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SUPPORTING INFORMATION

Synthesis and photophysics of new pyridyl end-capped 3D-dithia[3.3]paracyclophane-based Janus tectons: surface-confined self-assembly of their model pedestal on HOPG

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M. Auffray,^a F. Charra,^b L. Sosa Vargas,^a F. Mathevet^a, A-J. Attias^a and D. Kreher^{a*}

^a Sorbonne Université, UPMC Univ Paris 06, Institut Parisien de Chimie Moléculaire, UMR CNRS 8232, 4 Place Jussieu, 75252 Paris Cedex 05, France.

^b Service de Physique de l'Etat Condensé, CEA CNRS Université Paris-Saclay, CEA Saclay, F-91191 Gif-sur-Yvette Cedex, France.
corresponding author : david.kreher@sorbonne-universite.fr, andre-jean.attias@sorbonne-universite.fr

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¹H and ¹³C NMR spectra in CDCl₃ of the new intermediate synthons are reported here, except when too complicated due to isomer mixtures that could not be separated, as well as the high-resolution mass spectra of the target compounds **P**, **C** and **JT**. To end we report also the infrared (IR) spectra recorded on bulk after evaporation or filtration of the supramolecular complexes prepared in solution by simply mixing **P** with bis(benzonitrile)-palladium(II) for coordination (**P-Pd^{II}**), terephthalic acid for hydrogen bond (**P-TPA**) and finally 1,4-diiodobenzene for halogen bond (**P-IPhI**).

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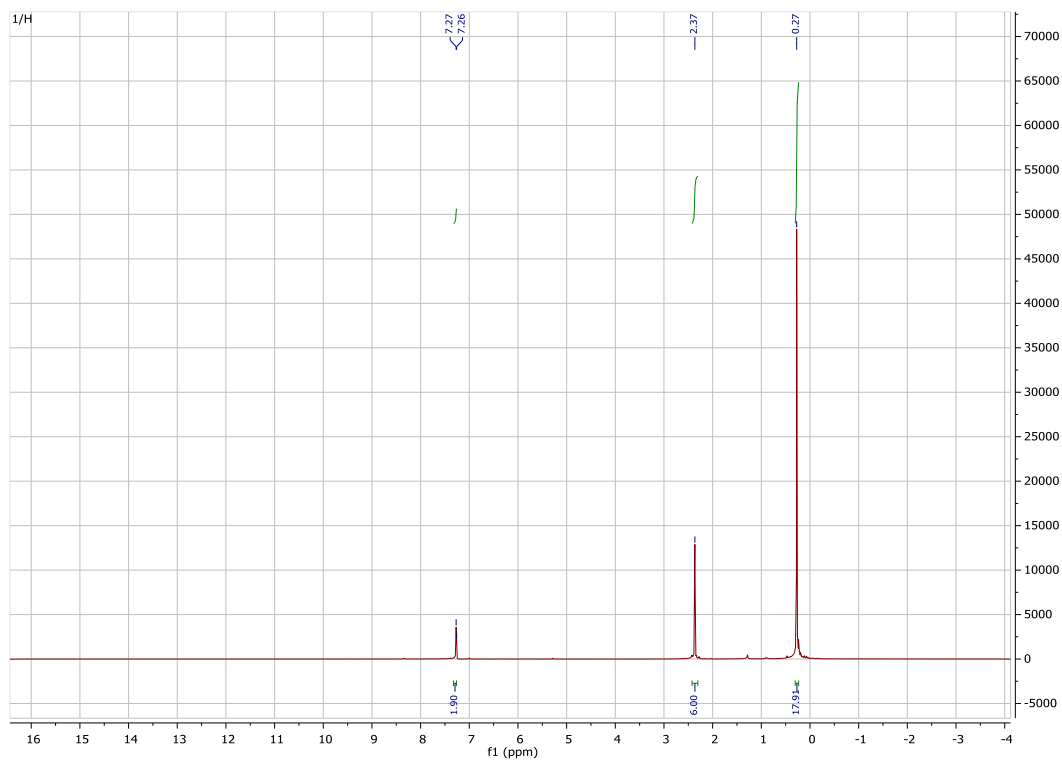
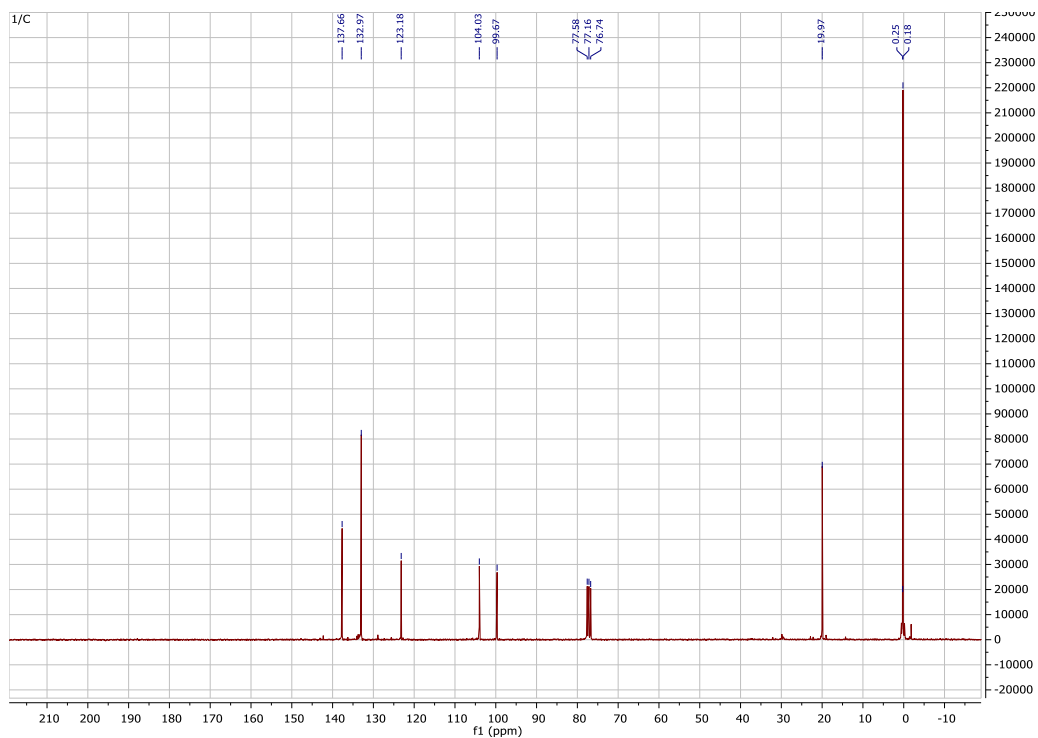
Figure S1. ^1H NMR (300 MHz, CDCl_3) spectrum of compound **1**Figure S2 : ^{13}C NMR (300 MHz, CDCl_3) spectrum of compound **1**

