Supporting Information

Pyridinium Modified β-Cyclodextrin: An Ionic Supramolecular Ligand for Palladium acetate in C-C Coupling Reactions in Water

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Spectrum data for pyridinium modified β-cyclodextrin:

NMR spectrum for *N*-octyl-pyridine-2-amine(2).

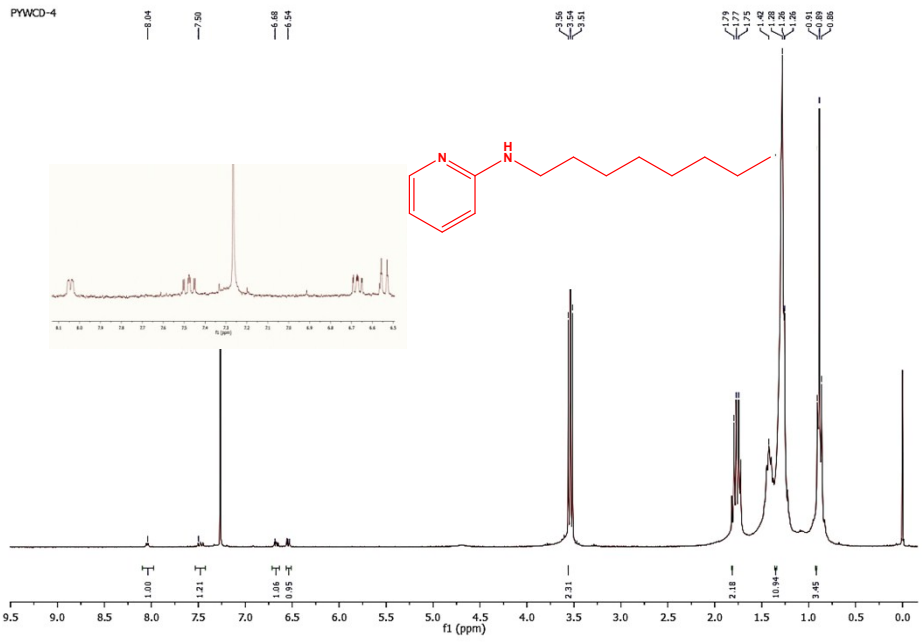

Figure S1. ^{1}H-NMR (300 MHz, $CDCl_3$) spectrum of *N*-octyl-pyridine-2-amine **(2).**

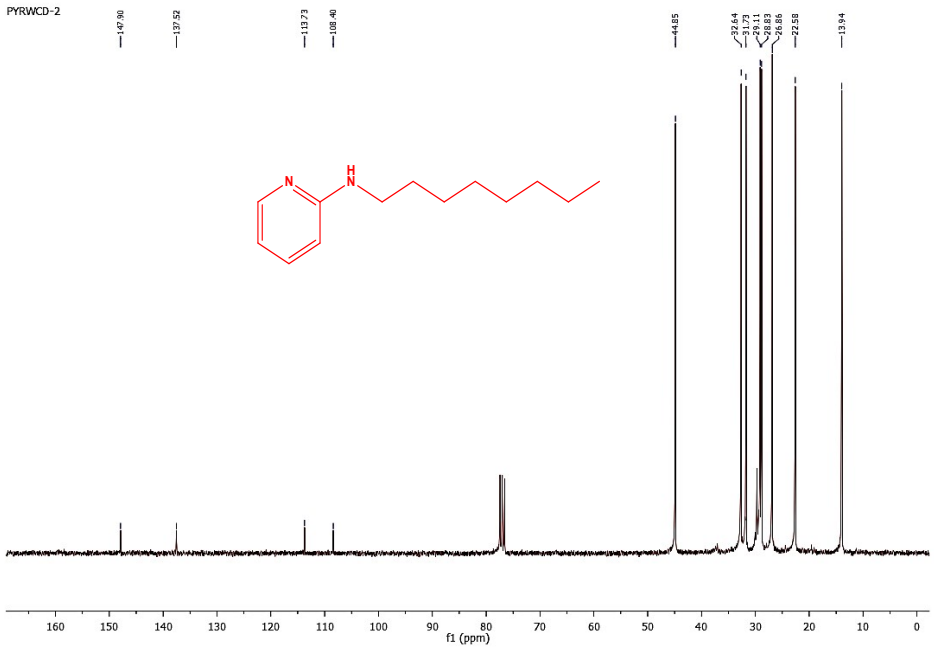

Figure S2. ^{13}C-NMR spectrum (75 MHz, $CDCl_3$) of *N*-octyl-pyridine-2-amine **(2).**

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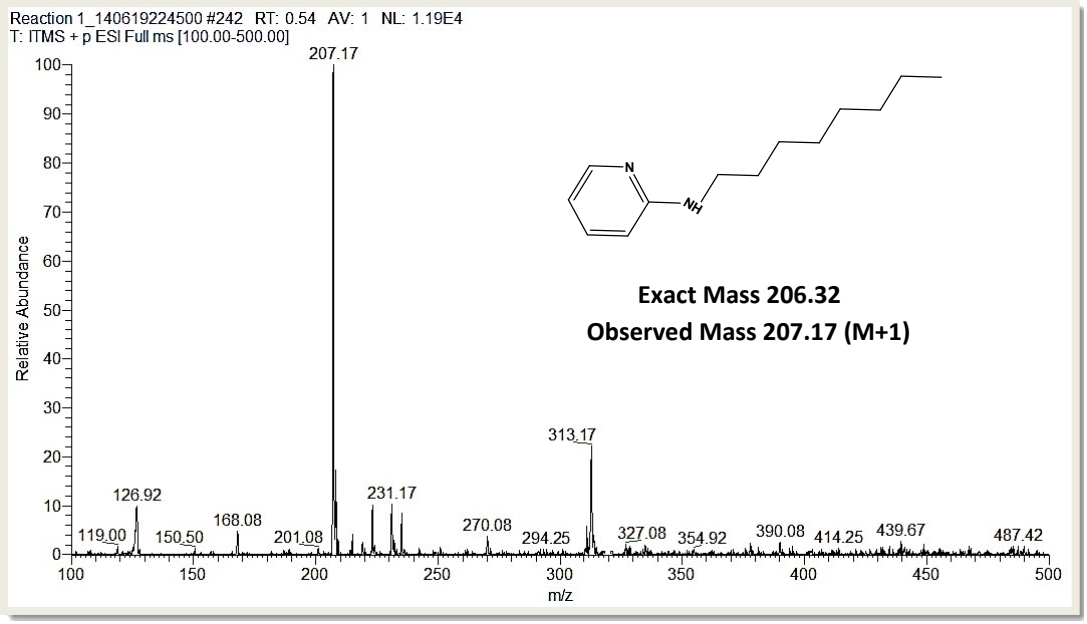


Figure S3. ESI-MS Spectra of *N*-octyl-pyridine-2-amine **(2).**

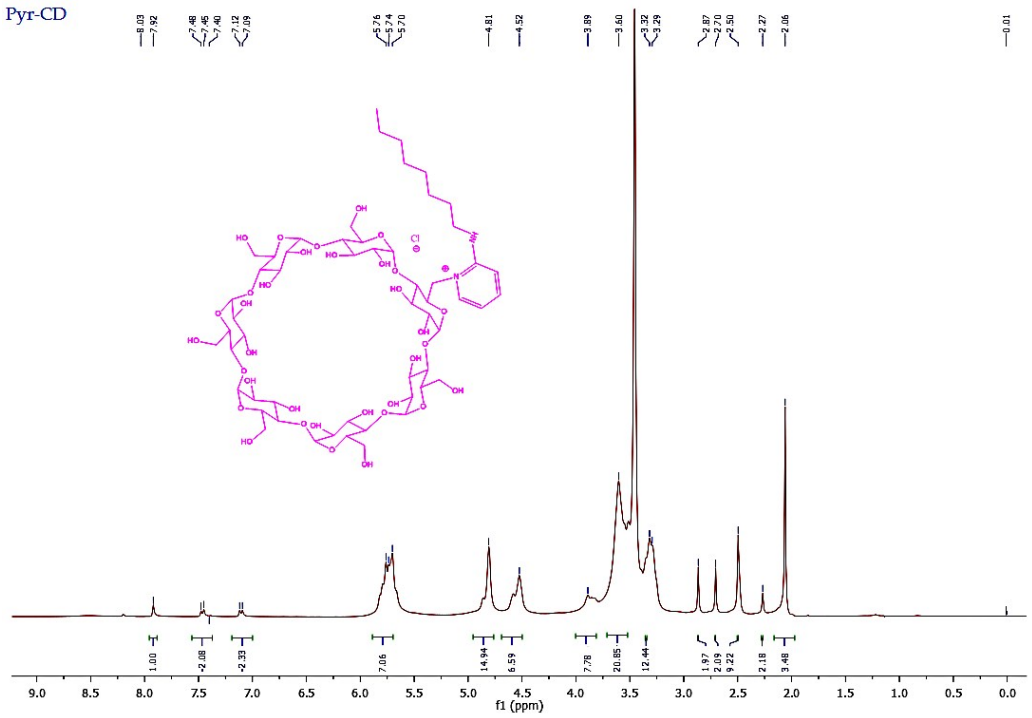


Figure S4. ^{1}H NMR (300 MHz, DMSO-d_6) for pyridinium modified β-cyclodextrin **(3)**.

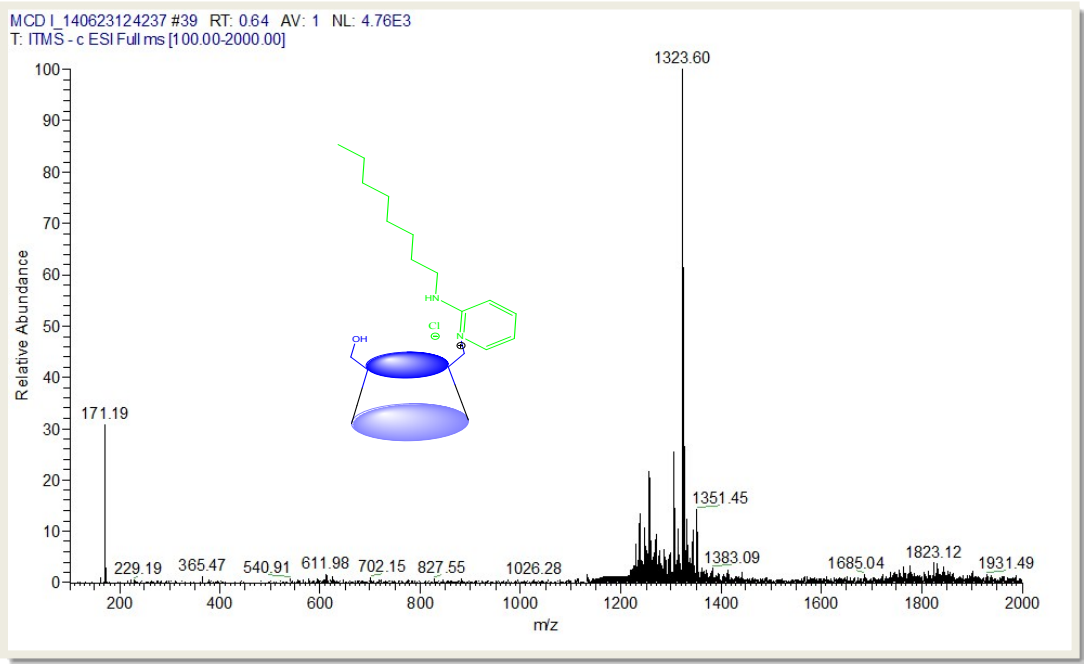


Figure S5. ESI-MS spectrum for pyridinium modified β –cyclodextrin **(3)** (M+1) adduct**.**

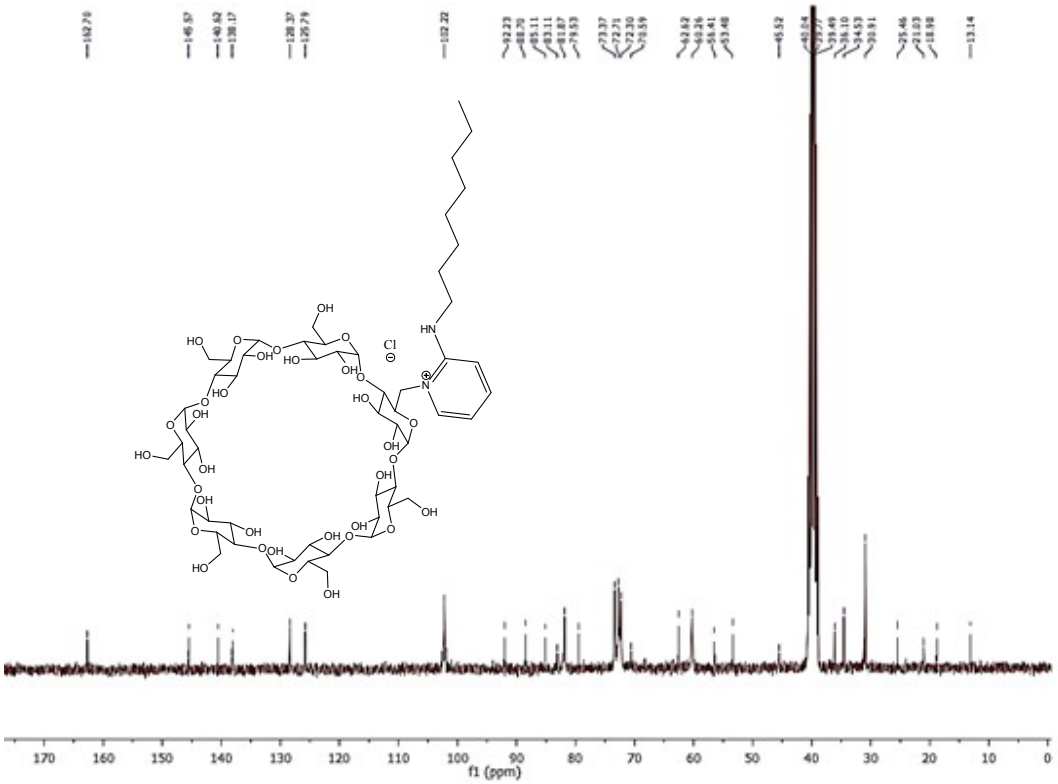


Figure S6. ^{13}C-NMR spectrum (75 MHz, DMSO-d_6) for pyridinium modified β-cyclodextrin **(3).**

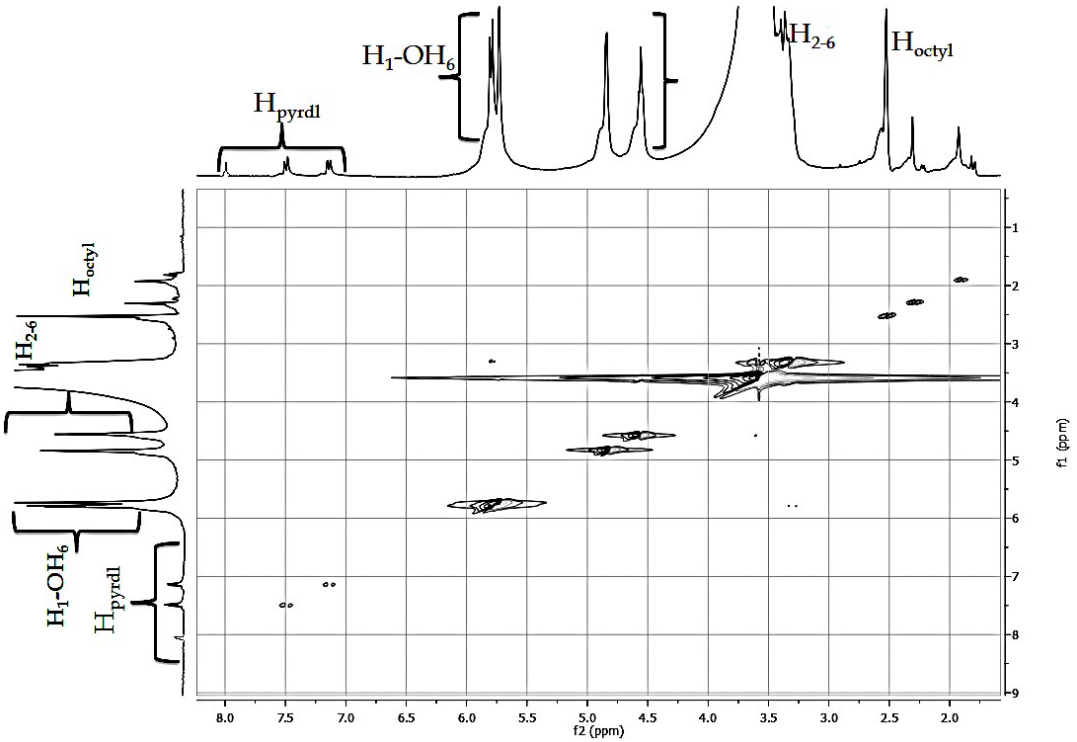


Figure S7. 2D-NOESY NMR spectrum of pyr:β-CD (3) (300 MHz in DMSO-d_6).

