Electronic Supplementary Material (ESI) for Dalton Transactions.
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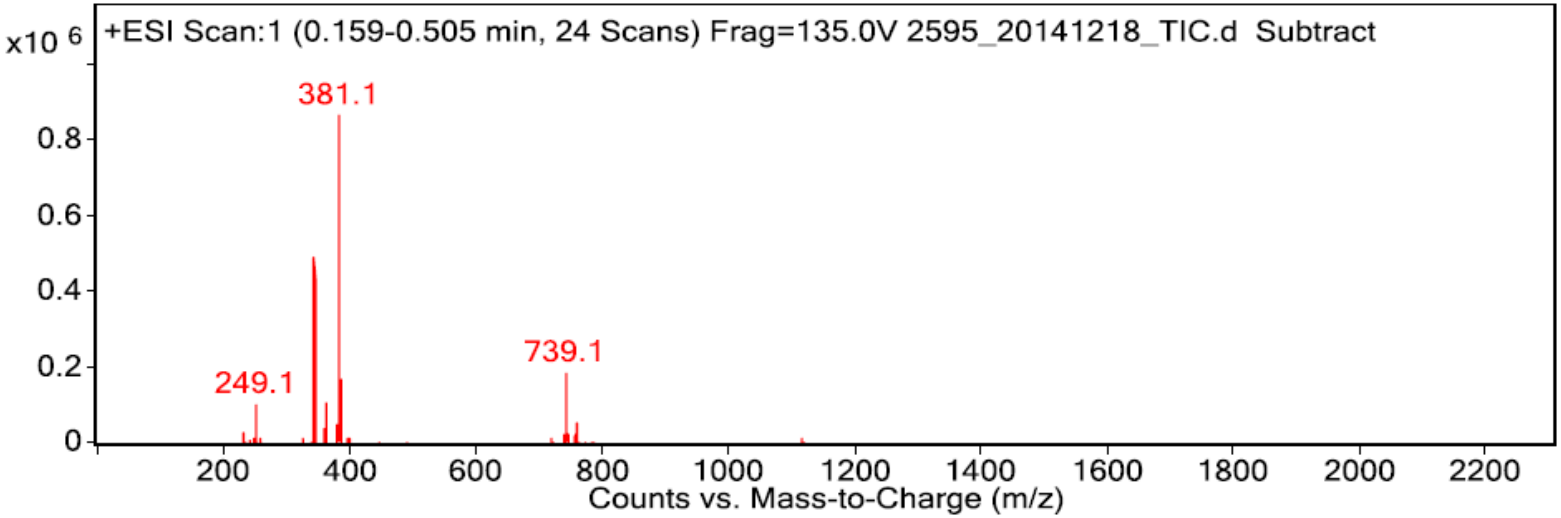
Compound 5



Peak List

m/z	z	Abund
249.1		104946.4
341.1	1	494078.5
342.1	1	108131.1
359.1		109946.5
379		68316.6
381.1	1	870123.6
382.1	1	173339.7
739.1	1	188025.3
740.1	1	91163.2
755		58995.4

Figure S1. ESI-MS spectrum of compound **5**

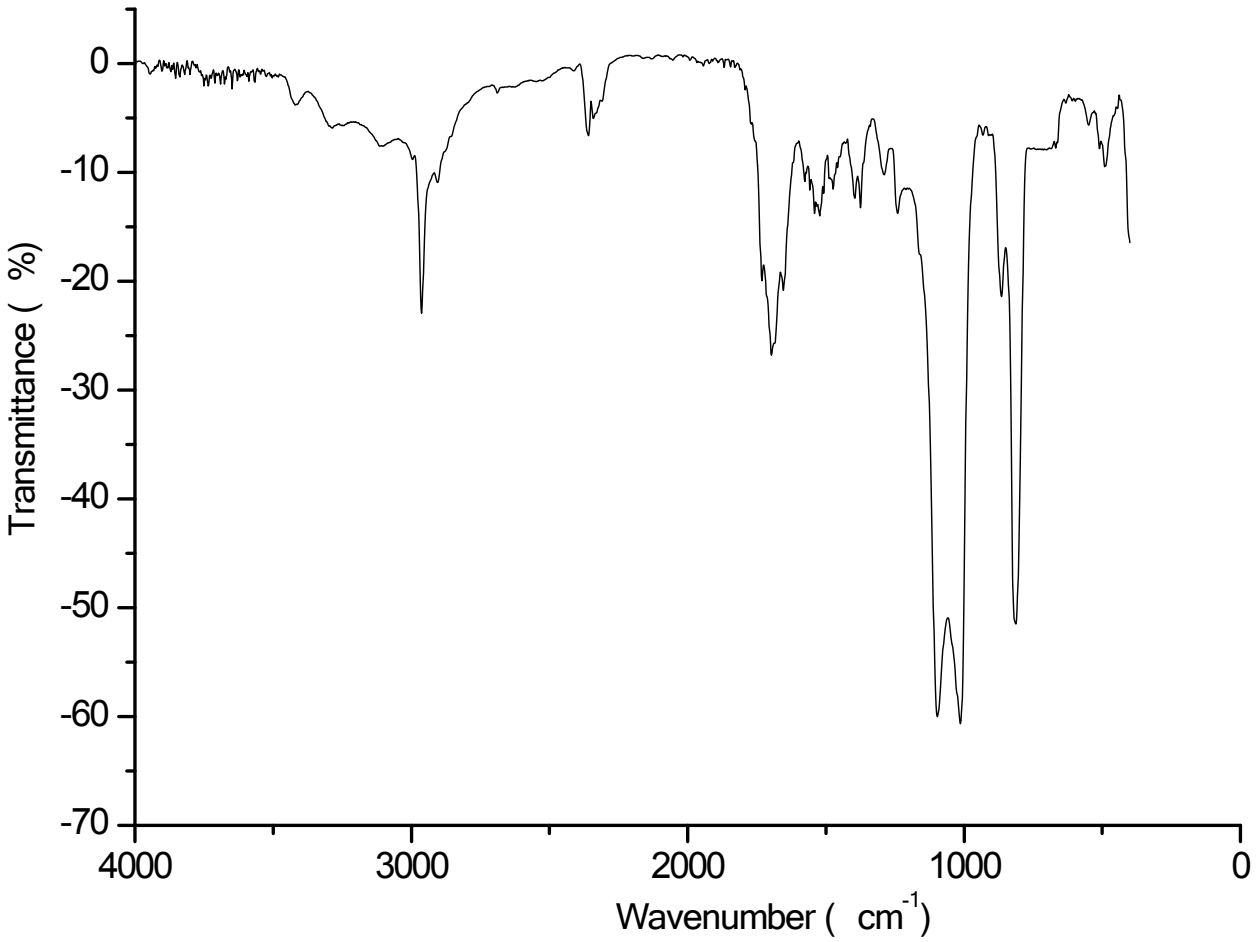


Figure S2. IR spectrum of compound **5** (c = 5 × 10^{-2}M)

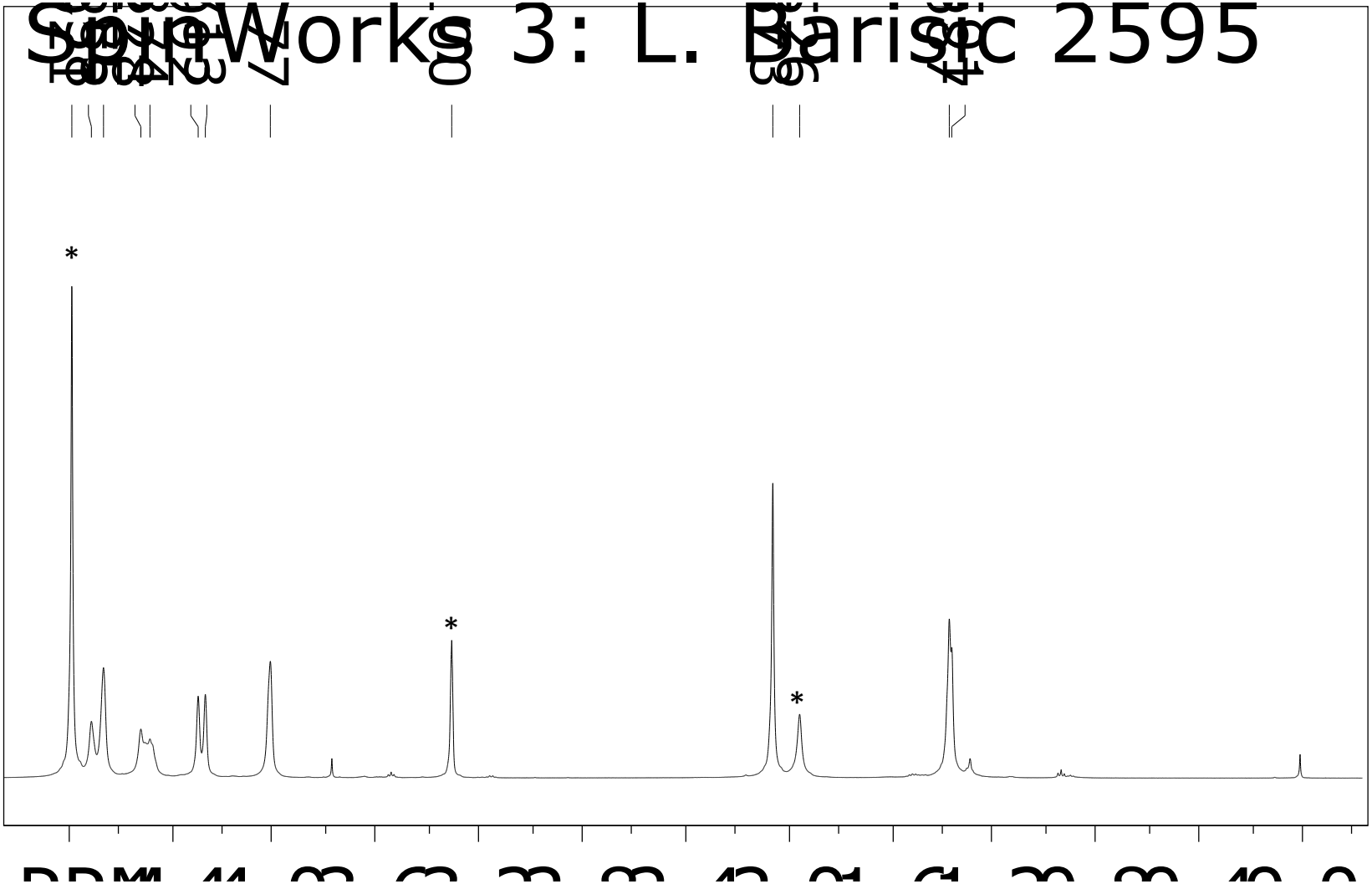


Figure S3. ^{1}H NMR spectrum of compound **5** (c = 2.5 × 10^{-2}M)

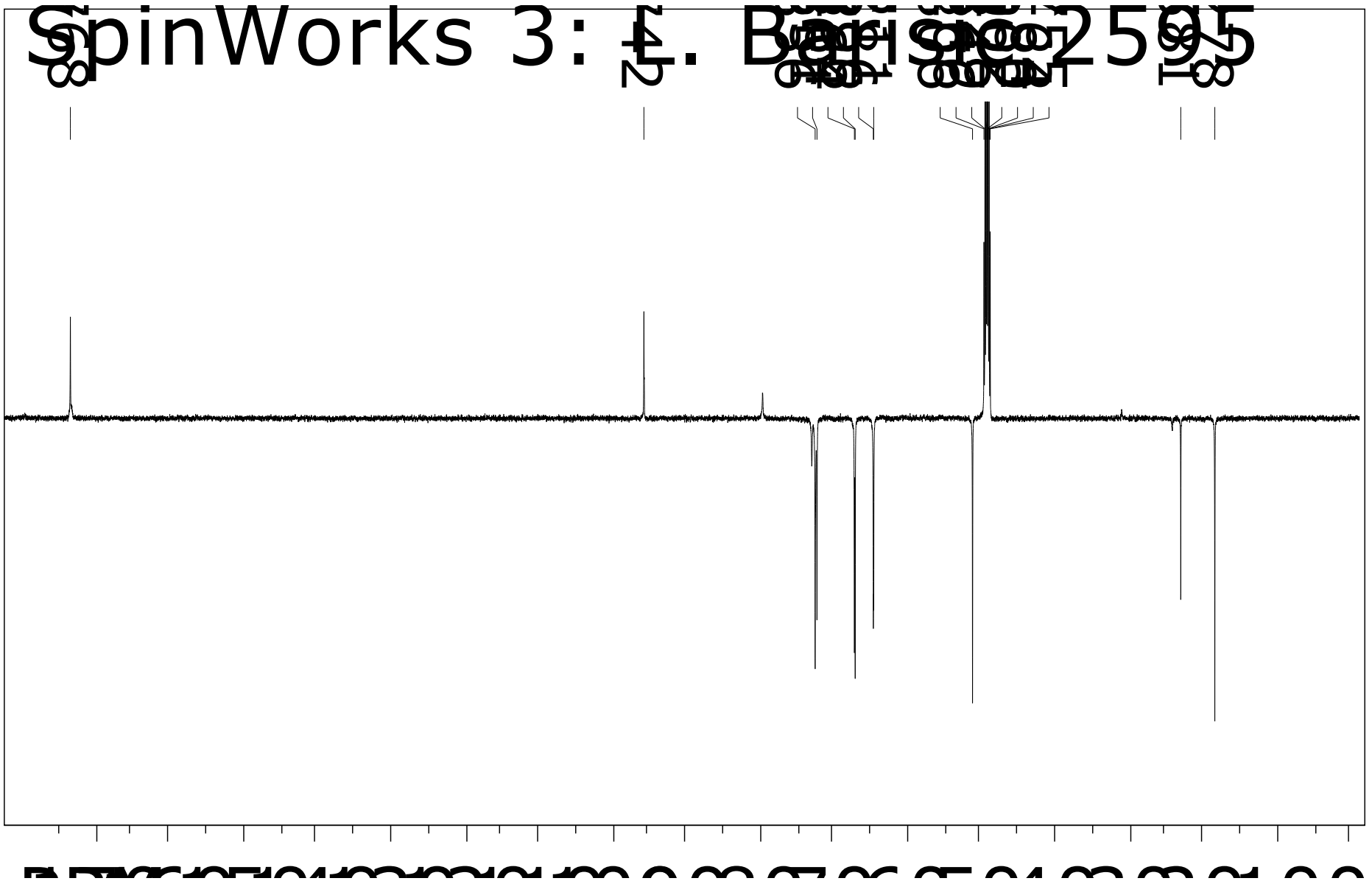


Figure S4. ^{13}C NMR spectrum of compound **5** (c = 5 × 10^{-2}M)