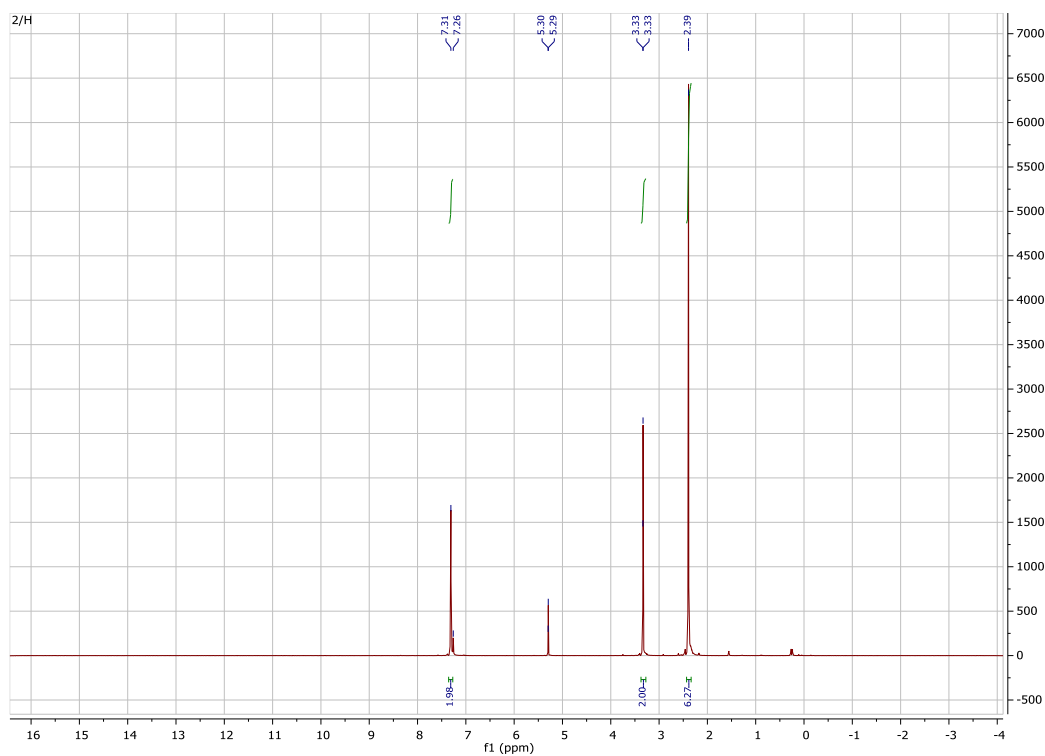
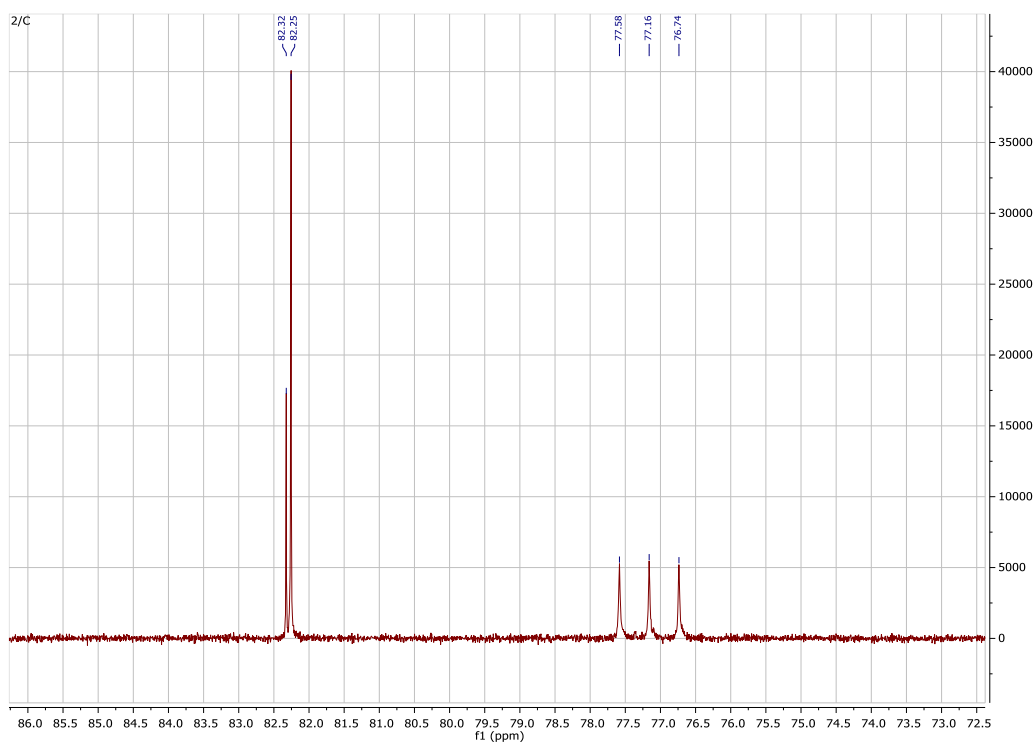
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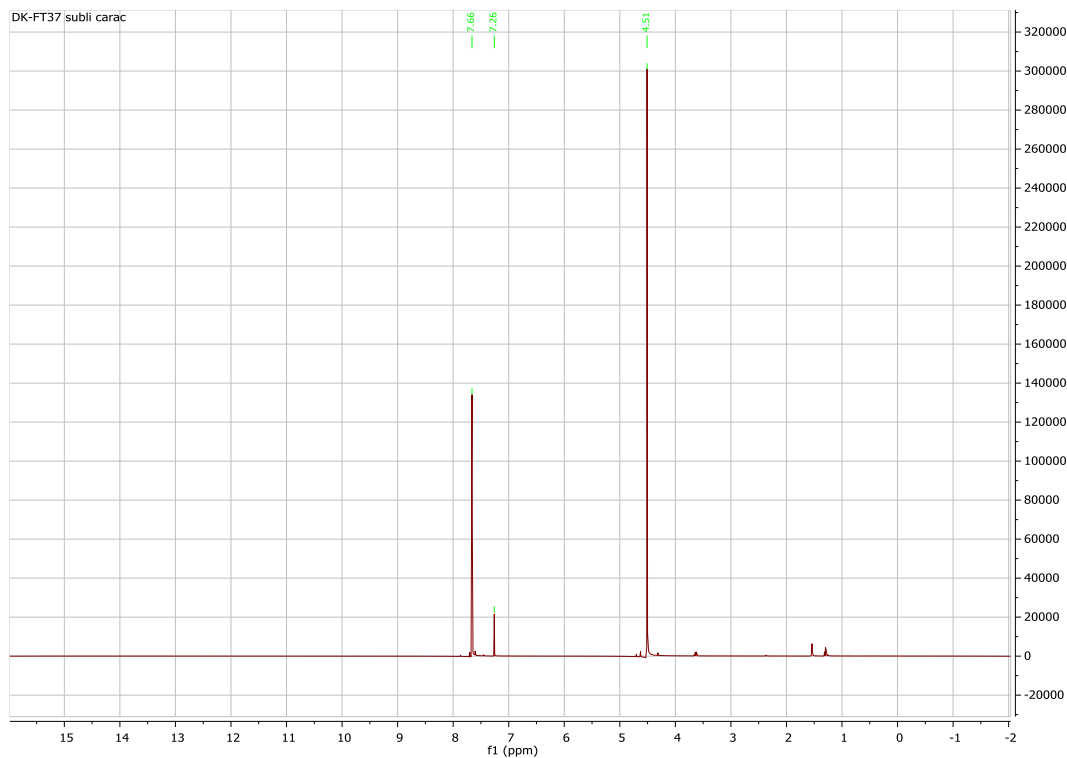
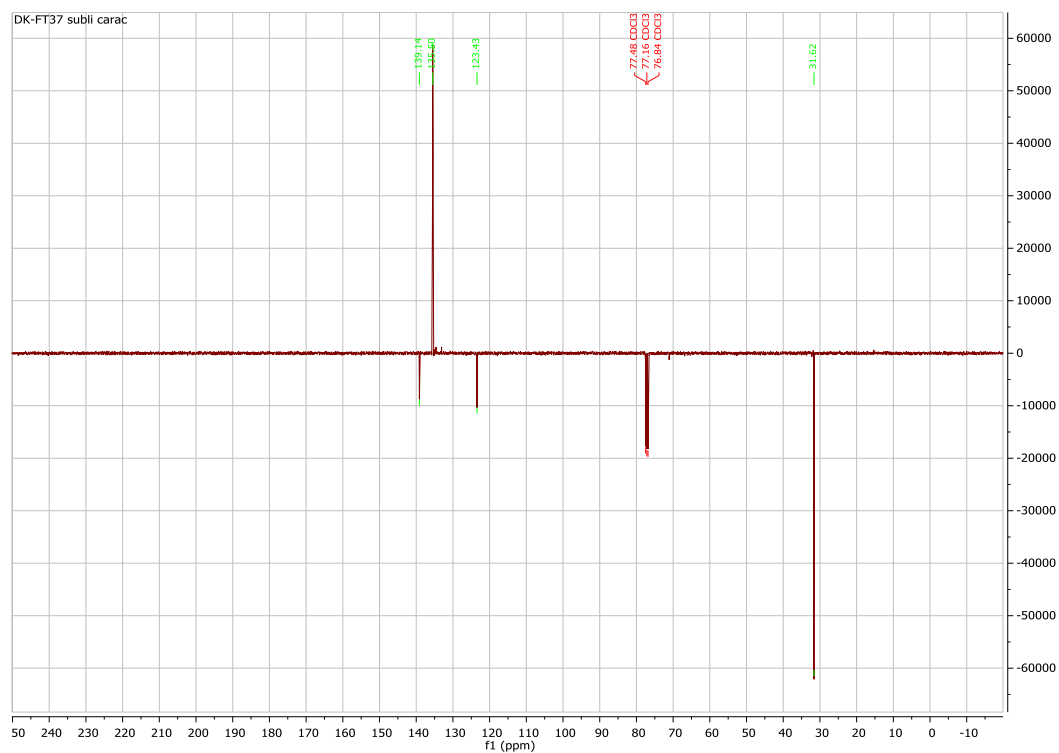
Figure S5 : ^1H NMR (300 MHz, CDCl_3) spectrum of compound **3**Figure S6 : ^{13}C NMR (300 MHz, CDCl_3) spectrum of compound **3**