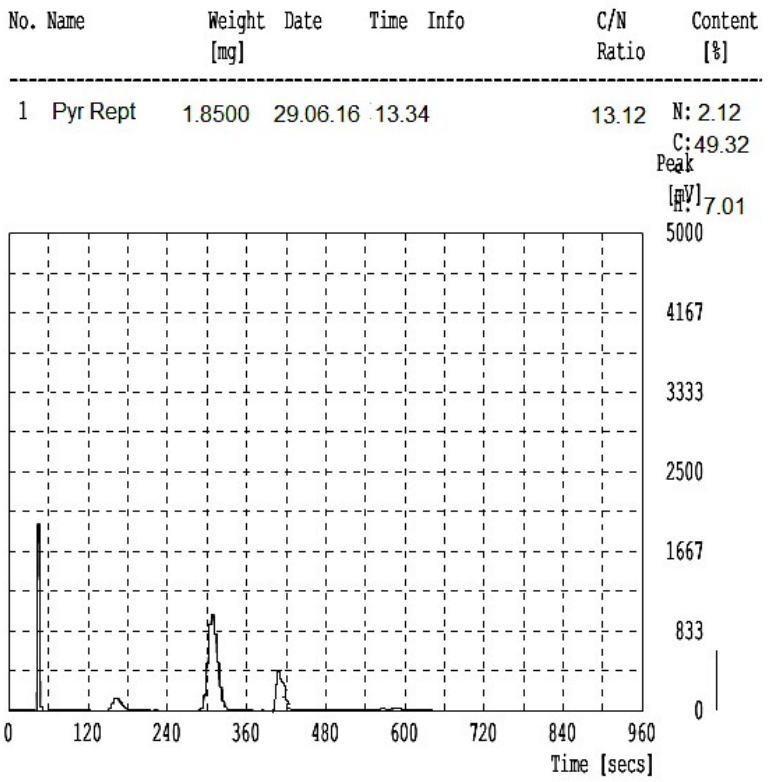


Figure S8. Elemental analysis of pyr:β-CD (3).

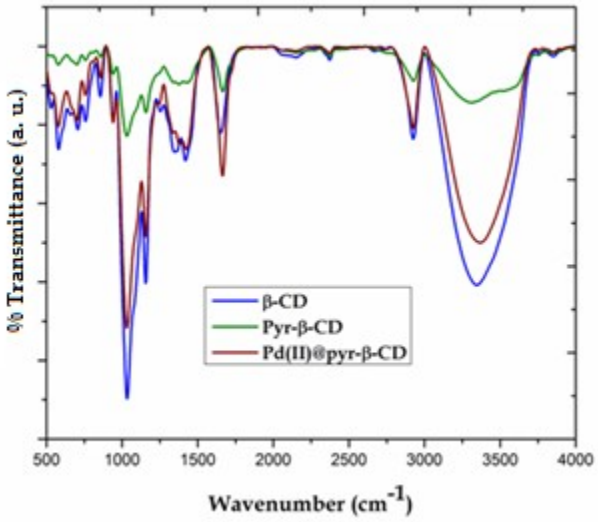


Figure S9. IR spectra for β-CD (blue), Pyr:β-CD (3) (green) and Pd@Pyr:β-CD (wine).

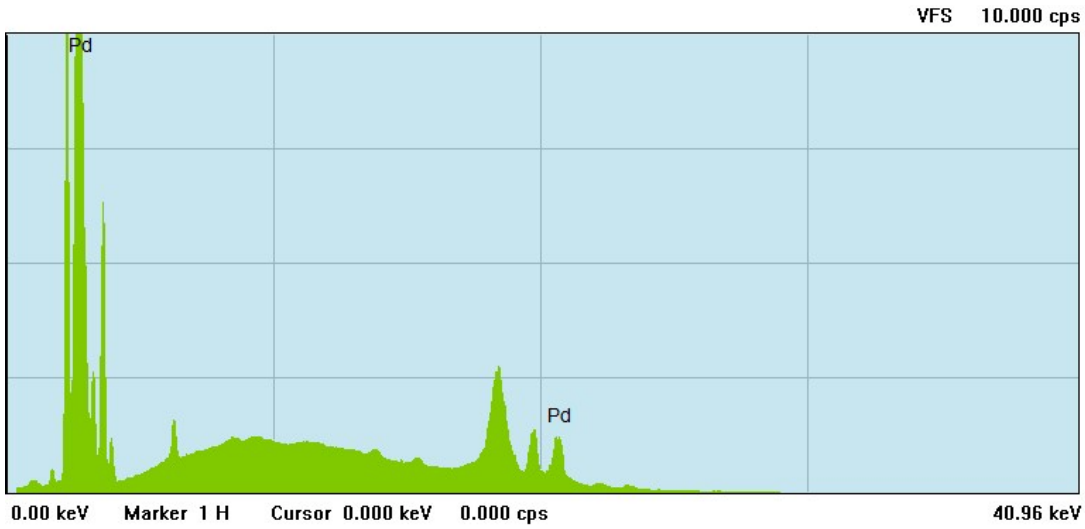


Figure S10. XRF image of Pd@pyr:β-CD complex

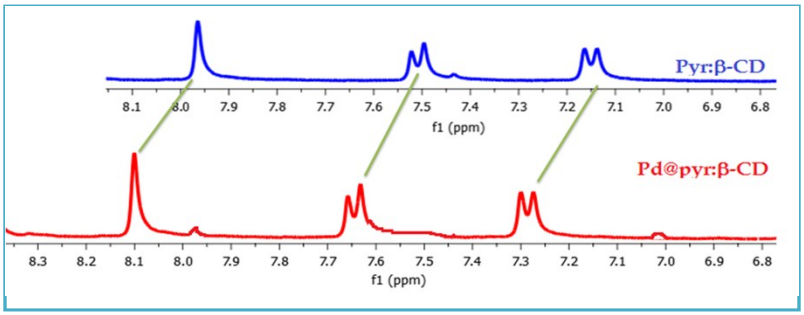


Figure S11. ^{1}H NMR (300 MHz, DMSO-d_6) for pyr:β-CD **(blue)** and Pd@pyr:β-CD **(red)**.

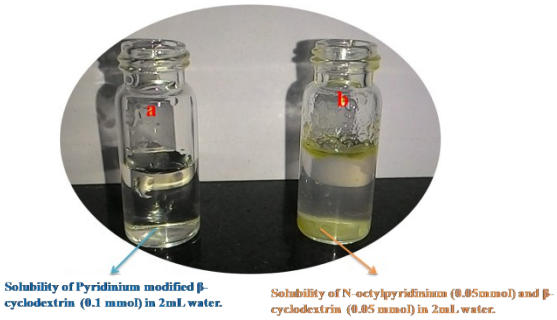


Figure S12 Water solubility of a) pyr:β-CD **(3)** (0.1 mmol in 2mL water), b) *N*-octyl-pyridine-2-amine **(2)** and β-cyclodextrin in 2mL water.

Theoretical Calculation

Molecular modeling studies of pyridinium and pyridinium modified *β*-cyclodextrin

Energy minimization studies

The complexation of pyridinium modified *β*-cyclodextrin was also confirmed from energy minimization studies. From this studies *N*-octyl-pyridine-2-amine **(2)** present in outside the modified β-cyclodextrin cavity (Figure S7 Mode A) which was more favored than that of inclusion of *N*-octyl-pyridine-2-amine **(2)** inside the modified β-cyclodextrin (Figure S8. Mode B), because lower complexation energy (Mode A) (ΔE) -64.8600 kcal M^{-1} is preferred more than that of mode B (ΔE) -50.8292 kcal M^{-1} .

Table S1: Molecular Modeling Studies of pyridinium modified *β*-cyclodextrin

Mode of Pyridinium	Mode of Inclusion	*β*-CD as Host (ΔE^a Kcal.M^{-1})
N-octyl-pyridine-2-amine present in outside the pyridinium modified β-cyclodextrin cavity	**Mode A**	**-64.8600**
N-octyl-pyridine-2-amine present in inside the pyridinium modified β-cyclodextrin cavity.	Mode B	-50.8292

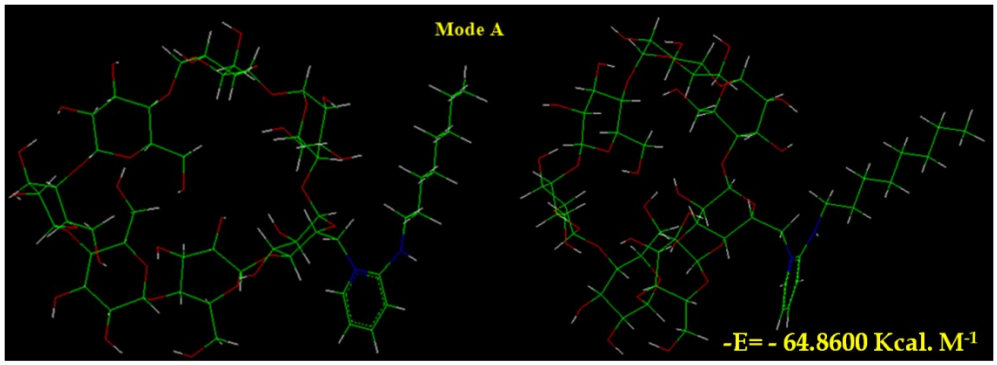


Figure S13 Mode A: CVFF optimized inclusion complex of *N*-octyl-pyridine-2-amine **(2)** group outside the Pyr:β-CD **(3).**

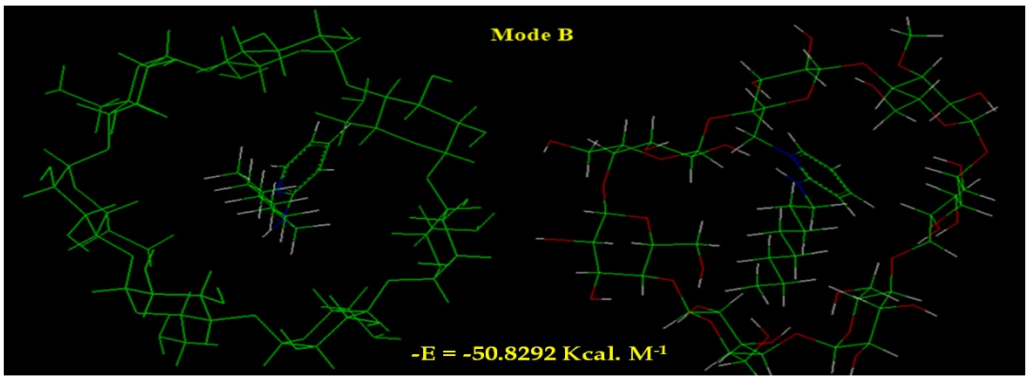


Figure S14 Mode B: CVFF optimized inclusion complex of *N*-octyl-pyridine-2-amine **(2)** group inside the Pyr:β-CD **(3)** cavity**.**

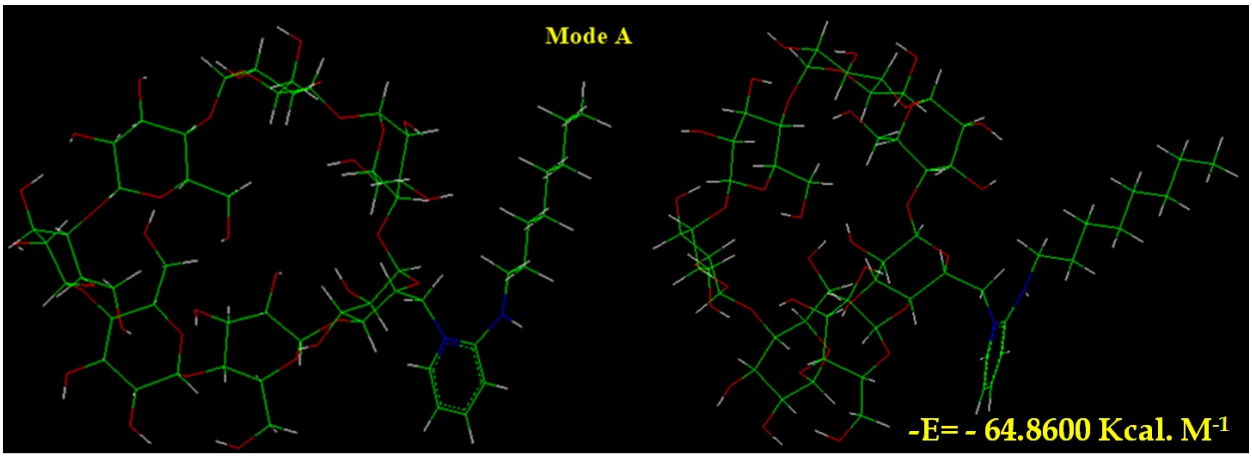


Figure S15. Mode A: CVFF optimized inclusion complex of *N*-octyl-pyridine-2-amine group outside the pyridinium modified *β*-cyclodextrin**.**

