

Supplementary Information

Homoleptic complexes of heterocyclic curcuminoids with Mg and Cu: first conformationally heteroleptic case, crystal structures and biological properties

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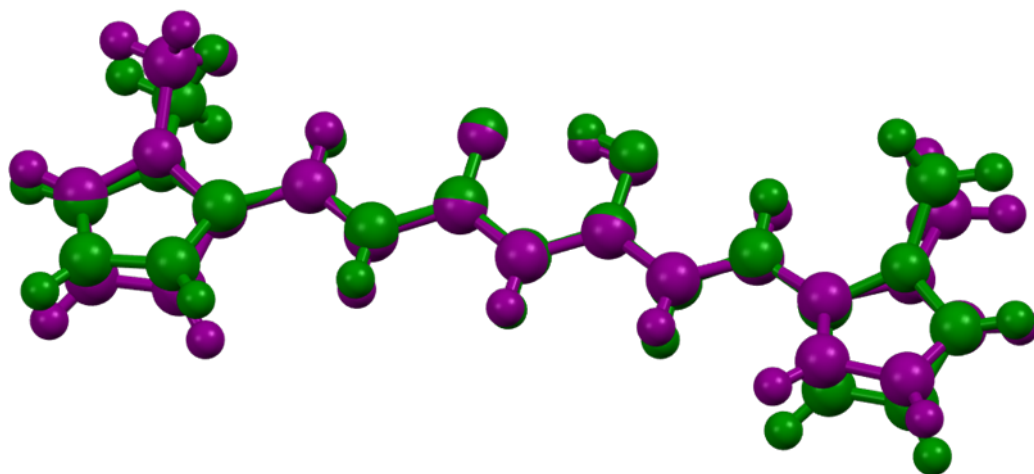


Figure S1. Calculated overlay (RMSD = 0.0764) of two polymorphs of ligand **1**.

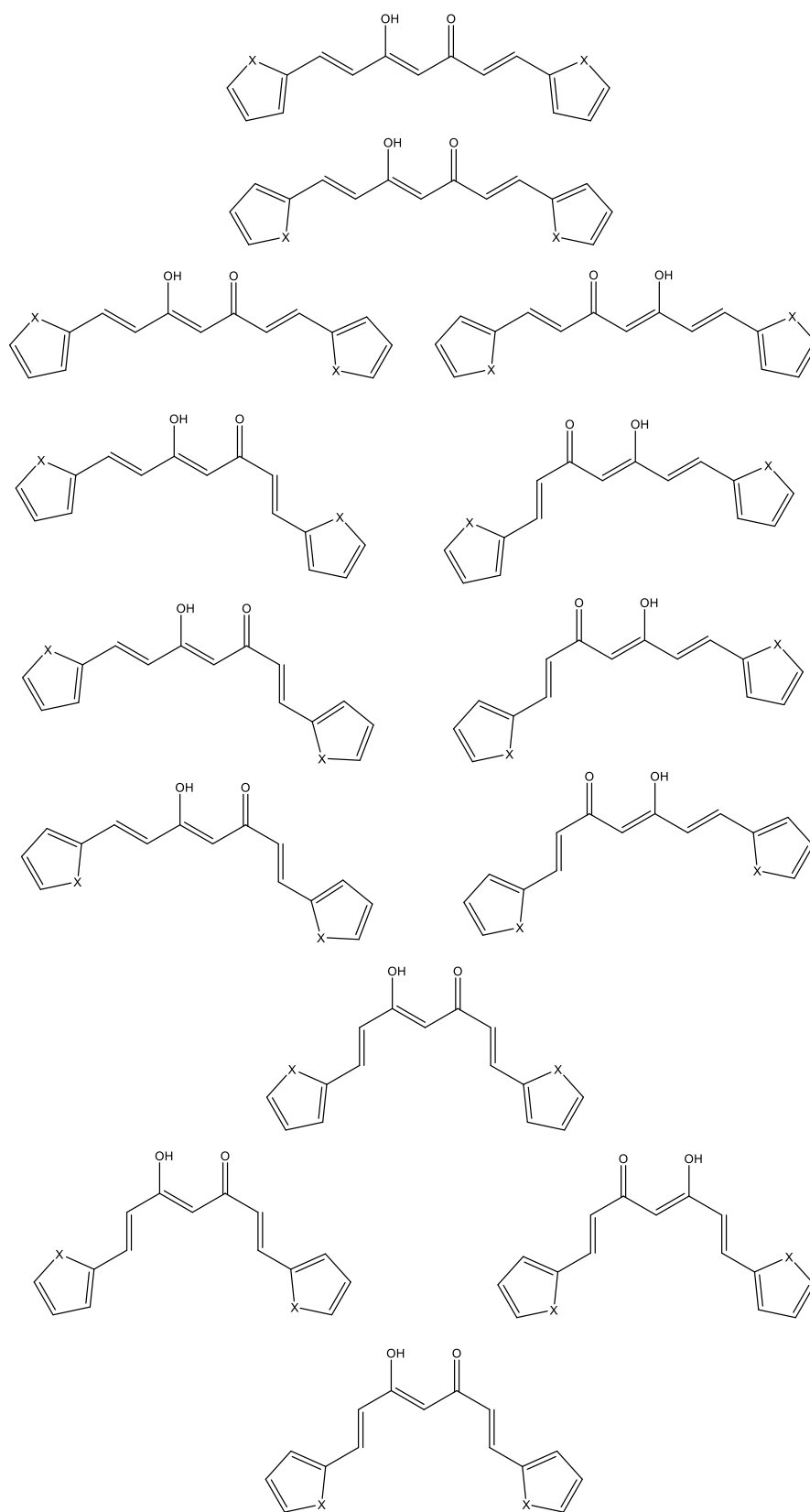
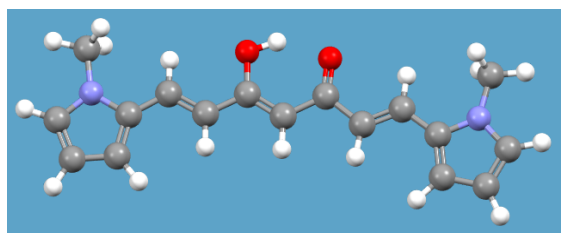
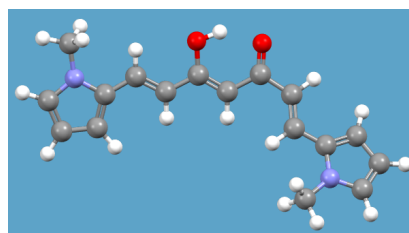


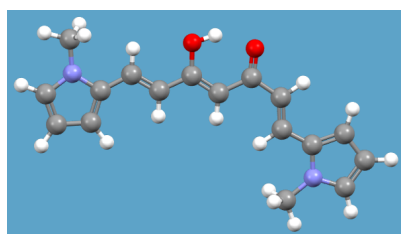
Figure S2. Theoretical extreme conformers for 1-3.



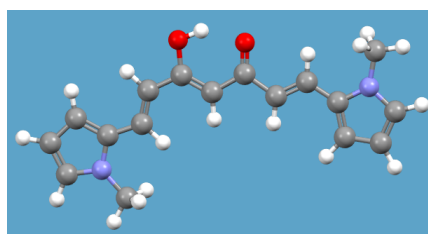
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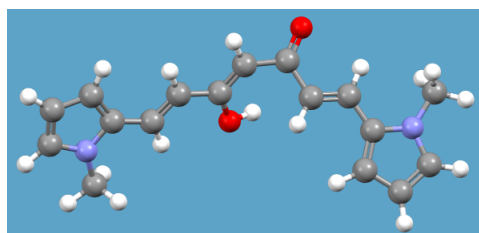
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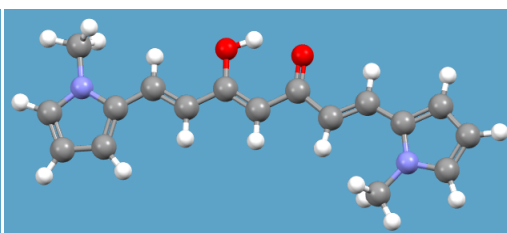
$\Delta E = 4.7476$



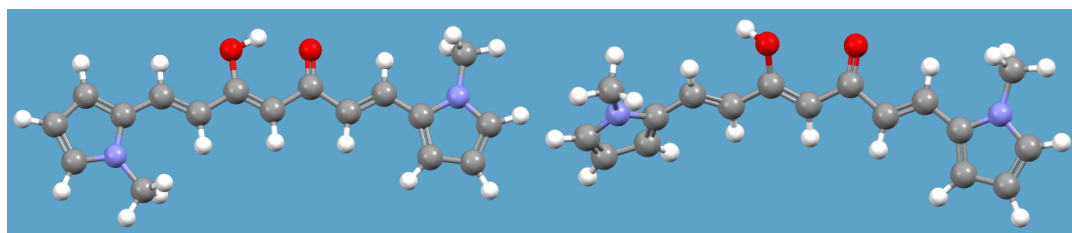
$\Delta E = 6.5320$



$\Delta E = 9.4600$



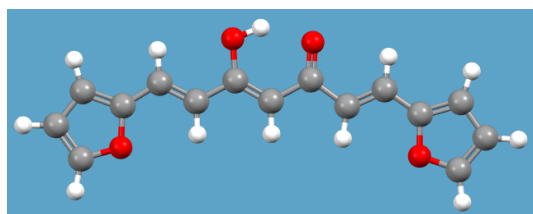
$\Delta E = 10.5589$



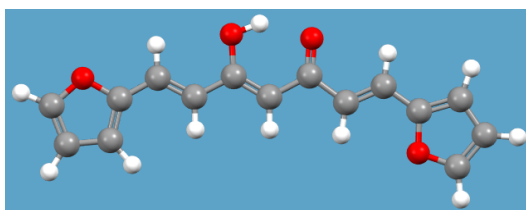
$\Delta E = 10.6842$

$\Delta E = 11.2770$

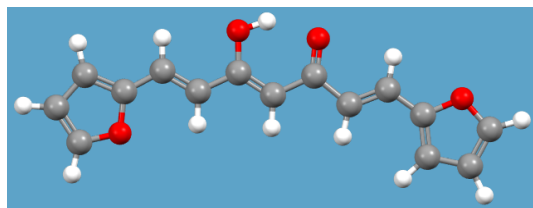
Figure S3. Structures of the lowest-energy (MMFF94S) conformers of **1**. Relative energies (Kcal/mol).



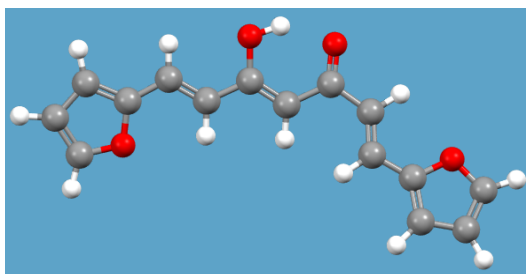
$\Delta E = 0.0$



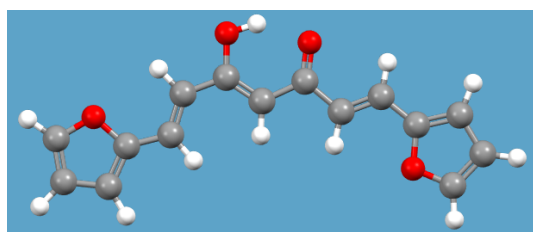
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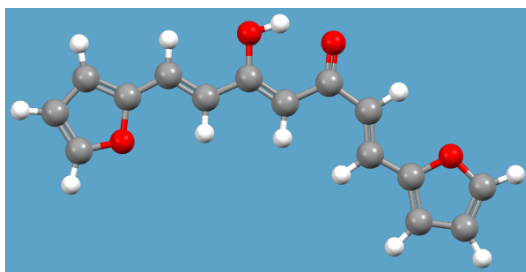
$\Delta E = 2.6490$



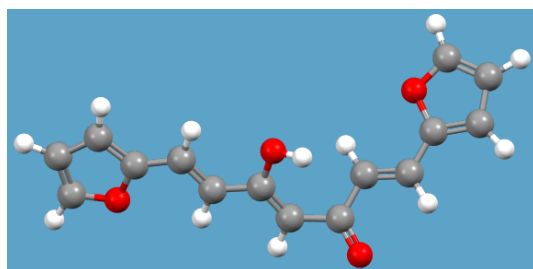
$\Delta E = 4.0078$



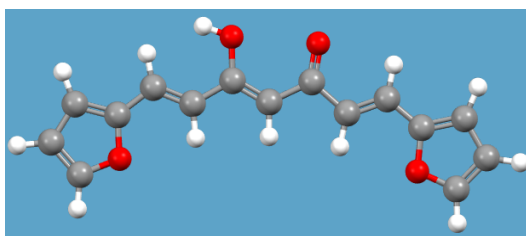
$\Delta E = 4.8899$



$\Delta E = 6.0404$

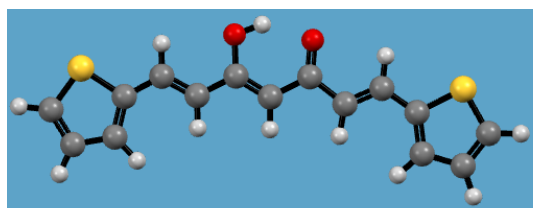


$\Delta E = 9.6297$

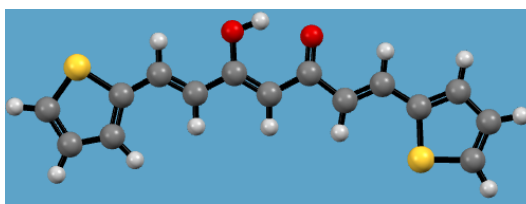


$\Delta E = 13.3214$

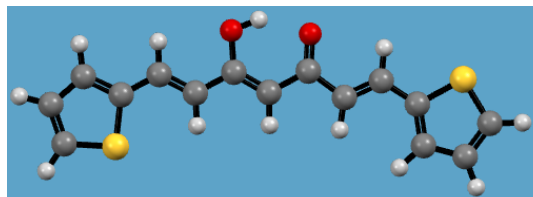
Figure S4. Structures of the lowest-energy (MMFF94S) conformers of **2**. Relative energies (Kcal/mol).



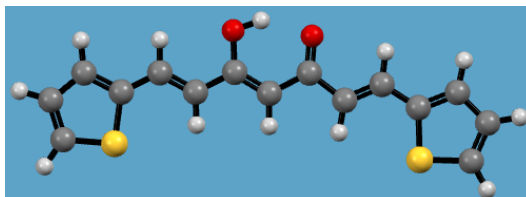
$\Delta E = 0.0$



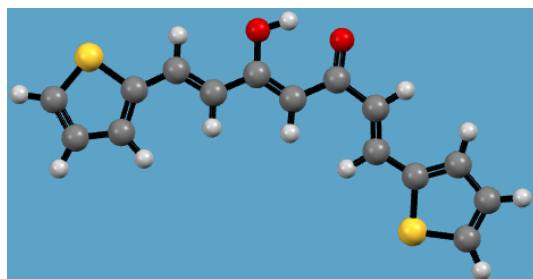
$\Delta E = 0.7707$



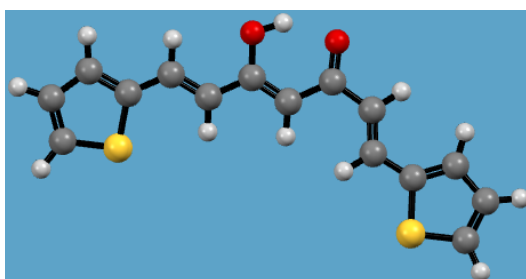
$\Delta E = 1.0669$



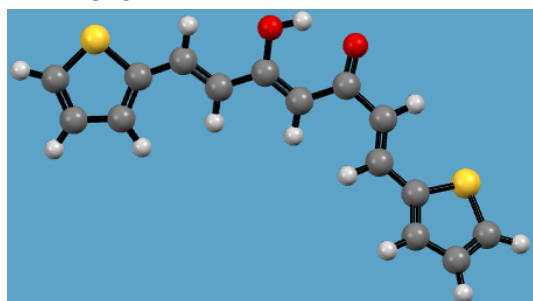
$\Delta E = 1.8976$



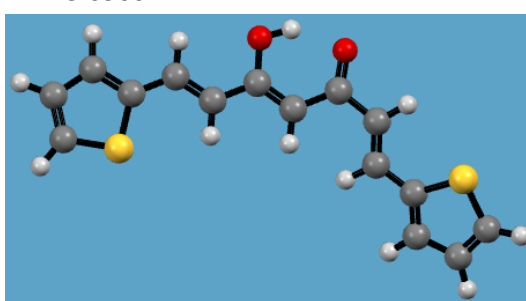
$\Delta E = 2.5407$



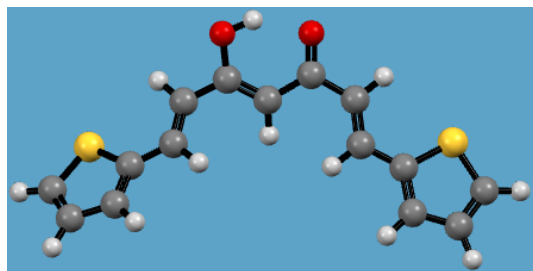
$\Delta E = 3.6560$



$\Delta E = 4.6575$



$\Delta E = 5.7026$



$\Delta E = 8.1190$

Figure S5. Structures of the lowest-energy (MMFF94S) conformers of **3**. Relative energies (Kcal/mol).

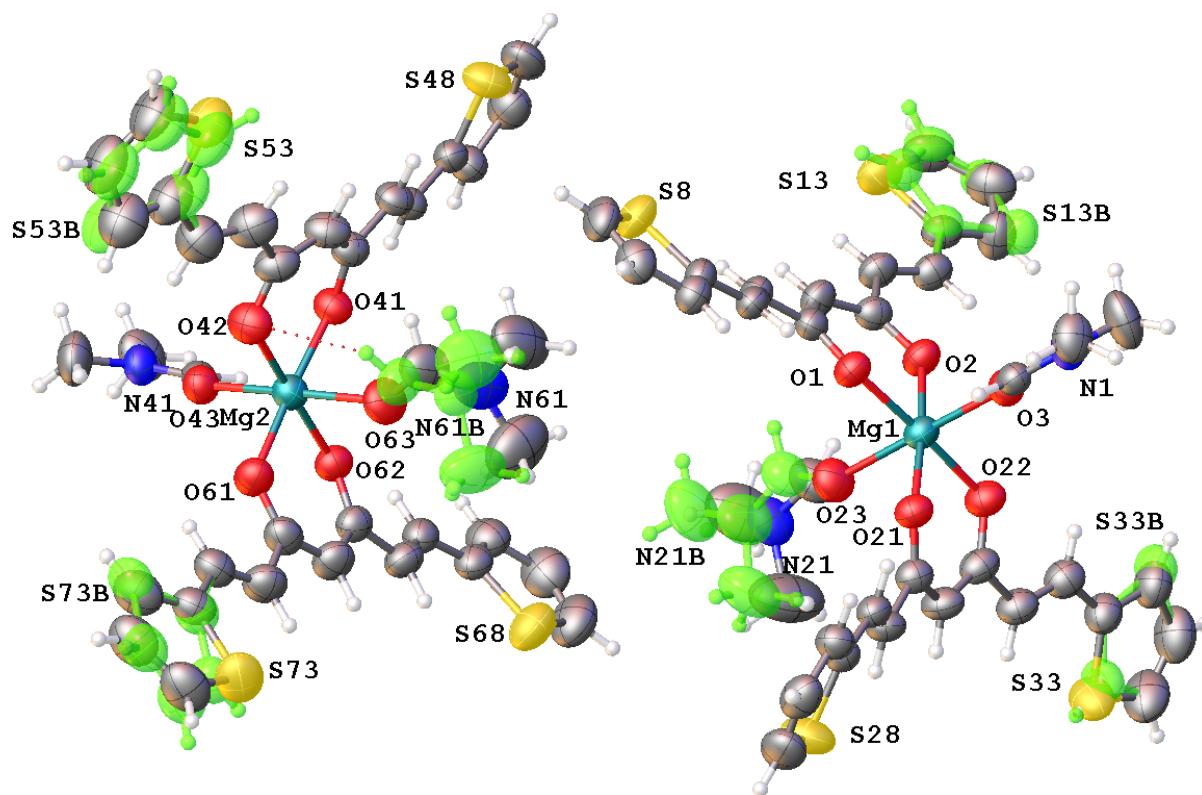


Figure S6. Crystal structures of complex 6.

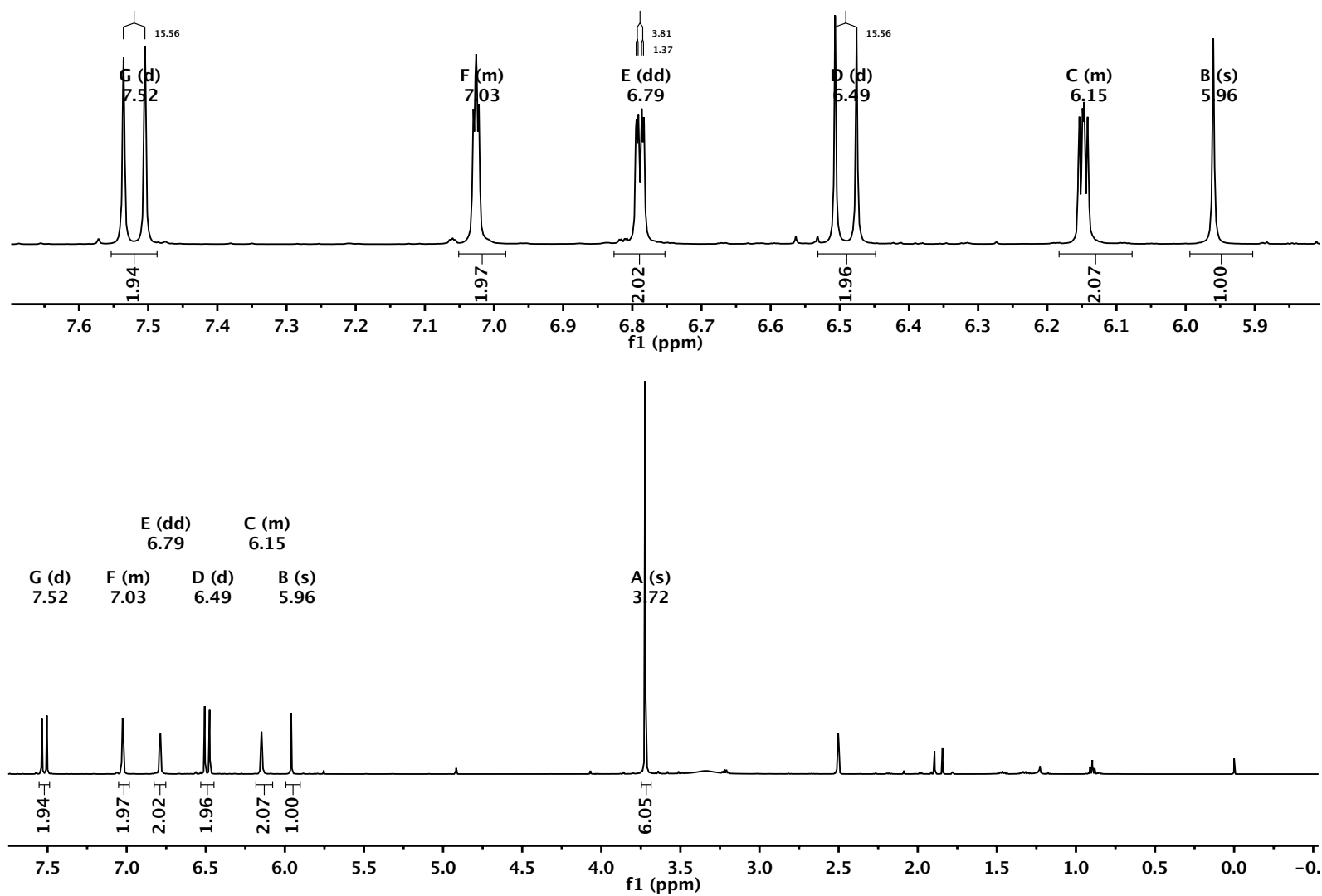


Figure S7. 500 MHz ^1H NMR spectrum of N-methyl-pyrCurc.

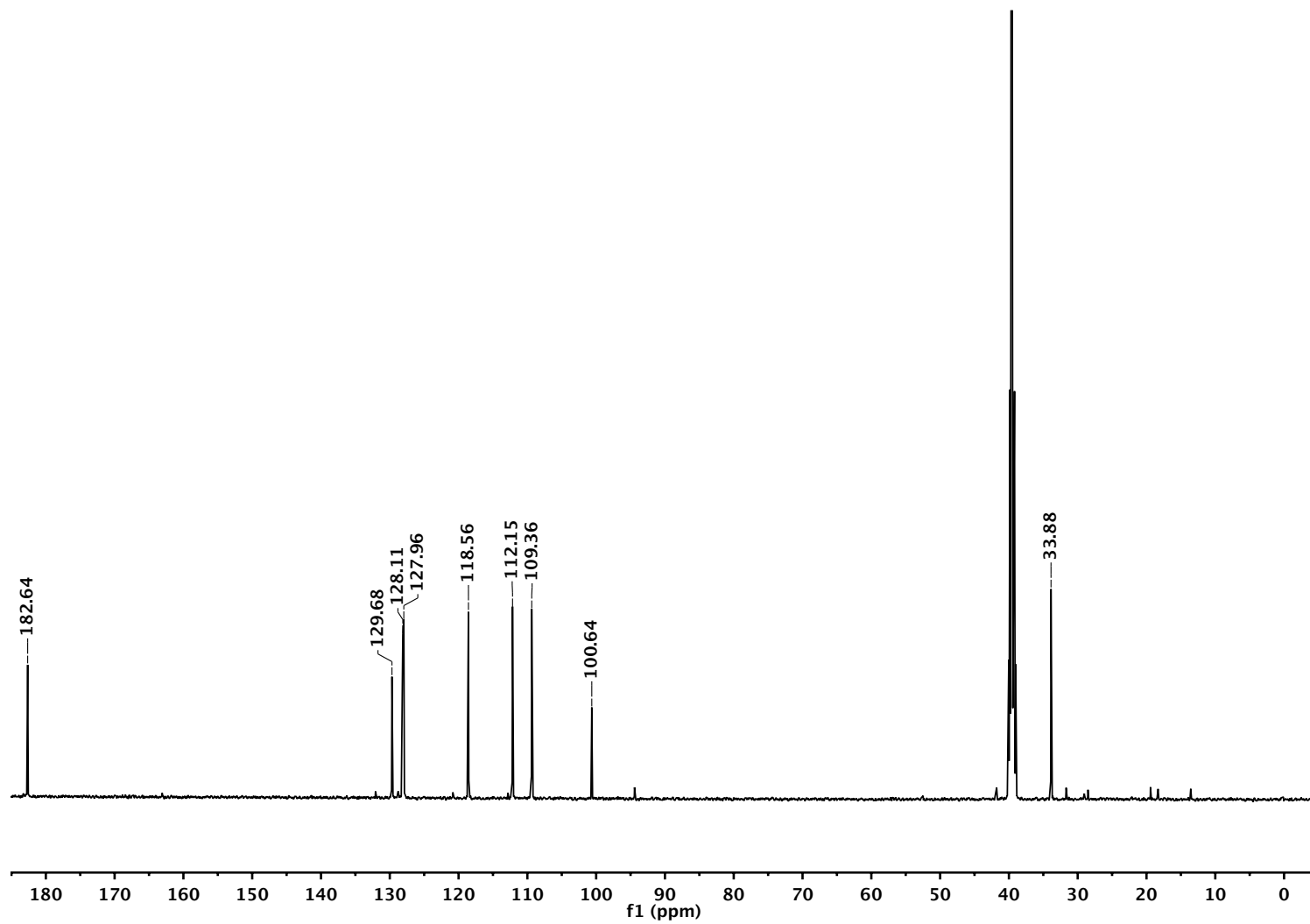


Figure S8. 125 MHz ^{13}C NMR spectrum of N-methyl-pyrCurc.

