

Supplementary Material

Regioselective reaction of imidazole-2-thiols with *N*-sulfonylphenyldichloroacetaldimines: en route to novel sulfonylamino- substituted imidazo[2,1-*b*]thiazoles and thiazolo[3,2-*a*]benzimidazoles

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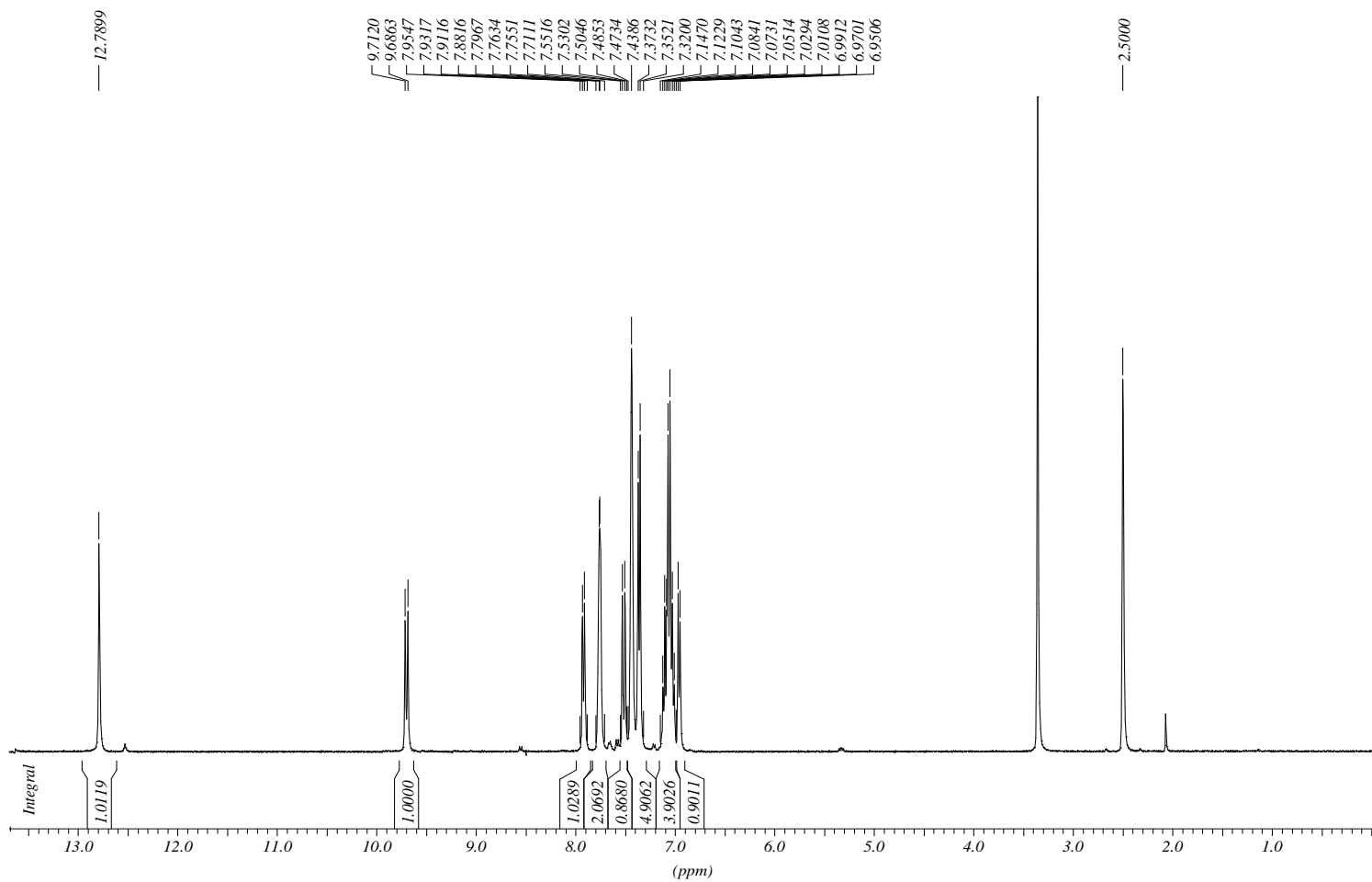
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Table of contents

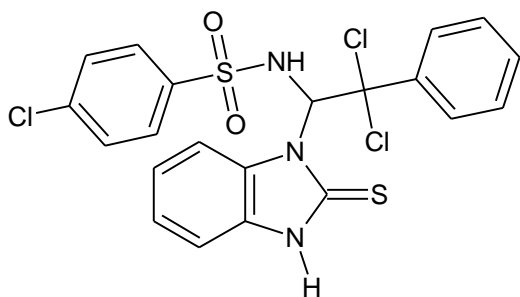
| | |
|--|-----|
| 1. X-Ray crystallographic data for compound 4ab , 4cd | S2 |
| 2. Copies of ¹ H, ¹³ C NMR spectra for compounds 3ac | S3 |
| 3. Copies of ¹ H and ¹³ C NMR spectra for compounds 4aa-4ac | S5 |
| 4. Copies of ¹ H, ¹³ C and 2D NMR spectra for compounds 4bc | S19 |
| 5. Copies of ¹ H, ¹³ C NMR spectra for compounds 4cc-4cd | S26 |

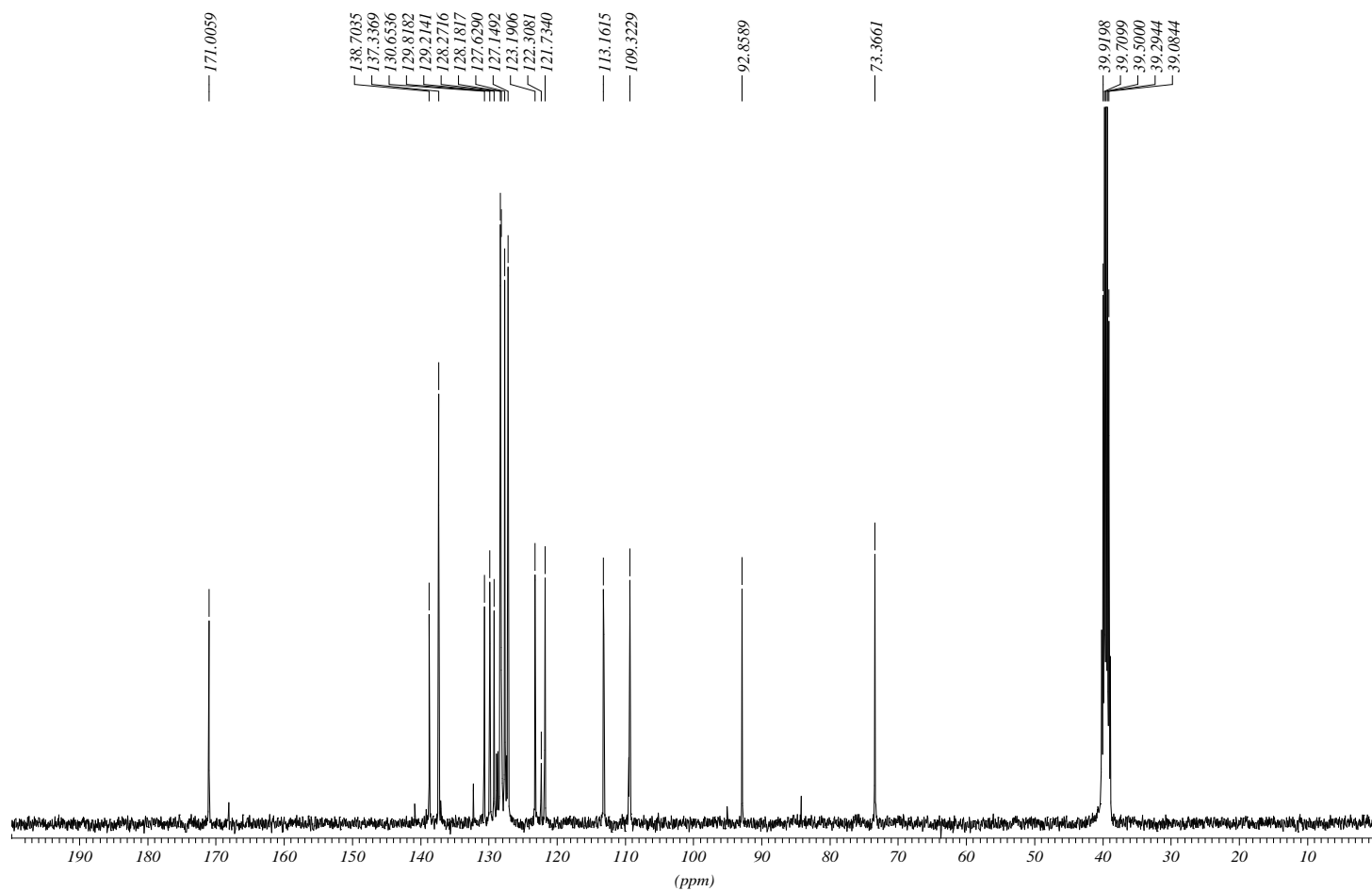
X-Ray crystallographic data for compound 4ab, 4cd

| Compound | 4ab | 4cd |
|--|--|---|
| CCDC | 1564758 | 1564759 |
| Empirical formula | C ₂₉ H ₂₁ N ₃ O ₂ S ₂ | C ₁₇ H ₁₂ N ₃ O ₂ S ₂ Cl |
| Formula mass [g/mol] | 507.61 | 389.87 |
| Temperature [K] | 100(2) | 100(2) |
| Crystal system | Monoclinic | Monoclinic |
| Space group | P2(1)/c | P2(1)/n |
| <i>a</i> [Å] | 11.2769(4) | 7.4393(3) |
| <i>b</i> [Å] | 15.6554(6) | 11.9777(4) |
| <i>c</i> [Å] | 13.8613(6) | 19.0799(7) |
| α [°] | 90.00 | 90 |
| β [°] | 105.831(2) | 99.957(2) |
| γ [°] | 90.00 | 90 |
| <i>V</i> [Å ³] | 2354.32(16) | 1674.52(11) |
| <i>Z</i> | 4 | 4 |
| <i>D</i> _{calcd.} [g·cm ⁻³] | 1.432 | 1.546 |
| μ [mm ⁻¹] | 0.261 | 0.494 |
| θ range [deg] | 2.01–28.00 | 2.02–28.00 |
| Reflections collected | 107937 | 32992 |
| Independent reflections | 5684 [R _{int} = 0.1627] | 4043 [R _{int} = 0.1109] |
| <i>R</i> ₁ , <i>wR</i> ₂ [<i>I</i> > 2 σ (<i>I</i>)] | 0.0473, 0.0898 | 0.0495, 0.0871 |
| <i>R</i> ₁ , <i>wR</i> ₂ (all data) | 0.0850, 0.1040 | 0.0953, 0.0999 |
| Completeness [%] | 100 | 100 |
| Crystalsize [mm] | 0.22×0.03×0.03 | 0.50×0.23×0.02 |
| Goodness of fit | 1.027 | 1.048 |

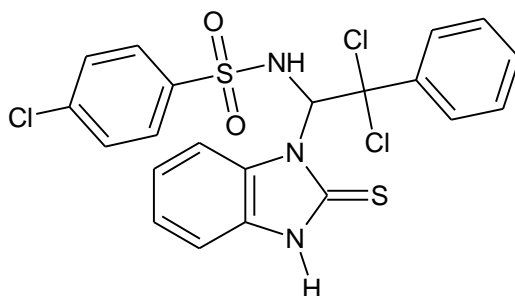


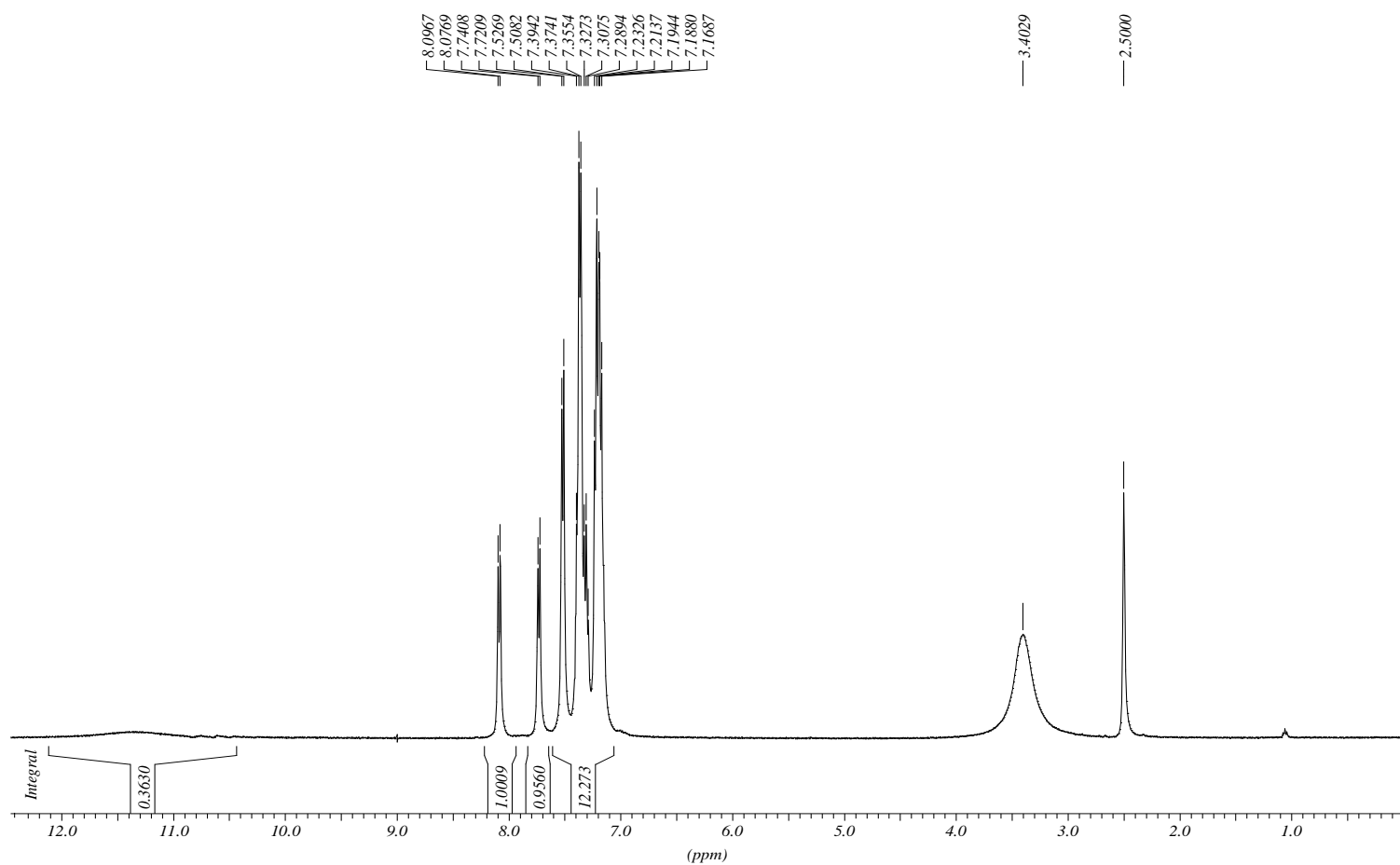
^1H NMR spectrum of **3ac** (400.13 MHz, $\text{DMSO-}d_6$)



