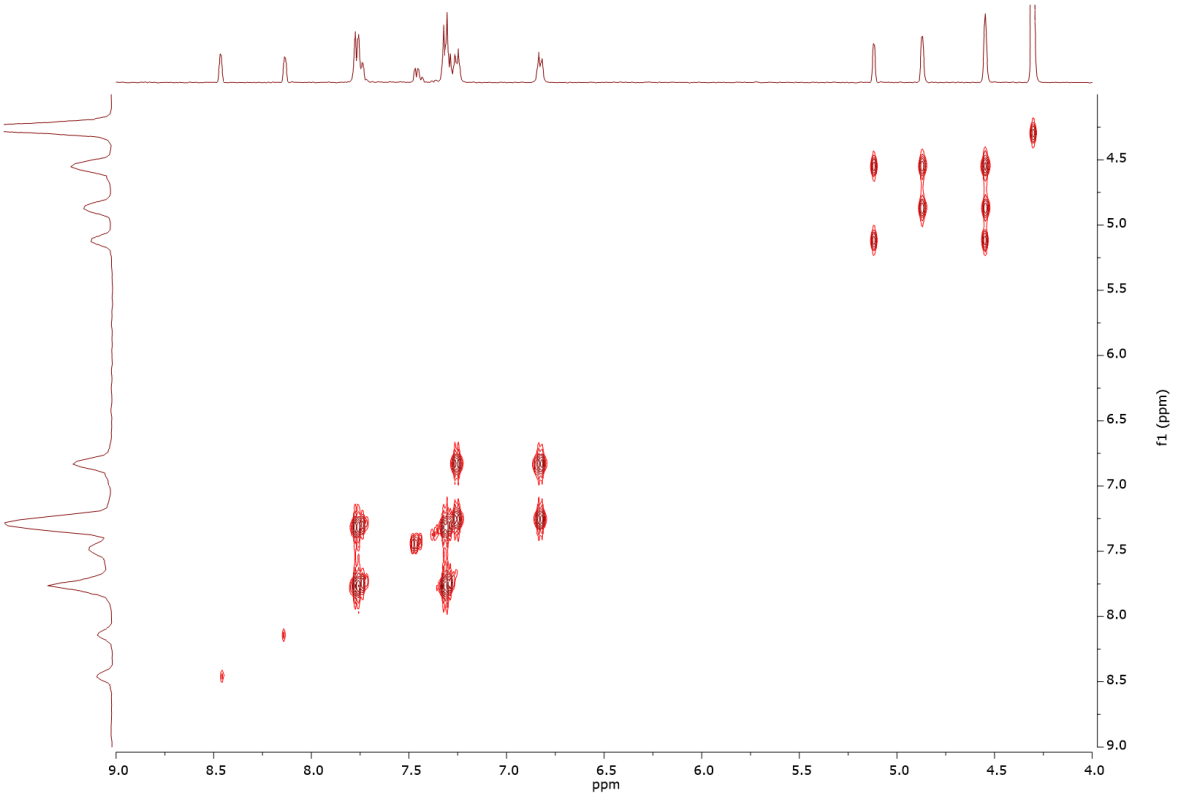

Figure S6. ^{1}H-^{1}H COSY NMR ($CDCl_3$, 500 MHz) spectrum of **Fc-den**.

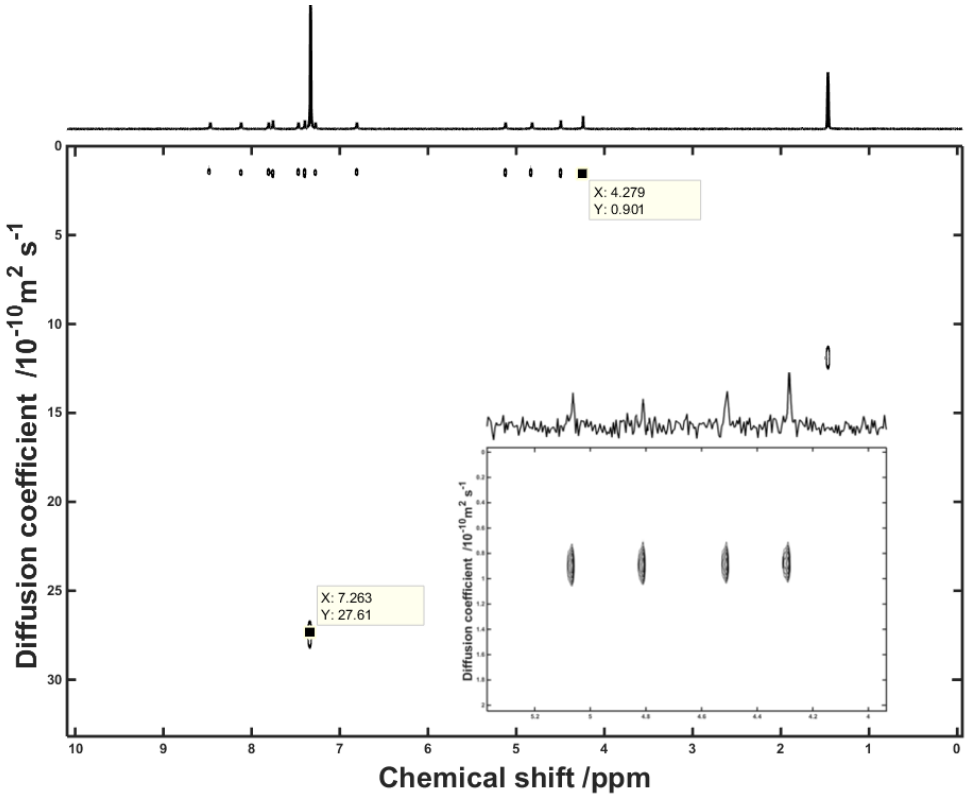

Figure S7. ^{1}H DOSY NMR ($CDCl_3$, 500 MHz, 0.7 mM) spectrum of **Fc-den**. 5.20-4.00 ppm inset of the spectrum is also presented.