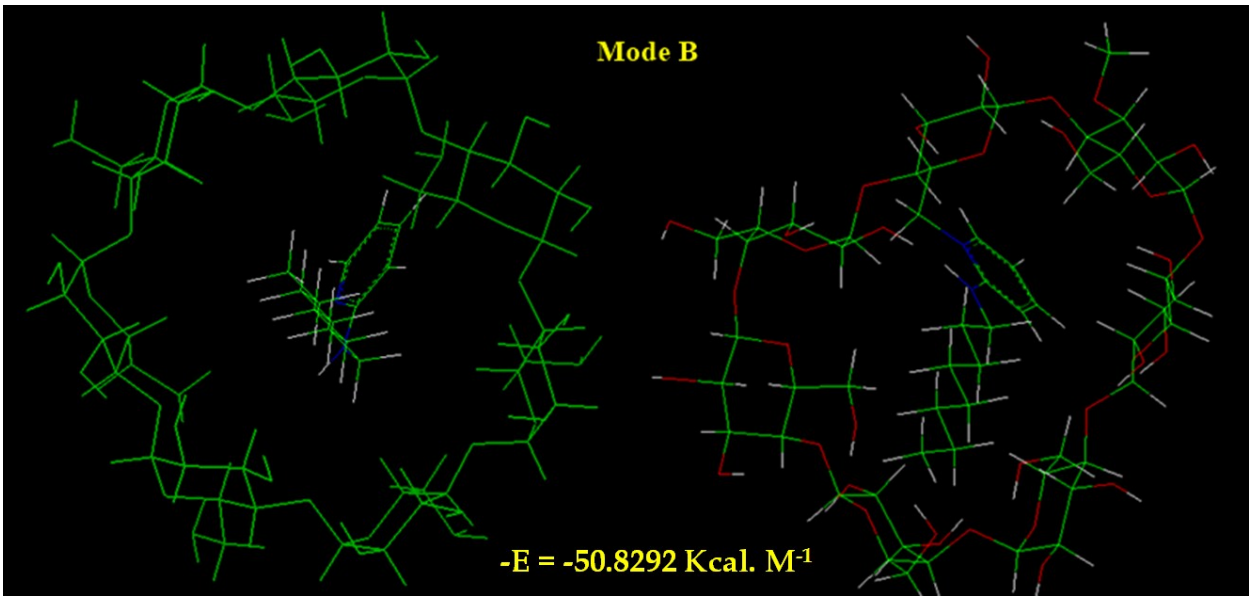


Figure S16. Mode A: CVFF optimized inclusion complex of *N*-octyl-pyridine-2-amine group inside the pyridinium modified *β*-cyclodextrin cavity**.**

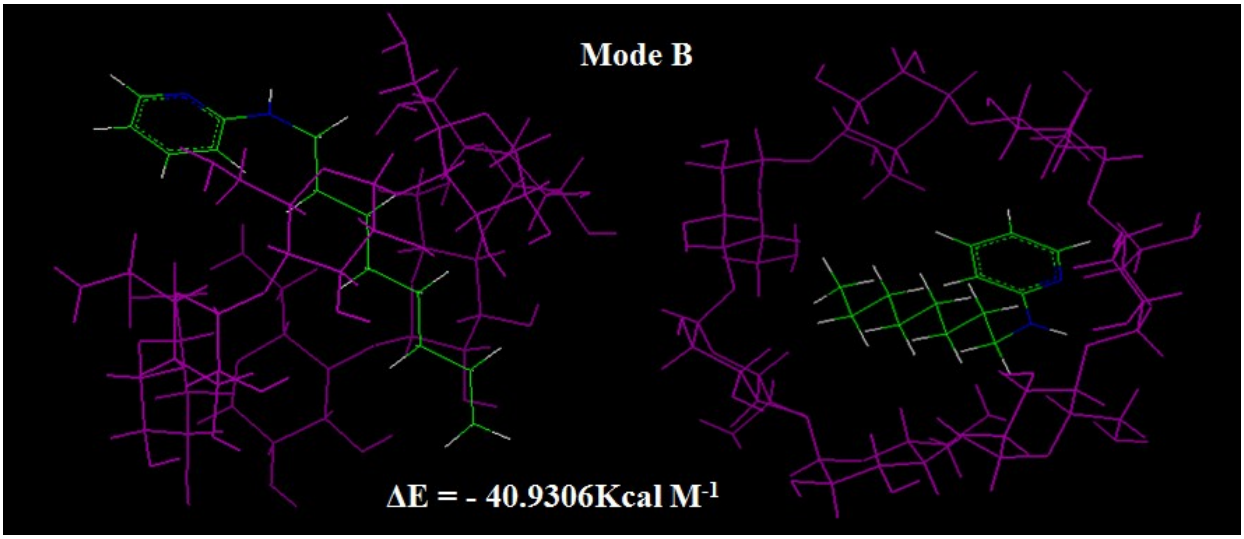


Figure S17. CVFF optimized inclusion complex of *β*-cyclodextrin with pyidinium; In mode B: with inclusion of *N*-octyl sides for pyridinium in *β*-cyclodextrin**.**

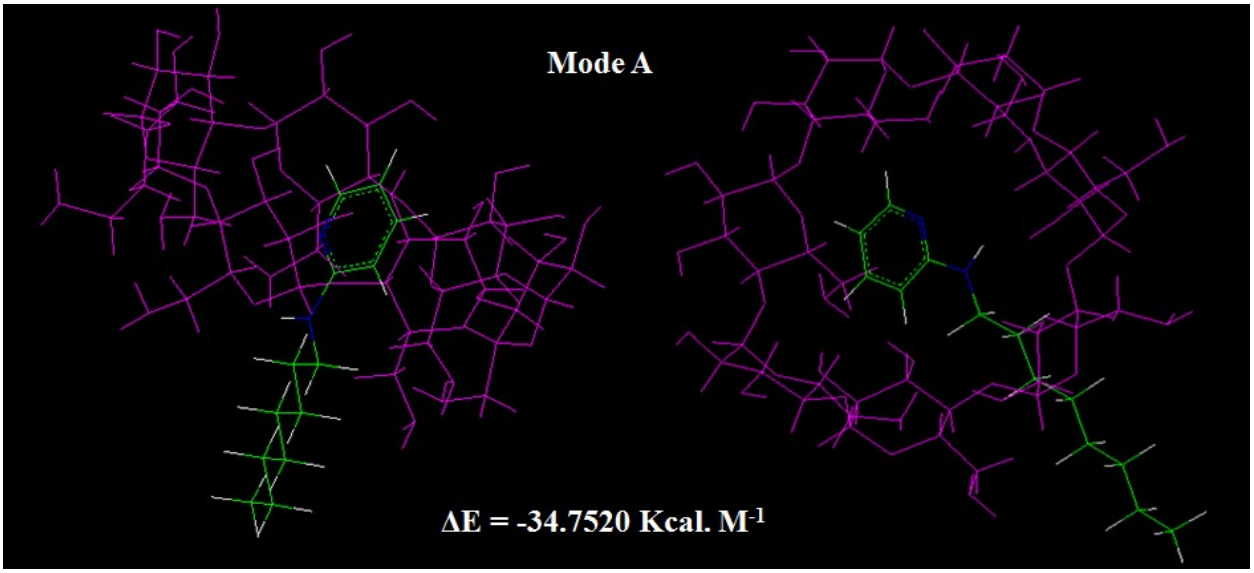


Figure S18. CVFF optimized inclusion complex of *β*-cyclodextrin with pyidinium; In mode A: with inclusion of pyridine sides for pyridinium in *β*-cyclodextrin**.**

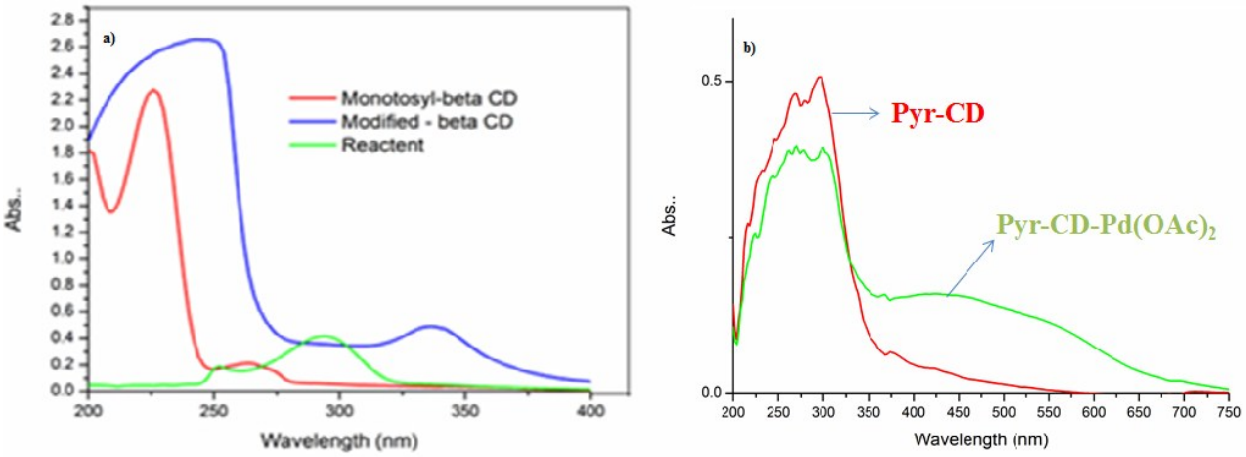


Figure S19. a) UV-Vis absorption spectra for Monotosyl-β-CD (Red), pyridinium modified- β-CD (Blue), *N*-octyl-pyridine-2-amine (Green), b) UV-DRS spectra for pyridinium modified- β-CD (Red), pyridinium modified- β-CD with $Pd(OAc)_2$ (Green).