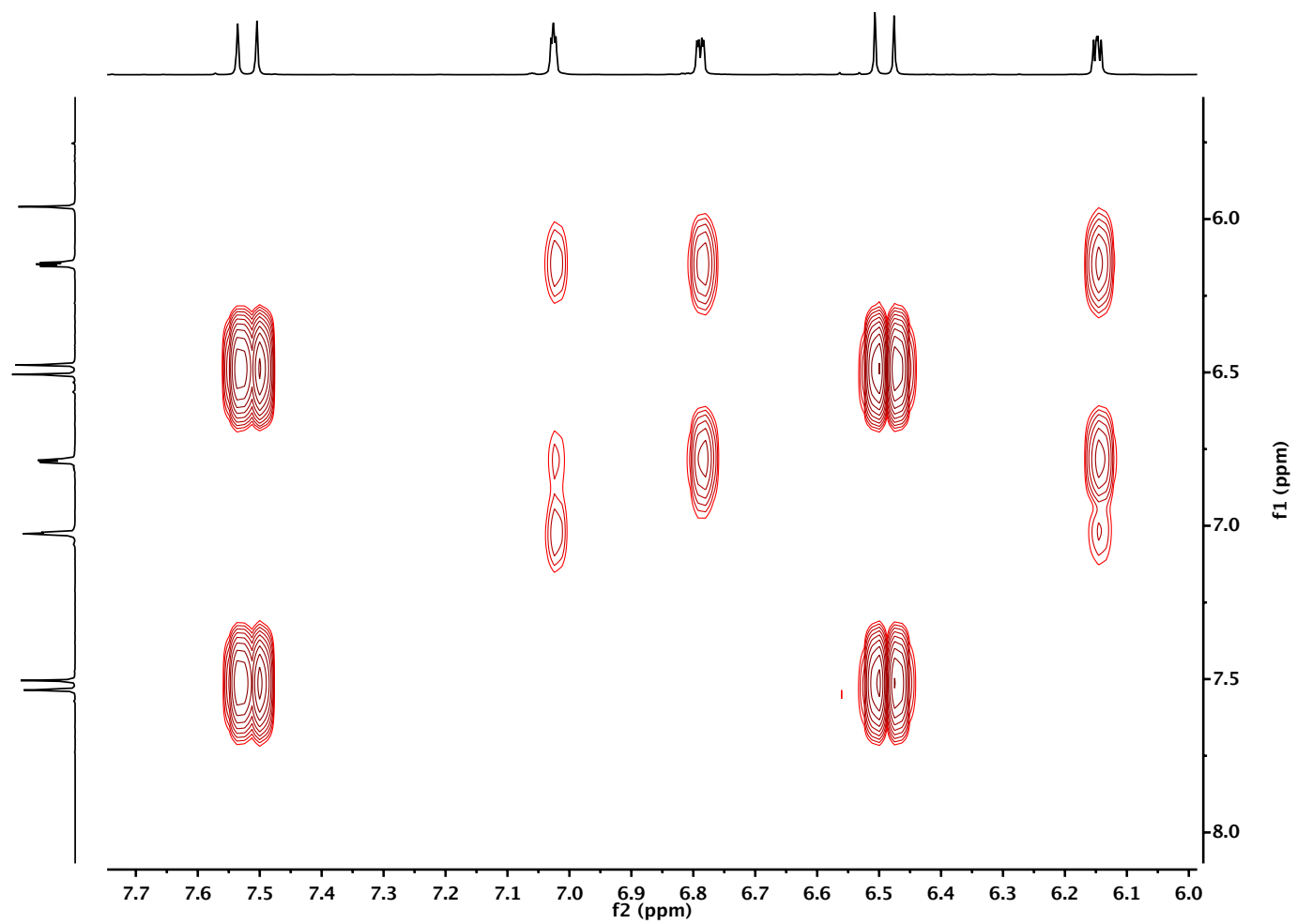


Figure S9. 500 MHz COSY NMR spectrum of N-methyl-pyrCurc.

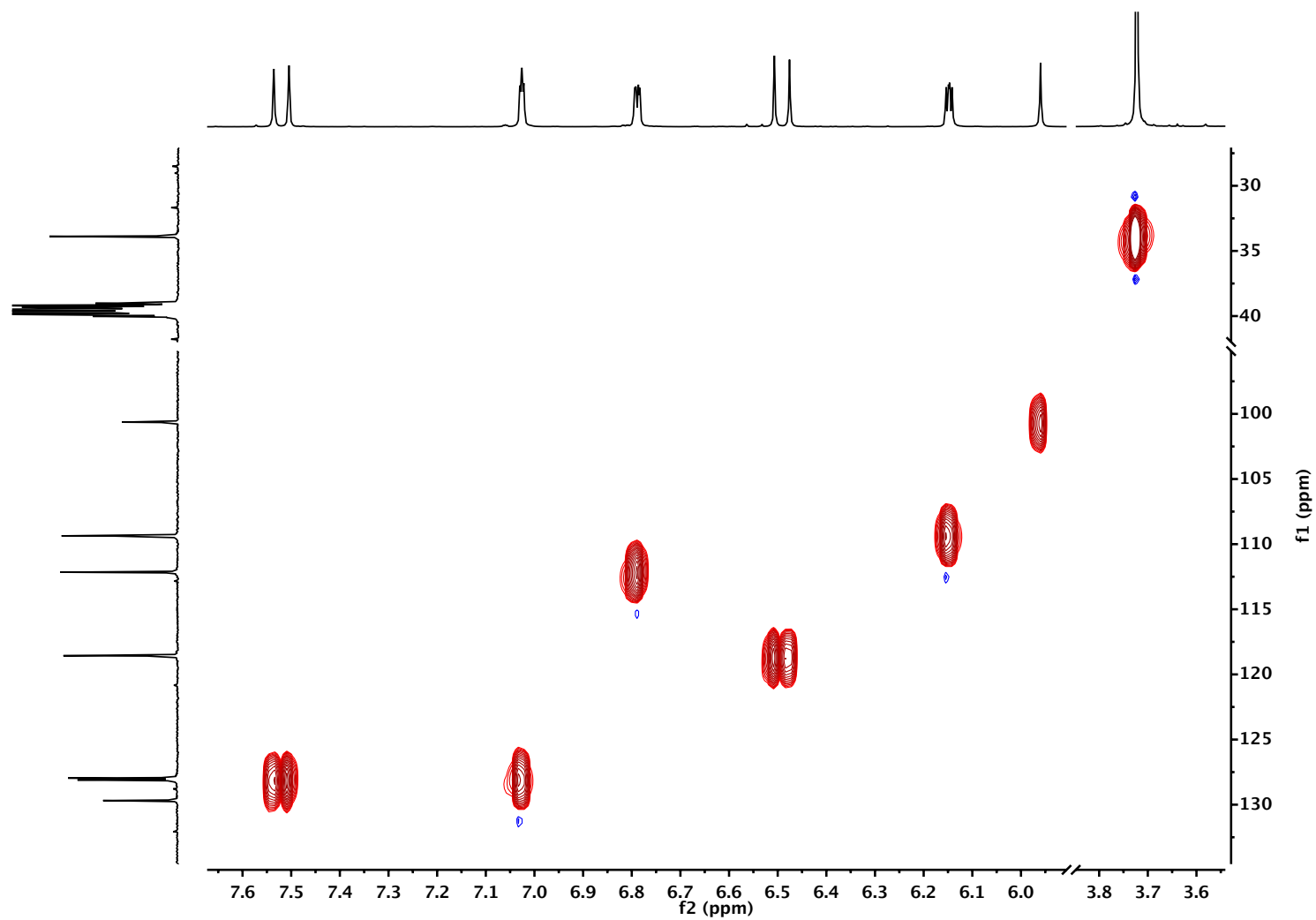


Figure S10. 500 MHz HSQC NMR spectrum of N-methyl-pyrCurc.

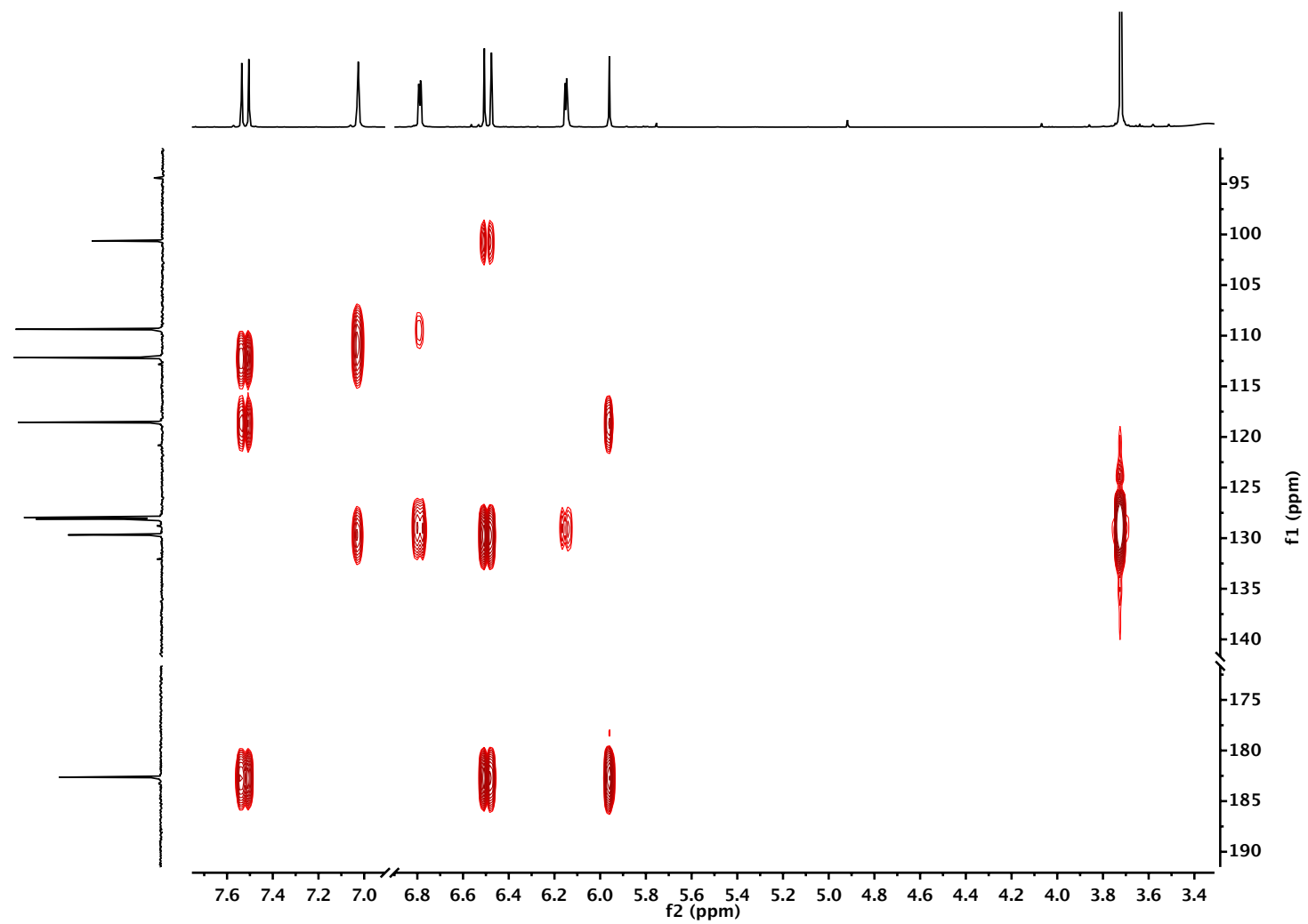


Figure S11. 500 MHz HMBC NMR spectrum of N-methyl-pyrCurc.

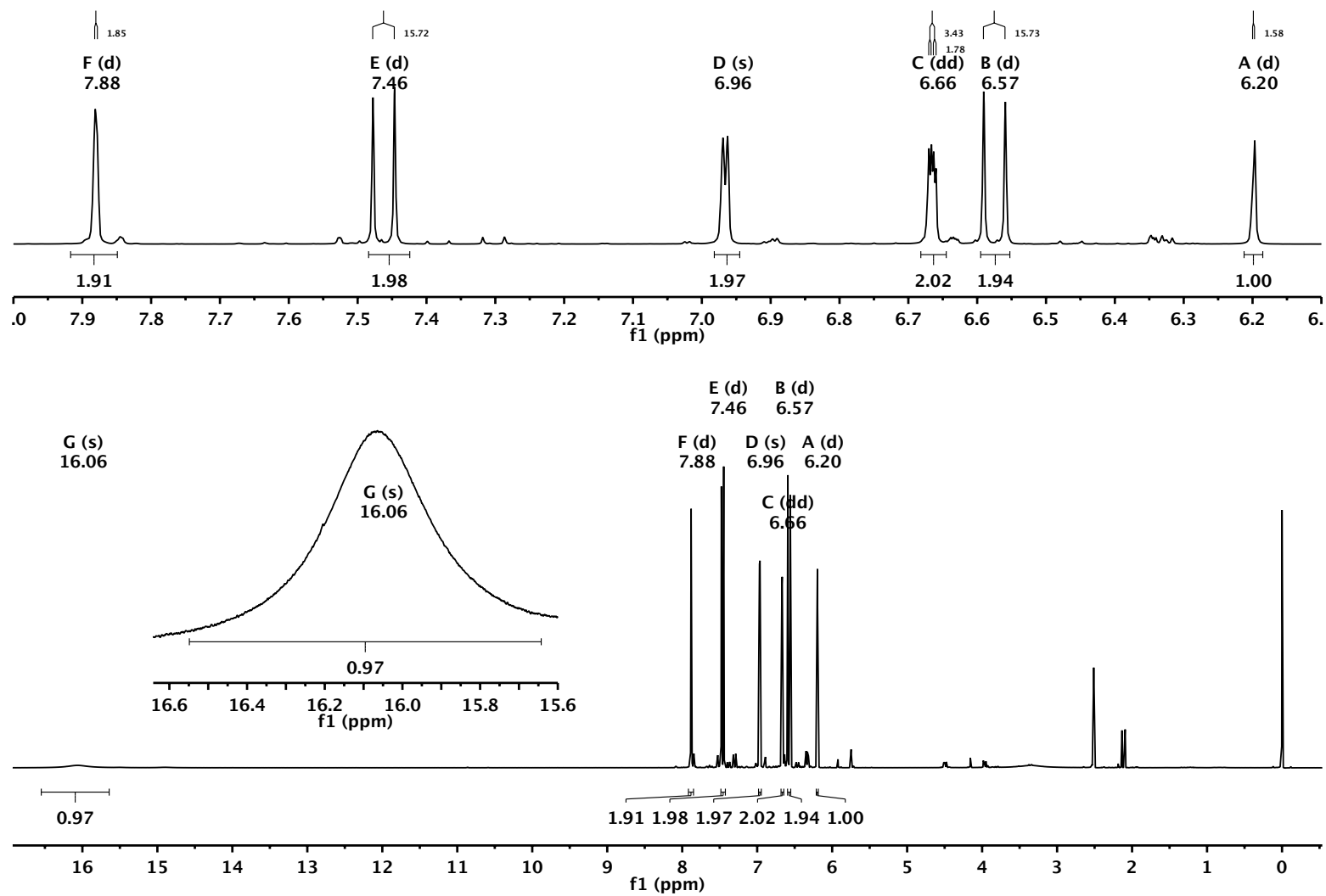


Figure S12. 500 MHz ^1H NMR spectrum of FuranCurc.

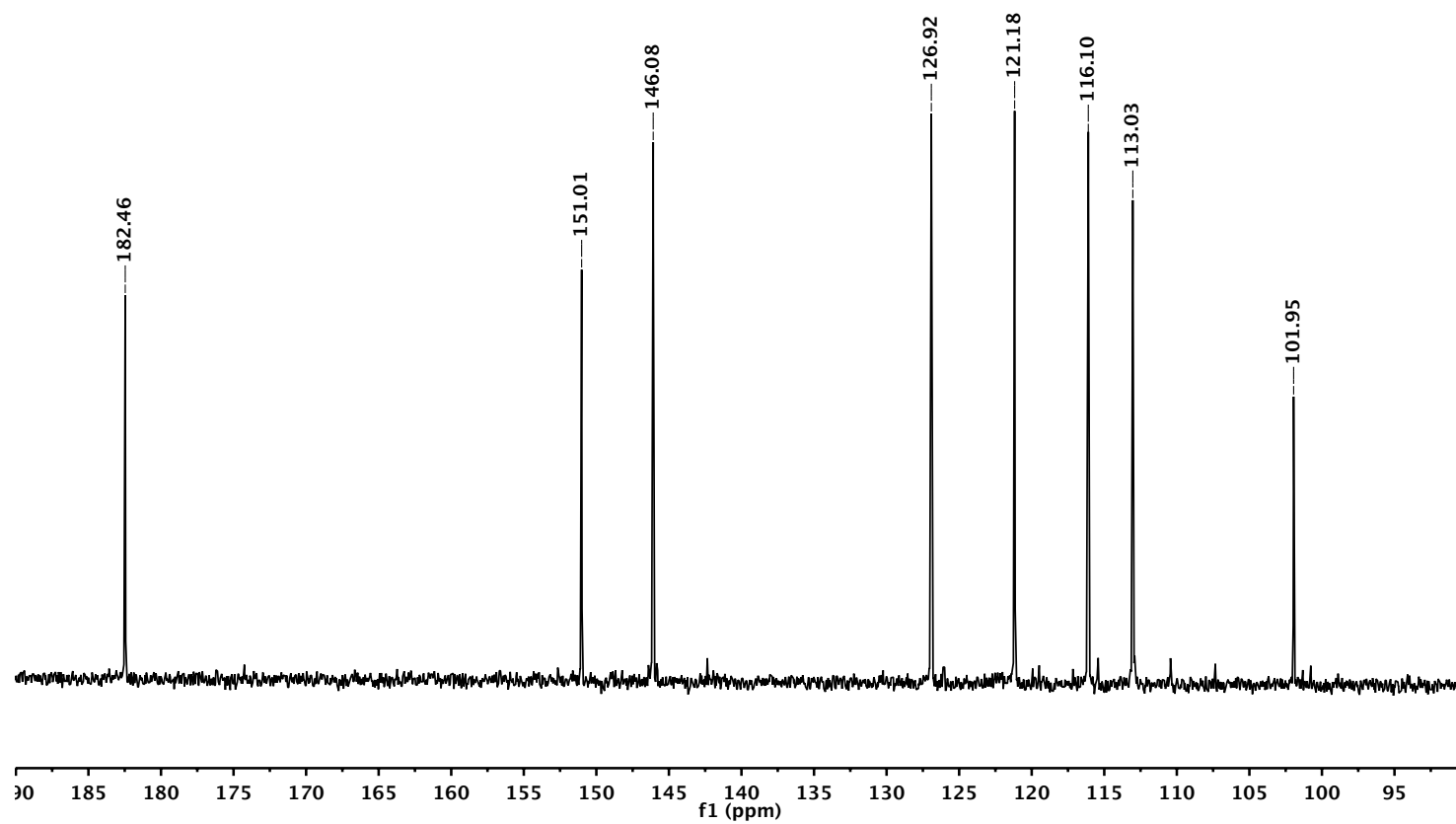


Figure S13. 125 MHz ^{13}C NMR spectrum of FuranCurc.

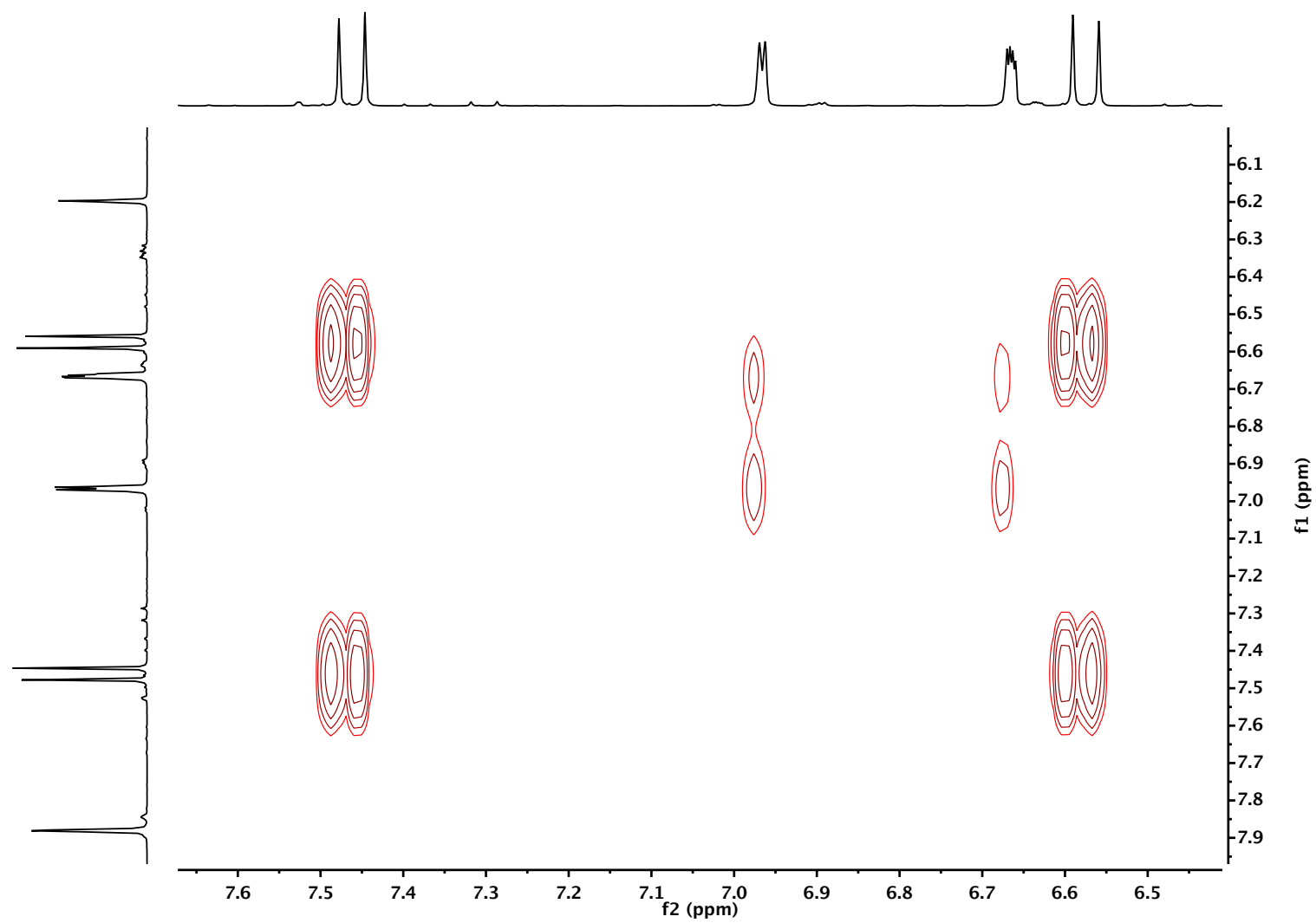


Figure S14. 500 MHz COSY NMR spectrum of FuranCurc.

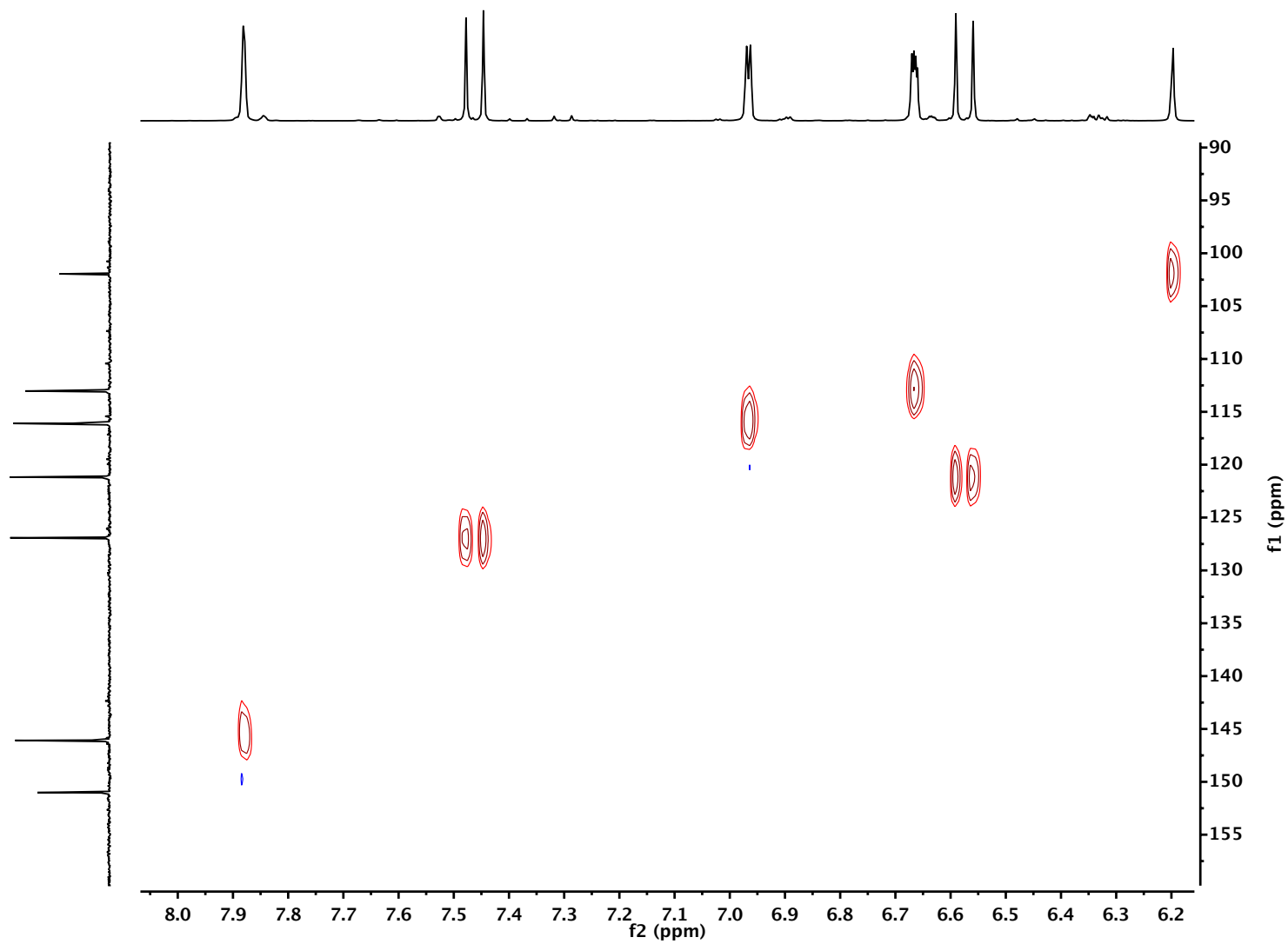


Figure S15. 500 MHz HSQC NMR spectrum of FuranCurc.

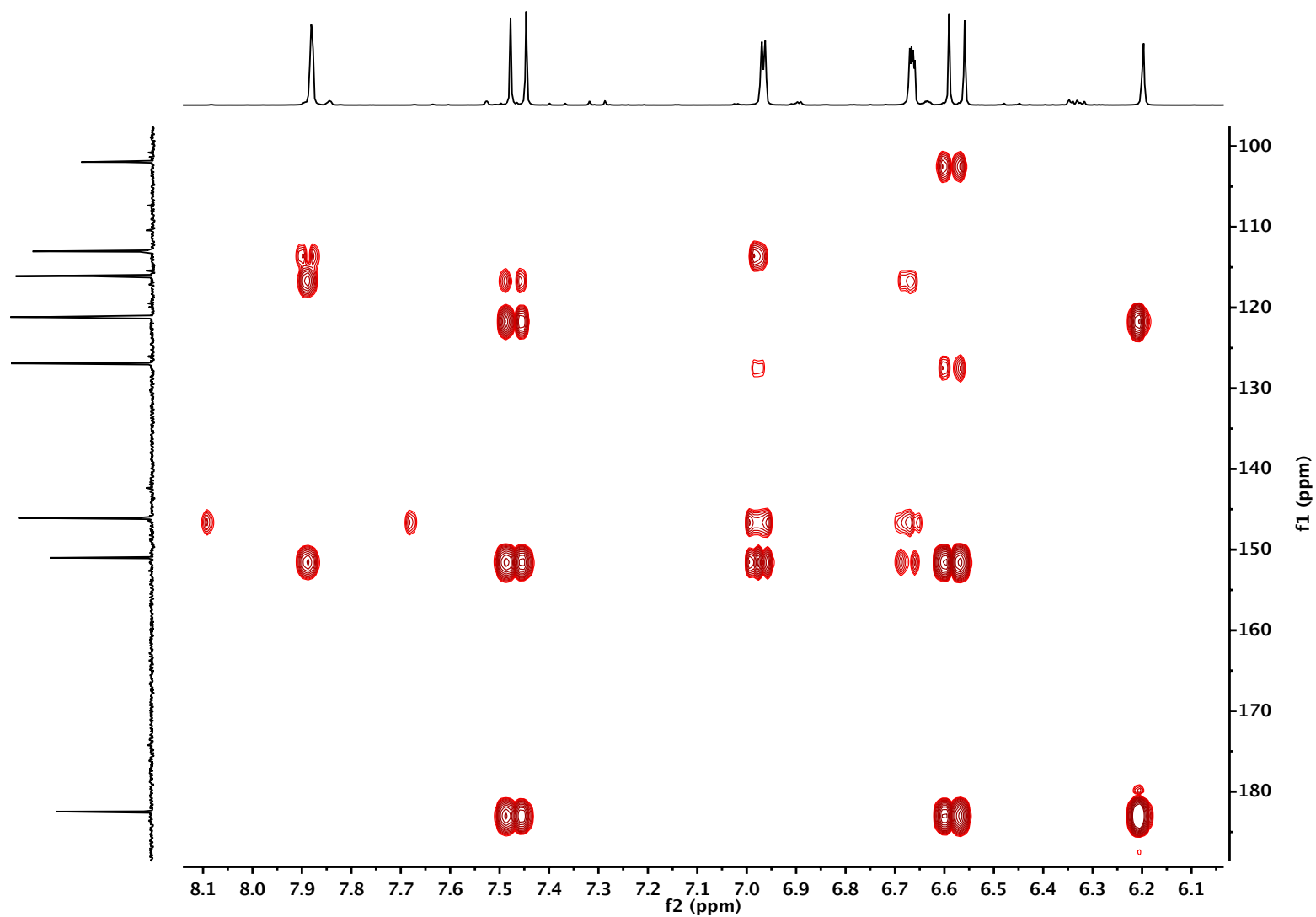


Figure S16. 500 MHz HMBC NMR spectrum of FuranCurc.