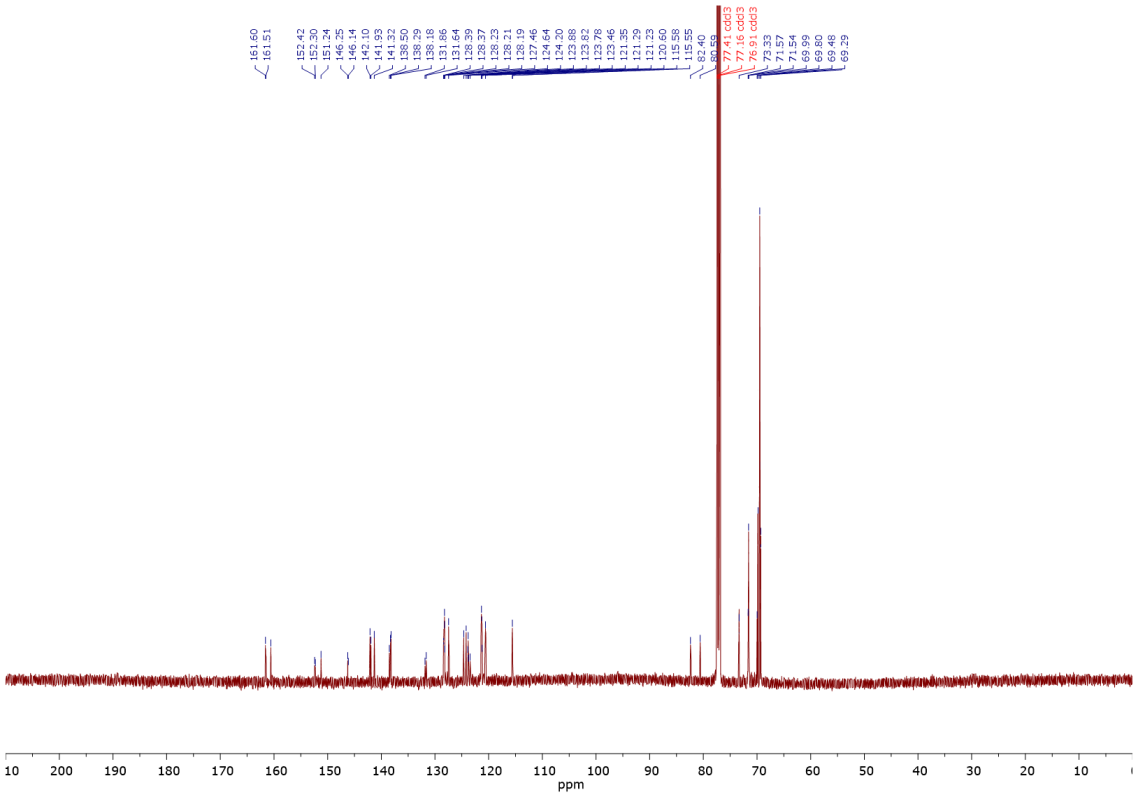

Figure S8. ^{13}C NMR ($CDCl_3$, 125 MHz) spectrum of **Fc-den**.

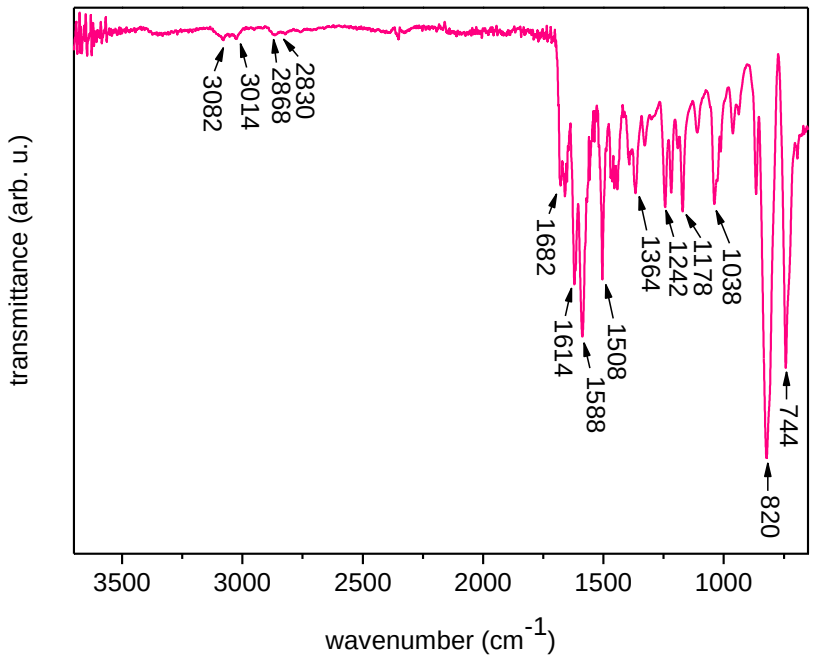

Figure S9. FT-IR (ATR) spectrum of **1**.

