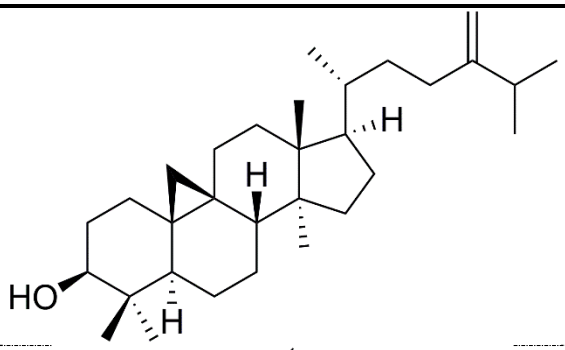
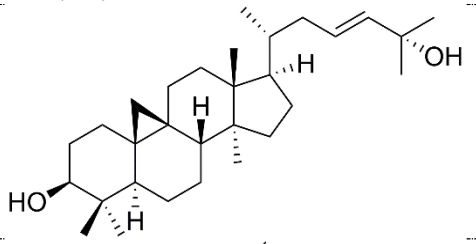
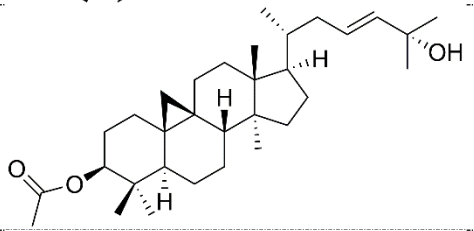
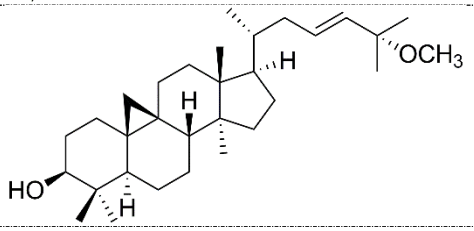
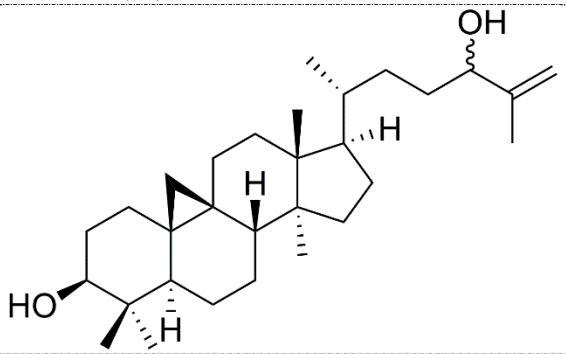
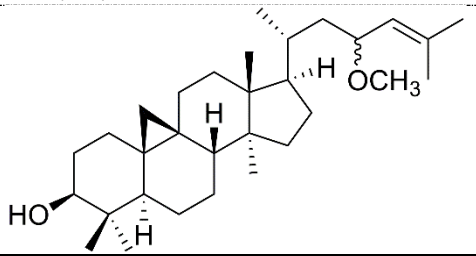
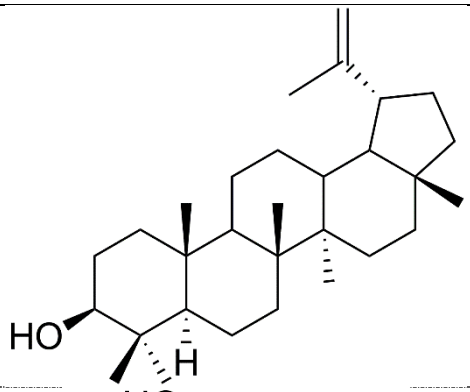
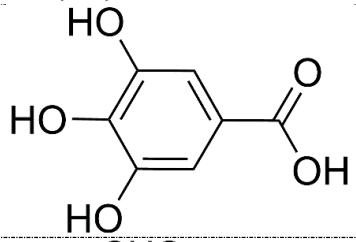
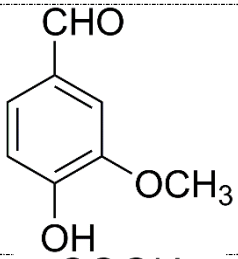
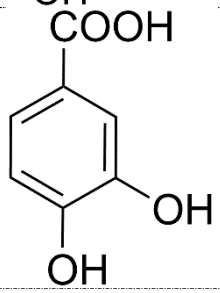
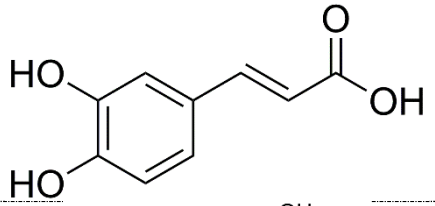
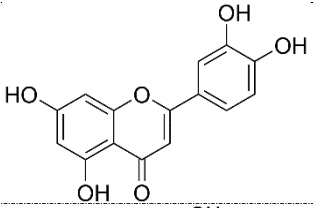
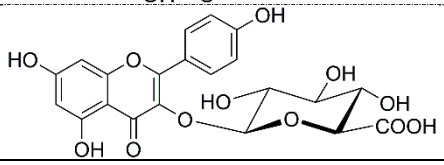
Supplementary material

Conducting the RBD of SARS-COV-2 Omicron Variant with Phytoconstituents from *Euphorbia dendroides* to Repudiate the Binding of Spike Glycoprotein Using Computational Molecular Search and Simulation Approach

Table S1. Compound name, 2D-chemical structure, and IUPAC name of the seventeen studied compounds.

Compound No.	2D-Chemical Structure	Compound Name
1		24-methylene cycloartan-3*β*-ol
2		Cycloart-23-ene-3*β*,25-diol
3		Cycloart-23-ene-3*β*,25-diol monoacetate
4		3*β*-hydroxy-cycloart-23-ene-25 methyl ether
5		24 *R*/*S*-3*β*-hydroxy-25-methylene cycloartan-24-ol
6		23 *R*/*S*-3*β* -hydroxycycloart-24-ene-23-methyl ether

7		Lupeol
8		Gallic acid
9		Vanillin
10		Protocatechuic acid
11		*trans*-caffeic acid
12		Luteolin
13		Kaempferol-3-*O*-*β*-D-glucuronopyranoside

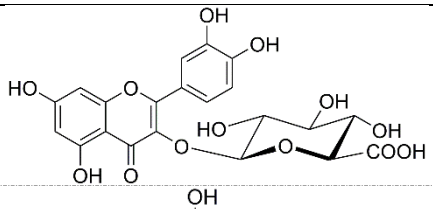
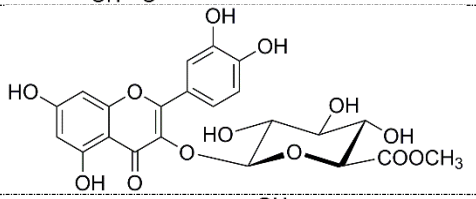
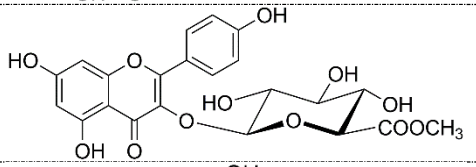
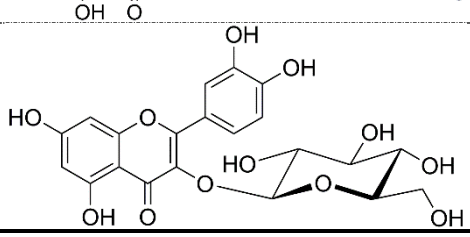
14		Quercetin-3-*O*-*β*-D-glucuronopyranoside
15		Quercetin-3-*O*-glucuronoide 6"-*O*-methyl ester
16		Kampferol-3-*O*-glucuronoide 6"-*O*-methyl ester
17		Quercetin-3-*O*-*β*-D-glucopyranoside

Table S2. Calculated docking scores (in kcal/mol) for the SARS-COV-2 Omicron drug candidates.

Compound No.	Docking Score (kcal/mol)
1	−4.4
2	−5.7
3	−6.4
4	−5.3
5	−4.7
6	−6.1
7	−5.0
8	−6.8
9	−7.2
10	−7.6
11	−7.7
12	−7.9
13	−8.1
14	−8.7
15	−8.8
16	−8.4
17	−8.3