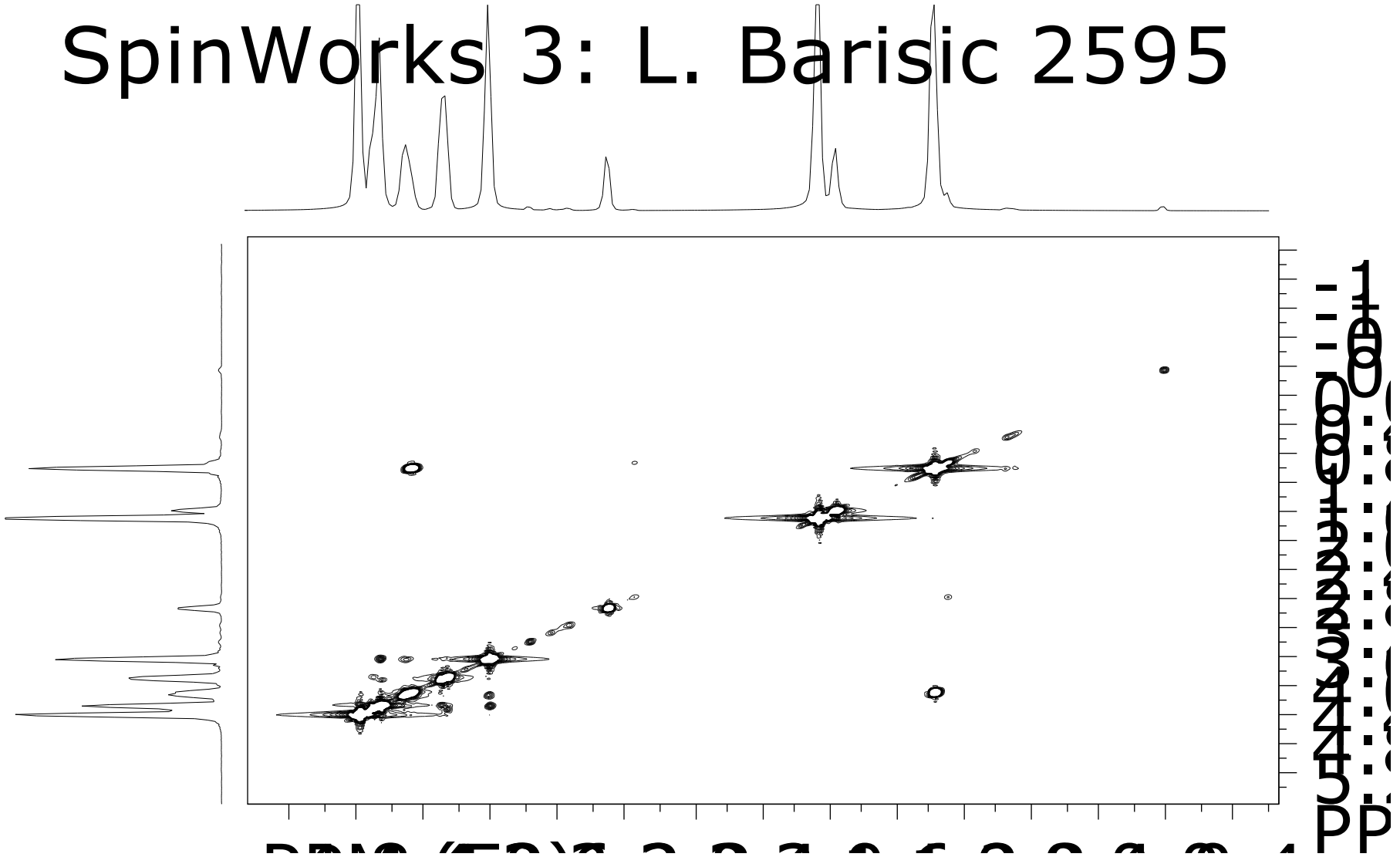
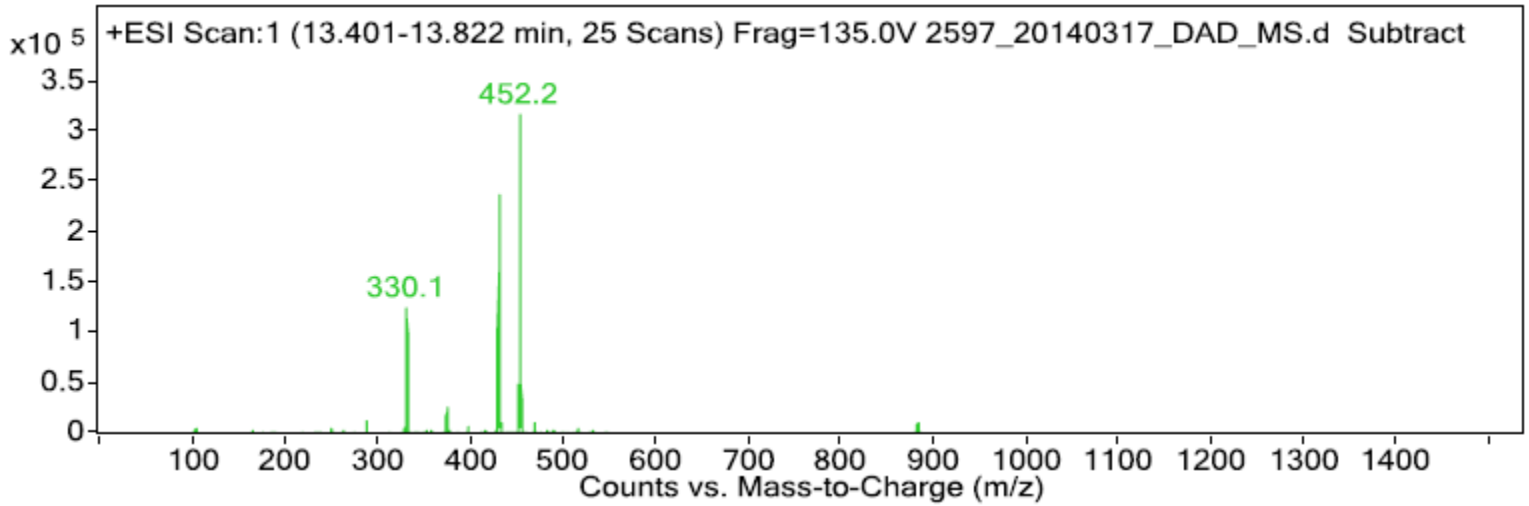


Figure S5. COSY NMR spectrum of compound **5** (c = 2.5 × 10^{-2}M)

Compound 7



Peak List

m/z	z	Abund
330.1	1	125219.8
331.2	1	24889
373.1		26764.7
374.1		23015.7
427.2		28753.2
429.1	1	237638.6
430.2	1	70686.9
450.1		50177.4
452.2	1	317638.1
453.2	1	72568.7

Figure S6. ESI-MS spectrum of compound **7**

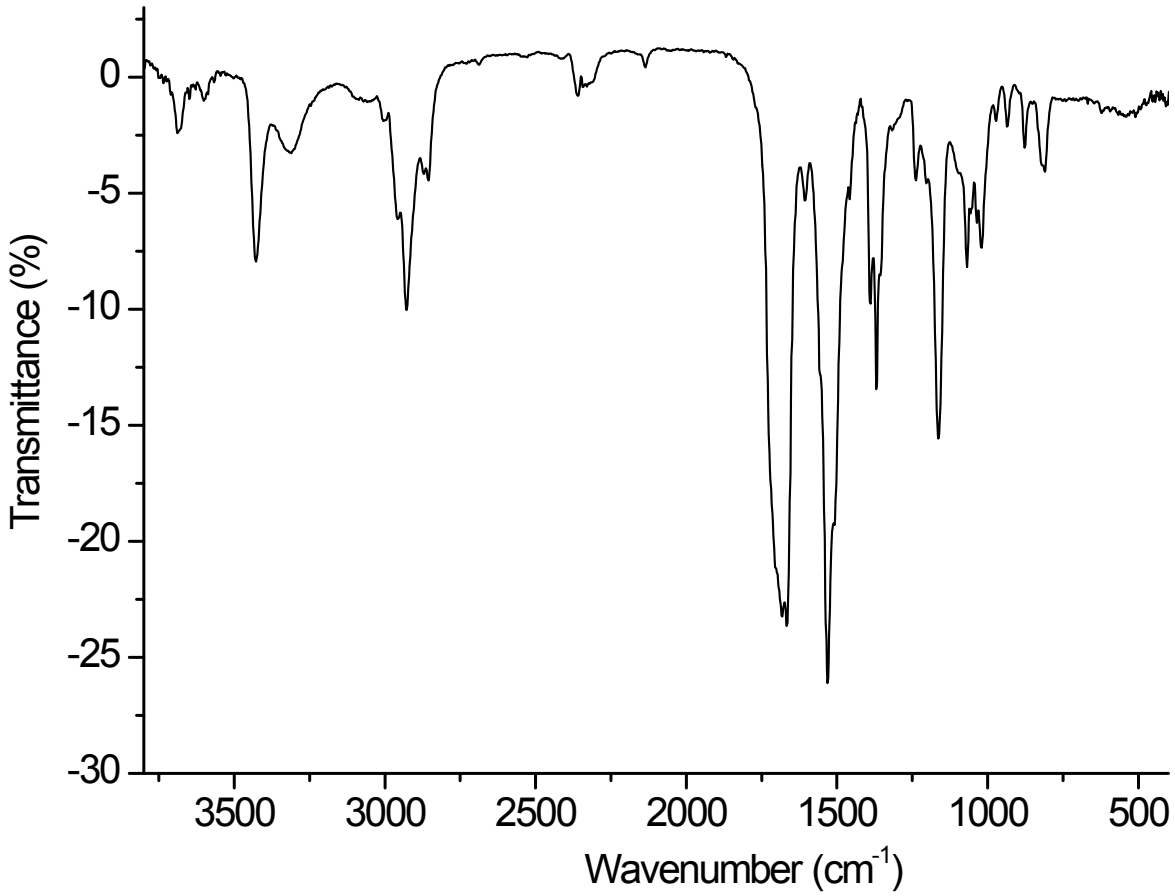


Figure S7. IR spectrum of compound **7** ($c = 5 \times 10^{-2}$M)

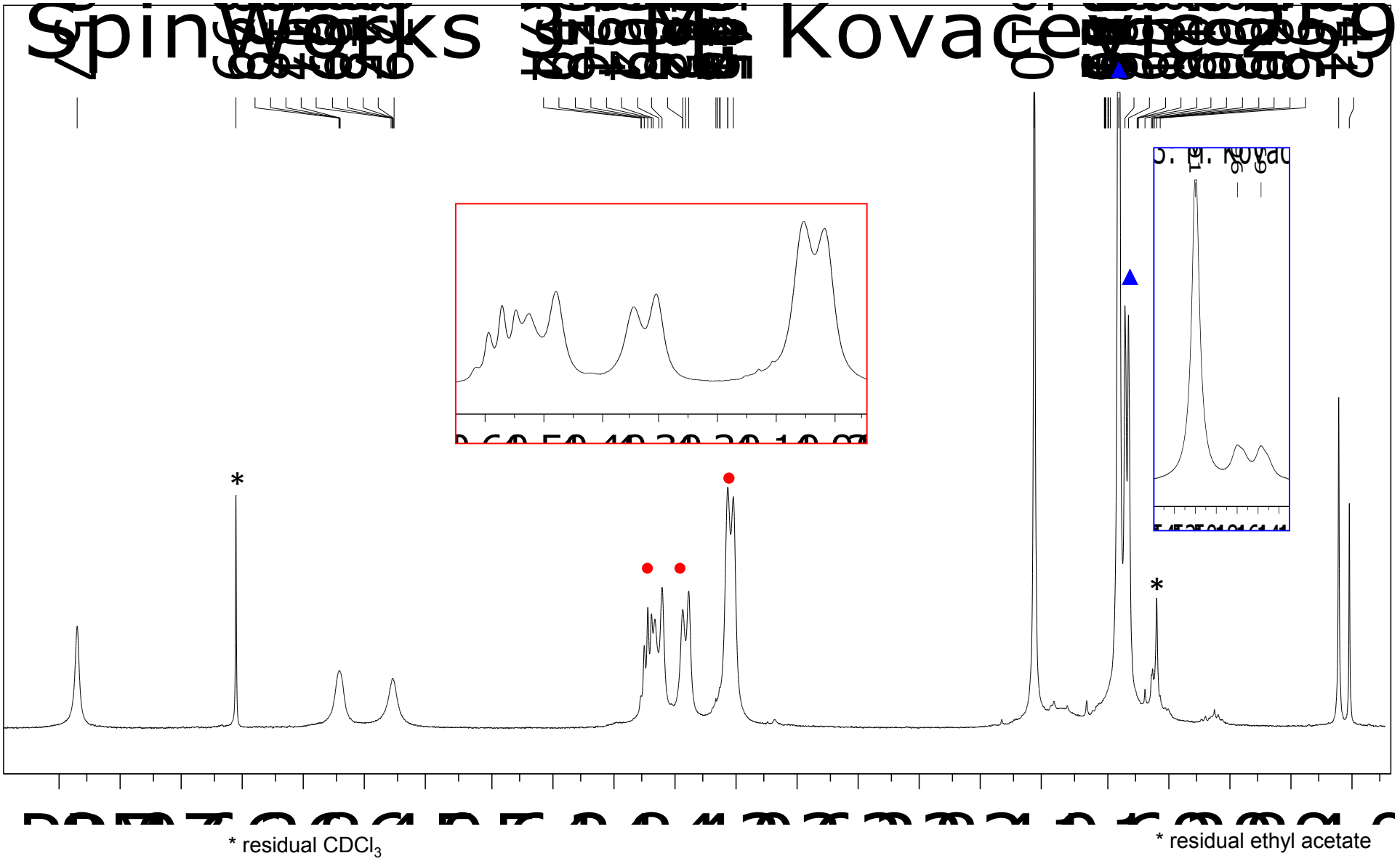


Figure S8. ^{1}H NMR spectrum of compound **7** (c = 2.5 × 10^{-2}M)

Figure S9. ^{13}C NMR spectrum of compound **7** ($c = 5 \times 10^{-2}$M)