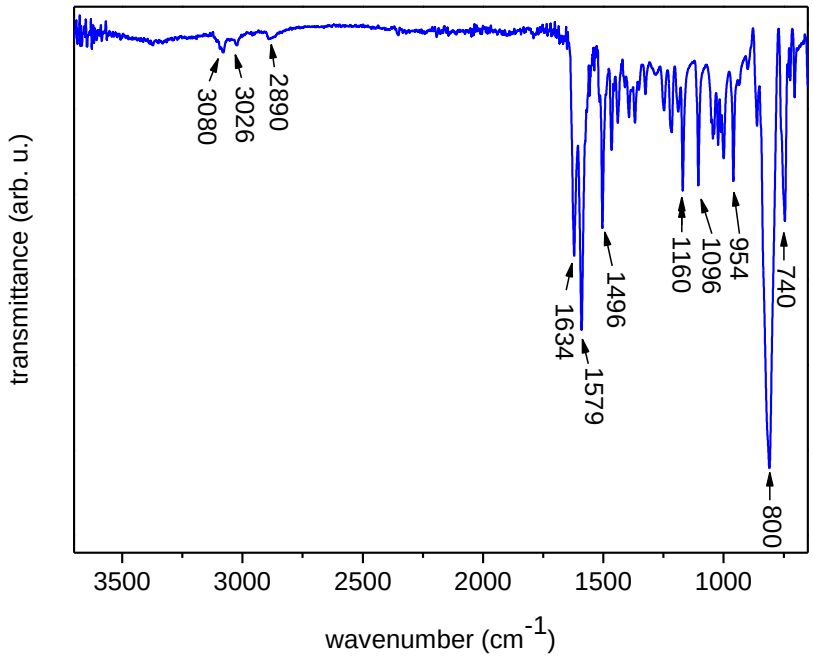

Figure S10. FT-IR (ATR) spectrum of **2**.

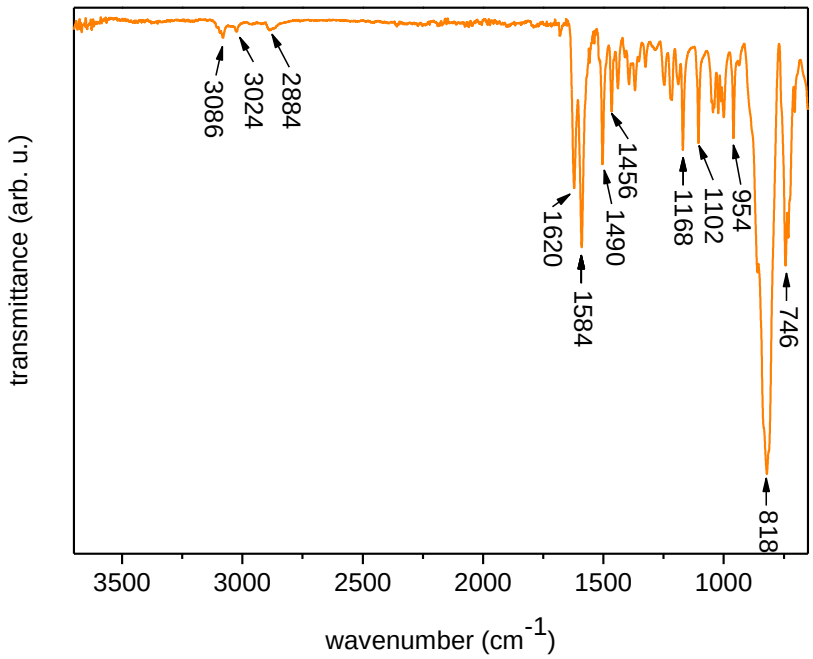

Figure S11. FT-IR (ATR) spectrum of **Fc-den**.