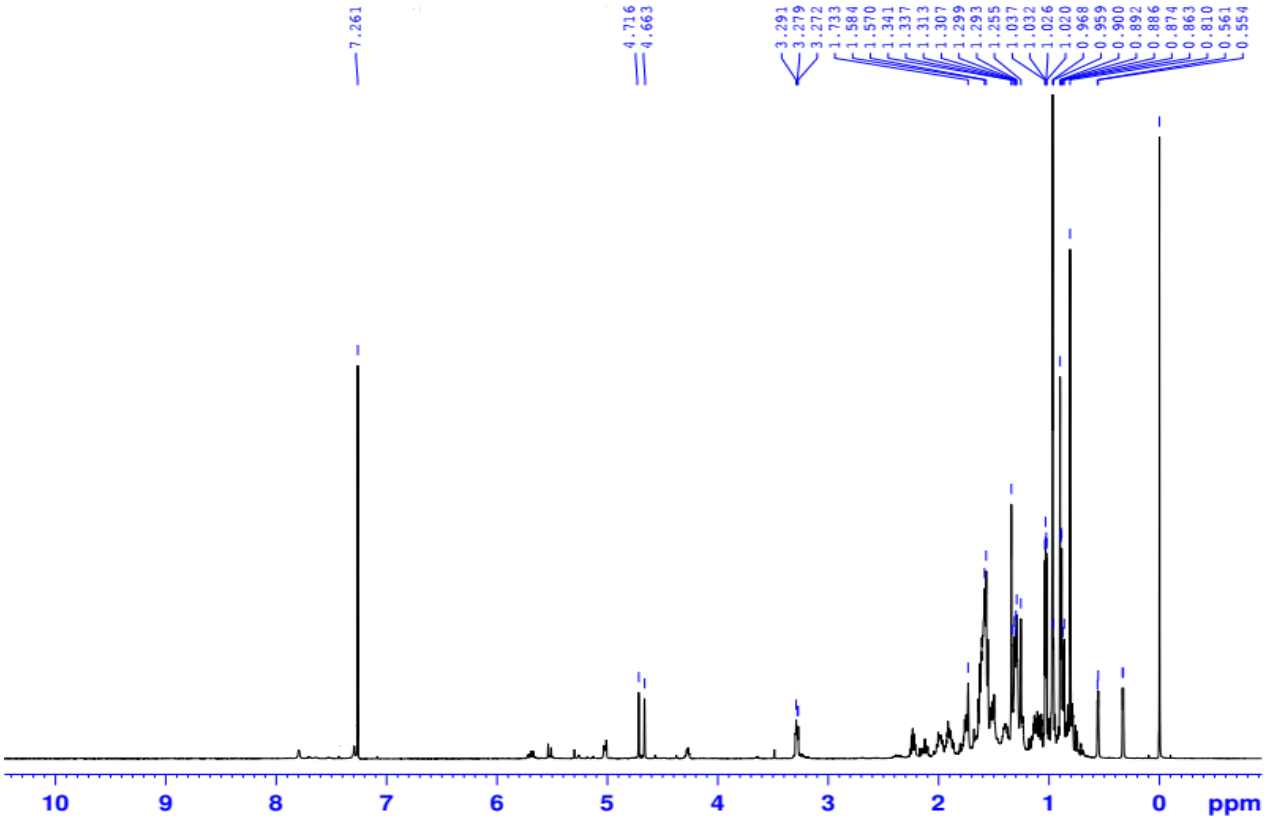


Figure S1. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of compound 1

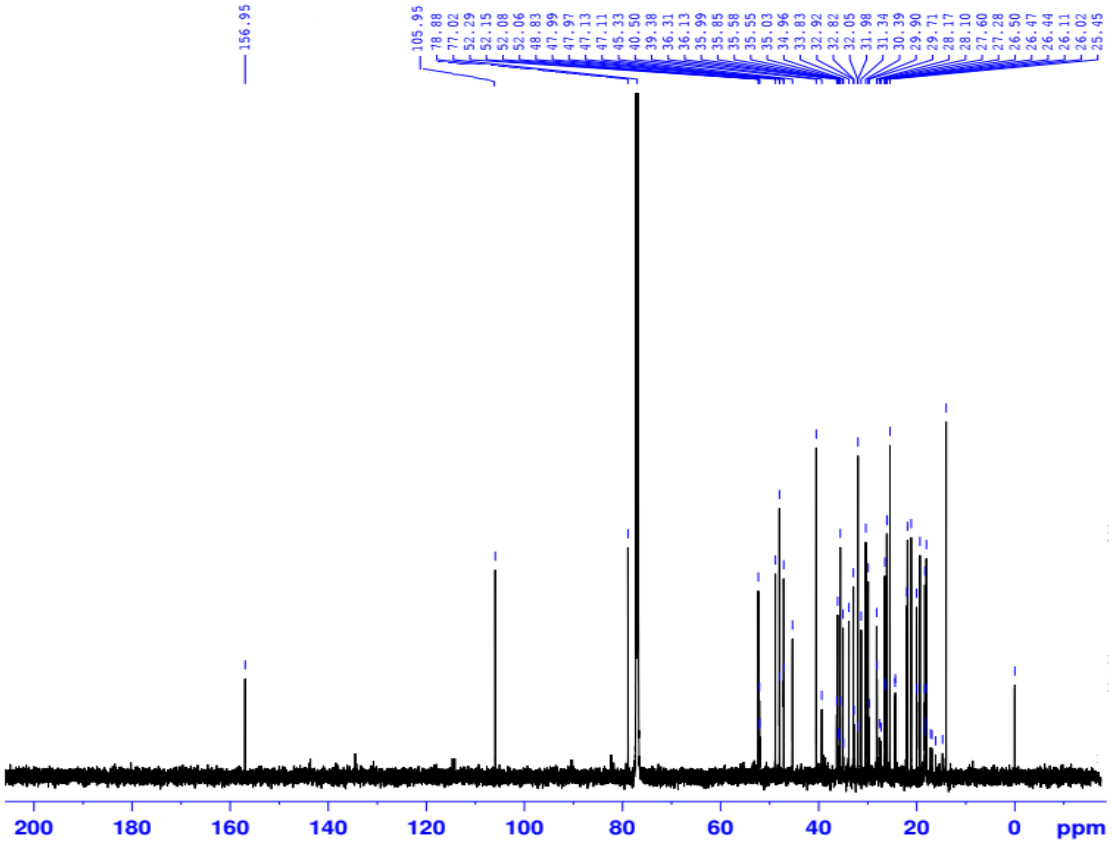


Figure S2. ^{13}C NMR spectrum (150 MHz, $CDCl_3$) of compound 1

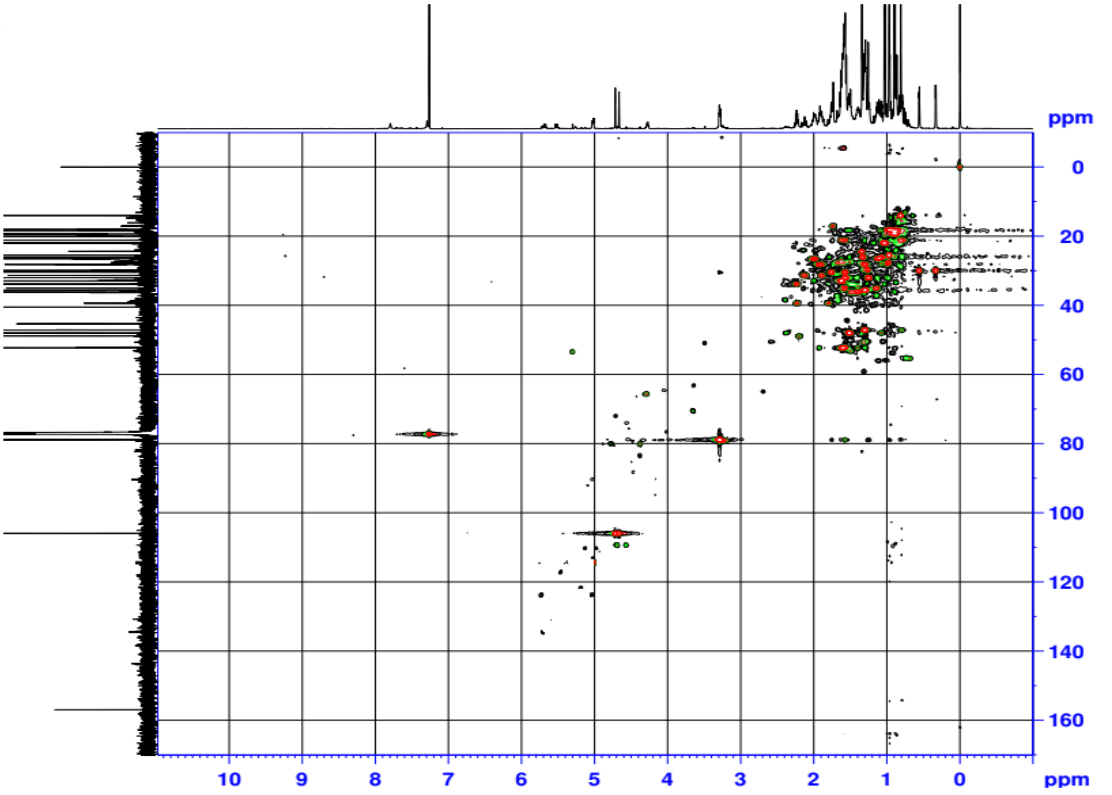


Figure S3. HSQC spectrum ($CDCl_3$) of compound 1

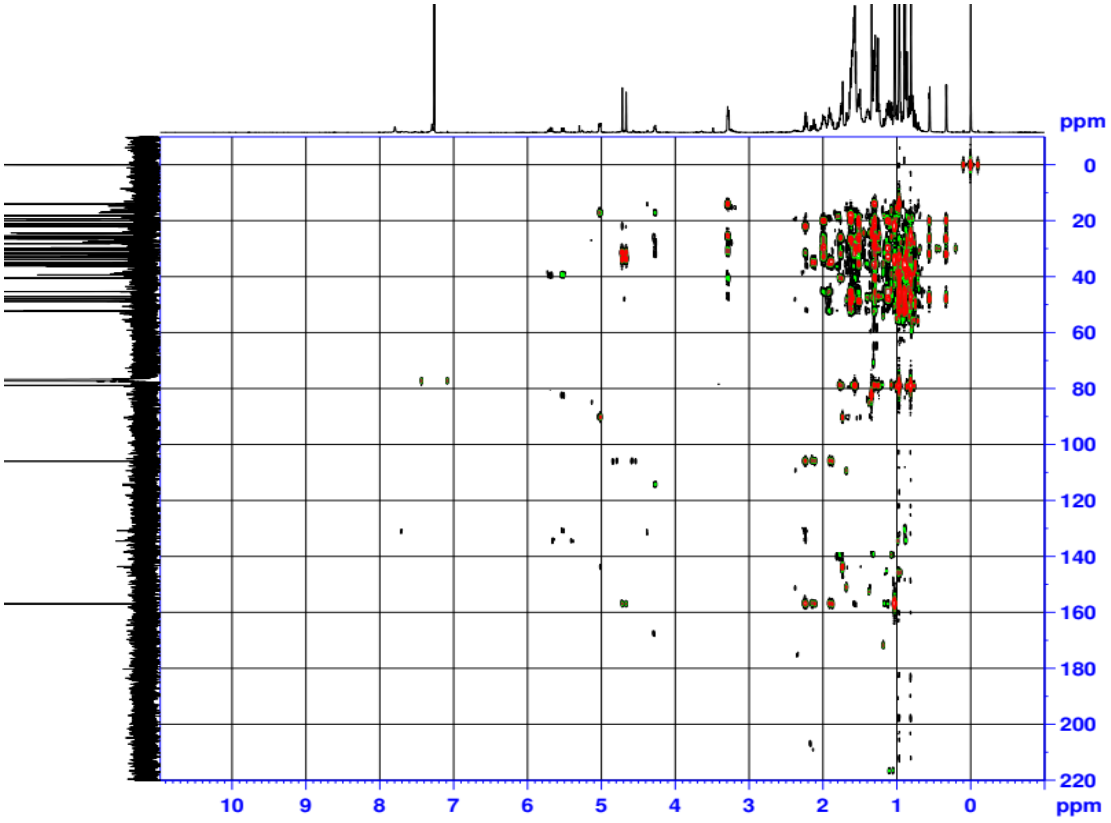


Figure S4. HMBC spectrum ($CDCl_3$) of compound 1

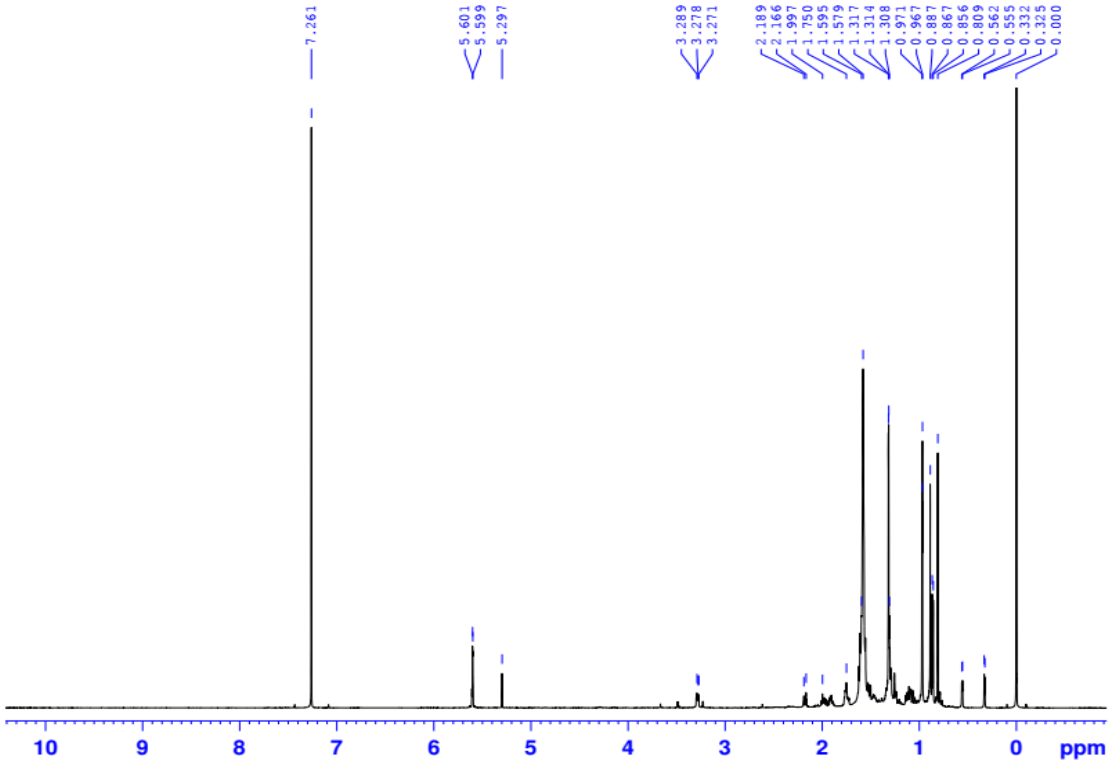


Figure S5. ^1H NMR spectrum (600 MHz, $CDCl_3$) of compound 2

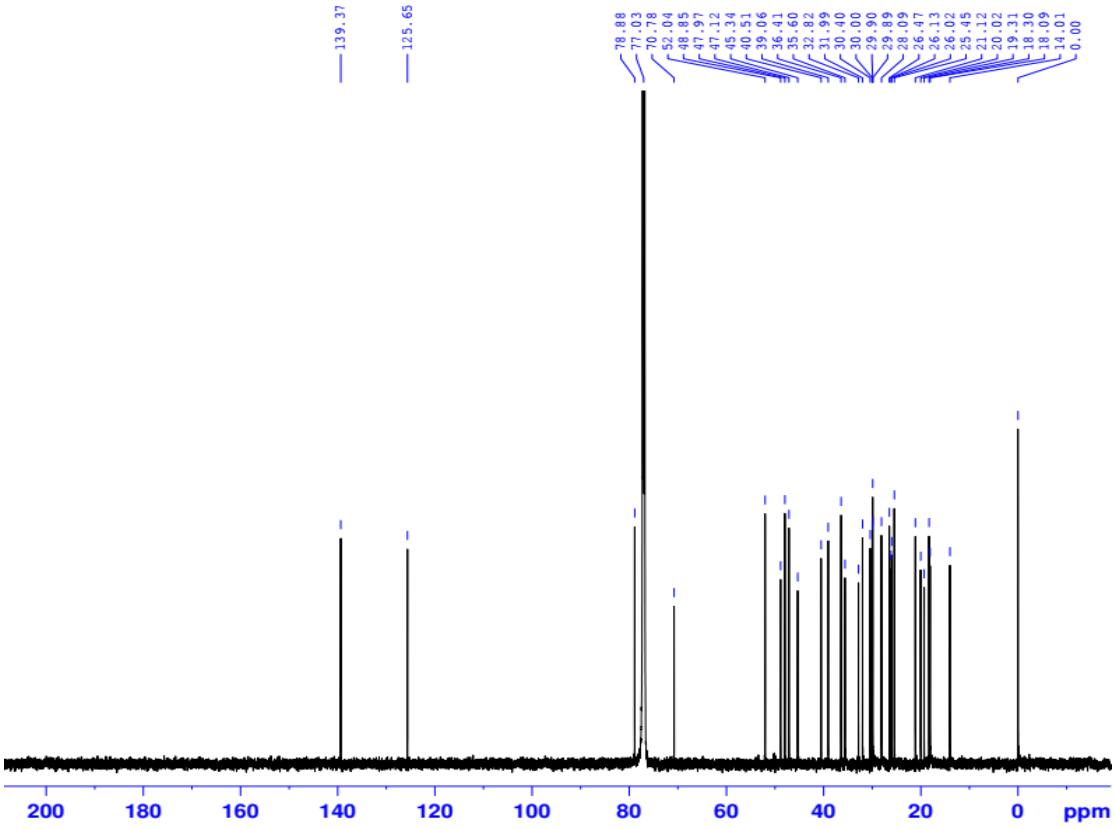


Figure S6. ^{13}C NMR spectrum (150 MHz, $CDCl_3$) of compound 2

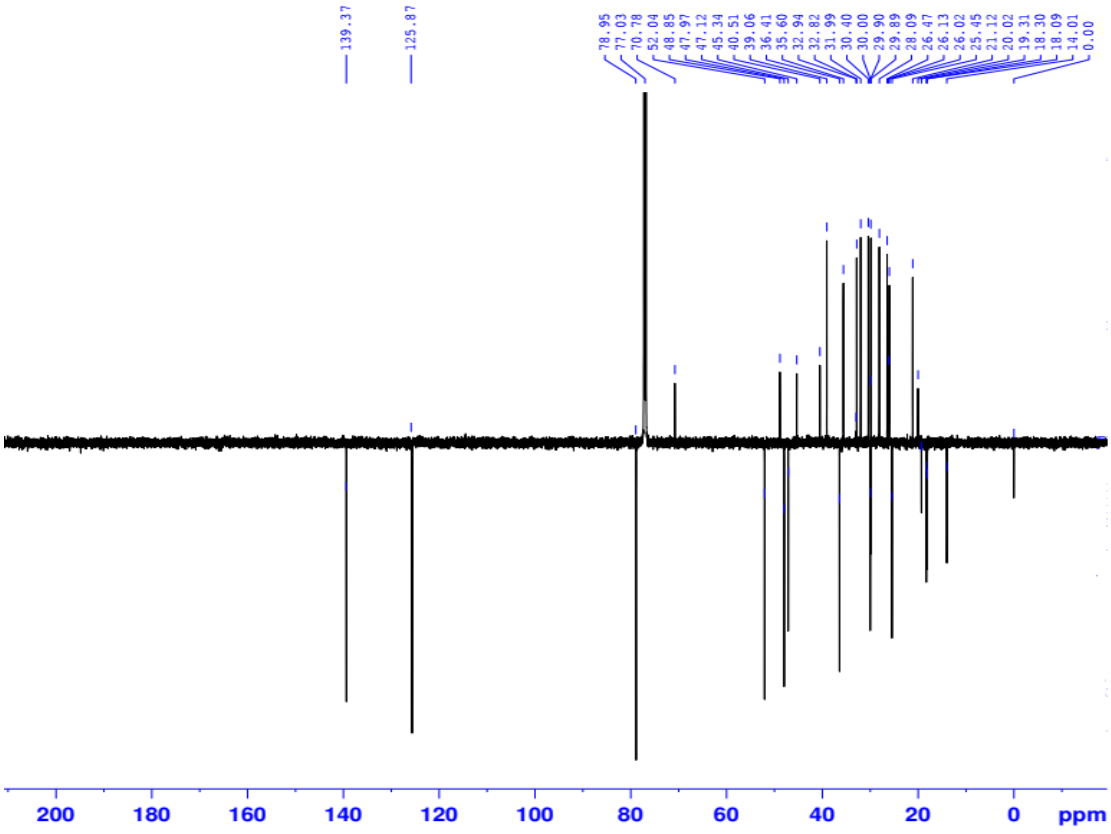


Figure S7. APT spectrum (150 MHz, $CDCl_3$) of compound 2

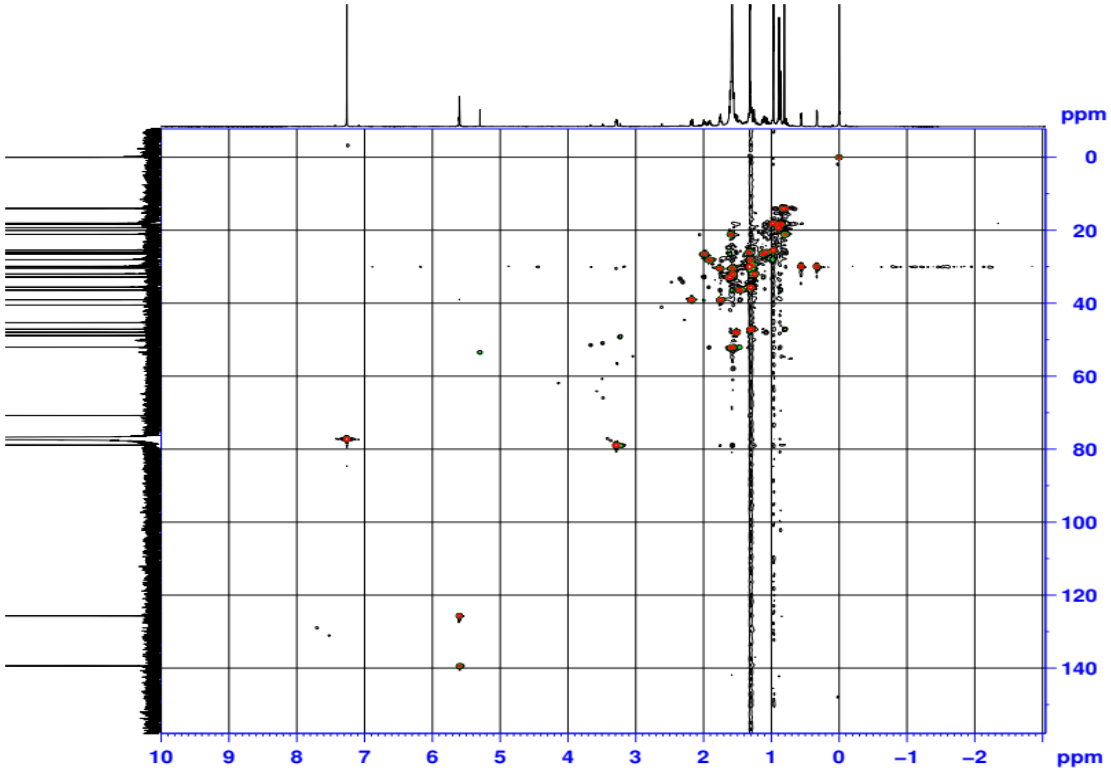