Spectroscopic data for compound 4a-r

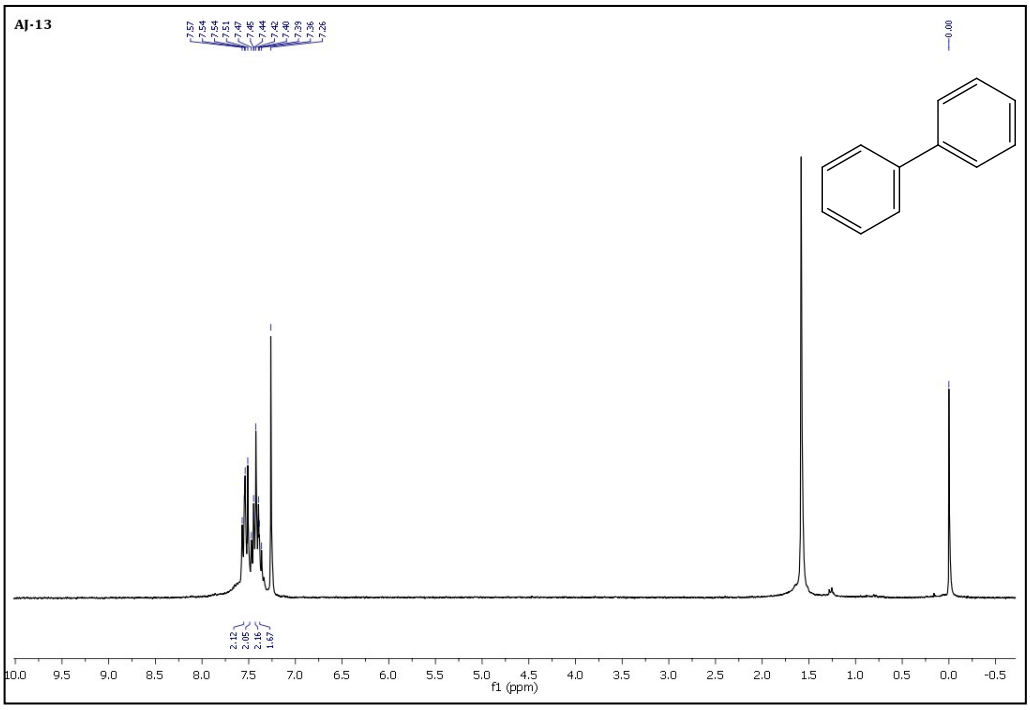


Figure S20. [1]H-NMR spectrum for 4a

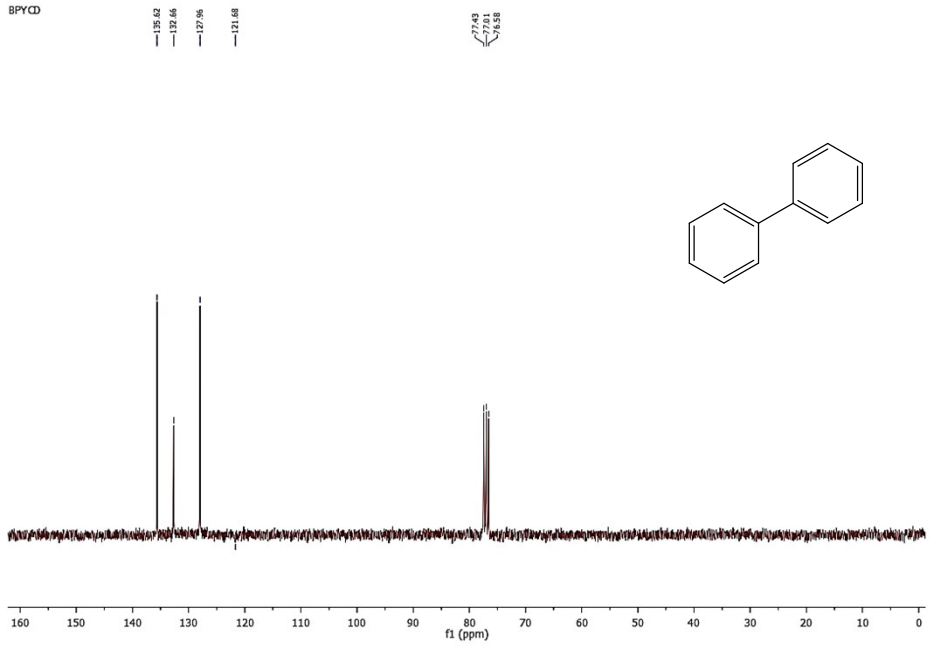


Figure S21. [13]**C**-NMR spectrum for 4a

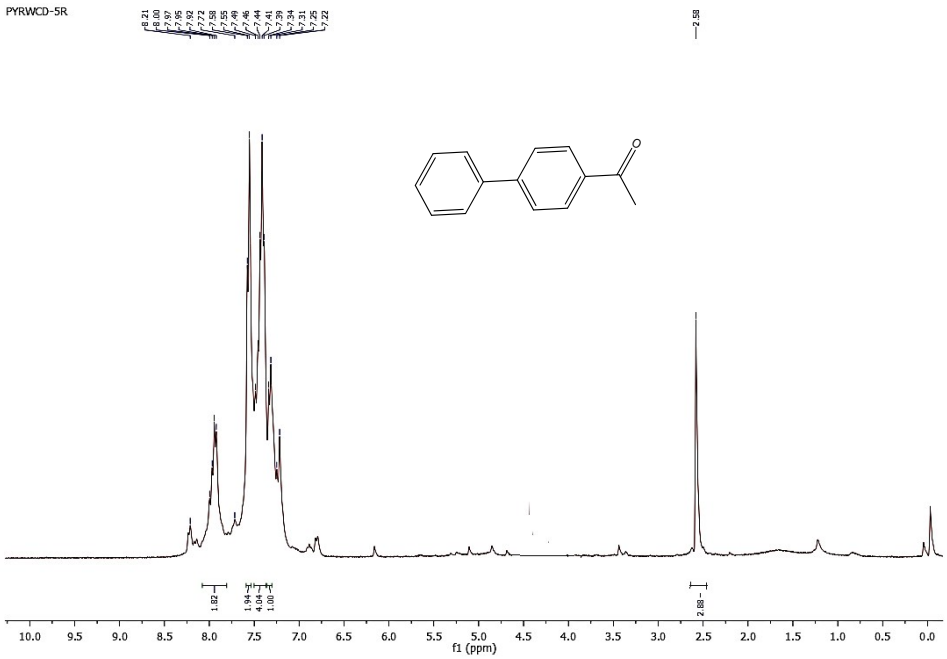


Figure S22. [1]H-NMR spectrum for 4b

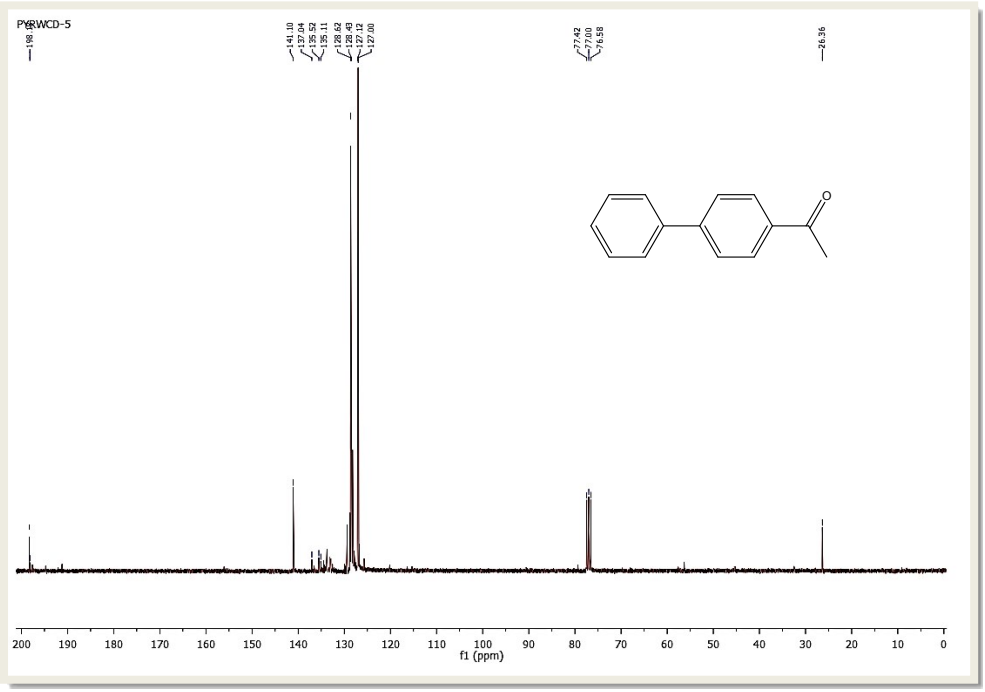


Figure S23. ^{13}C-NMR spectrum for 4b

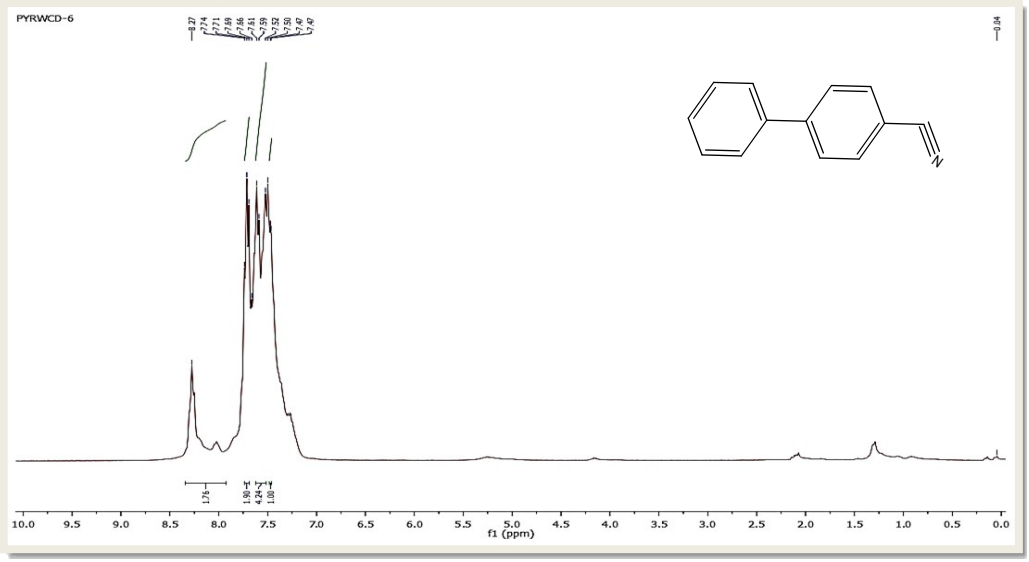


Figure S24. ^{1}H-NMR spectrum for 4c

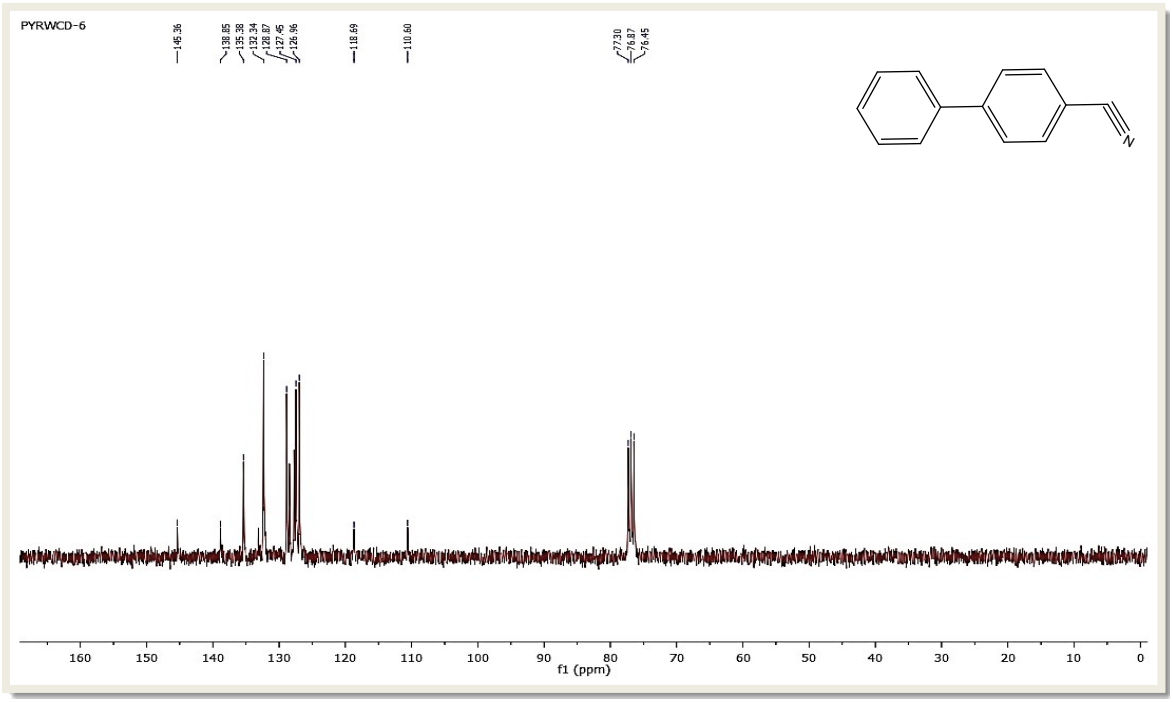


Figure S25. ^{13}C-NMR spectrum for 4c

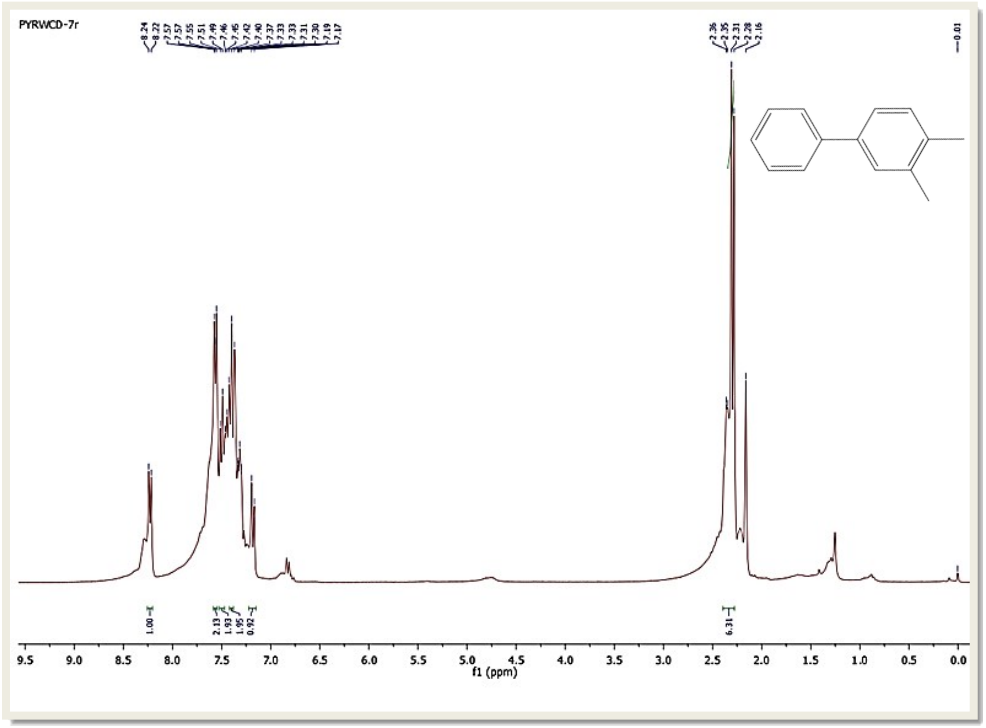


Figure S26. ^{1}H-NMR spectrum for 4d

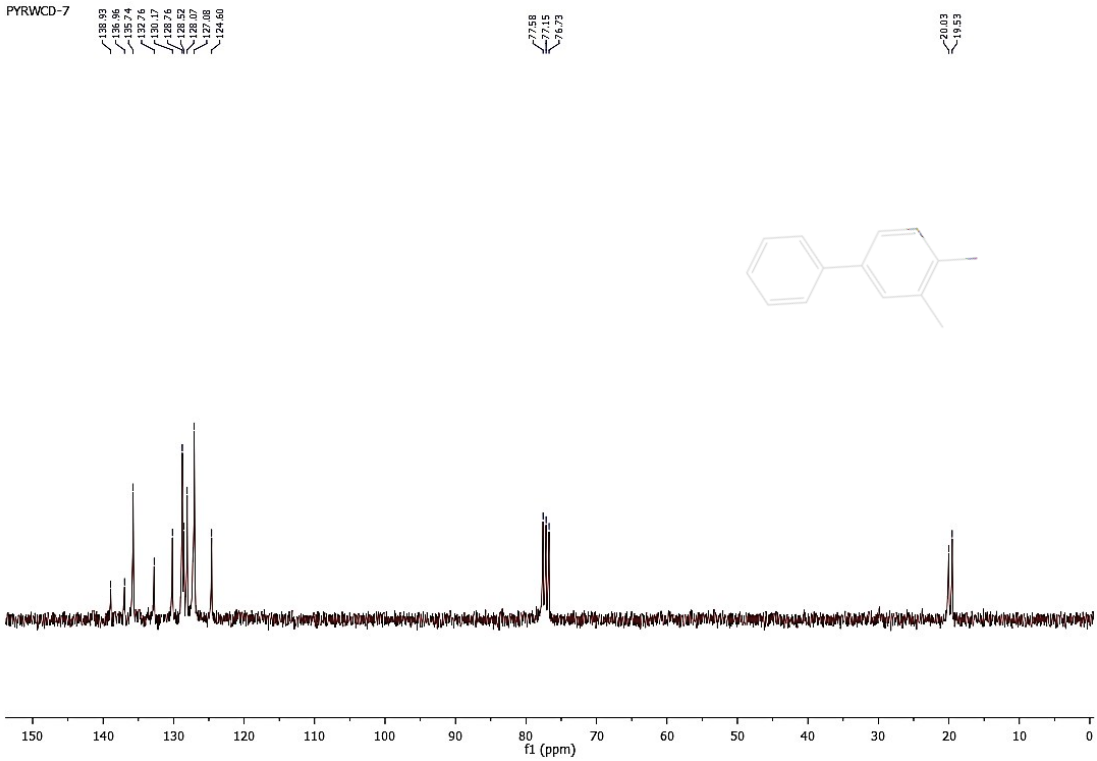


Figure S27. ^{13}C-NMR spectrum for 4d

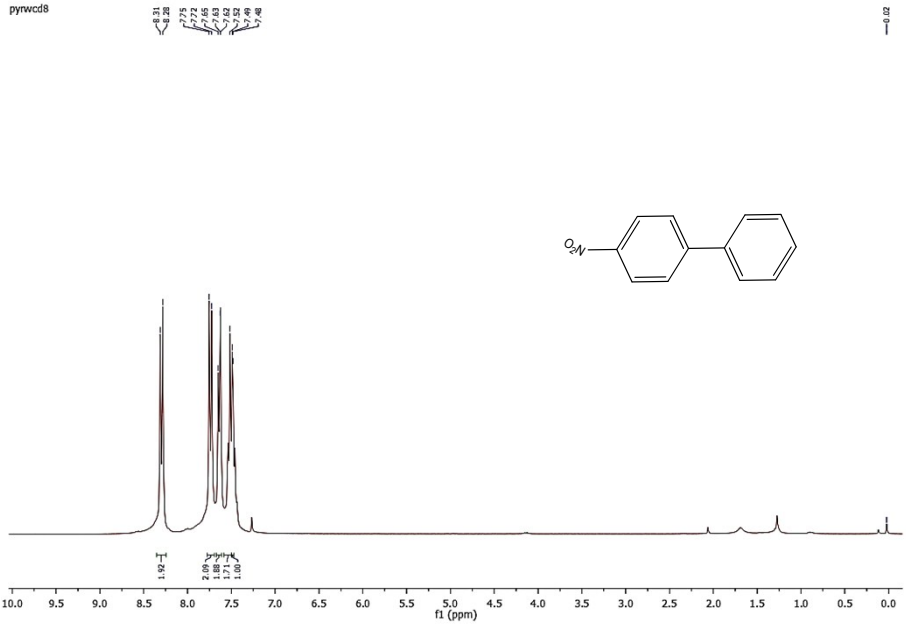


Figure S28. ^{1}H-NMR spectrum for 4e