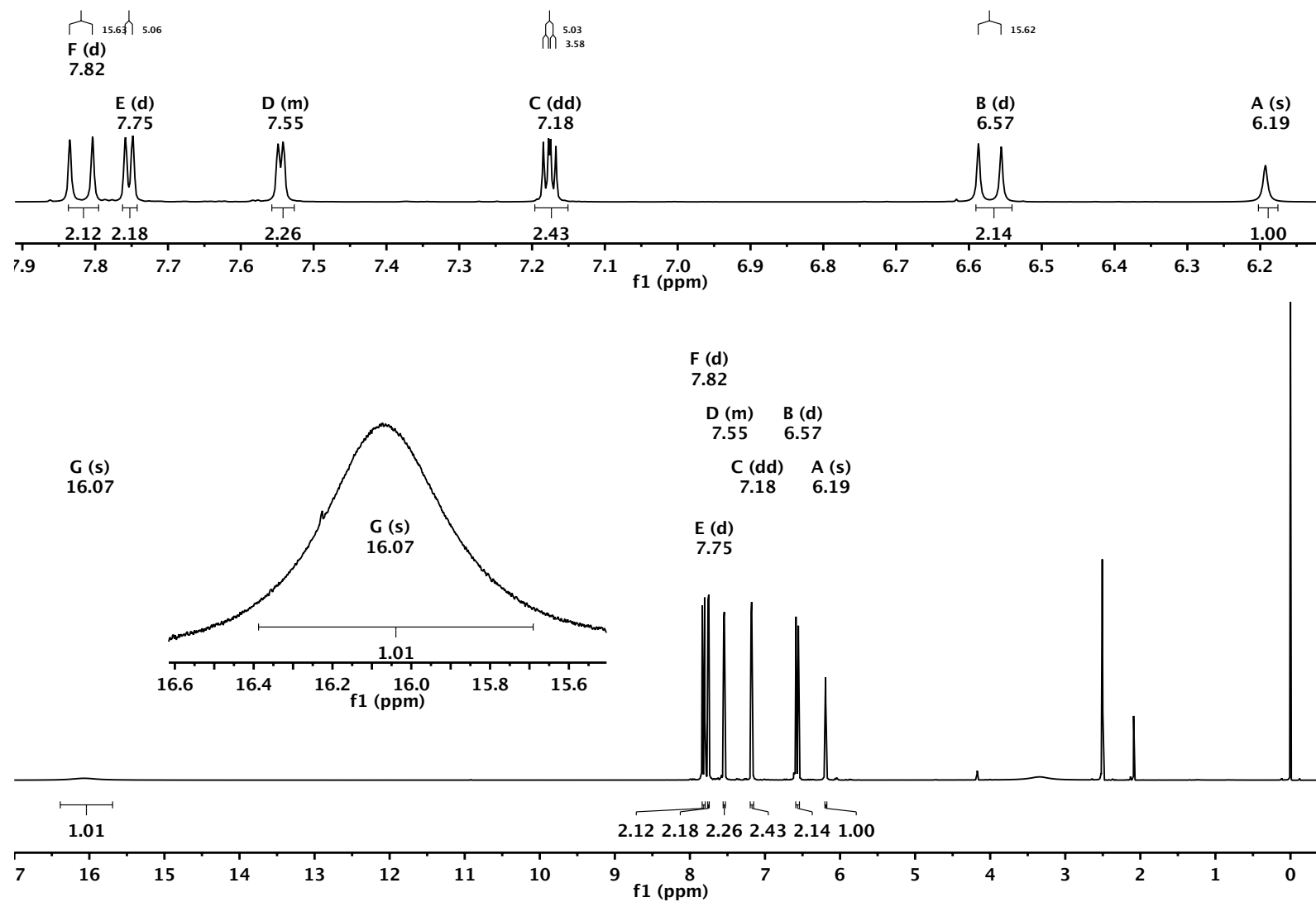


Figure S17. 500 MHz ^1H NMR spectrum of ThiopheneCurc.

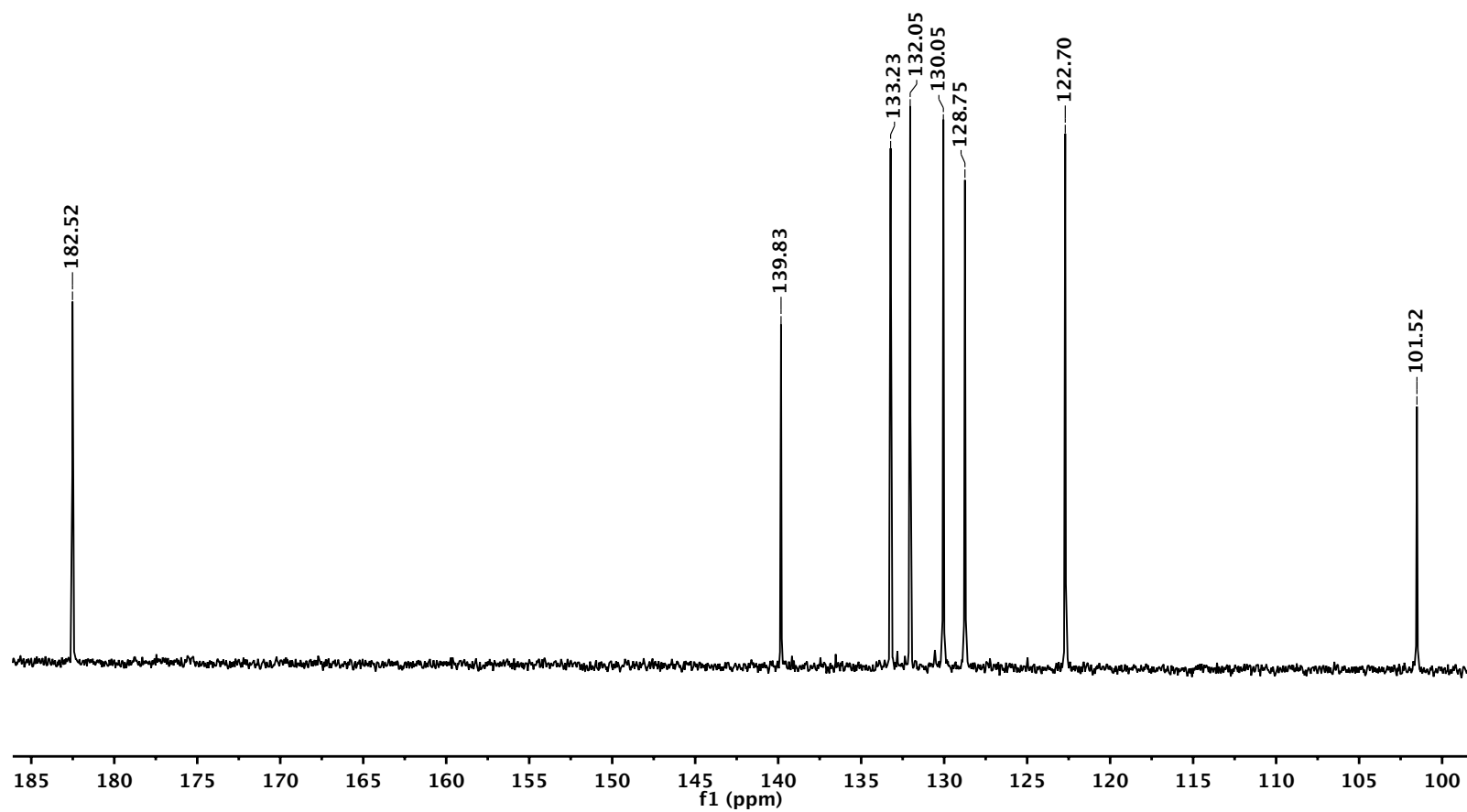


Figure S18. 125 MHz ^{13}C NMR spectrum of ThiopheneCurc.

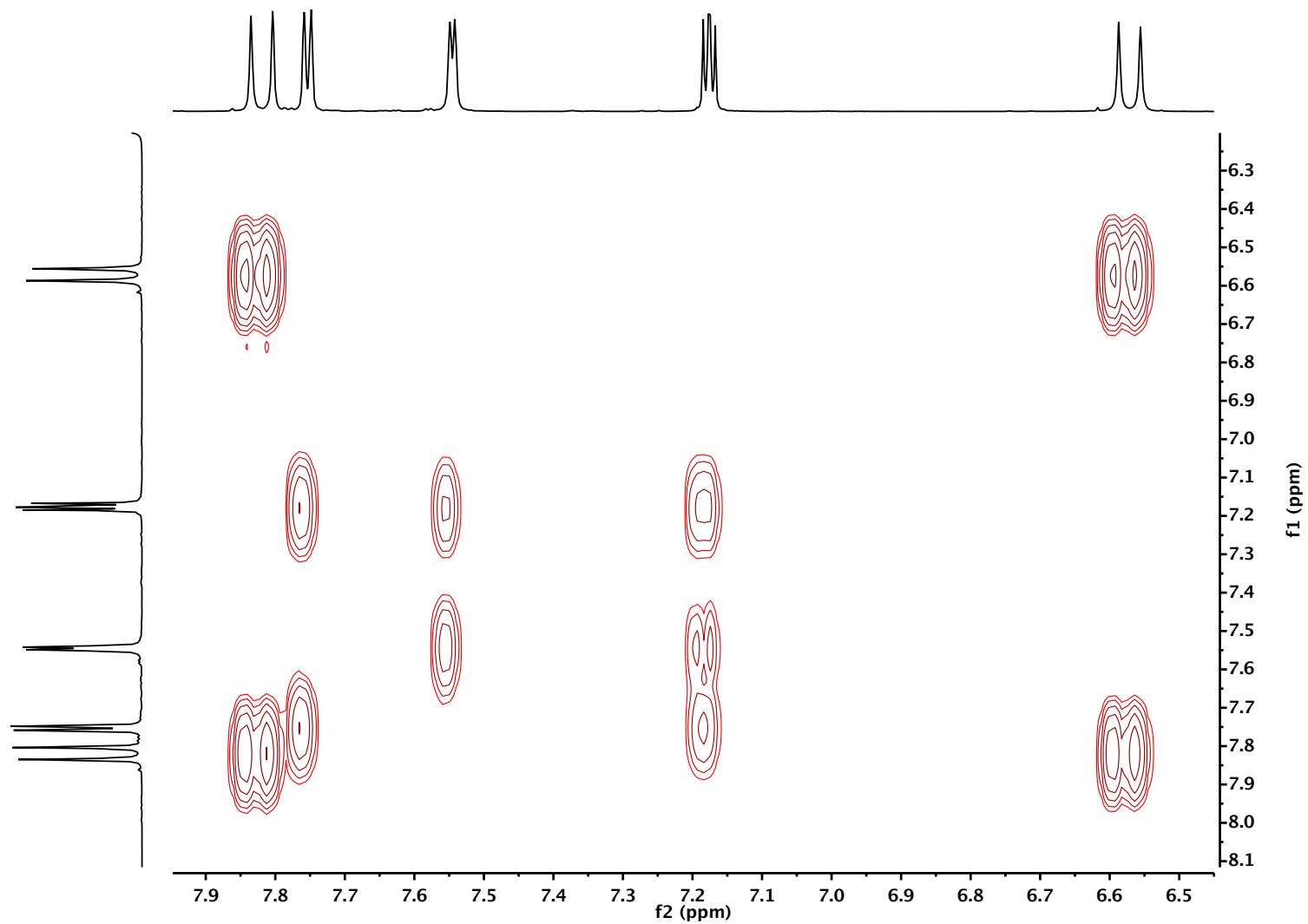


Figure S19. 500 MHz COSY NMR spectrum of ThiopheneCurc.

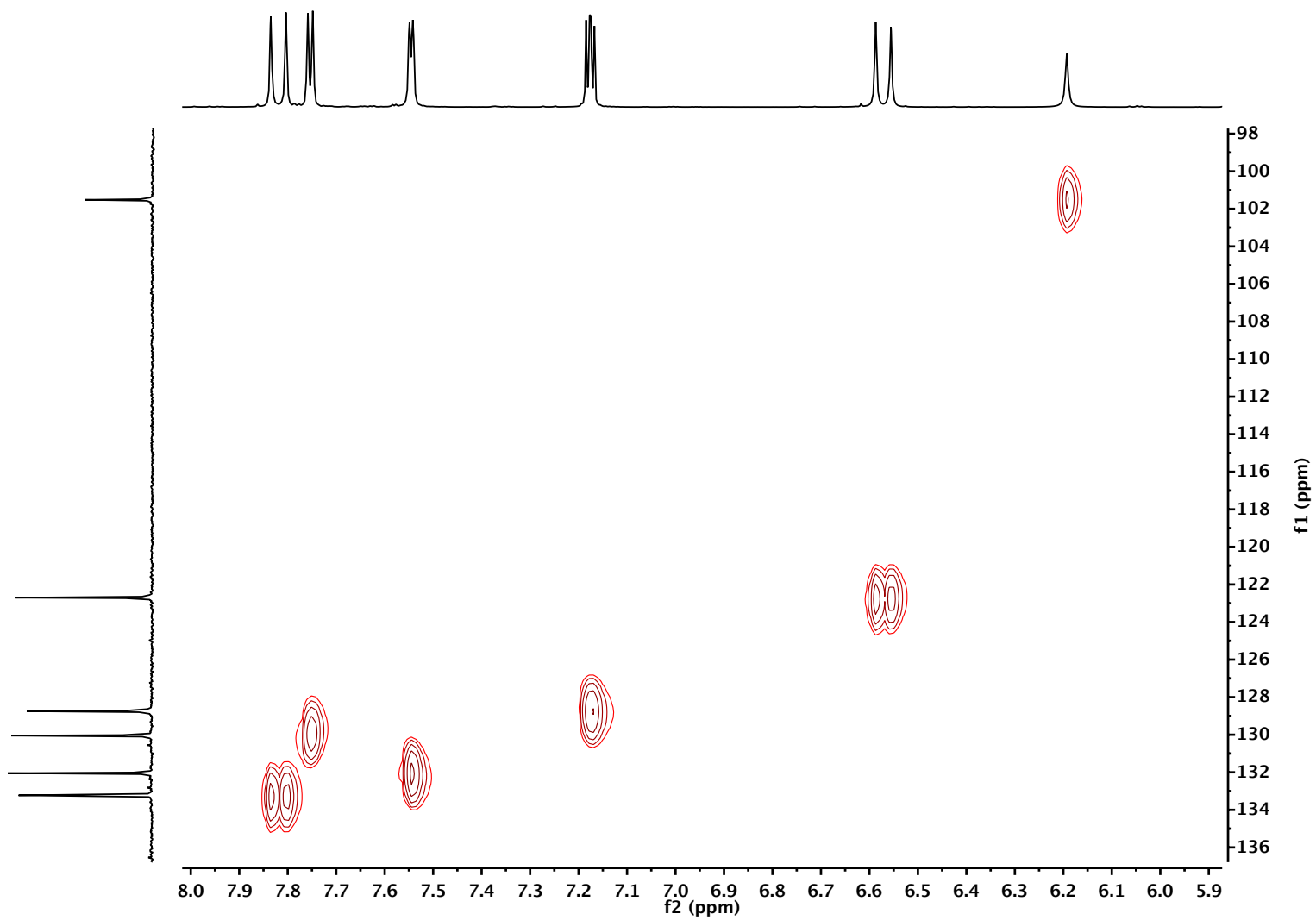


Figure S20. 500 MHz HSQC NMR spectrum of ThiopheneCurc.

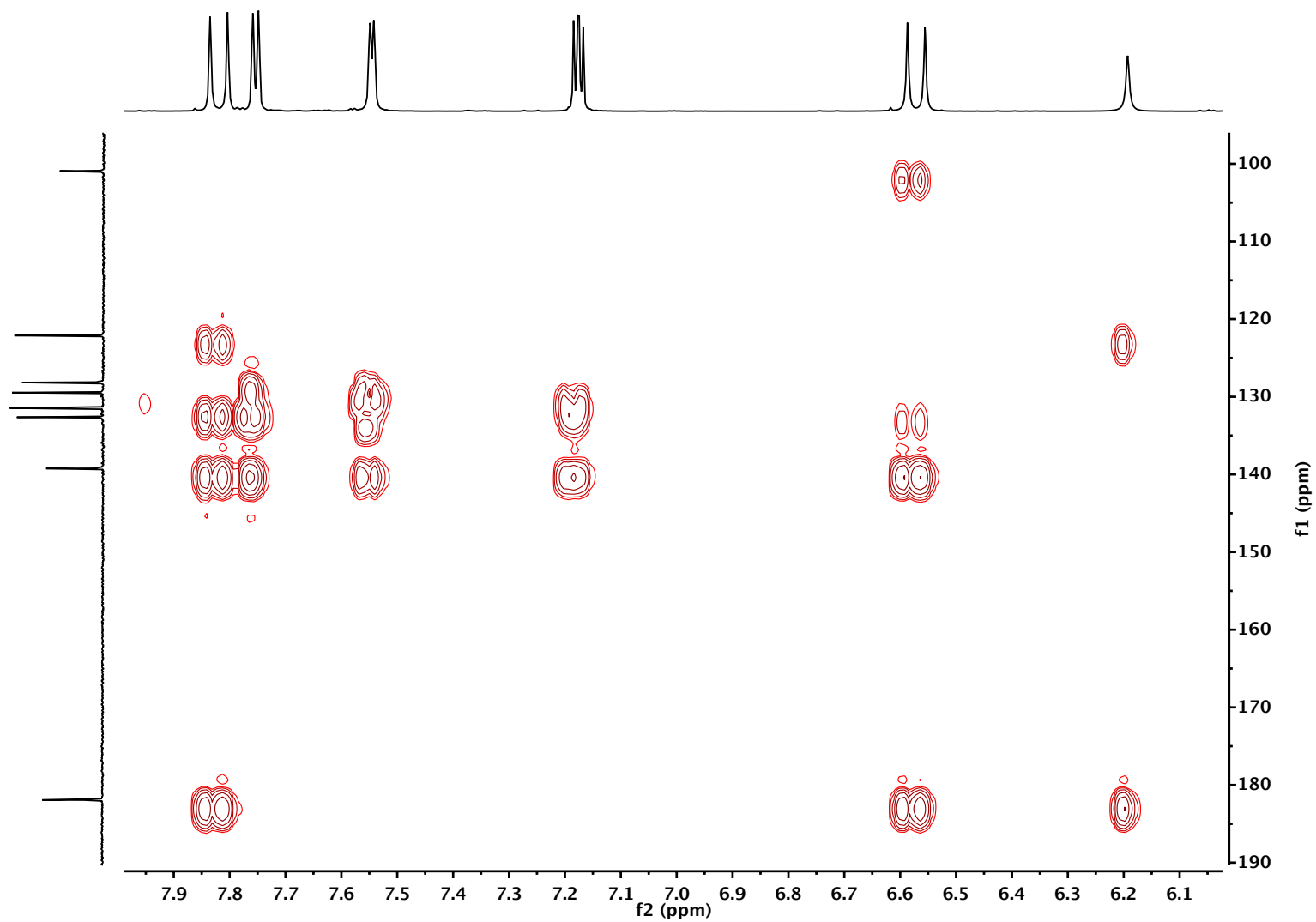


Figure S21. 500 MHz HMBC NMR spectrum of ThiopheneCurc.

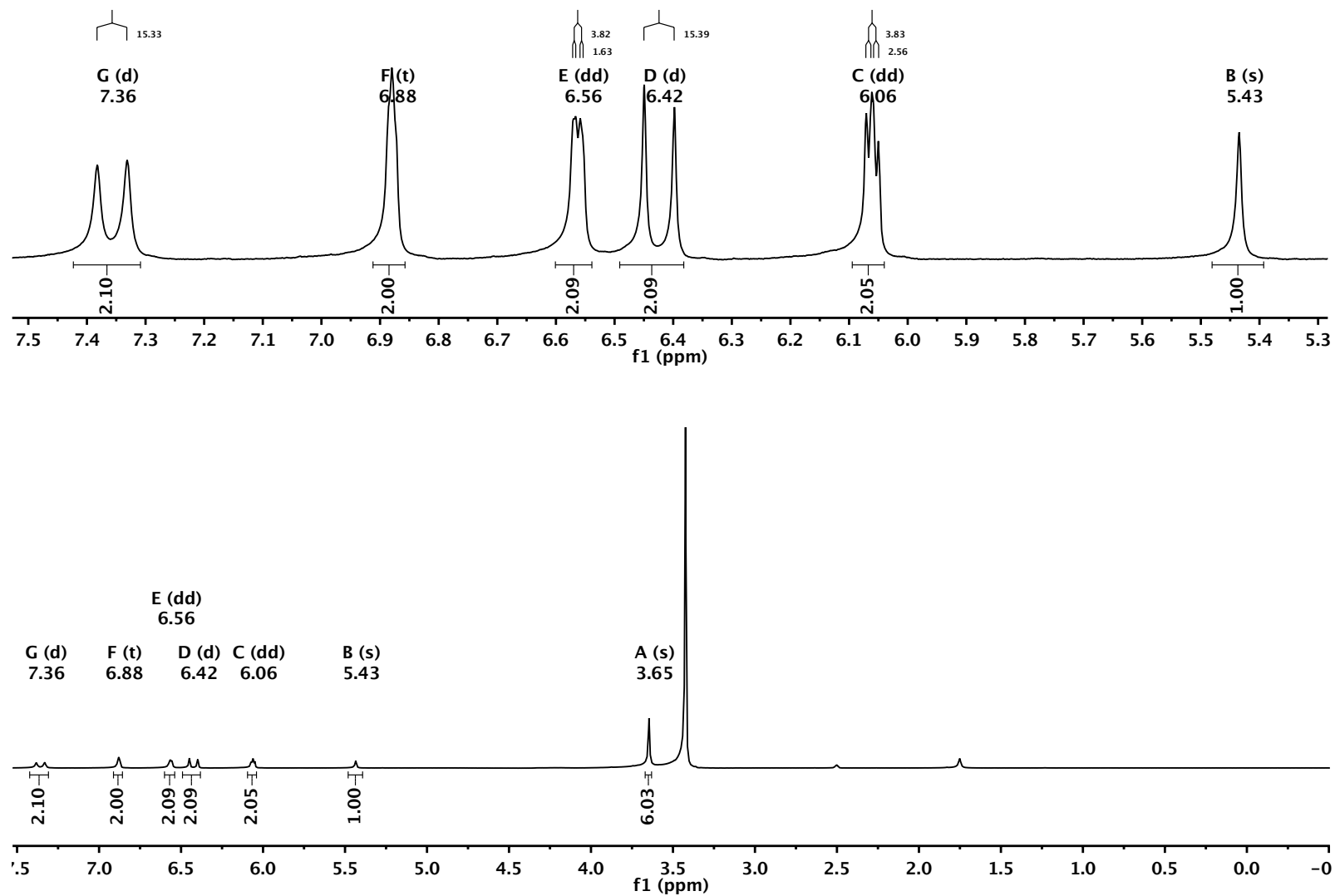


Figure S22. 500 MHz ¹H NMR spectrum of N-methyl-pyrCurc-Mg.

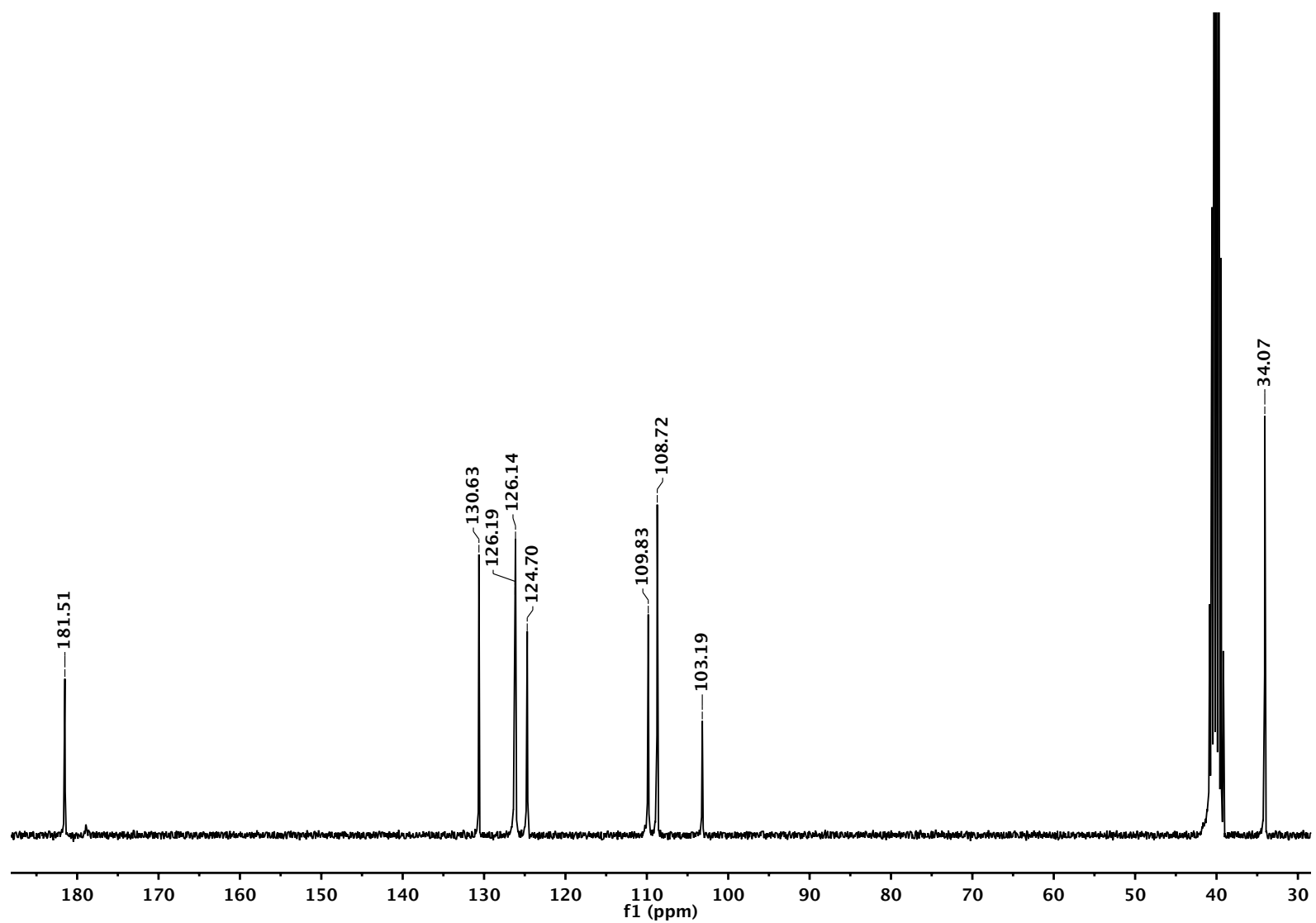


Figure S23. 125 MHz ^{13}C NMR spectrum of N-methyl-pyrCurc-Mg.

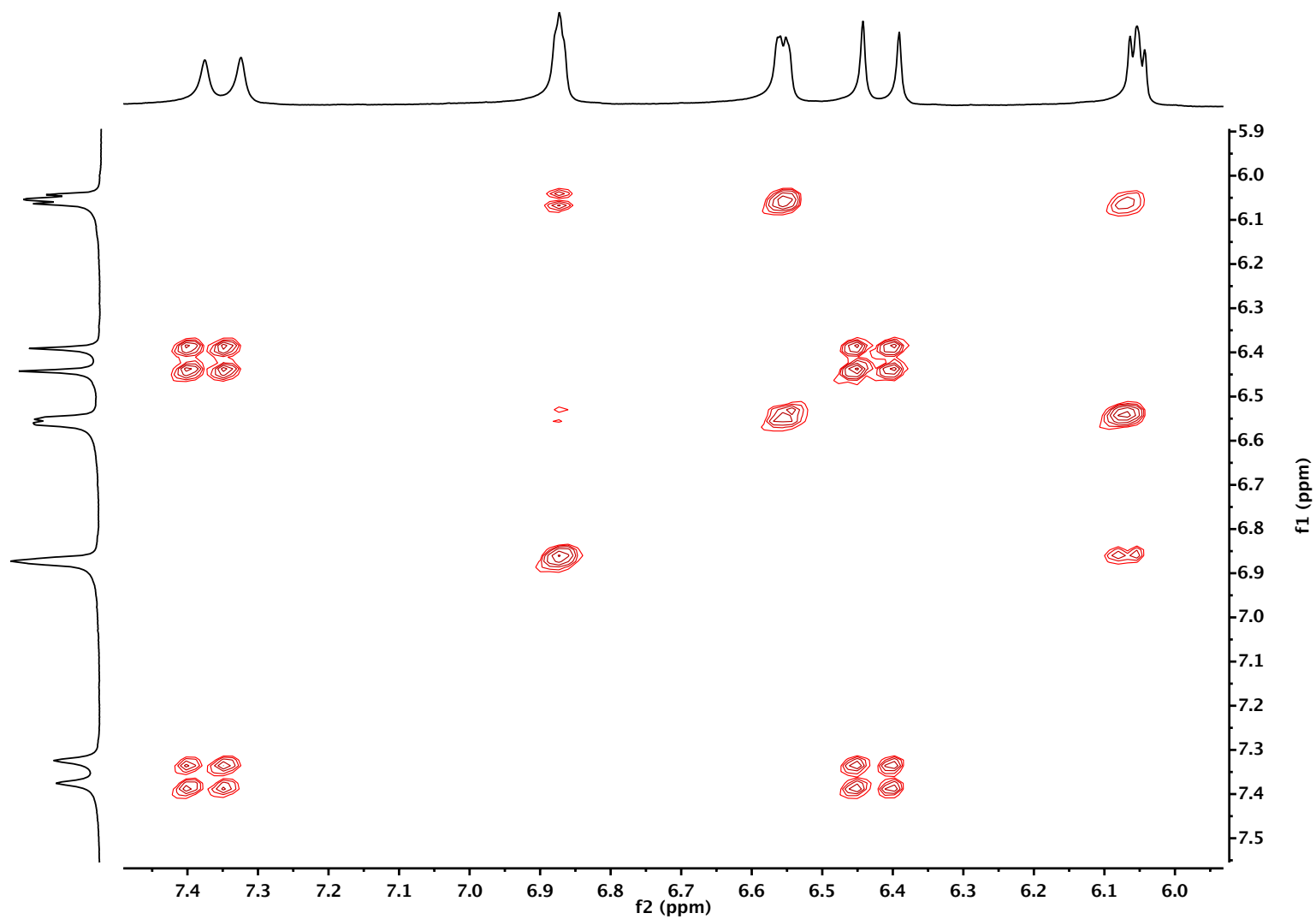


Figure S24. 500 MHz COSY NMR spectrum of N-methyl-pyrCurc-Mg.