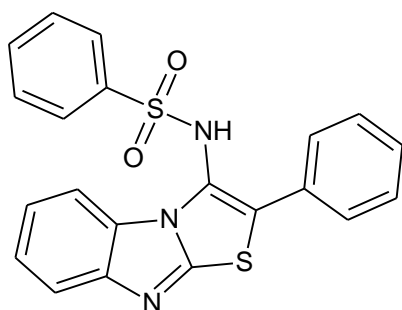


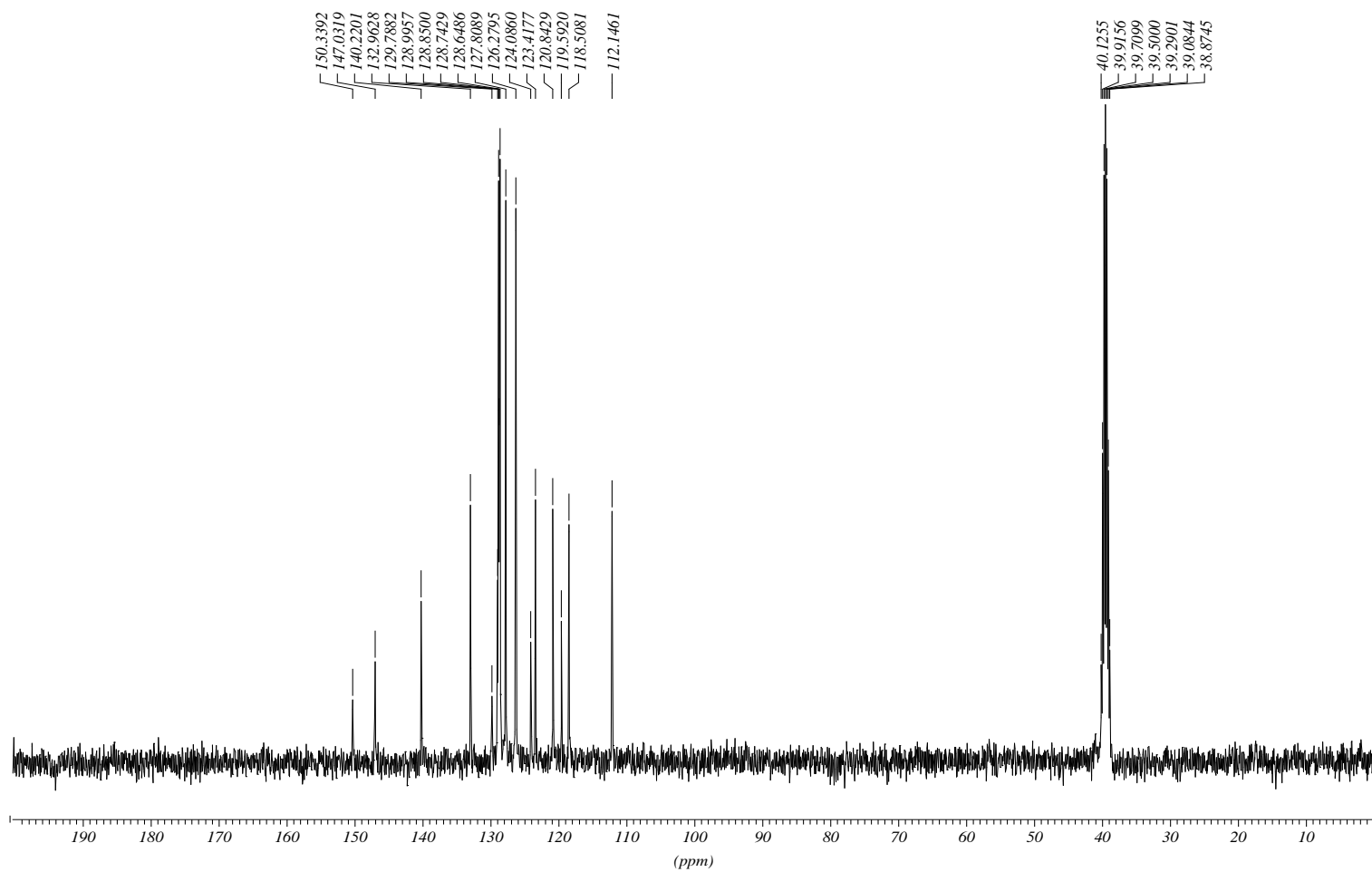
^{13}C NMR spectrum of **3ac** (100.61 MHz, $\text{DMSO-}d_6$)



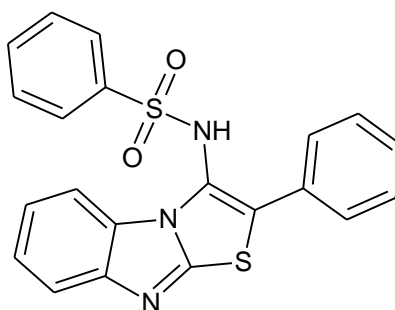


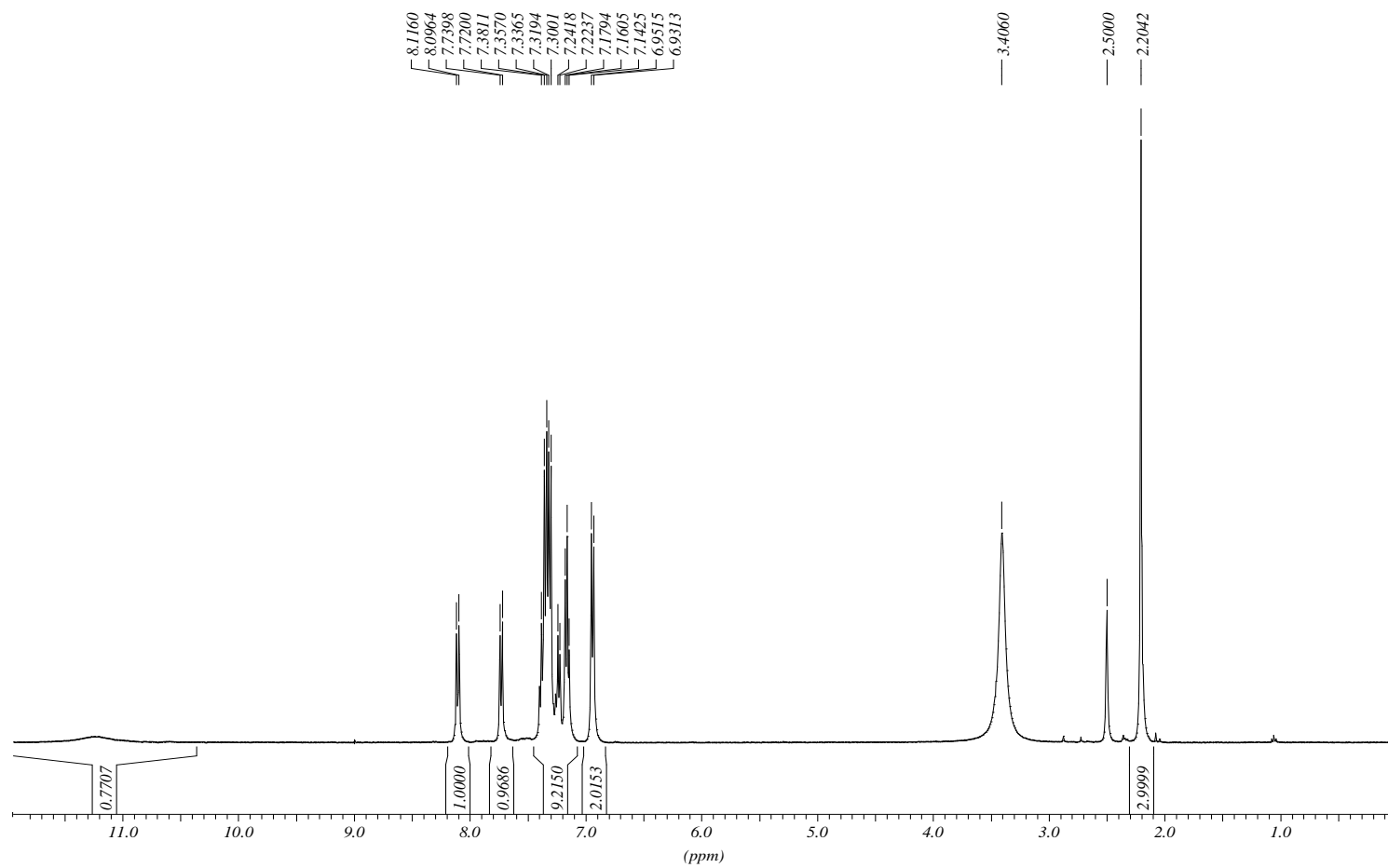
^1H NMR spectrum of **4aa** (400.13 MHz, $\text{DMSO-}d_6$)



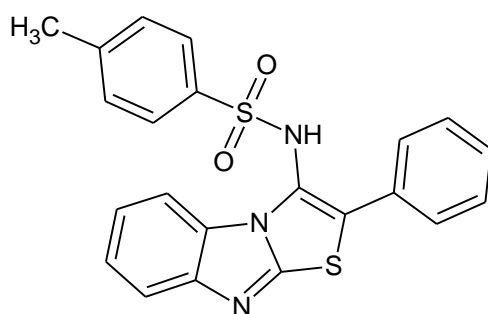


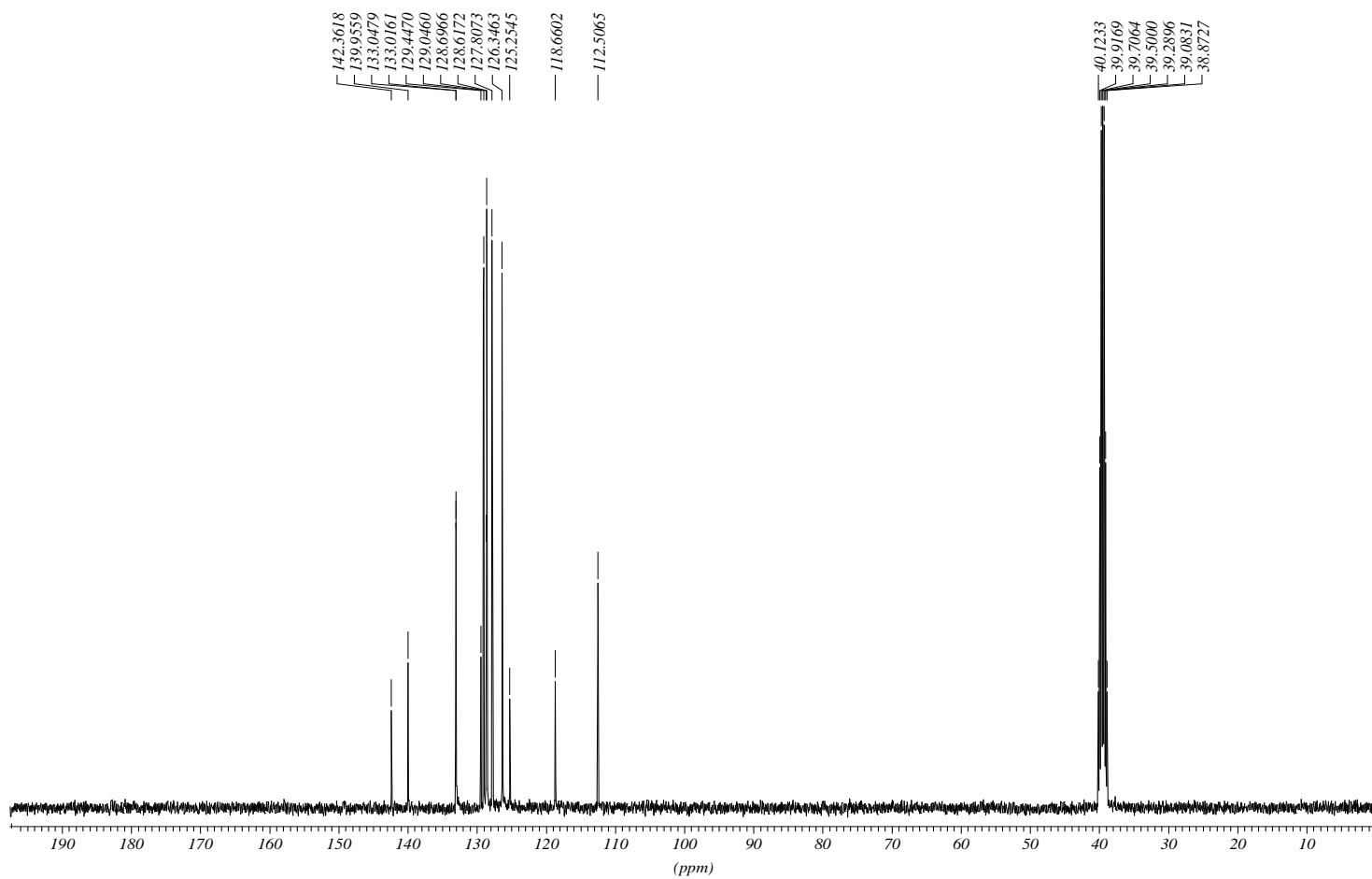
^{13}C NMR spectrum of **4aa** (100.61 MHz, $\text{DMSO-}d_6$)



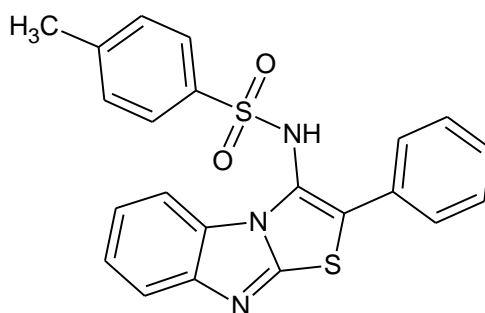


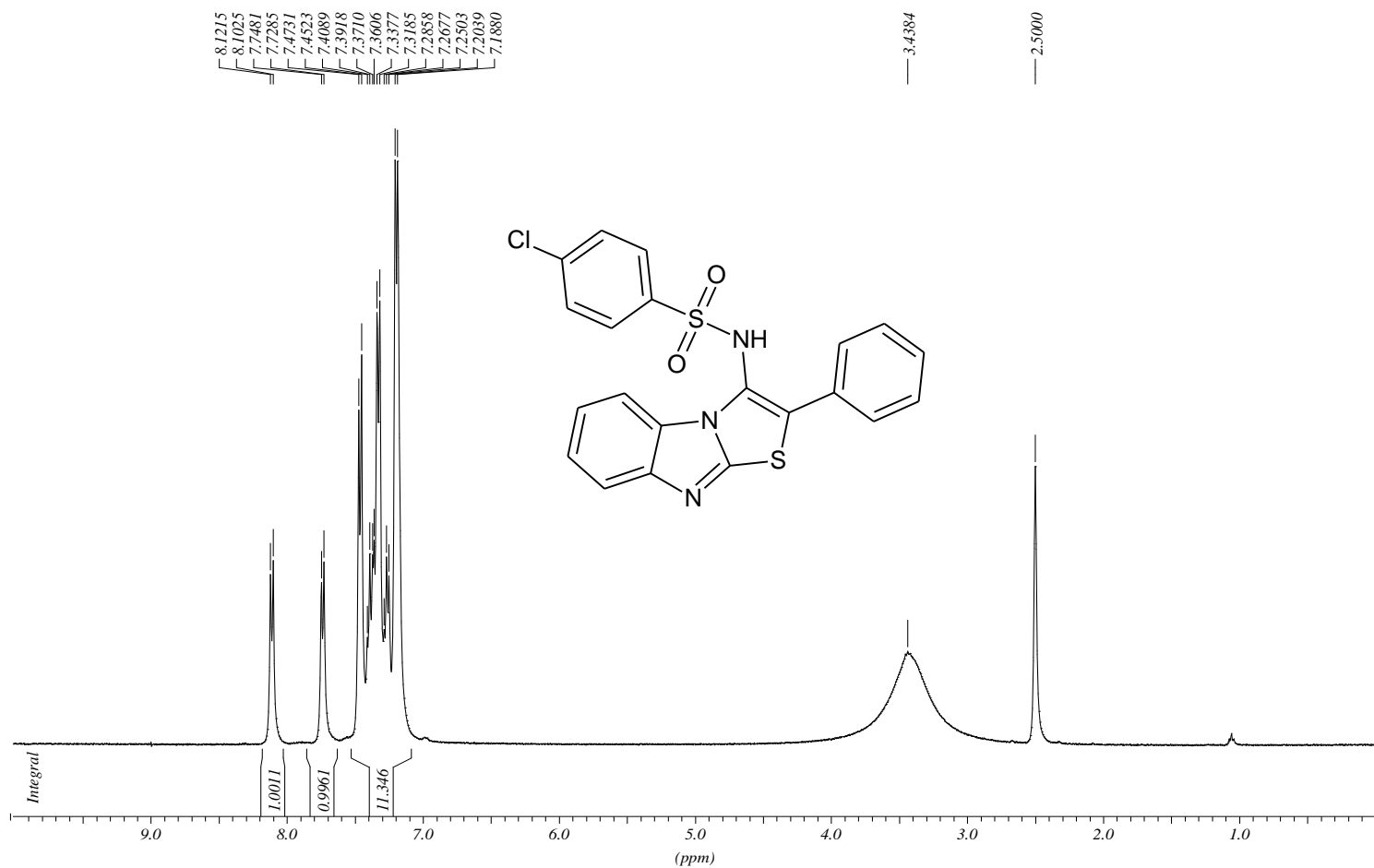
^1H NMR spectrum of **4ba** (400.13 MHz, $\text{DMSO-}d_6$)