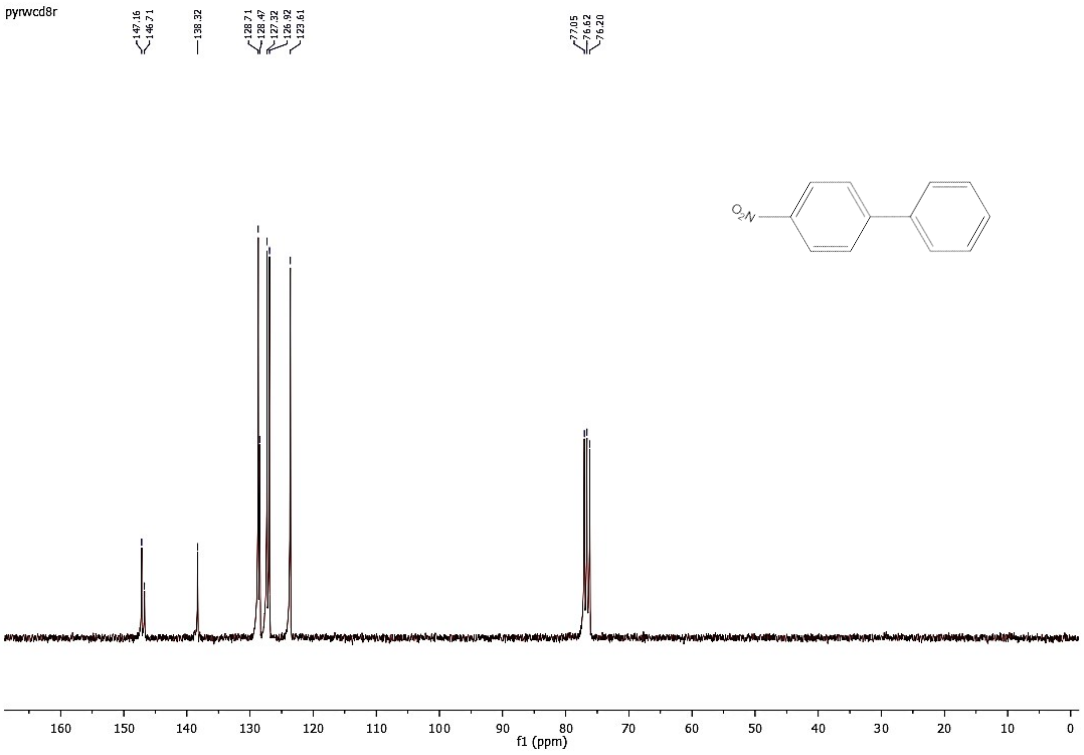


Figure S29. ^{13}C-NMR spectrum for 4e

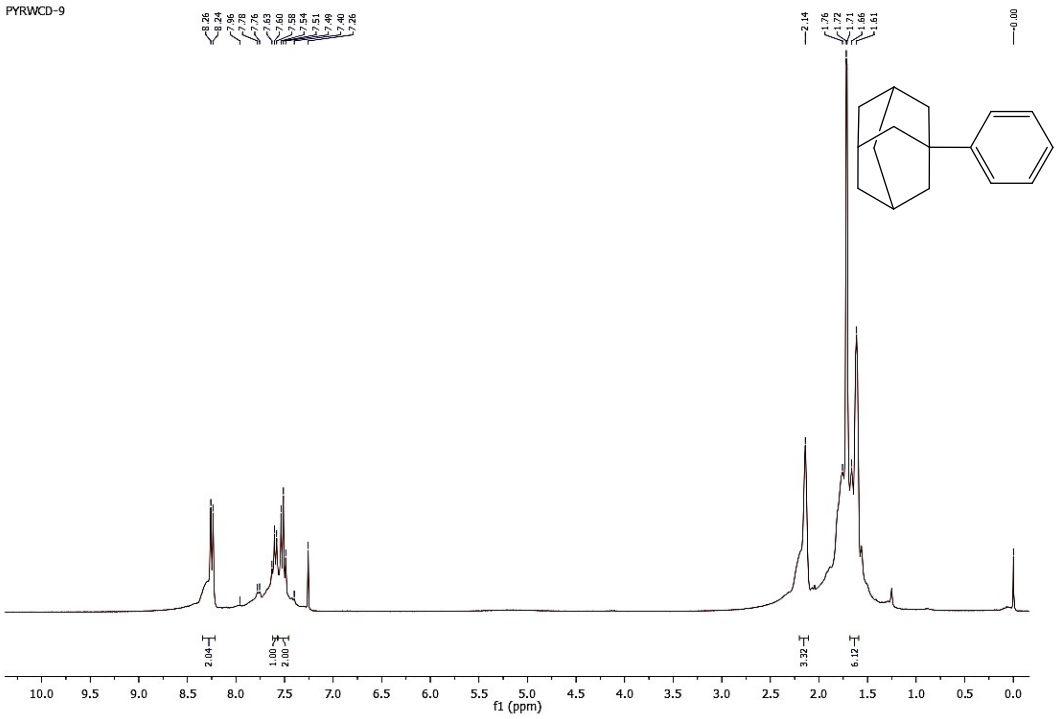


Figure S30. ^{1}H-NMR spectrum for 4f

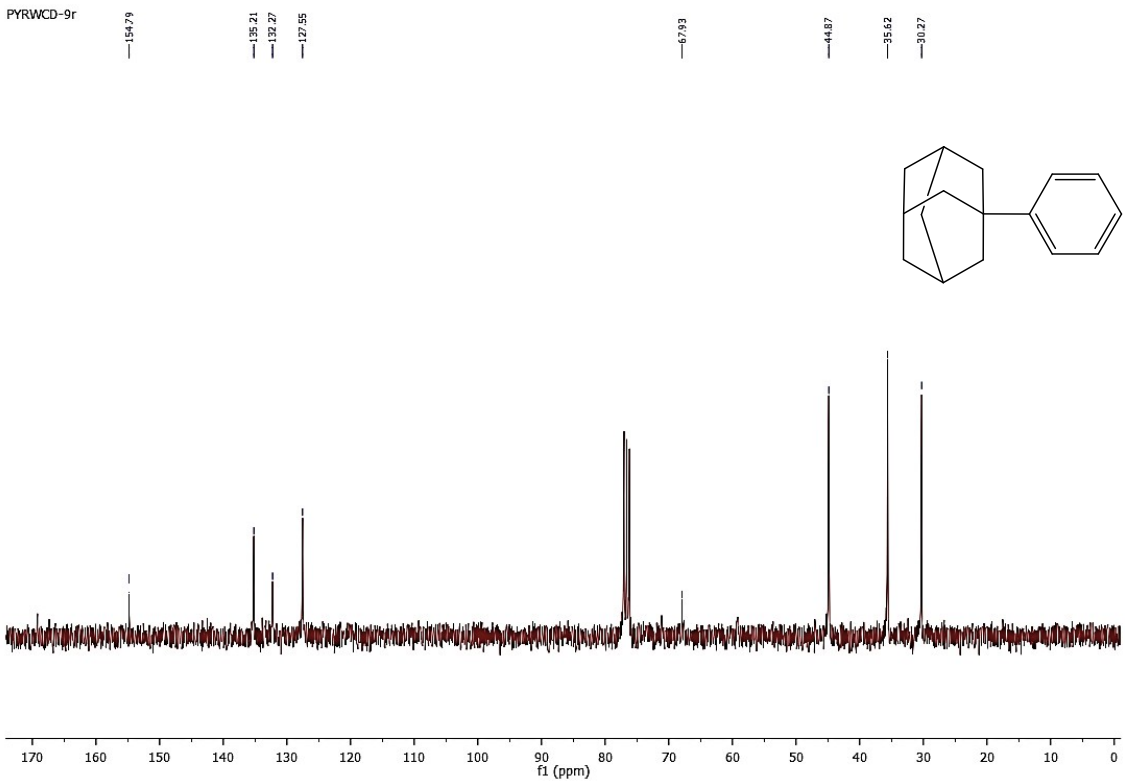


Figure S31. ^{13}C-NMR spectrum for 4f

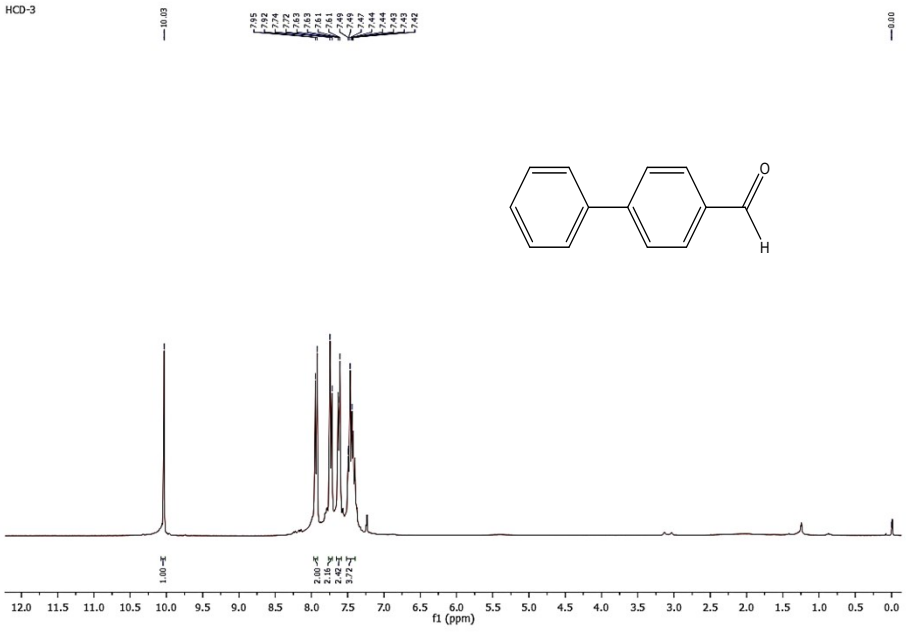


Figure S32. ^{1}H-NMR spectrum for 4i

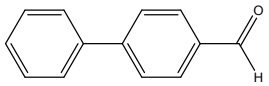


Figure S33. ^{13}C-NMR spectrum for 4i

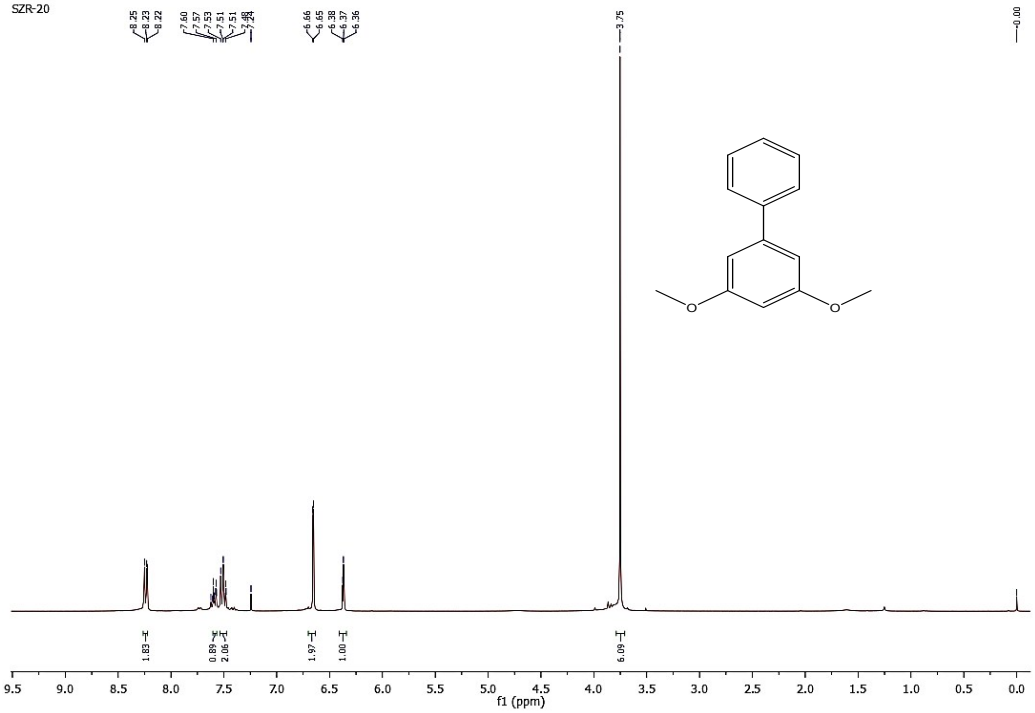


Figure S34. ^{1}H-NMR spectrum for 4i

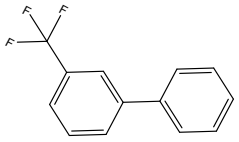


Figure S35. [1]H-NMR spectrum for 4K

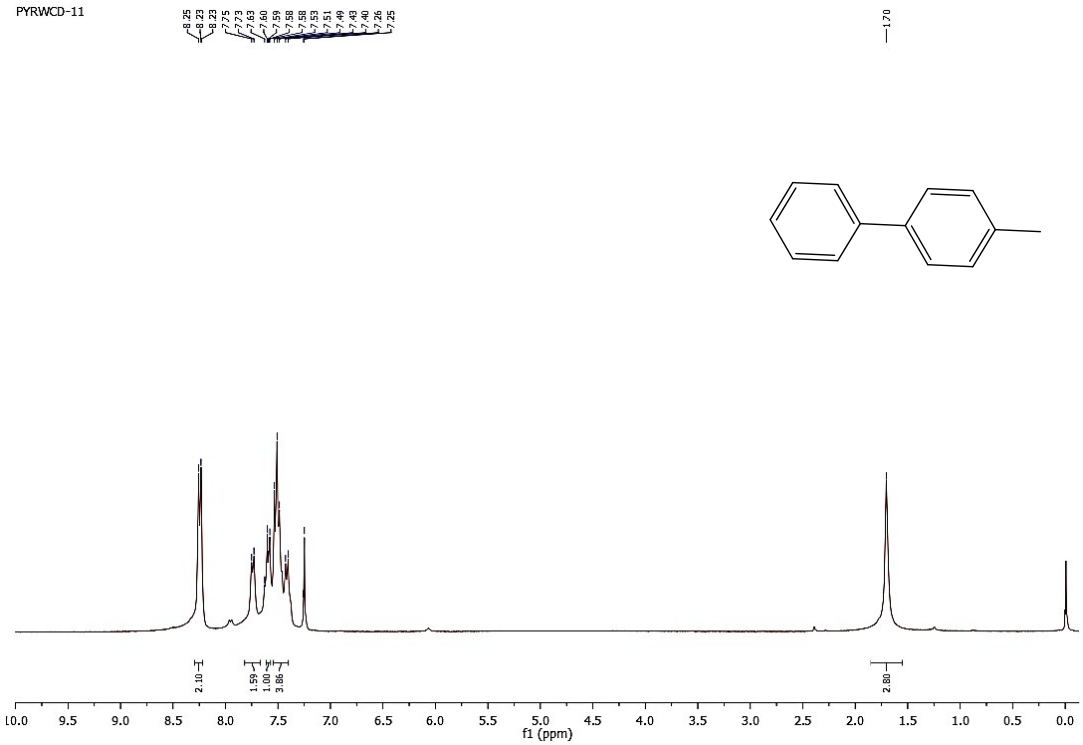


Figure S36. [1]H-NMR spectrum for 4l

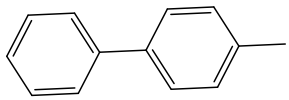


Figure S37. ^{13}C-NMR spectrum for 4l

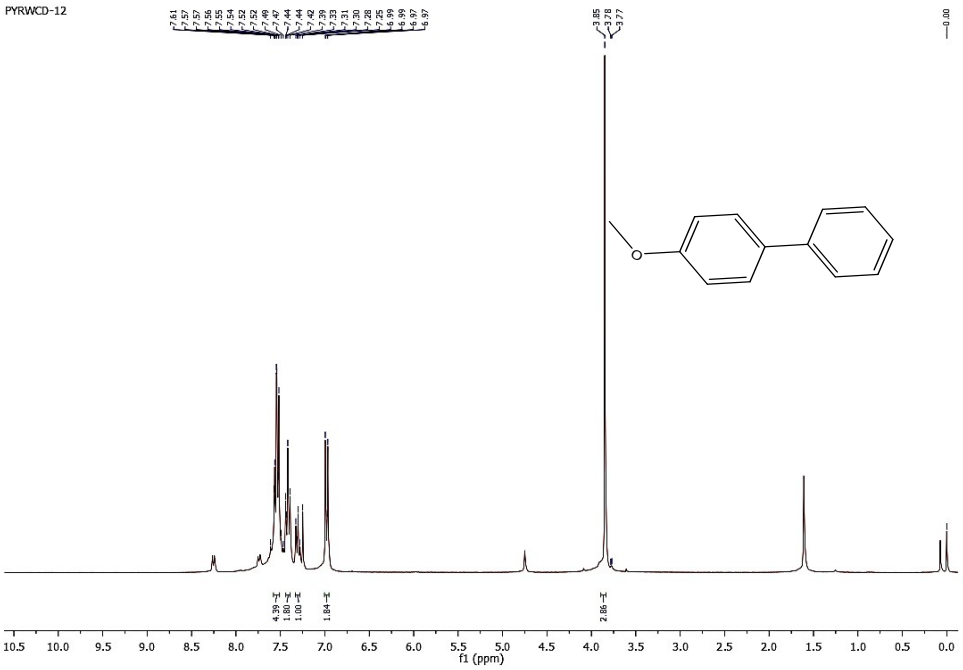
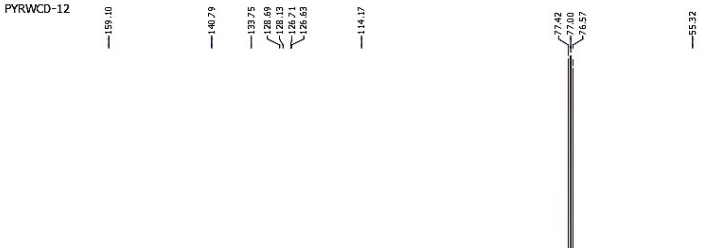