Figure S8. HSQC spectrum ($CDCl_3$) of compound 2

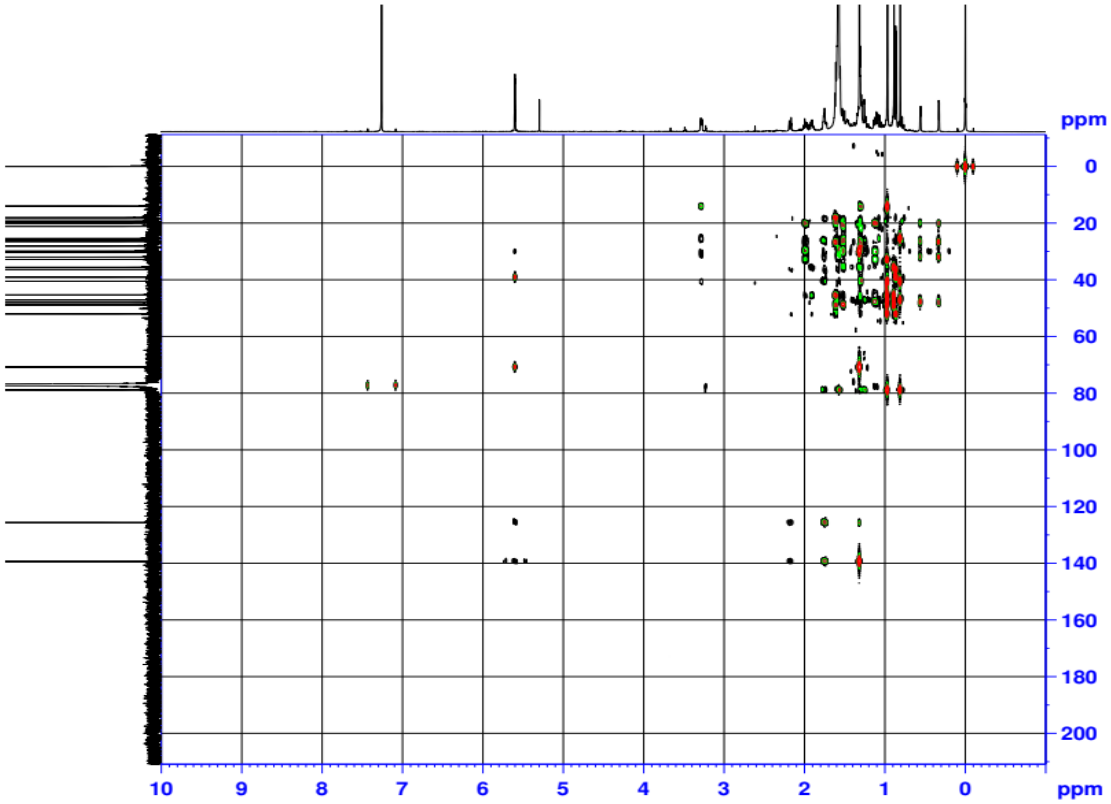


Figure S9. HMBC spectrum ($CDCl_3$) of compound 2

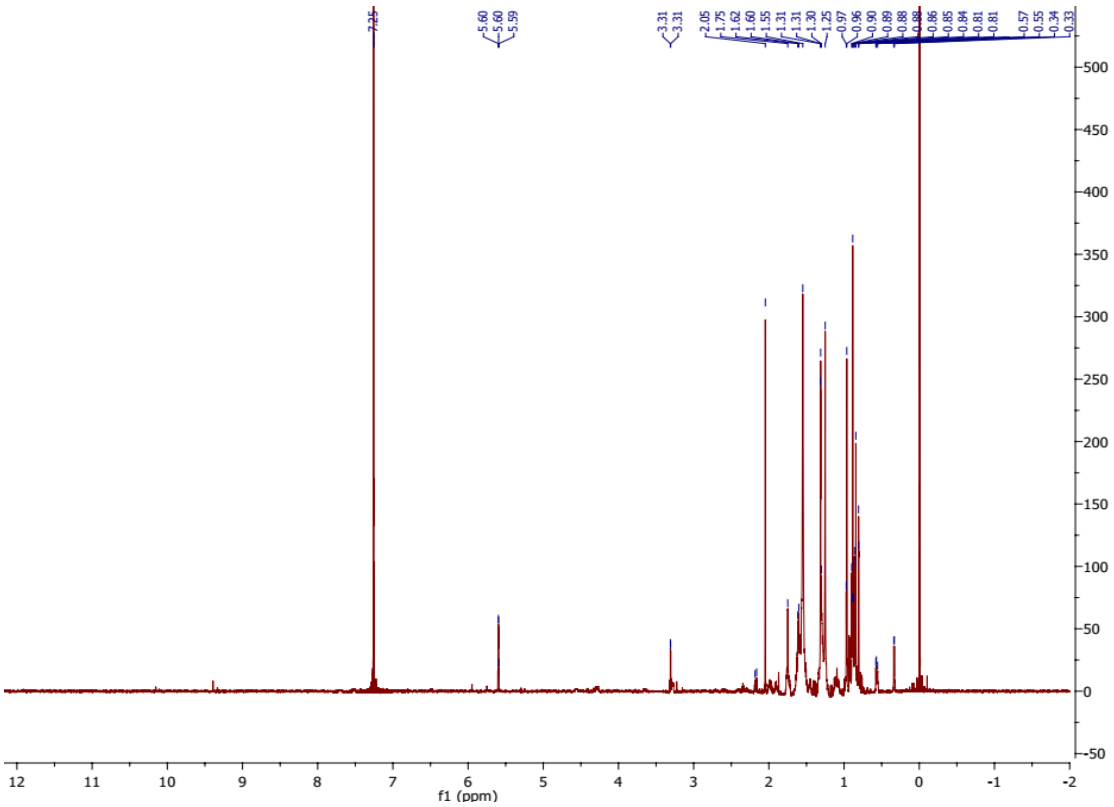


Figure S10. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of compound 3

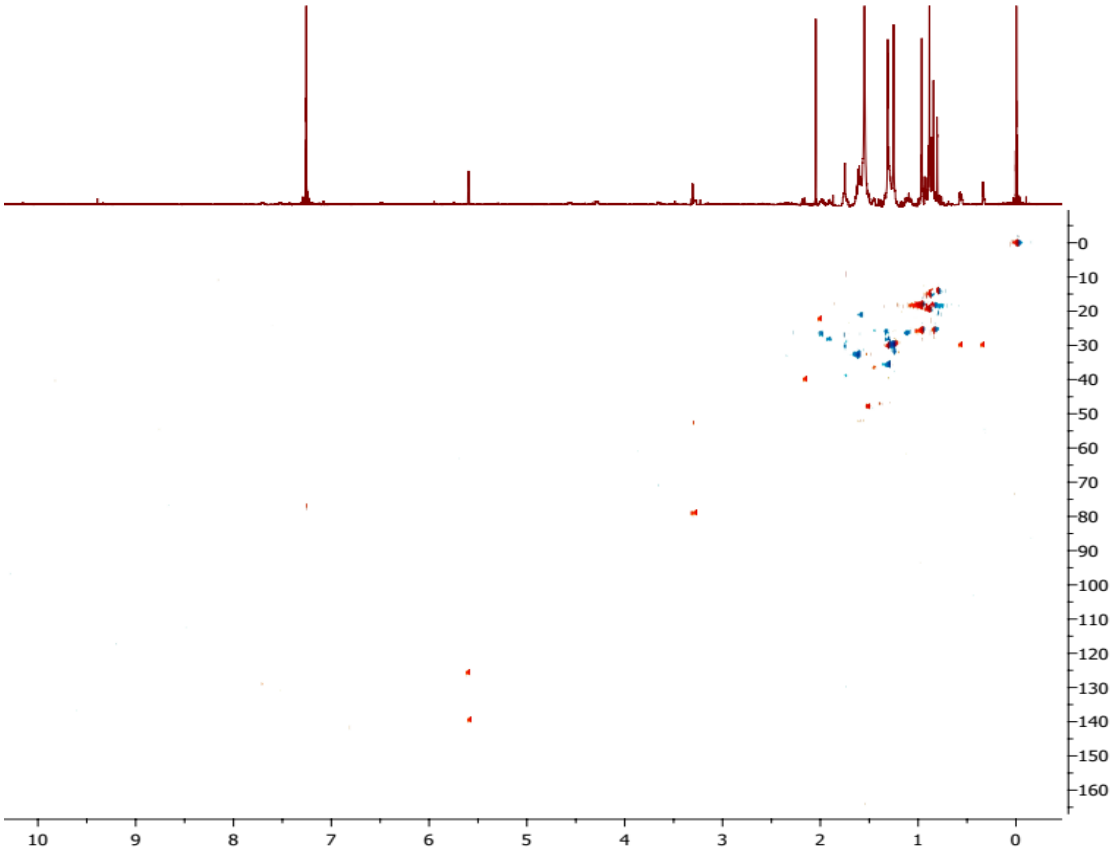


Figure S11. HSQC spectrum ($CDCl_3$) of compound 3

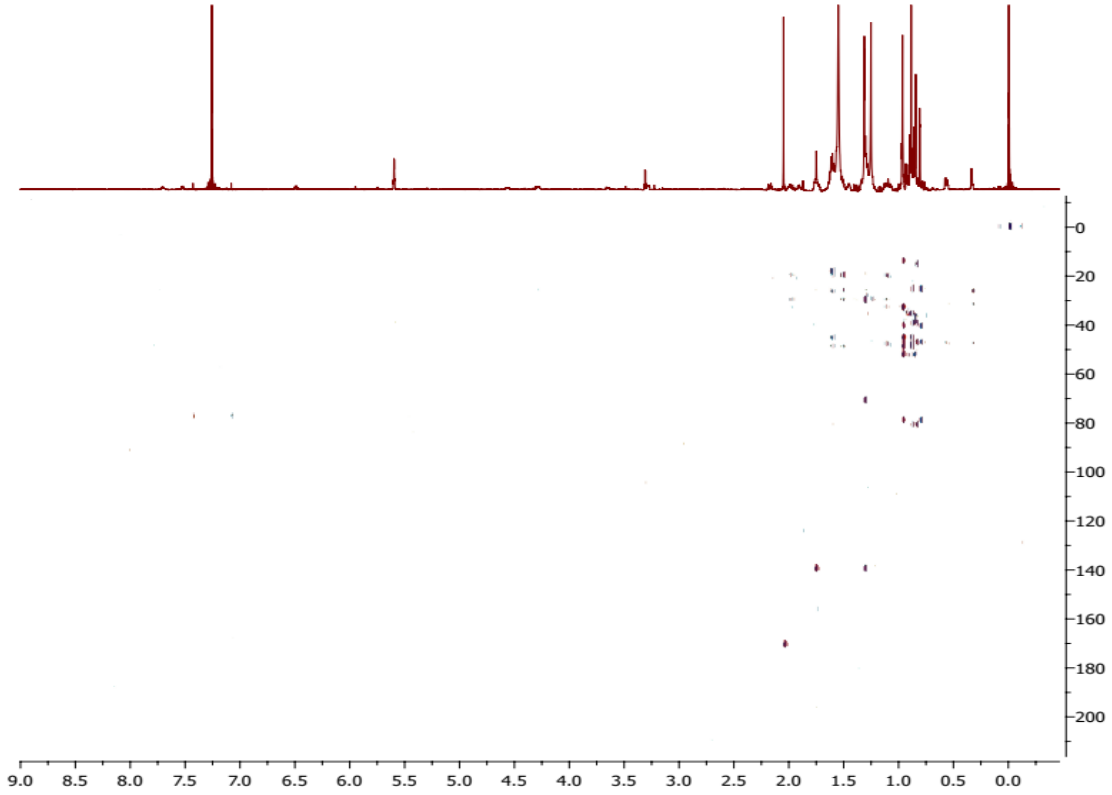


Figure S12. HMBC spectrum ($CDCl_3$) of compound 3

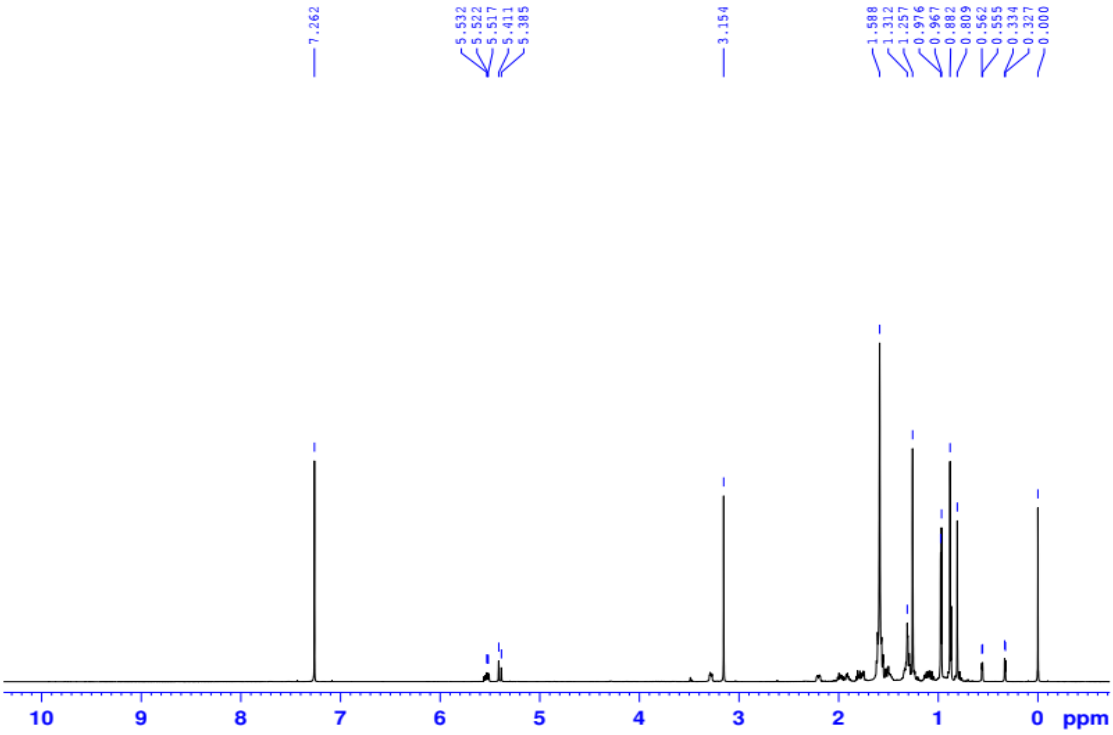


Figure S13. ^1H NMR spectrum (600 MHz, $CDCl_3$) of compound 4

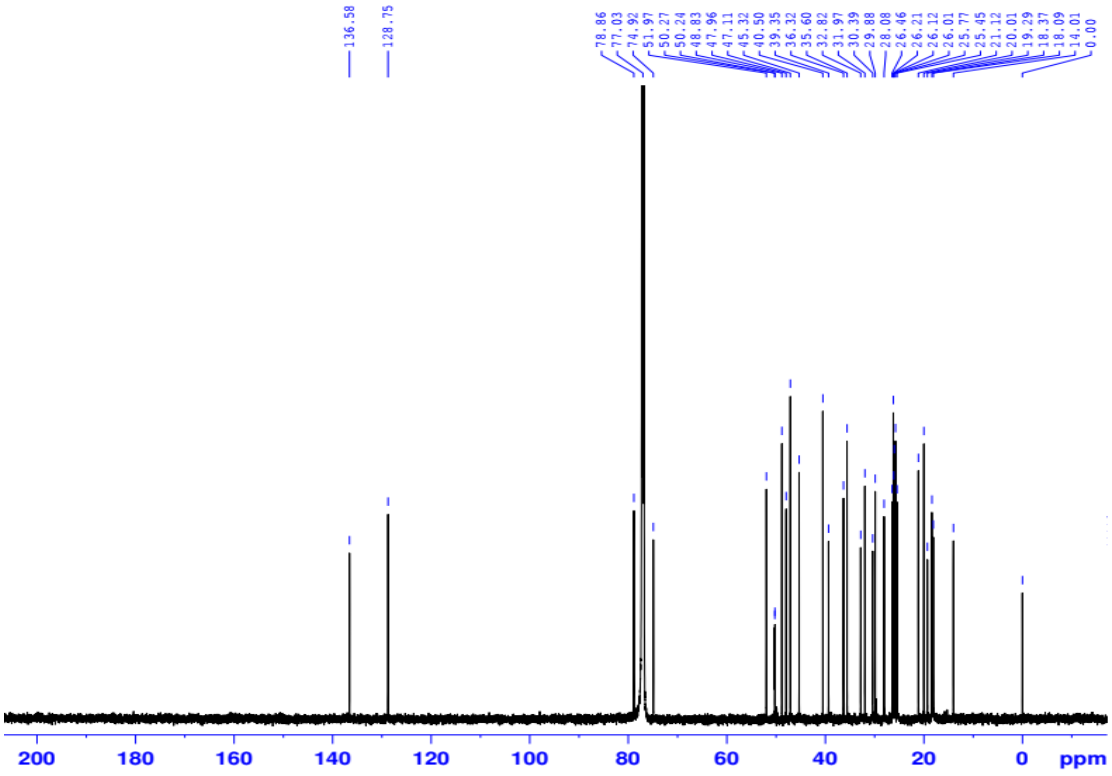


Figure S14. ^{13}C NMR spectrum (150 MHz, $CDCl_3$) of compound 4

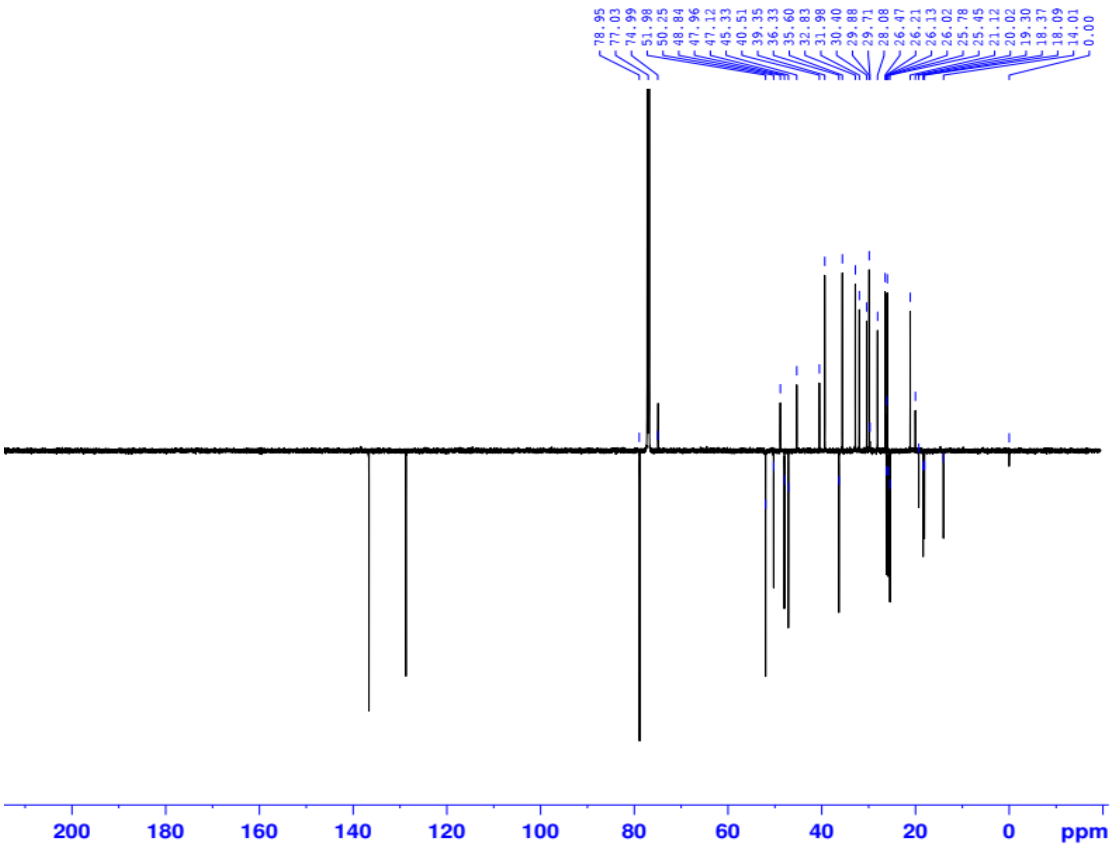


Figure S15. APT spectrum (150 MHz, $CDCl_3$) of compound 4

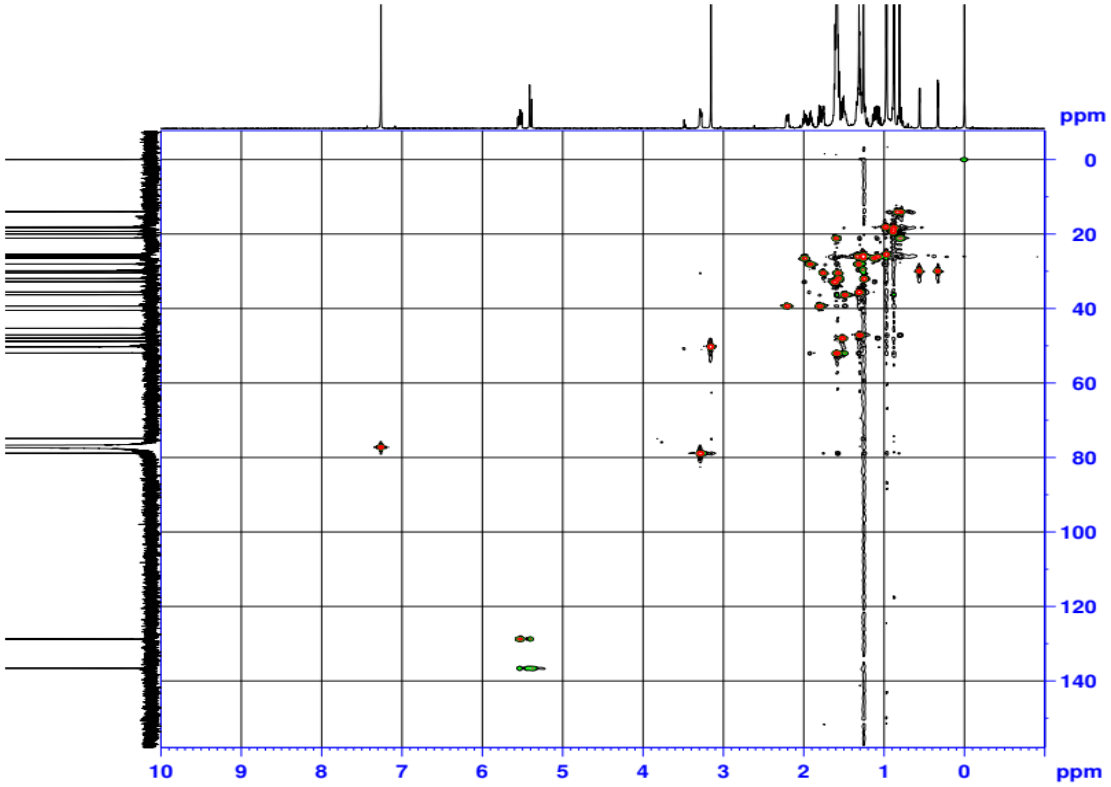