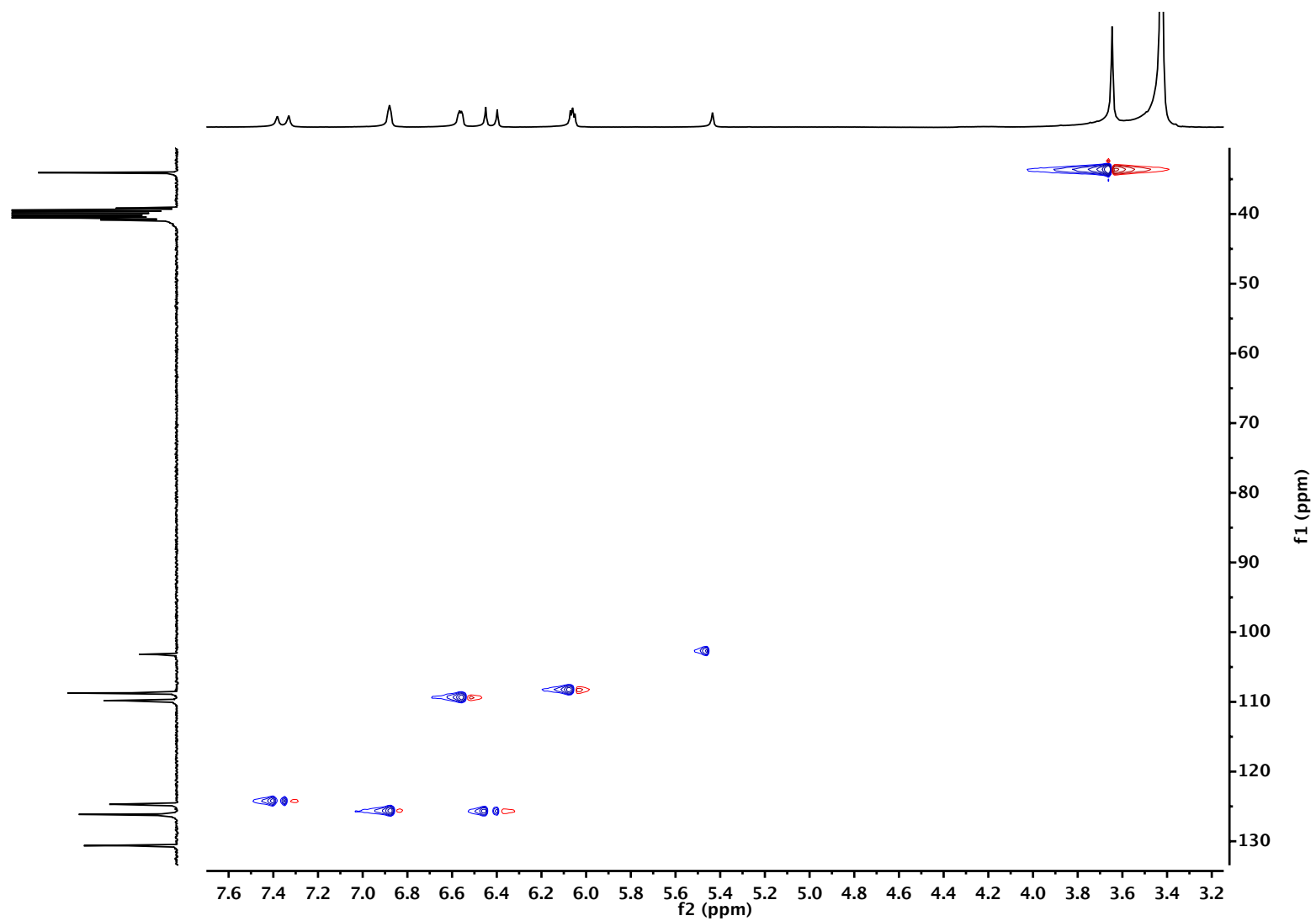


Figure S25. 500 MHz HSQC NMR spectrum of N-methyl-pyrCurc-Mg.

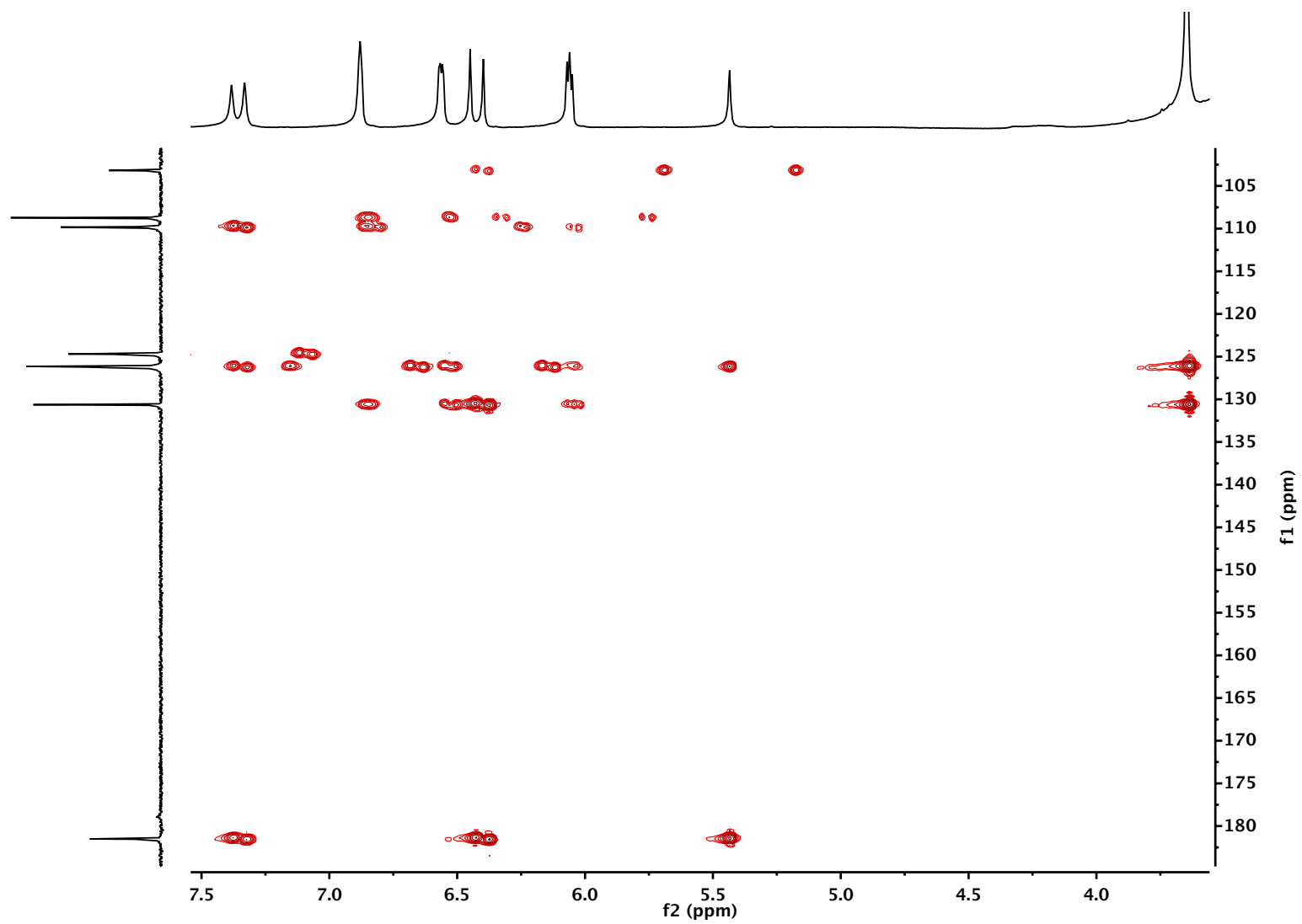


Figure S26. 500 MHz HMBC NMR spectrum of N-methyl-pyrCurc-Mg.

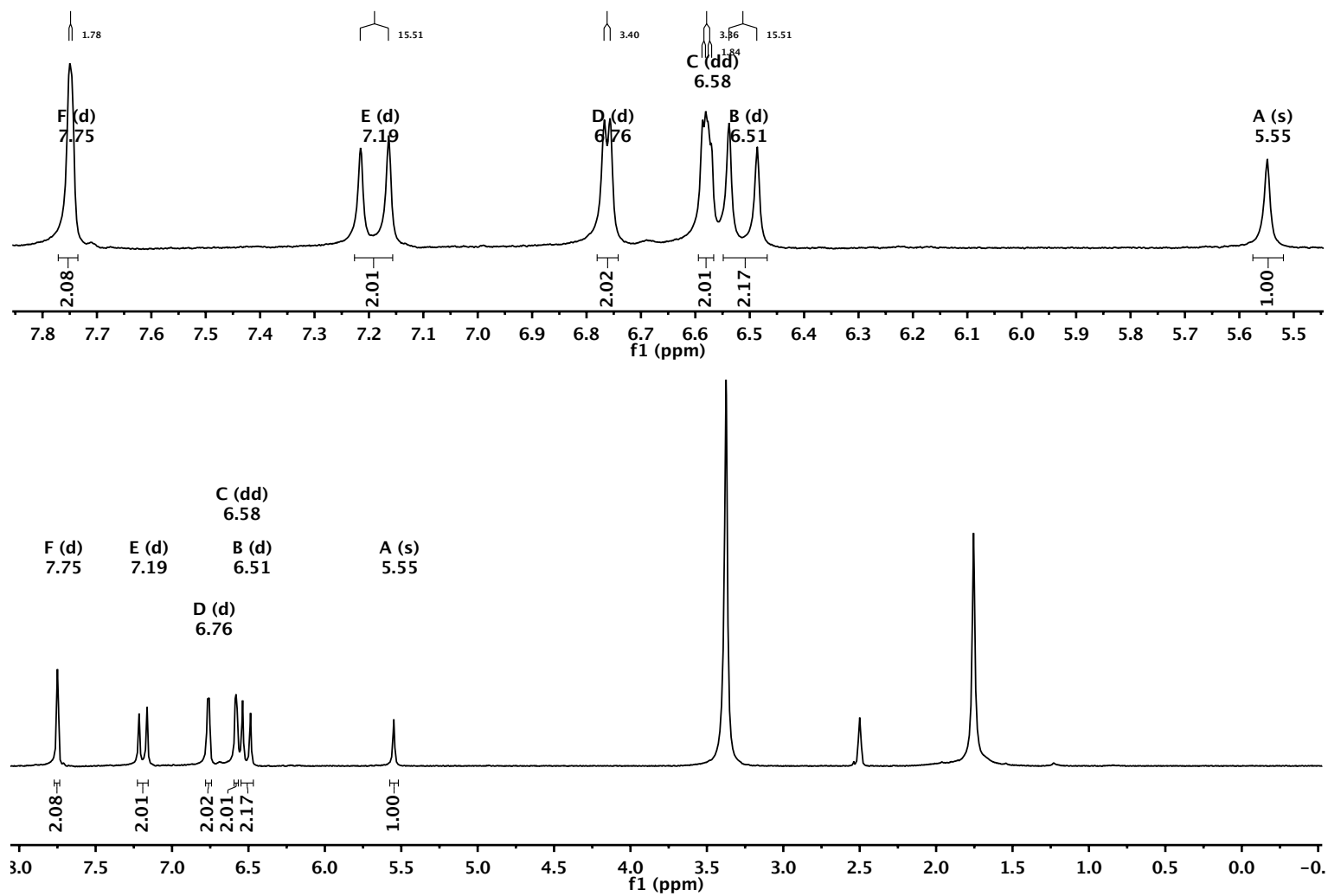


Figure S27. 500 MHz ¹H NMR spectrum of FuranCurc-Mg.

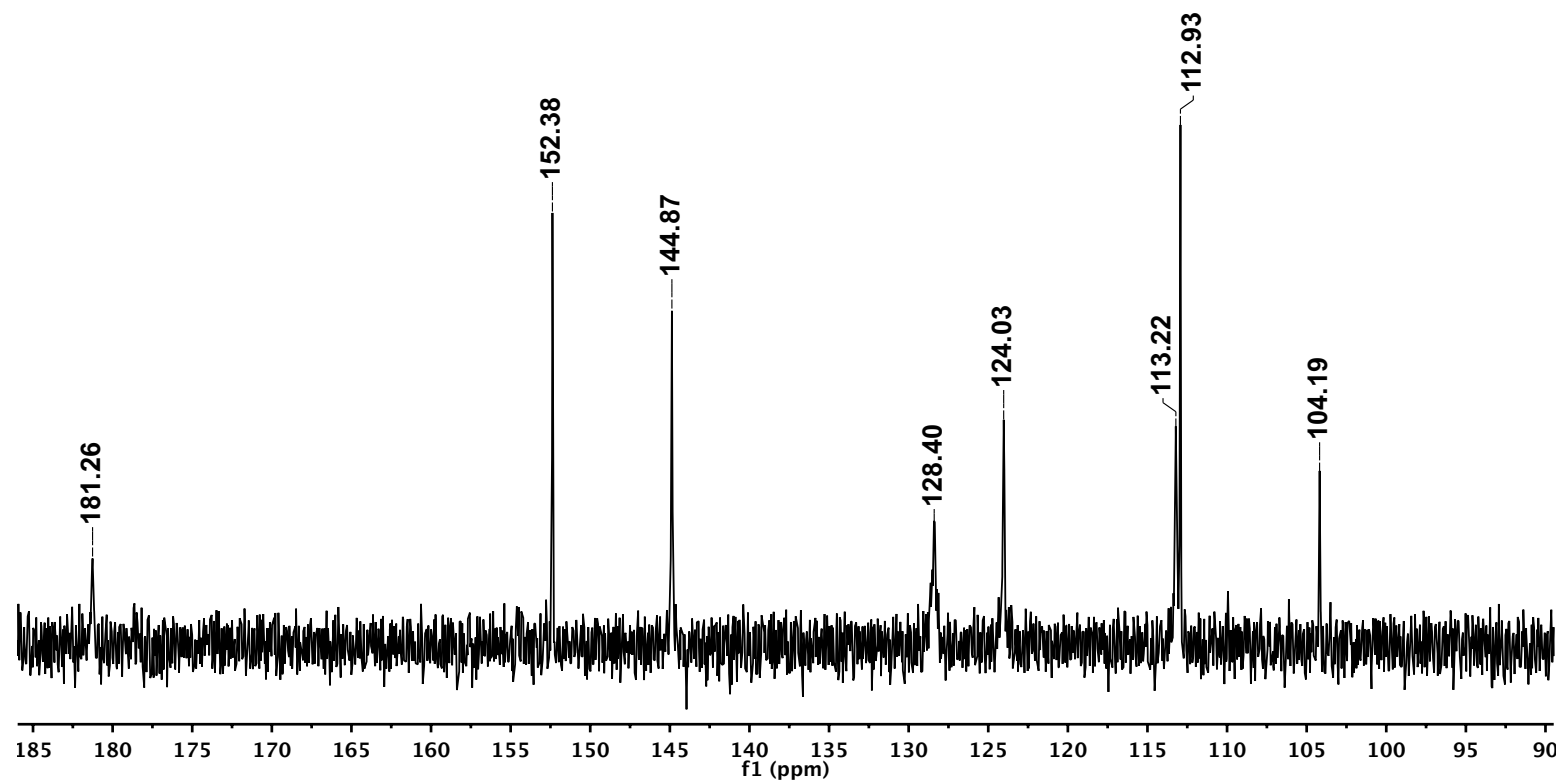


Figure S28. 125 MHz ^{13}C NMR spectrum of FuranCurc-Mg.

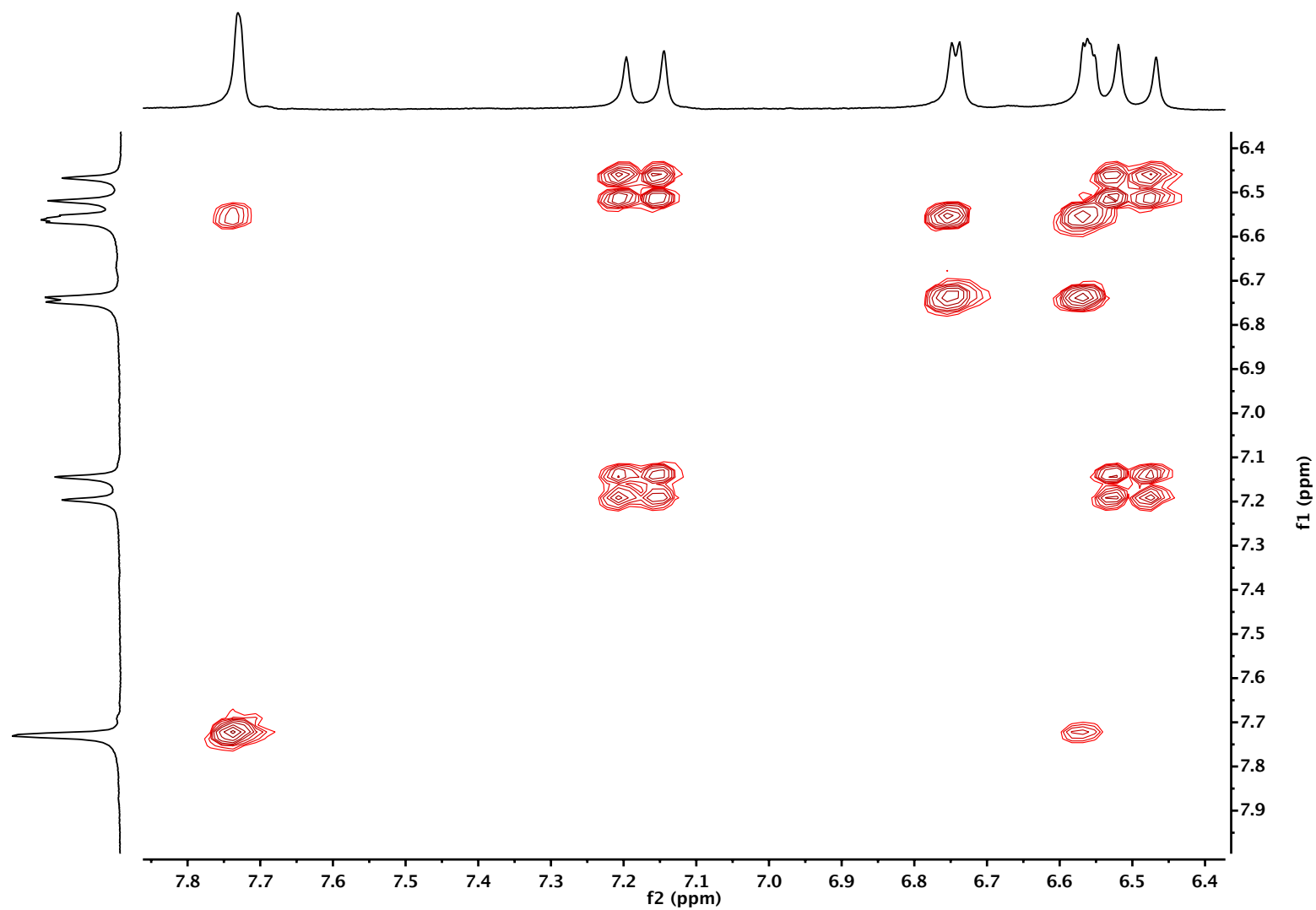


Figure S29. 500 MHz COSY NMR spectrum of FuranCurc-Mg.

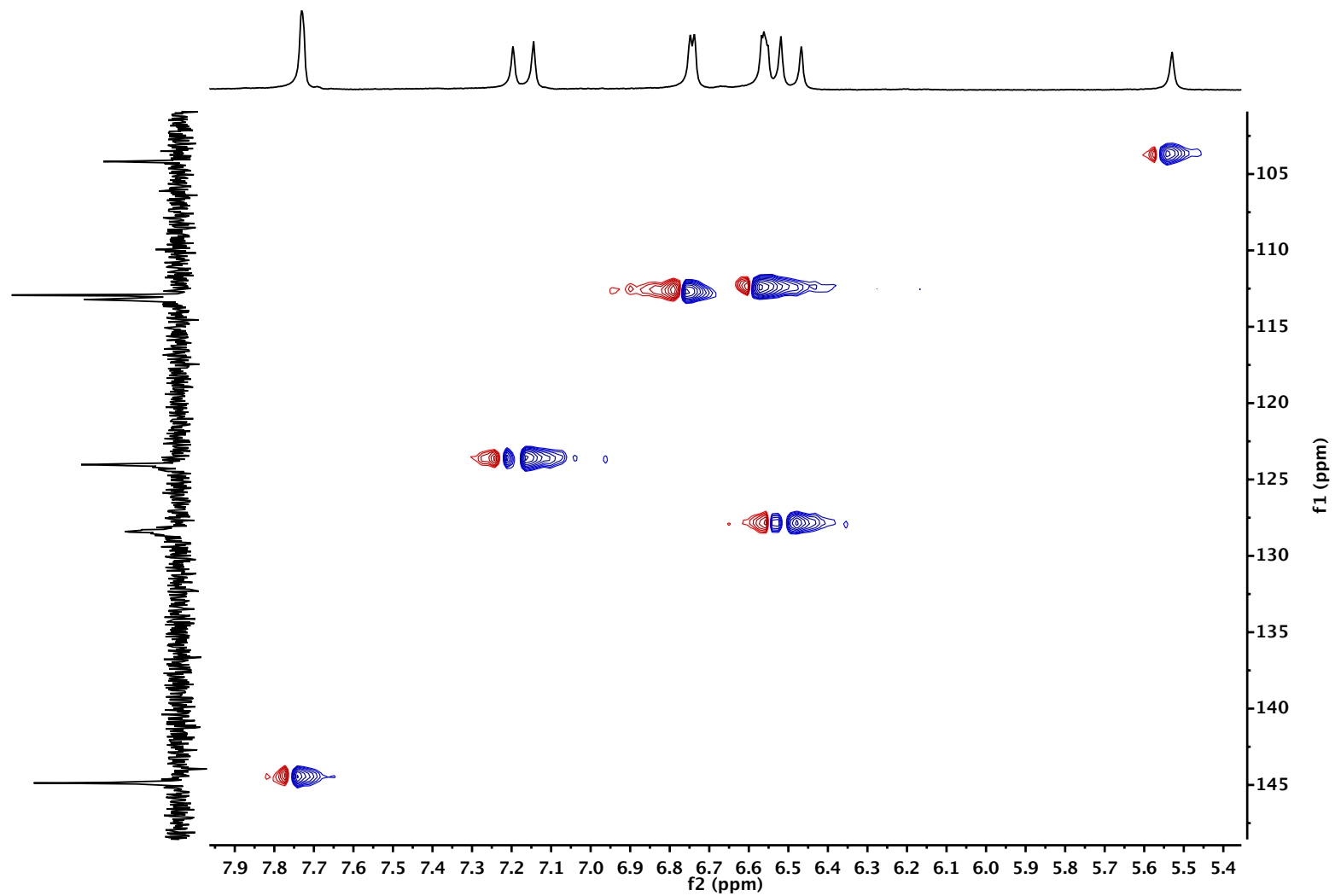


Figure S30. 500 MHz HSQC NMR spectrum of FuranCurc-Mg.

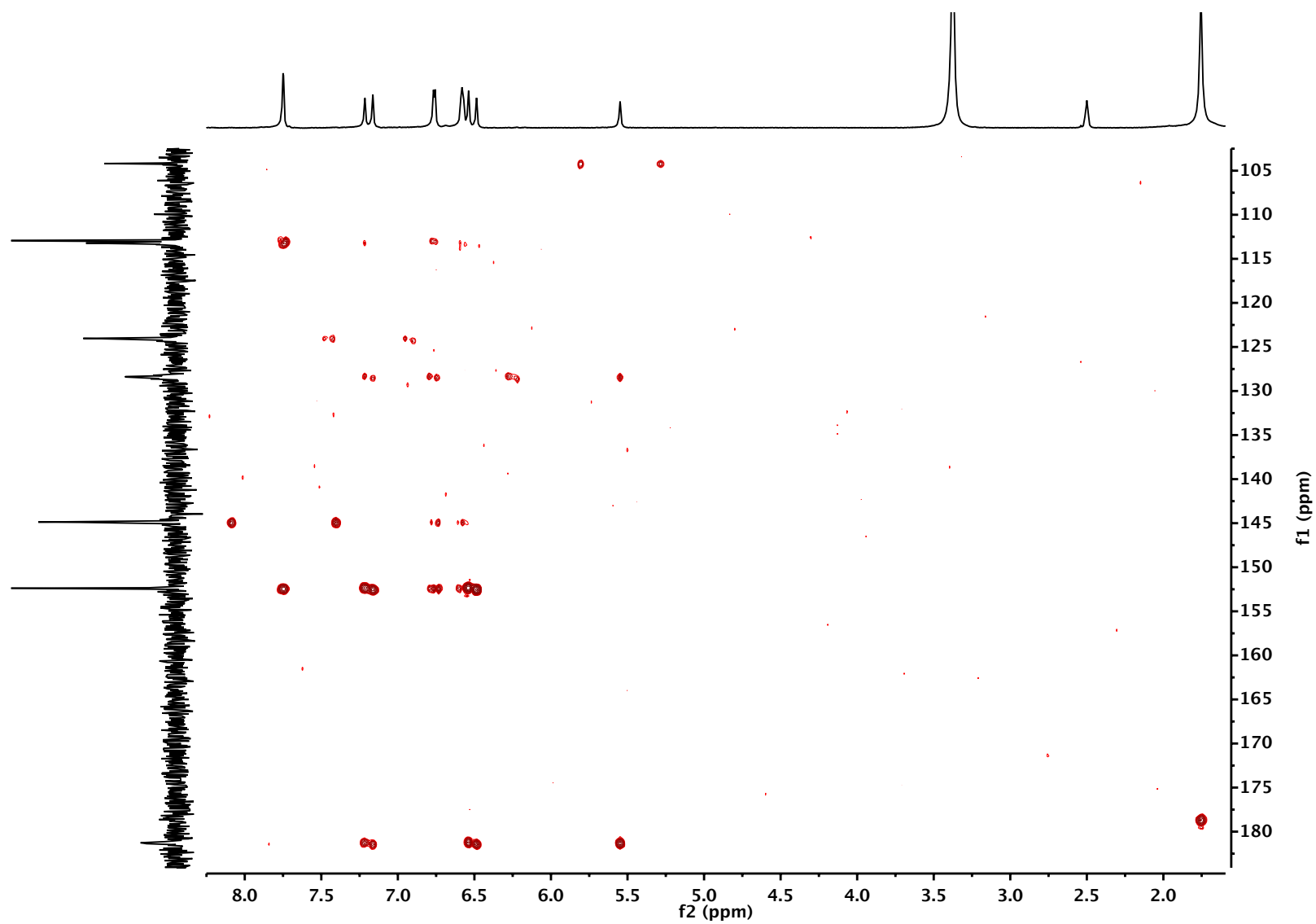


Figure S31. 500 MHz HMBC NMR spectrum of FuranCurc-Mg.