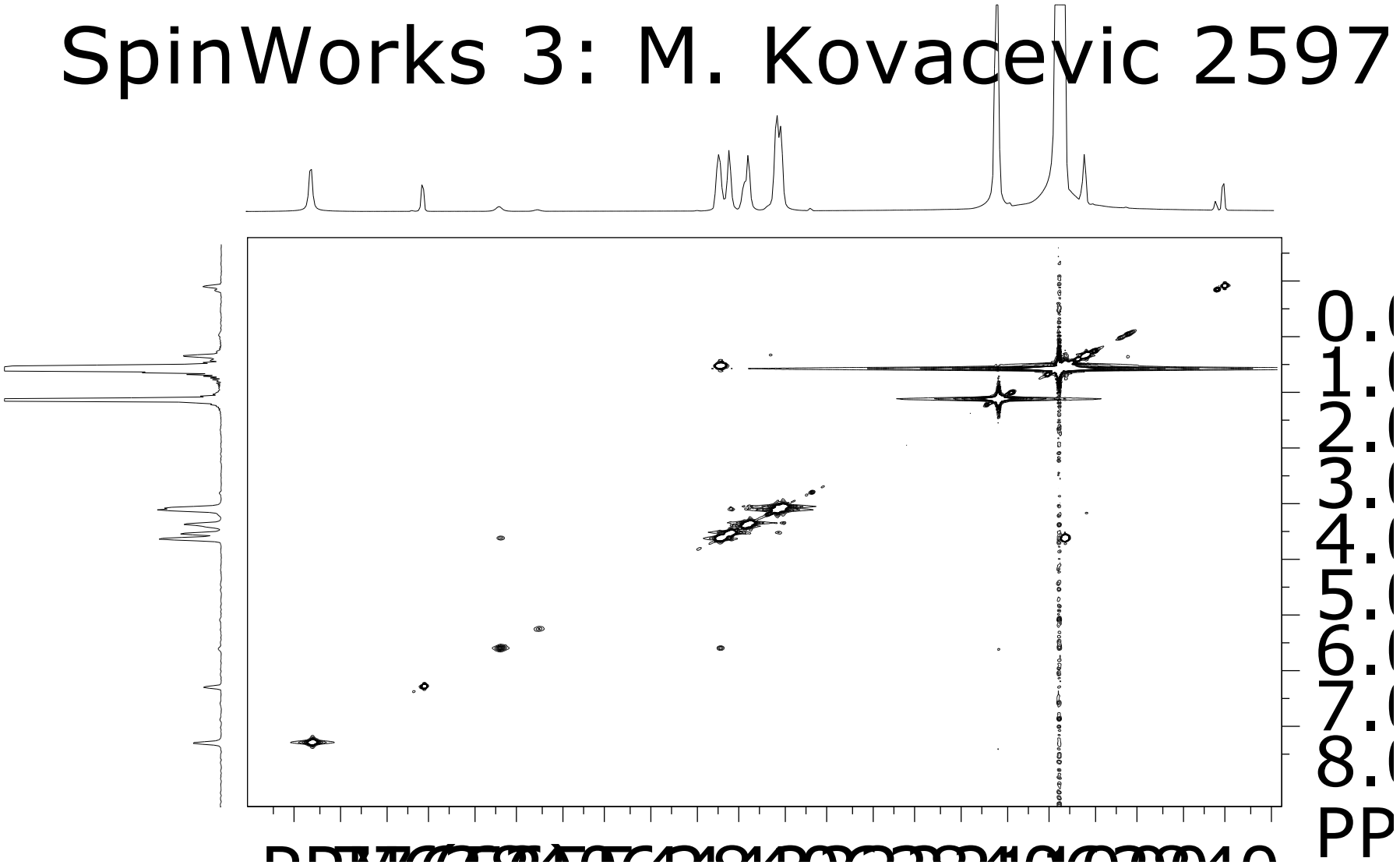


Figure S10. COSY NMR spectrum of compound **7** (*c* = 2.5 × 10^{-2}M)

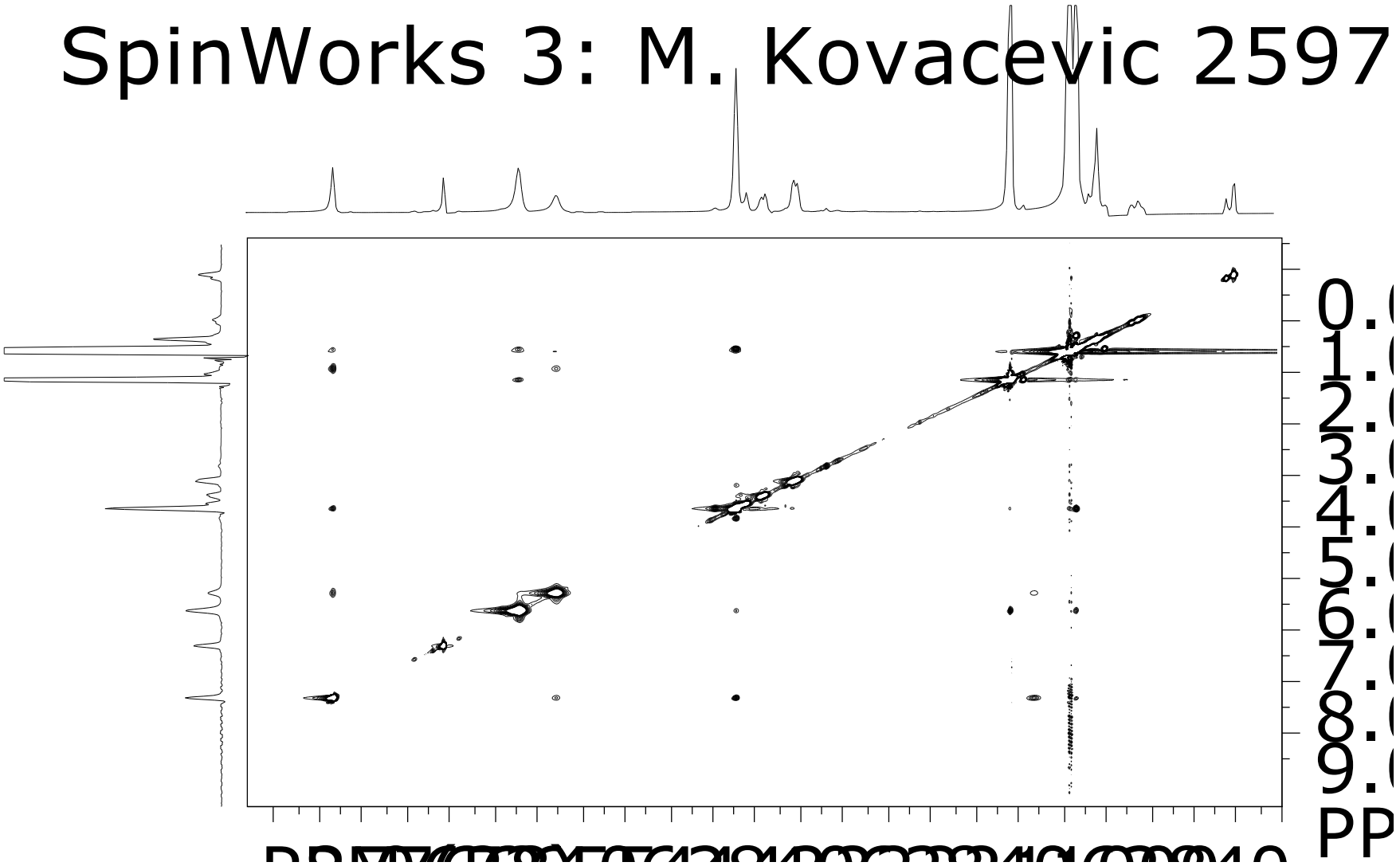


Figure S11. NOESY NMR spectrum of compound **7** (c = 2.5 × 10^{-2}M)

Compound 3b

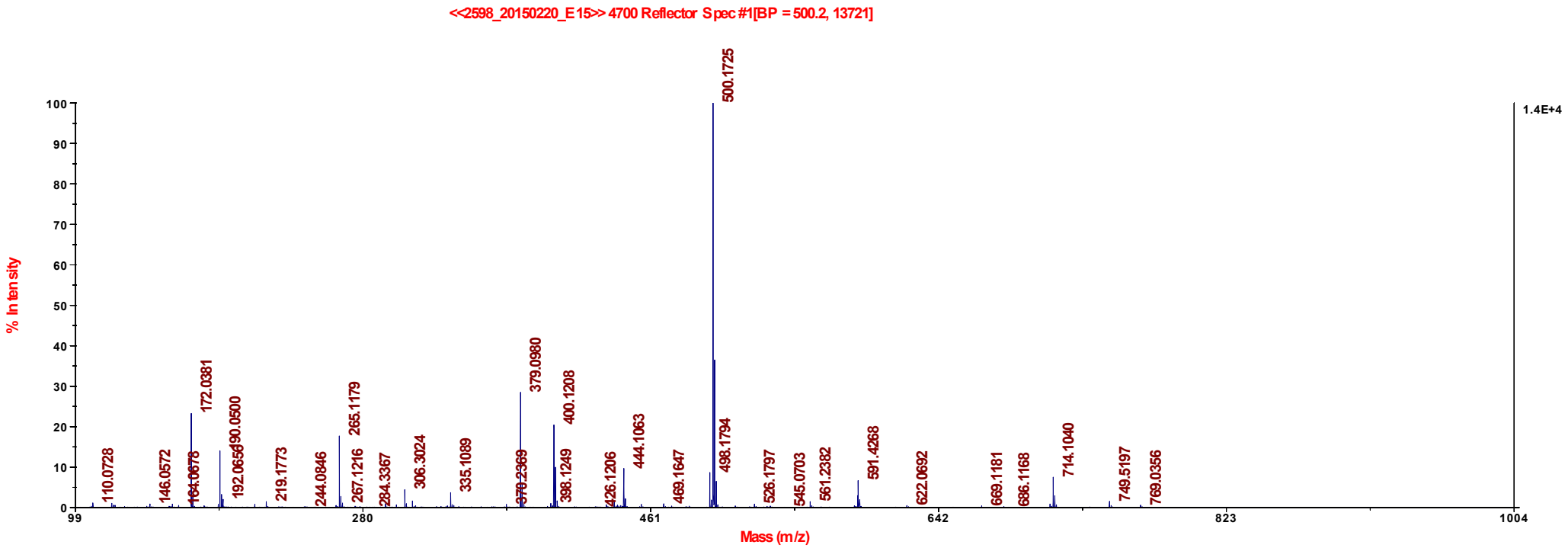


Figure S12. HRMS spectrum of compound **3b**

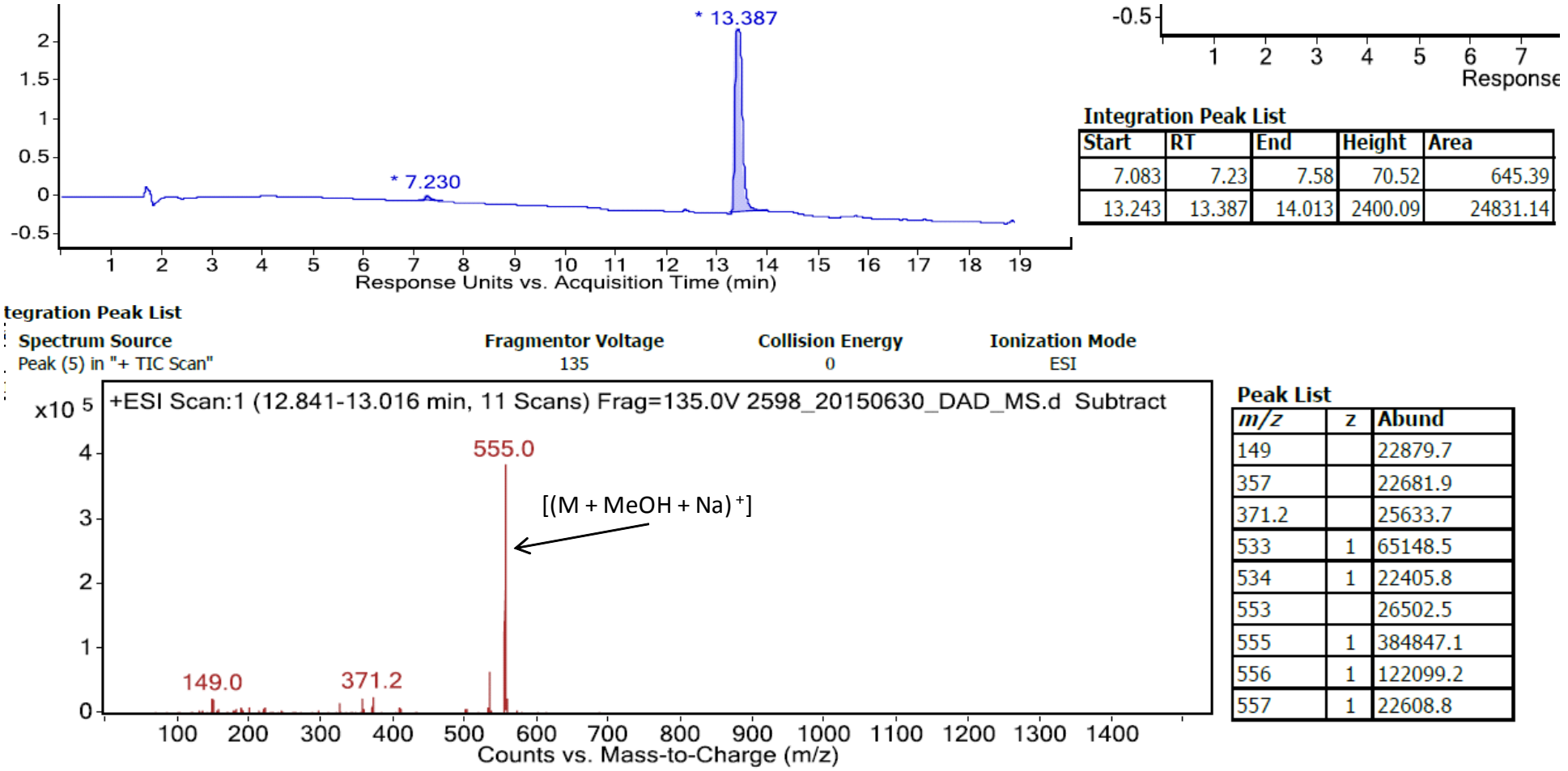


Figure S13. LC-MS assessment of purity of **3b** (97%) dissolved in MeOH. Elution conditions: 30-70% gradient elution system with H2O + 0.1% FA (solvent A) and MeOH + 0.1% FA (solvent B) over 20 min at 0.5 mL/min.
Coloumn used: Zorbax C18 XDB 3.5 um, 4.6x75 mm (Agilent, palo Alto, CA, USA).