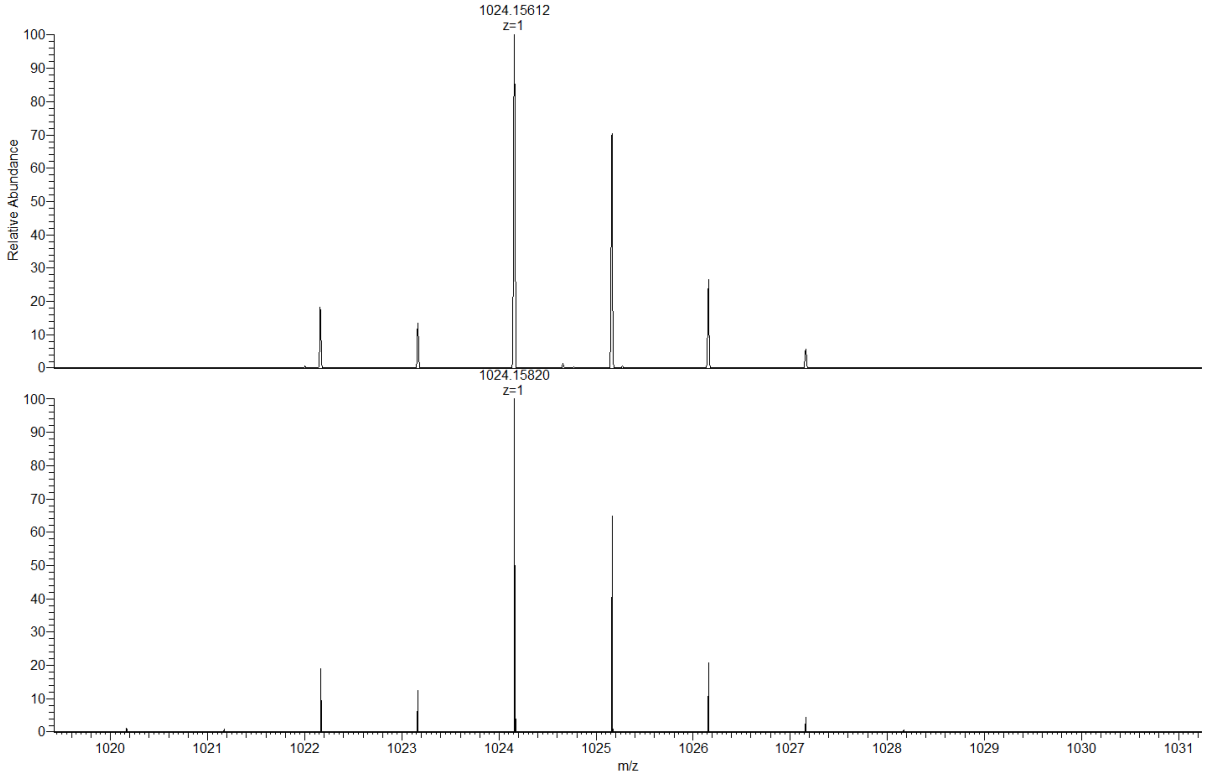

Figure S12. HRMS (TOF) spectrum of **1** (top: measured, bottom: calculated).

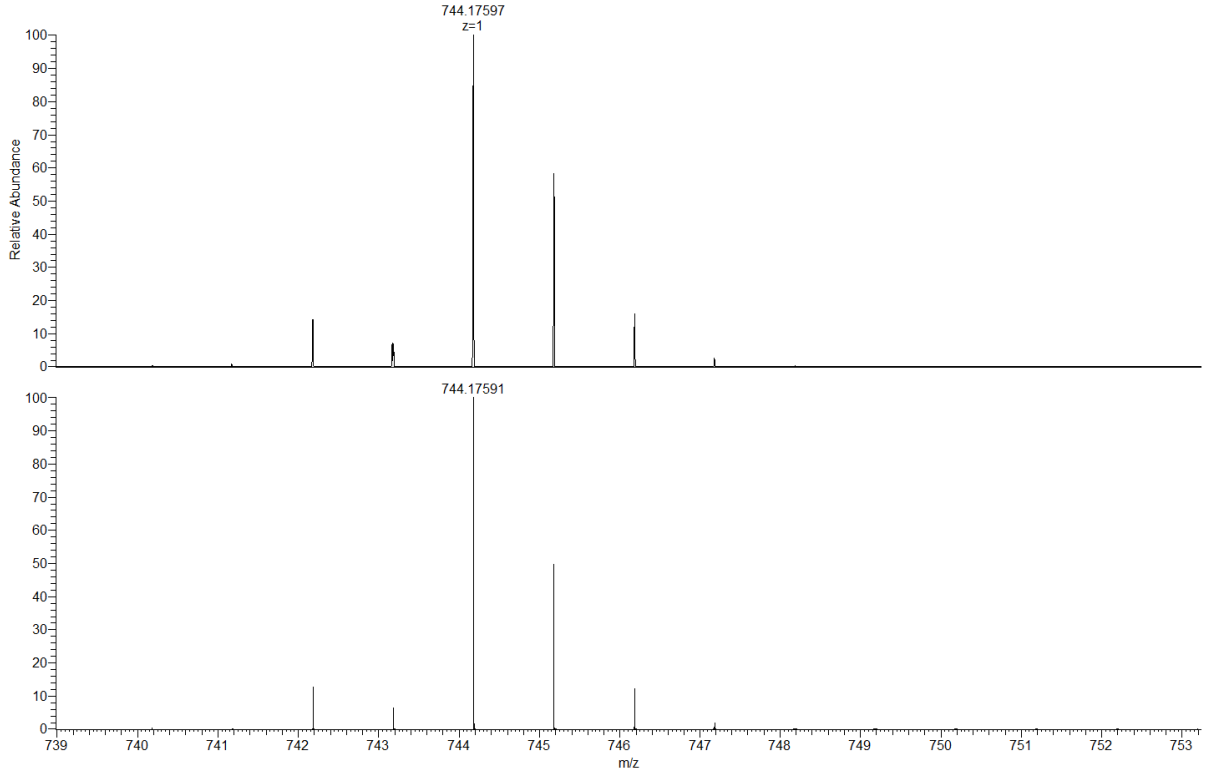

Figure S13. HRMS (TOF) spectrum of **2** (top: measured, bottom: calculated).