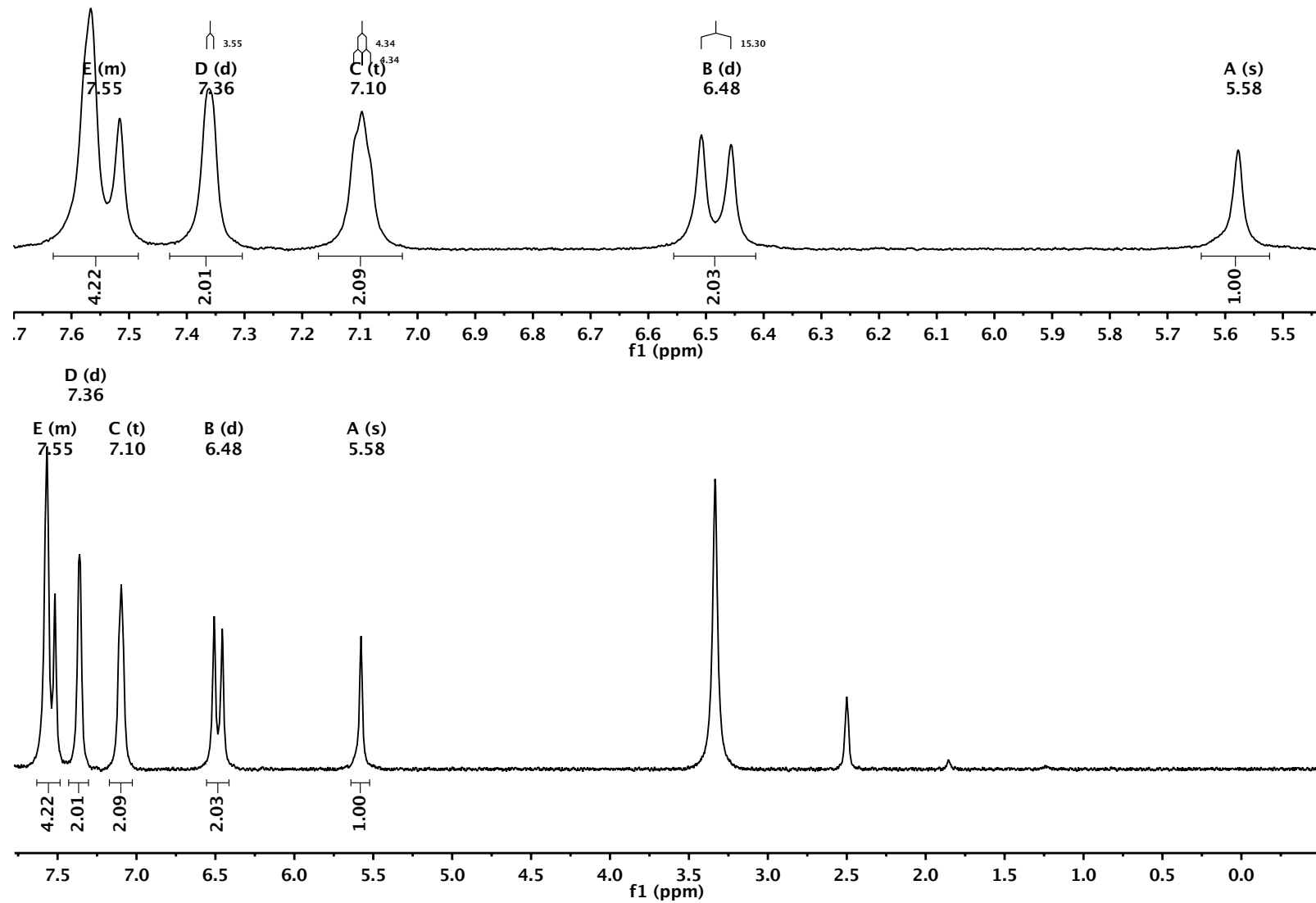


Figure S32. 500 MHz ¹H NMR spectrum of ThiopheneCurc-Mg.

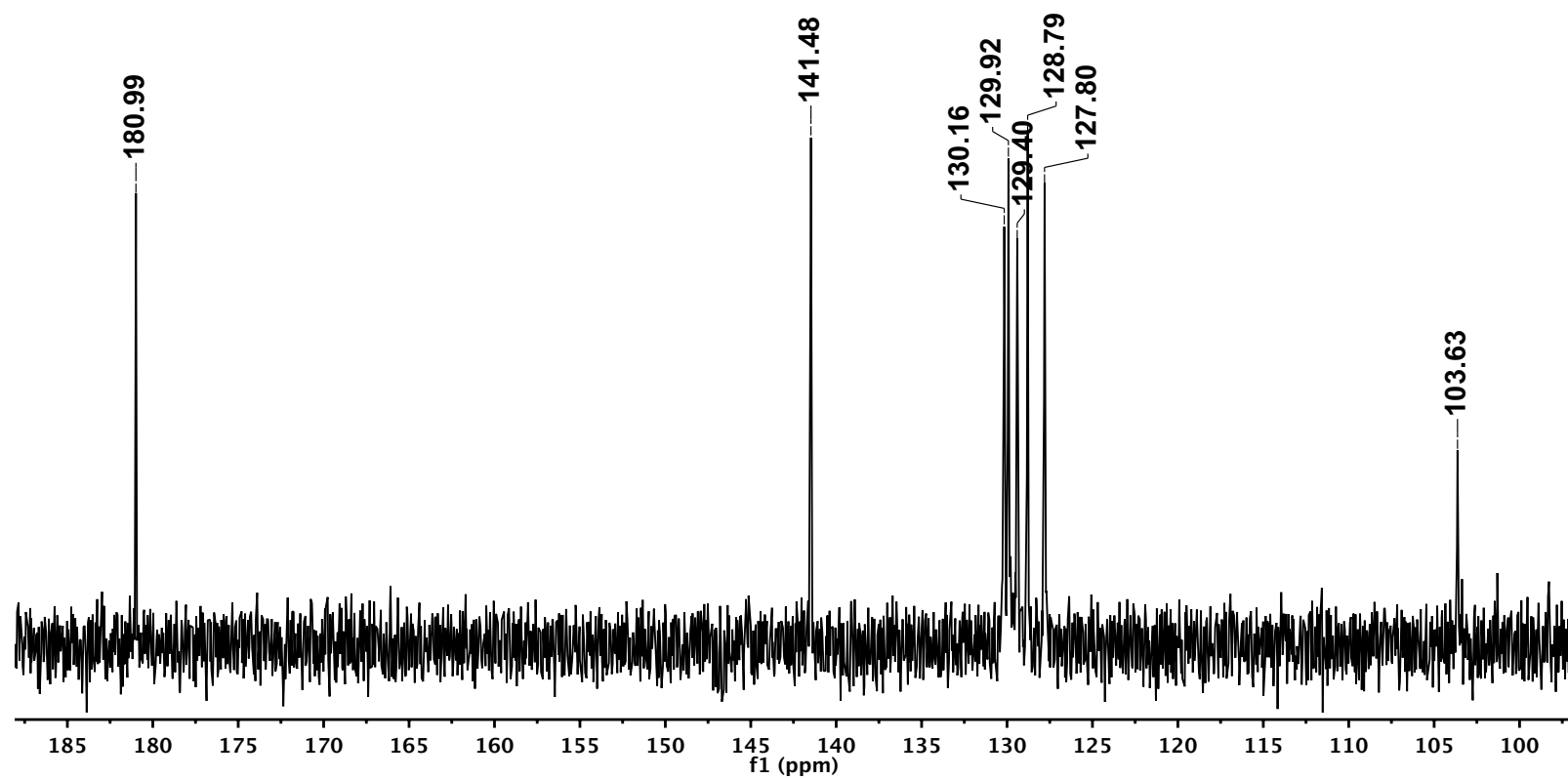


Figure S33. 125 MHz ^{13}C NMR spectrum of ThiopheneCurc-Mg.

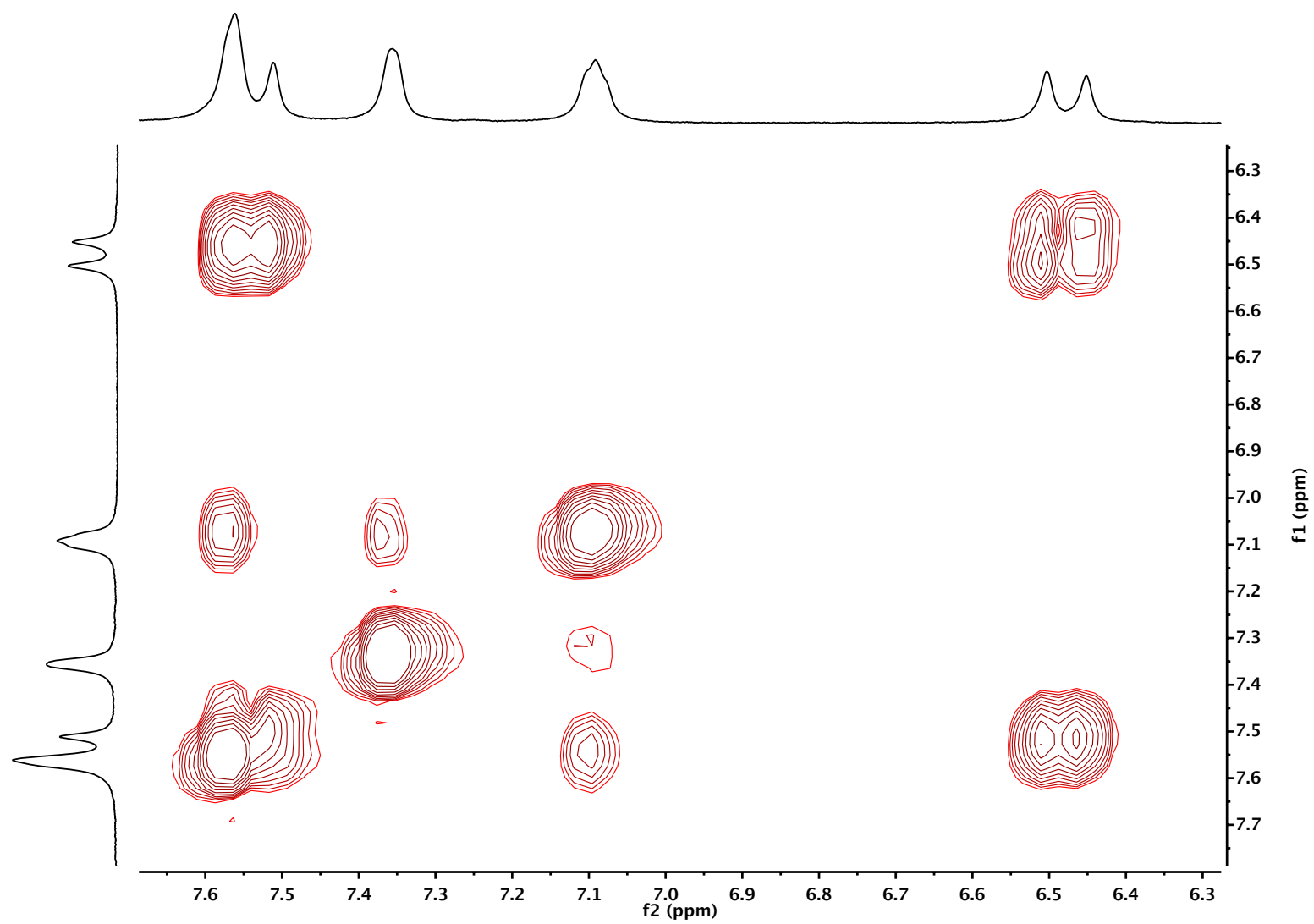


Figure S34. 500 MHz HSQC NMR spectrum of ThiopheneCurc-Mg.

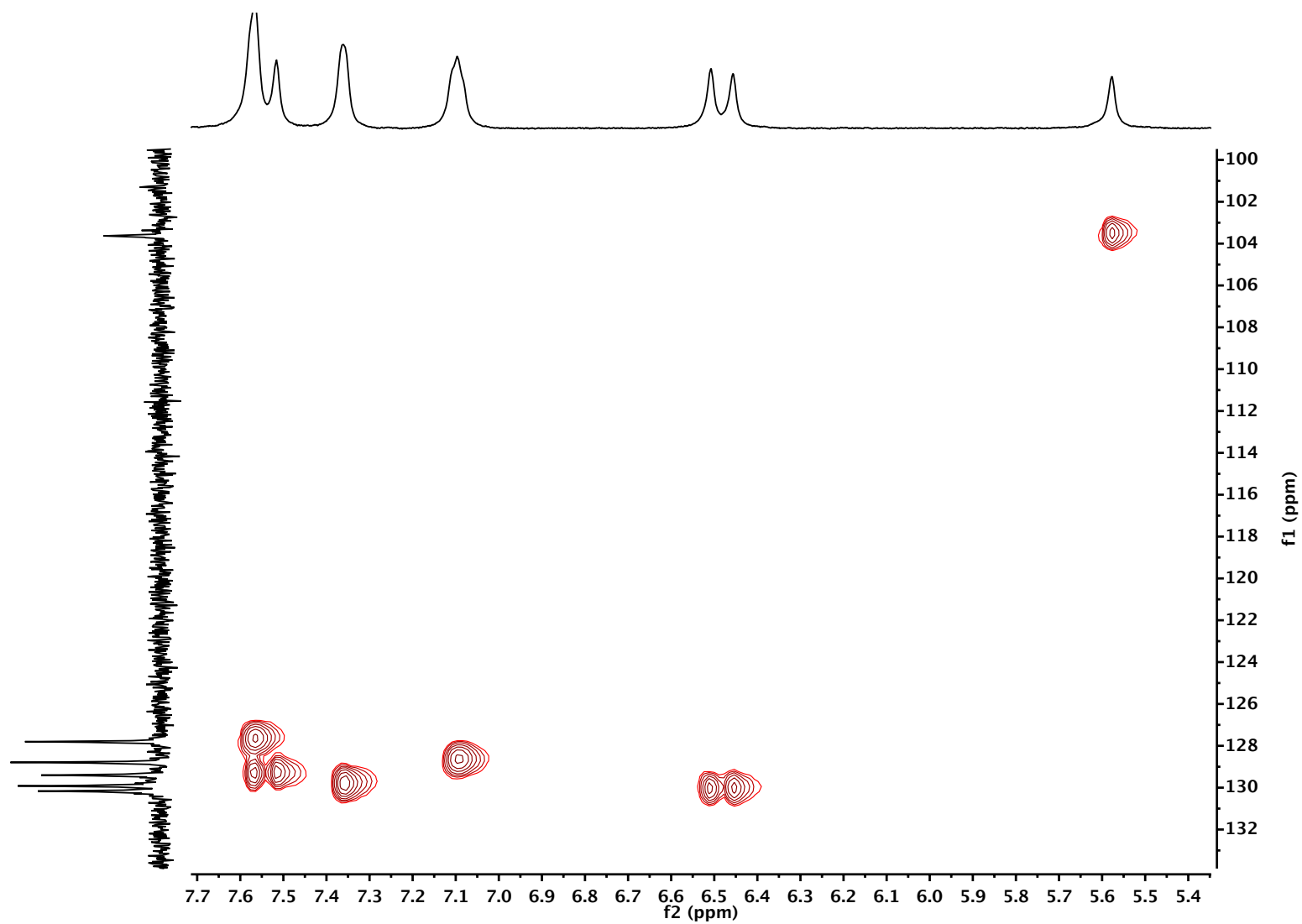


Figure S35. 500 MHz HSQC NMR spectrum of ThiopheneCurc-Mg.

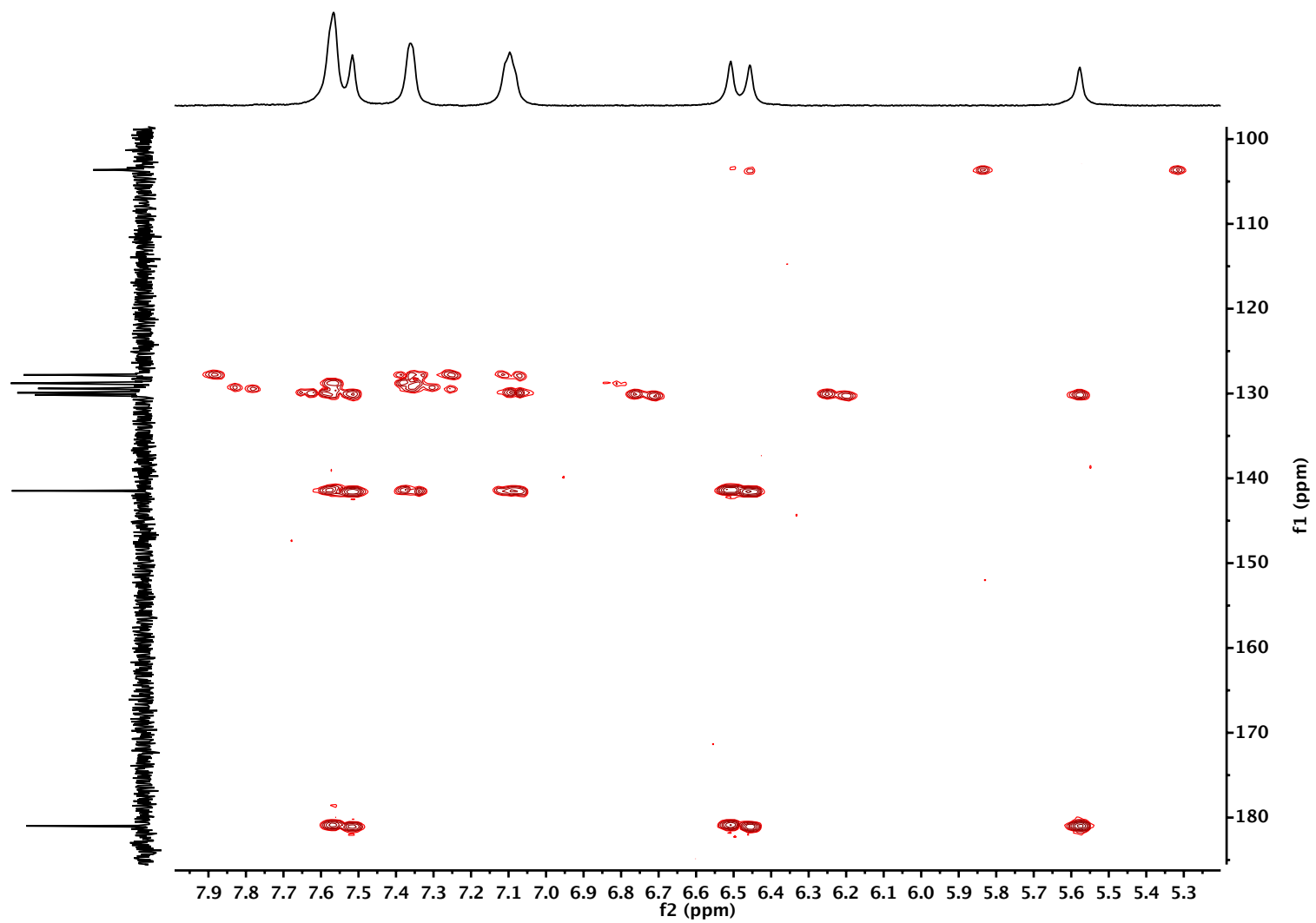


Figure S36. 500 MHz HMBC NMR spectrum of ThiopheneCurc-Mg.

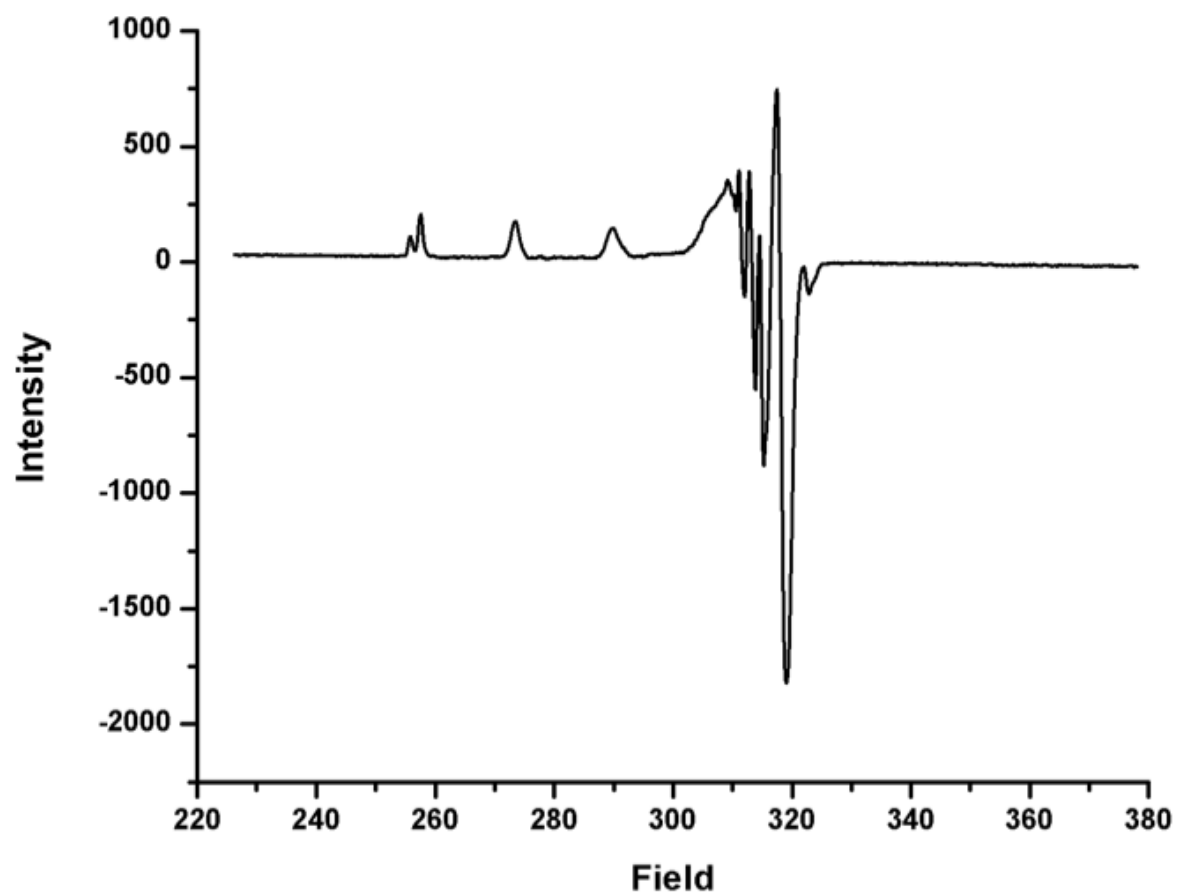


Figure S37. EPR Spectrum of N-methyl-pyrCurc-Cu.

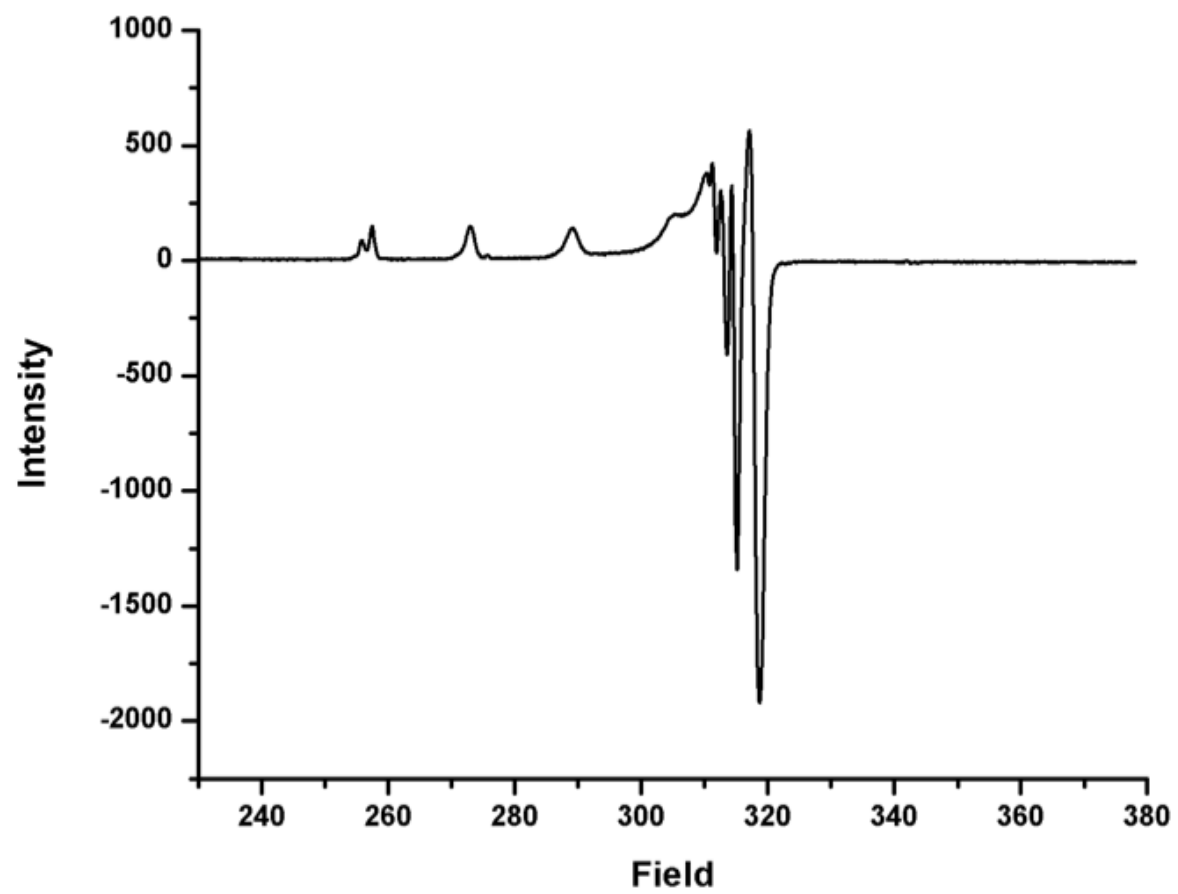


Figure S38. EPR Spectrum of FuranCurc-Cu.

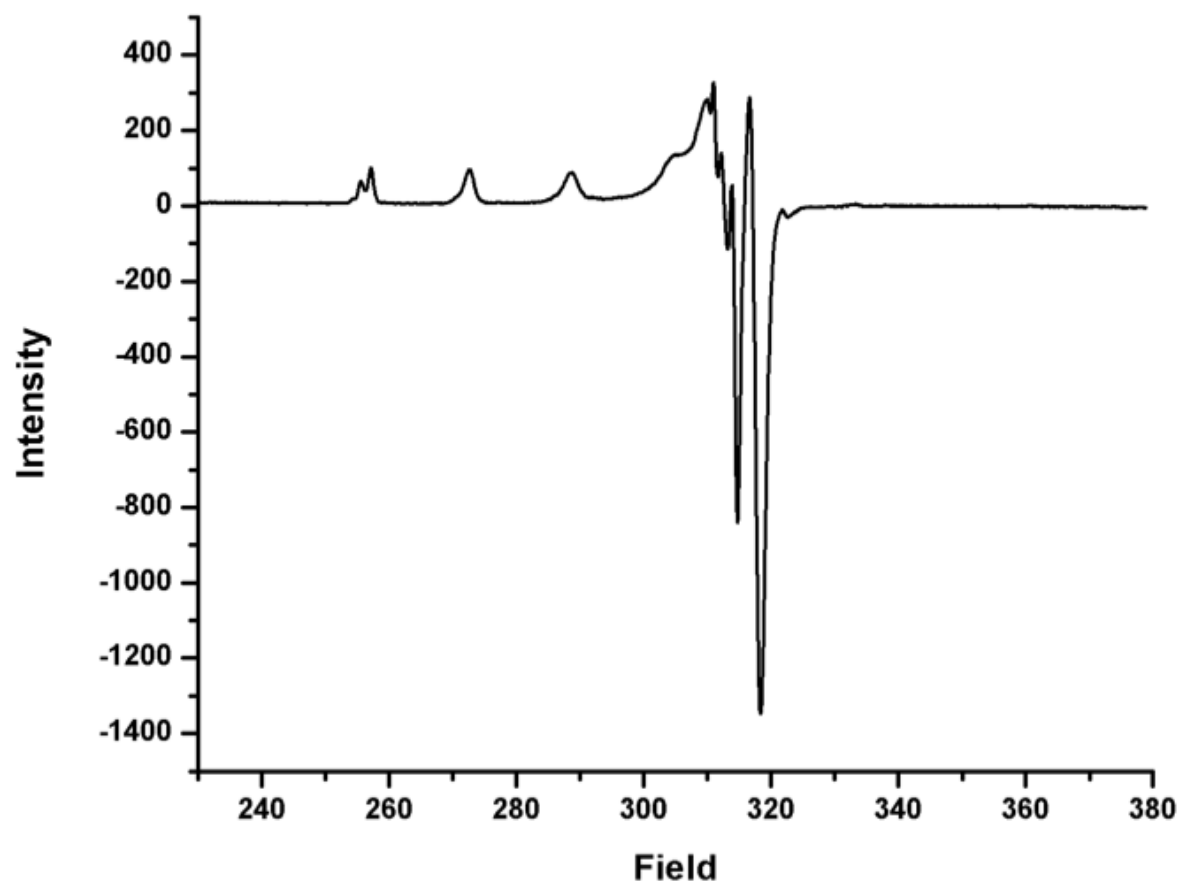
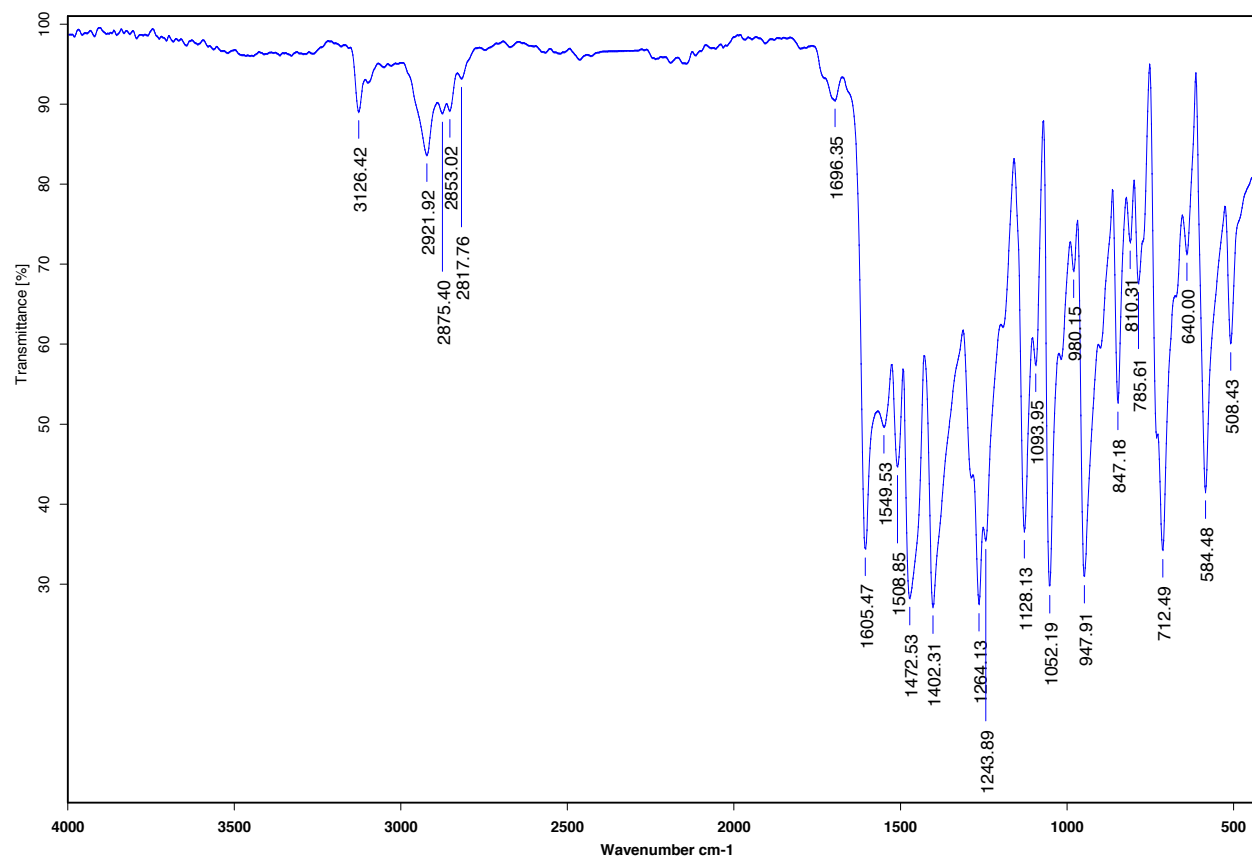


Figure S39. EPR Spectrum of ThiopheneCurc-Cu.