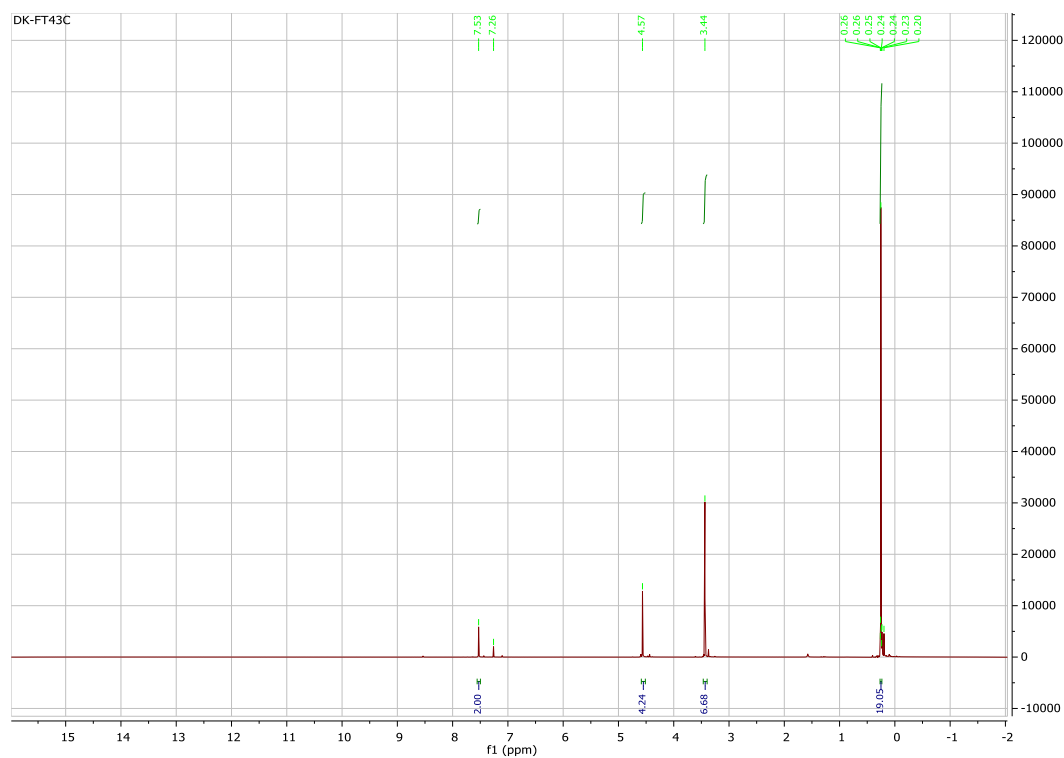
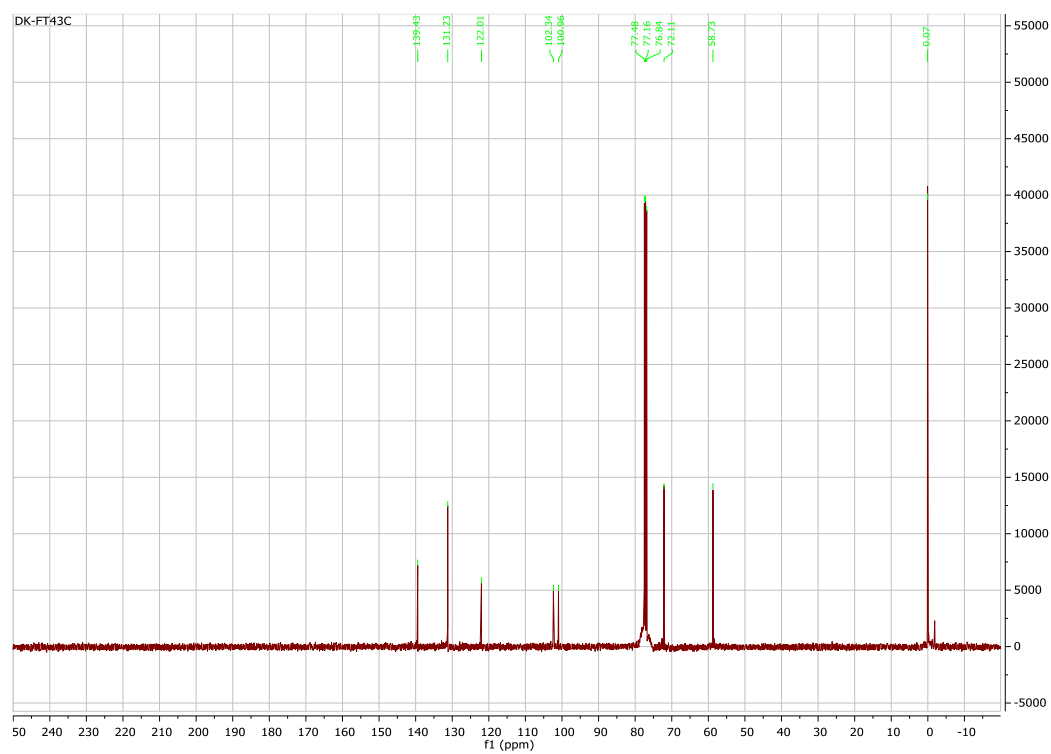
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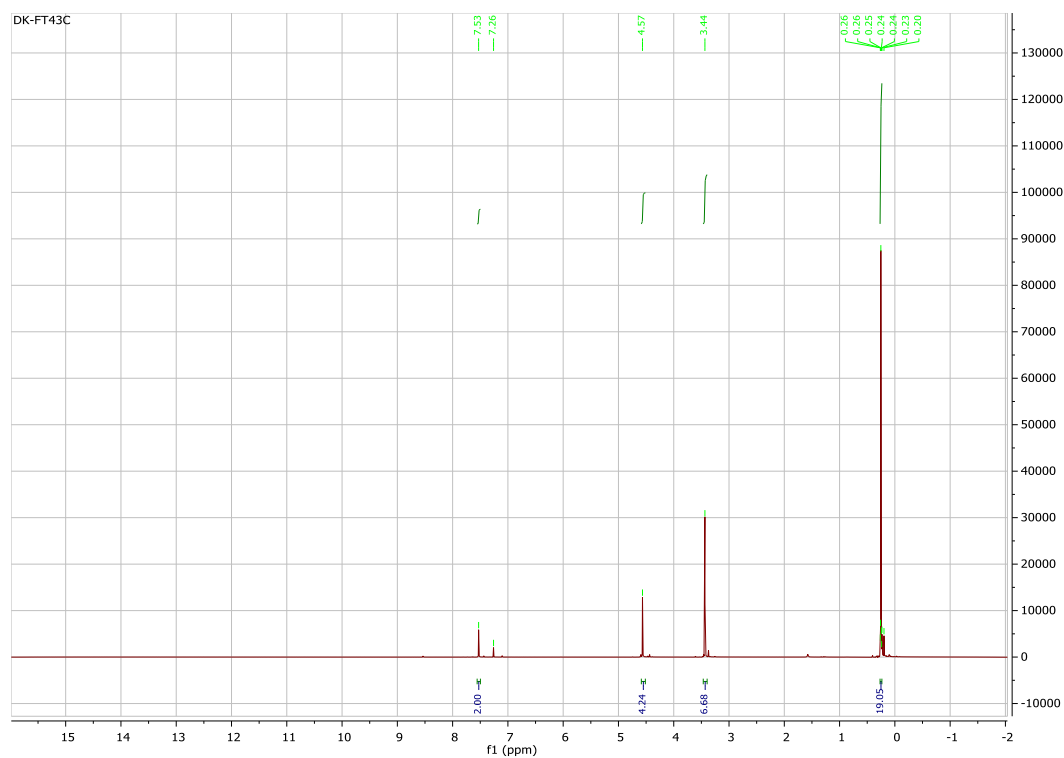
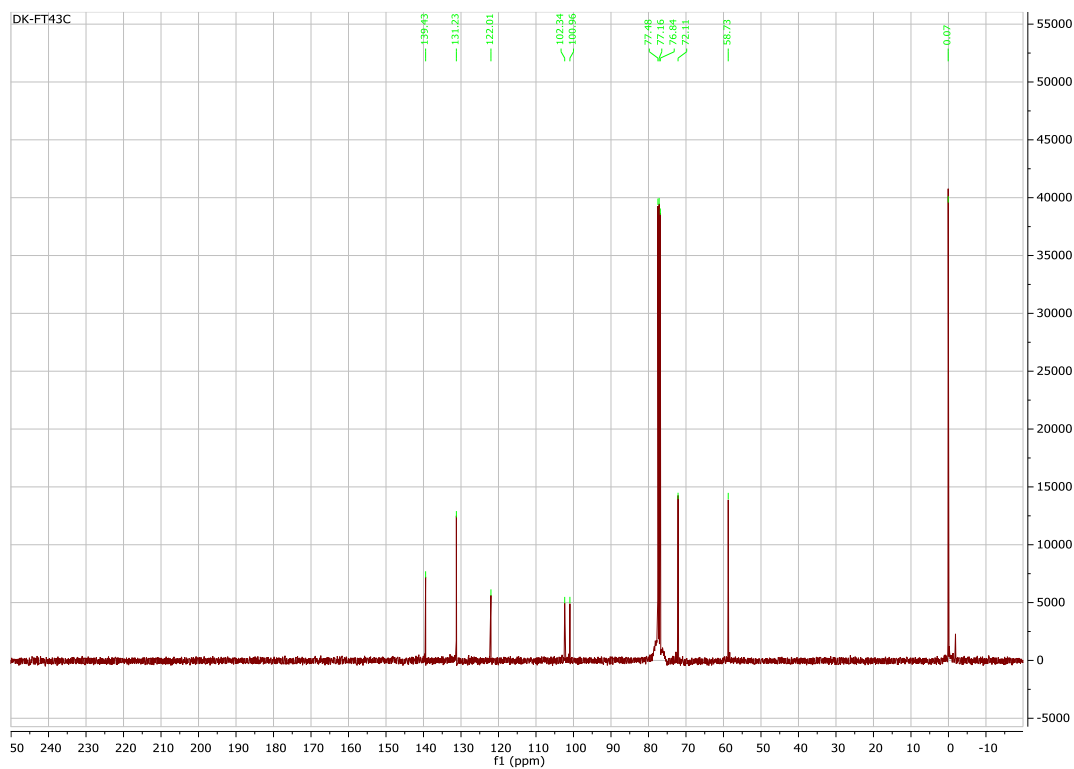
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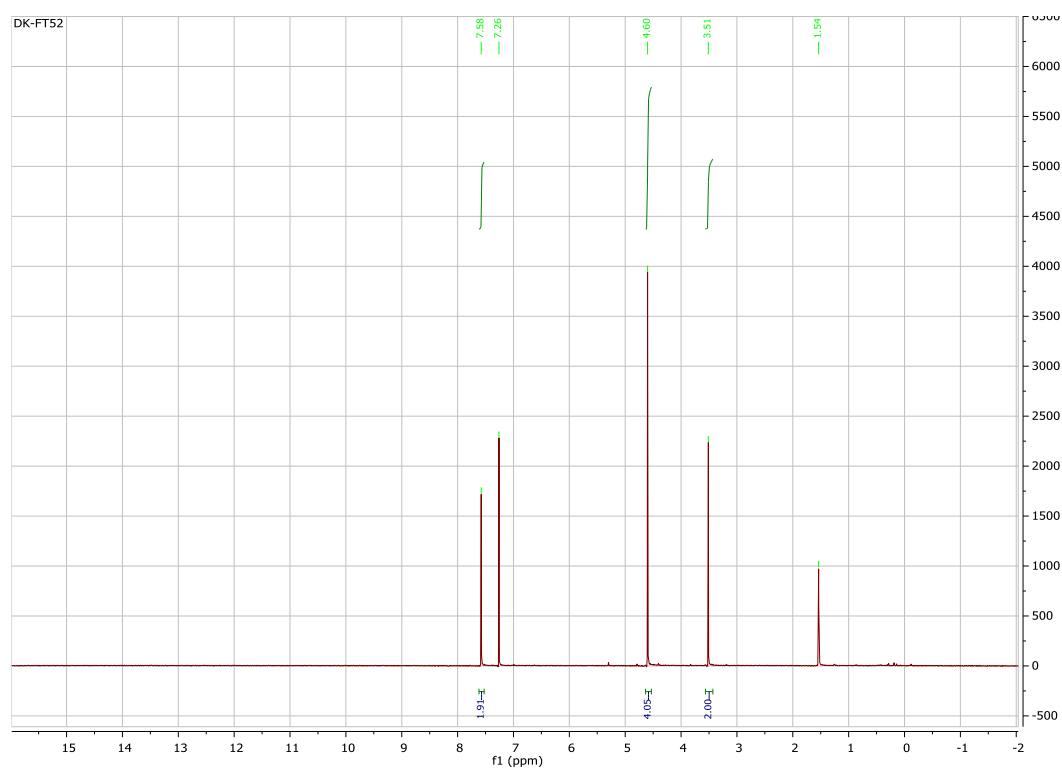
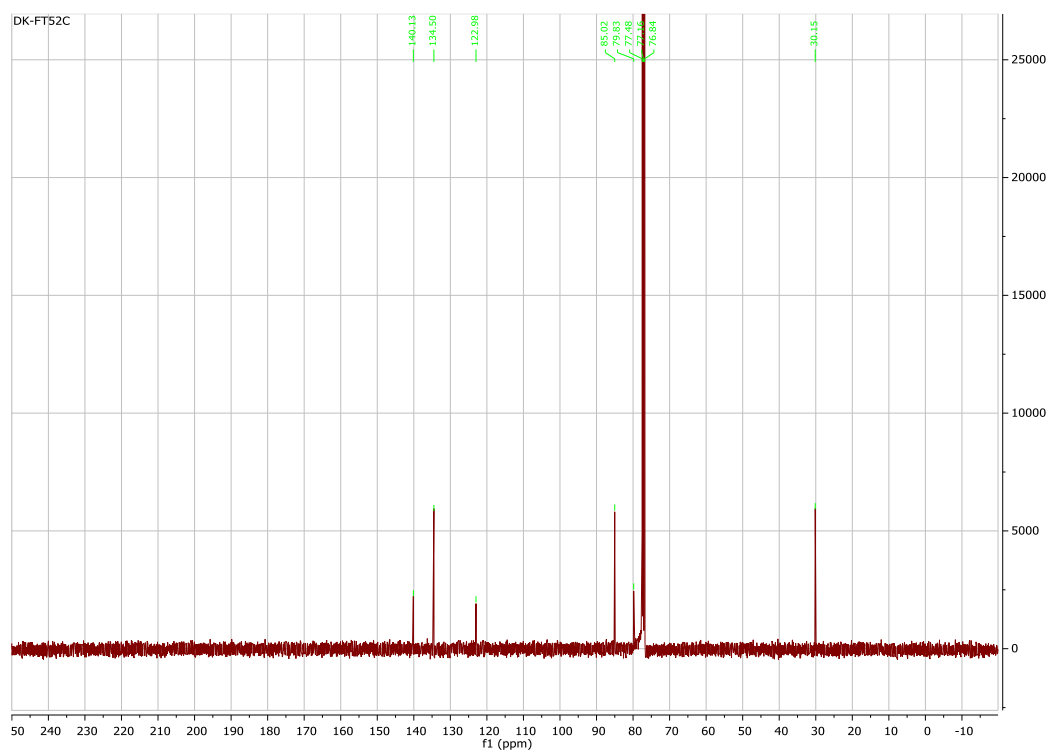
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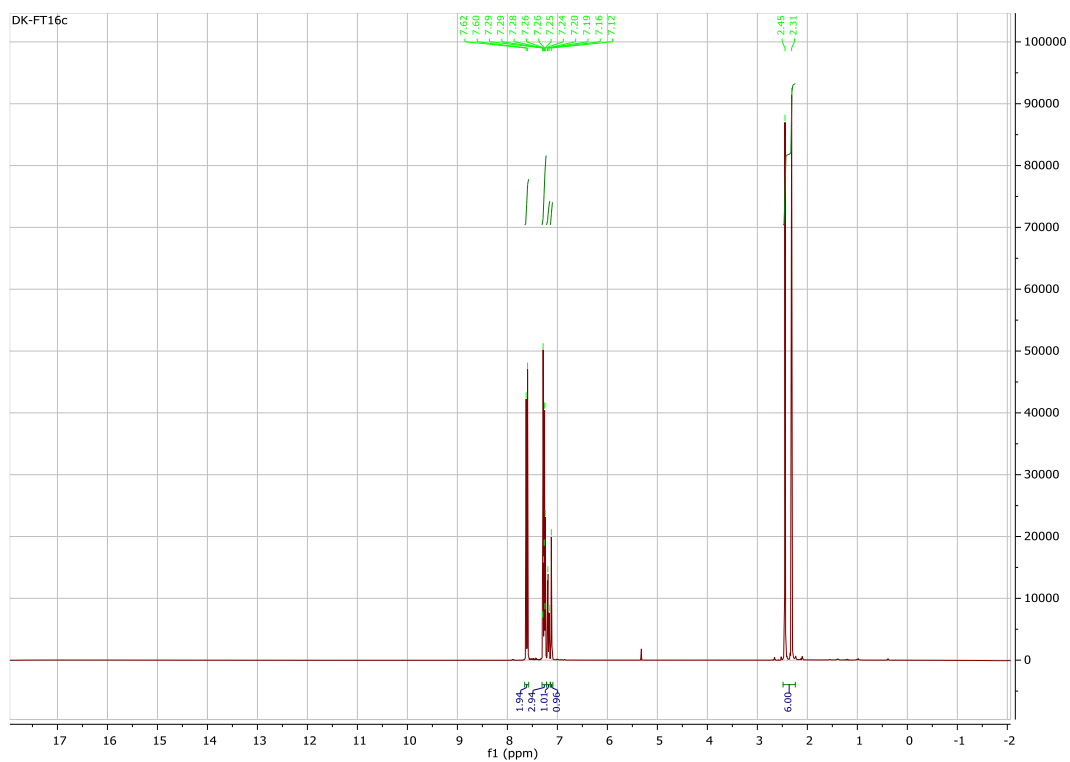
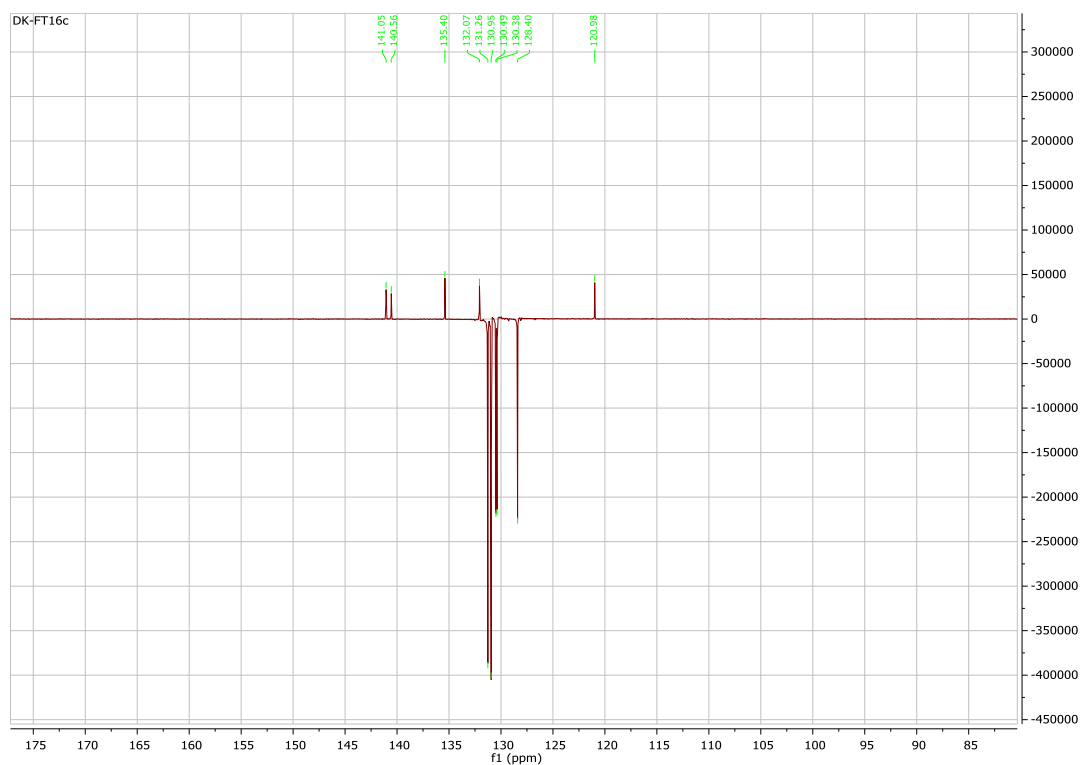
Figure S13 : ^1H NMR (300 MHz, CDCl_3) spectrum of compound **7**Figure S14 : ^{13}C NMR (300 MHz, CDCl_3) spectrum of compound **7**