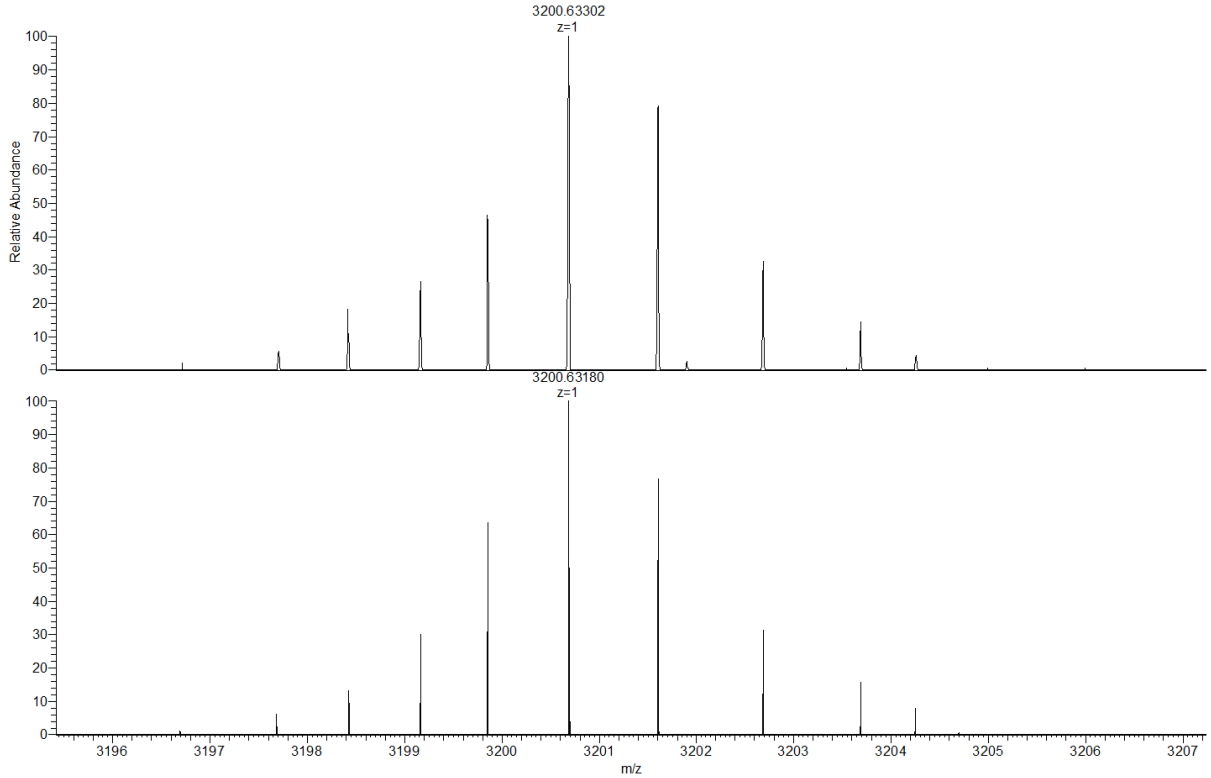

Figure S14. HRMS (TOF) spectrum of **Fc-den** (top: measured, bottom: calculated).

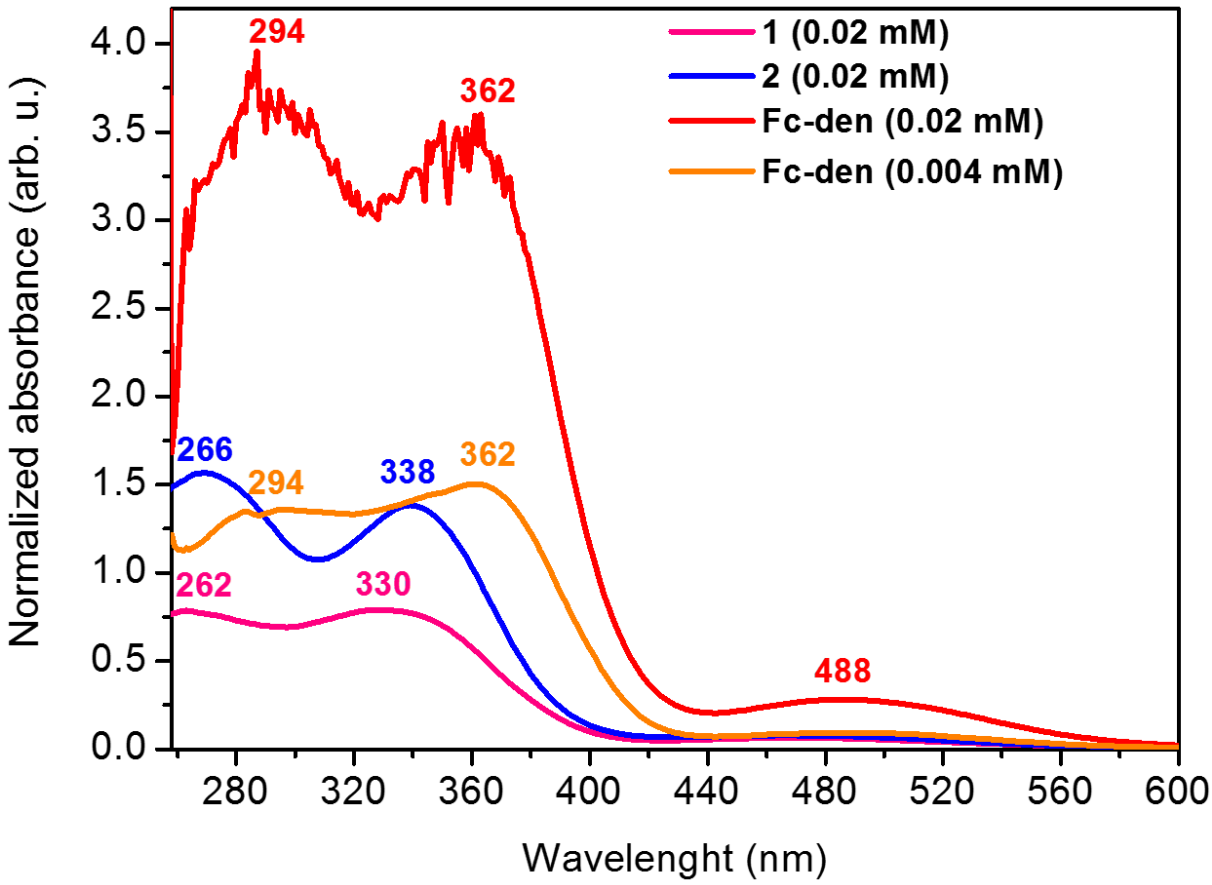

Figure S15. UV-Vis spectra ($CHCl_3$) of **1**, **2** and **Fc-den**.