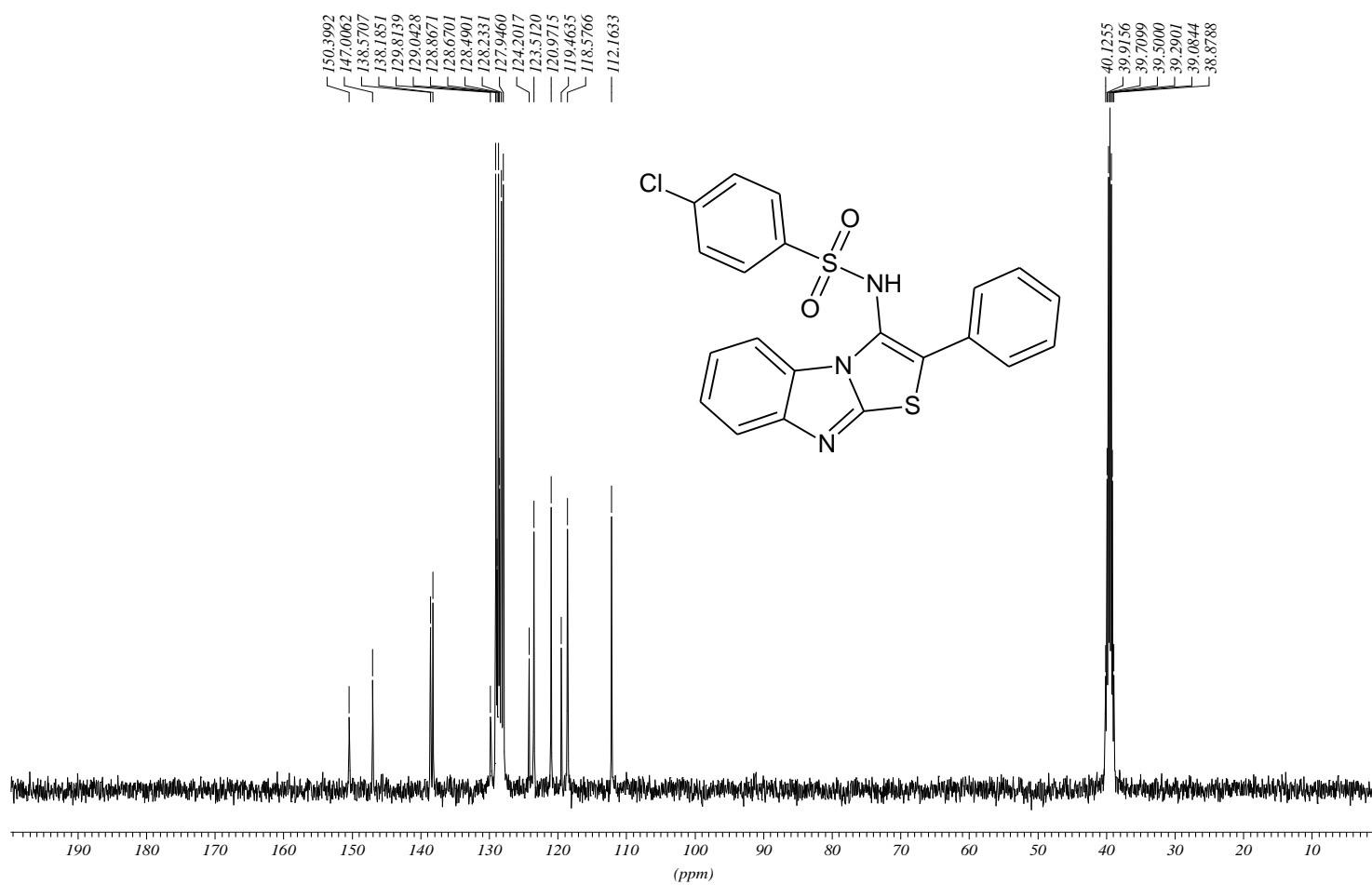


¹³C NMR spectrum of **4ba** (100.61 MHz, DMSO-*d*₆)

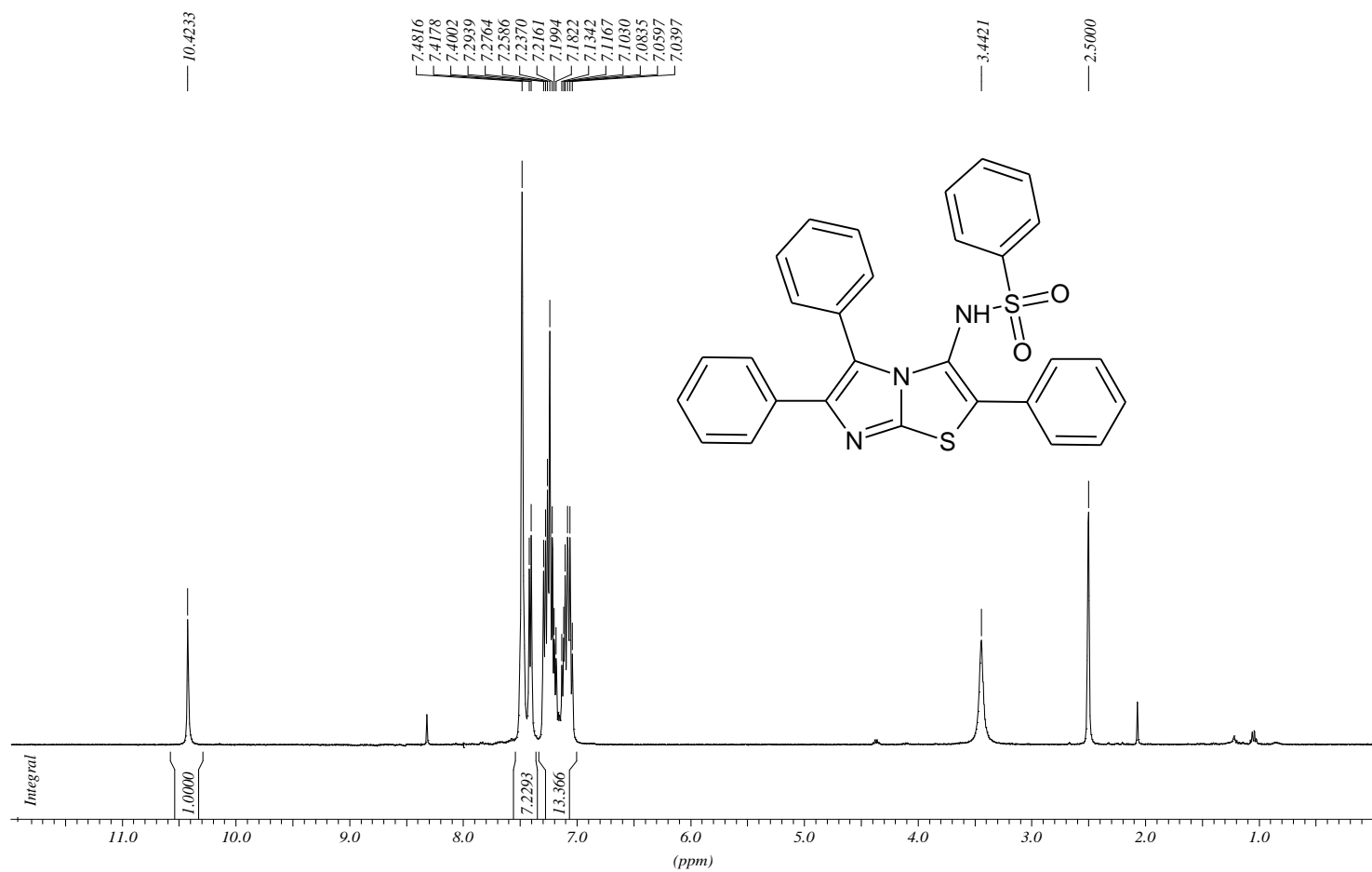




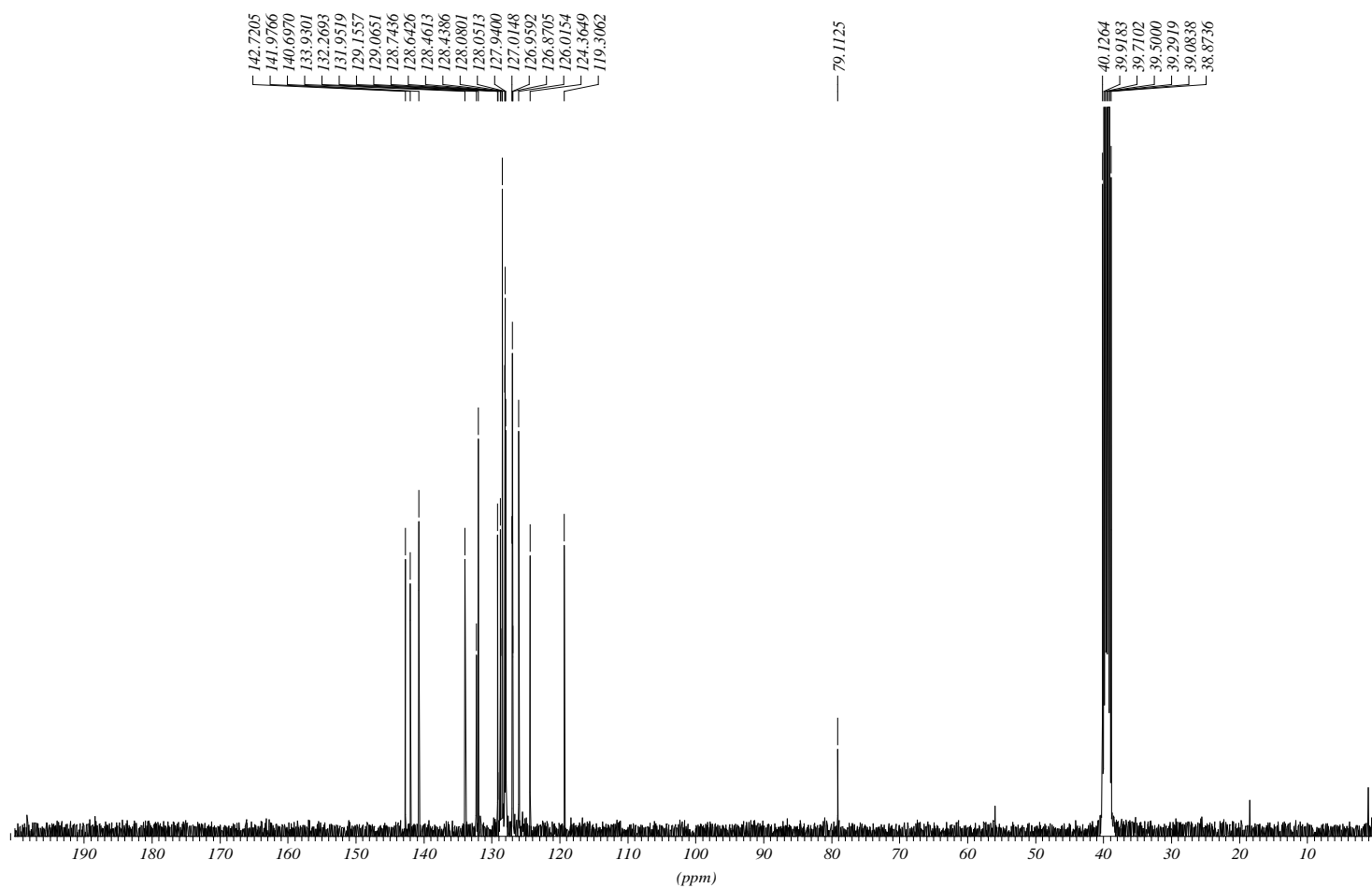
¹H NMR spectrum of **4ca** (400.13 MHz, DMSO-*d*₆)



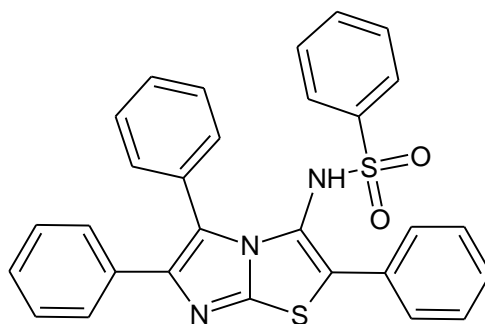
¹³C NMR spectrum of **4ca** (100.61 MHz, DMSO-*d*₆)

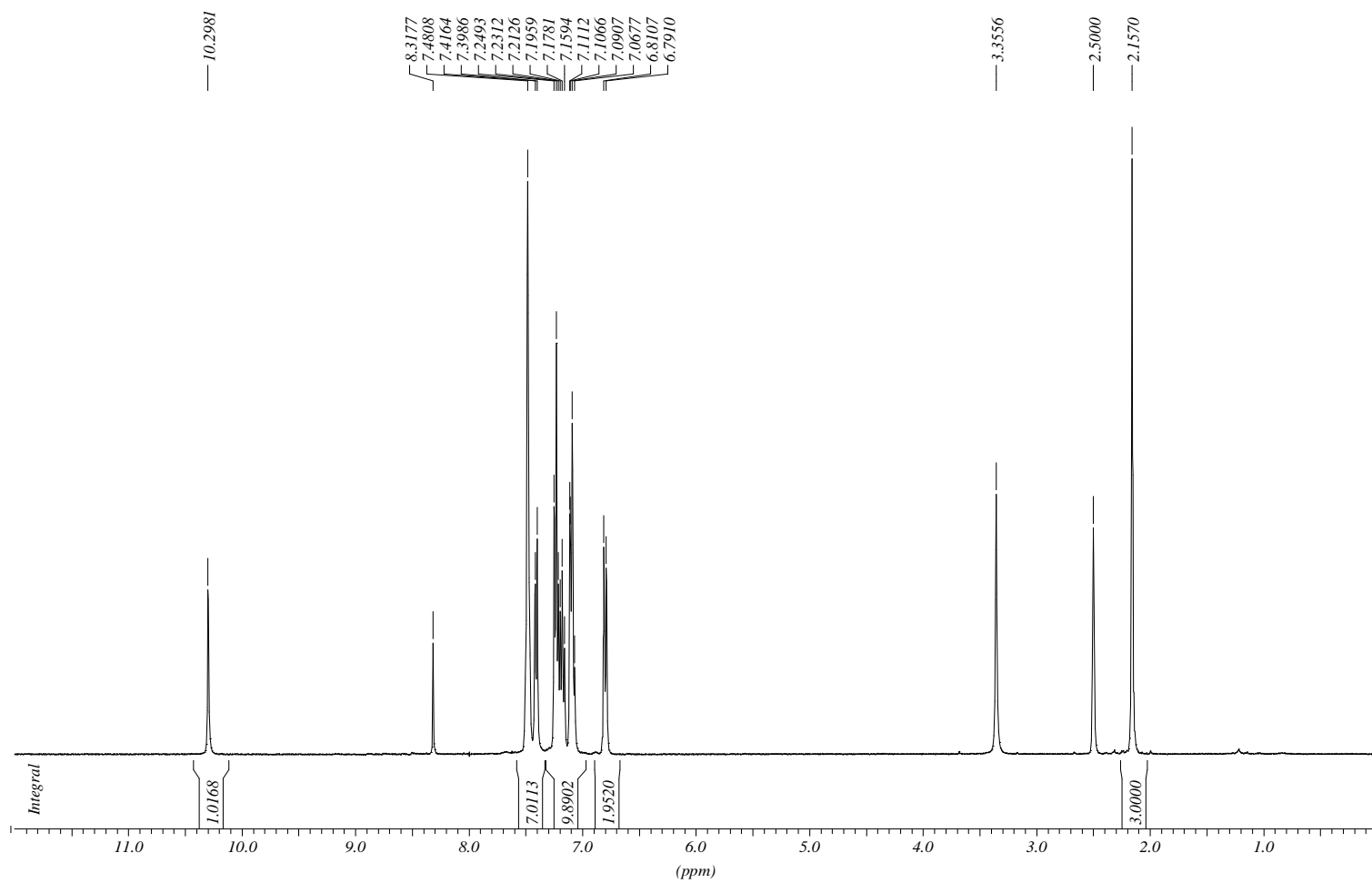


^1H NMR spectrum of **4ab** (400.13 MHz, $\text{DMSO-}d_6$)