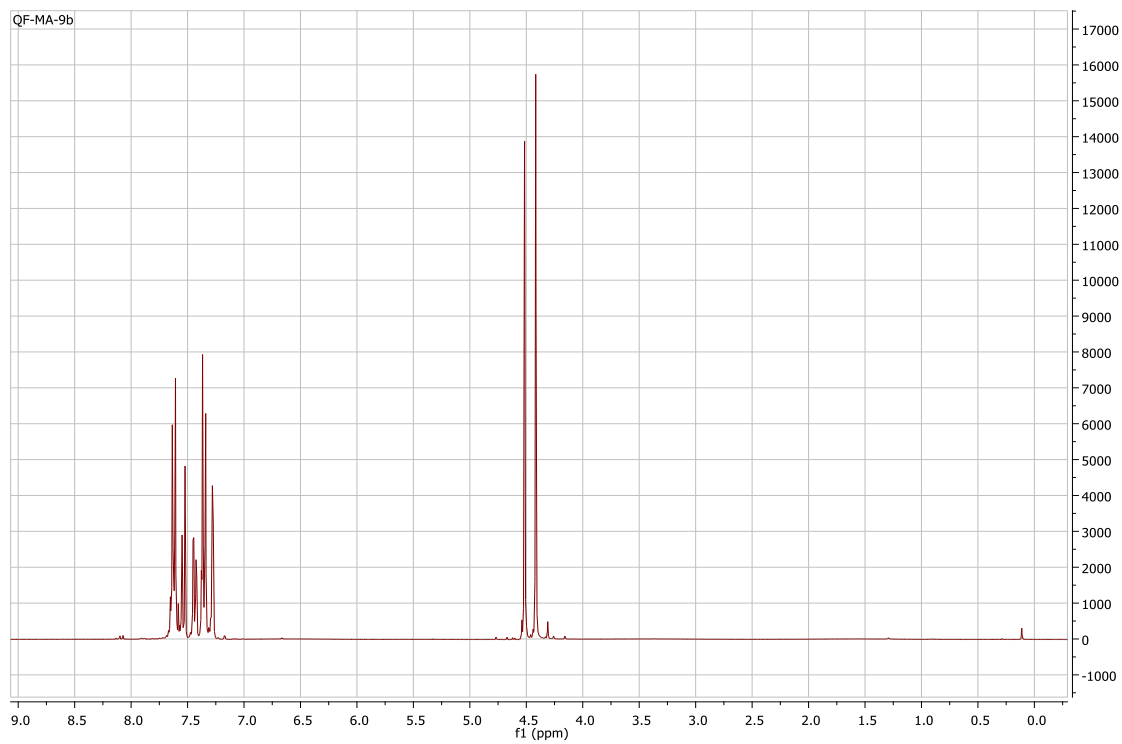
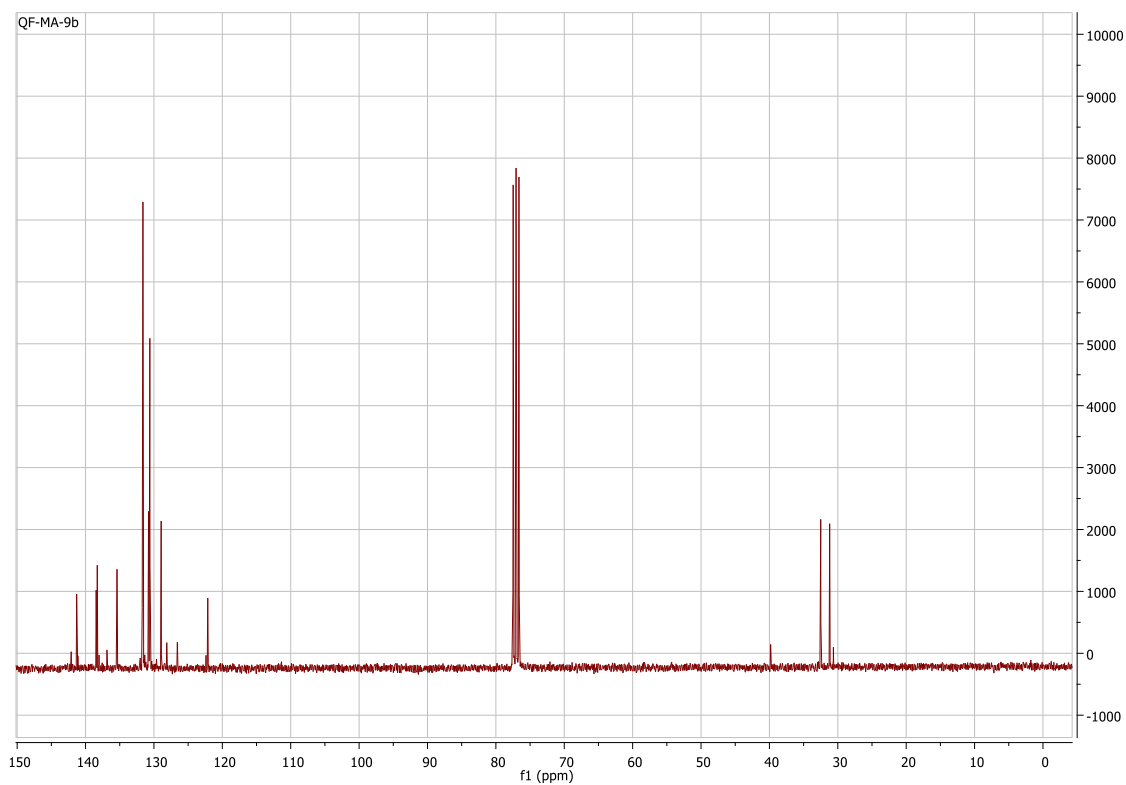
Figure S15 : ^1H NMR (300 MHz, CDCl_3) spectrum of compound **8b**Figure S16 : ^{13}C NMR (300 MHz, CDCl_3) spectrum of compound **8b**