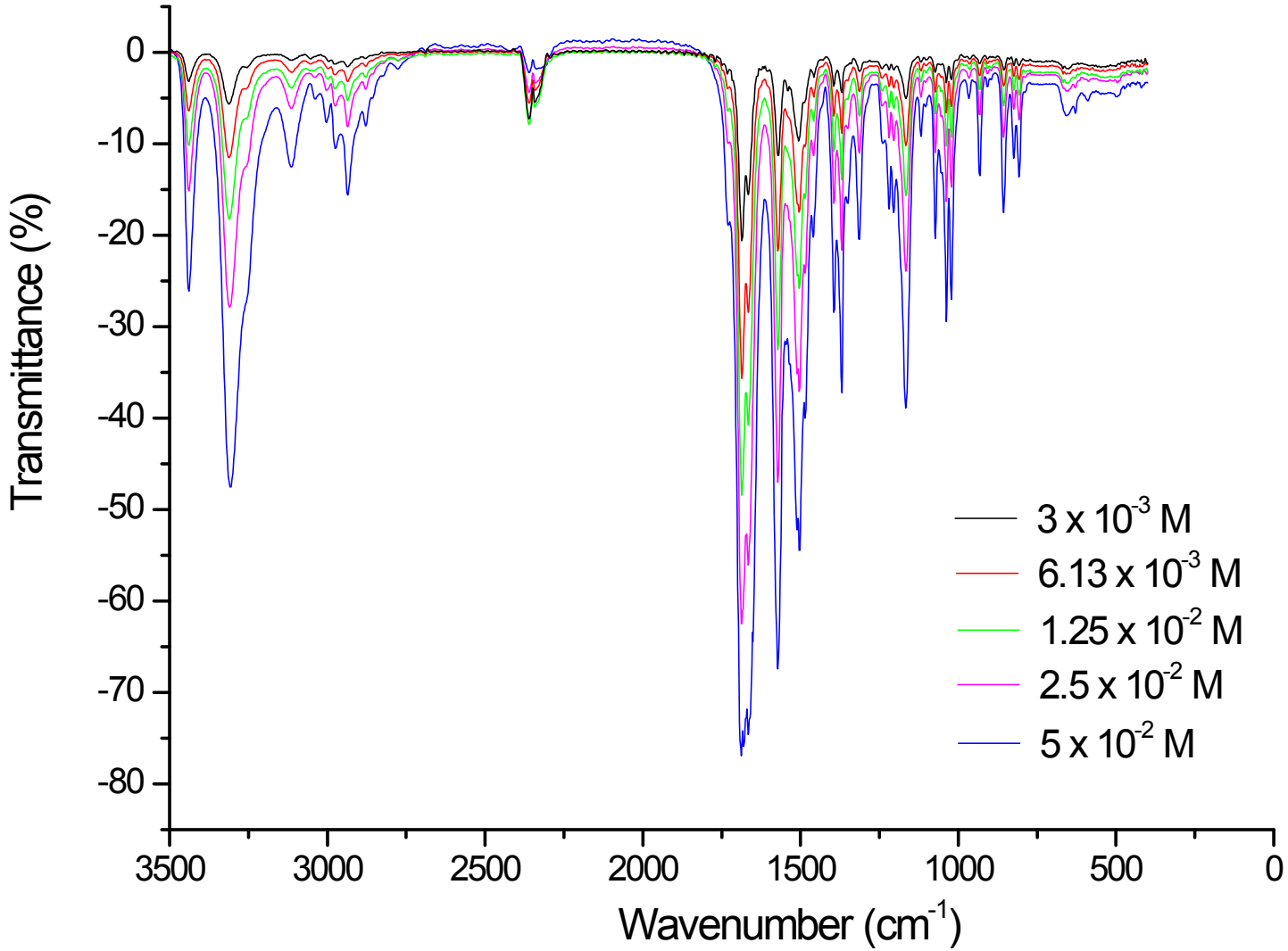


Figure S14. Concentration-dependent IR spectra of compound **3b**

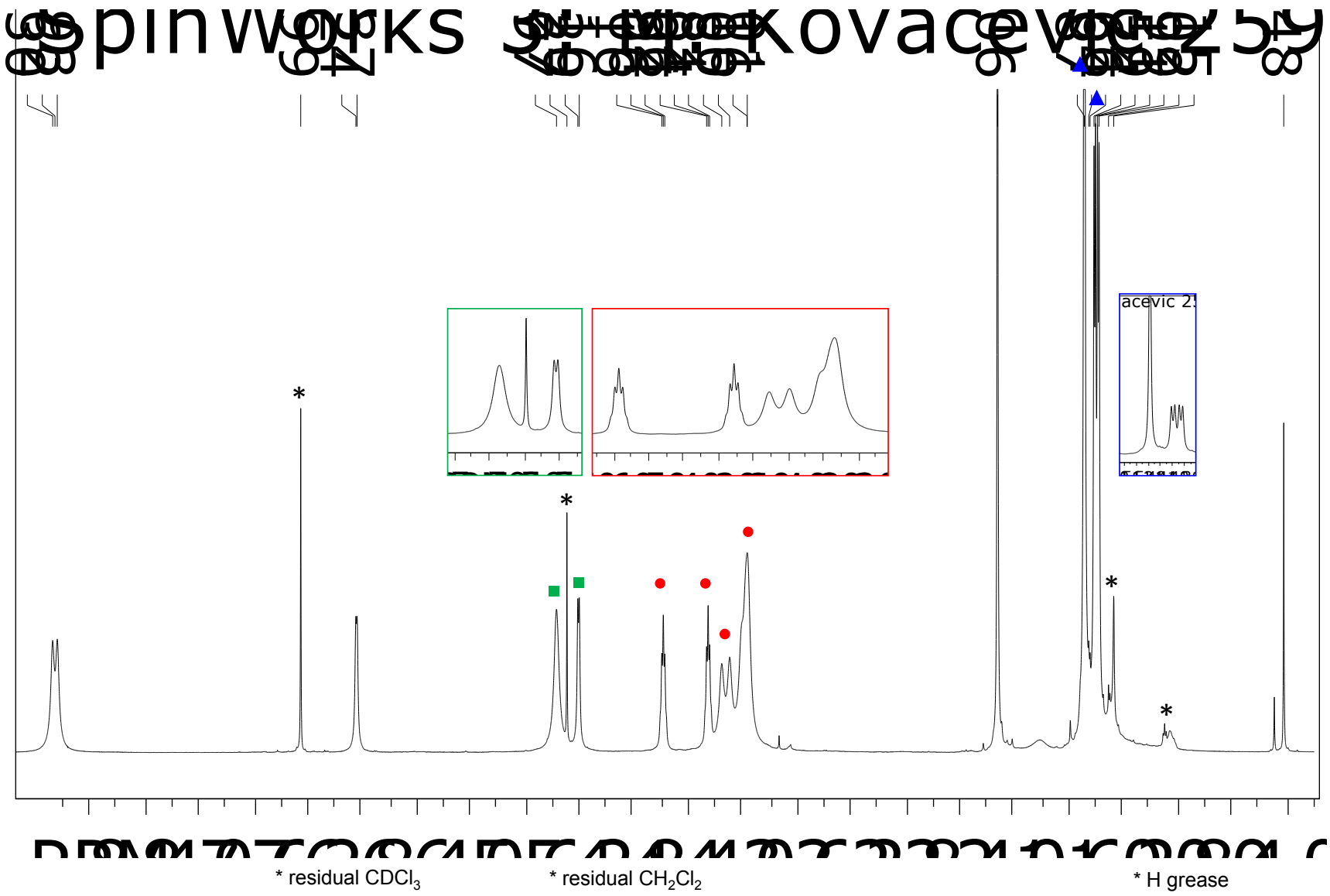


Figure S15. ^{1}H NMR spectrum of compound **3b** (c = 5 × 10^{-2}M)

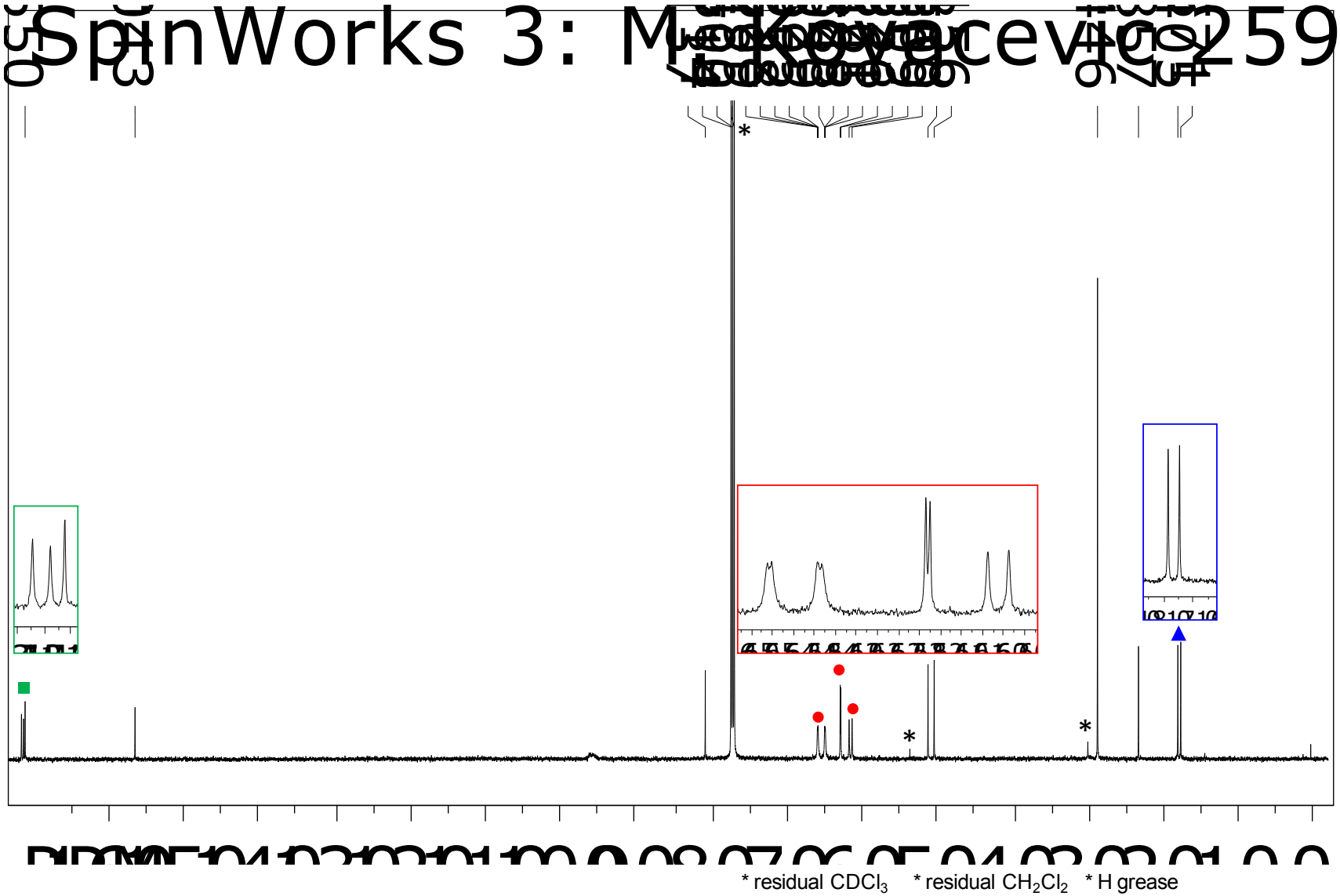


Figure S16. ^{13}C NMR spectrum of compound **3b** (*c* = 5 × 10^{-2}M)