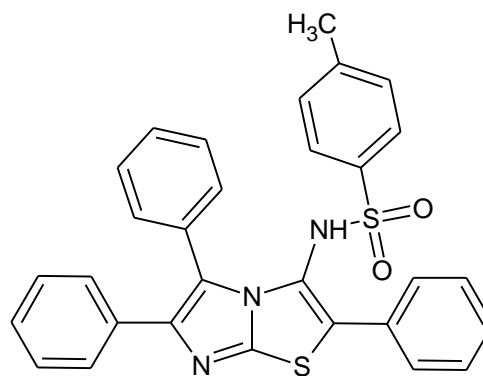


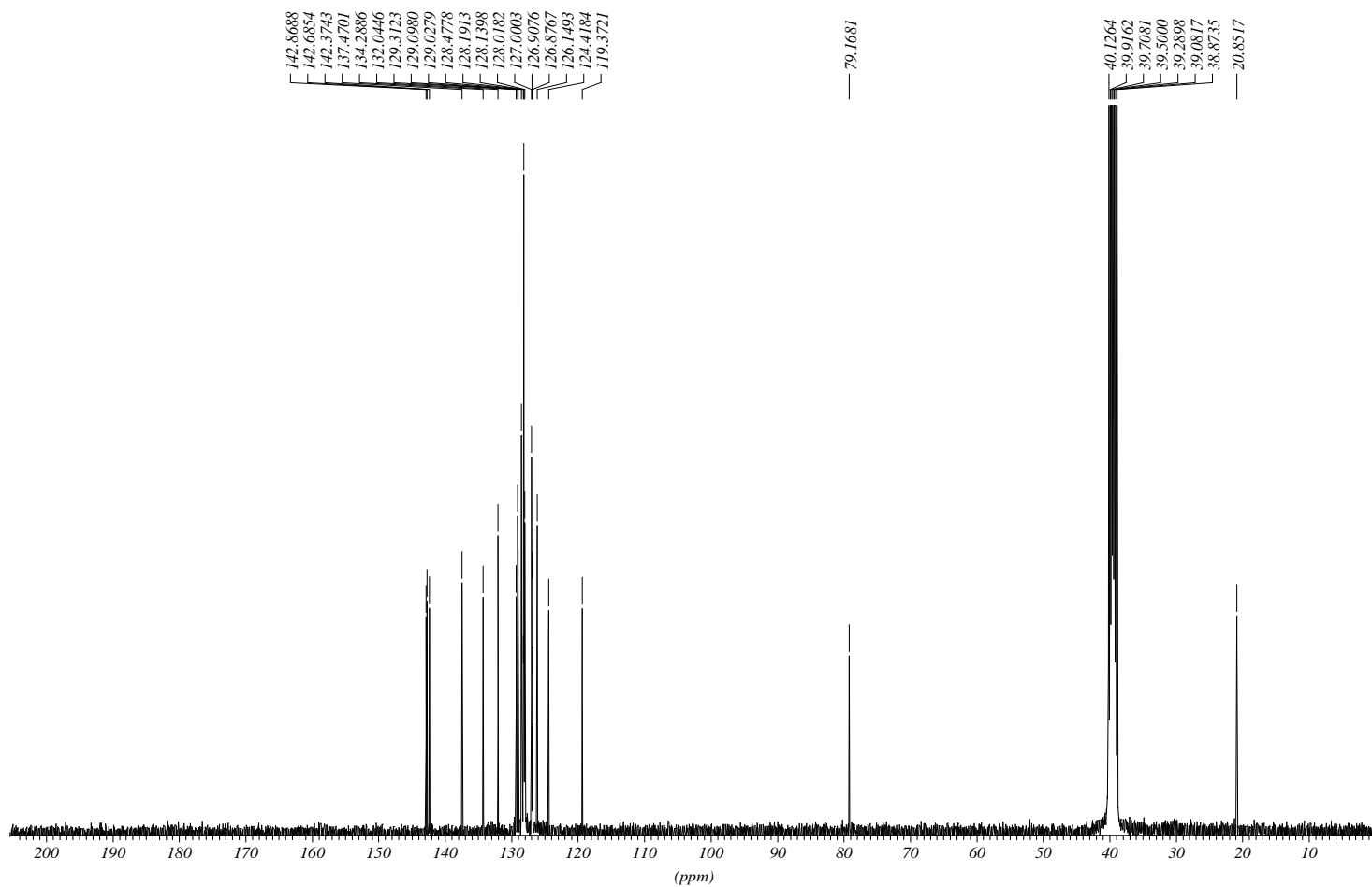
^{13}C NMR spectrum of **4ab** (100.61 MHz, $\text{DMSO-}d_6$)



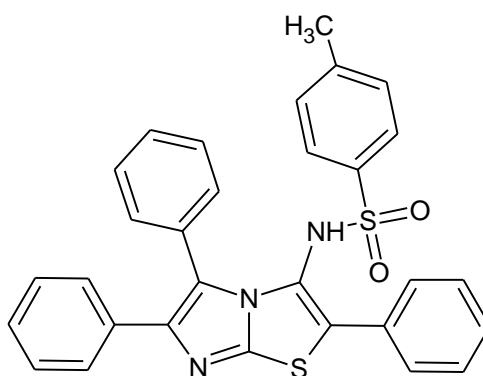


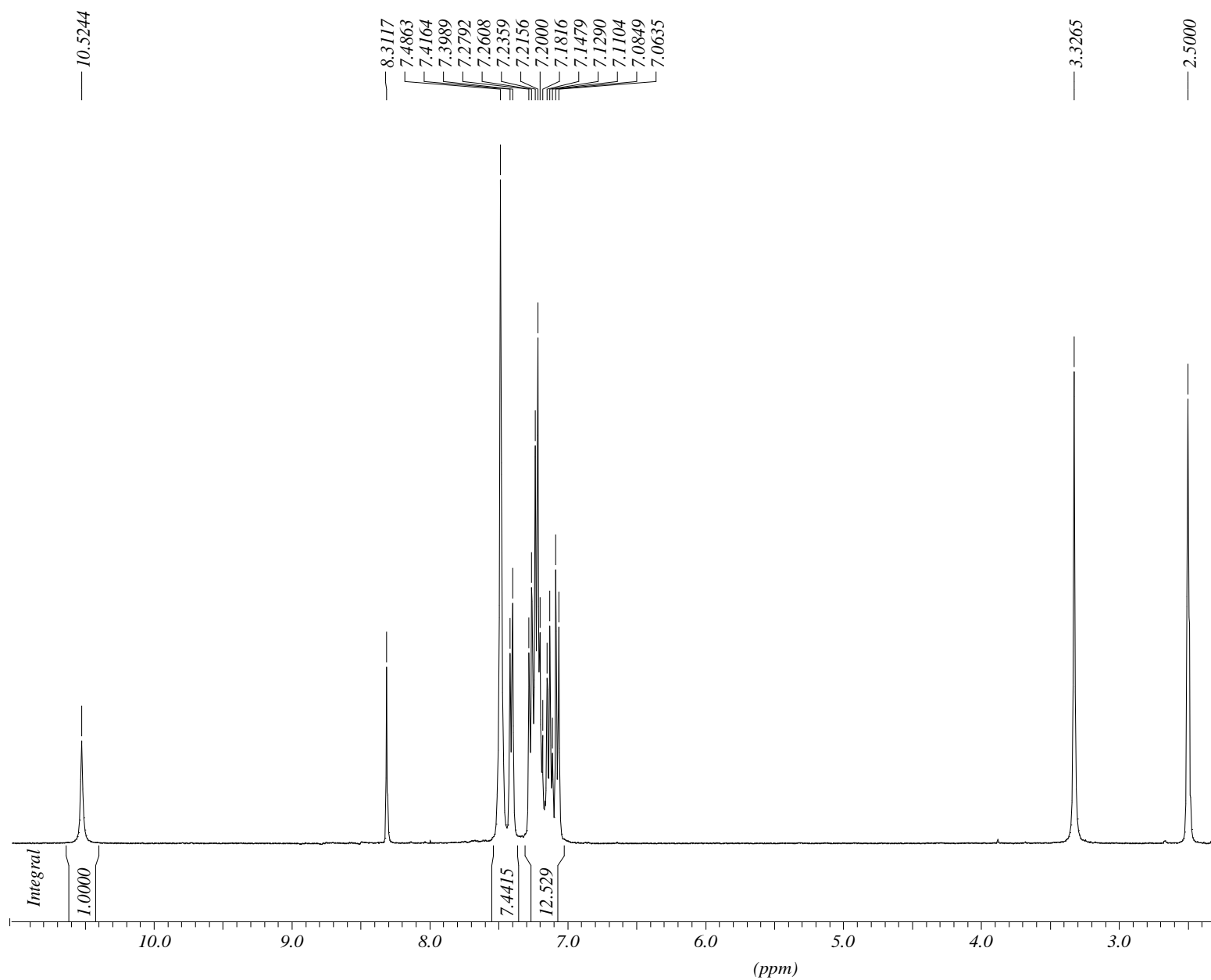
¹H NMR spectrum of **4bb** (400.13 MHz, DMSO-*d*₆)



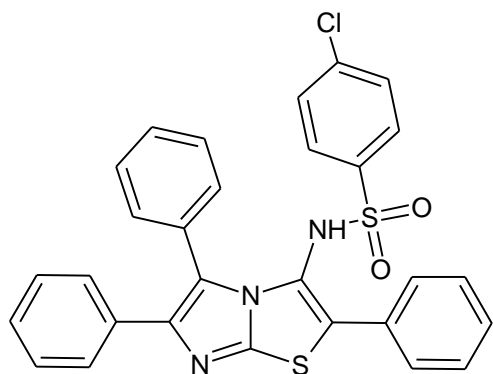


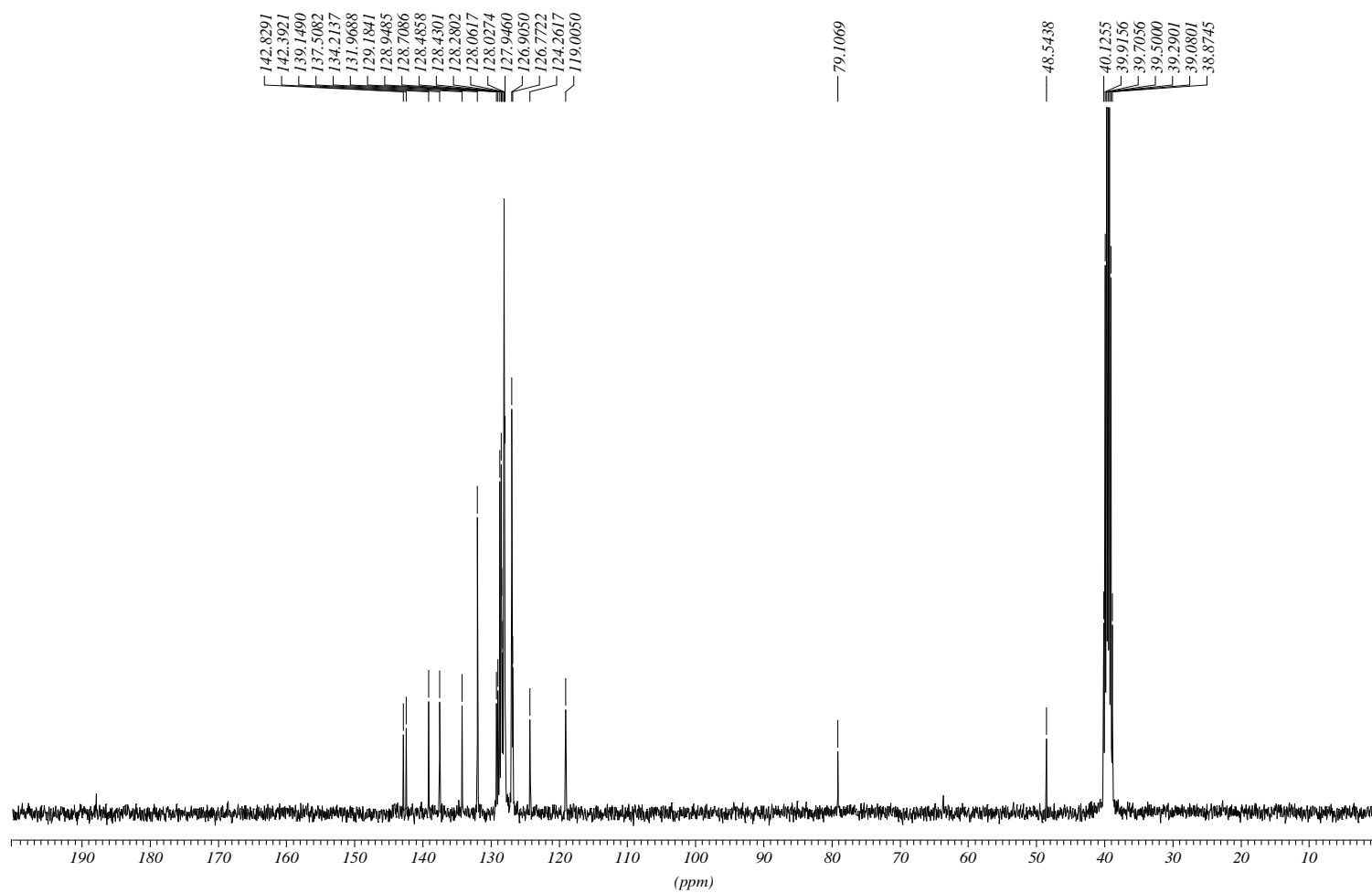
^{13}C NMR spectrum of **4bb** (100.61 MHz, $\text{DMSO-}d_6$)



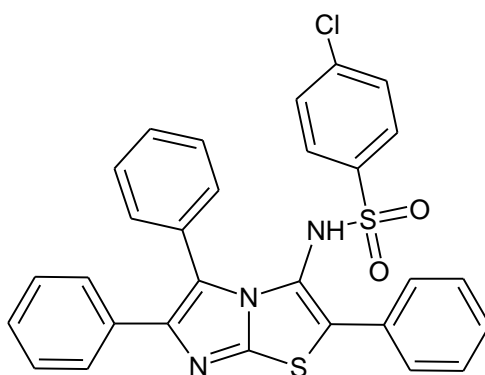


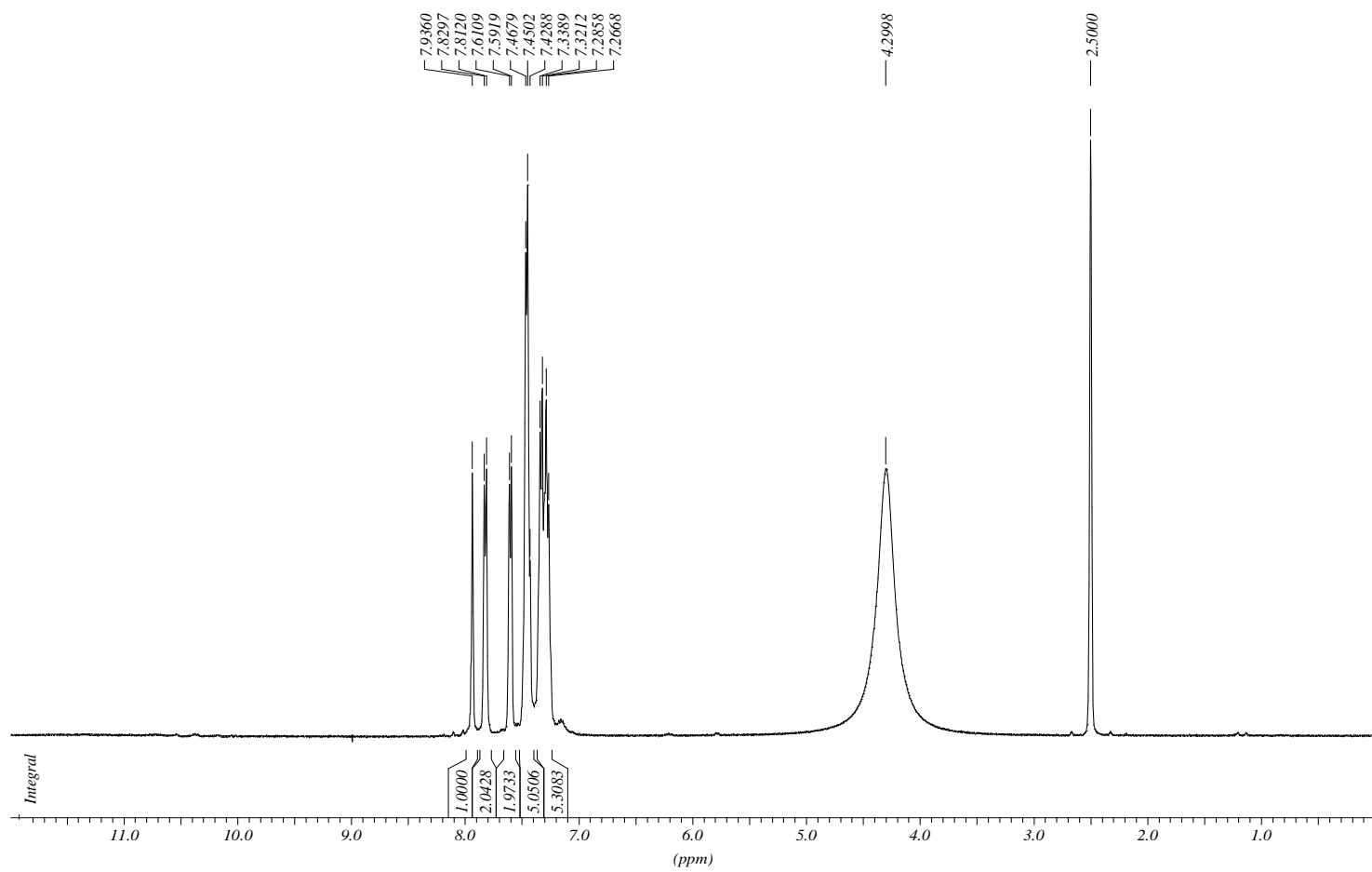
^1H NMR spectrum of **4cb** (400.13 MHz, $\text{DMSO-}d_6$)