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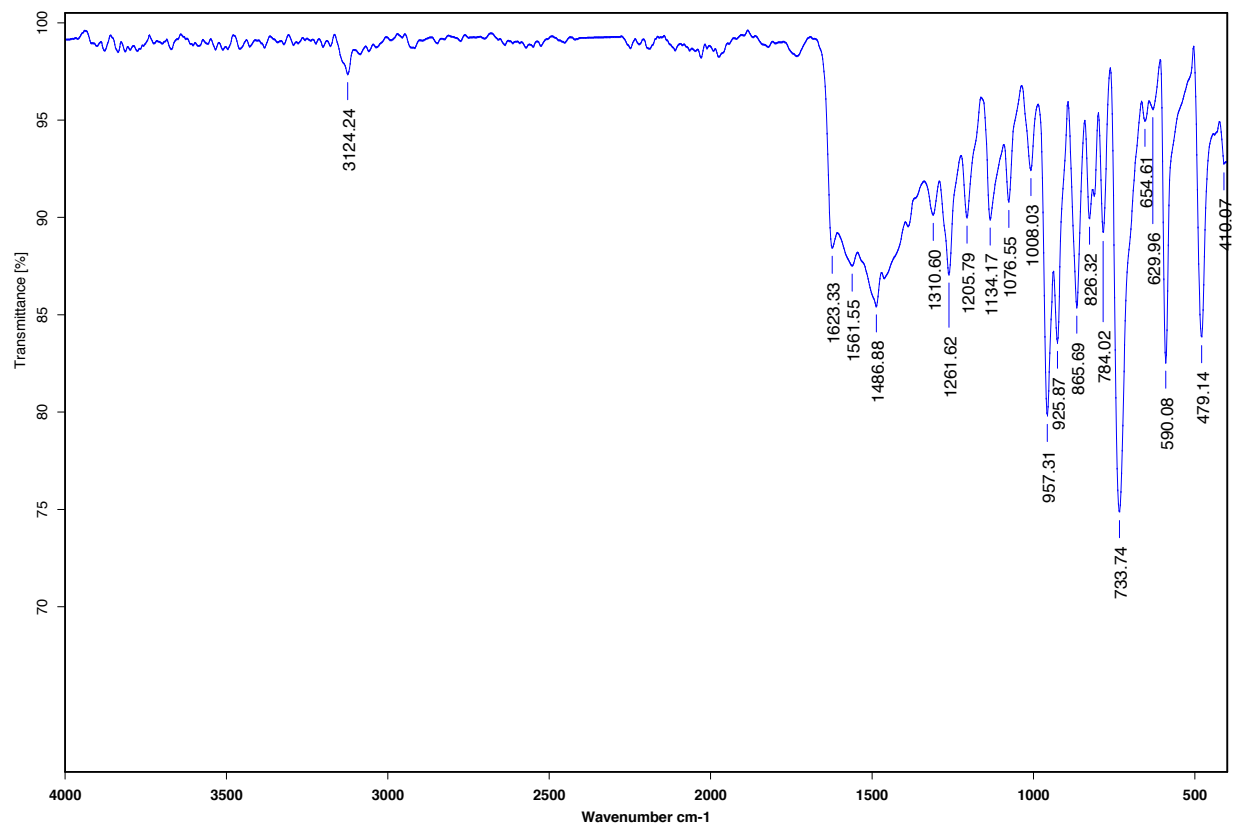
Dr.R.Enriquez

N-met-Pirrol-Curcu

KBr/Pastilla

25/01/2019

Figure S40. IR Spectrum of N-methyl-pyrCurc.



C:\Infrarrojo\AIR-LEP-IQUI-007_18\Rocio\1483.0

Dr.R.Enriquez FuranC

KBr/Pastilla RPM

28/11/2018

Figure S41. IR Spectrum of FuranCurc.

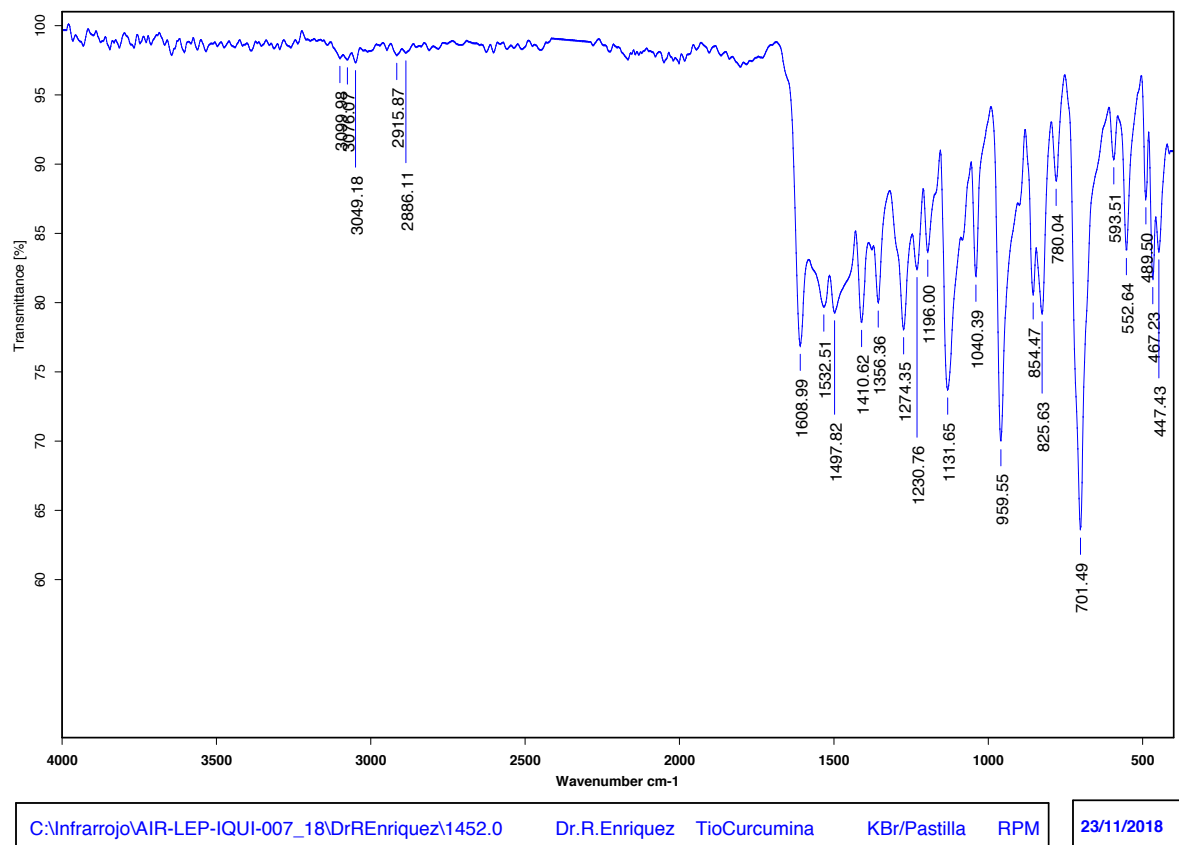
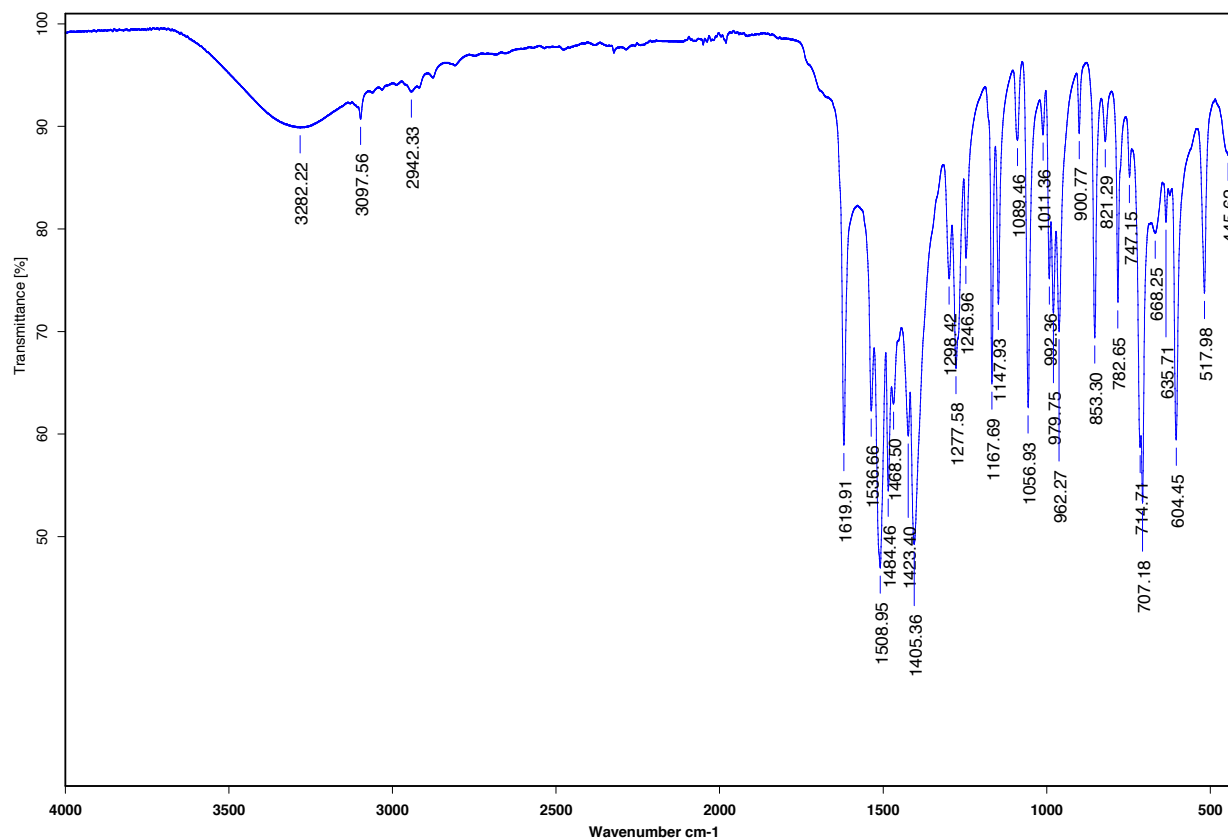


Figure S42. IR Spectrum of ThiopheneCurc.



E:\LEP-IQUI-IR2-2019\DrREnriquez\1575.SPA

Dr.R.Enriquez Nmpcurc-Mg

KBr/Pastilla

RPM

No1575

18/10/2019

Figure S43. IR Spectrum of N-methyl-pyrCurc-Mg.

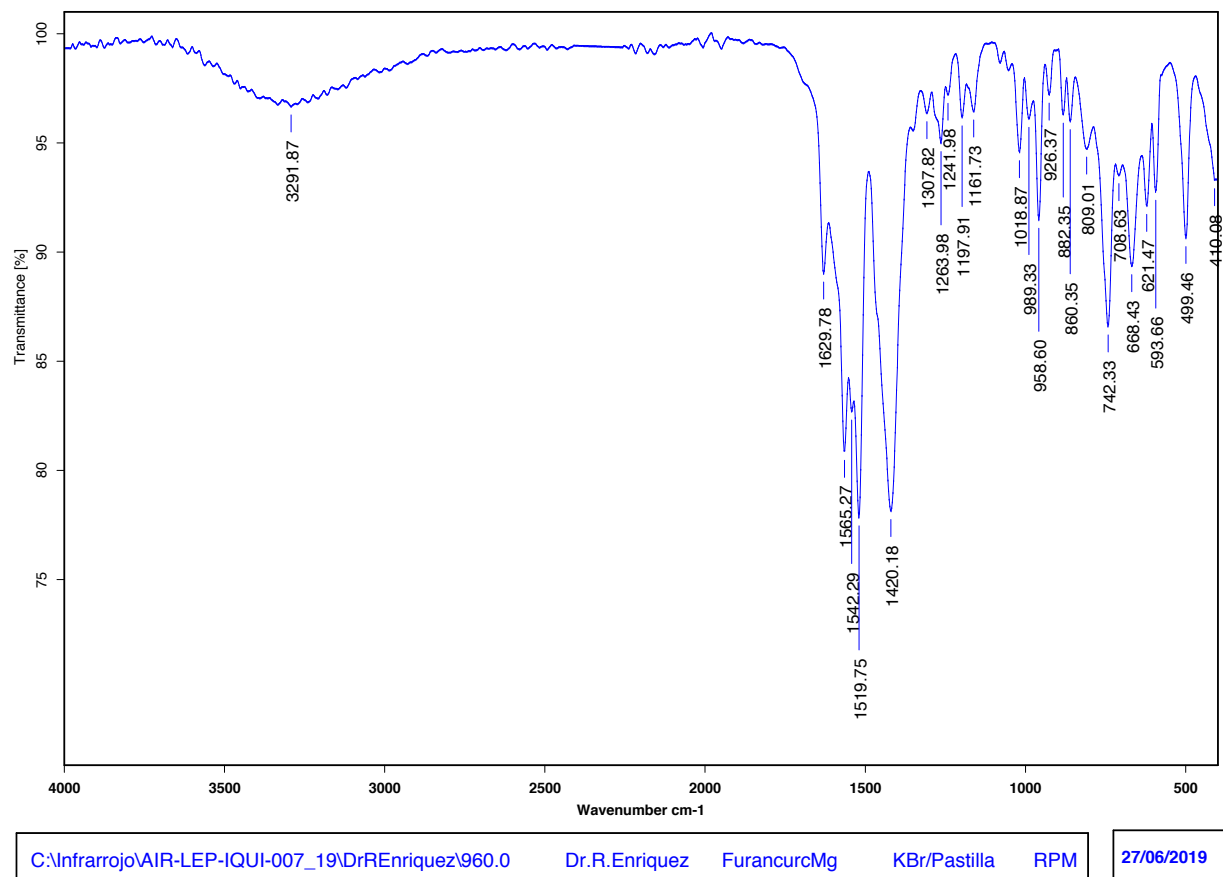


Figure S44. IR Spectrum of FuranCurc-Mg.

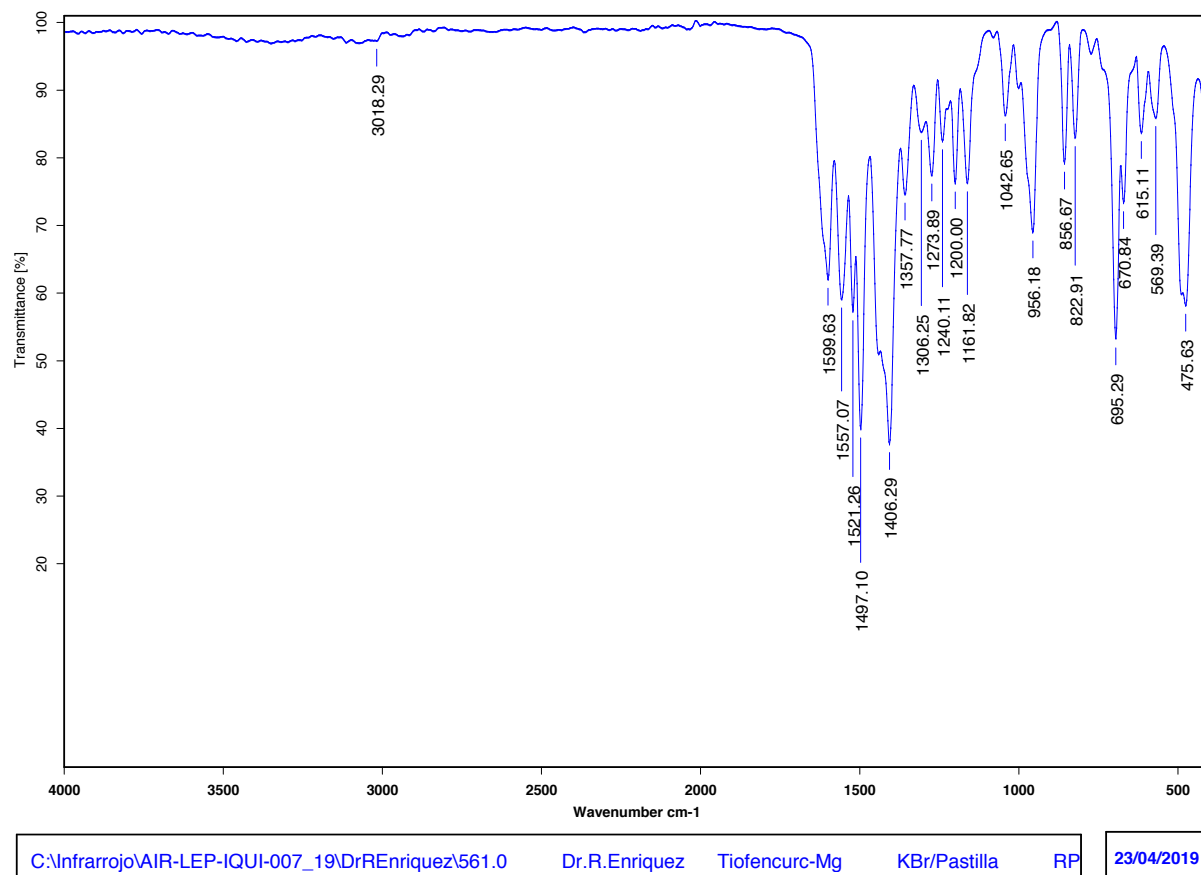
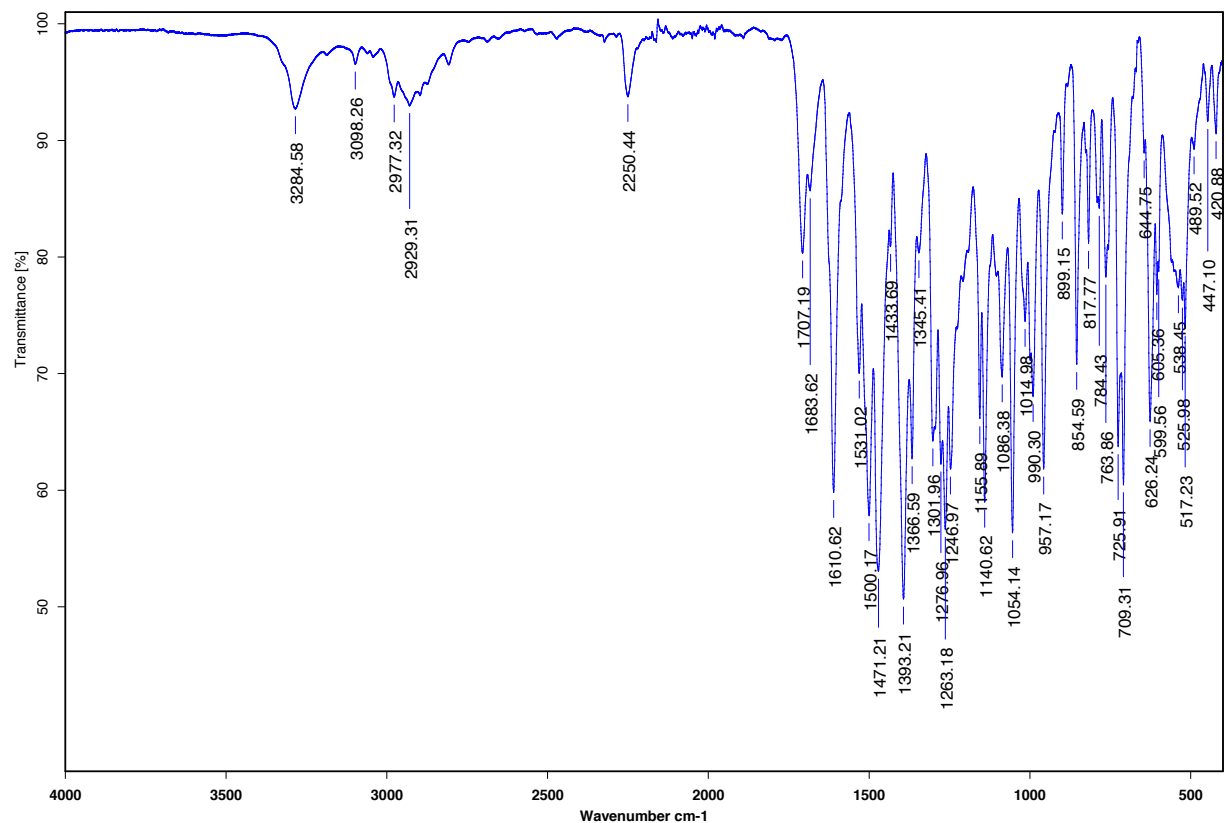


Figure S45. IR Spectrum of ThiopheneCurc -Mg.



C:\Infrarrojo\AIR-LEP-IQUI-007_19\DrREnriquez\120.SPA.0 Dr.R.Enriquez N-metpirolC-Cu KBr/Pastilla No

06/02/2019

Figure S46. IR Spectrum of N-methyl-pyrCurc-Cu.

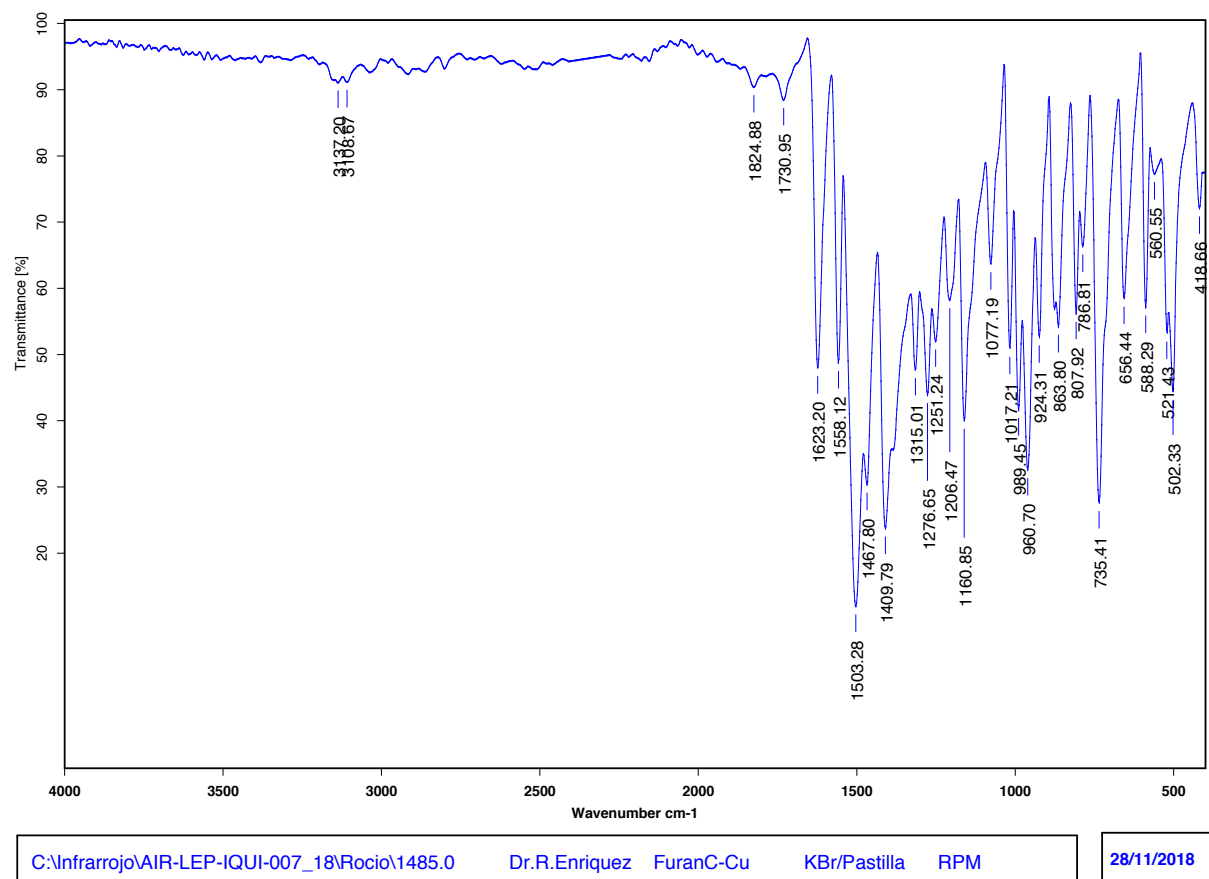
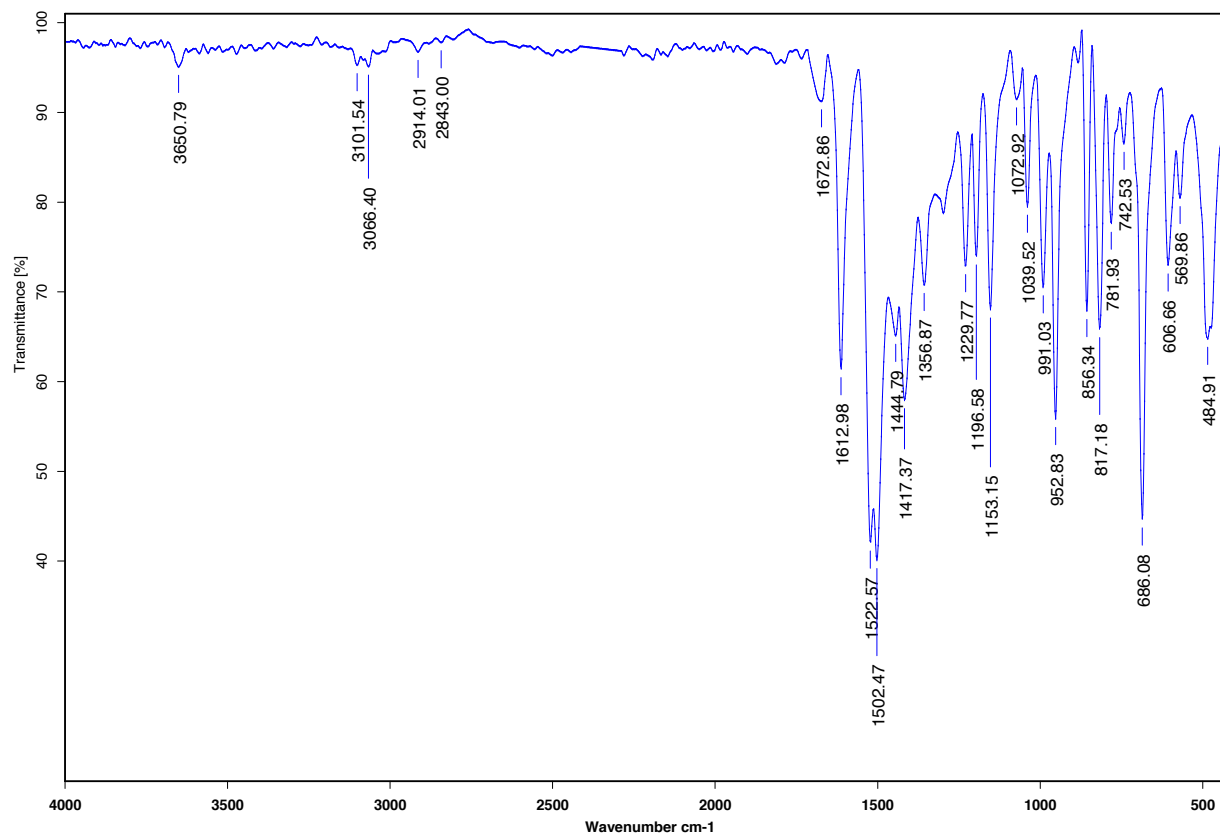


Figure S47. IR Spectrum of FuranCurc-Cu.