Figure S38· ^{1}H-NMR spectrum for 4m



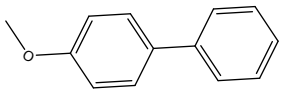


Figure S39. ^{13}C-NMR spectrum for 4m

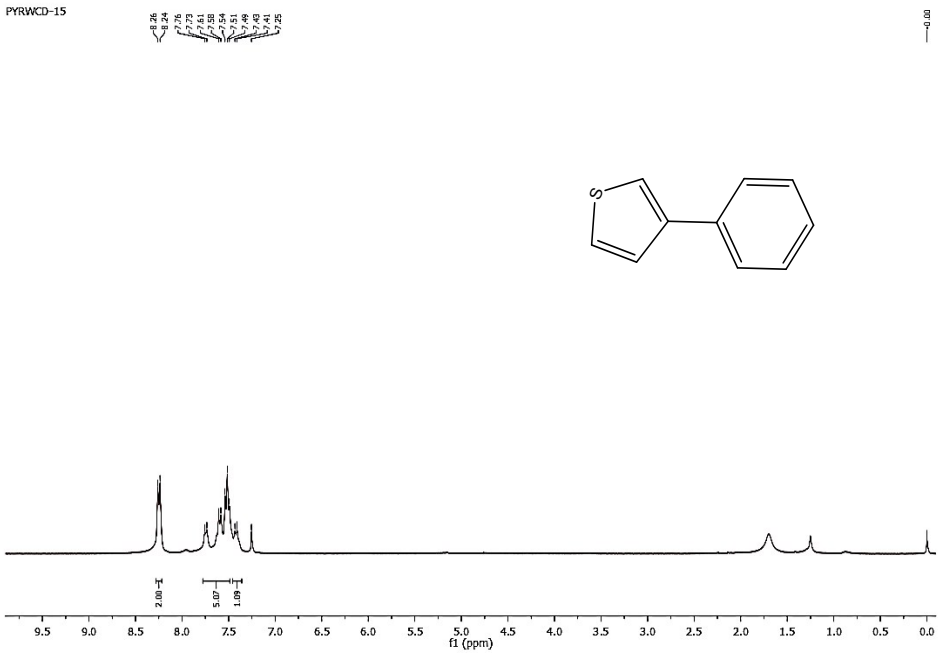


Figure S40. ^{1}H-NMR spectrum for 4o

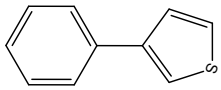


Figure S41. ^{13}C-NMR spectrum for 4o

Spectroscopic data for compound 5a-k

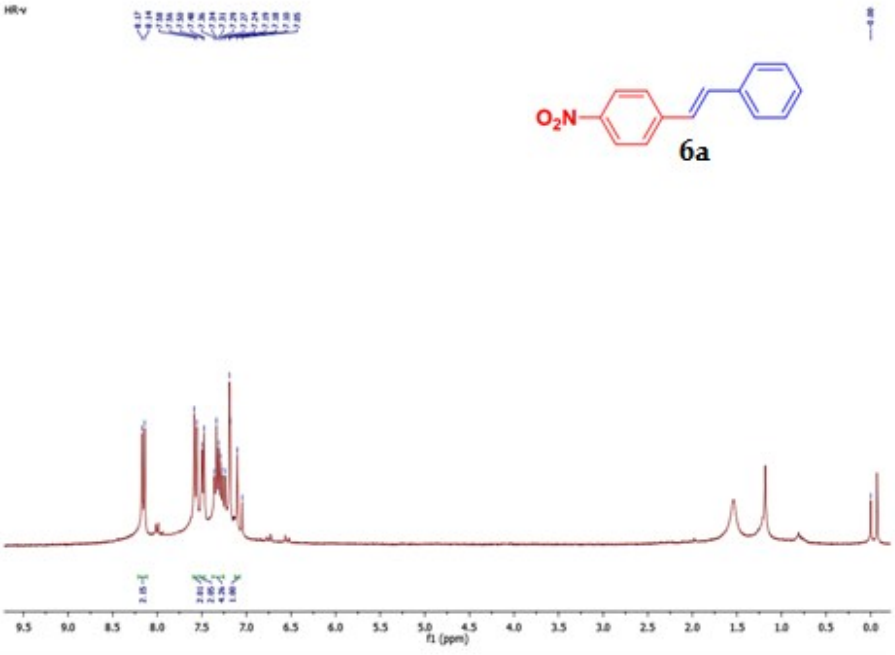


Figure S42. ^{1}H-NMR spectrum for 6a

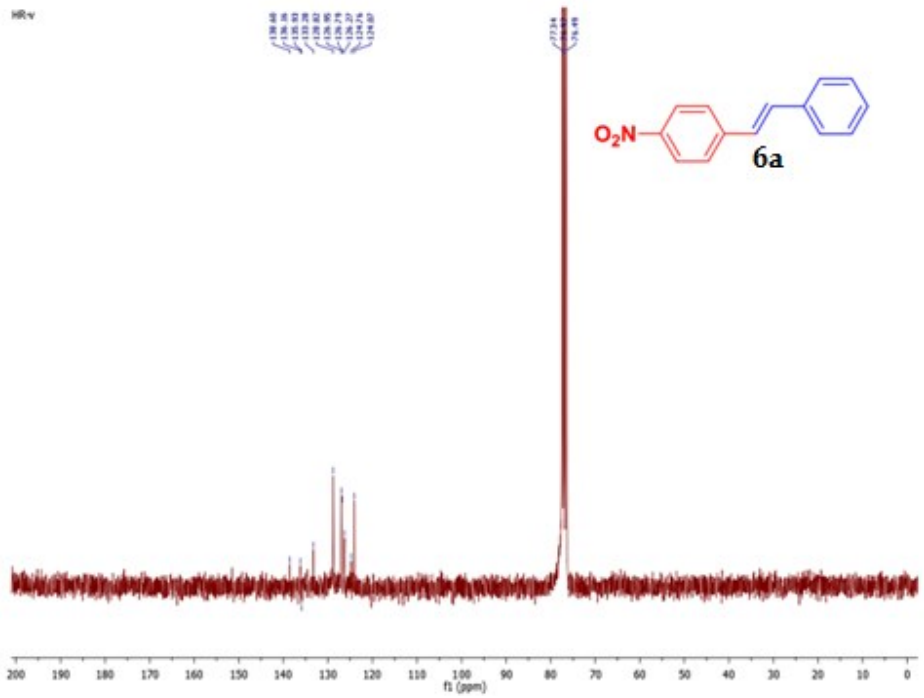


Figure S43. ^{13}C-NMR spectrum for 6a

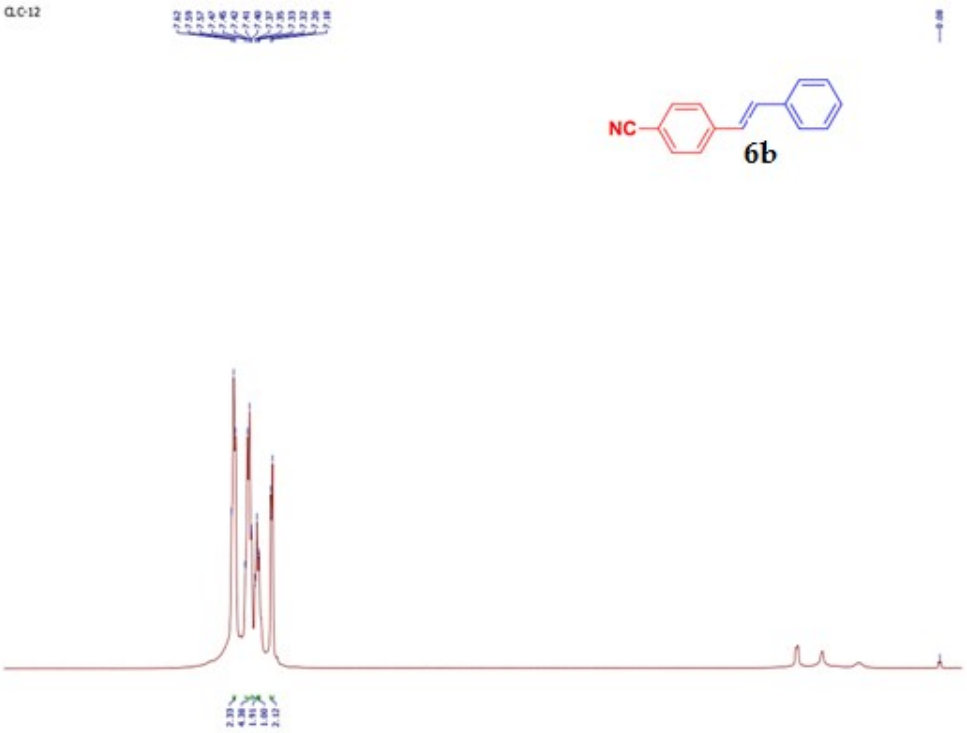


Figure S44. ^{1}H-NMR spectrum for 6b

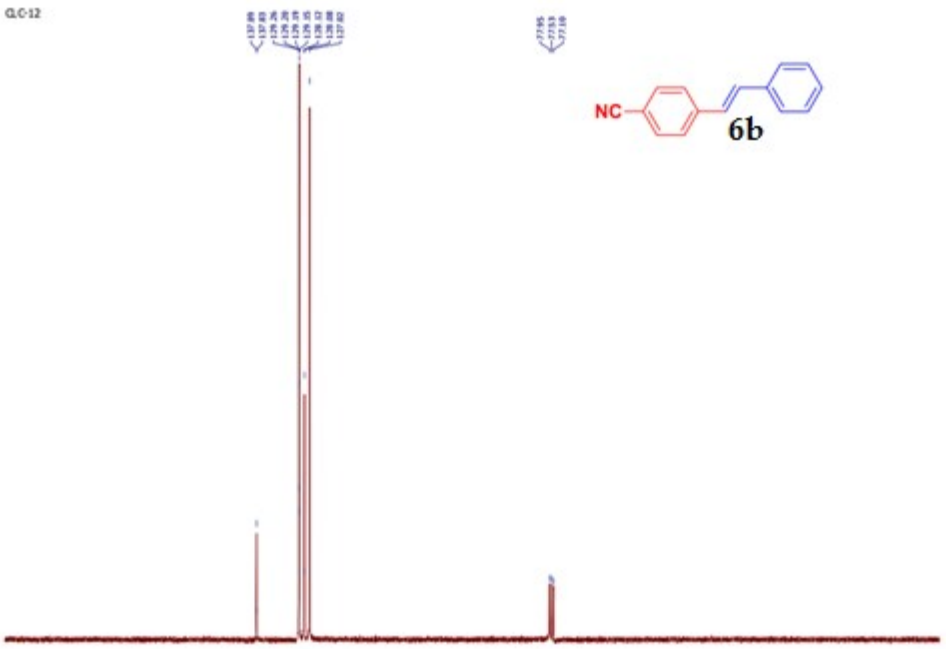