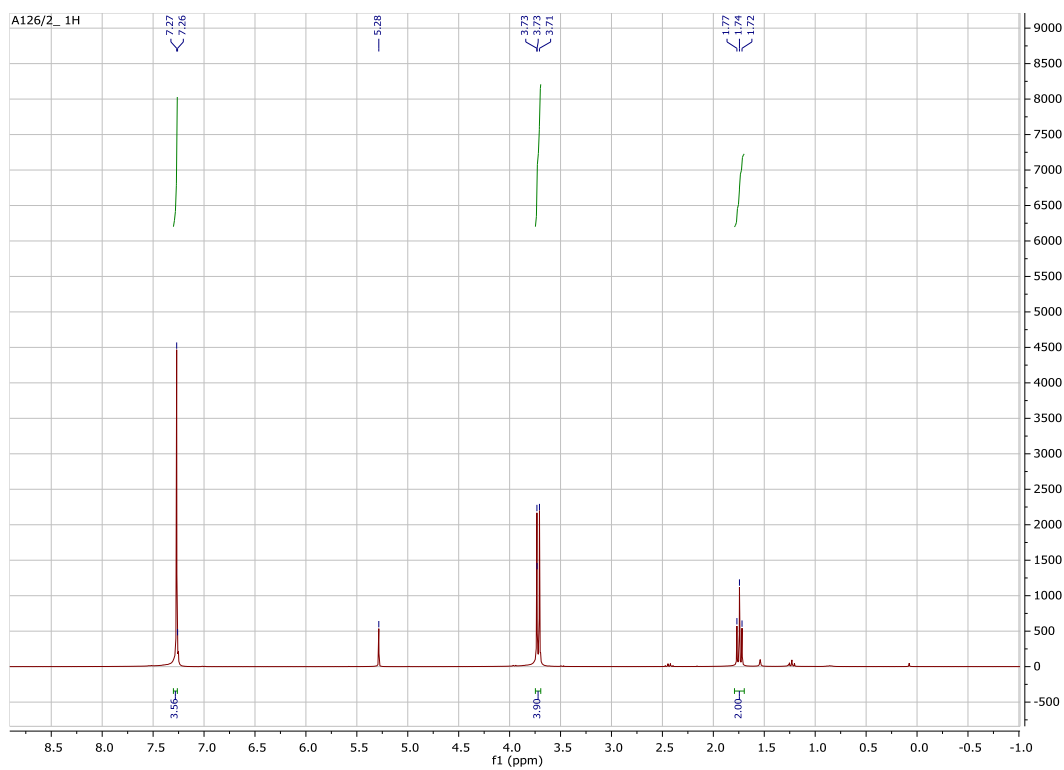
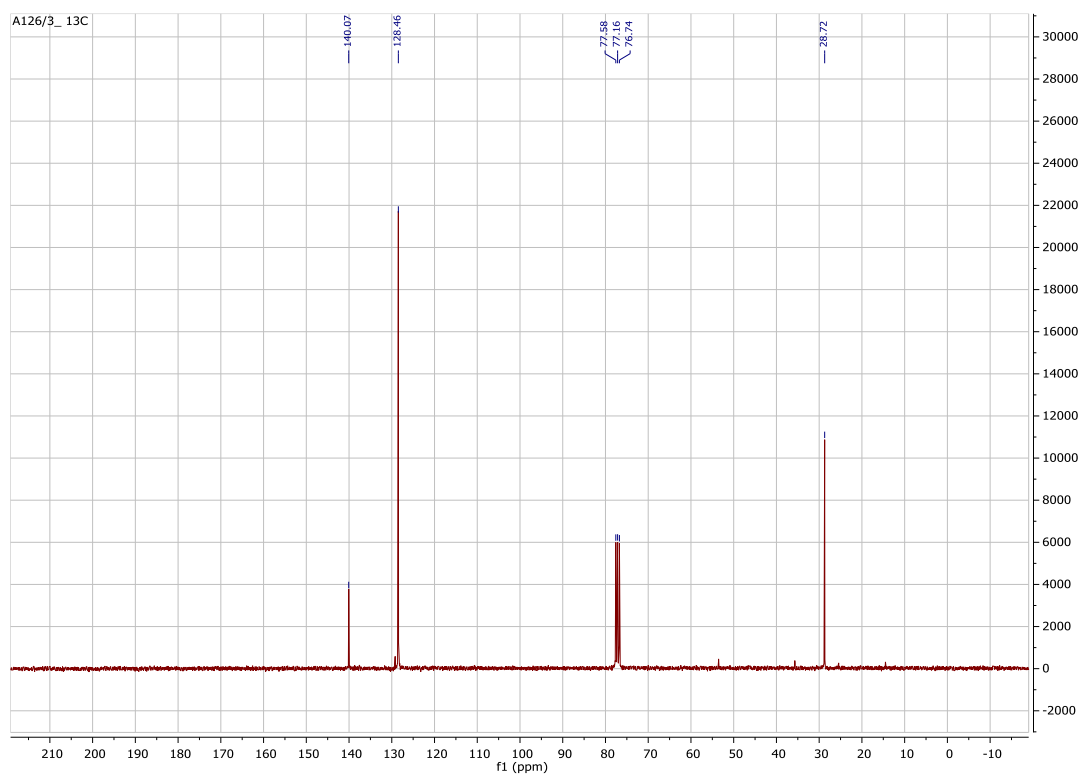
Figure S17 : ^1H NMR (300 MHz, CDCl_3) spectrum of compound **9a**Figure S18 : ^{13}C NMR (300 MHz, CDCl_3) spectrum of compound **9a**

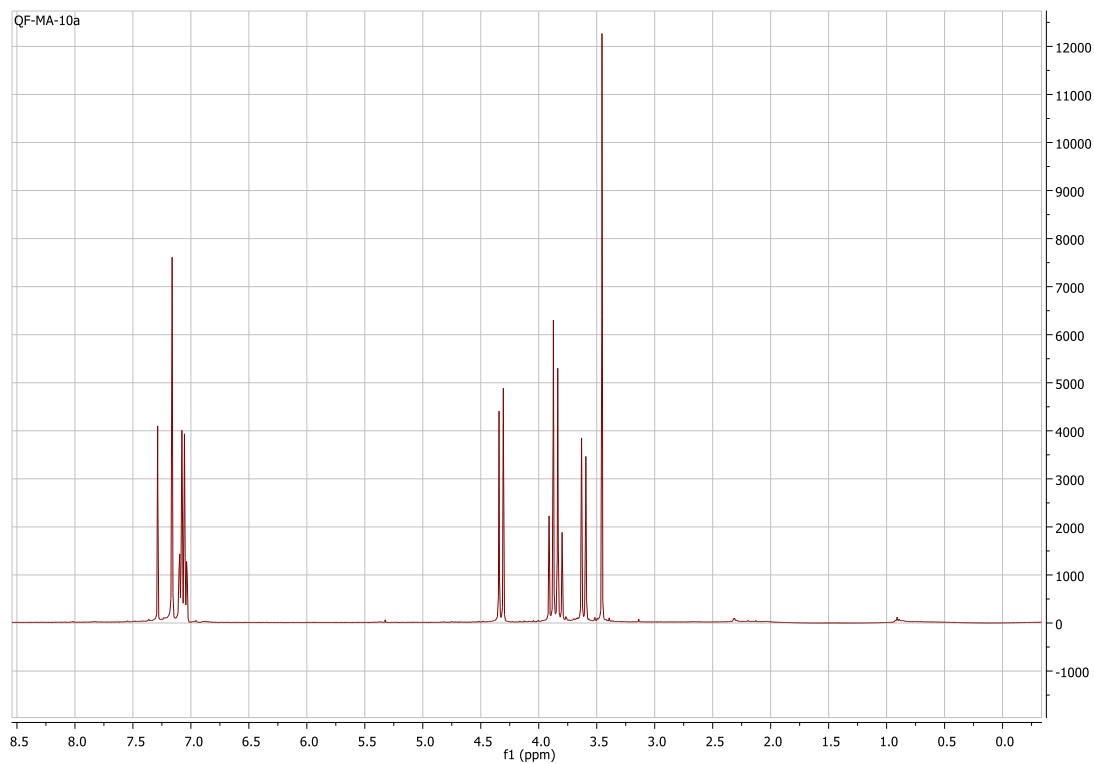
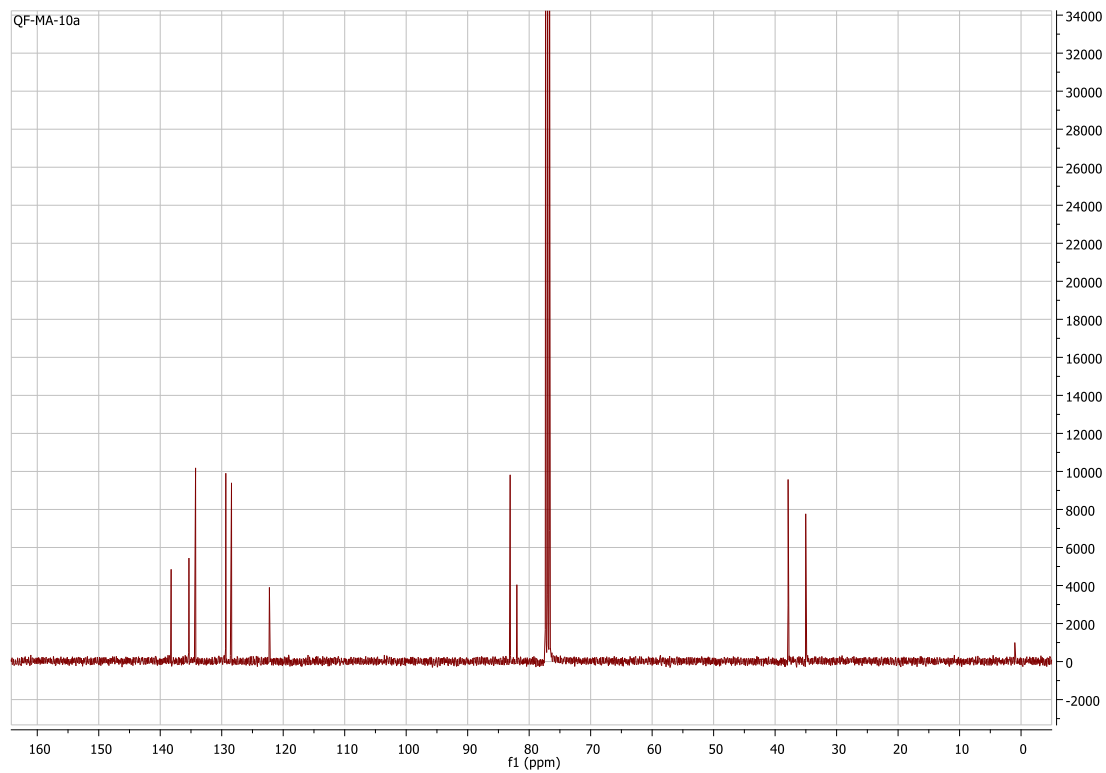
Figure S19 : ^1H NMR (300 MHz, CDCl_3) spectrum of compound **10a**Figure S20 : ^{13}C NMR (300 MHz, CDCl_3) spectrum of compound **10a**