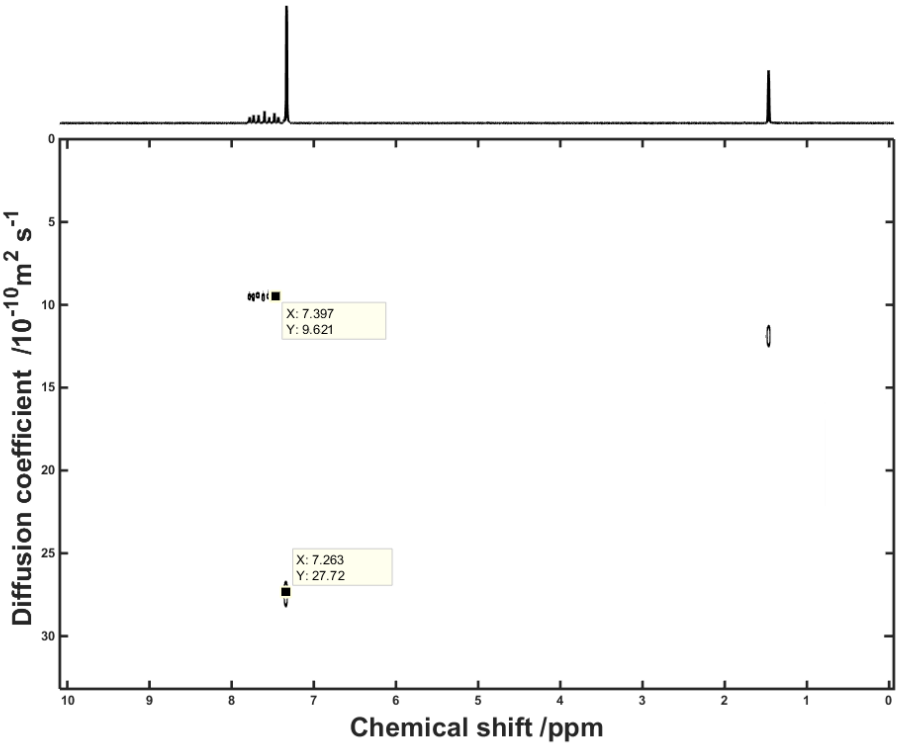

Figure. S16. ^1H DOSY NMR ($CDCl_3$, 500 MHz, 10.0 mM) spectrum of native 9,10-diphenylantracene.

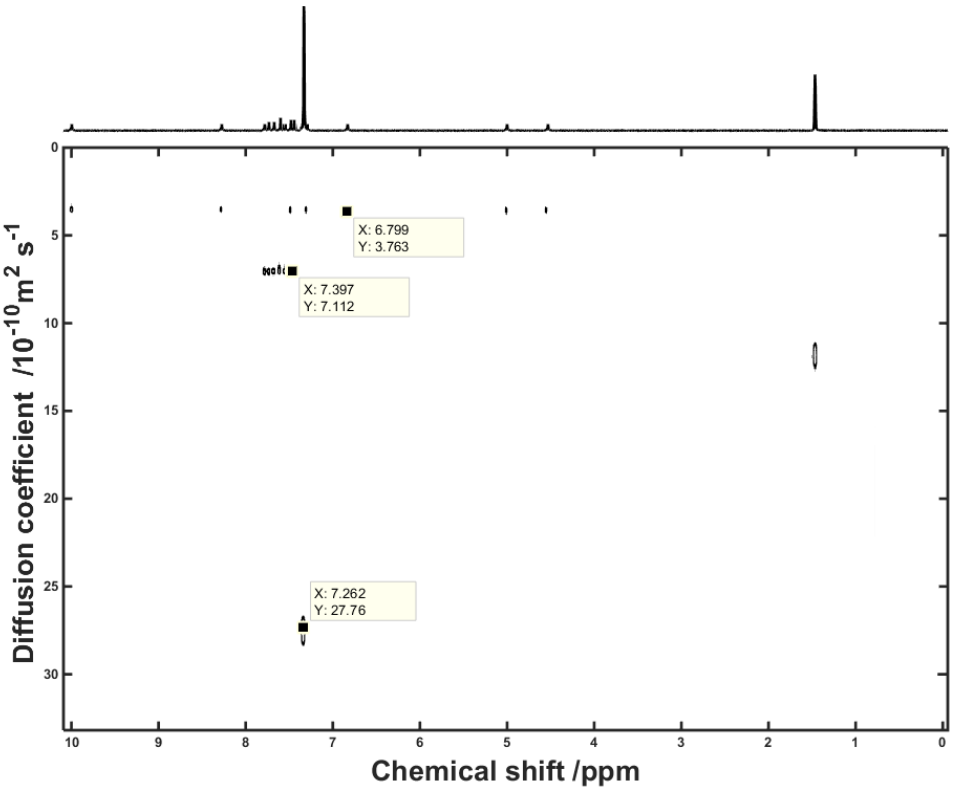

Figure. S17. ^{1}H DOSY NMR ($CDCl_3$, 500 MHz, 10.0 mM) spectrum of 9,10-diphenylantracene in the presence of compound **1** (10.0 mM).