Figure S45. ^{13}C-NMR spectrum for 6b

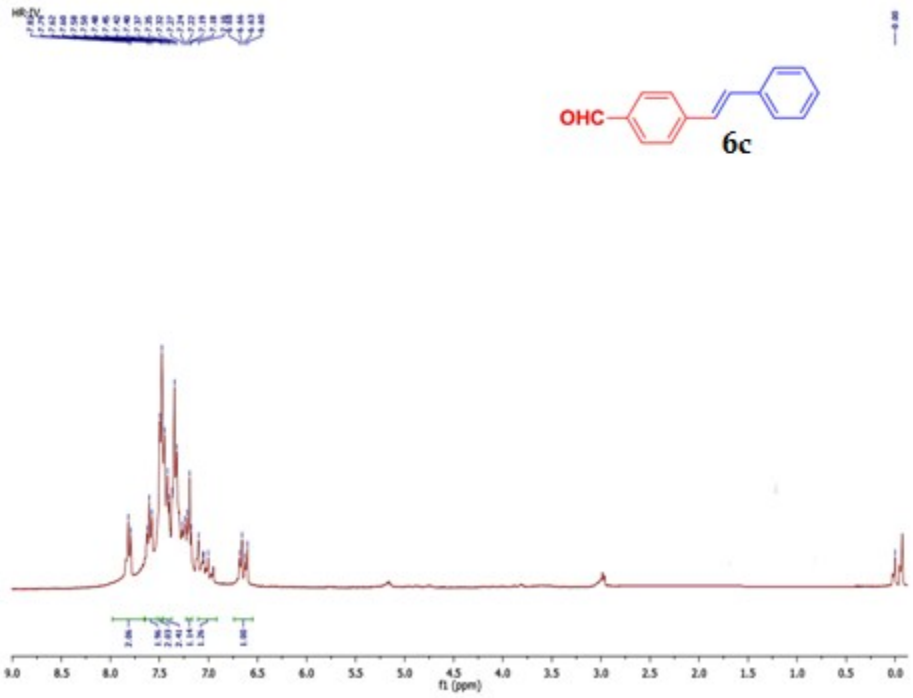


Figure S46. ^{1}H-NMR spectrum for 6c

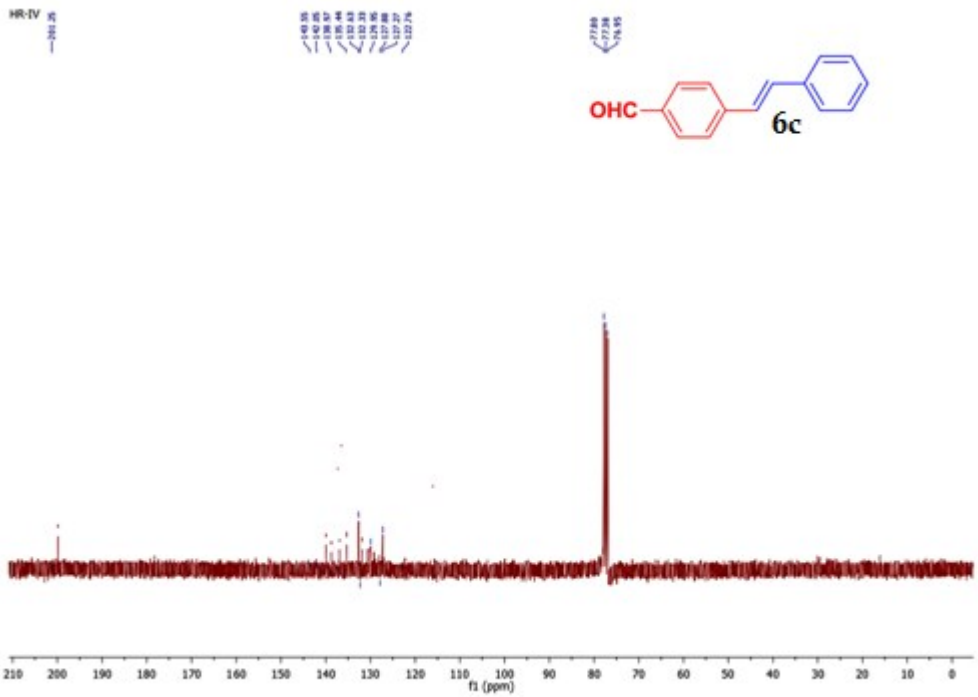


Figure S47. ^{13}C-NMR spectrum for 6c

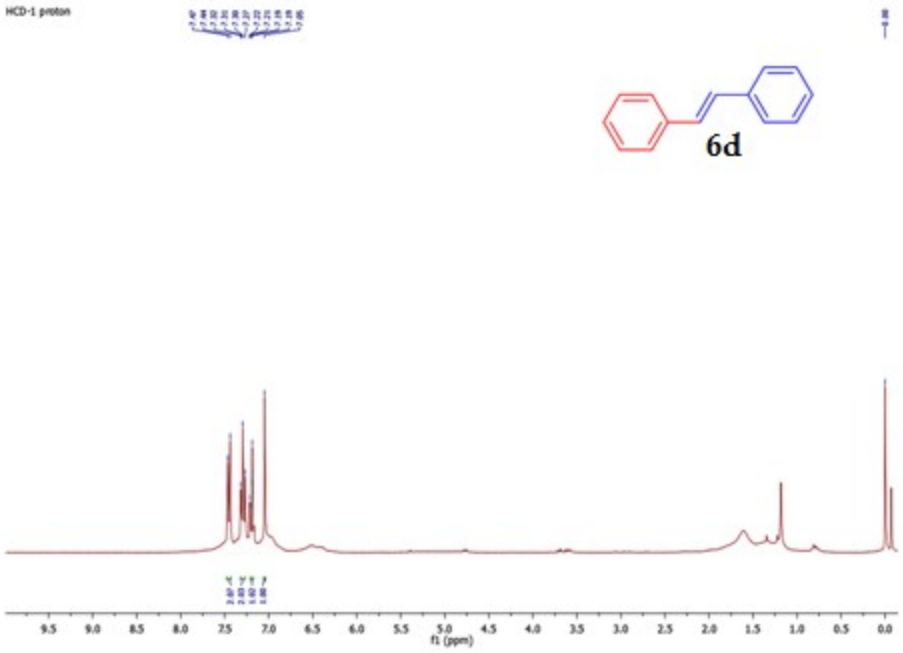


Figure S48. ^{1}H-NMR spectrum for 6d

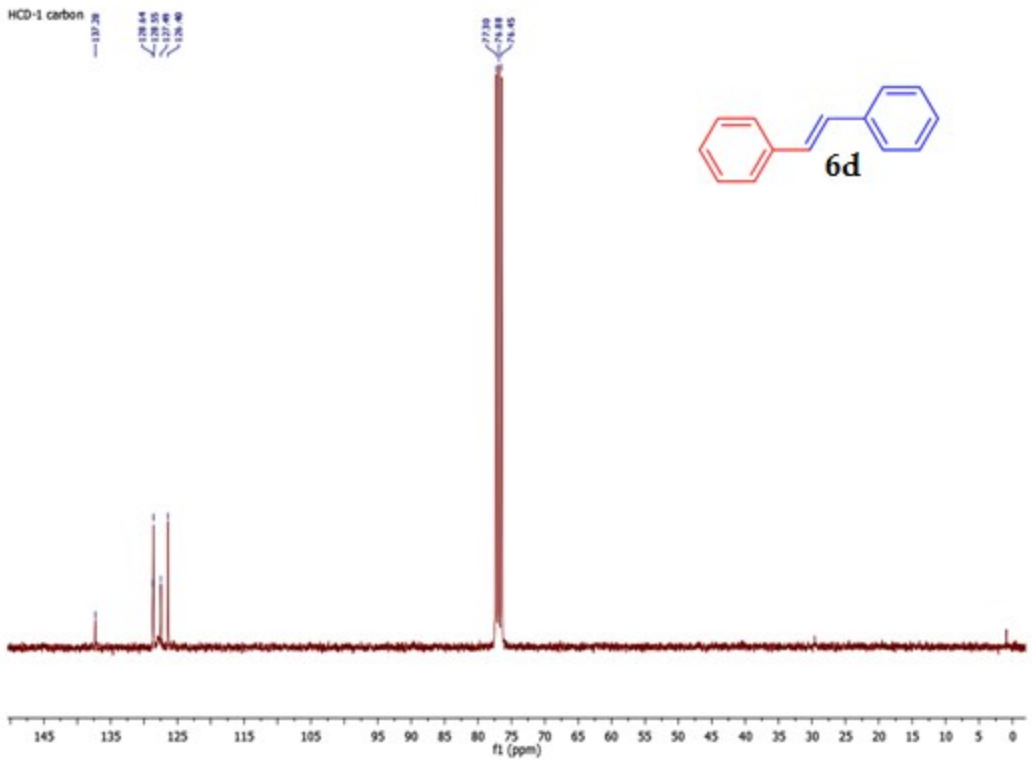


Figure S49. ^{13}C-NMR spectrum for 6d

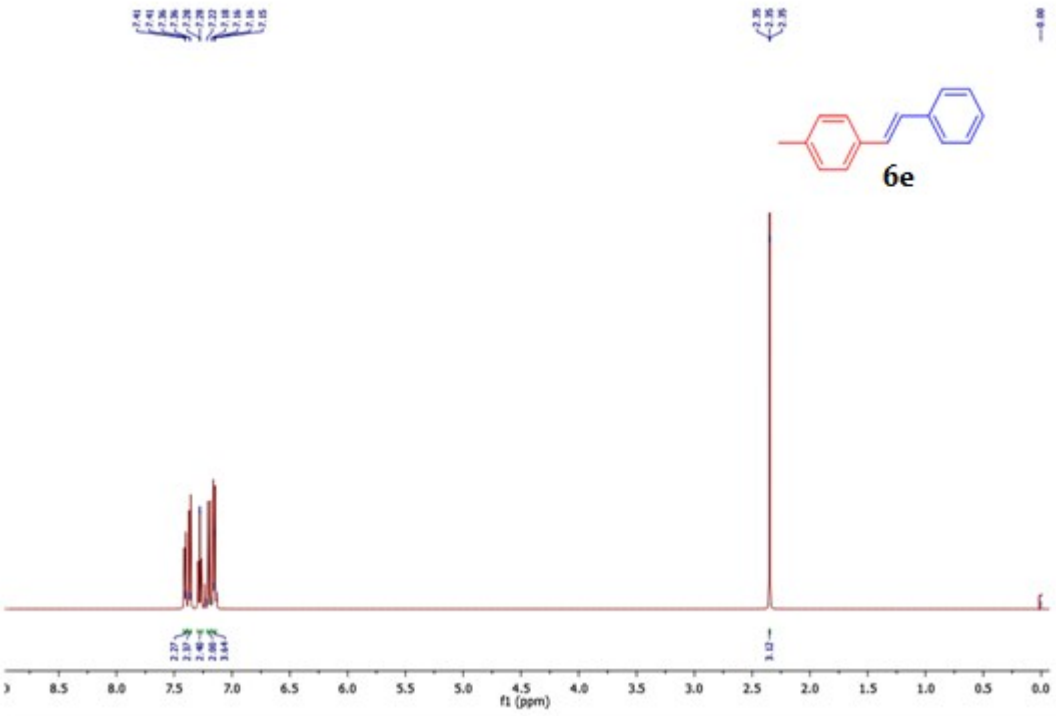


Figure S50. ^{1}H-NMR spectrum for 6e

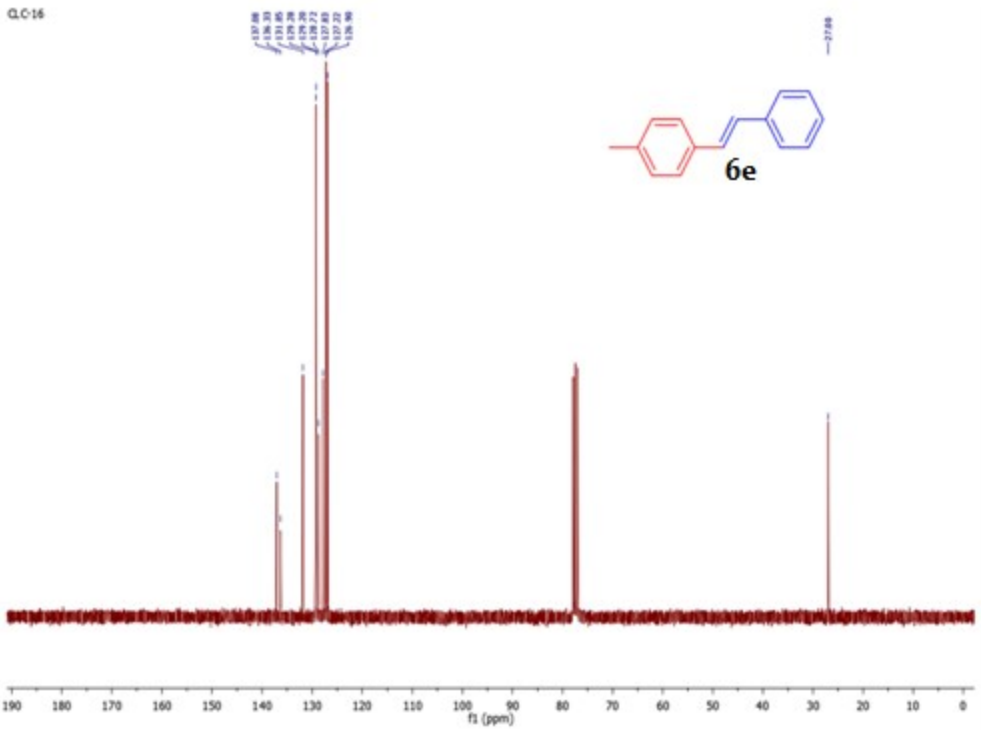


Figure S51. ^{13}C-NMR spectrum for 6e

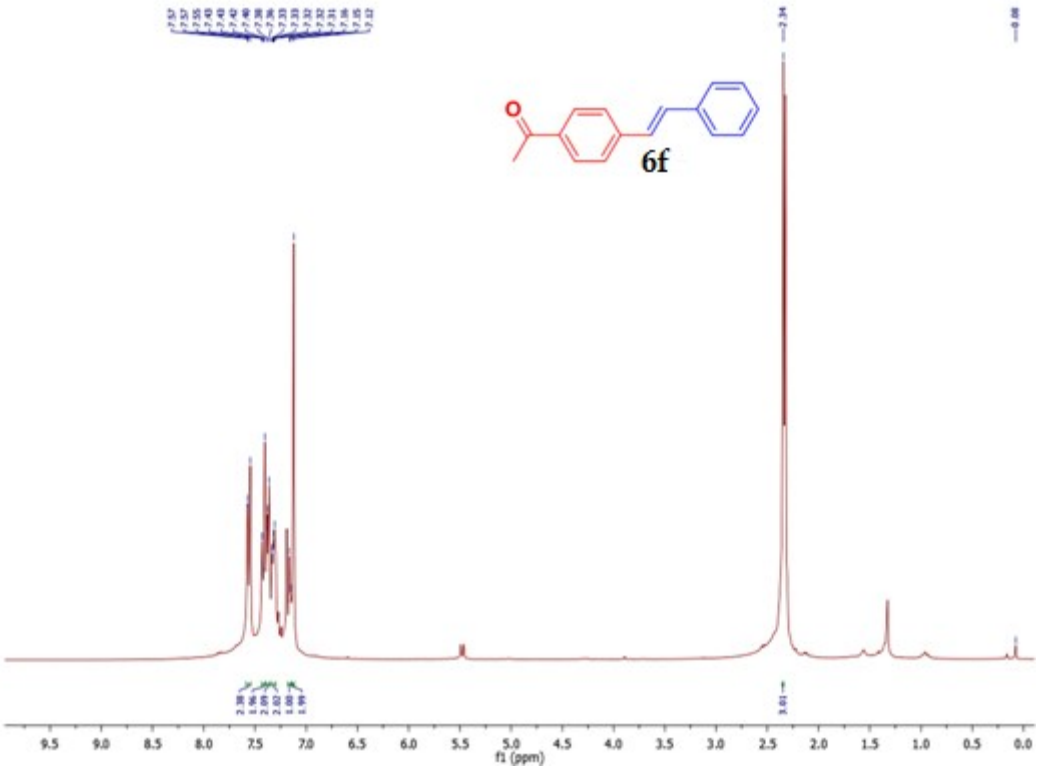