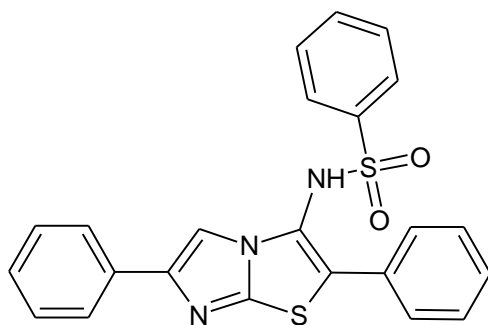


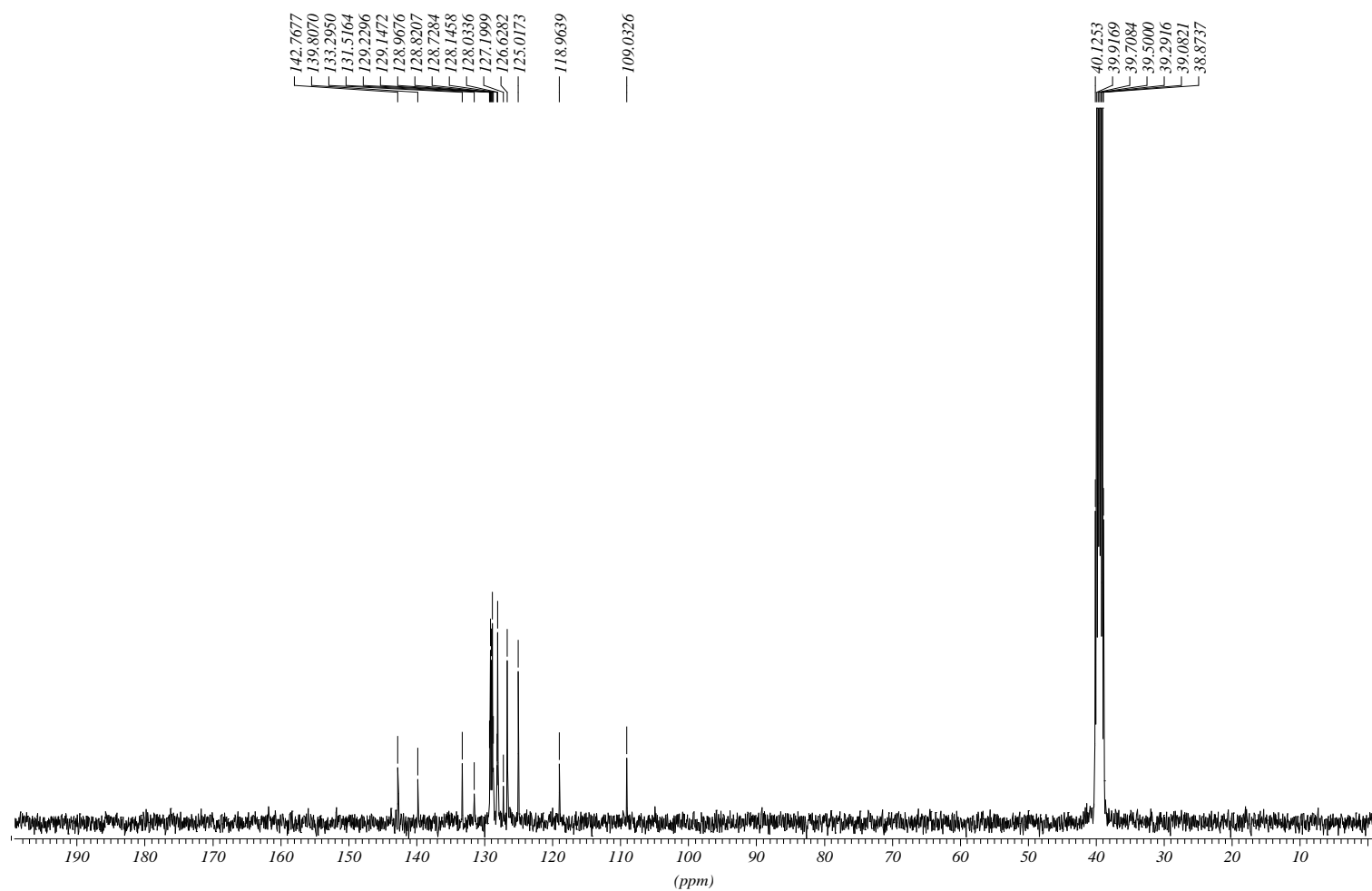
¹³C NMR spectrum of **4cb** (100.61 MHz, DMSO-*d*₆)



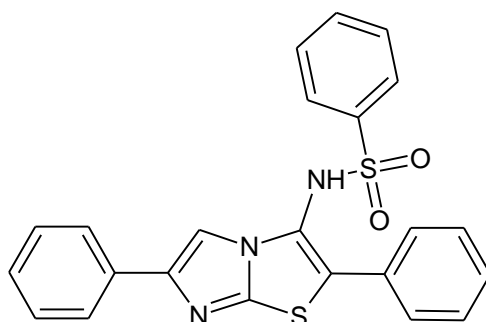


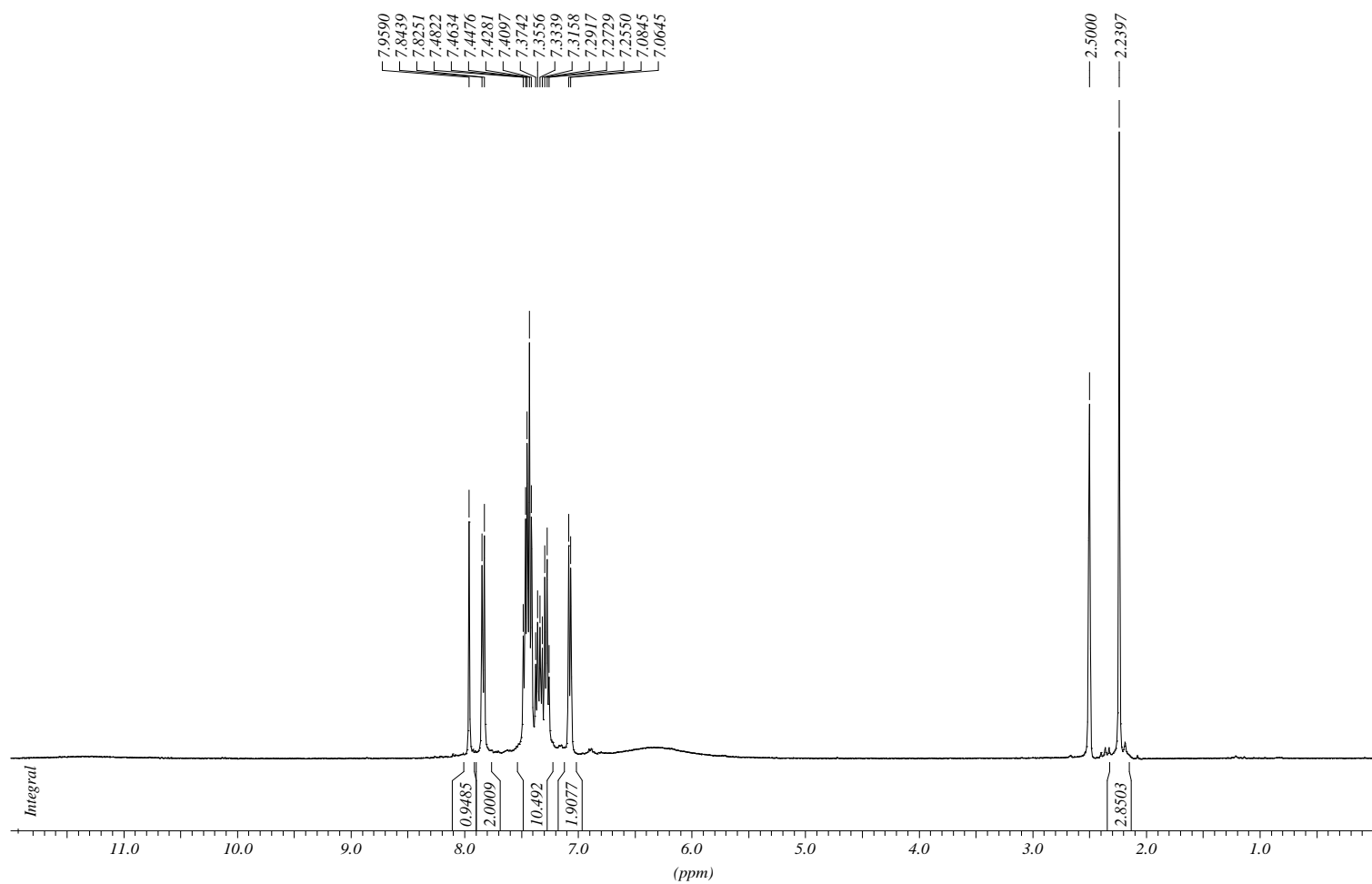
¹H NMR spectrum of **4ac** (400.13 MHz, DMSO-*d*₆)



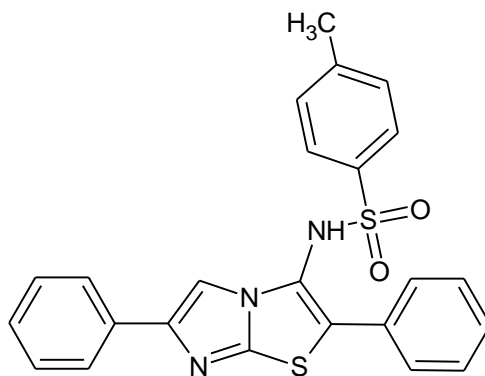


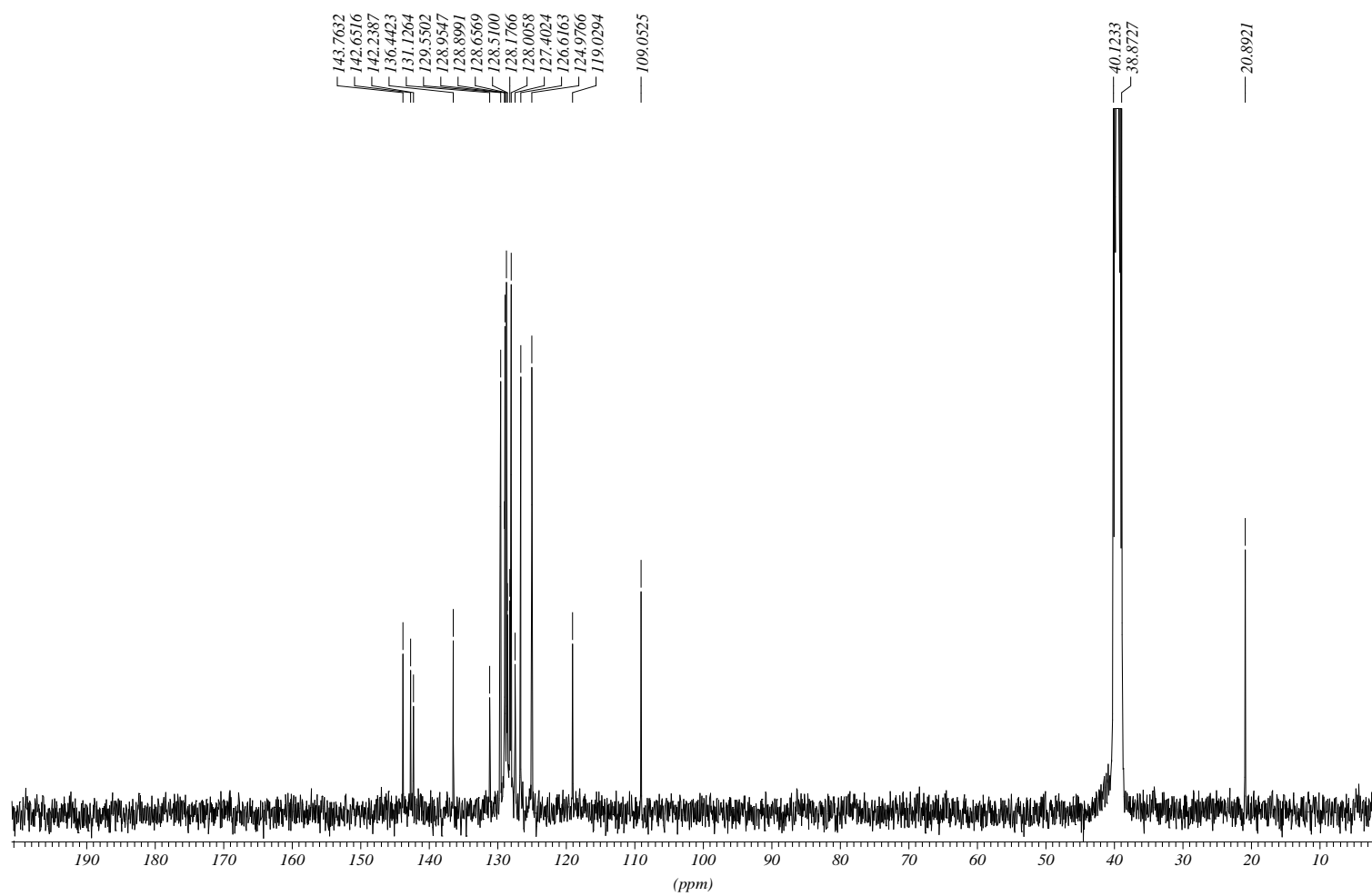
^{13}C NMR spectrum of **4ac** (100.61 MHz, $\text{DMSO-}d_6$)