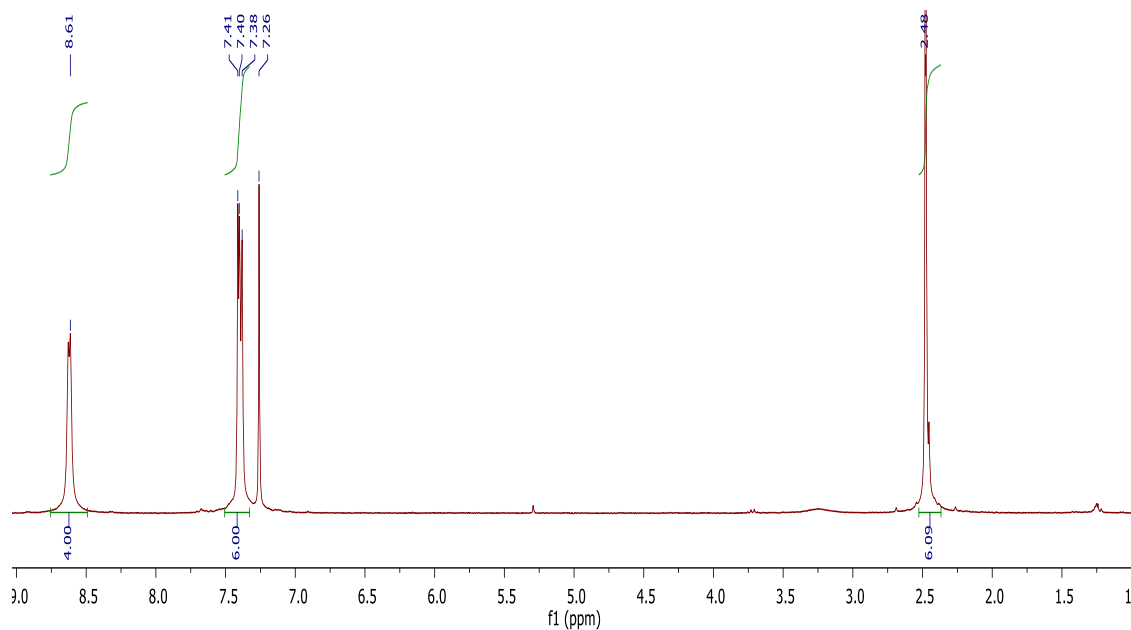
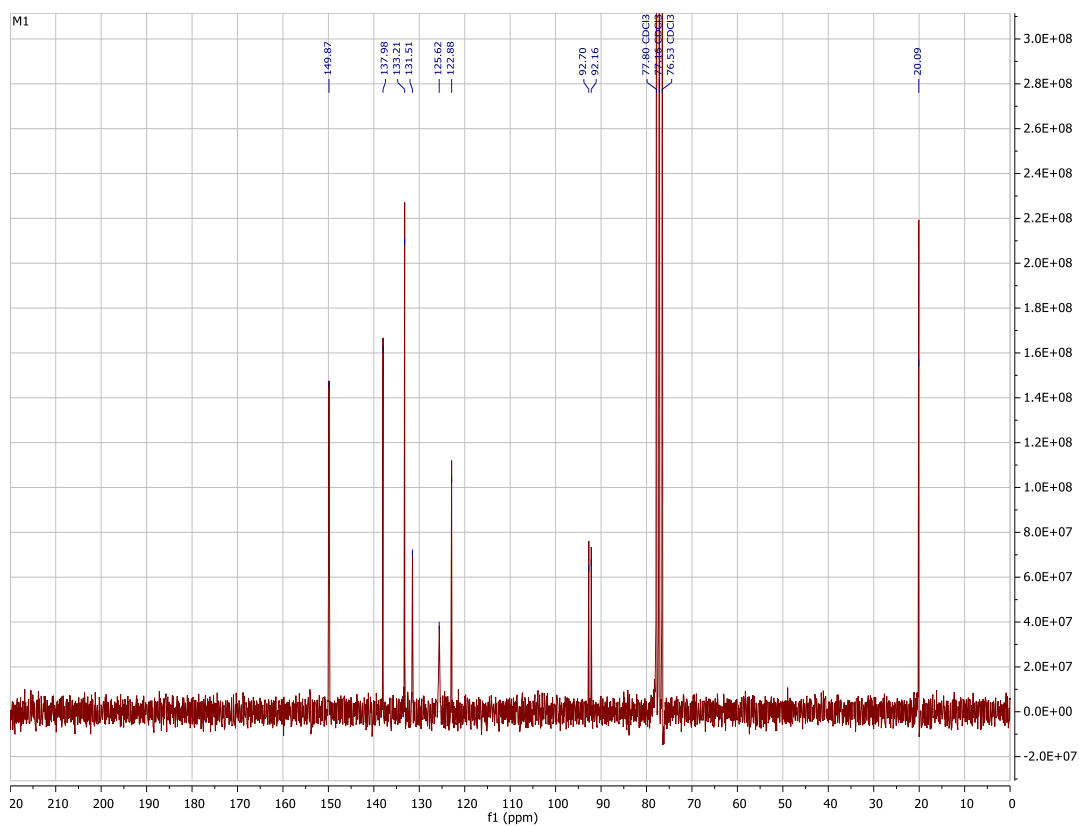
Figure S21 : ^1H NMR (300 MHz, CDCl_3) spectrum of compound PFigure S22 : ^{13}C NMR (300 MHz, CDCl_3) spectrum of compound P

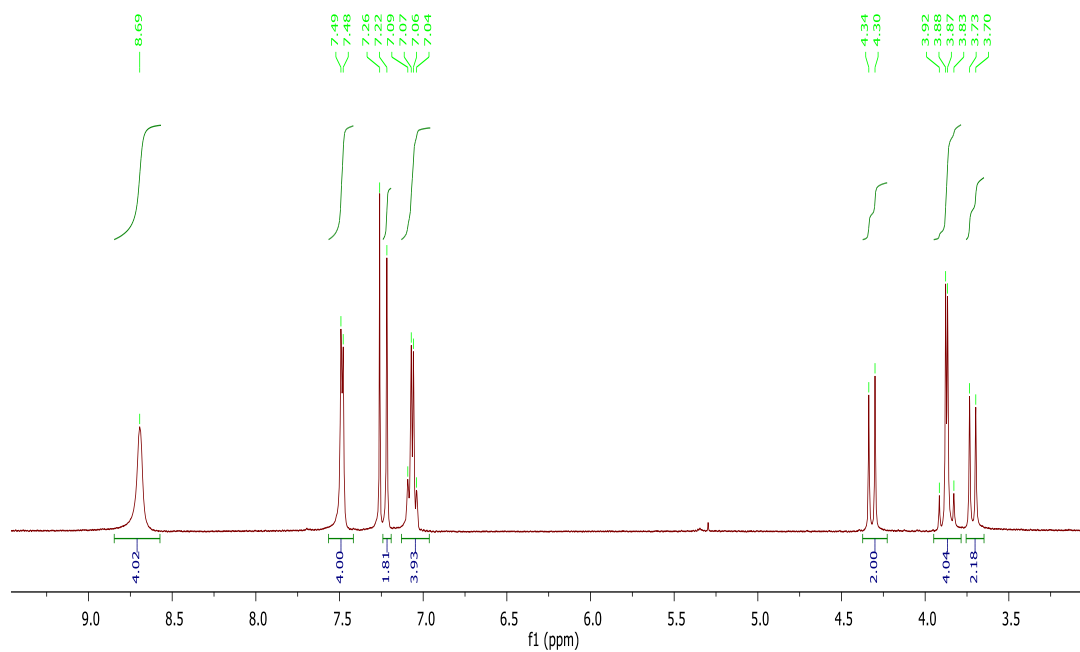
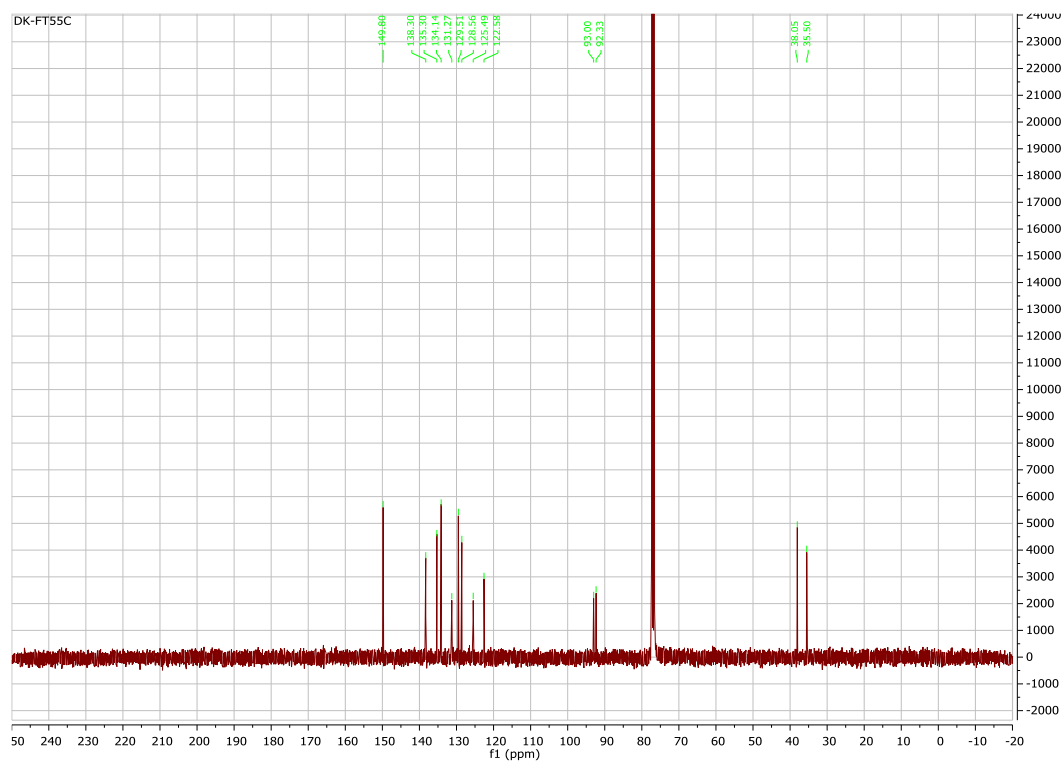
Figure S23 : ^1H NMR (300 MHz, CDCl_3) spectrum of compound CFigure S24 : ^{13}C NMR (300 MHz, CDCl_3) spectrum of compound C