Figure S52. ^{1}H-NMR spectrum for 6f

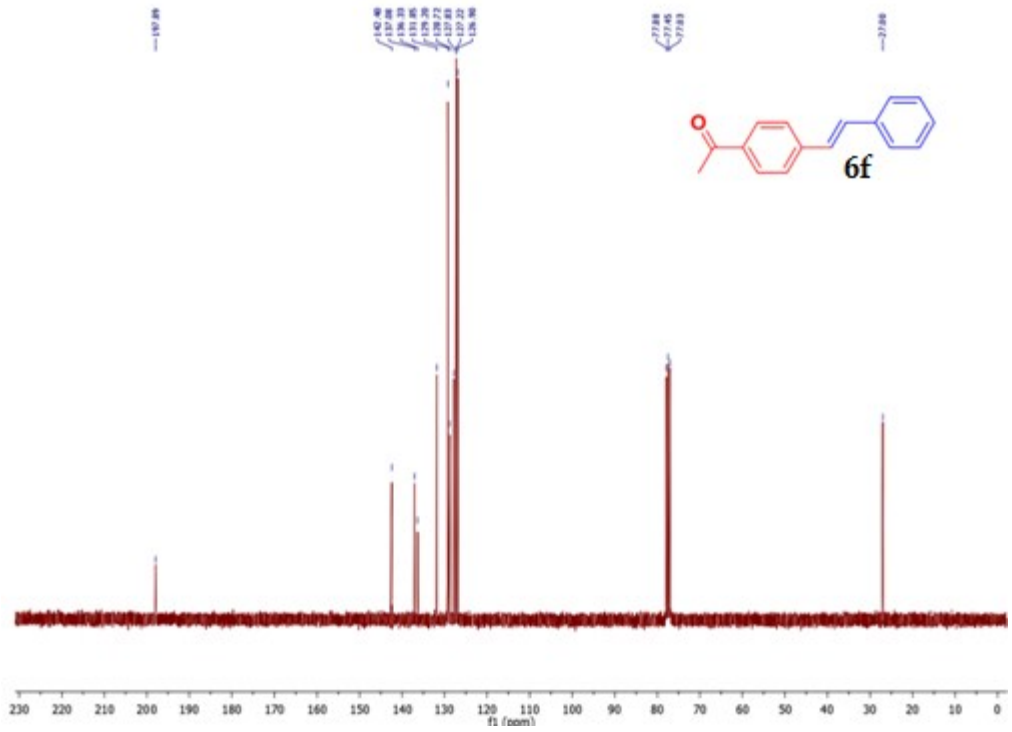


Figure S53. ^{13}C-NMR spectrum for 6f

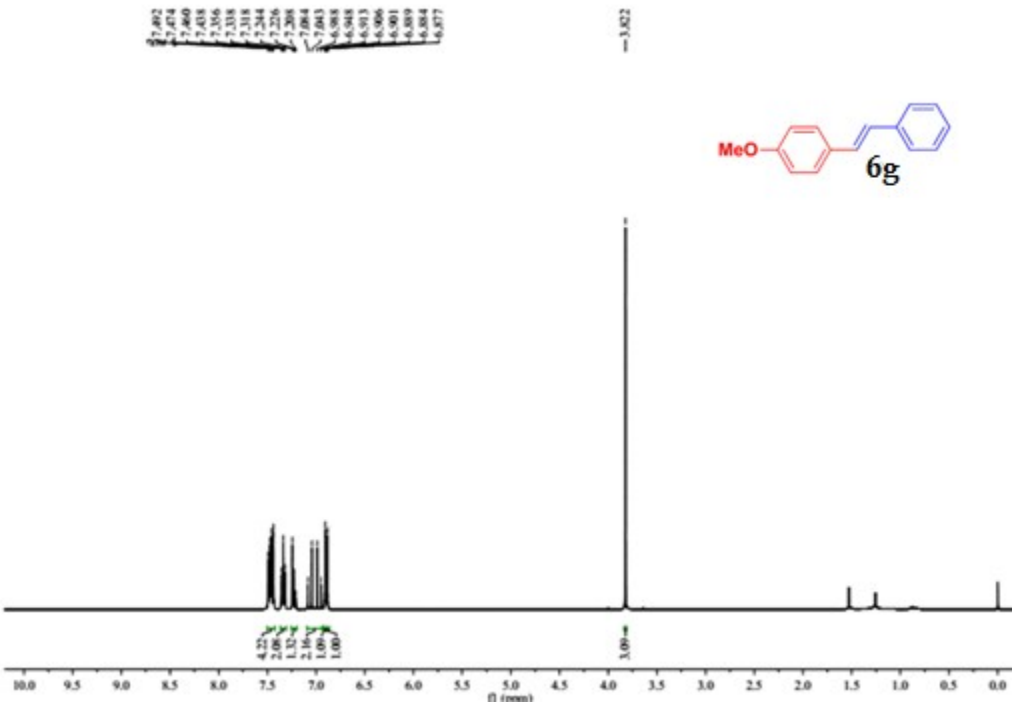


Figure S54. ^{1}H-NMR spectrum for 6g

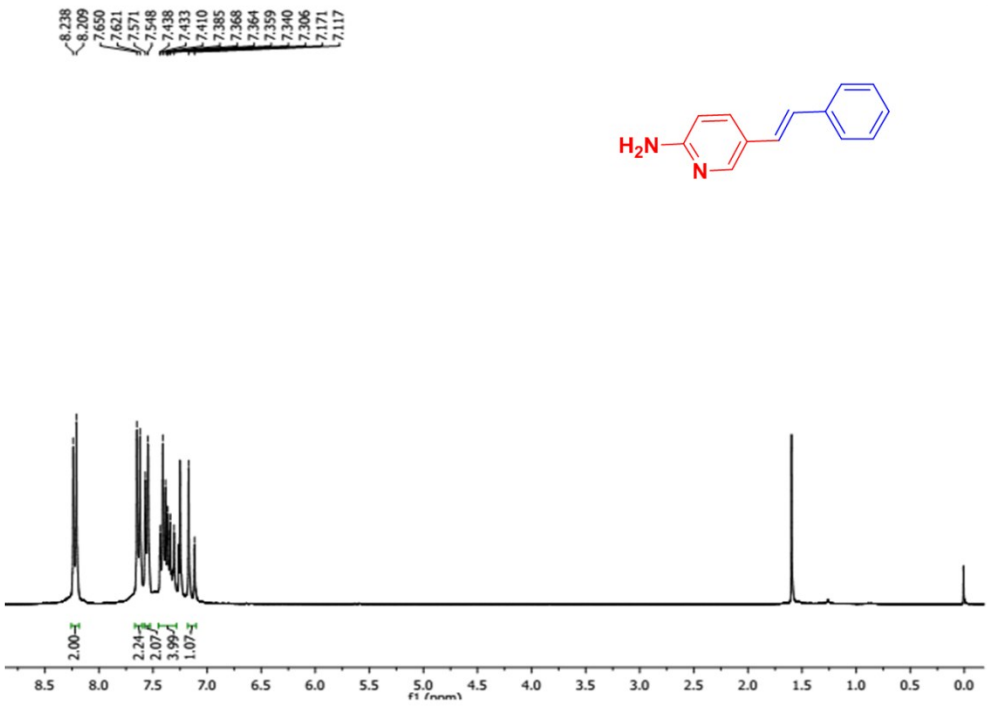


Figure S55. [1]H-NMR spectrum for 6h

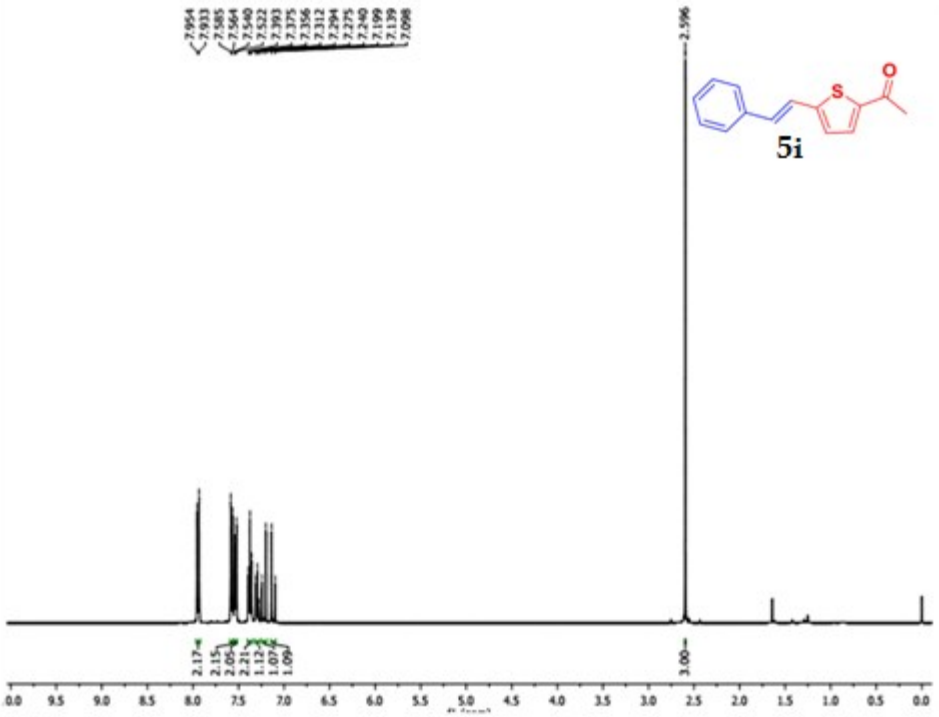


Figure S56. [1]H-NMR spectrum for 6i

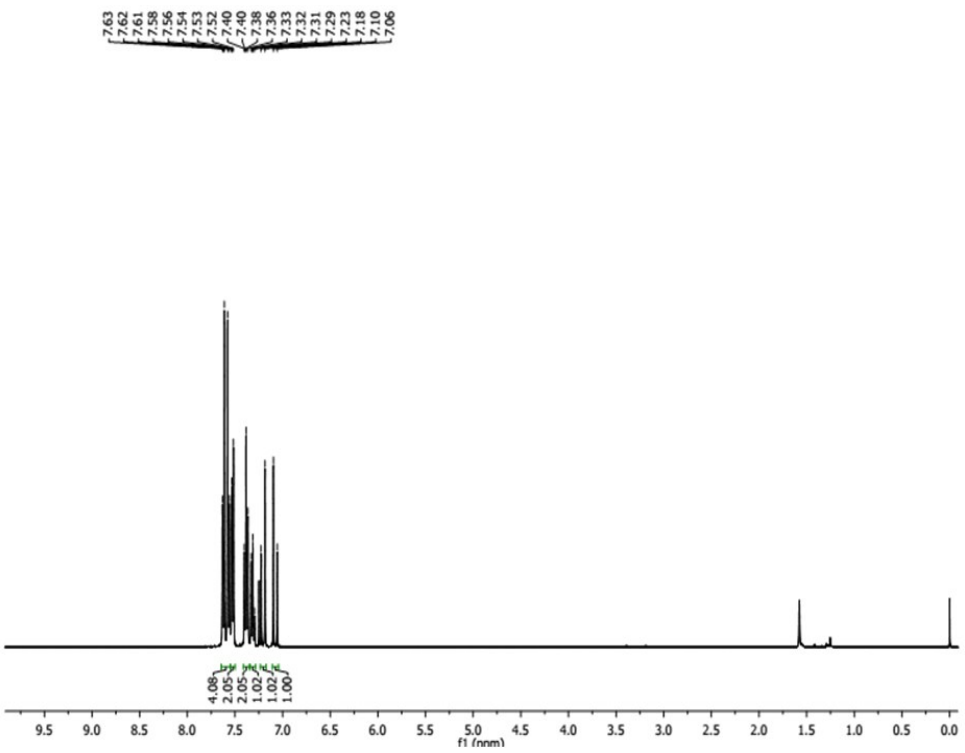


Figure S57. [1]H-NMR spectrum for 6j

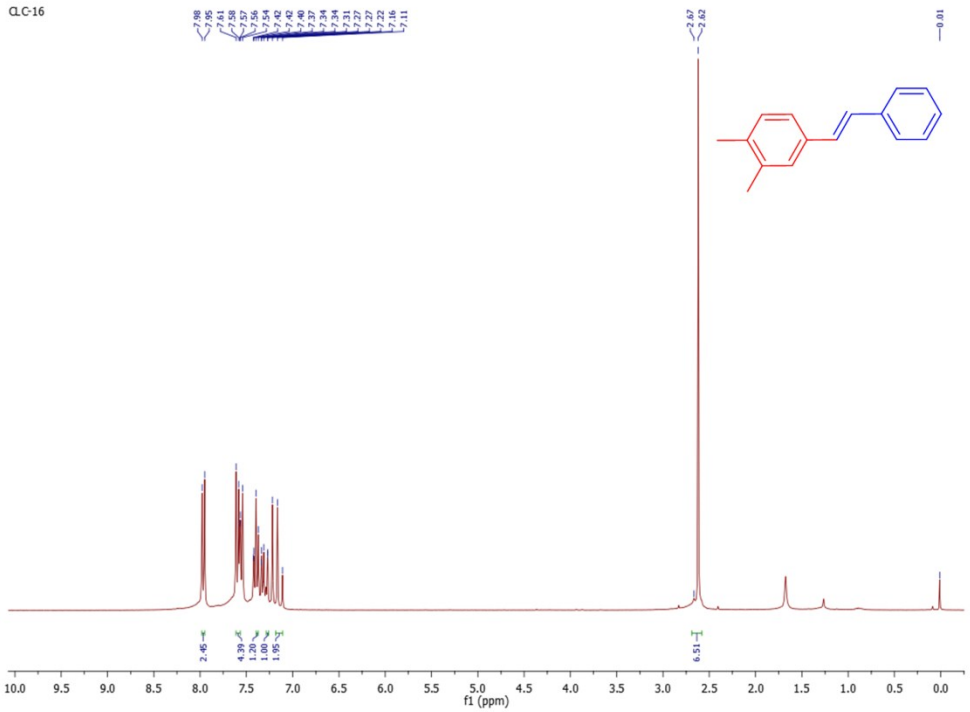


Figure S58. [1]H-NMR spectrum for 6k

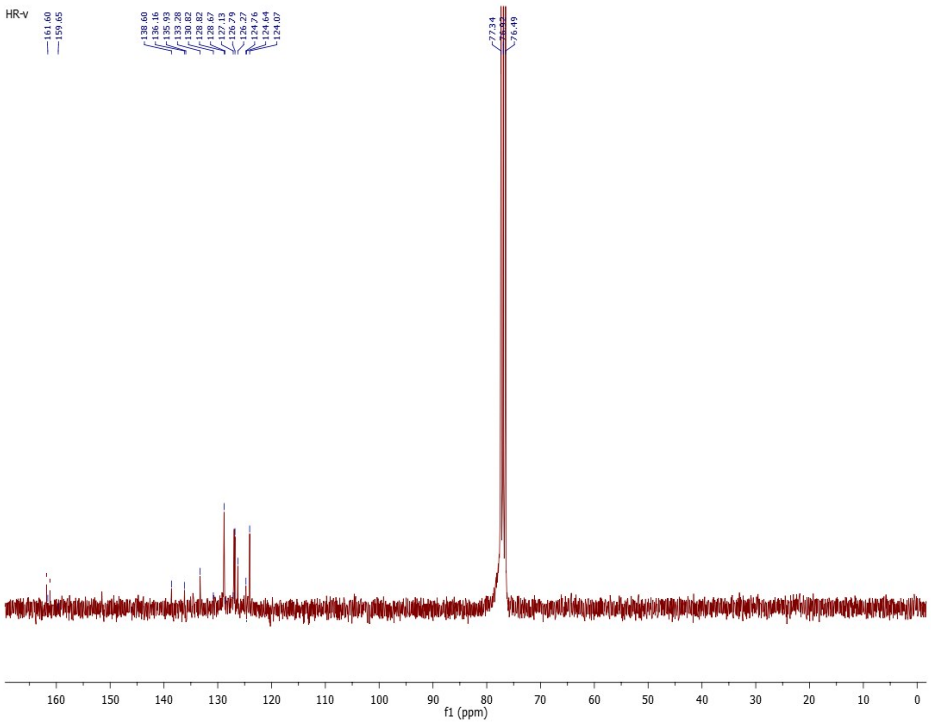


Figure S59. ^{13}C-NMR spectrum for 6k