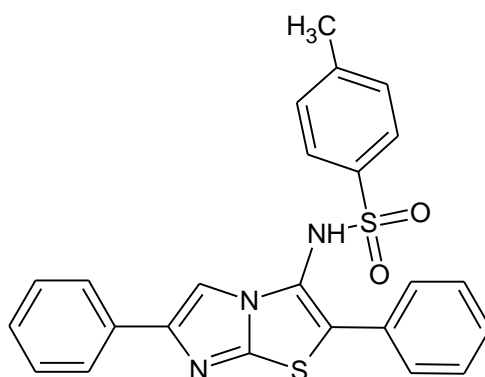


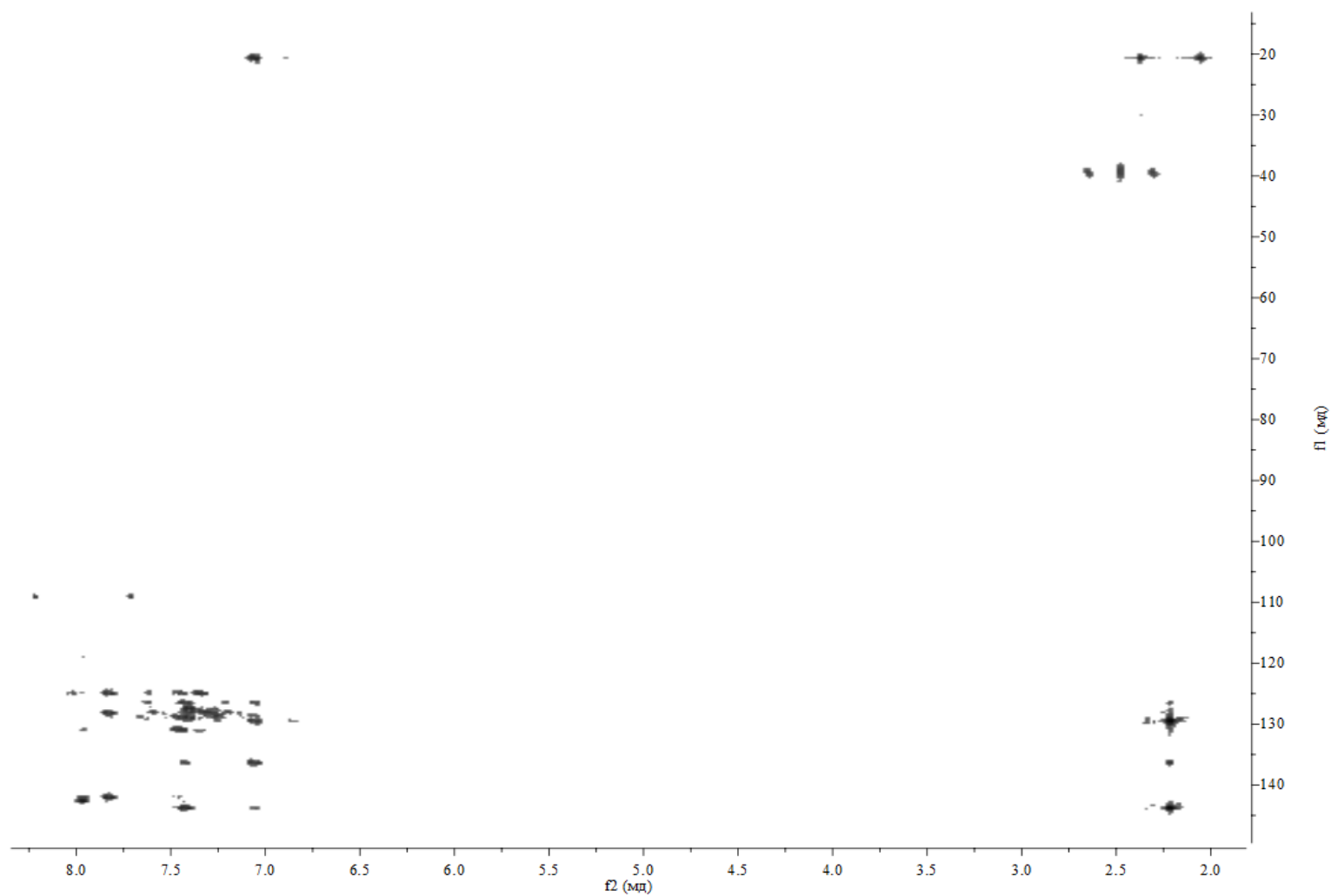
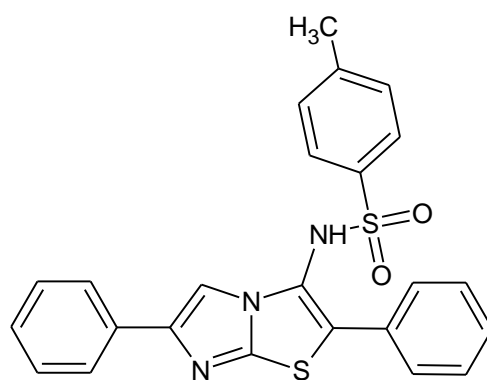
¹H NMR spectrum of **4bc** (400.13 MHz, DMSO-*d*₆)

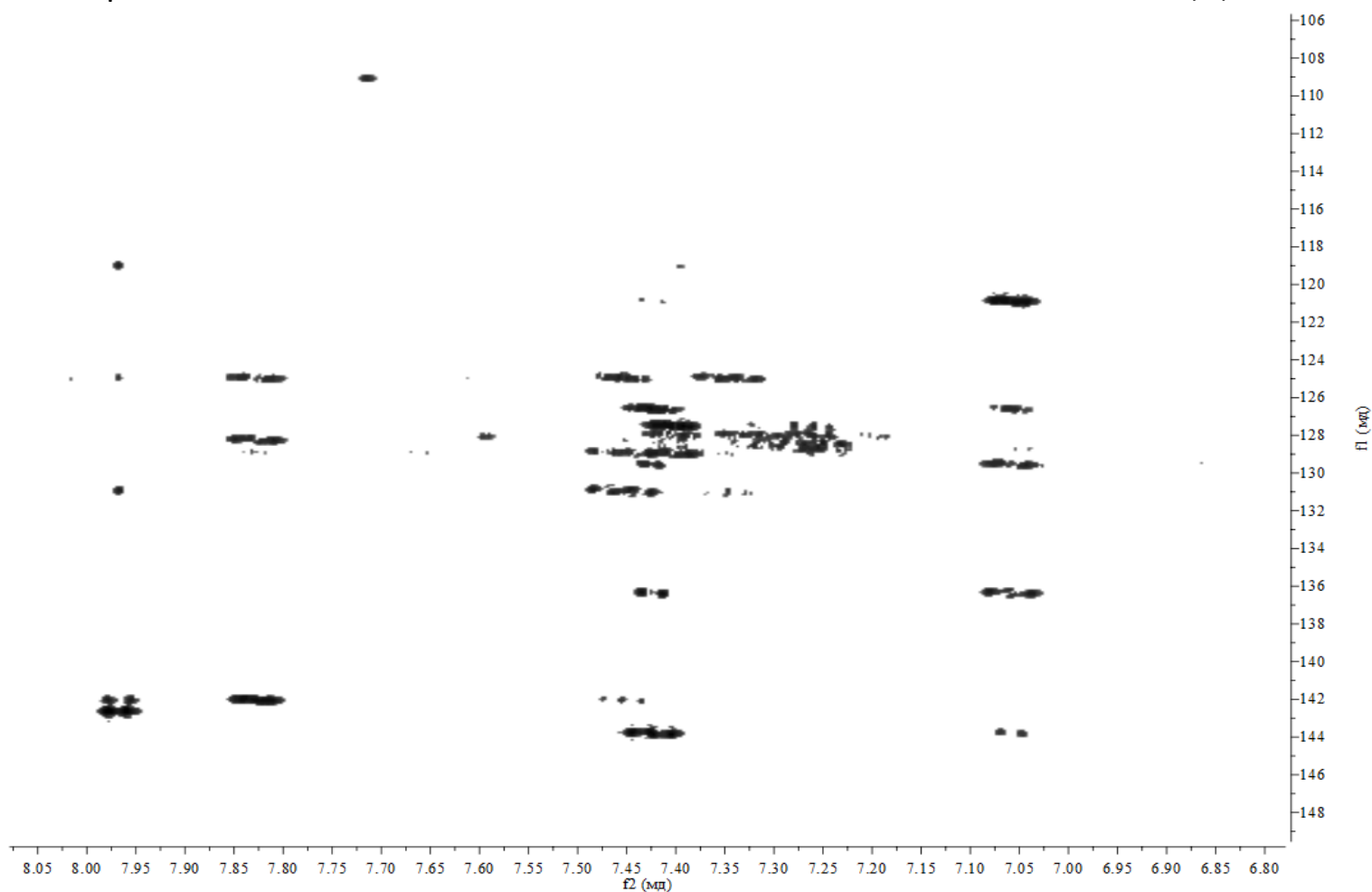




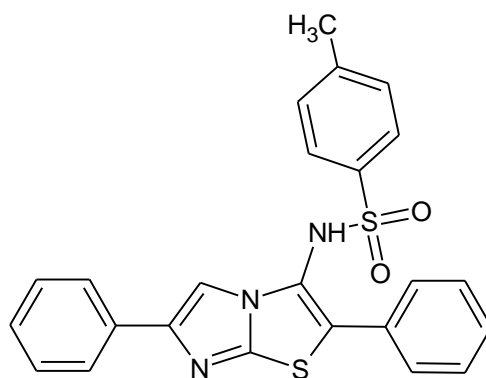
^{13}C NMR spectrum of **4bc** (100.61 MHz, $\text{DMSO-}d_6$)

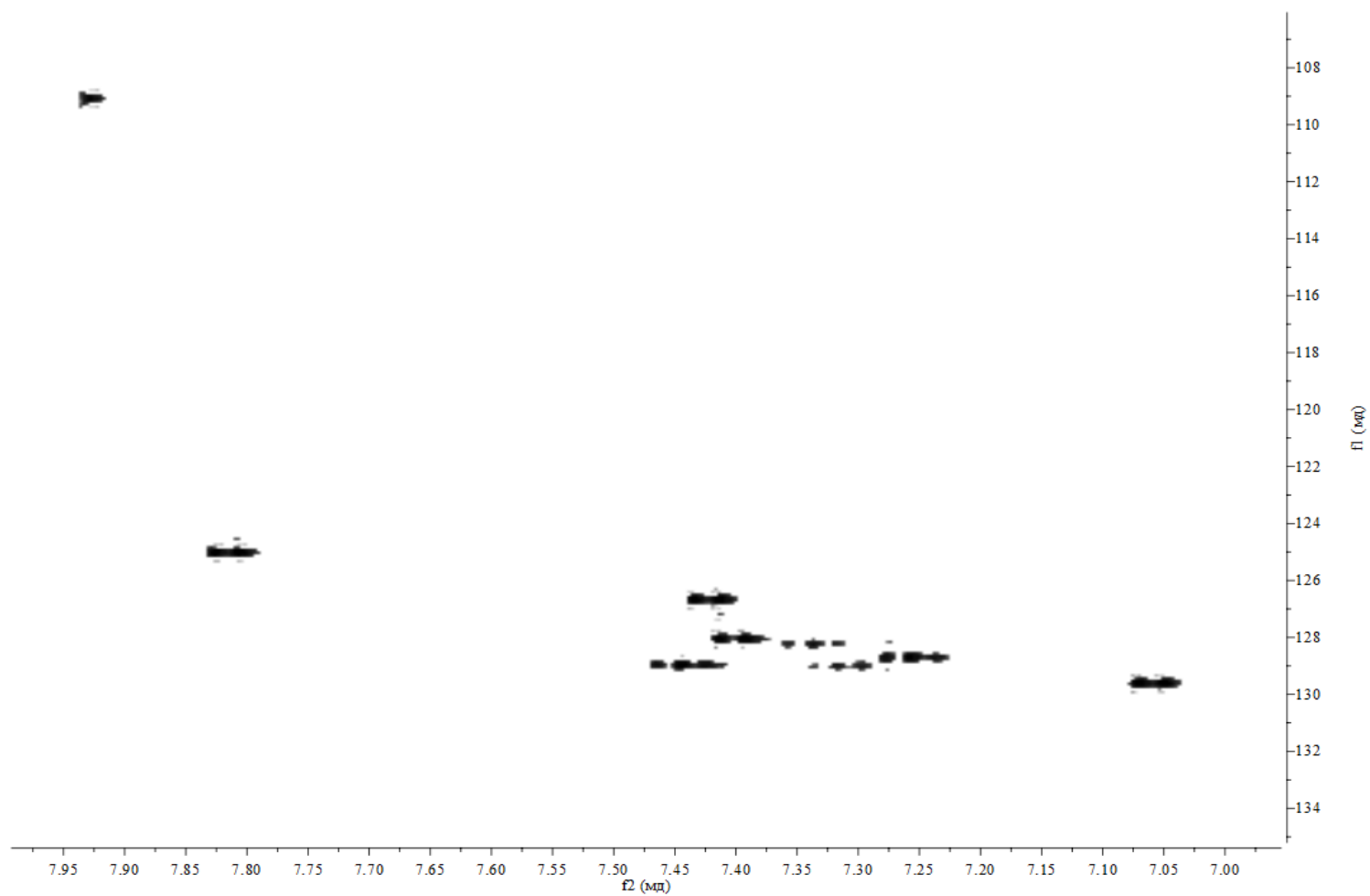
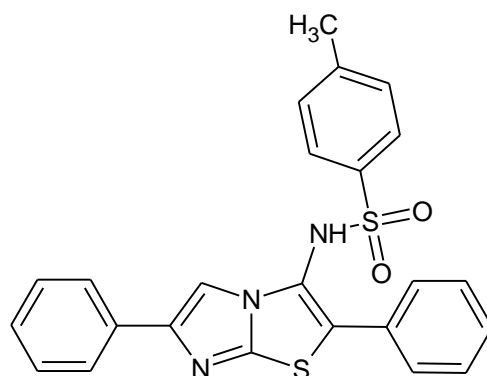


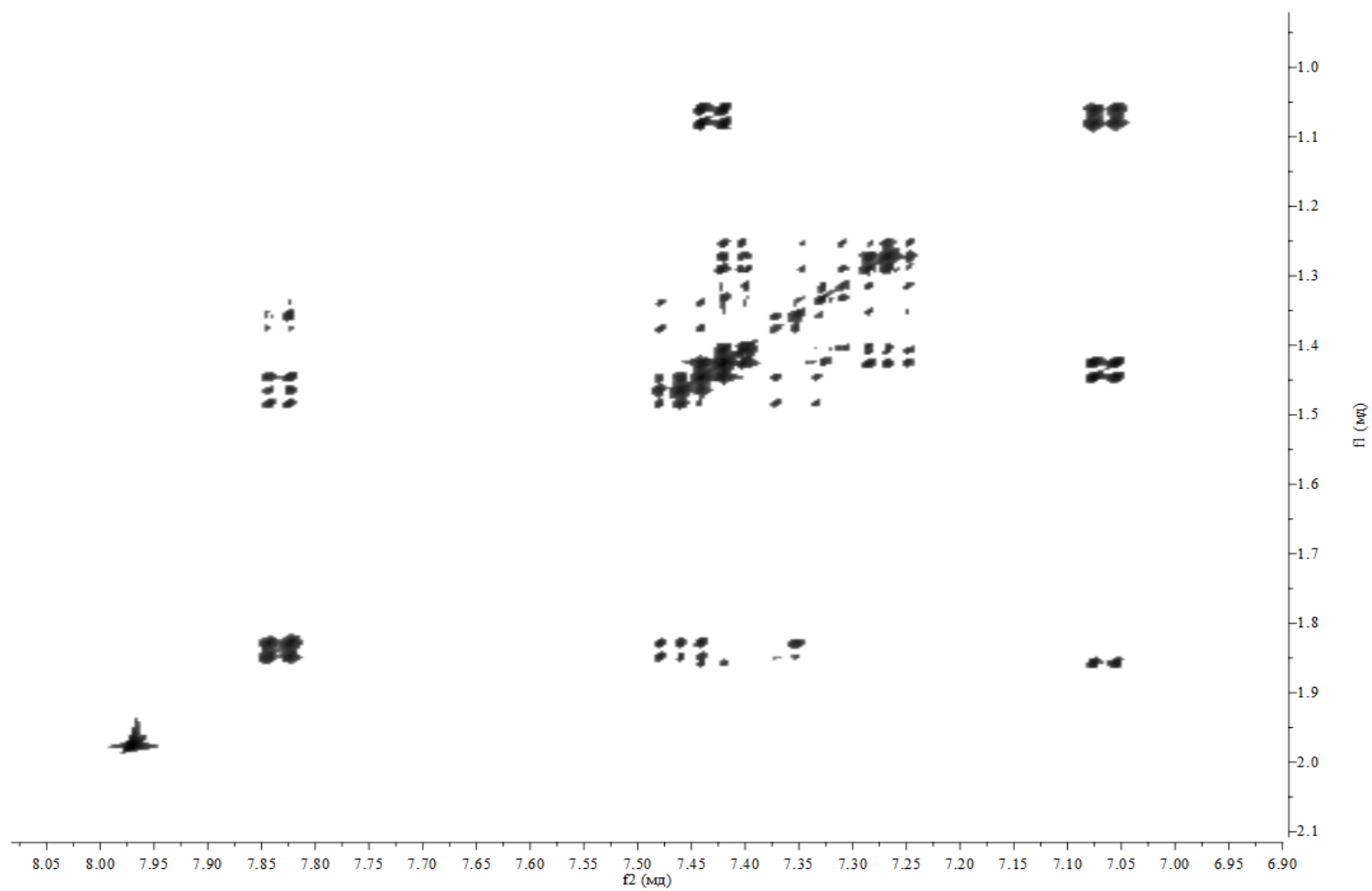
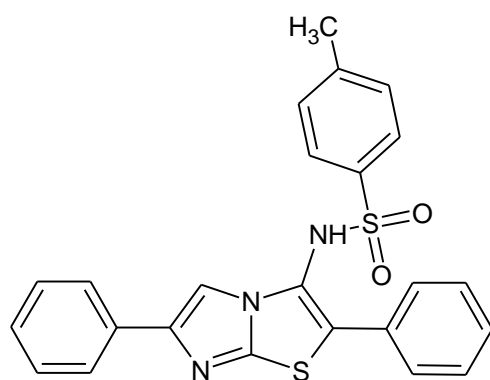
2D ^1H - ^{13}C HMBC spectrum of **4bc**(DMSO- d_6)