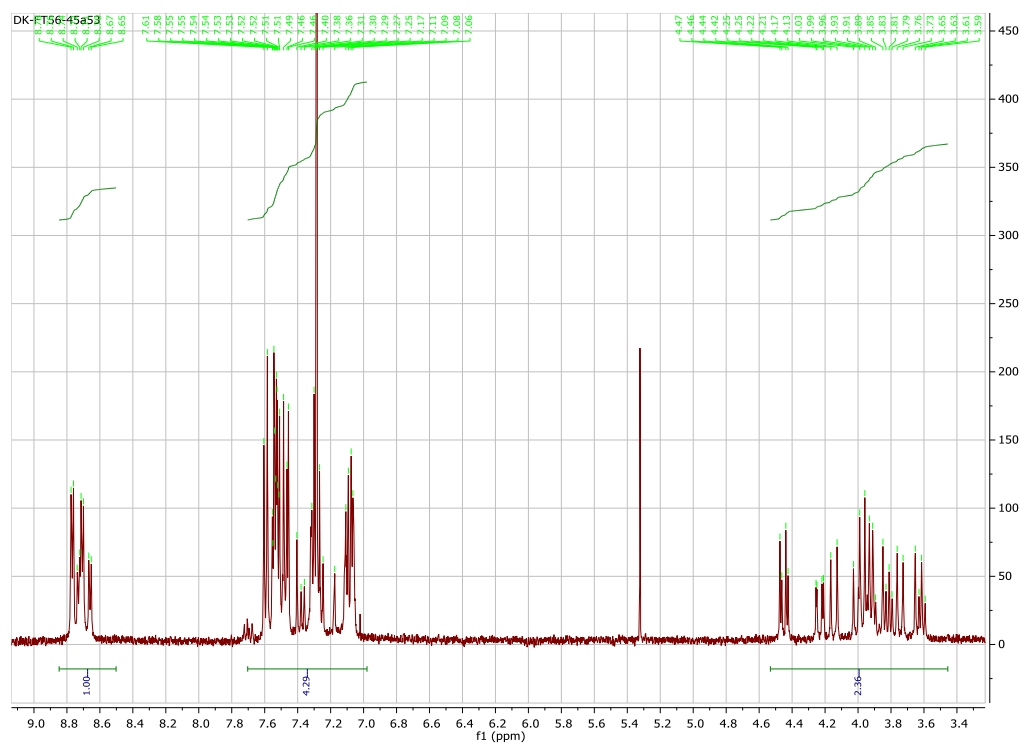
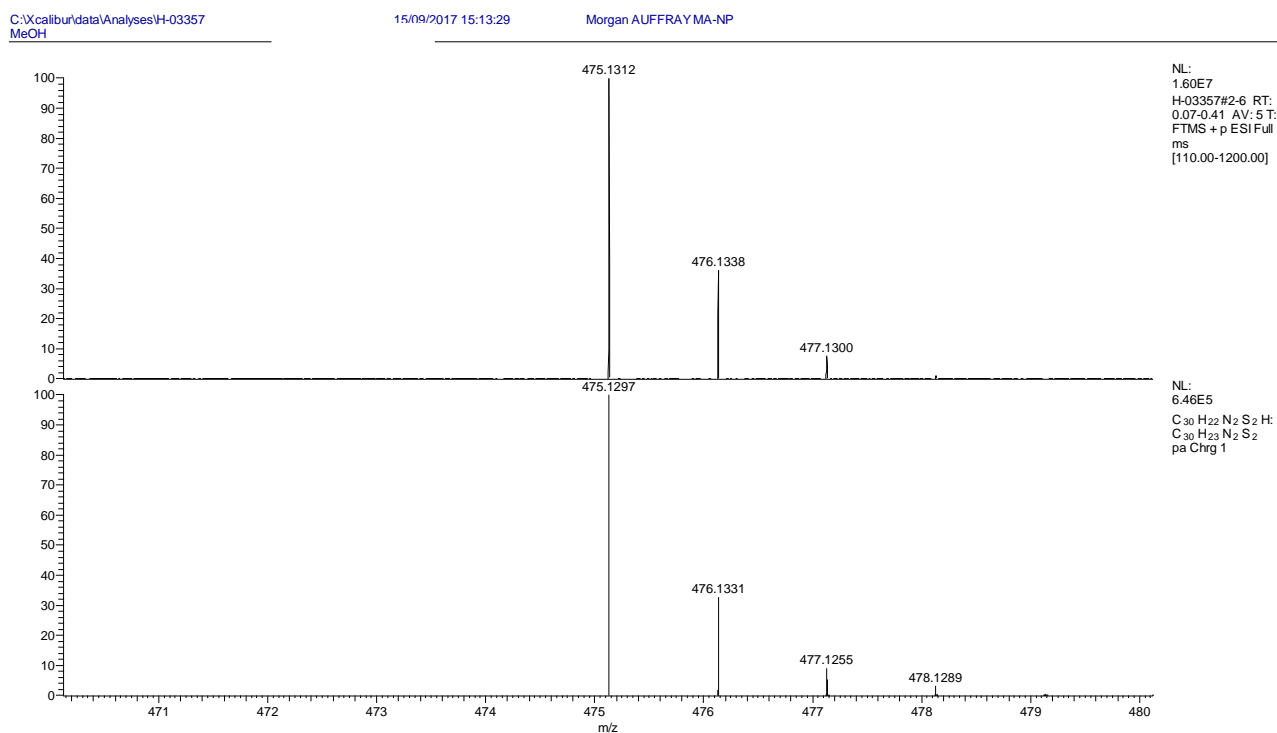
Figure S25 : ^1H NMR (300 MHz, CDCl_3) spectrum of compound JT

Figure S26 : HRMS for compound P : (EI) m/z (%) for C₂₂H₁₆N₂; calcd 308.1313; found 308.1315.

Error = 3.1 ppm Relative intensity (%) 100

Calcul of monoisotopic masses – 1.00728 Th (-H⁺).
– 22.98922 Th (-Na⁺).
– 38.96316 Th (-K⁺).

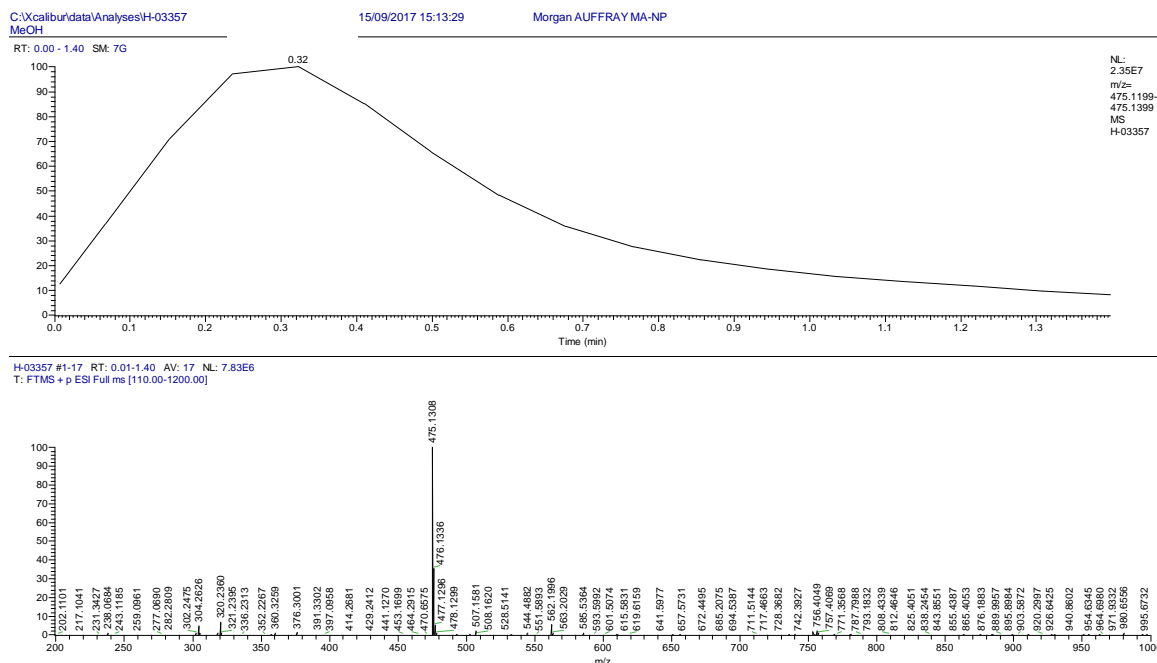
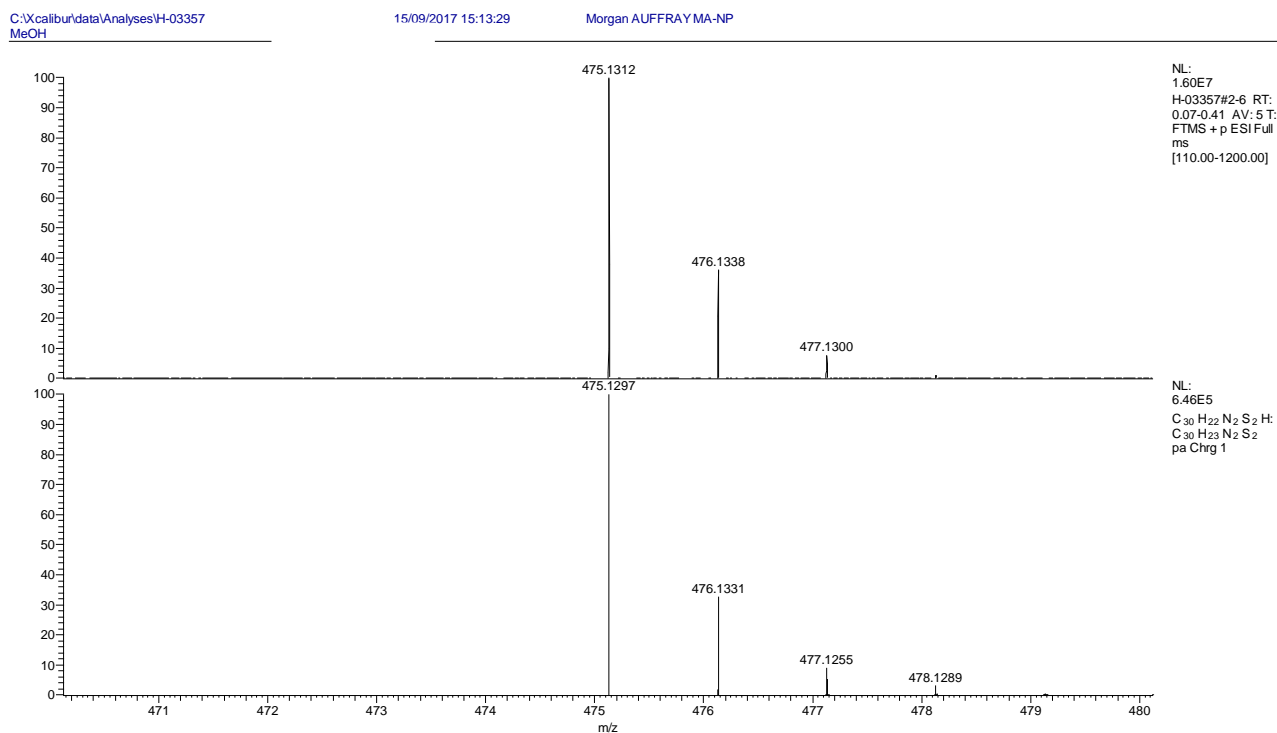


Figure S27: HRMS for compound C : (EI) m/z (%) for C₃₀H₂₂N₂S₂; calcd 474.1224; found 474.1224.