Figure S16. HSQC spectrum ($CDCl_3$) of compound 4

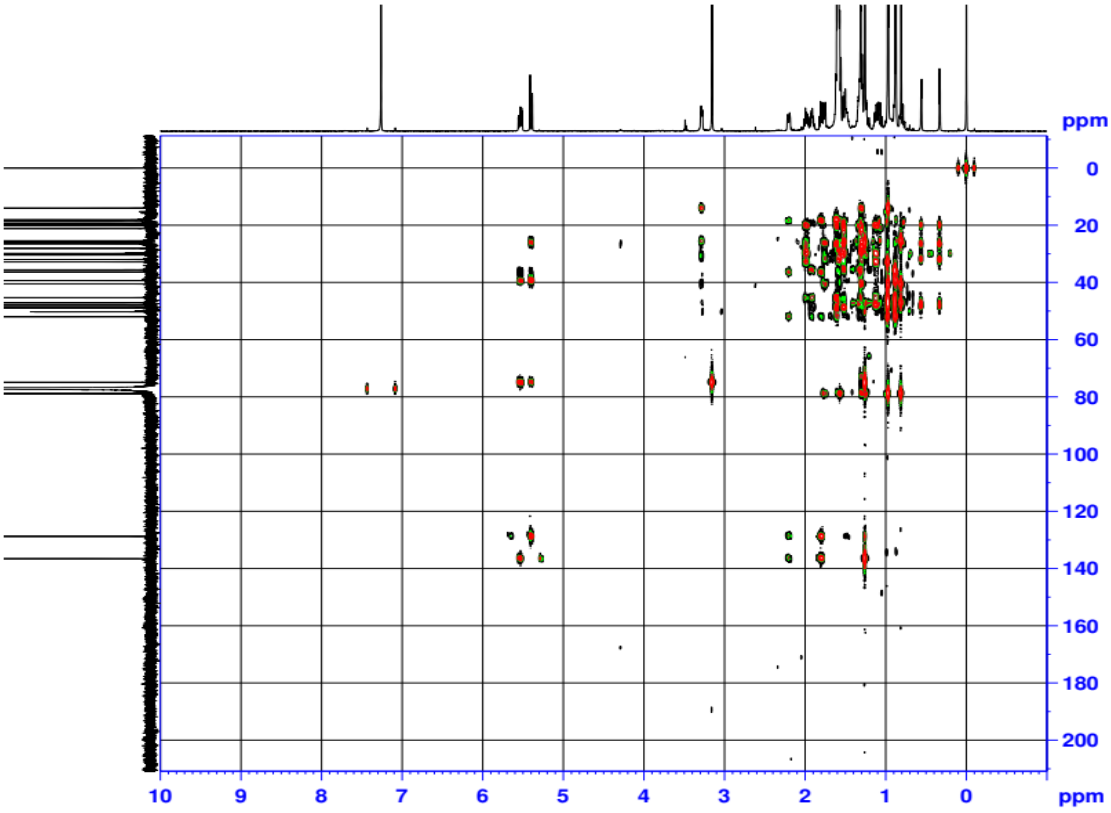


Figure S17. HMBC spectrum ($CDCl_3$) of compound 4

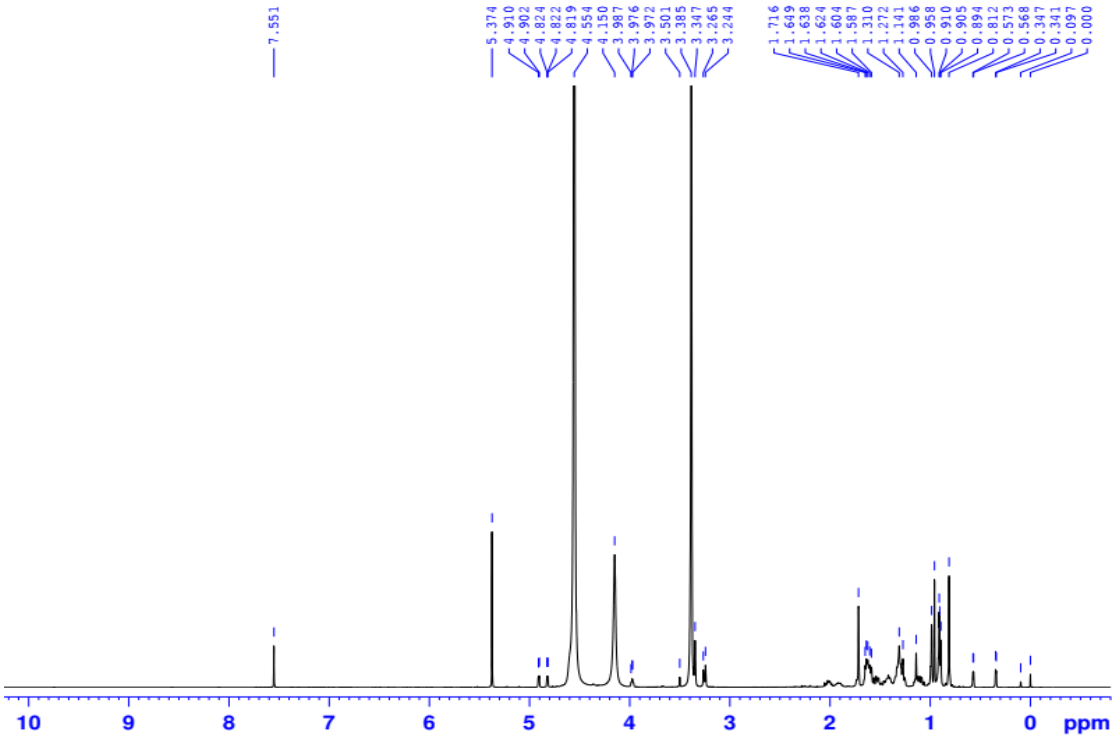


Figure S18. ^{1}H NMR spectrum (600 MHz, CD_3OD & $CDCl_3$) of compound 5

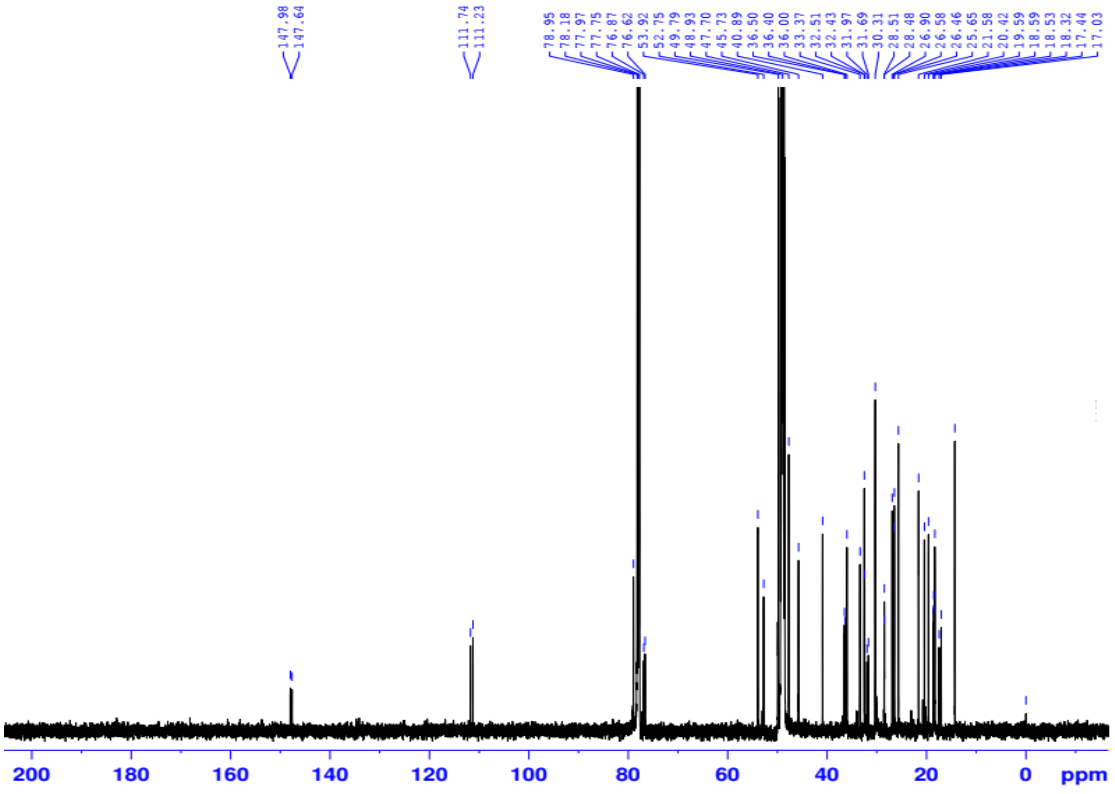


Figure S19. ^{13}C NMR spectrum (150 MHz, CD_3OD & $CDCl_3$) of compound 5

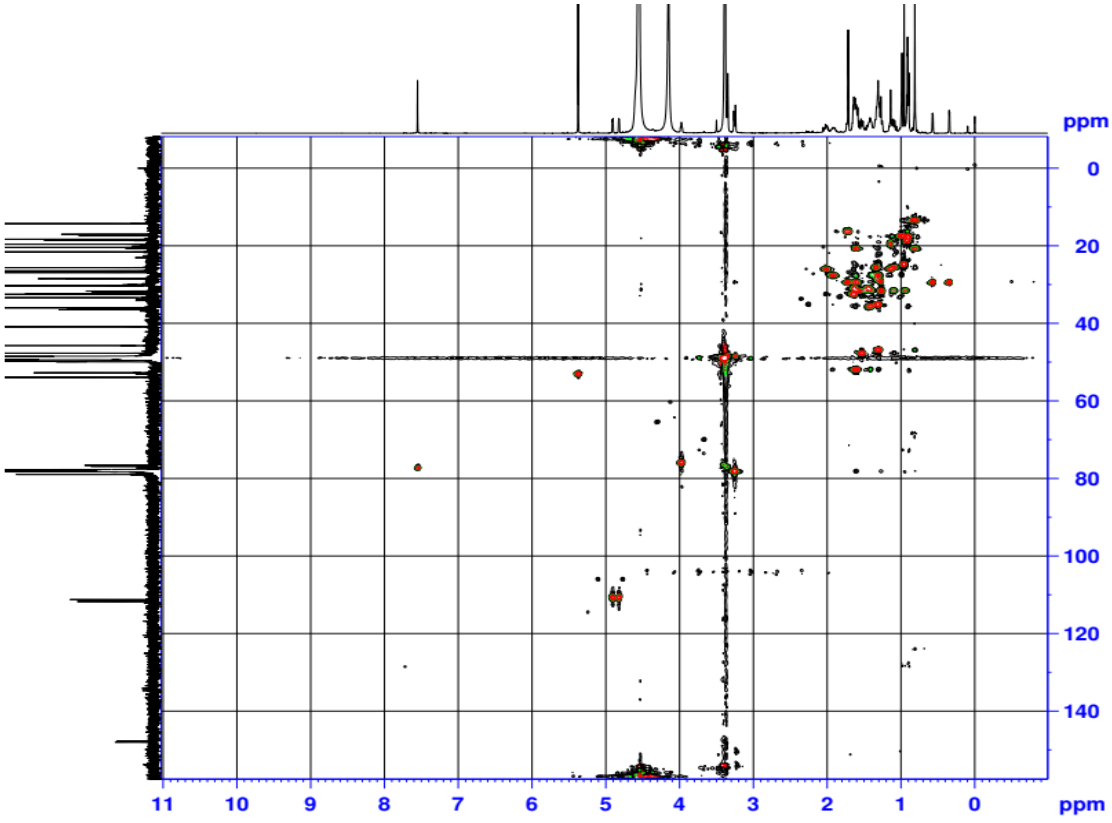


Figure S20. HSQC spectrum (CD_3OD & $CDCl_3$) of compound 5

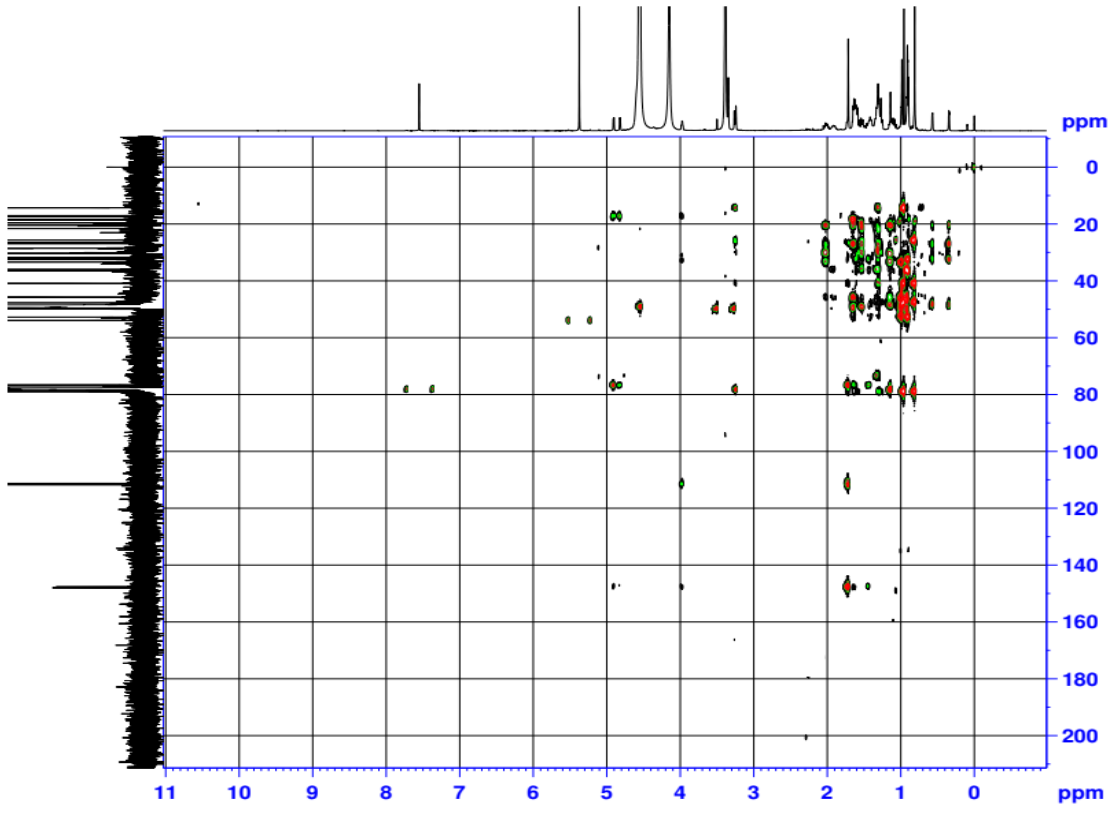


Figure S21. HMBC spectrum (CD_3OD & $CDCl_3$) of compound 5

EEA-6-1H

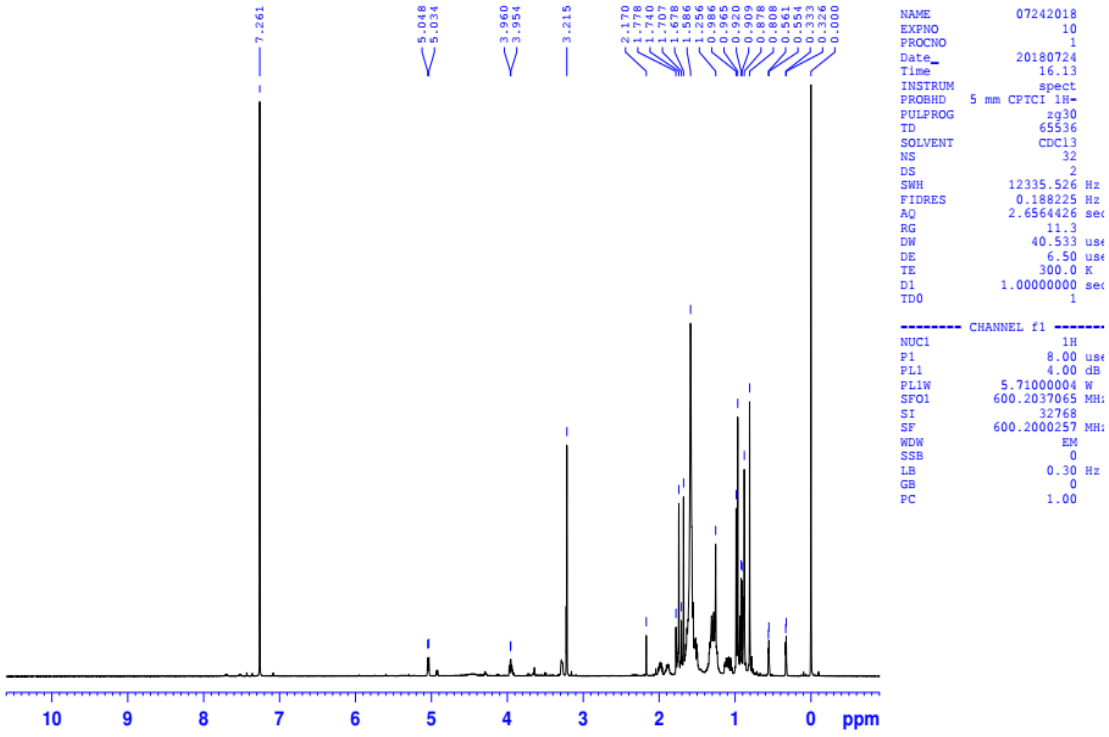


Figure S22. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of compound 6

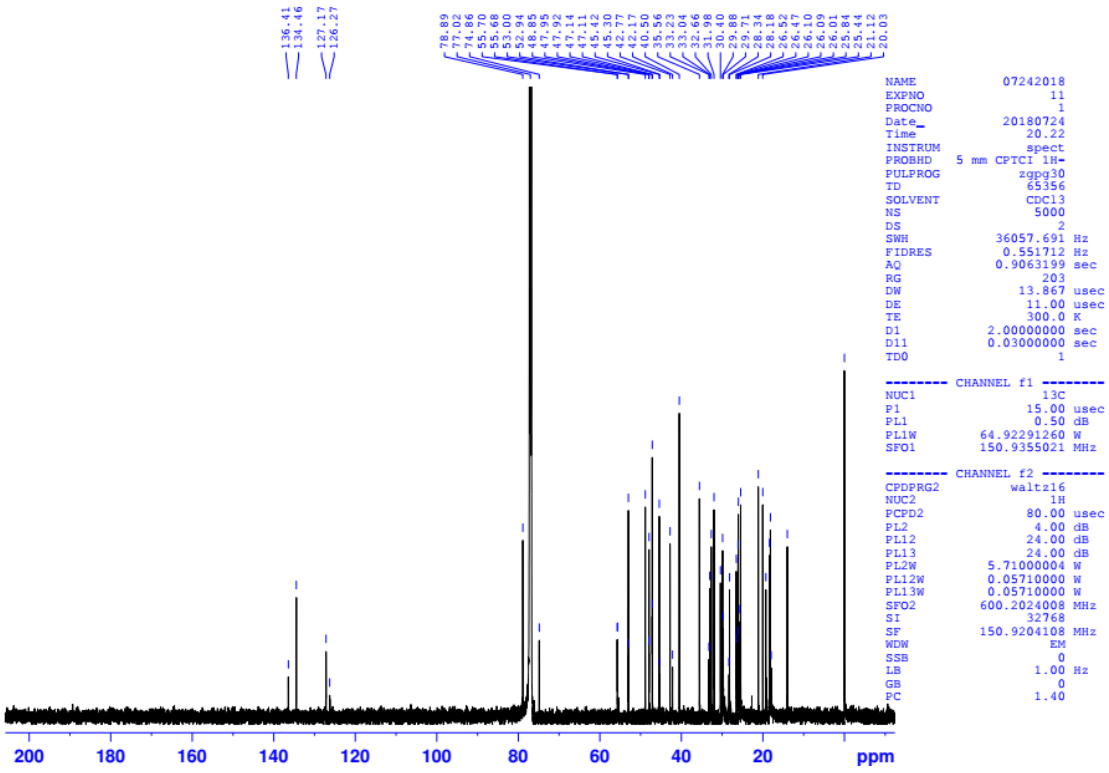