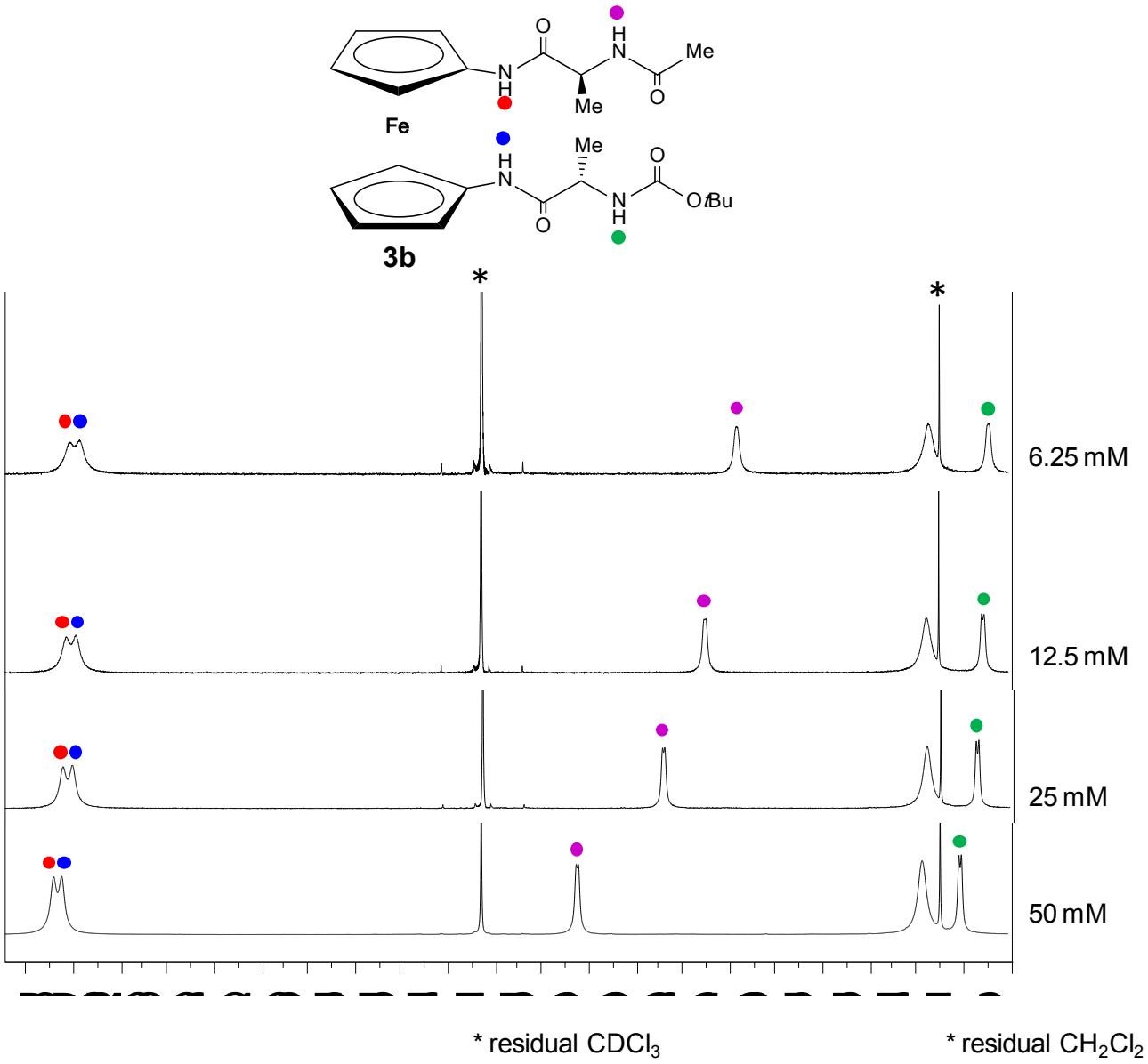


Figure S17. Concentration-dependent NH chemical shifts of compound **3b**

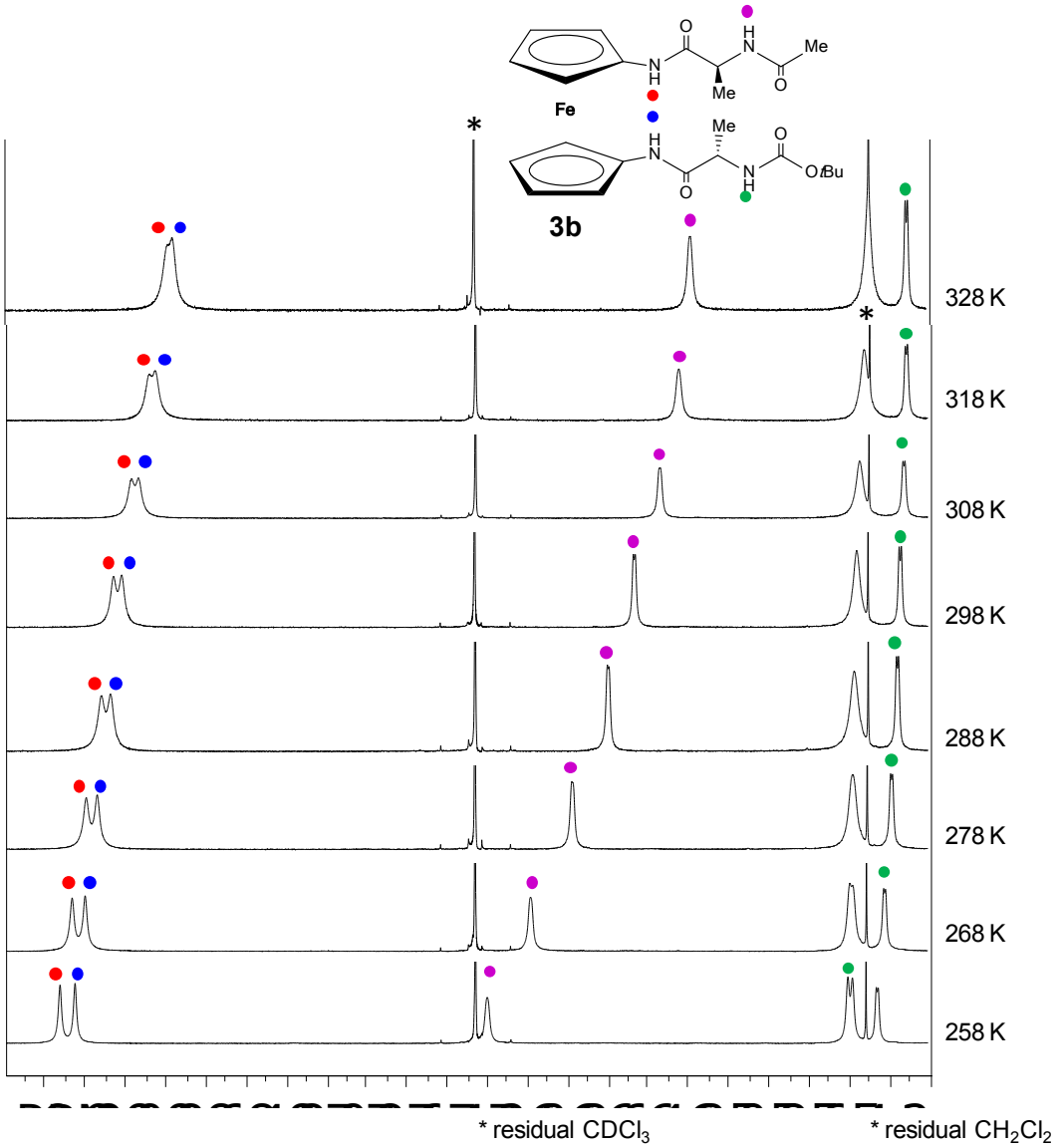


Figure S18. Temperature-dependent NH chemical shifts of compound **3b** (c = 2.5 × 10^{-2}M)

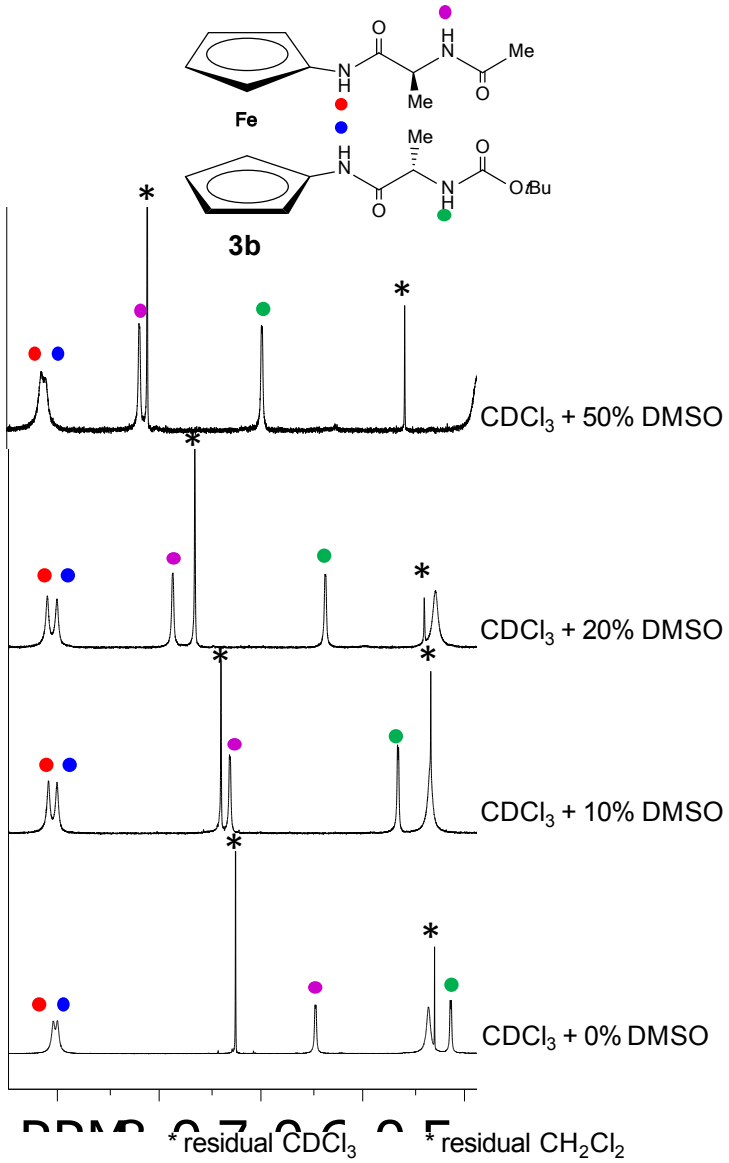


Figure S19. Solvent dependence of NH chemical shifts of compound **3b** at varying concentrations of d_6-DMSO in $CDCl_3$ (c = 2.5 × 10^{-2}M)

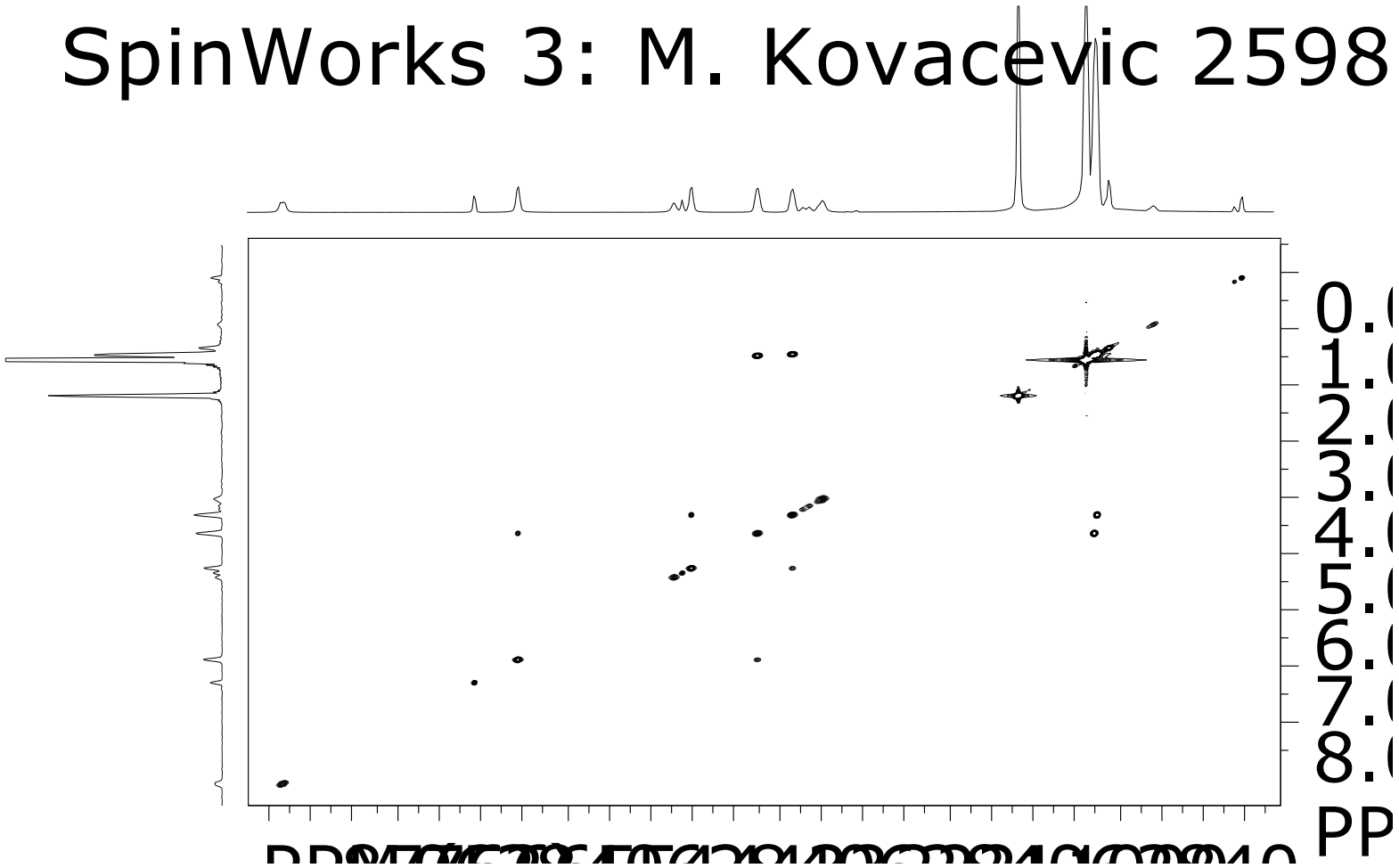


Figure S20. COSY NMR spectrum of compound **3b** (c = 5 × 10^{-2}M)

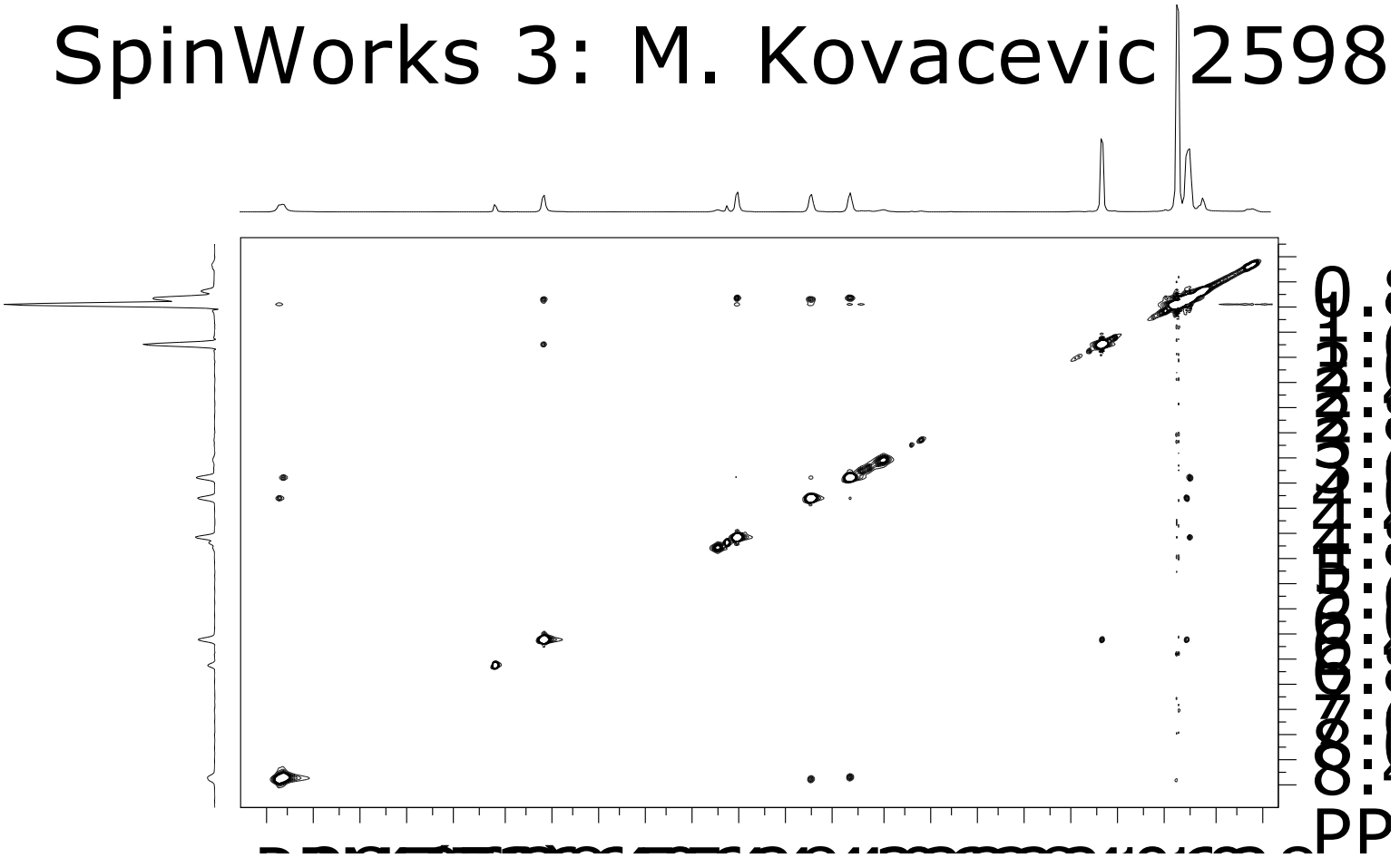


Figure S21. NOESY NMR spectrum of compound **3b** ($c = 5 \times 10^{-2}$M)