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Dr.R.Enriquez

TioCurcumina-Cu

KBr/Pastilla

RF

23/11/2018

Figure S48. IR Spectrum of ThiopheneCurc-Cu.

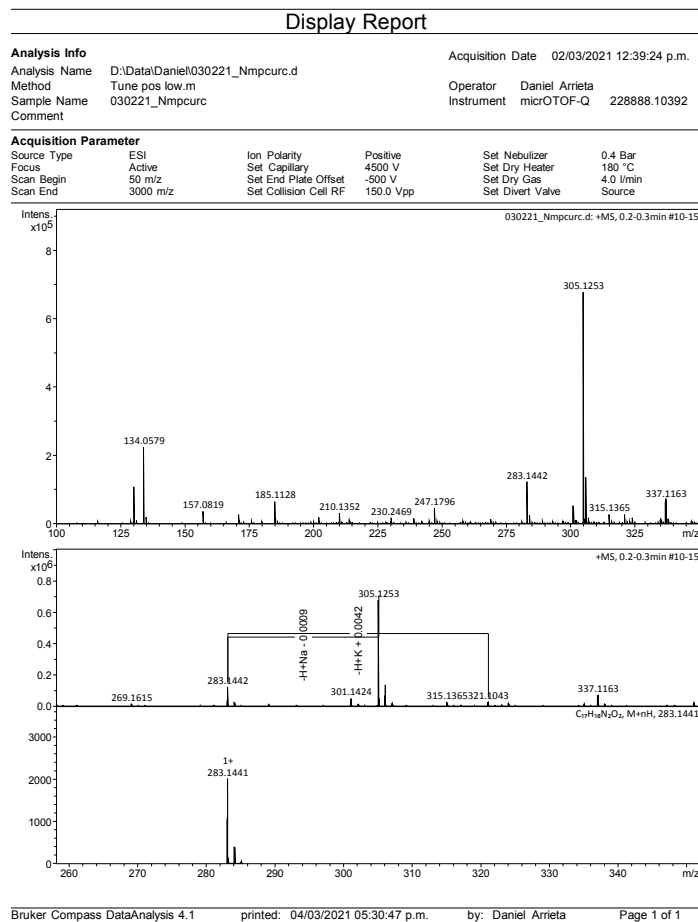
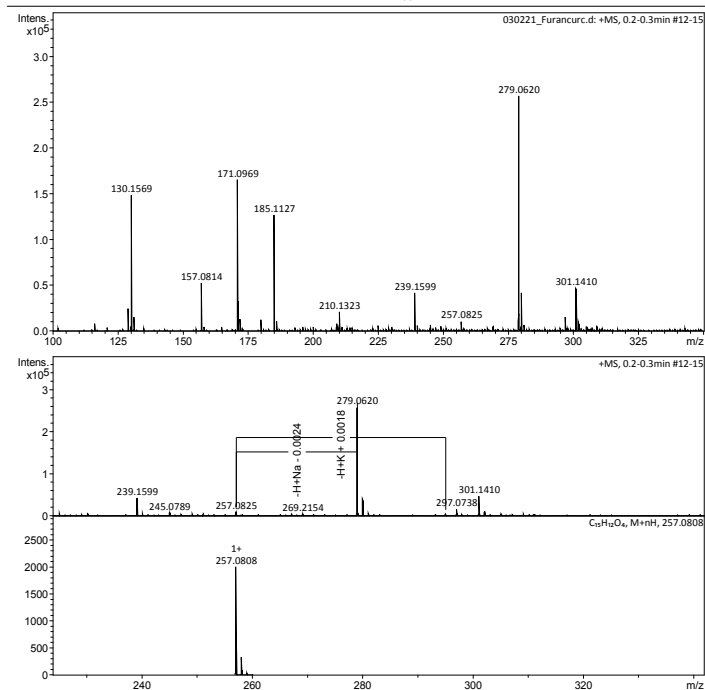


Figura S49. Mass Spectrum of N-methyl-pyrCurc.

Analysis Info		Acquisition Date	
Analysis Name	D:\Data\Daniel\030221_Furancurc.d	02/03/2021 12:56:21 p.m.	
Method	Tune pos low.m	Operator	Daniel Arieta
Sample Name	030221_Furancurc	Instrument	micrOTOF-Q 228888.10392
Comment			

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



50

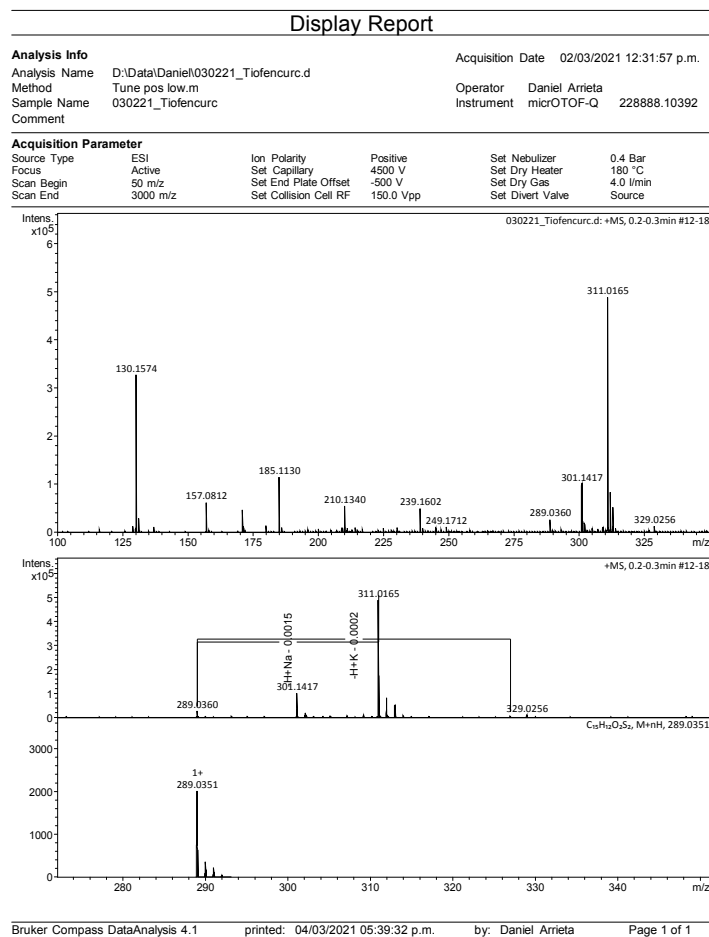


Figura S51. Mass Spectrum of ThiopheneCurc.



Date of Acquisition 2021-01-26T12:47:54.624-06:00
Acquisition method D:\Methods\flexControlMethods\LP_700-5000_Da_ULTRA.par
Processing method
File Name D:\Data\2021\Julia\012621_Nmpcurc-Mg_SDHB_LP7005000\0_G12\1

BRUKER
DALTONICS

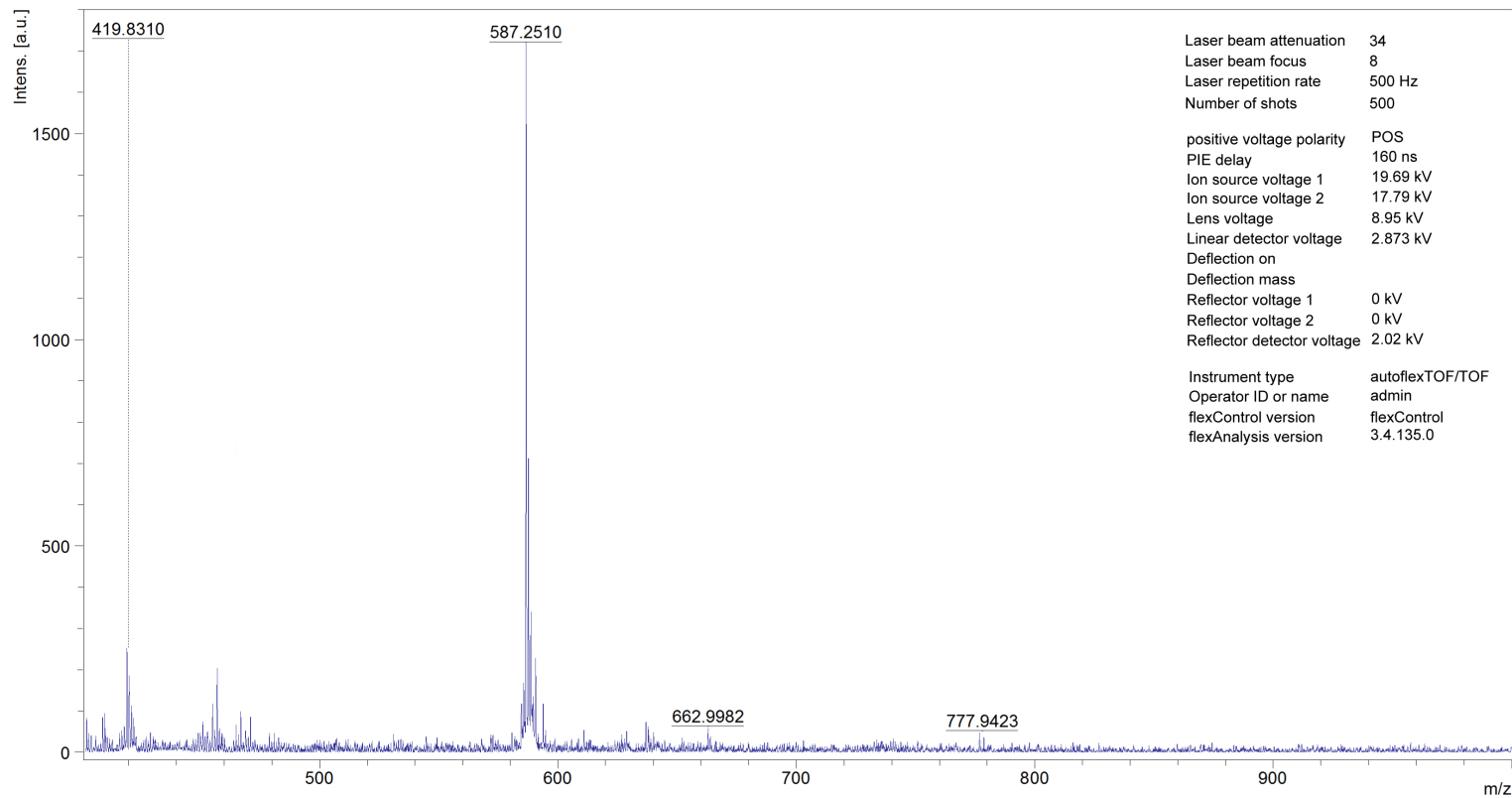


Figura S52. Mass Spectrum of N-methyl-pyrCurc-Mg.



Date of Acquisition 2021-01-26T13:00:25.257-06:00
Acquisition method D:\Methods\flexControlMethods\LP_700-5000_Da_ULTRA.par
Processing method
File Name D:\Data\2021\Julia\012621_Furancurc-Cu_SDHB_LP7005000_01\0_G20\1

BRUKER
DALTONICS

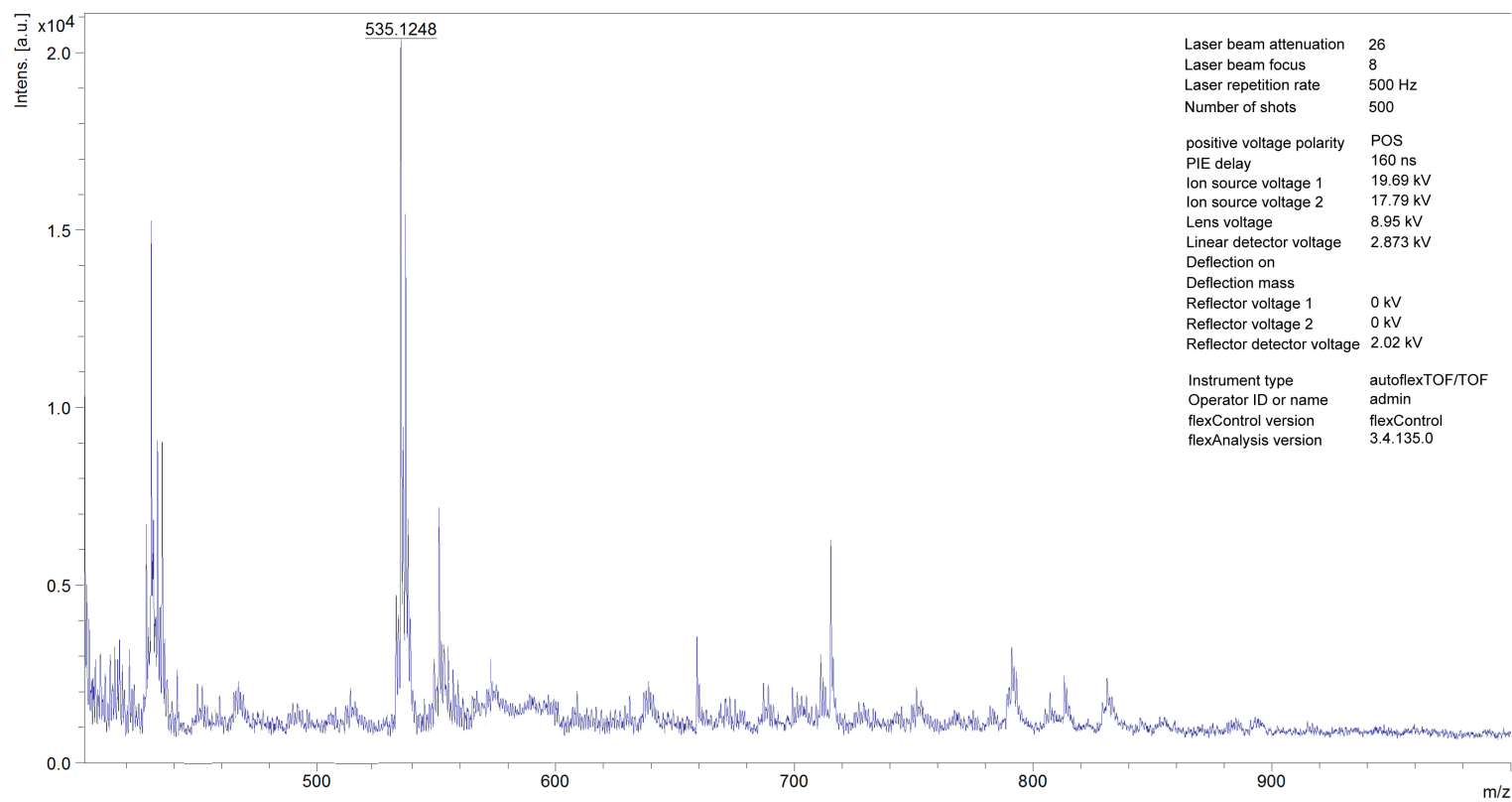


Figura S53. Mass Spectrum of mass exact of FuranCurc-Mg.



Date of Acquisition 2021-01-26T12:51:45.705-06:00
Acquisition method D:\Methods\flexControlMethods\LP_700-5000_Da_ULTRA.par
Processing method
File Name D:\Data\2021\Julia\012621_Tiofencurcc-Mg_SDHB_LP7005000\0_G14\1

BRUKER
DALTONICS

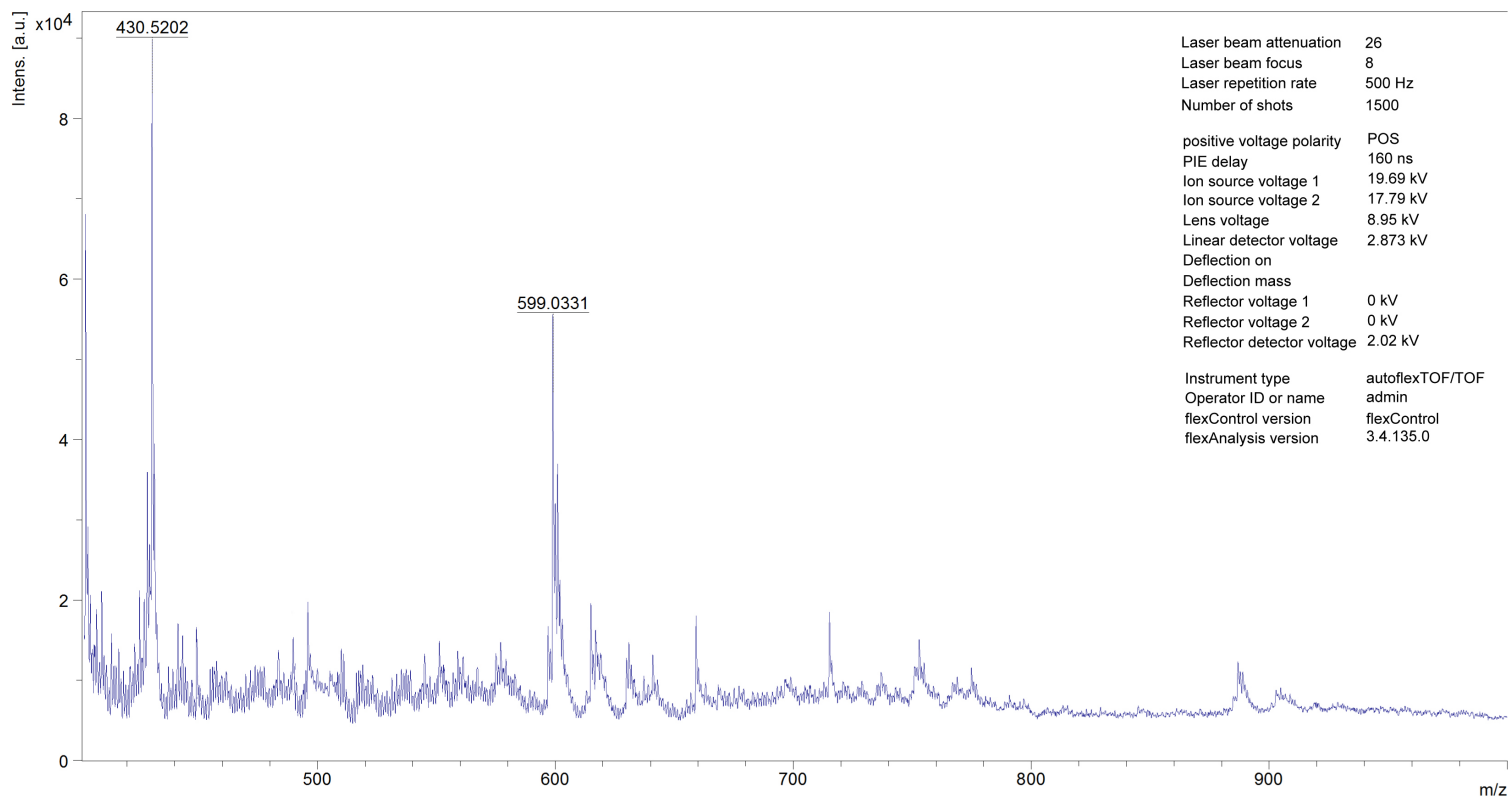
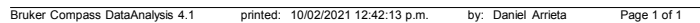


Figura S54. Mass Spectrum of mass exact of ThiopheneCurc-Mg.

Display Report

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



55

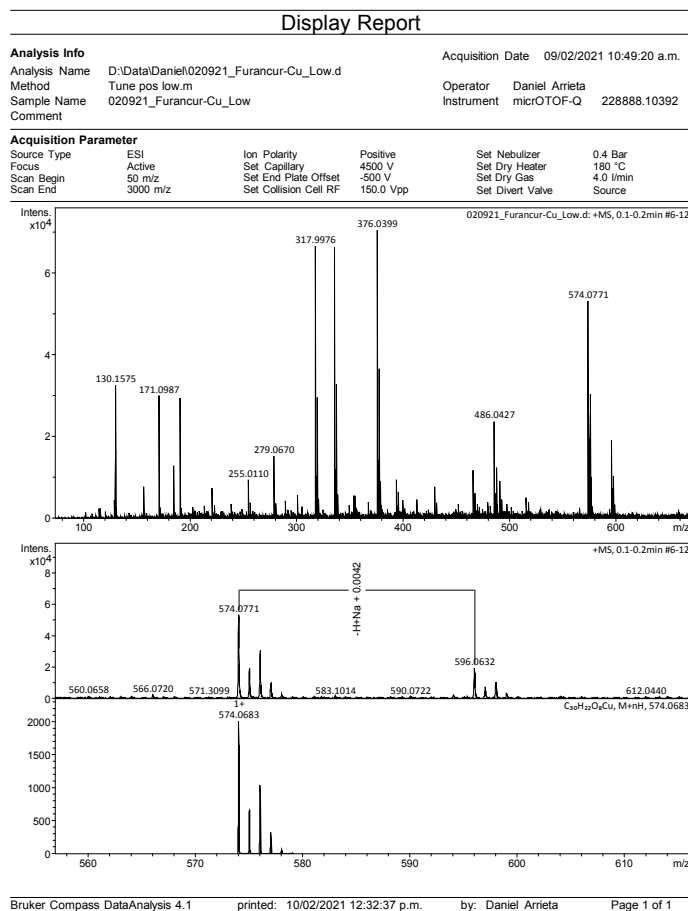


Figure S56. Mass Spectrum of FuranCurc-Cu.

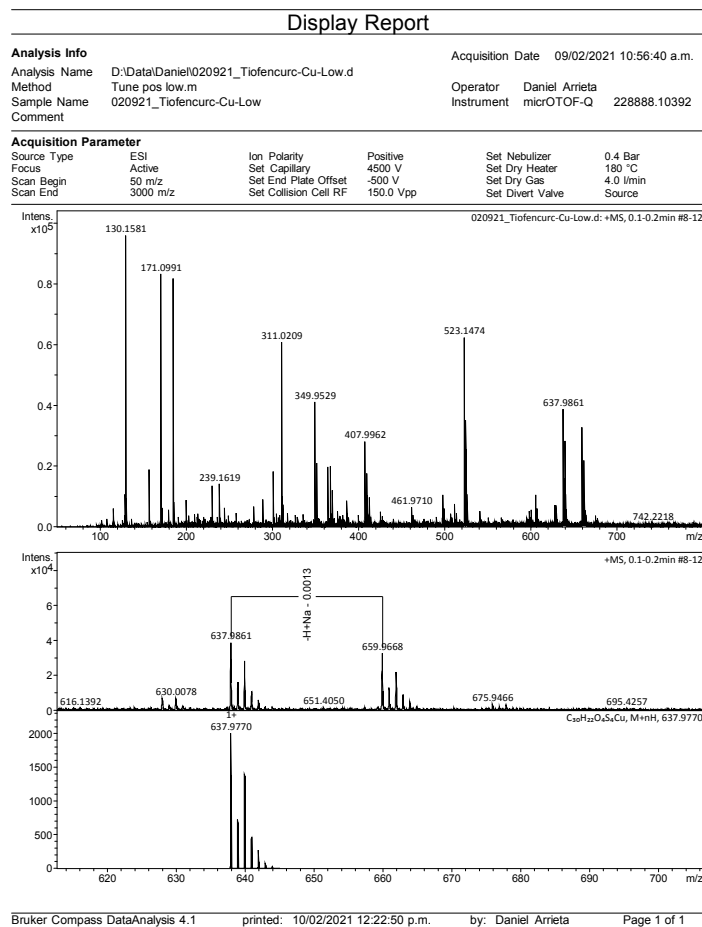


Figura S57. Mass Spectrum of ThiopheneCurc-Cu.

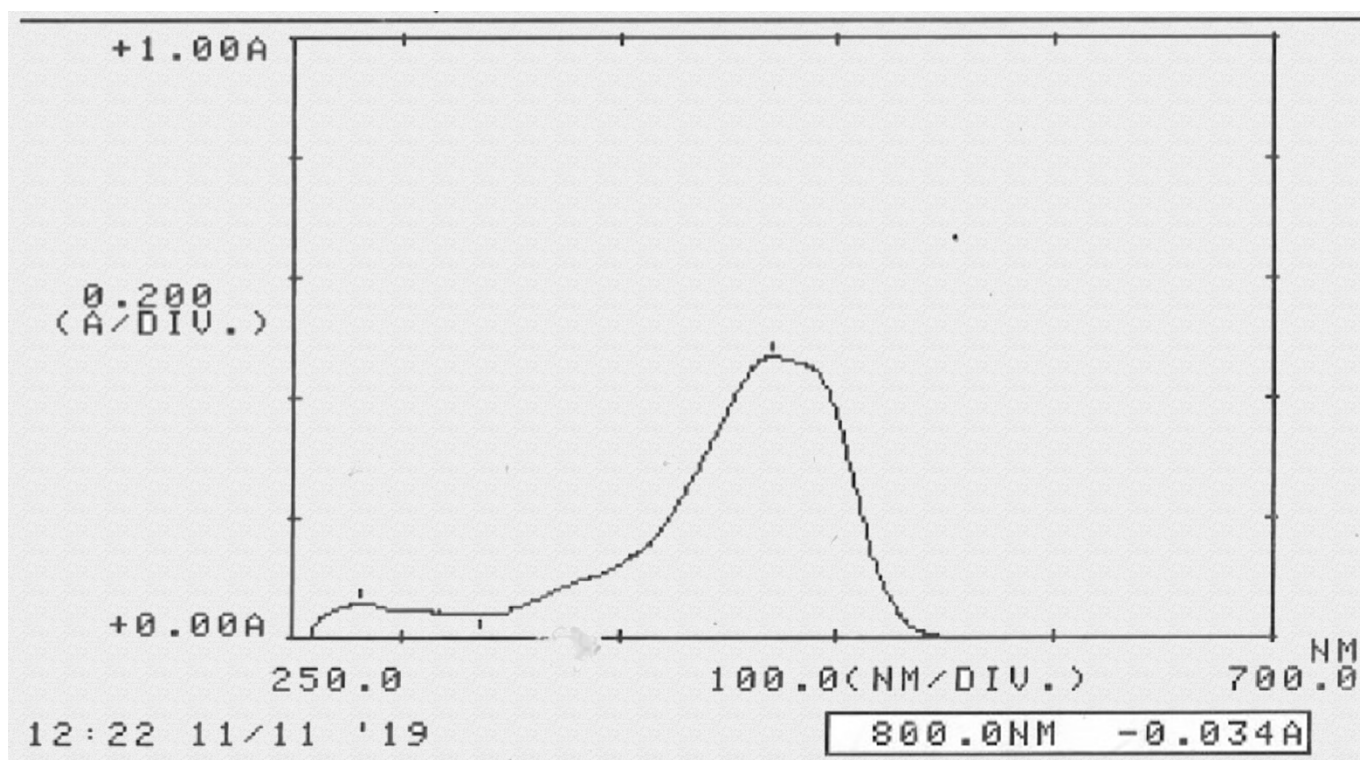


Figure S58. UV-Vis spectra of N-methyl-pyrCurc.