Error = 3.1 ppm Relative intensity (%) 100

Calcul of monoisotopic masses – 1.00728 Th (-H⁺).
–22.98922 Th (-Na⁺).
–38.96316 Th (-K⁺).

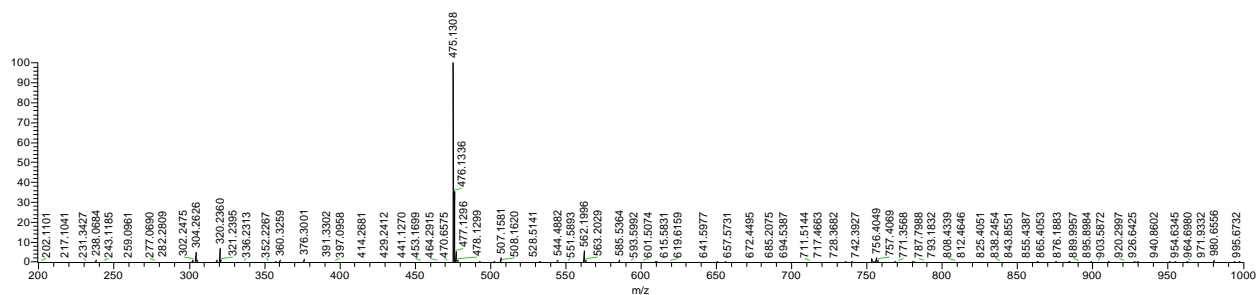
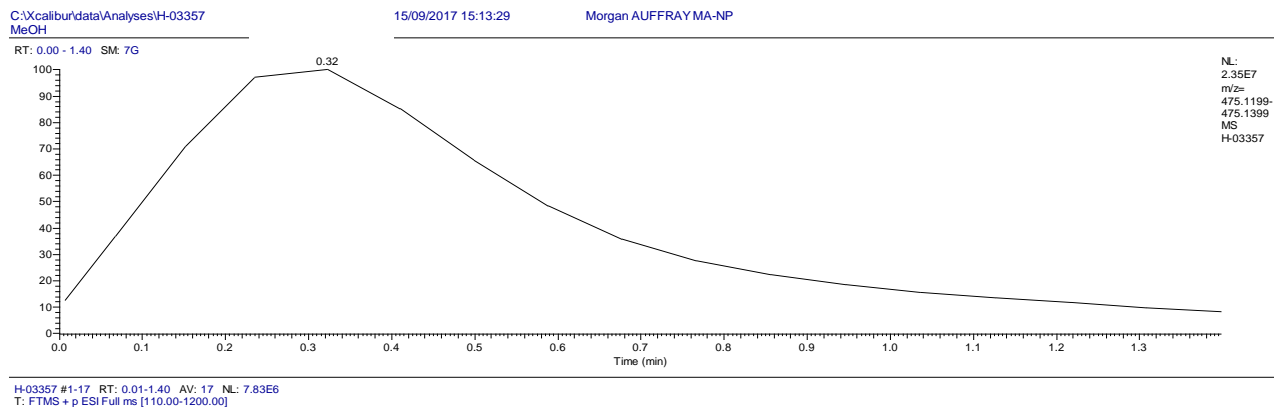
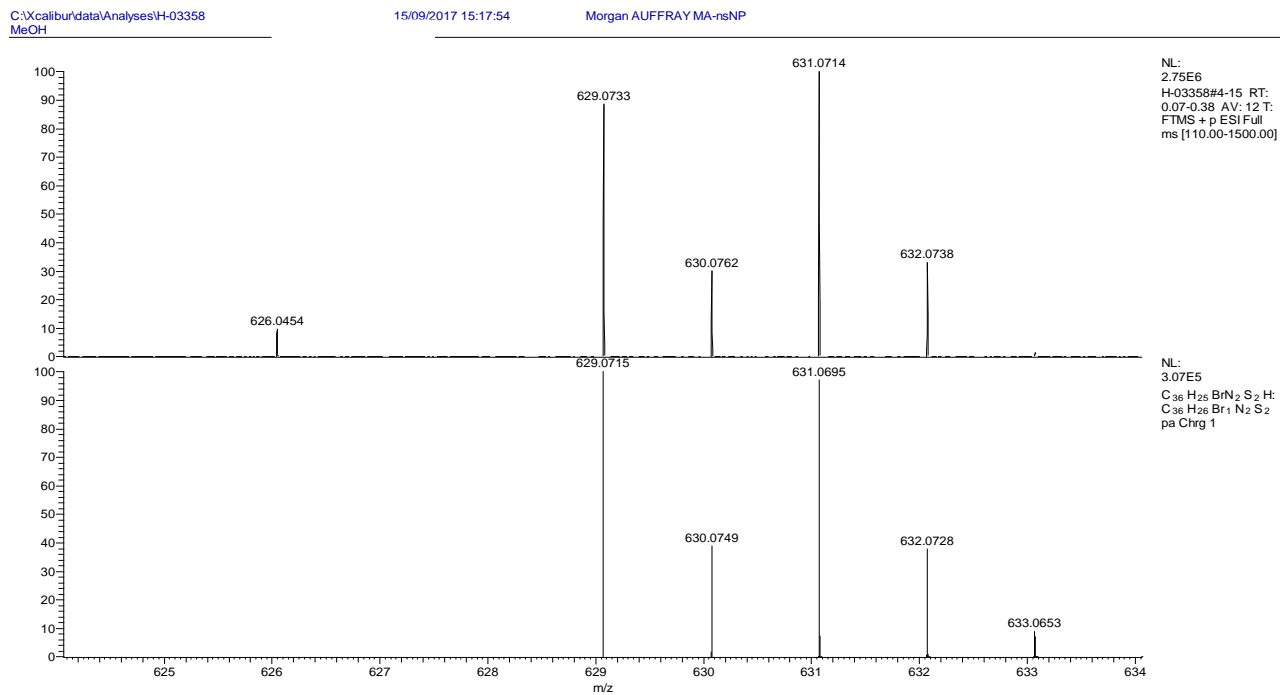
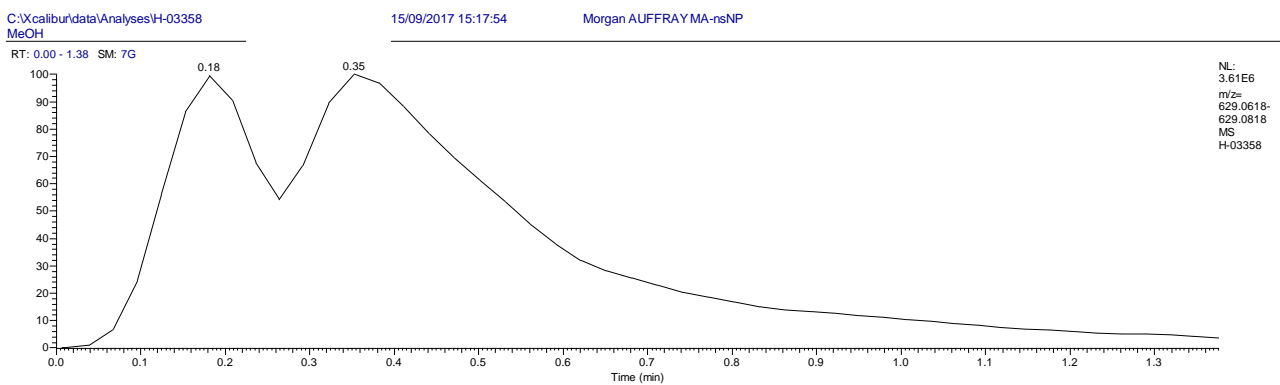


Figure S28 : HRMS for compound JT : (EI) m/z (%) for C₃₆H₂₅N₂S₂; calcd 628.0643; found 628.0642.

Error = 2.8 ppm ; Relative intensity (%) 100

Calcul of monoisotopic masses – 1.00728 Th (-H⁺),
– 22.98922 Th (-Na⁺),
– 38.96316 Th (-K⁺).



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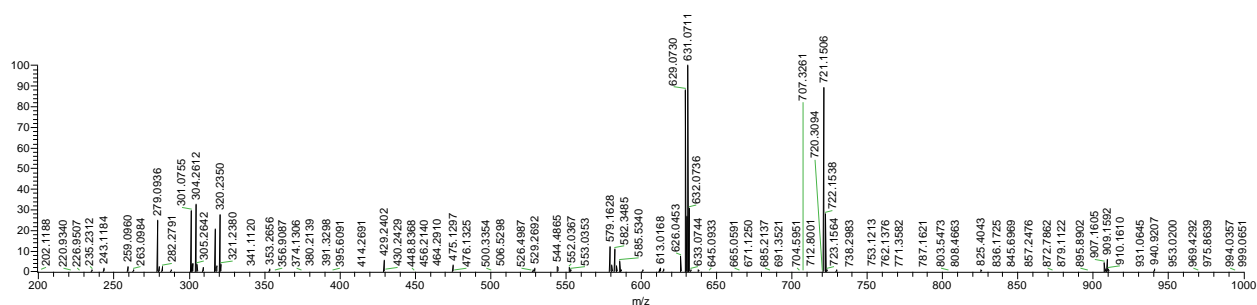


Figure S29 : IR spectra spectra recorded on bulk after evaporation or filtration of the supramolecular complexes prepared.....18 in solution by simply mixing P with bis(benzonitrile)-palladium(II) for coordination (P-PdII), terephthalic acid for hydrogen bond (P-TPA) and finally 1,4-diiodobenzene for halogen bond (P-IPI).