Compound 3c

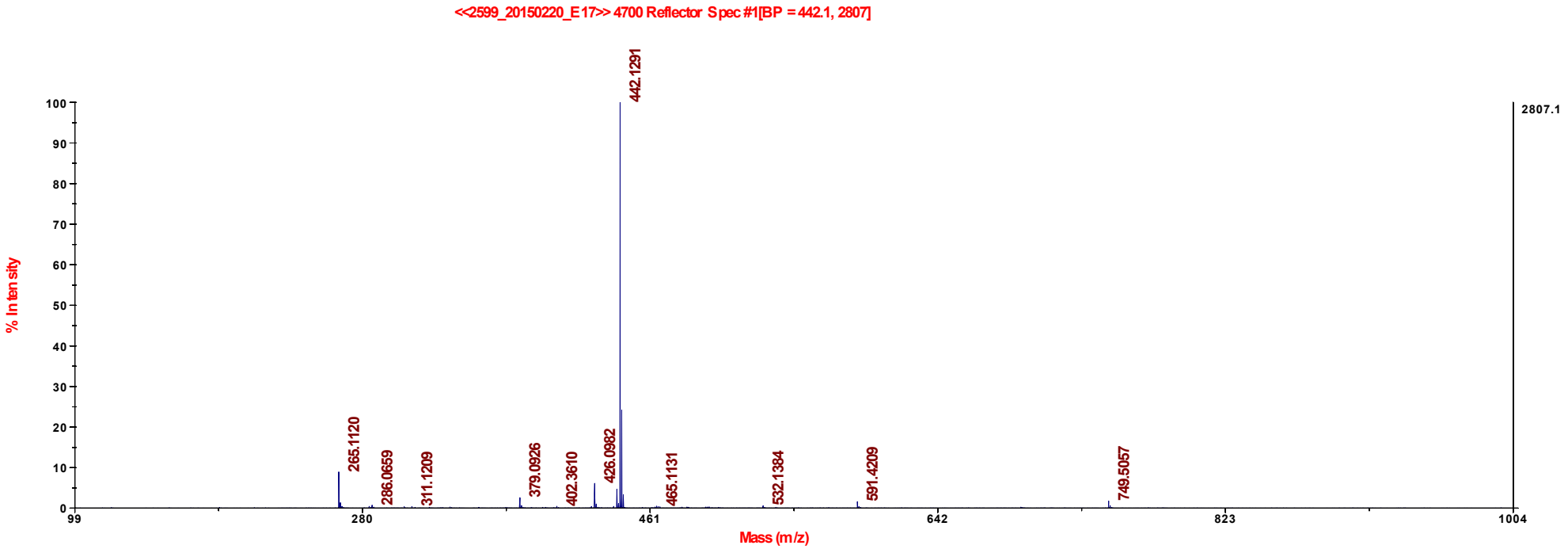
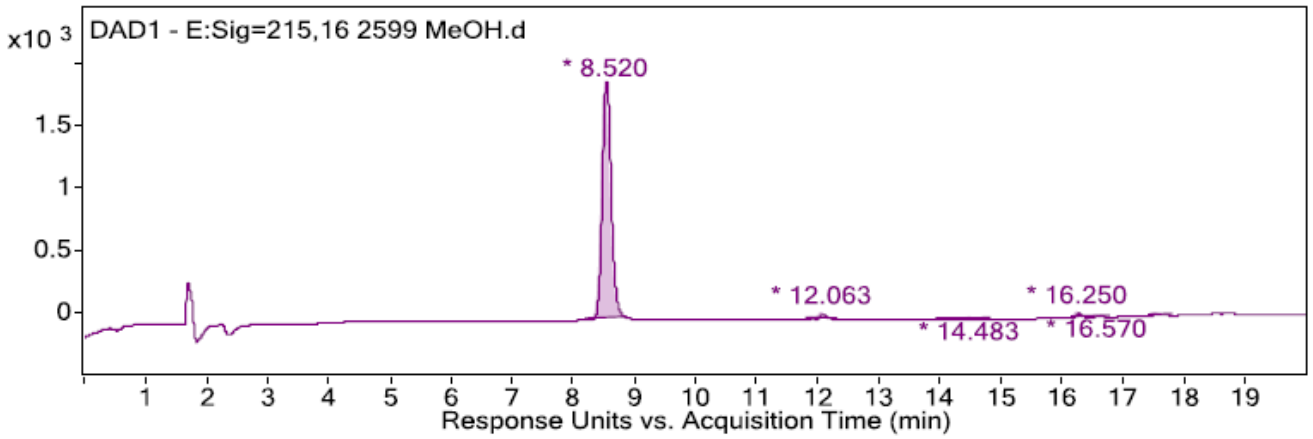


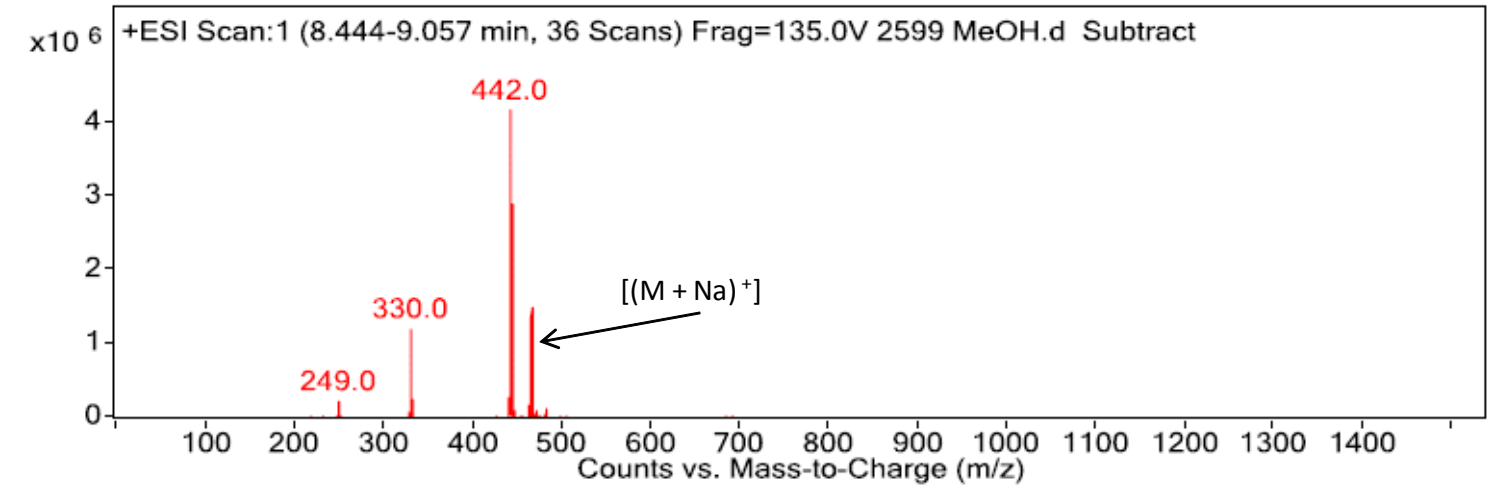
Figure S22. HRMS spectrum of compound **3c**



Integration Peak List

Start	RT	End	Height	Area
8.19	8.52	8.883	1894.37	19465.4
11.803	12.063	12.33	45.62	419.62
13.937	14.483	14.837	8.17	154.78
16.153	16.25	16.483	36.72	259.43
16.493	16.57	16.79	12.85	94.45
17.42	17.53	17.82	16.98	141.34

Spectrum Source Peak (2) in "+ TIC Scan" | **Fragmentor Voltage** 135 | **Collision Energy** 0 | **Ionization Mode** ESI



Peak List

m/z	z	Abund
249		223026.7
330	1	1210599.9
331	1	241481.3
440.1		271536.1
442		4188175.8
443.1	1	2901169.5
444.1	1	668026.3
465	1	1513849.4
466.1	1	375245.8

Figure S23. LC-MS assessment of purity of **3c** (95%) dissolved in MeOH. Elution conditions: 30-70% gradient elution system with H2O + 0.1% FA (solvent A) and MeOH + 0.1% FA (solvent B) over 20 min at 0.5 mL/min.
Coloumn used: Zorbax C18 XDB 3.5 um, 4.6x75 mm (Agilent, palo Alto, CA, USA).

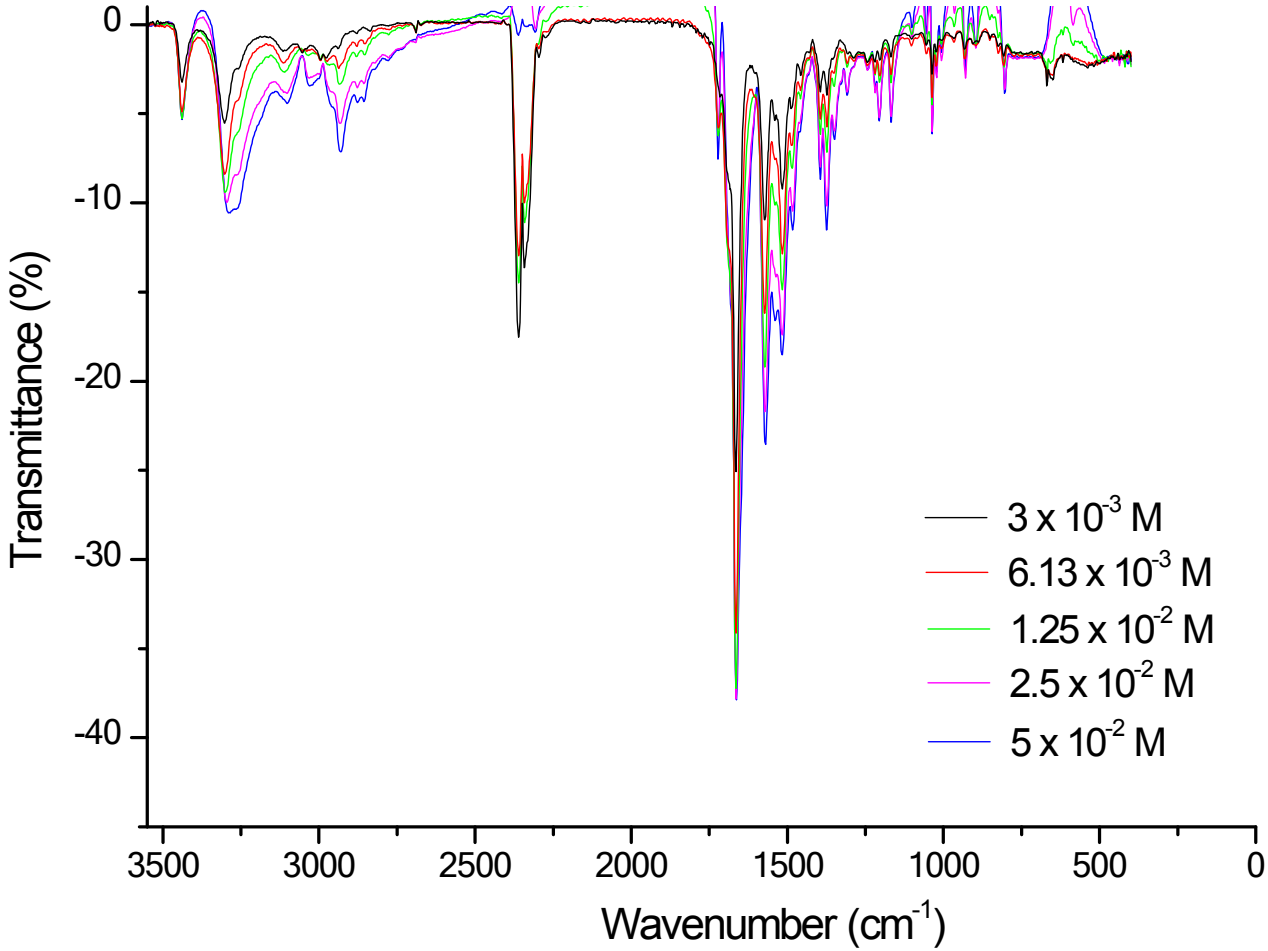


Figure S24. Concentration-dependent IR spectra of compound **3c**

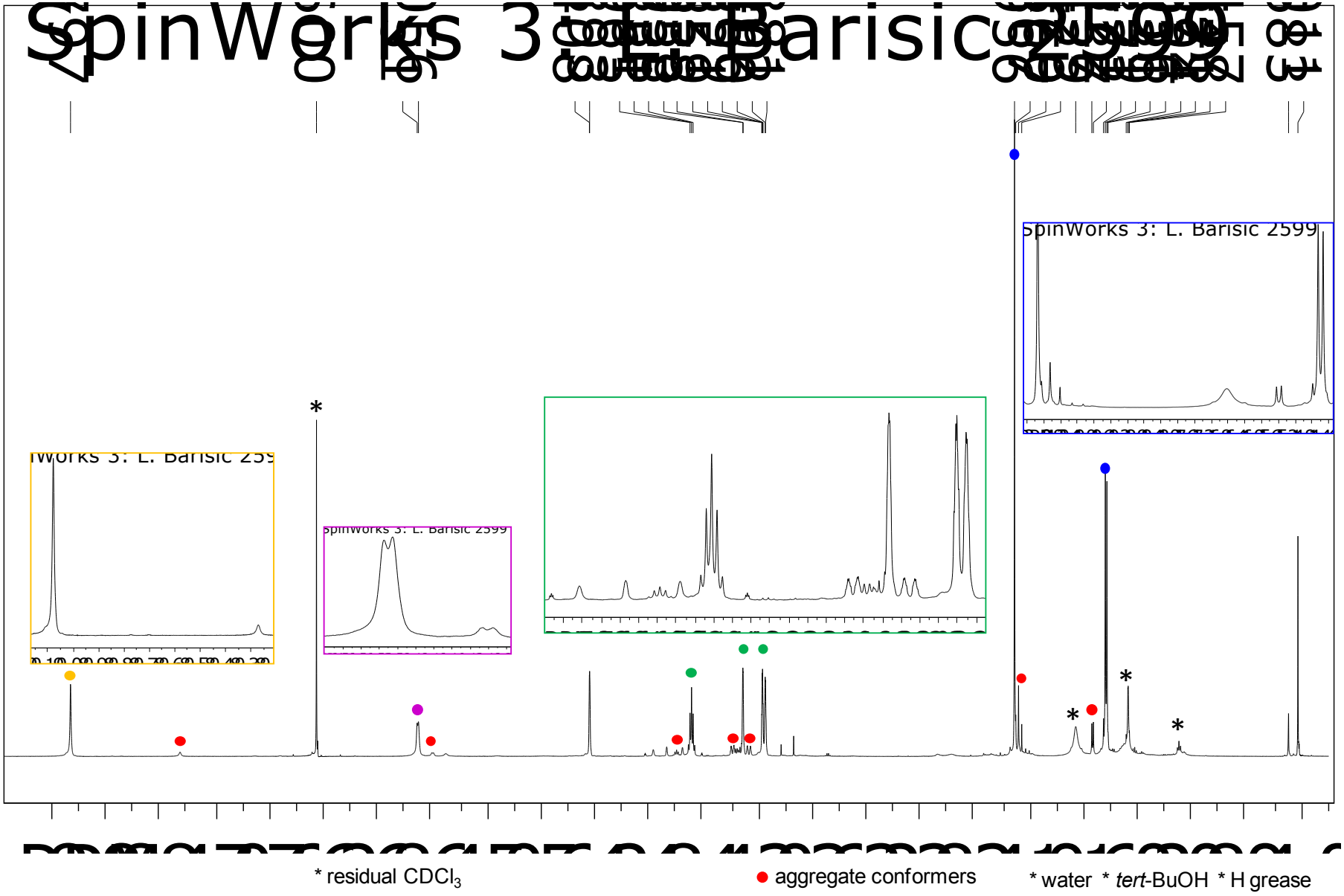


Figure S25. ^{1}H NMR spectrum of compound **3c** (c = 5 × 10^{-2}M)