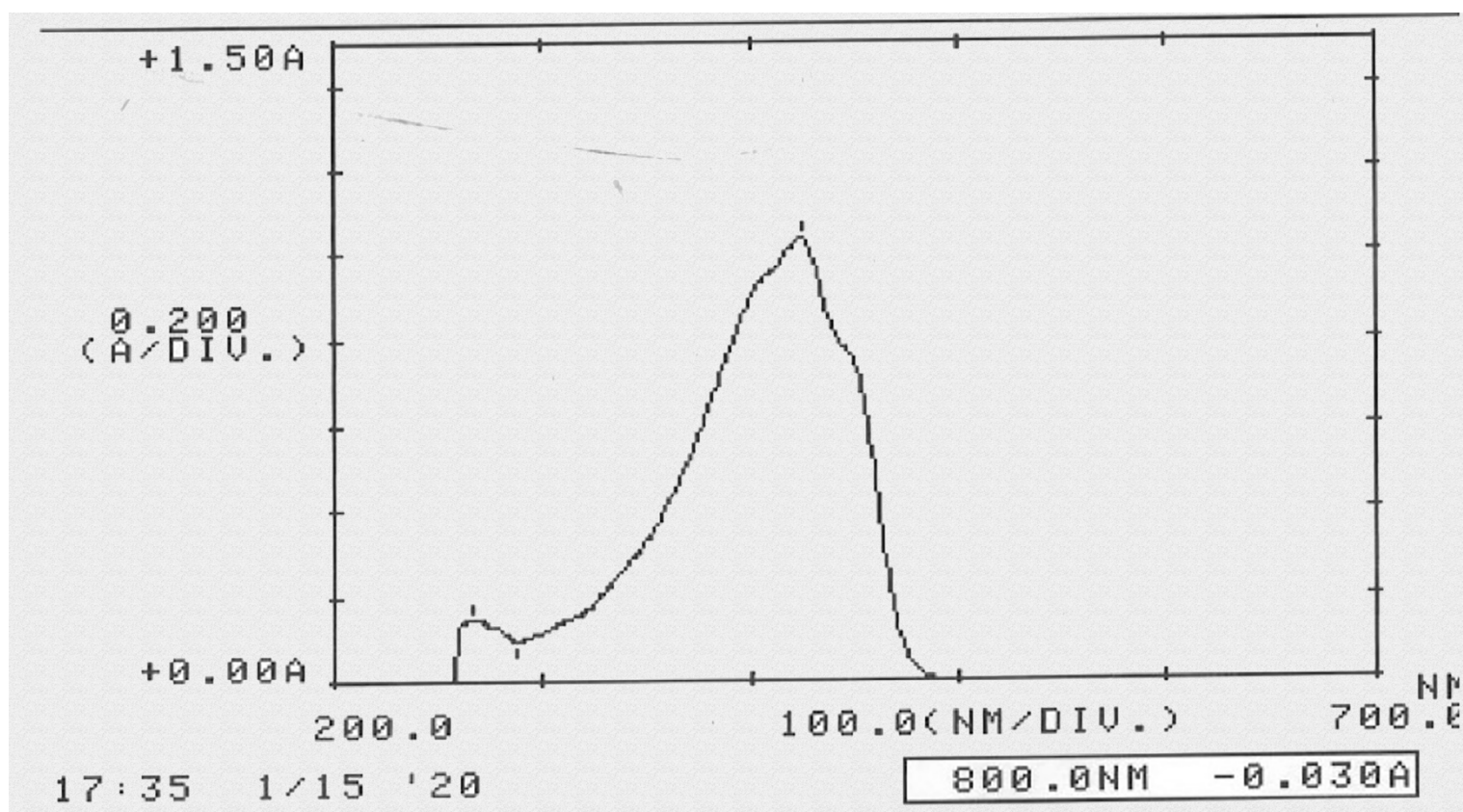


Figure S59. UV-Vis spectra of FuranCurc.

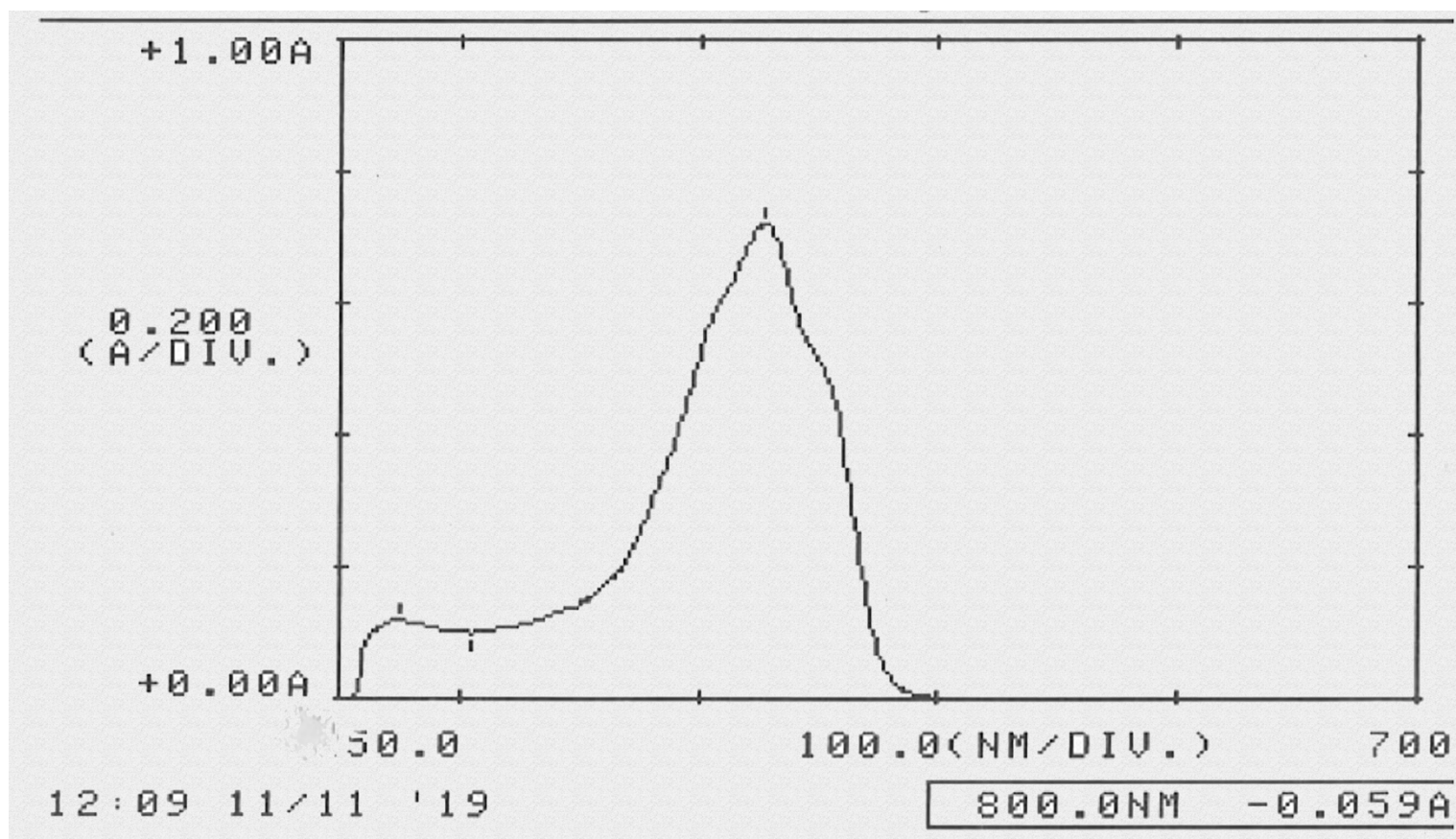


Figure S60. UV-Vis spectra of ThiopheneCurc.

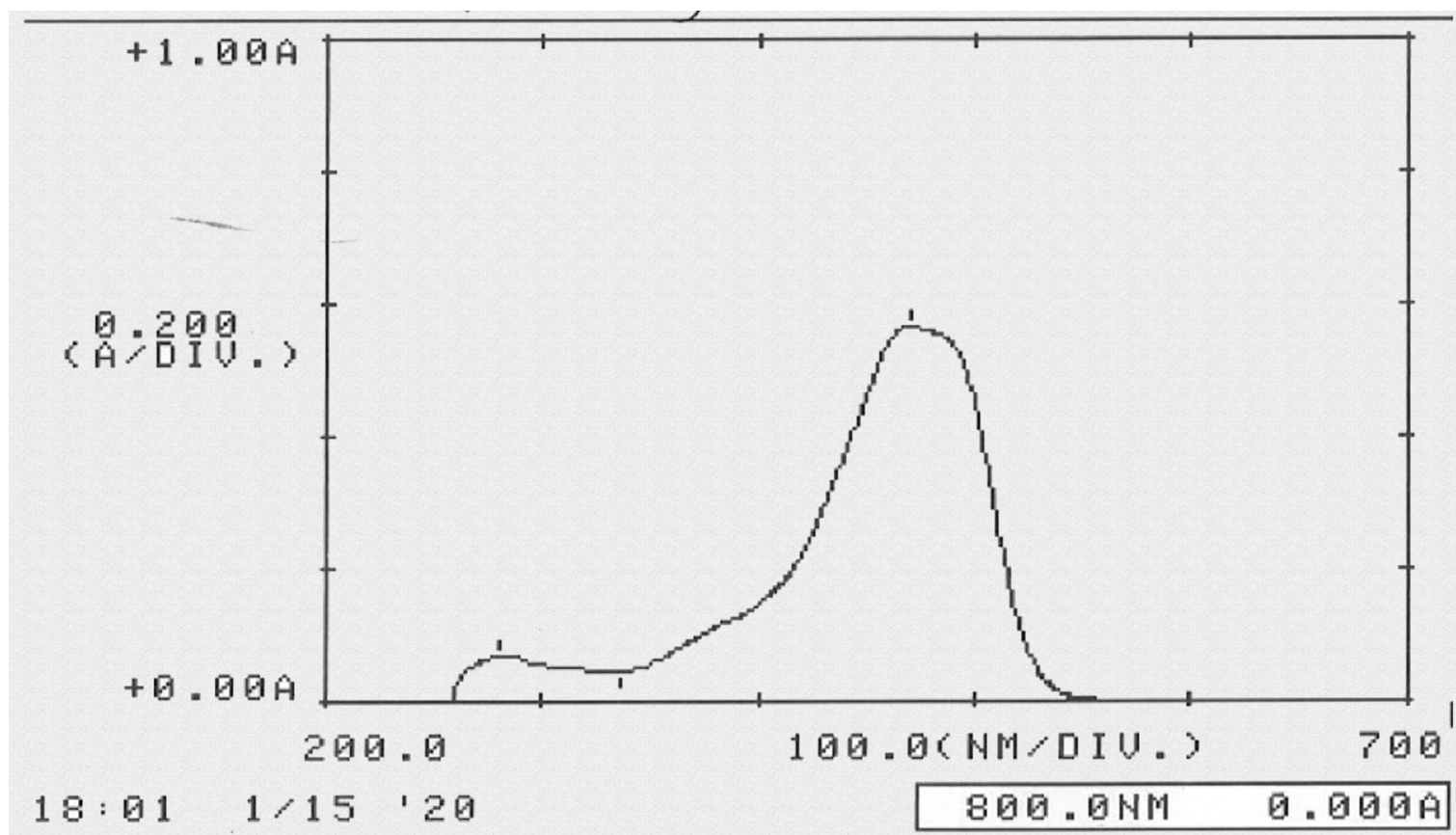


Figure S61. UV-Vis spectra of N-methyl-pyrCurc-Mg.

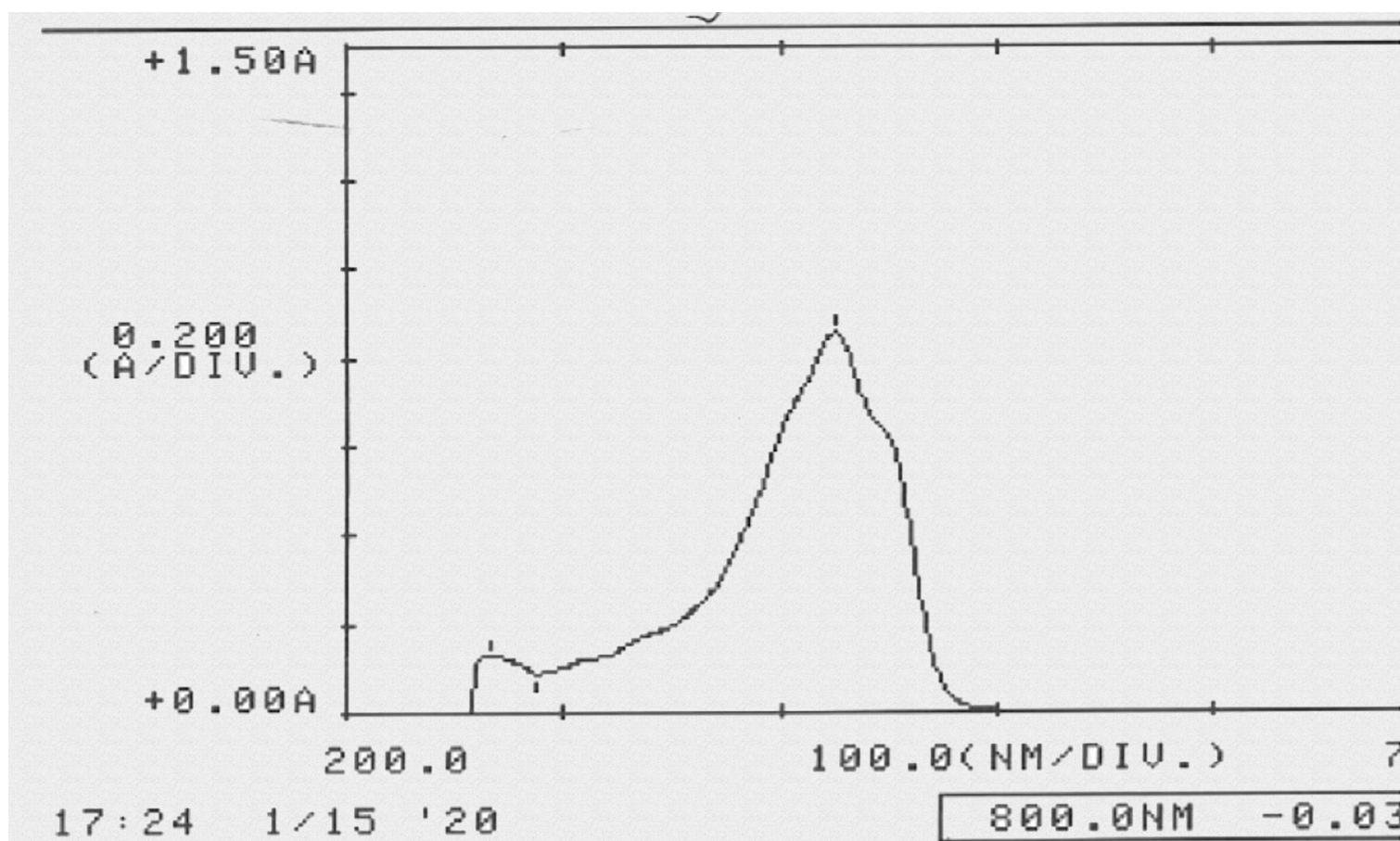


Figure S62. UV-Vis spectra of FuranCurc-Mg.

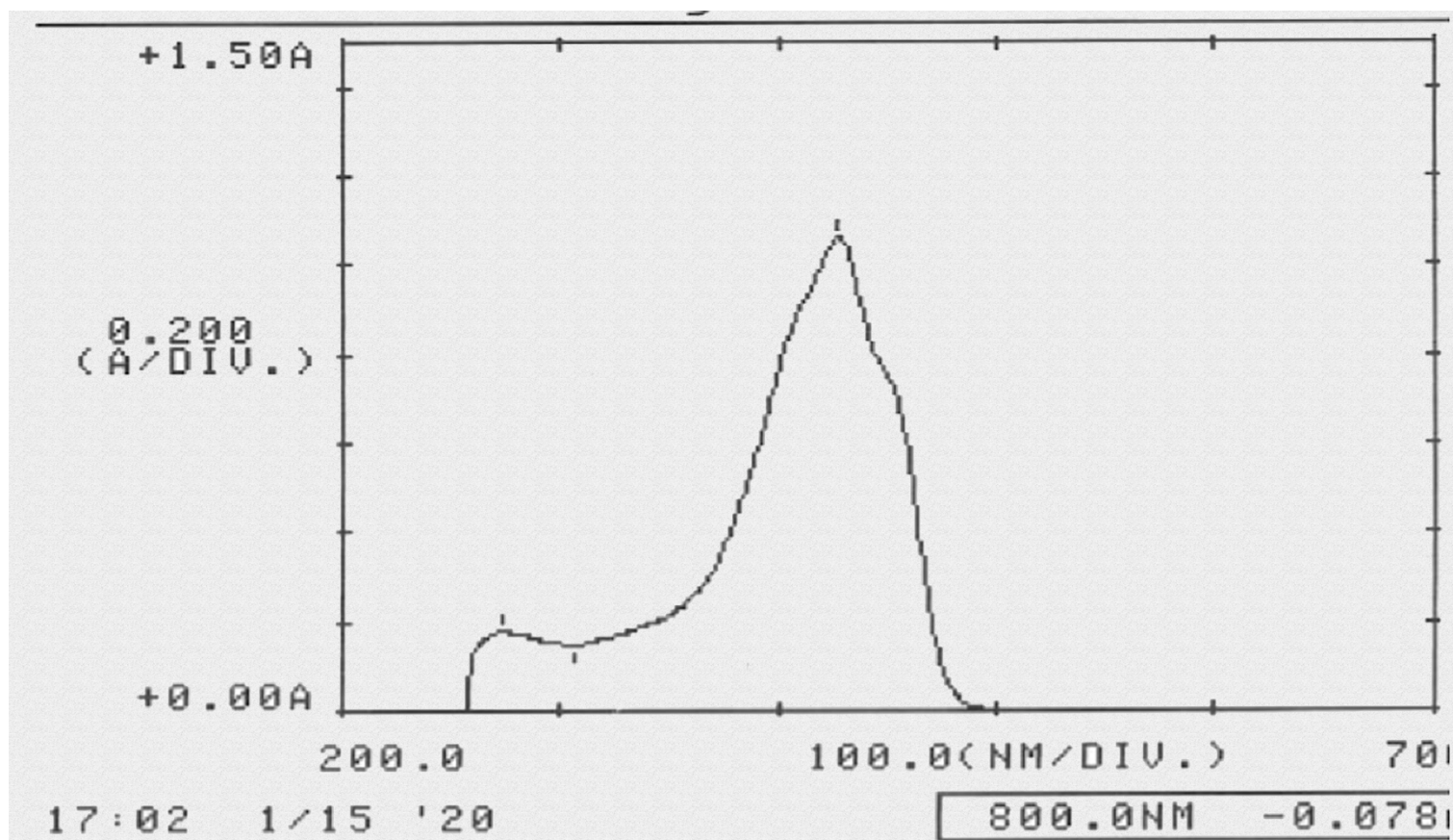


Figure S63. UV-Vis spectra of ThiopheneCurc-Mg.

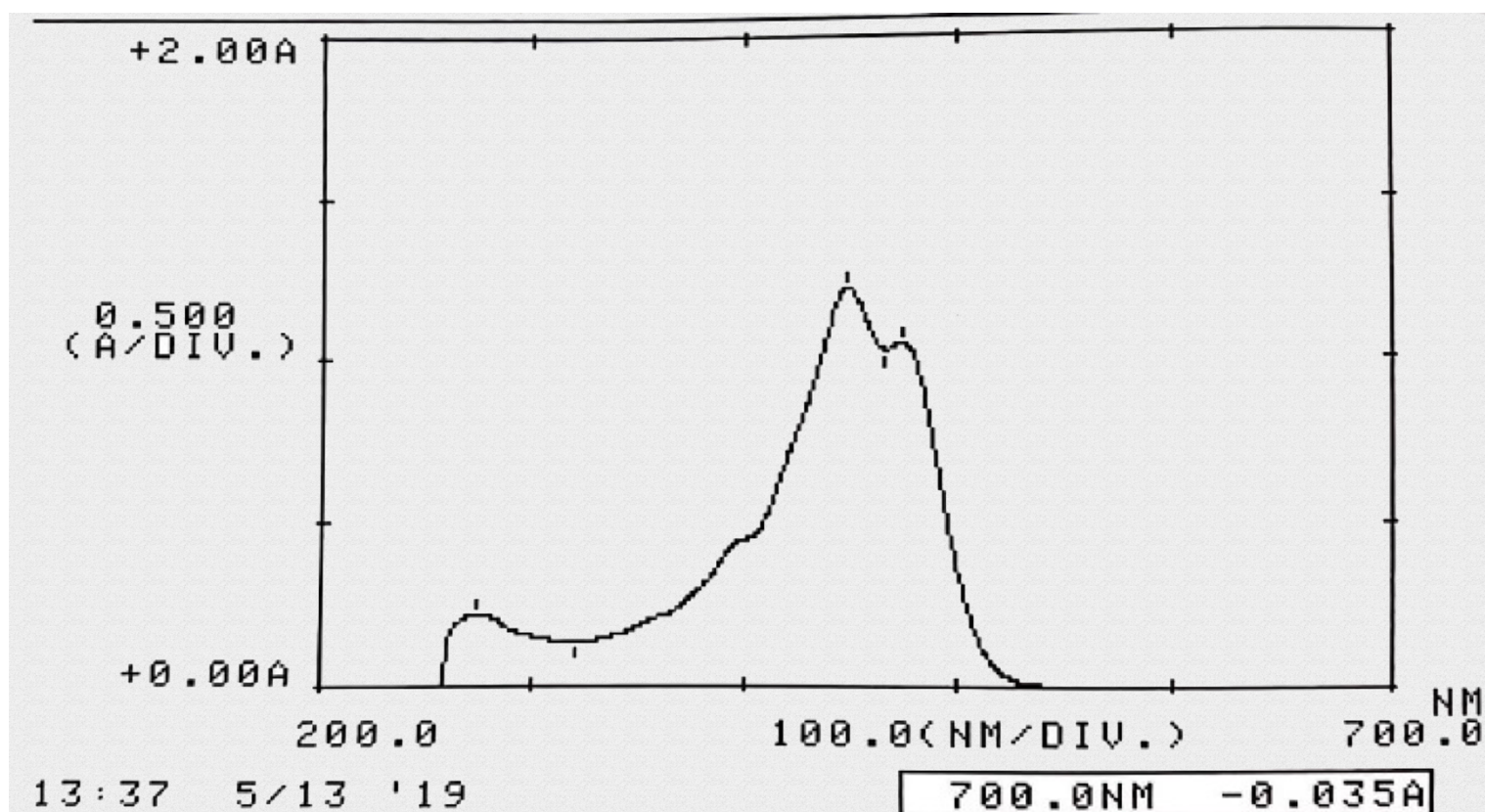


Figure S64. UV-Vis spectra of N-methyl-pyrCurc-Cu.

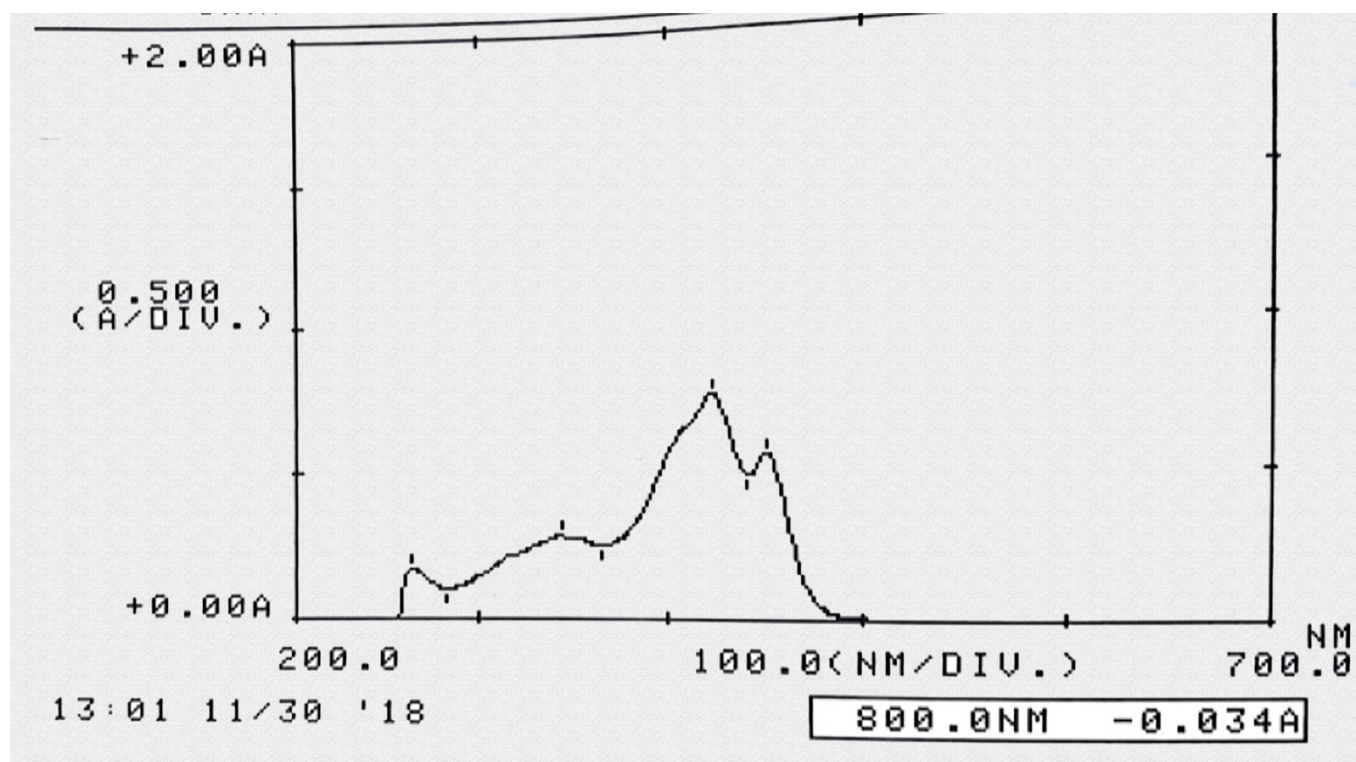


Figure S65. UV-Vis spectra of FuranCurc-Cu.

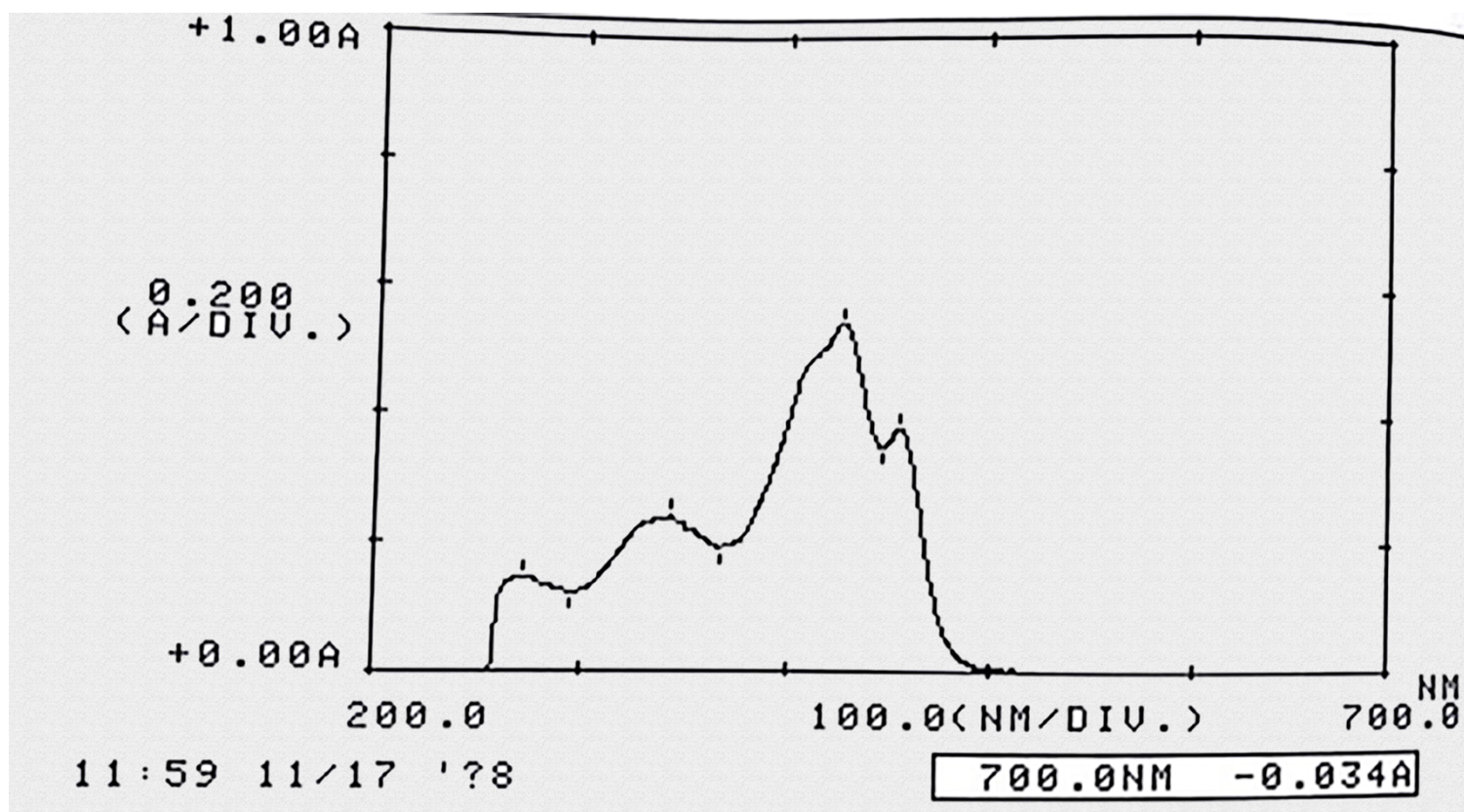


Figure S66. UV-Vis spectra of ThiopheneCurc-Cu.