Figure S23. ^{13}C NMR spectrum (150 MHz, $CDCl_3$) of compound 6

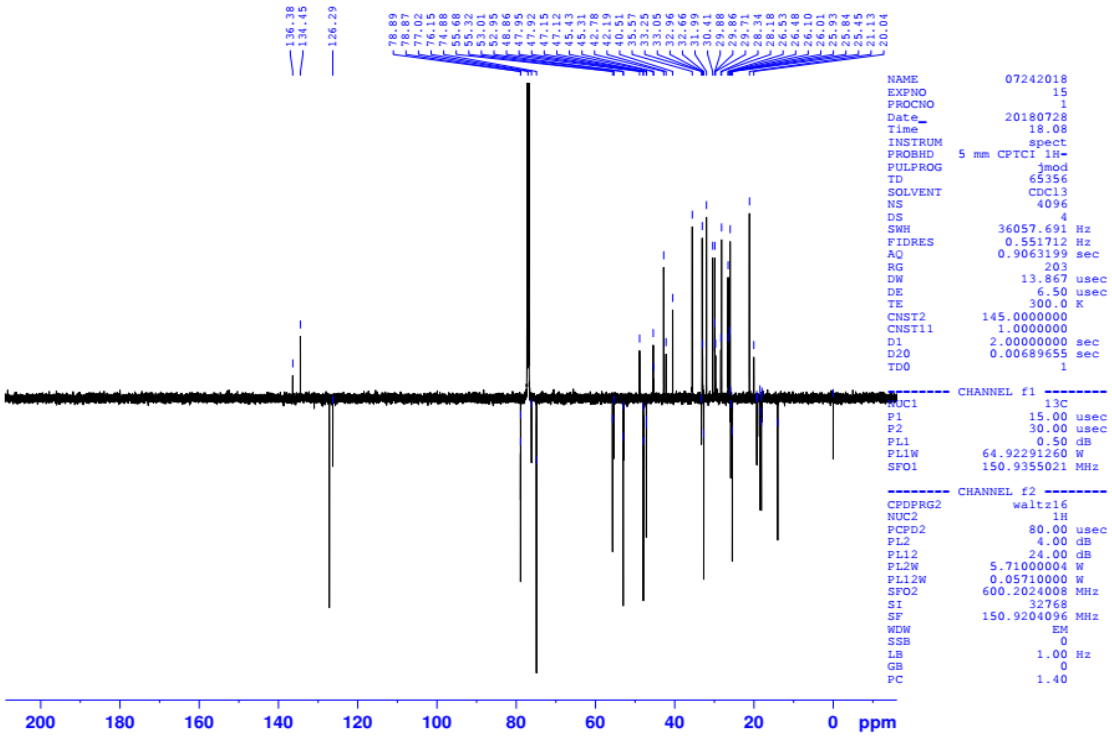


Figure S24. APT spectrum (150 MHz, $CDCl_3$) of compound 6

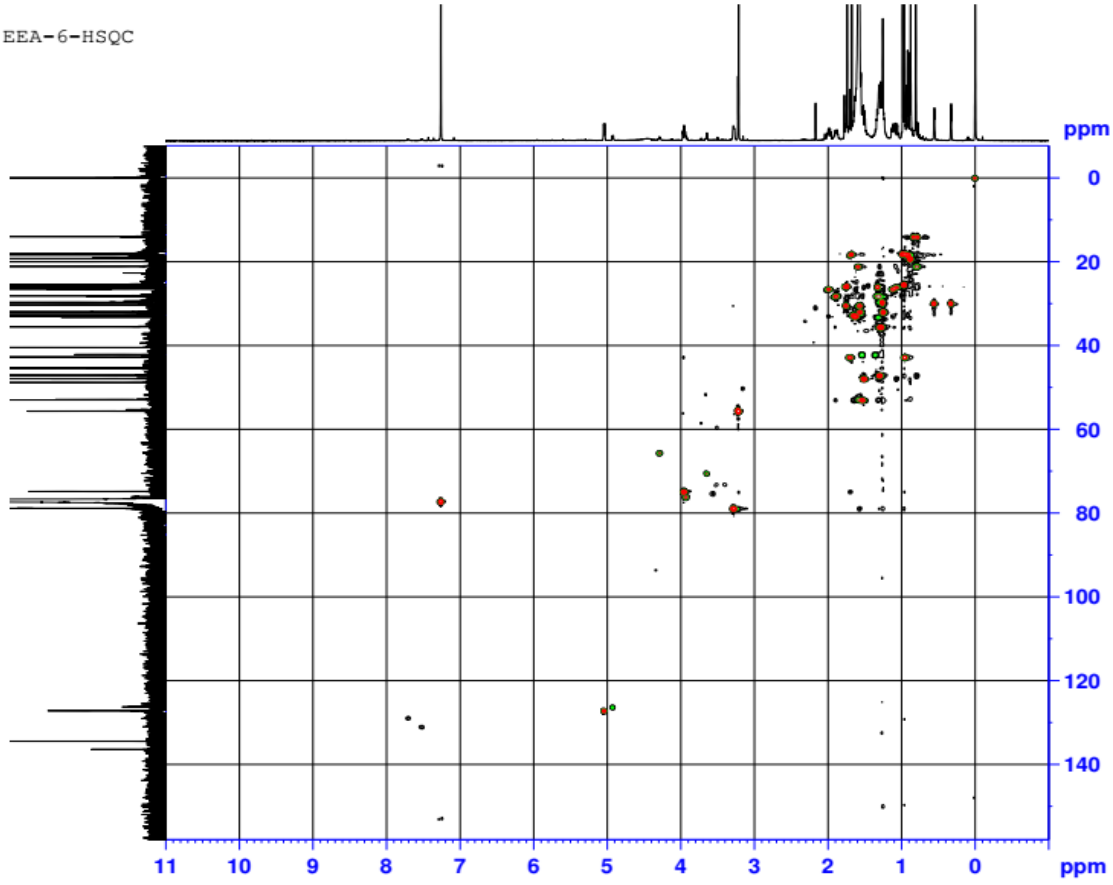


Figure S25. HSQC spectrum ($CDCl_3$) of compound 6

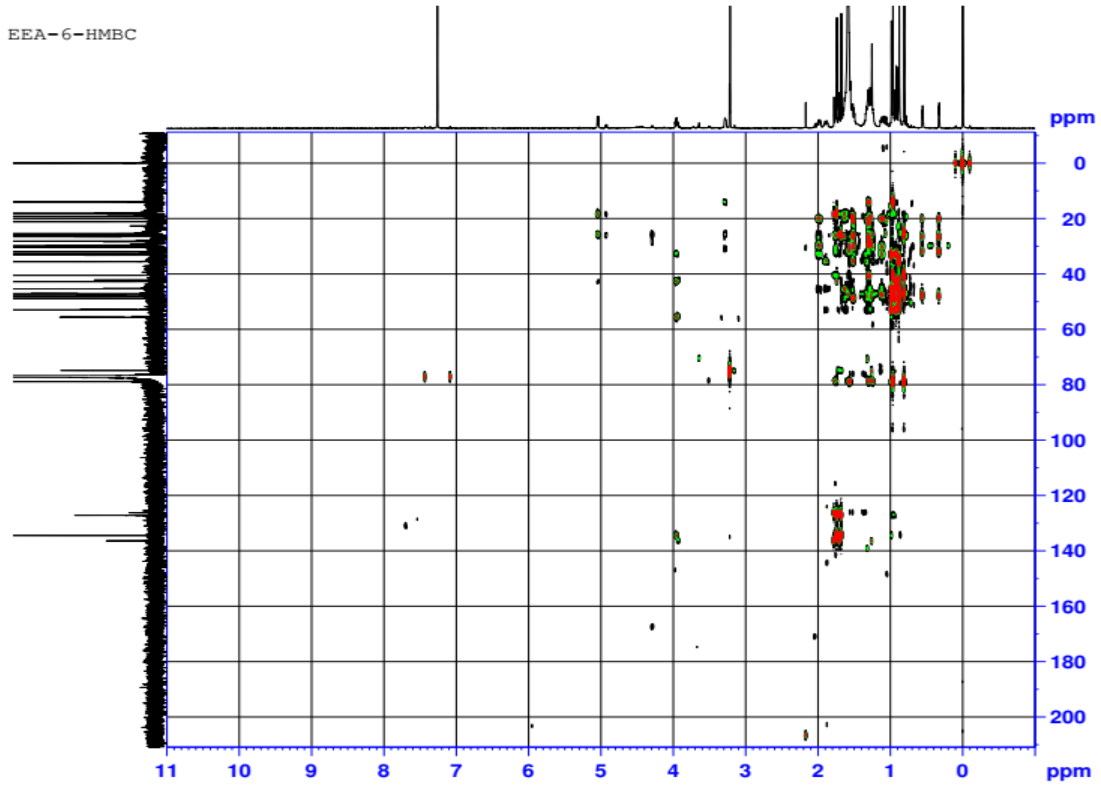


Figure S26. HMBC spectrum ($CDCl_3$) of compound 6

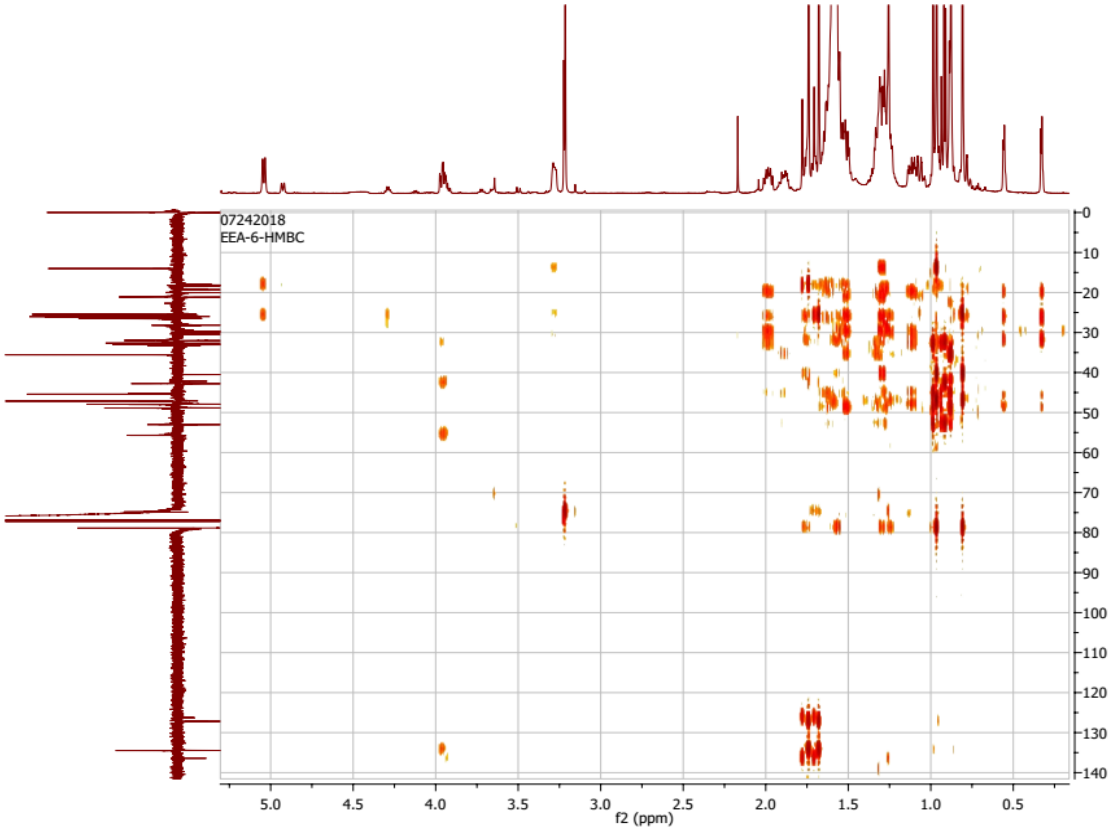


Figure S26-1. Expanded HMBC spectrum ($CDCl_3$) of compound 6

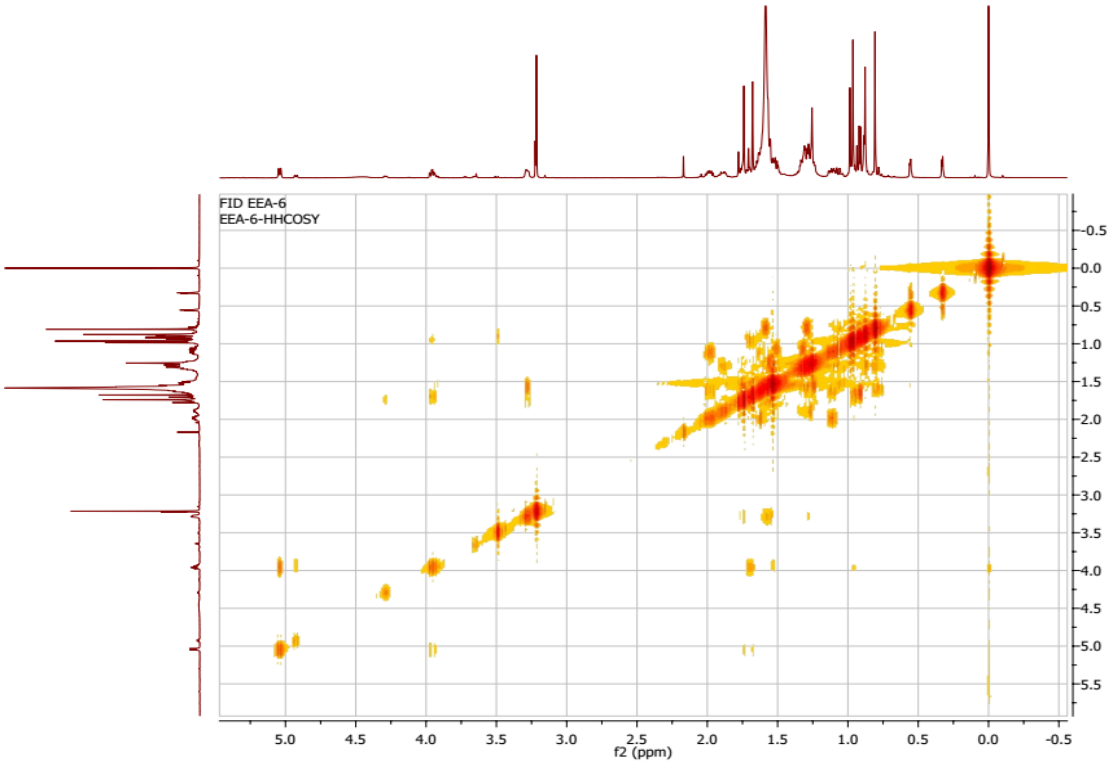


Figure S27. ^{1}H-^{1}H COSY spectrum ($CDCl_3$) of compound 6

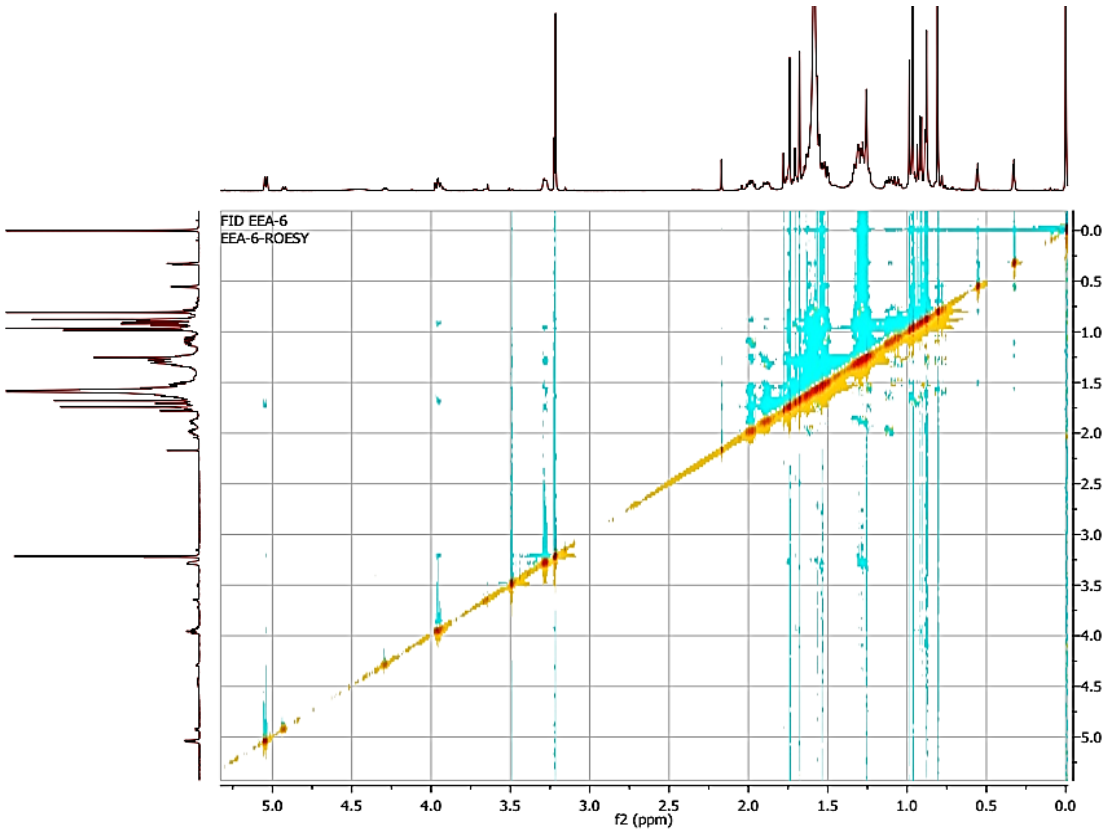


Figure S28. ROESY spectrum ($CDCl_3$) of compound 6

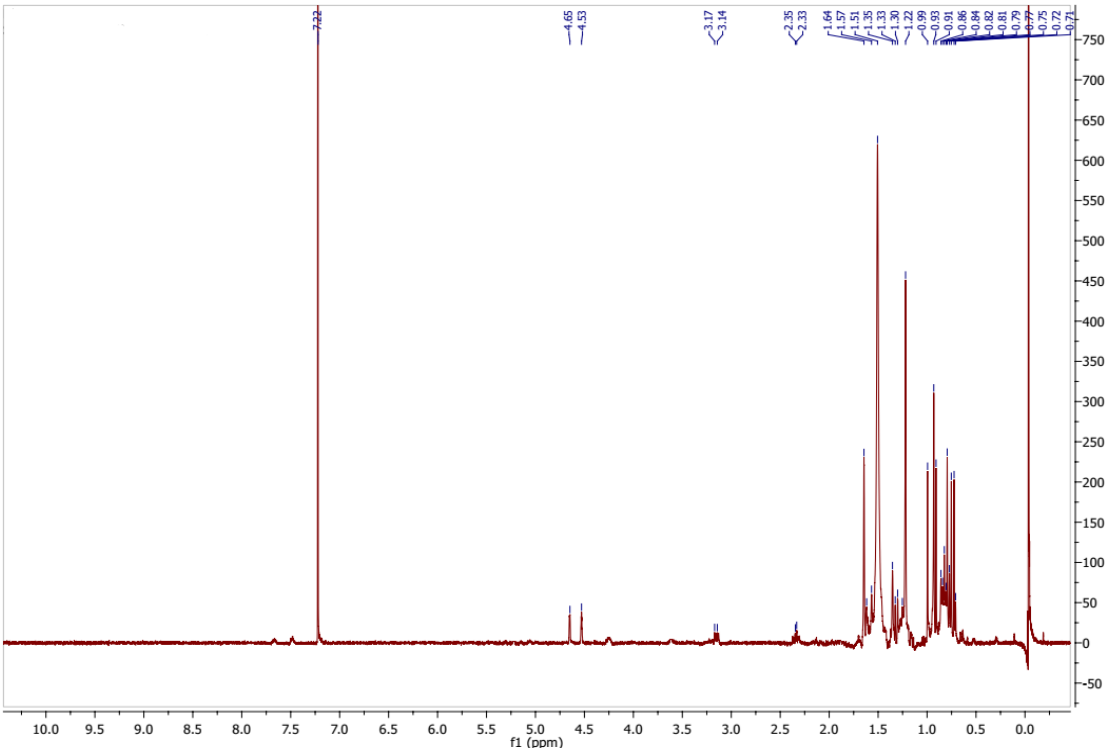


Figure S29. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of compound 7

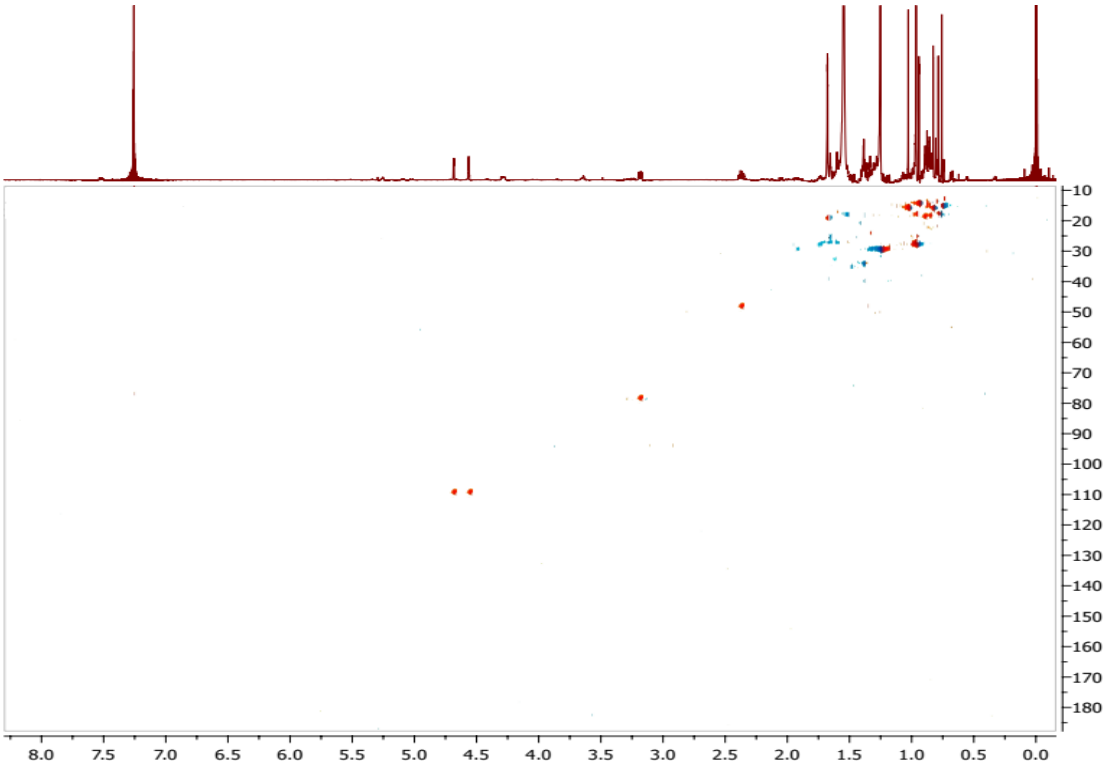