Table S1. Calculation of K_{app} for the 9,10-diphenylantracene:**1** non-covalent system. For the details of this methodology, see: A. Kasprzak, M. Koszytkowska-Stawińska, A. M. Nowicka, W. Buchowicz, M. Poplawska. *J. Org. Chem*., **2019**, *84*, 15900–15914. Diffusion coefficient values are given in 10^{-10} m^2s^{-1}. Molar fraction of the bound 9,10-diphenylanthracene (x_b) was calculated as follows: $x_b = (D_{free} - D_{obs}) \cdot [(D_{free} - D_{bound})^{-1}]$, where x_b is a molar fraction value of the bound 9,10-diphenylanthracene, D_{free} is a diffusion coefficient value for the native 9,10-diphenylanthracene, D_{obs} stands for a diffusion coefficient value for the 9,10-diphenylanthracene in the non-covalent system, D_{bound} is a diffusion coefficient value for compound **1** in the non-covalent system. K_{app} value was calculated as follows: $K_{app} = x_b \cdot [(1- x_b) \cdot (0.01\ M - x_b \cdot 0.01\ M)]^{-1}$, where K_{app} [M^{-1}] is an apparent binding constant, x_b is a molar fraction of the 9,10-diphenylanthracene in the non-covalent system, 0.01 M is a concentration of 9,10-diphenylanthracene and compound **1** in the sample.

D_{free}	D_{obs}	D_{bound}	x_b	K_{app} [M^{-1}]
9.621	7.112	3.763	0.428	131.045

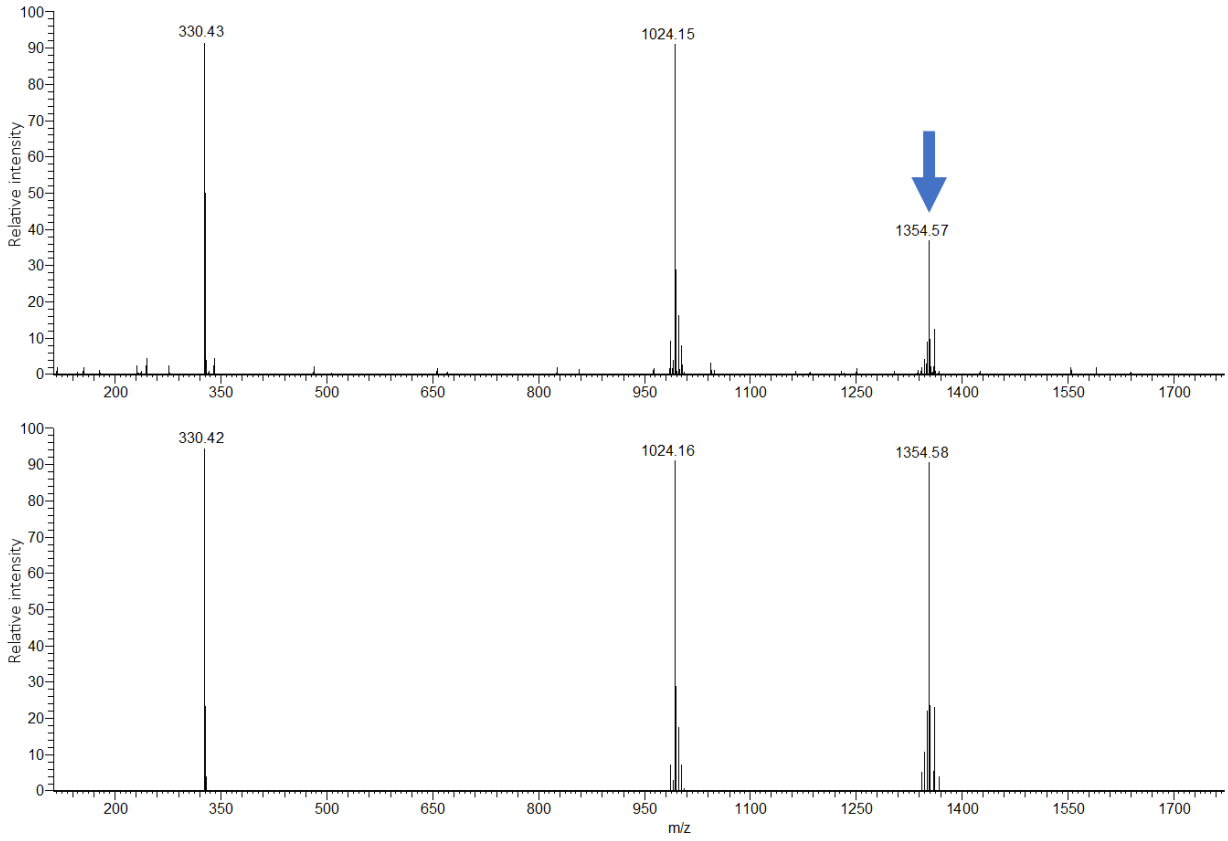

Figure. S18. Cold-spray ESI-MS spectrum of the 9,10-diphenylantracene in the presence of 1 equiv of **1** (top: measured, bottom: calculated). The peak originating from the presence of 1:1 non-covalent system is marked with blue arrow.