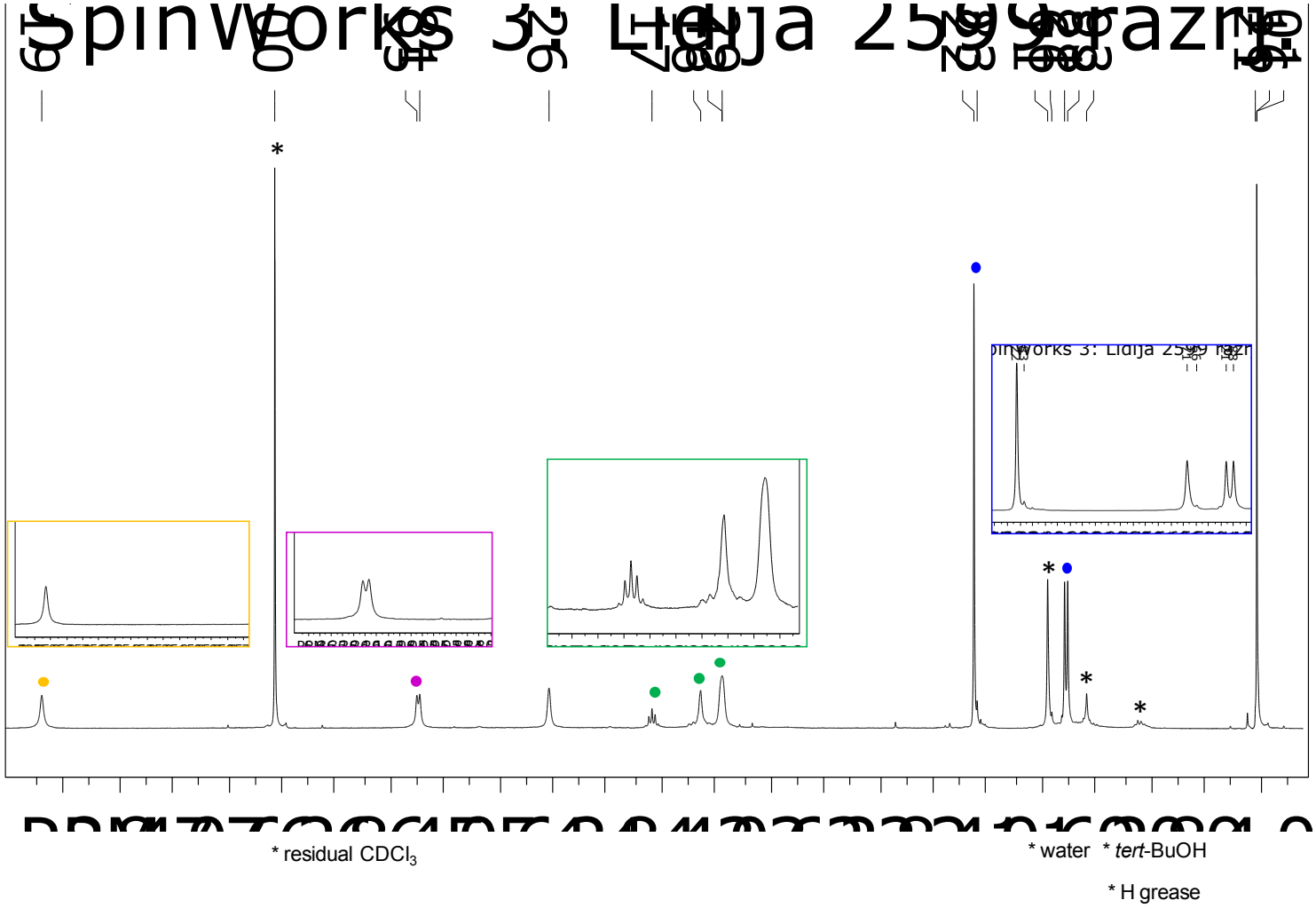


Figure S26. ^{1}H NMR spectrum of compound **3c** (c = 2.5 × 10^{-2}M)

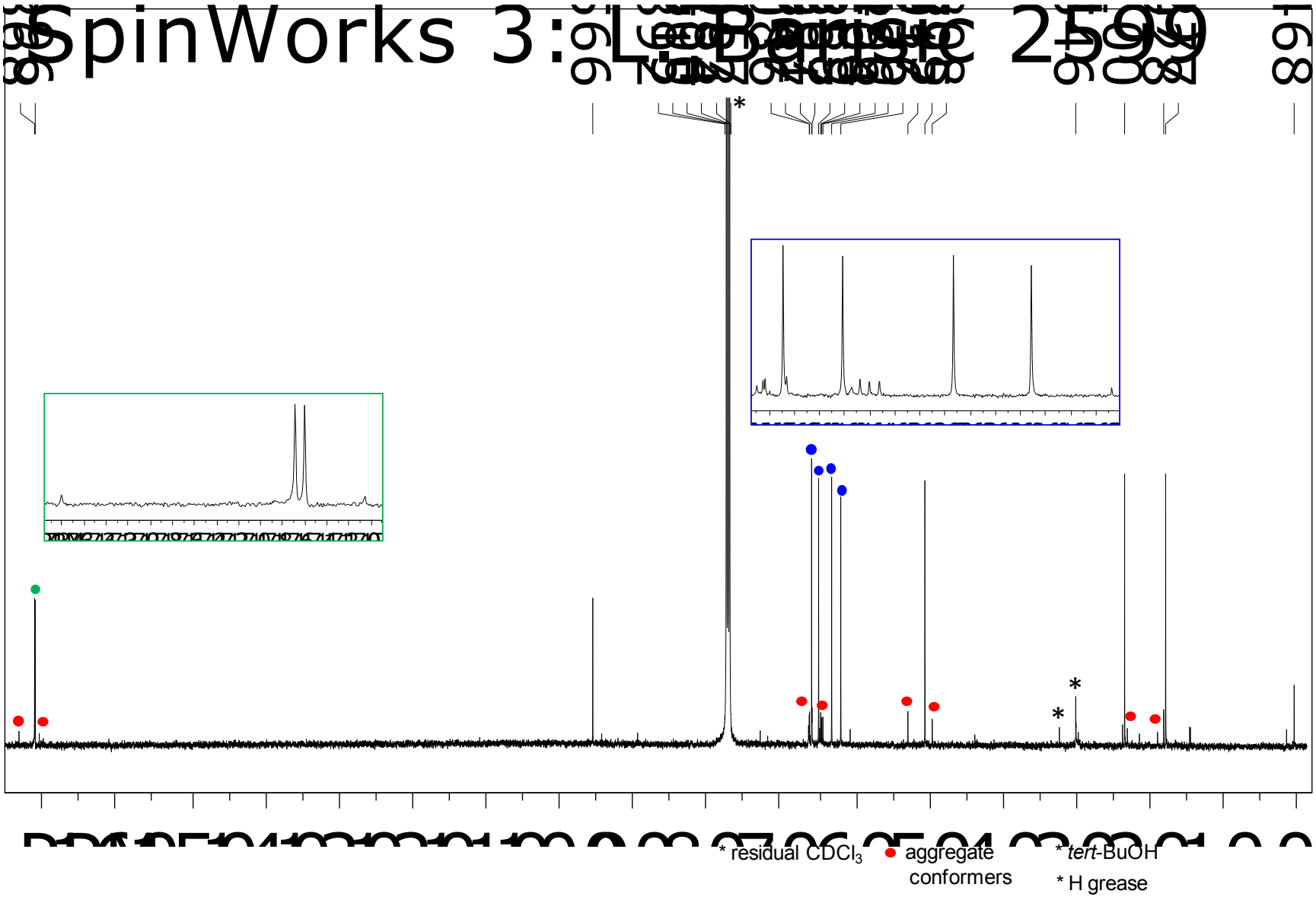


Figure S27. ^{13}C NMR spectrum of compound **3c** (c = 5 × 10^{-2}M)

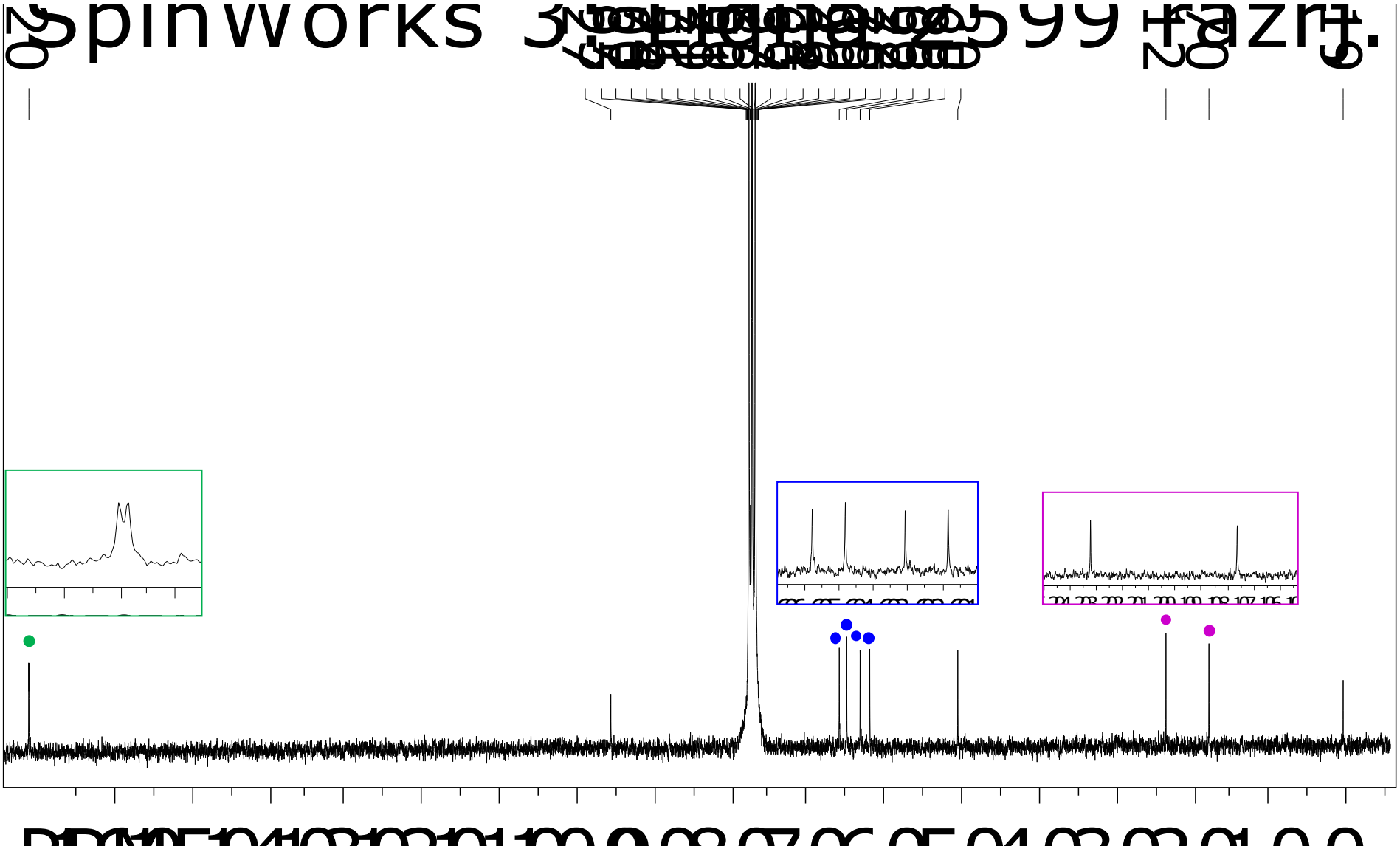


Figure S28. ^{13}C NMR spectrum of compound **3c** (c = 2.5 × 10^{-2}M)