Figure S30. HSQC spectrum ($CDCl_3$) of compound 7

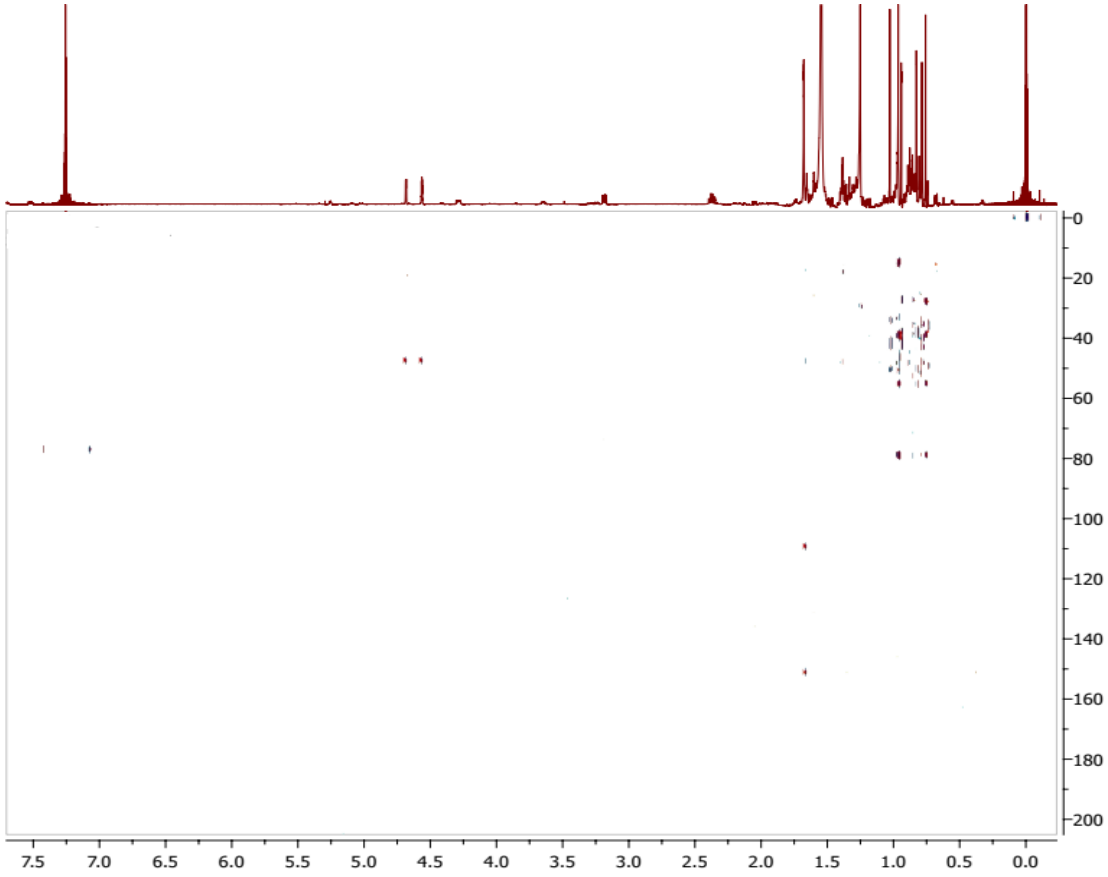


Figure S31. HMBC spectrum ($CDCl_3$) of compound 7

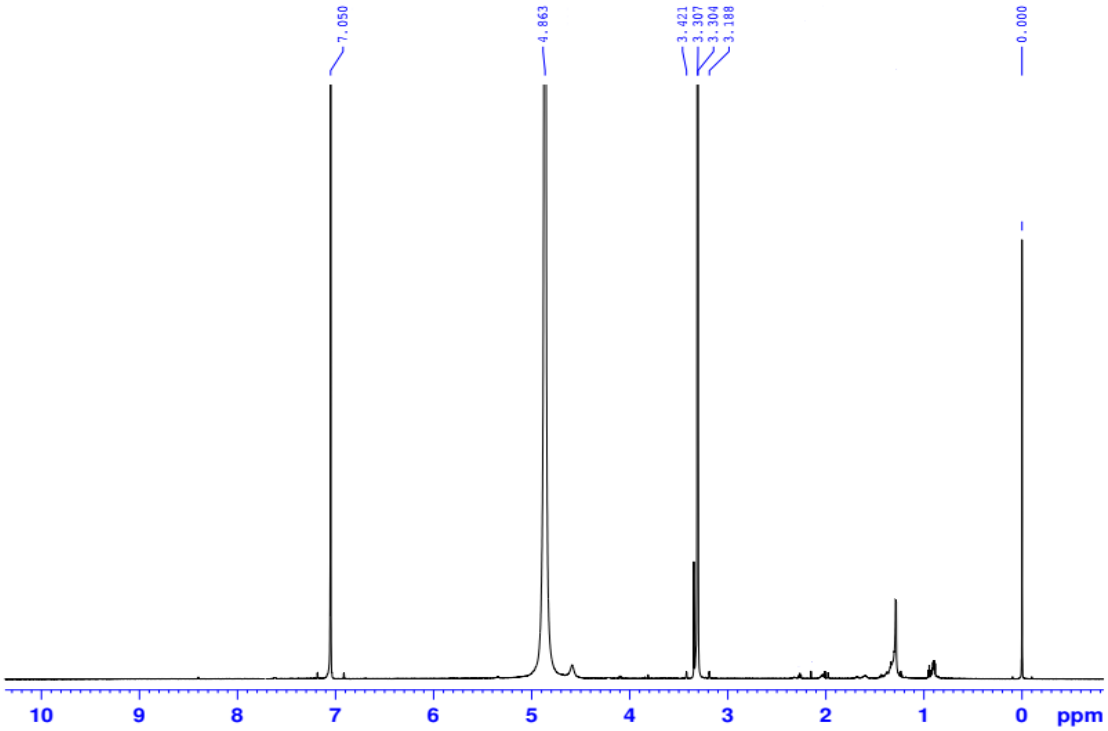


Figure S32. ^1H NMR spectrum (600 MHz, CD_3OD) of compound 8

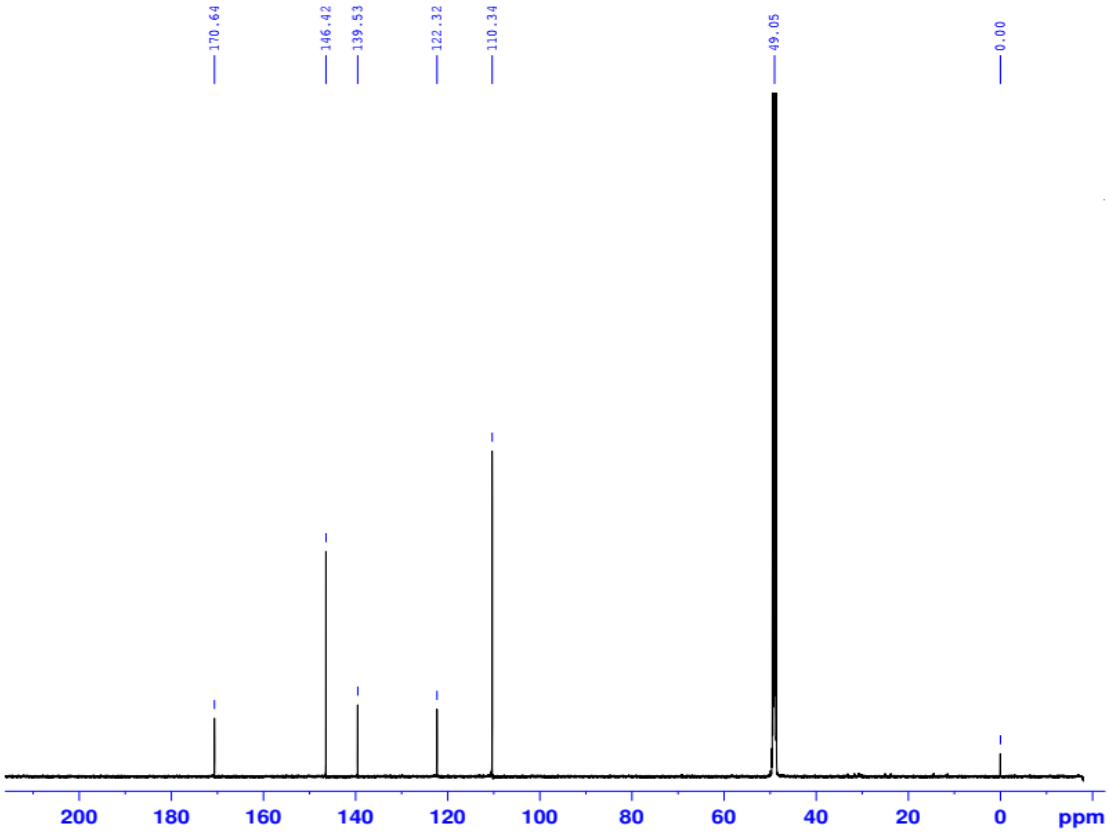


Figure S33. ^{13}C NMR spectrum (150 MHz, CD_3OD) of compound 8

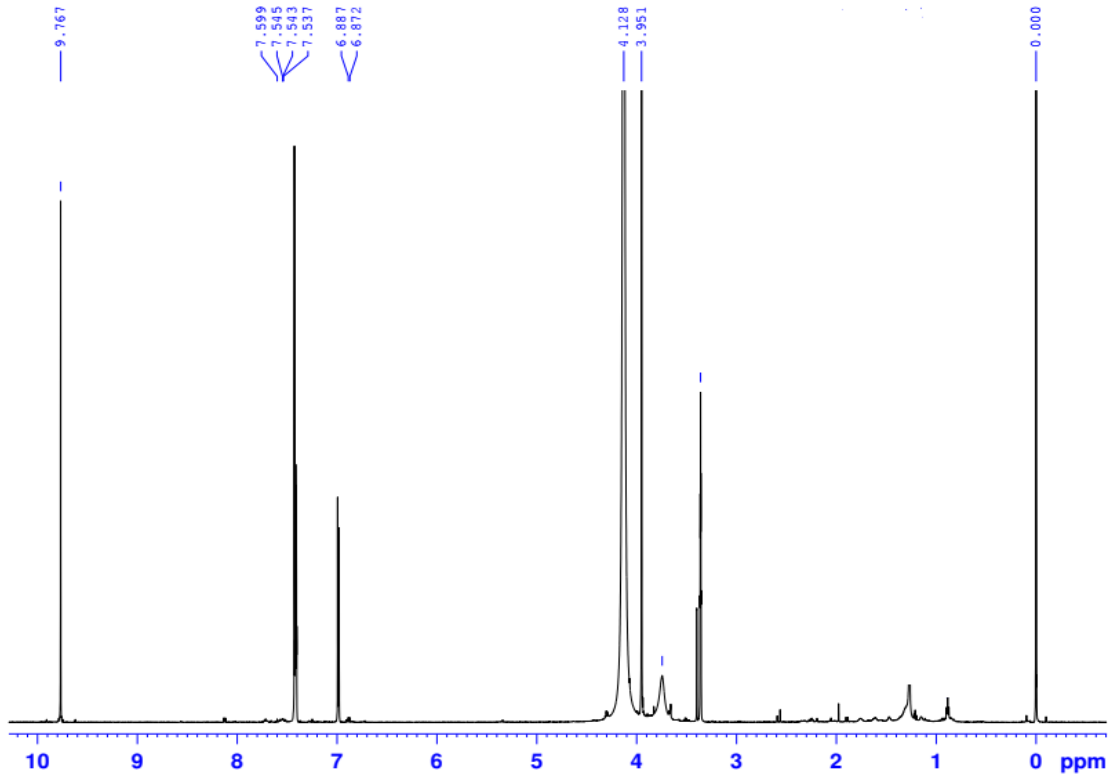


Figure S34. ^{1}H NMR spectrum (600 MHz, CD_3OD & $CDCl_3$) of compound 9

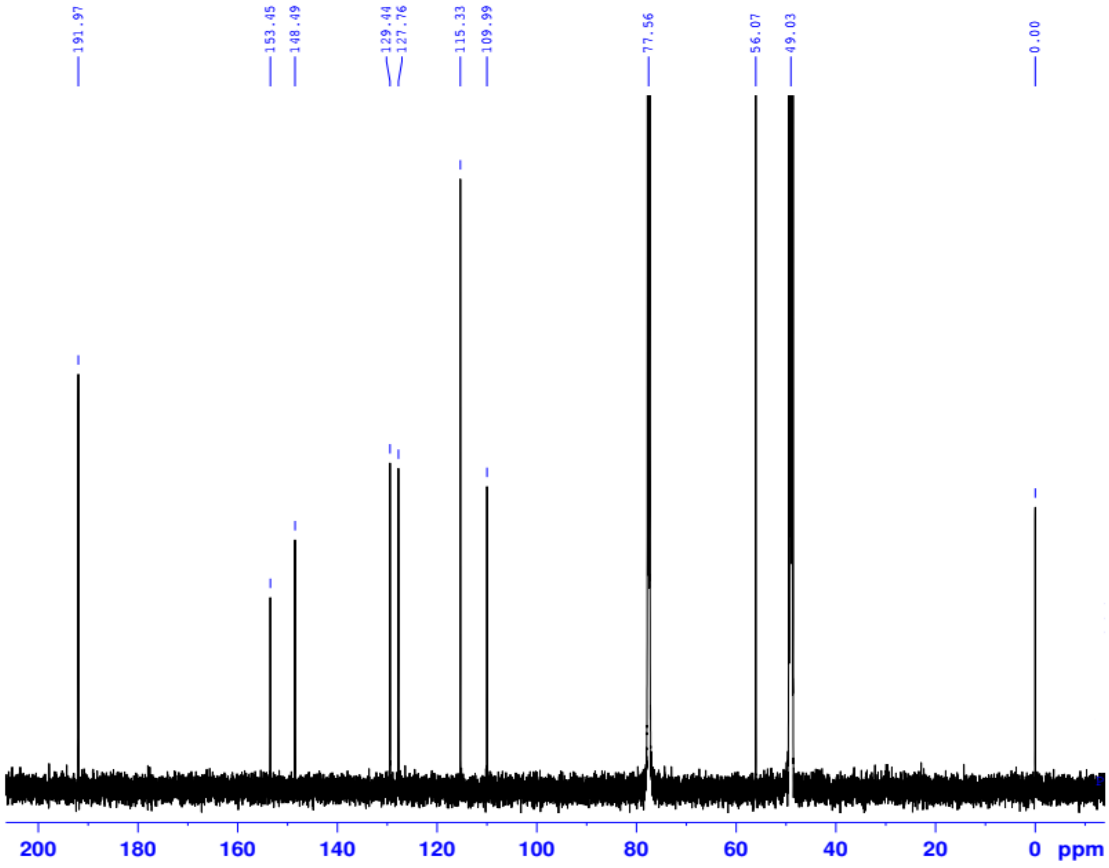


Figure S35. ^{13}C NMR spectrum (150 MHz, CD_3OD & $CDCl_3$) of compound 9

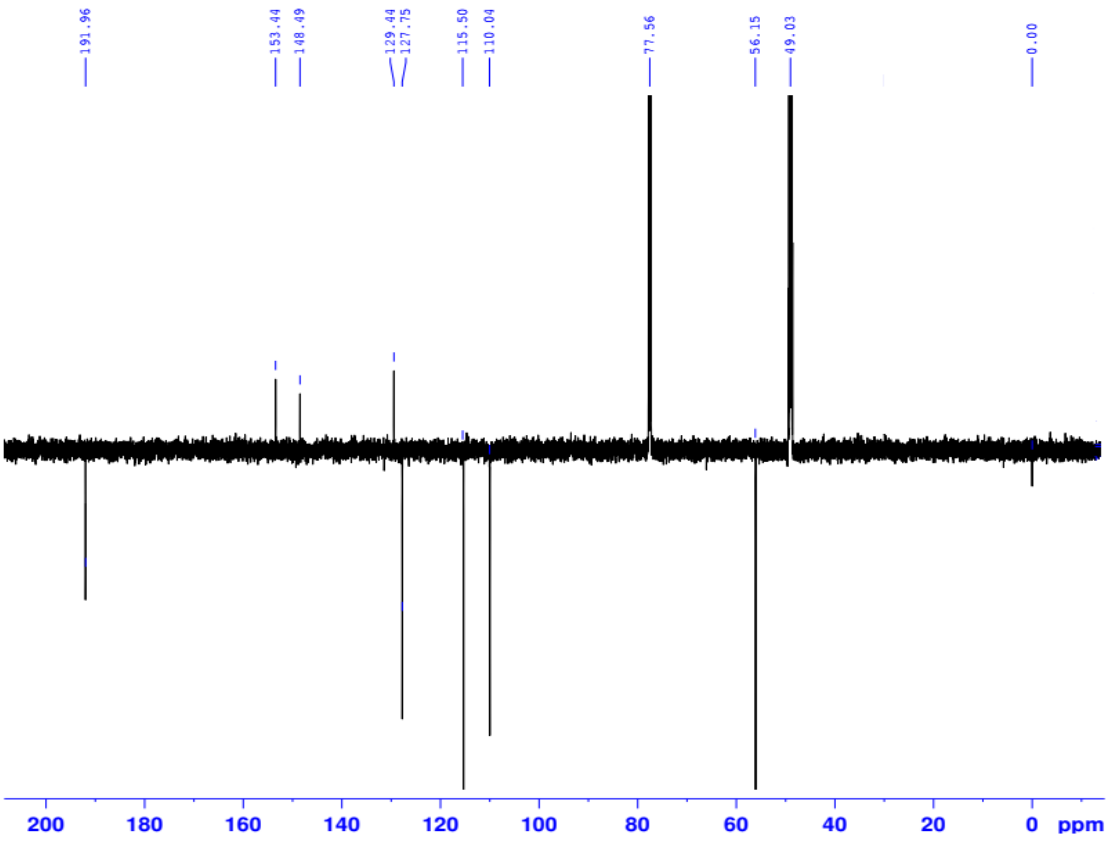


Figure S36. APT spectrum (150 MHz, CD_3OD & $CDCl_3$) of compound 9

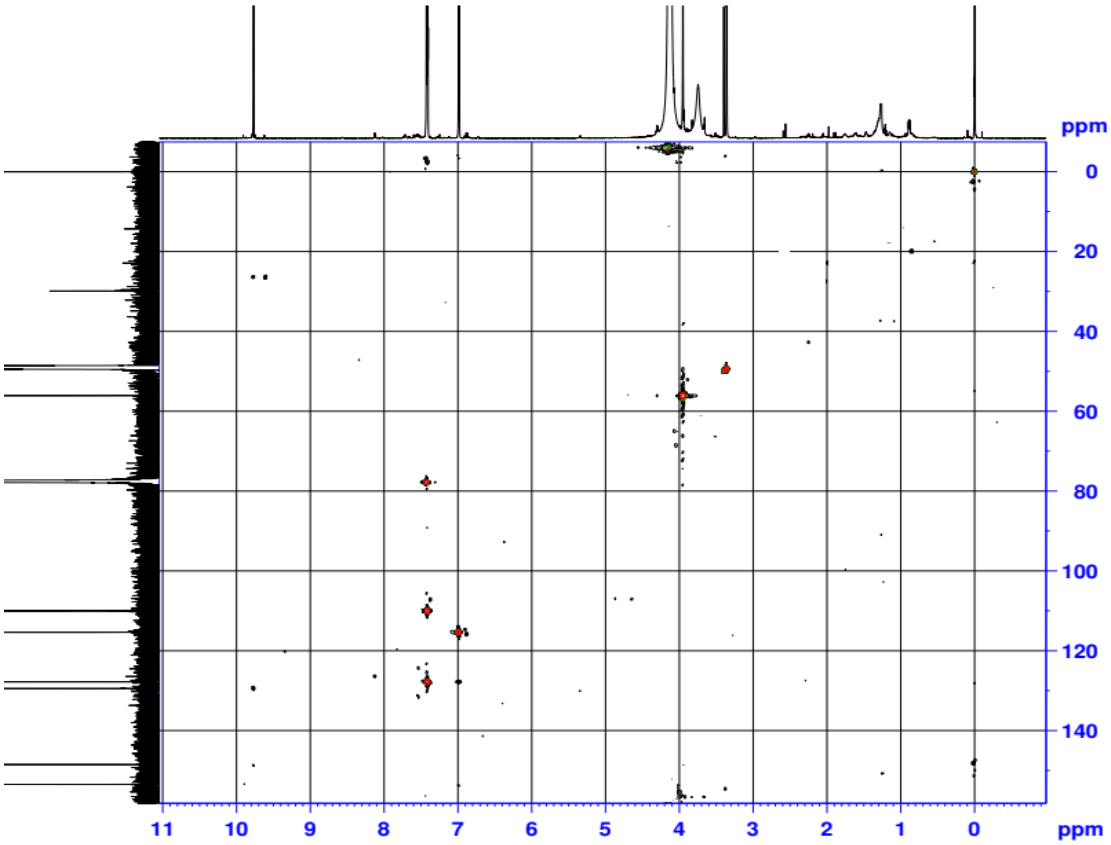