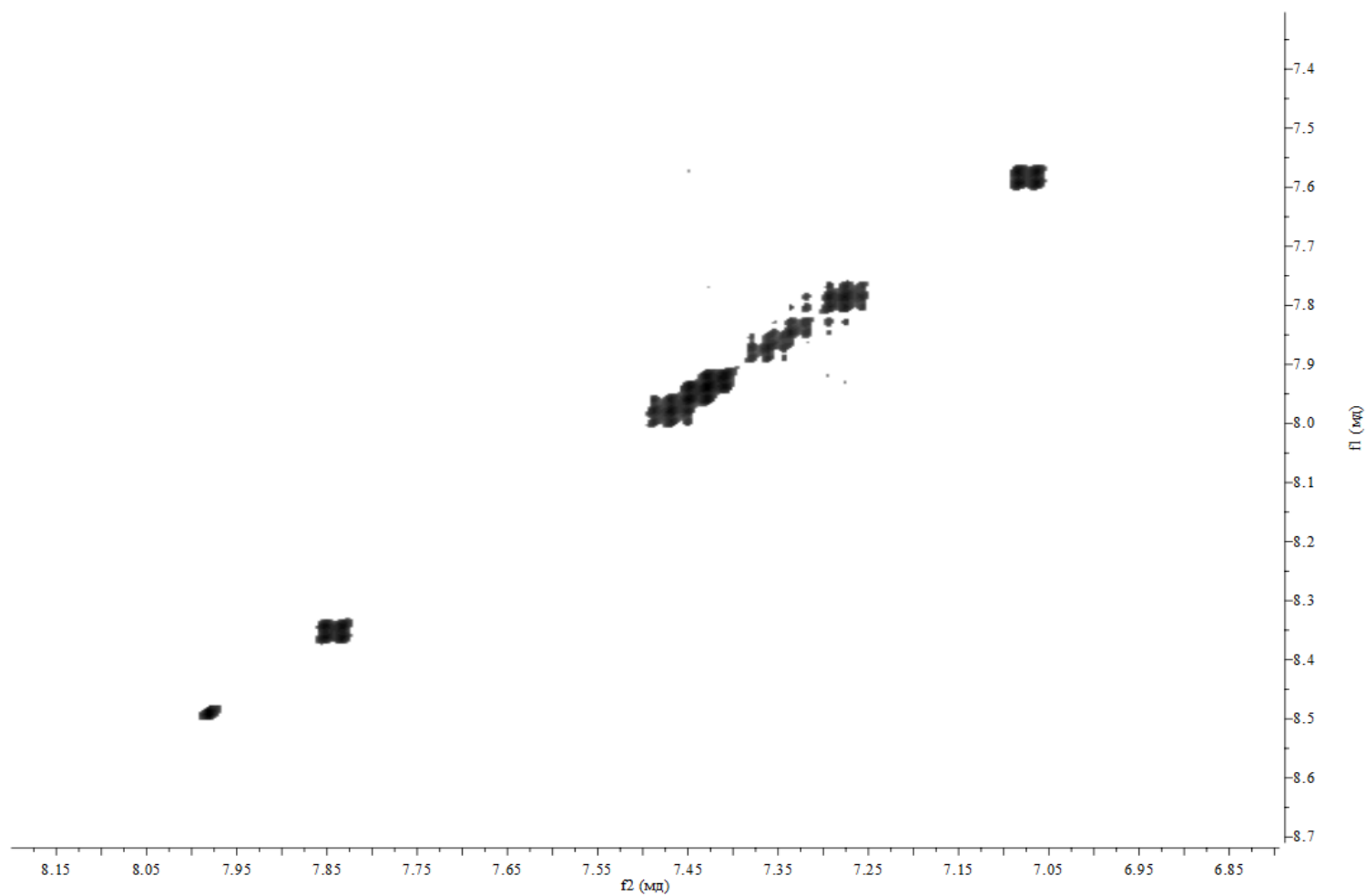
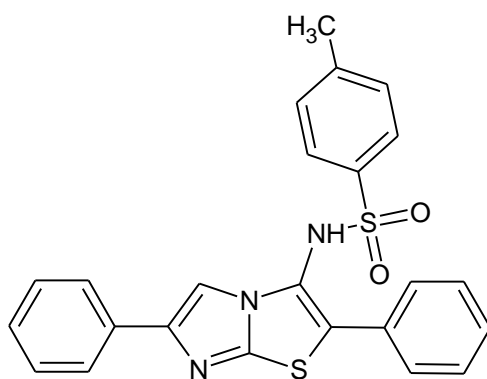


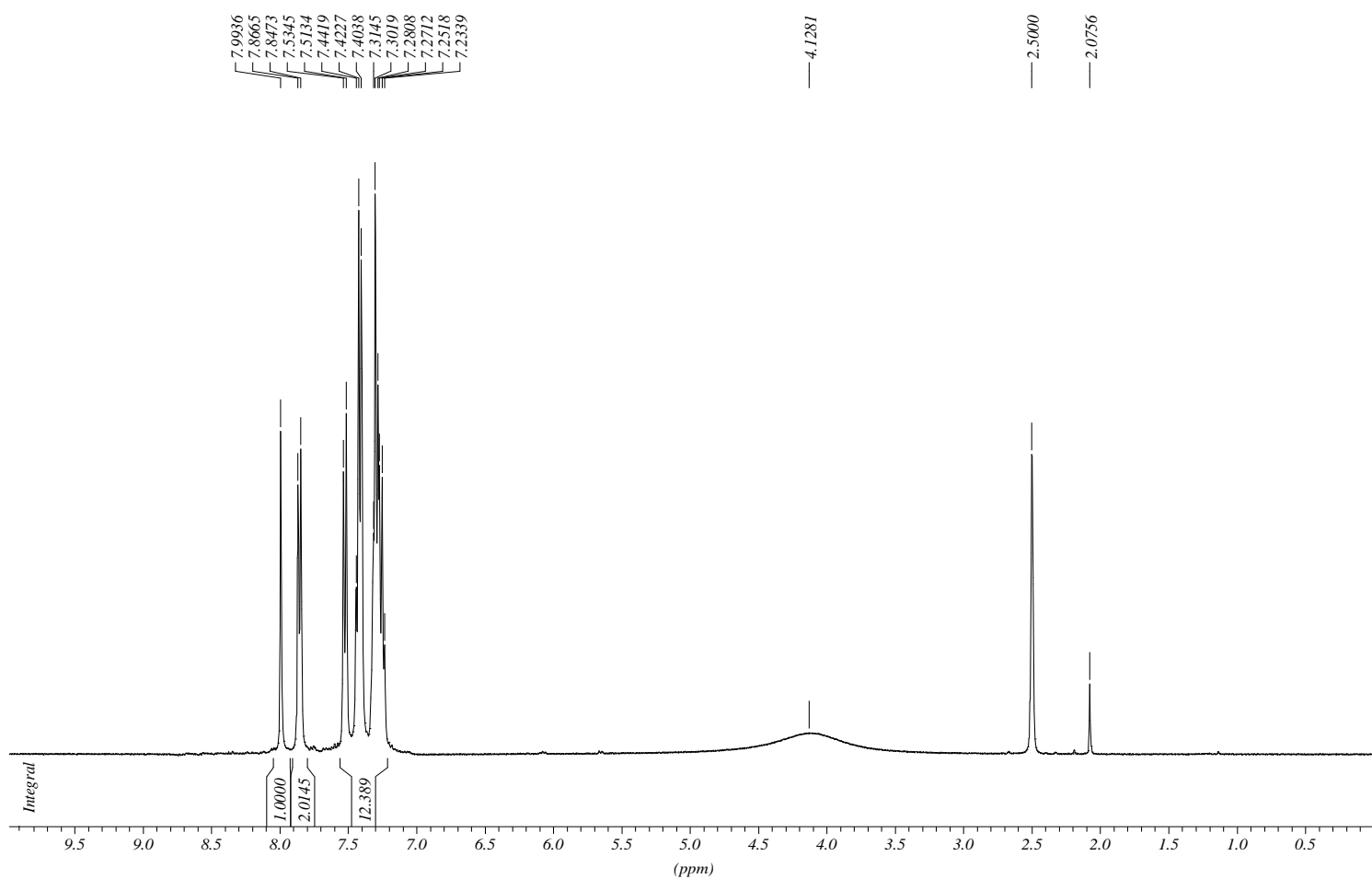
2D ^1H - ^{13}C HMBC spectrum of **4bc**(DMSO- d_6) -low field region



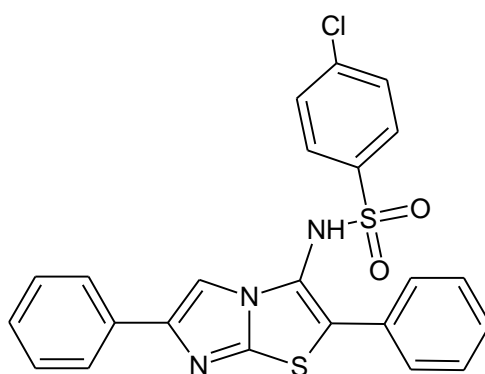
2D ^1H - ^{13}C HSQC spectrum of **4bc**(DMSO- d_6)

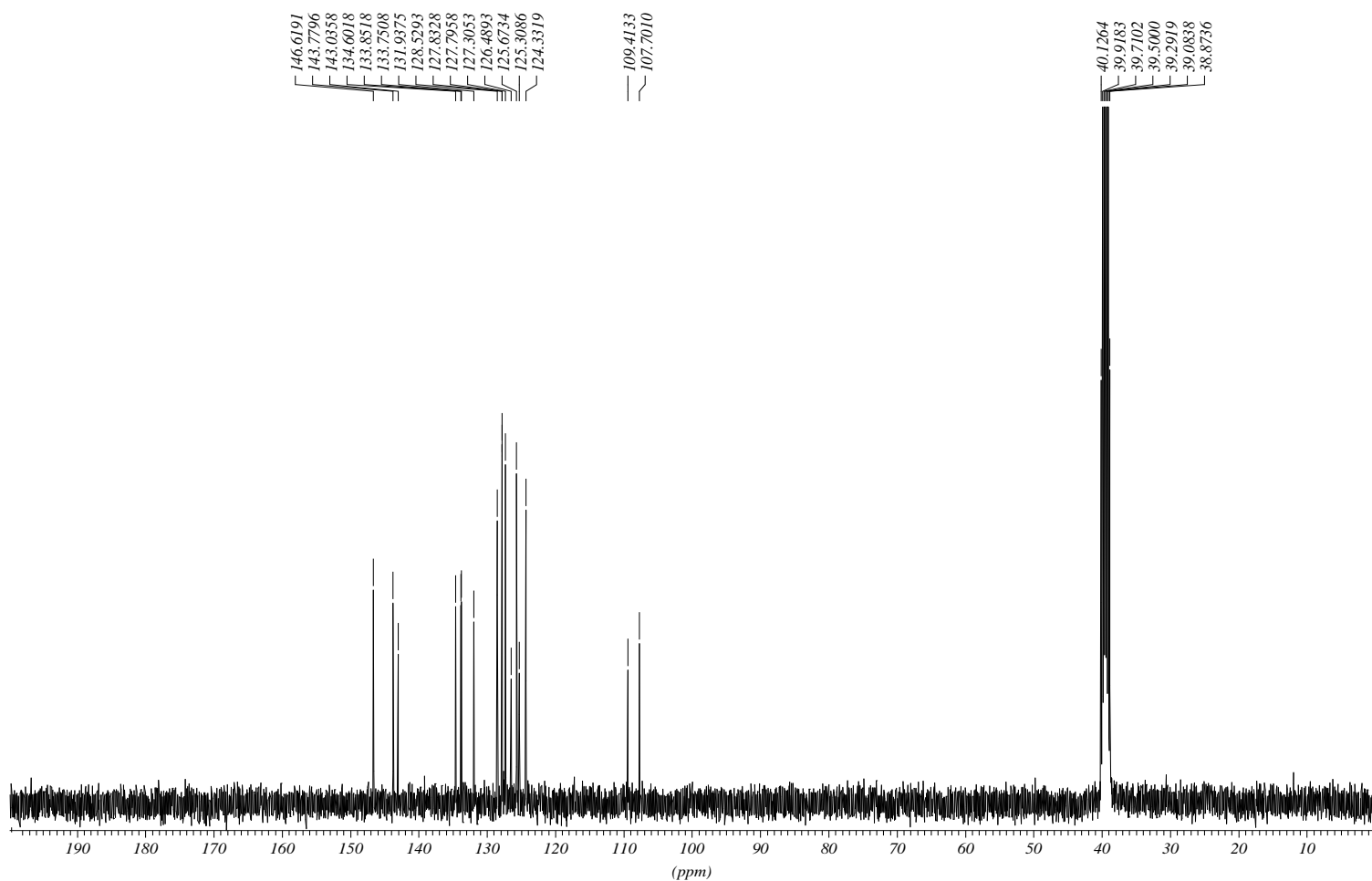
2D ^1H - ^1H COSY spectrum of **4bc**(DMSO- d_6)

2D ^1H - ^1H NOESY spectrum of **4bc**(DMSO- d_6)

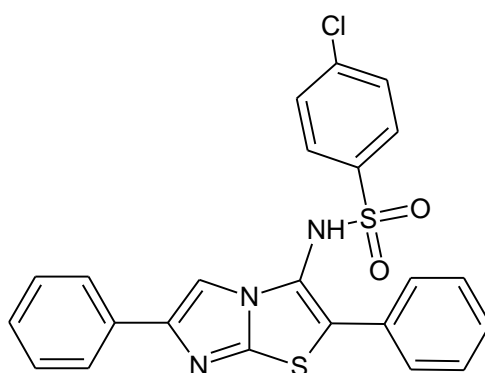


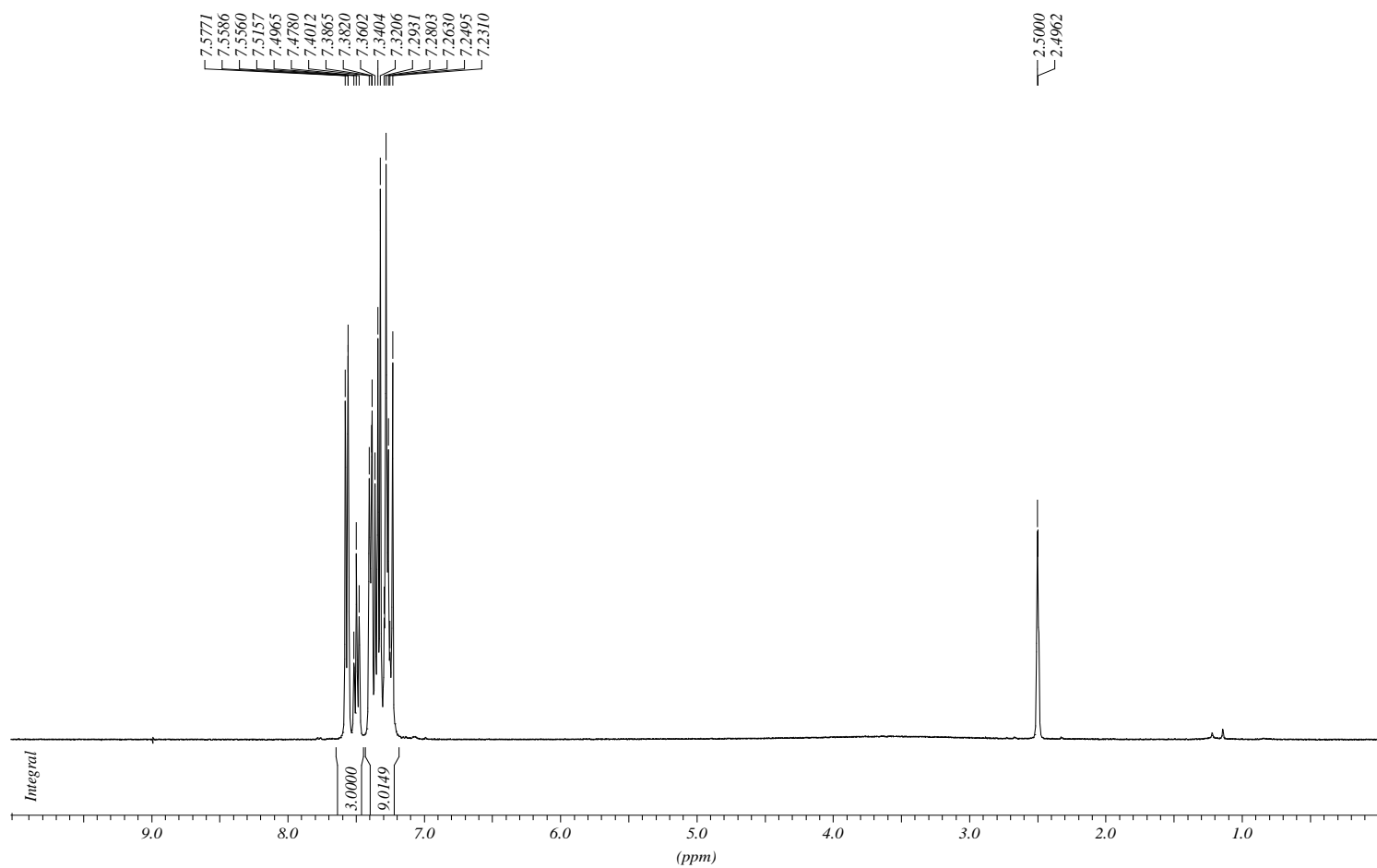
¹H NMR spectrum of **4cc** (400.13 MHz, DMSO-*d*₆)