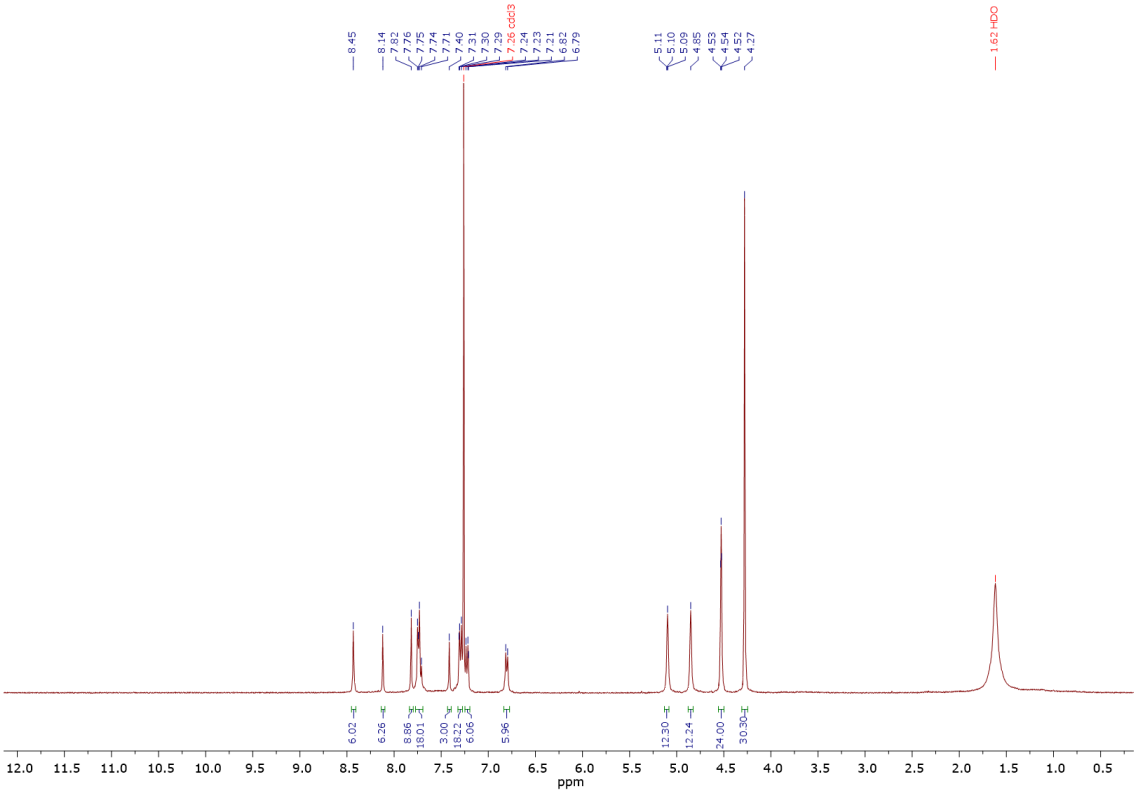

Figure S19. ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of **Fc-den** after keeping the sample on air for 3 months.

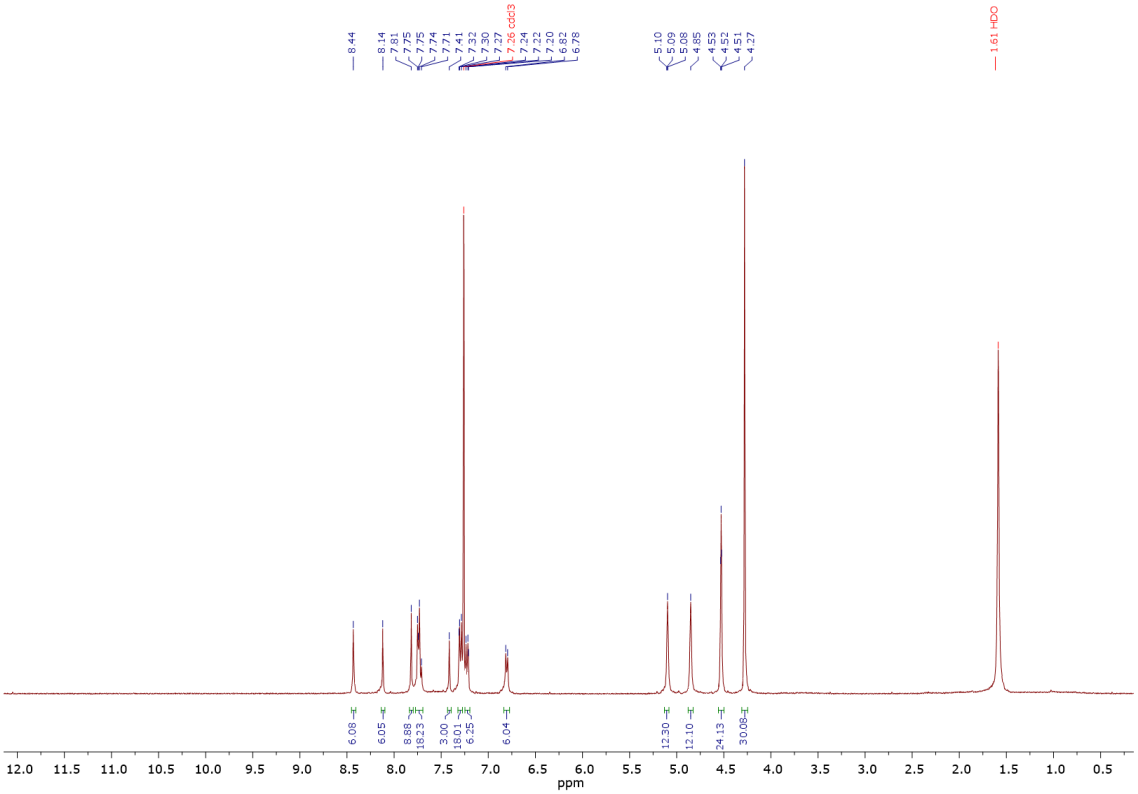

Figure S20. ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of **Fc-den** after the treatment with water (solid **Fc-den** was shaken in distilled water for 6 hours, filtered, washed with methanol, dried under high vacuum and ^{1}H NMR spectrum was acquired).