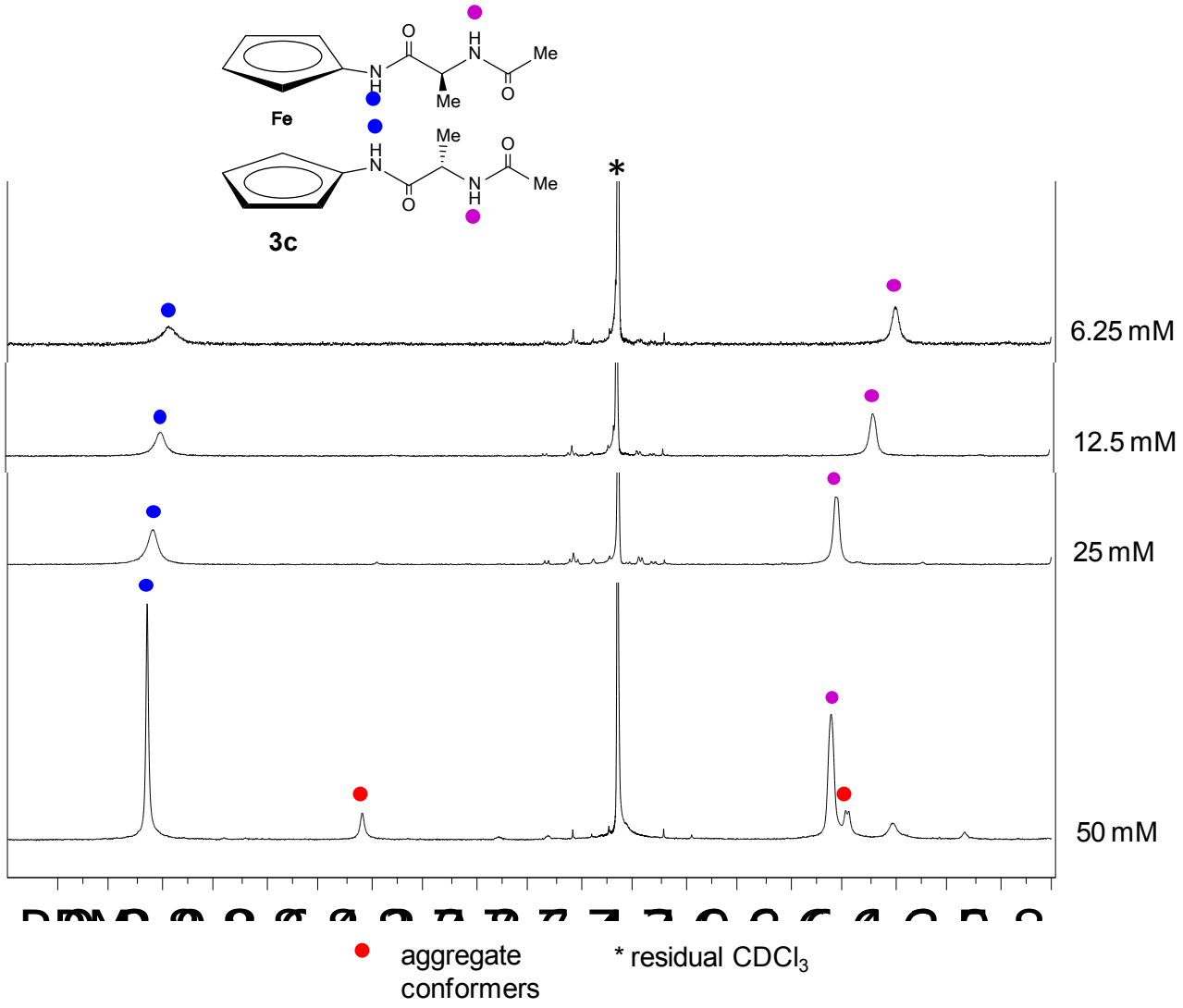


Figure S29. Concentration-dependent NH chemical shifts of compound **3c**

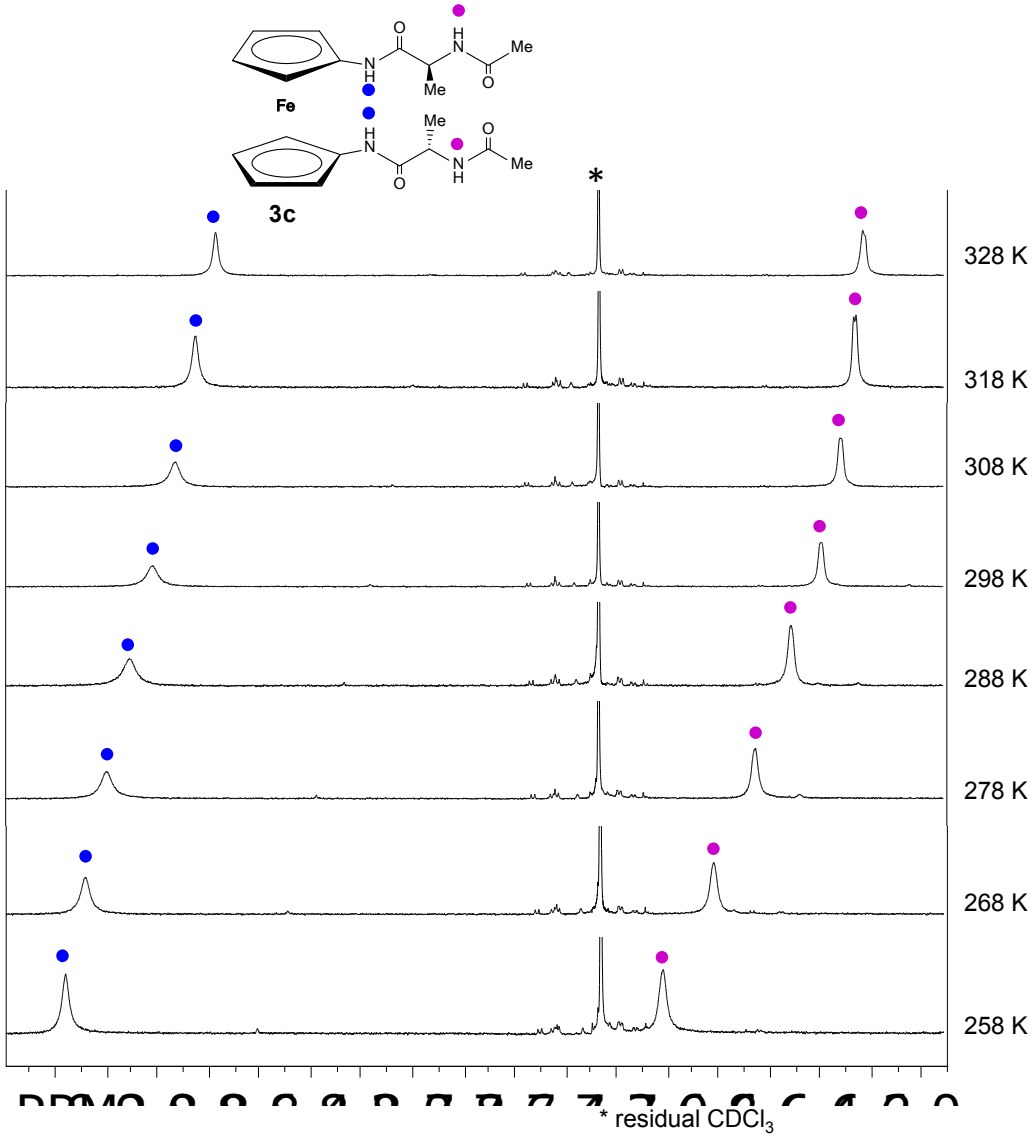


Figure S30. Temperature-dependent NH chemical shifts of compound **3c** (c = 2.5 × 10^{-2}M)

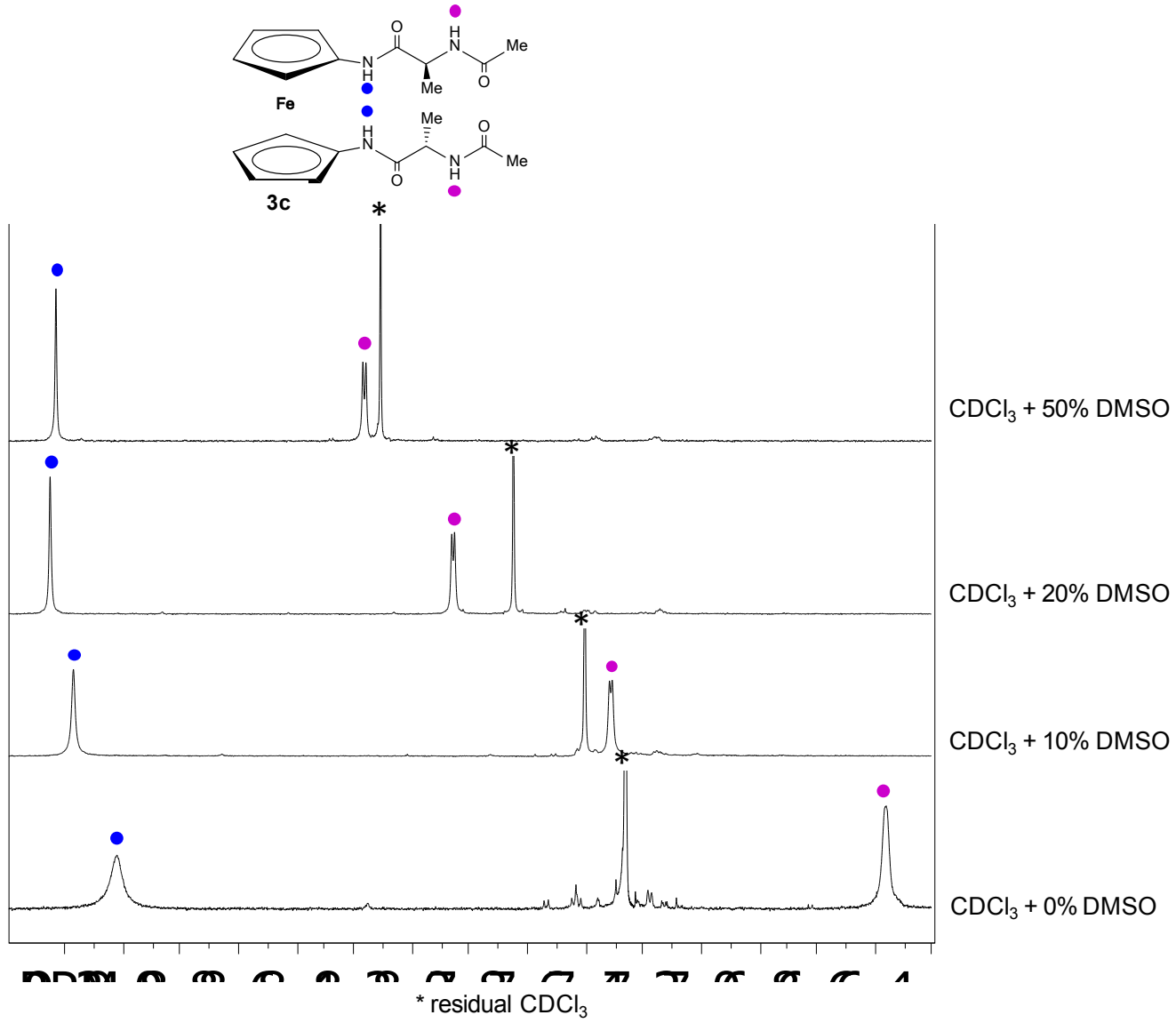


Figure S31. Solvent dependence of NH chemical shifts of compound **3c** at varying concentrations of d_6-DMSO in $CDCl_3$ (c = 2.5 × 10^{-2}M)

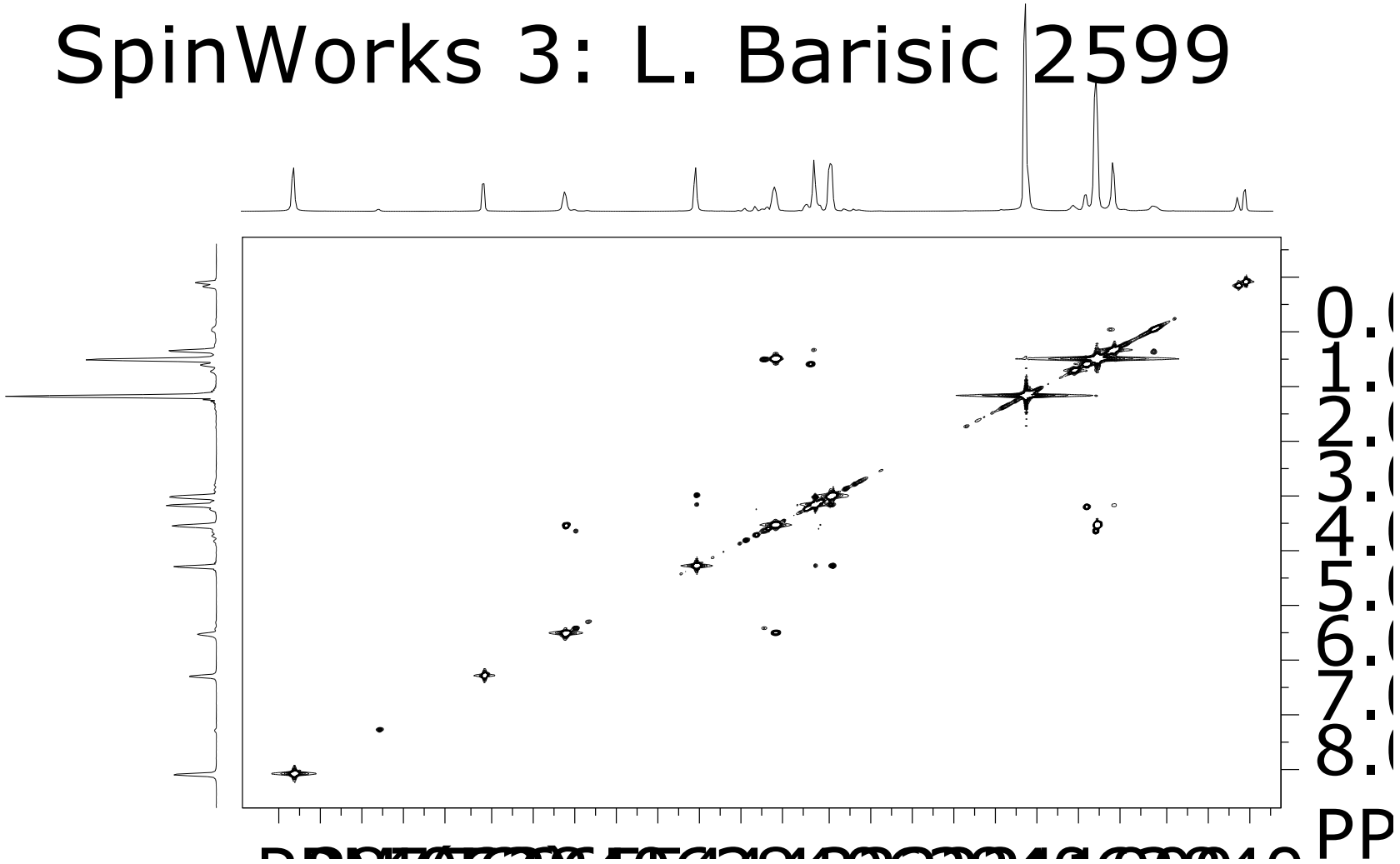


Figure S32. COSY NMR spectrum of compound **3c** ($c = 5 \times 10^{-2}$M)

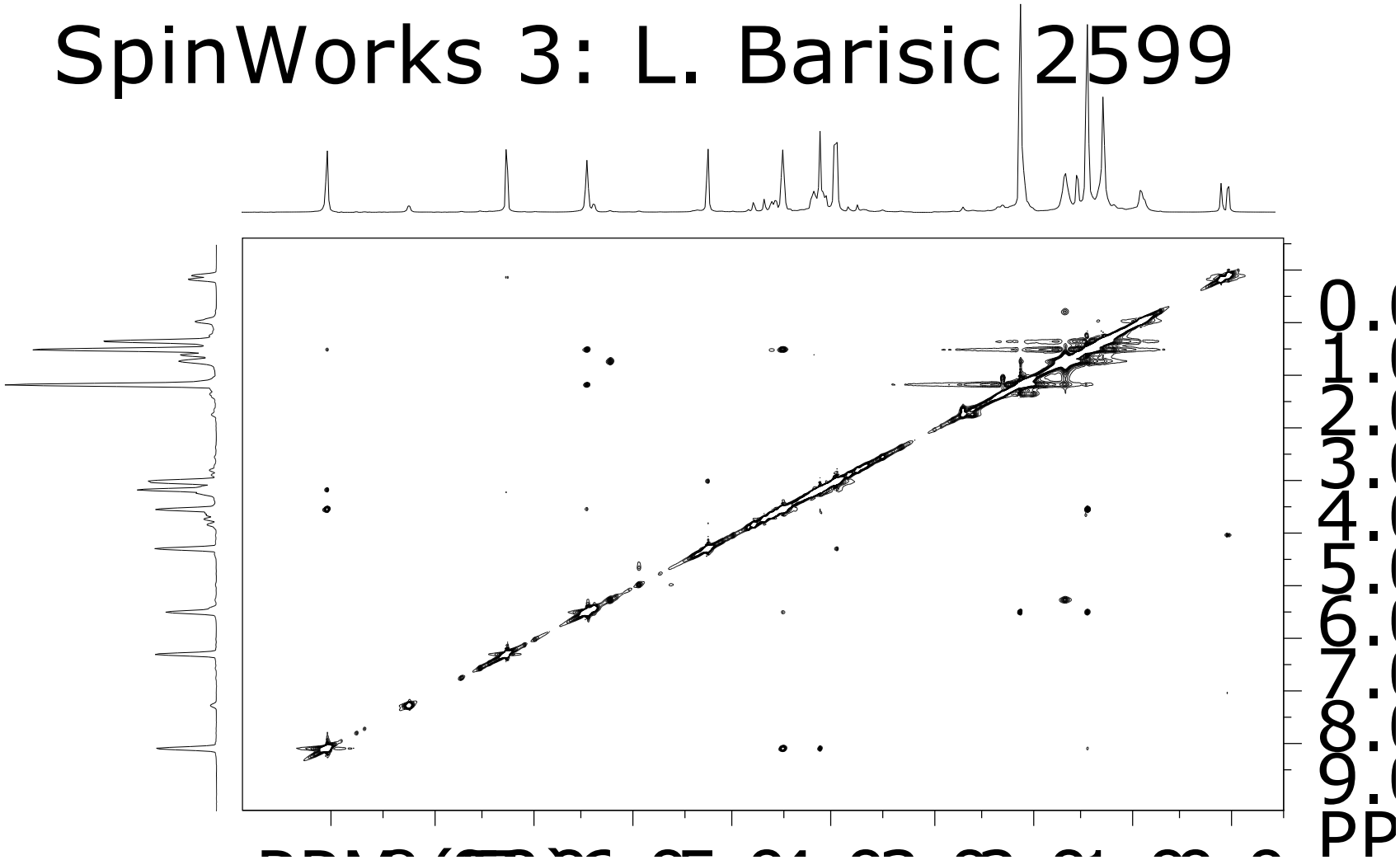


Figure S33. NOESY NMR spectrum of compound **3c** ($c = 5 \times 10^{-2}$M)