Figure S37. HSQC spectrum (CD_3OD & $CDCl_3$) of compound 9

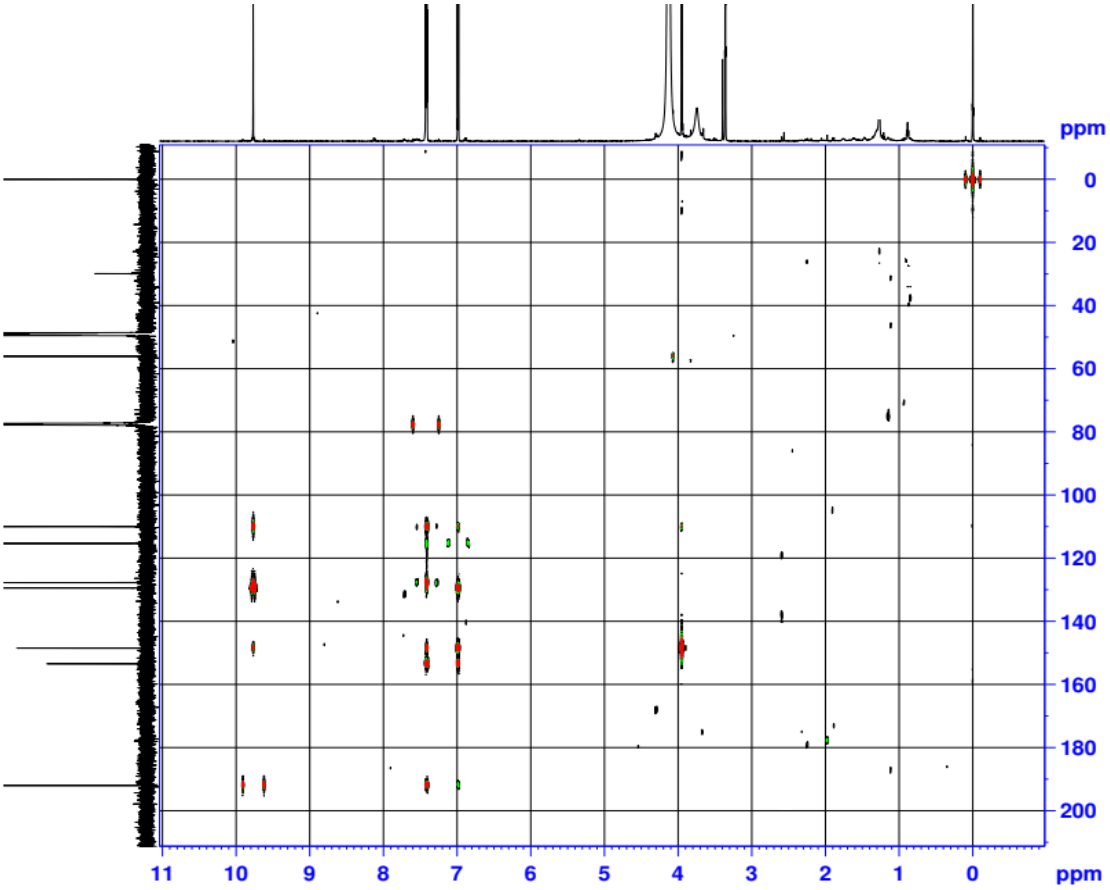


Figure S38. HMBC spectrum (CD_3OD & $CDCl_3$) of compound 9

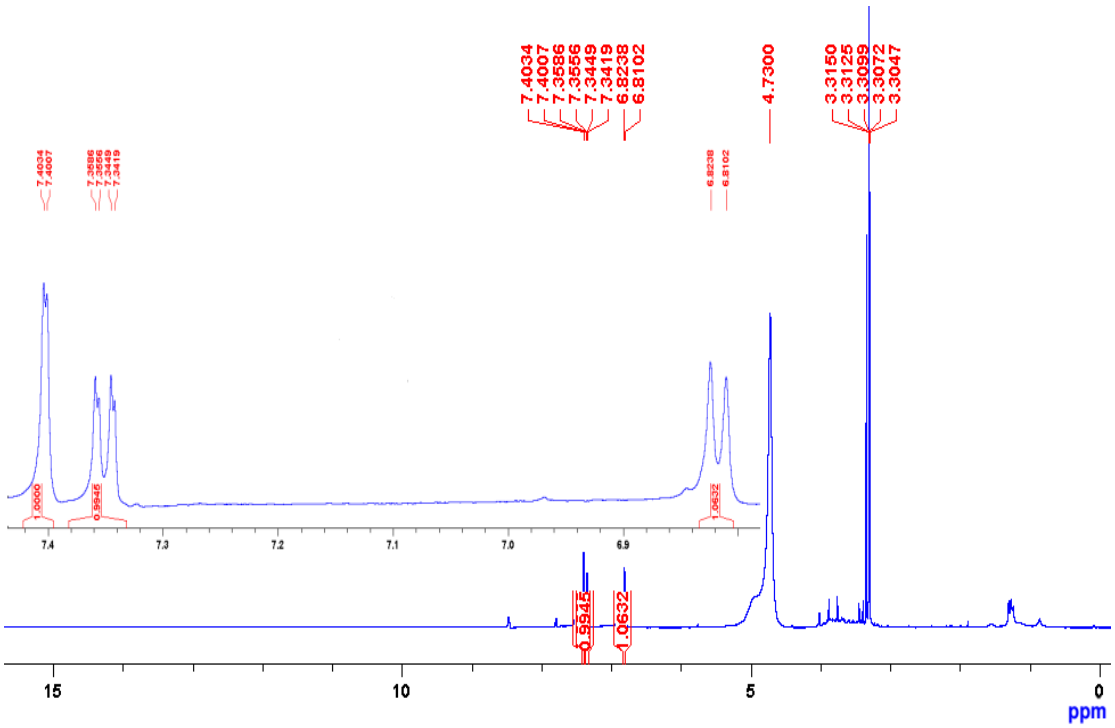


Figure S39. ^1H NMR spectrum (600 MHz, CD_3OD) of compound 10

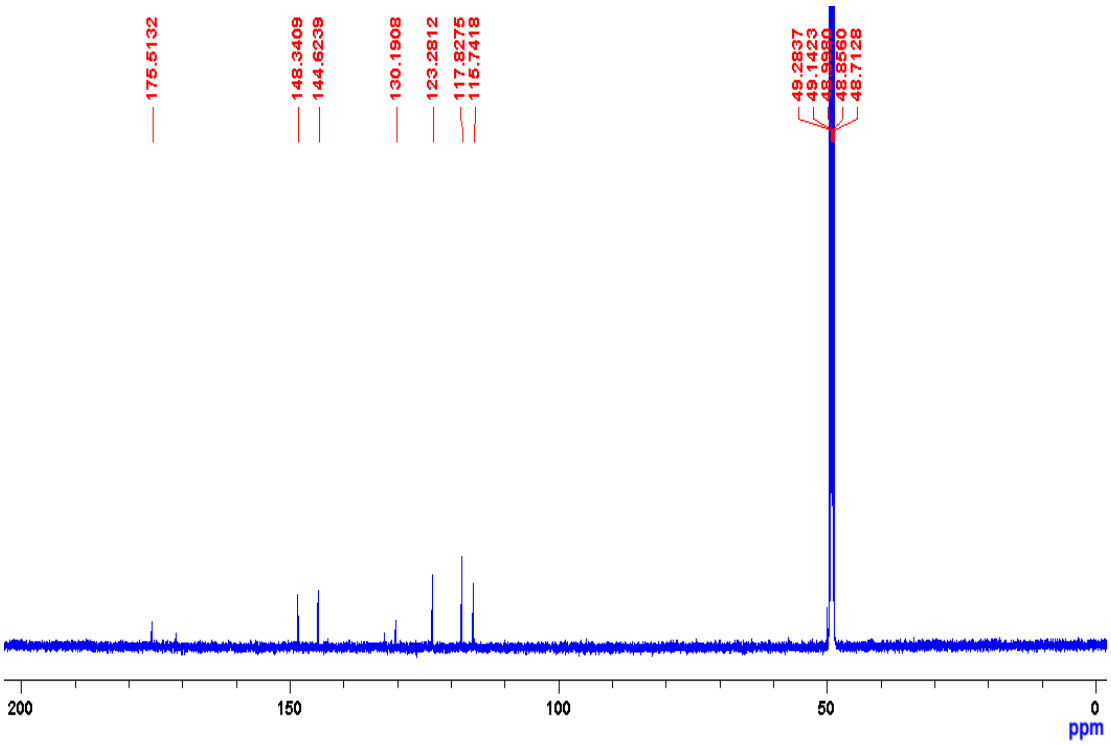


Figure S40. ^{13}C NMR spectrum (150 MHz, CD_3OD) of compound 10

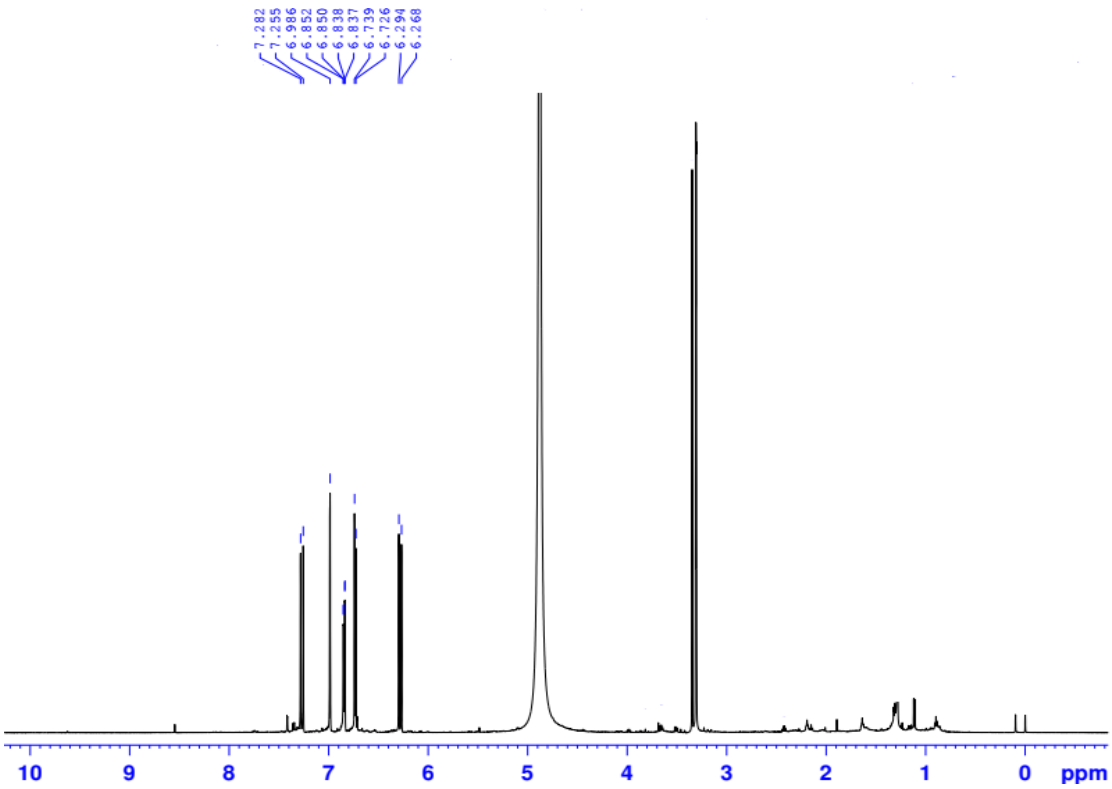


Figure S41. ^{1}H NMR spectrum (600 MHz, CD_3OD) of compound 11

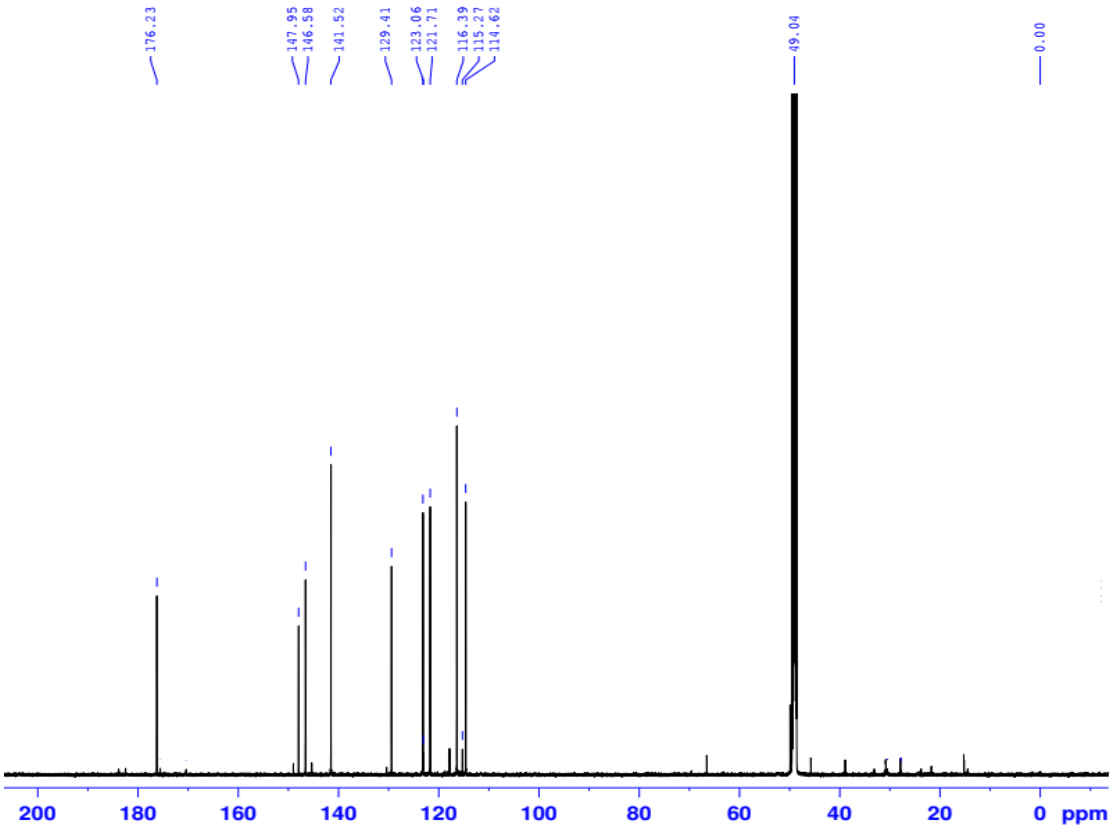


Figure S42. ^{13}C NMR spectrum (150 MHz, CD_3OD) of compound 11

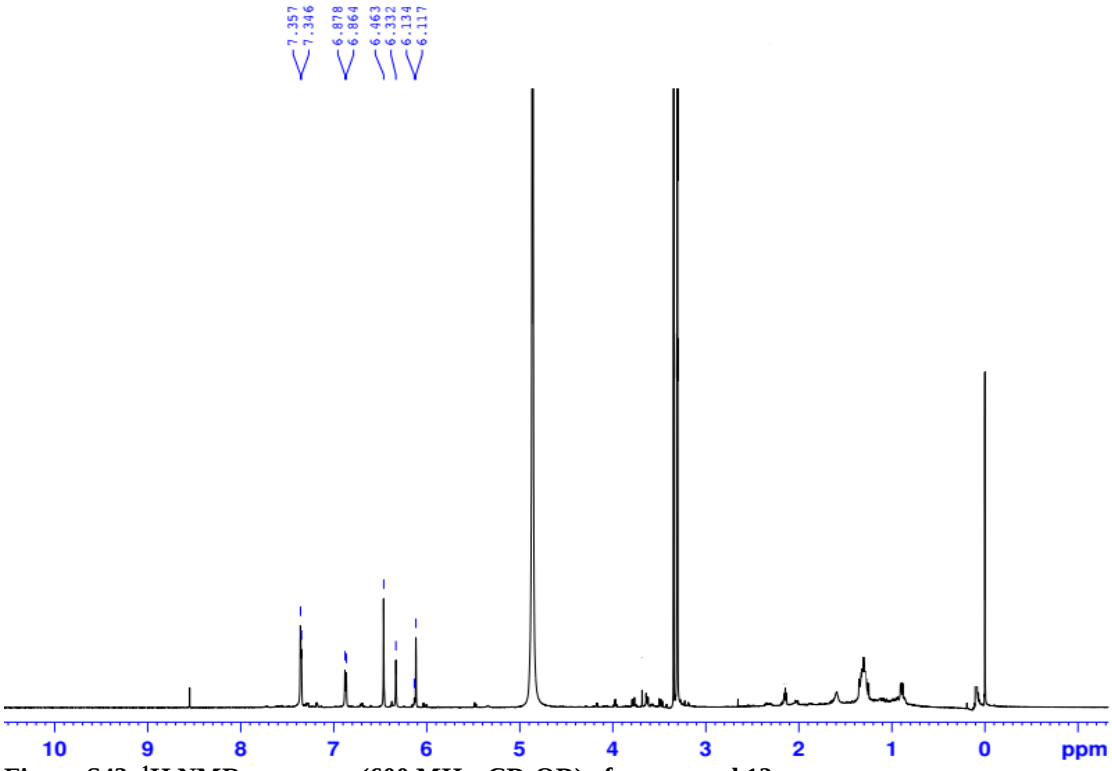


Figure S43. ^{1}H NMR spectrum (600 MHz, CD_3OD) of compound 12

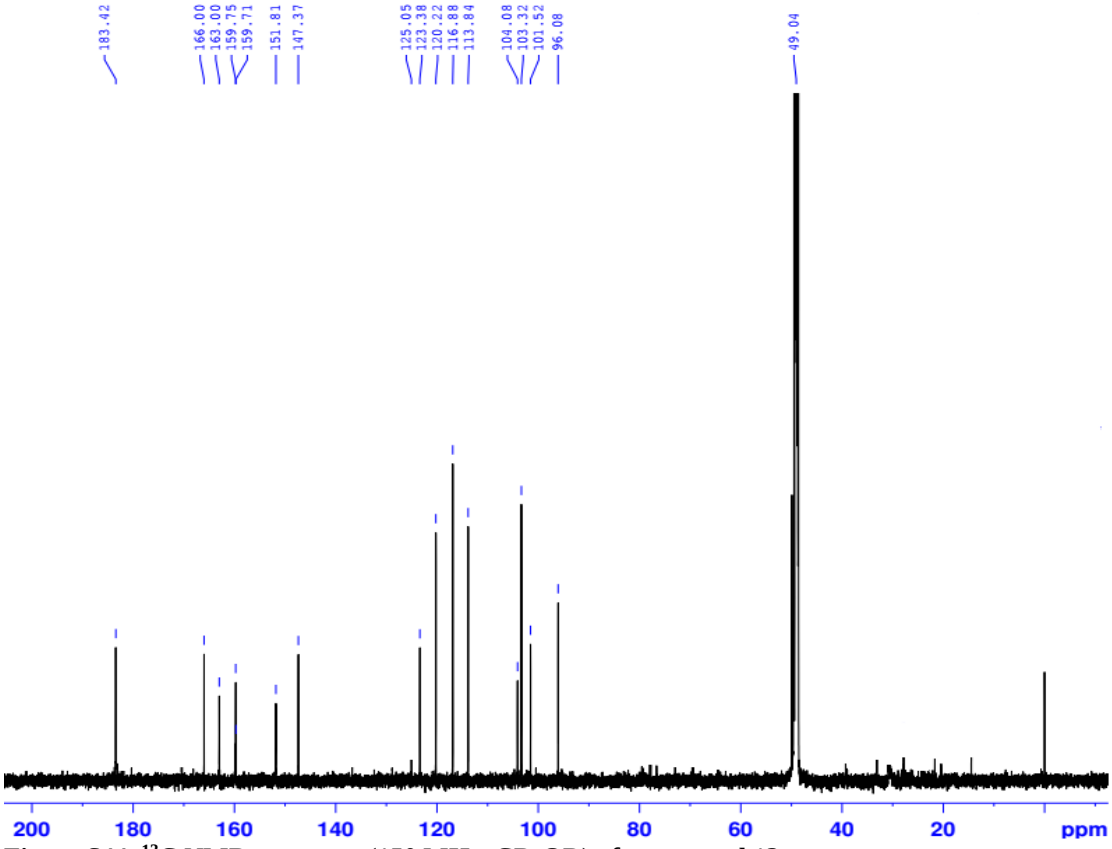


Figure S44. ^{13}C NMR spectrum (150 MHz, CD_3OD) of compound 12

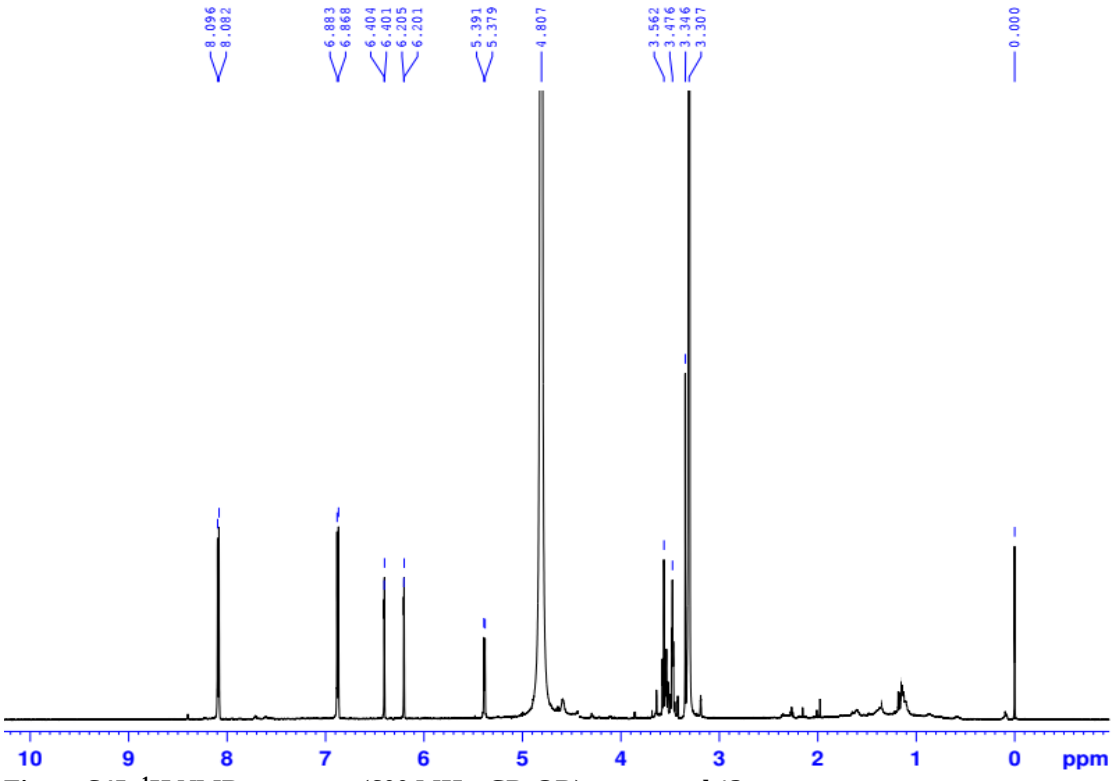


Figure S45. ^{1}H NMR spectrum (600 MHz, CD_3OD) compound 13

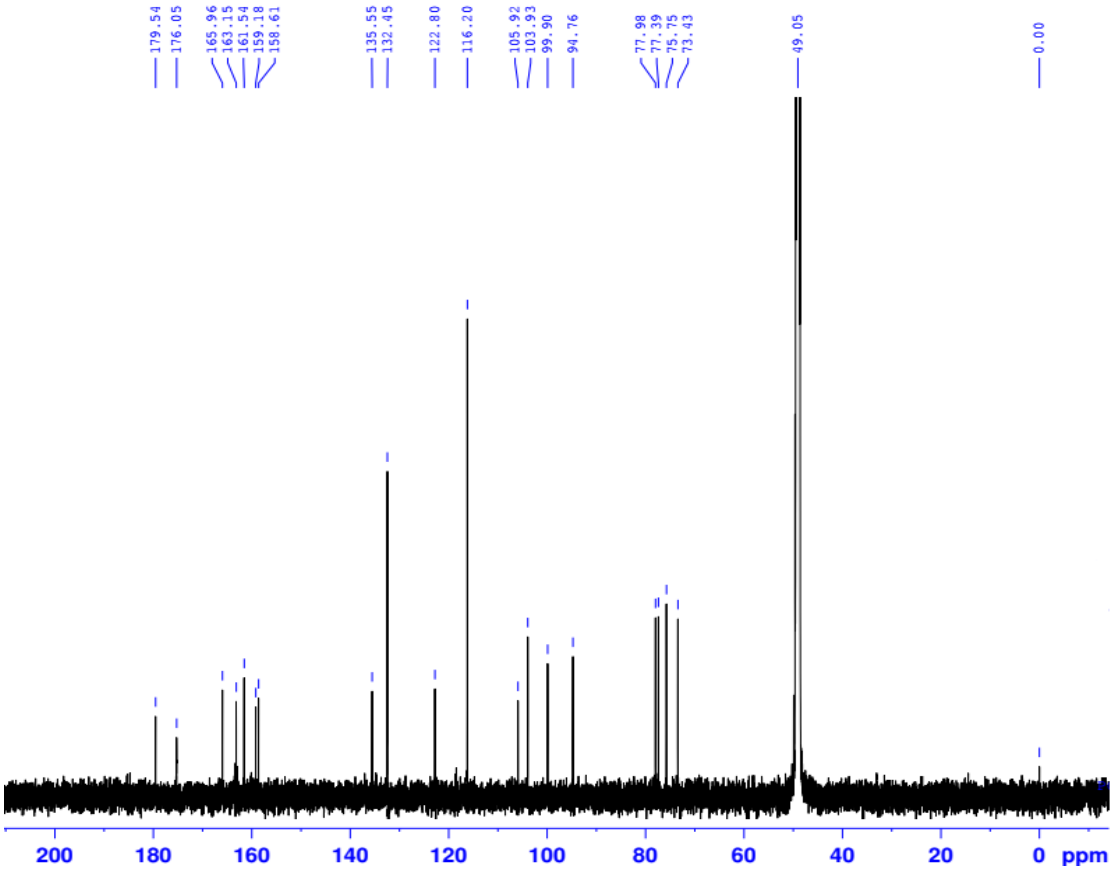


Figure S46. ^{13}C NMR spectrum (150 MHz, CD_3OD) of compound 13

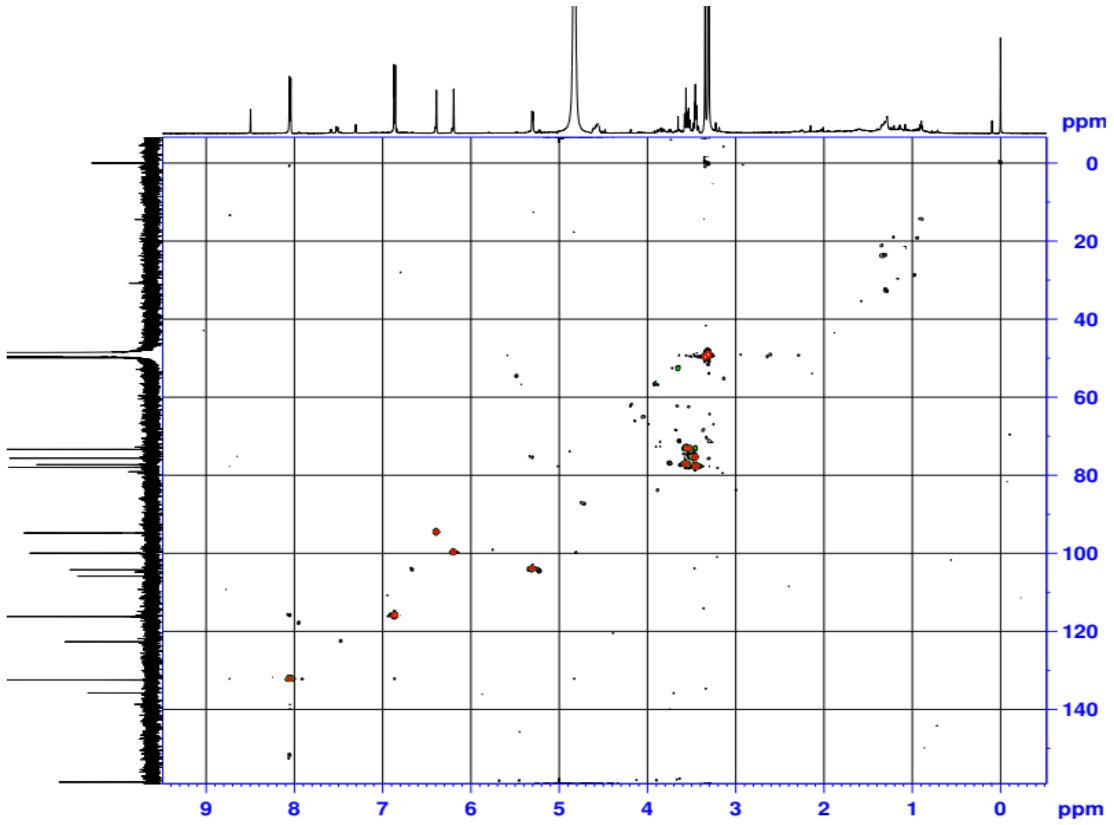


Figure S47. HSQC spectrum (CD_3OD) of compound 13

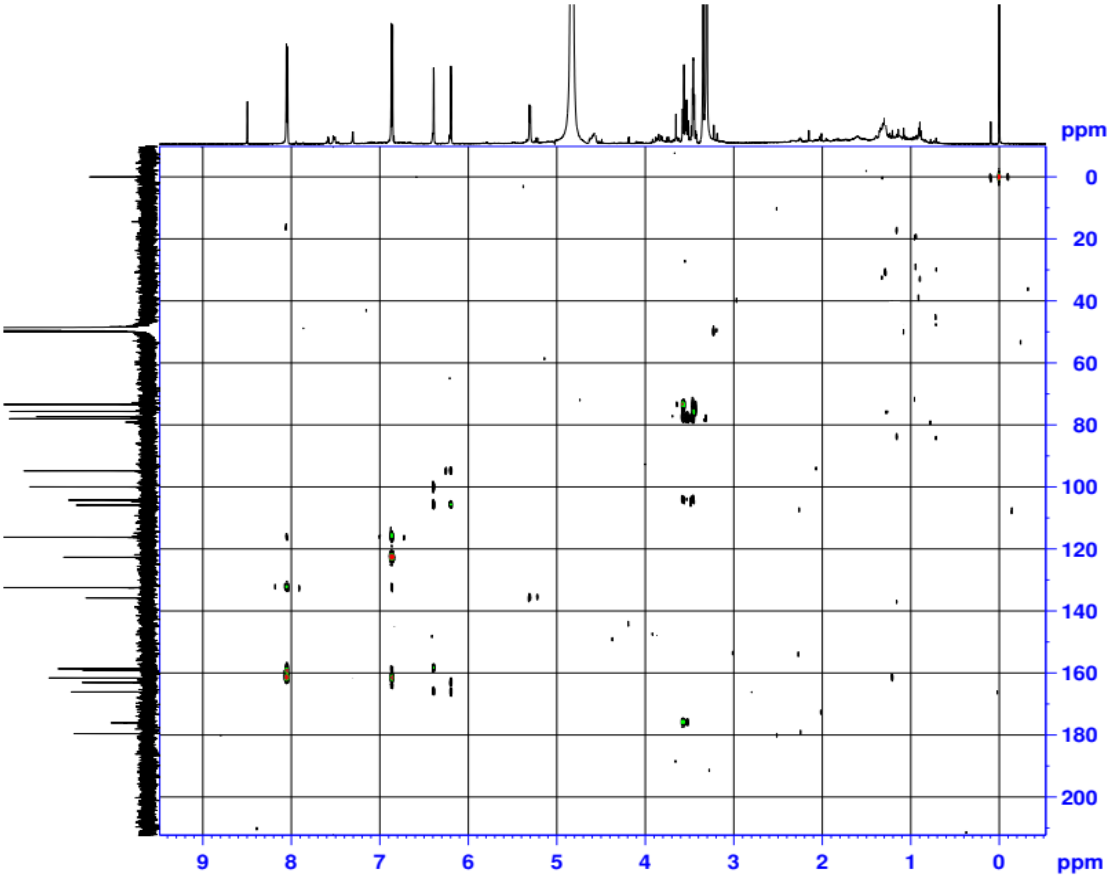


Figure S48. HMBC spectrum (CD_3OD) of compound 13

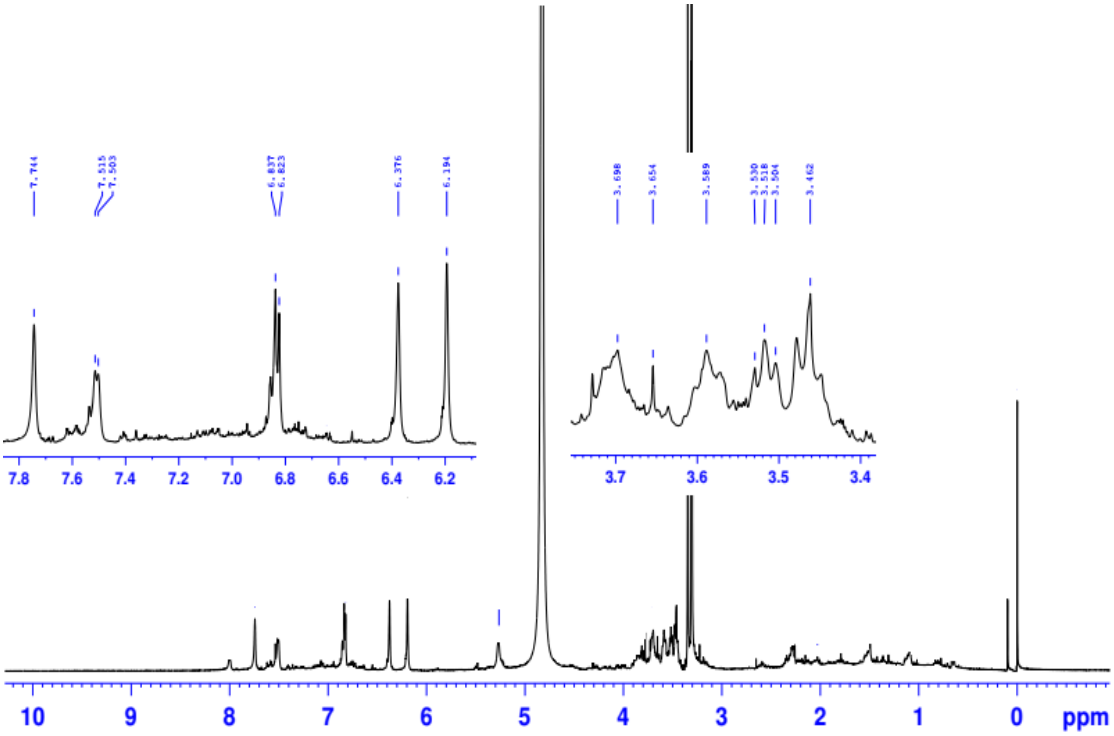


Figure S49. ^1H NMR spectrum (600 MHz, CD_3OD) of compound 14

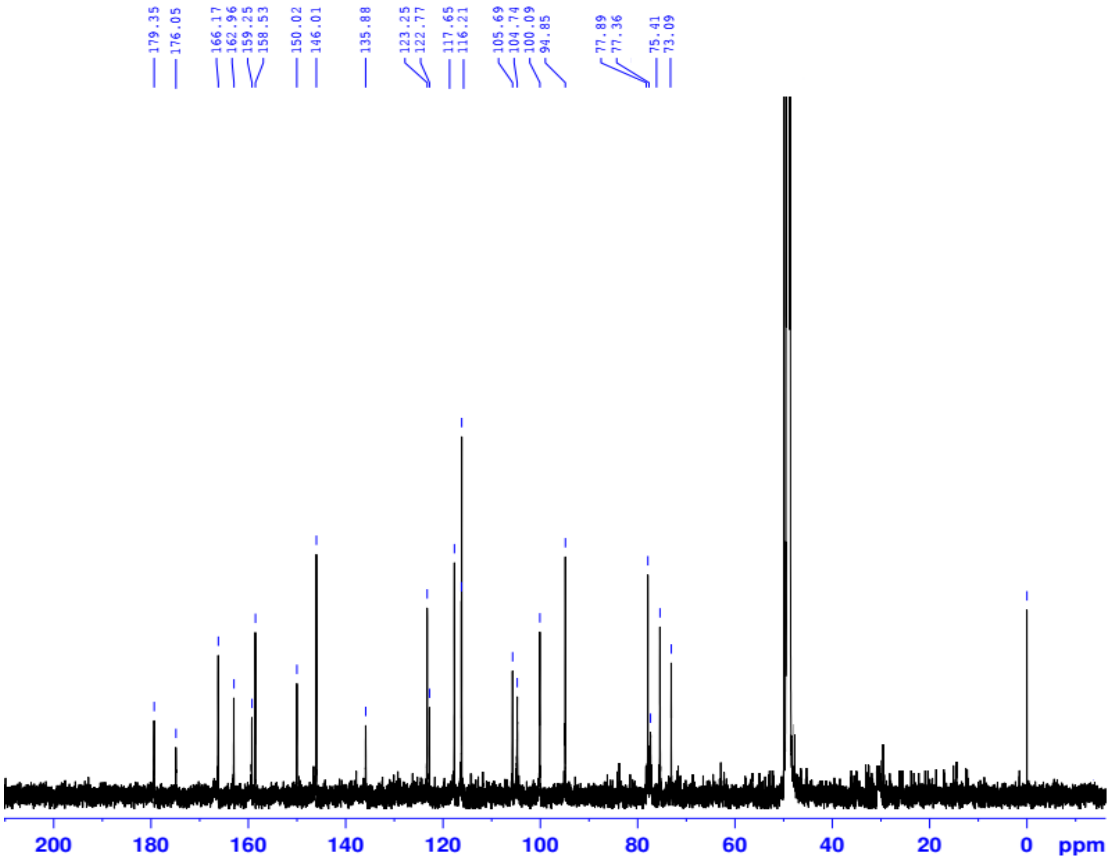


Figure S50. ^{13}C NMR spectrum (150 MHz, CD_3OD) of compound 14

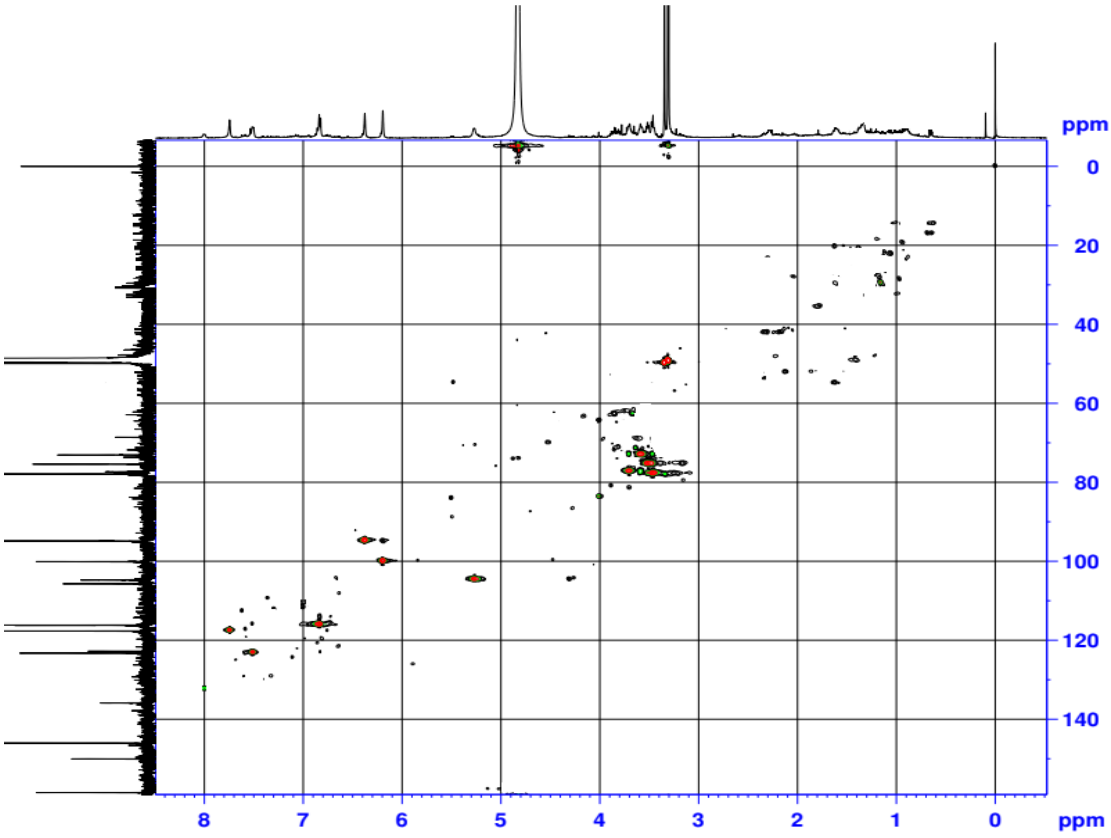


Figure S51. HSQC spectrum (CD_3OD) of compound 14

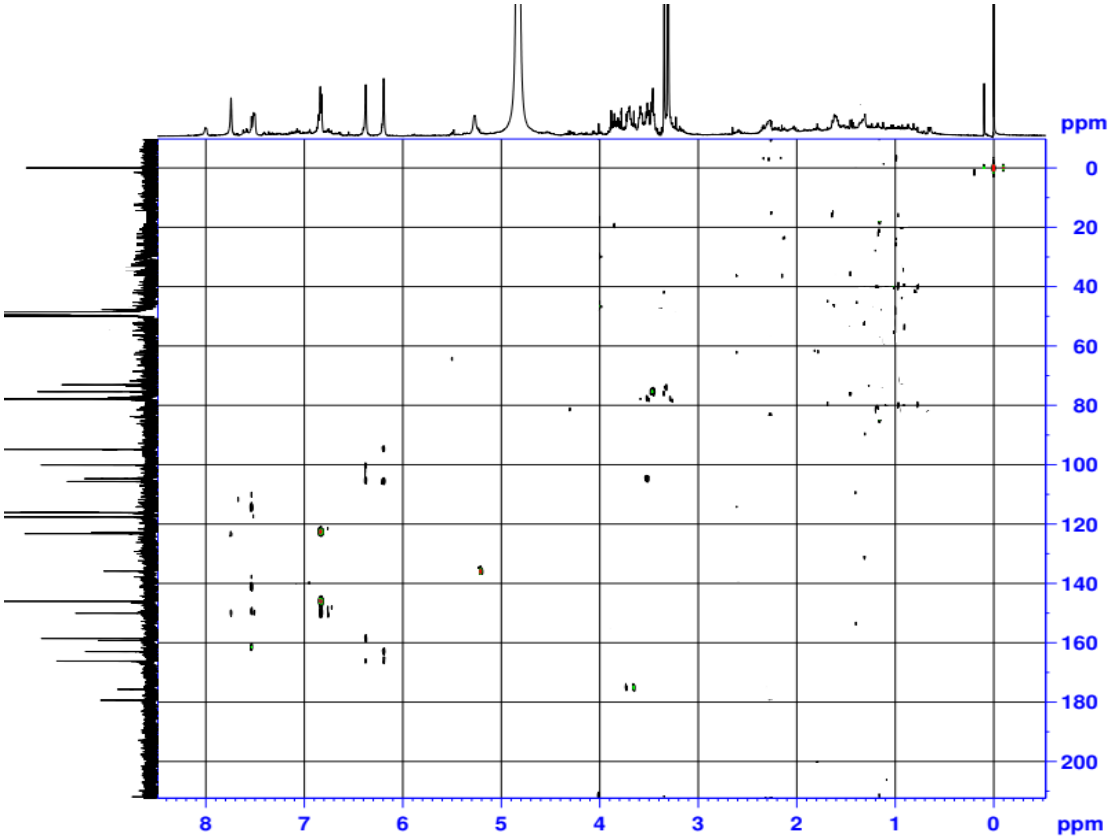


Figure S52. HMBC spectrum (CD_3OD) of compound 14