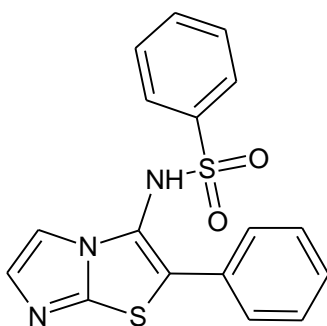


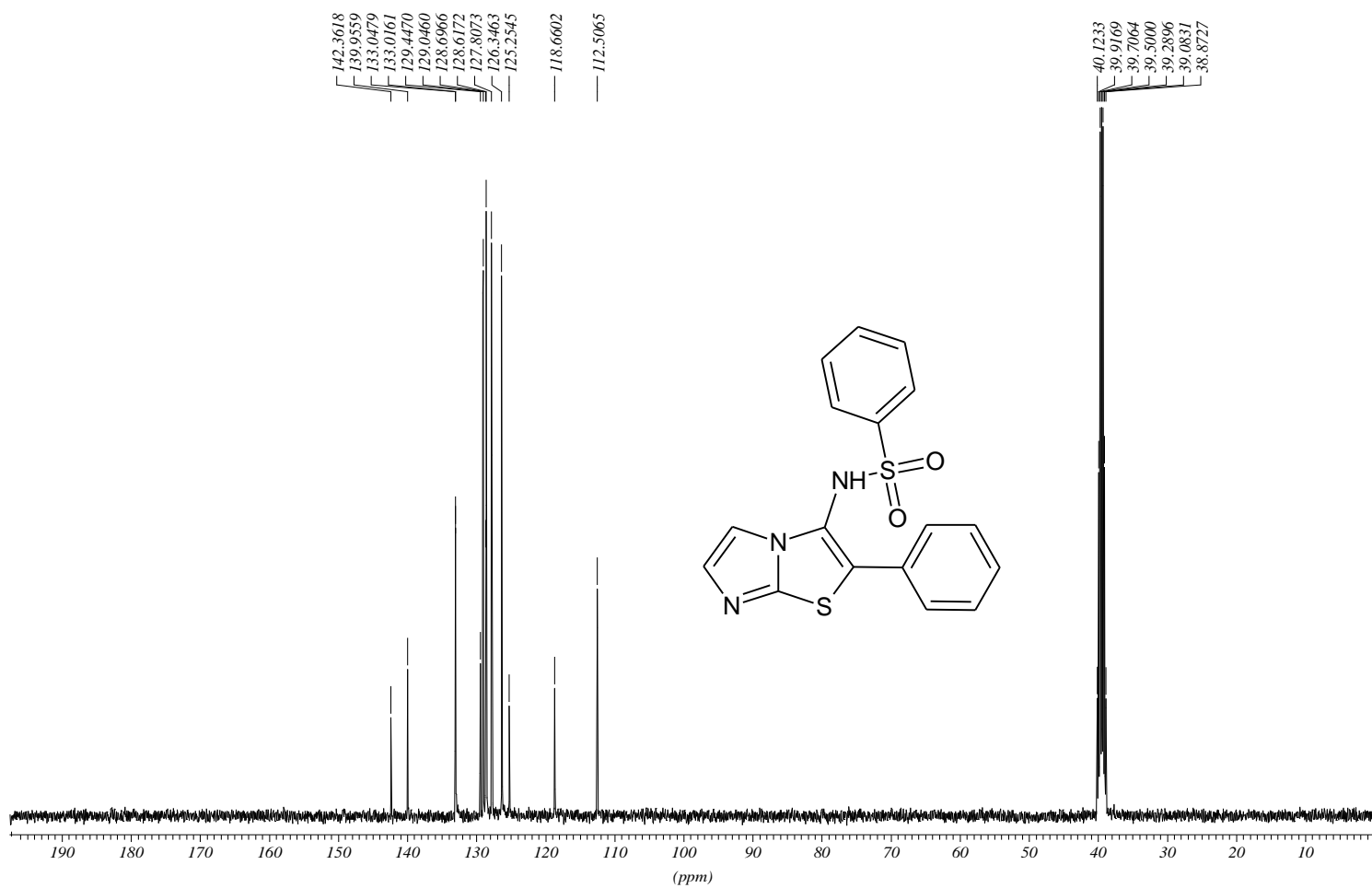
^{13}C NMR spectrum of **4cc** (100.61 MHz, $\text{DMSO-}d_6$)



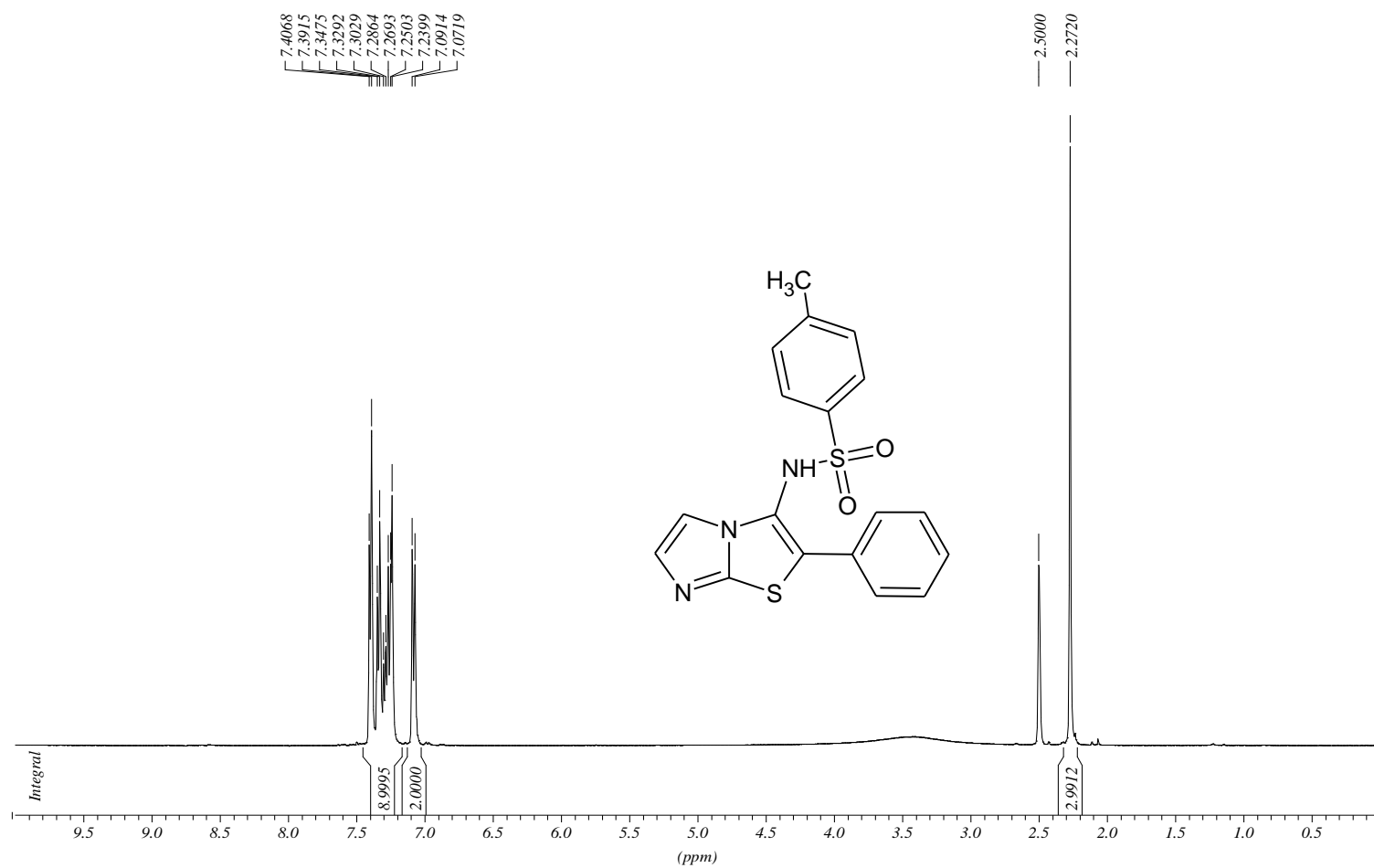


¹H NMR spectrum of **4ad** (400.13 MHz, DMSO-*d*₆)

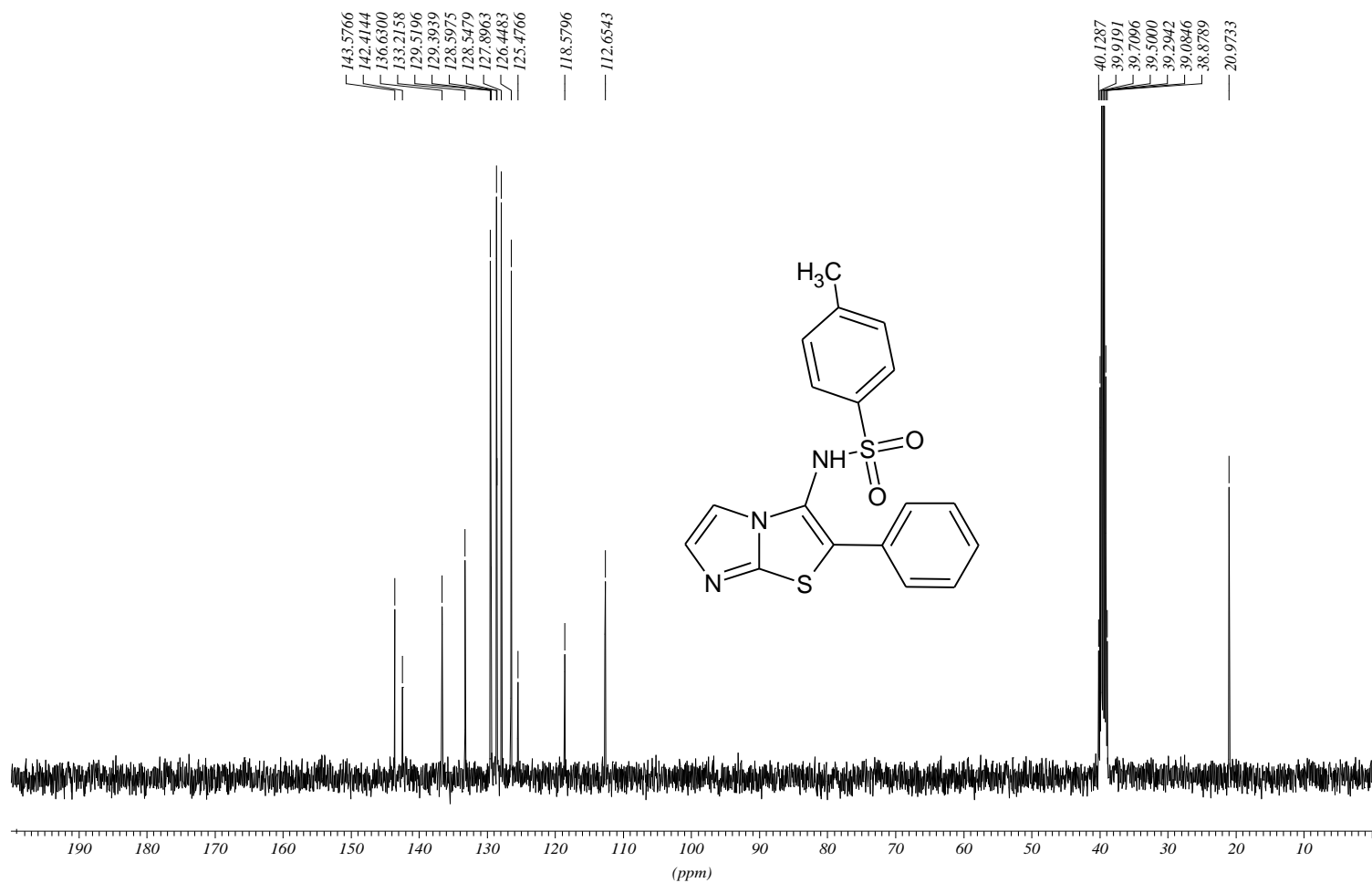




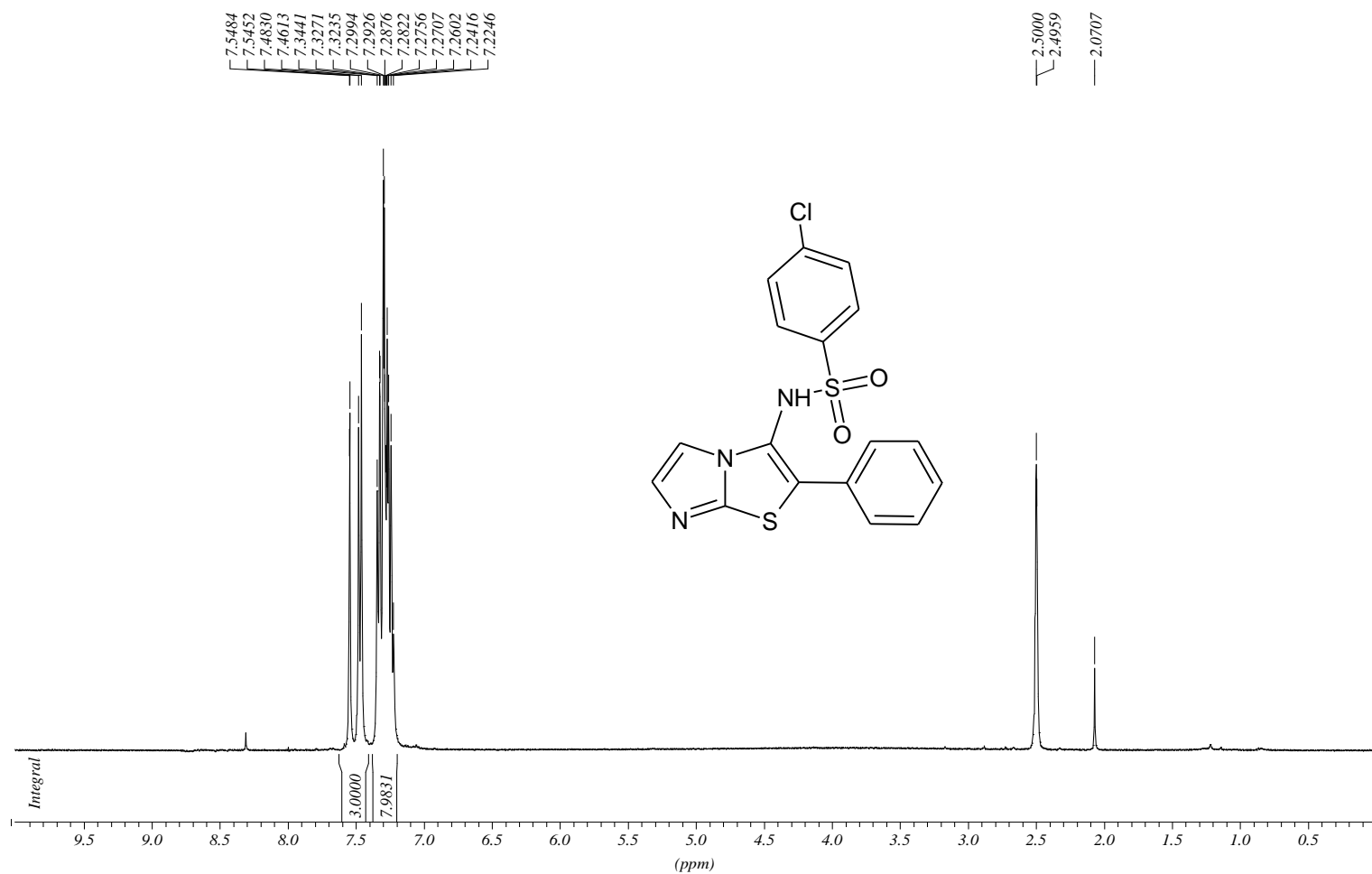
¹³C NMR spectrum of **4ad** (100.61 MHz, DMSO-*d*₆)



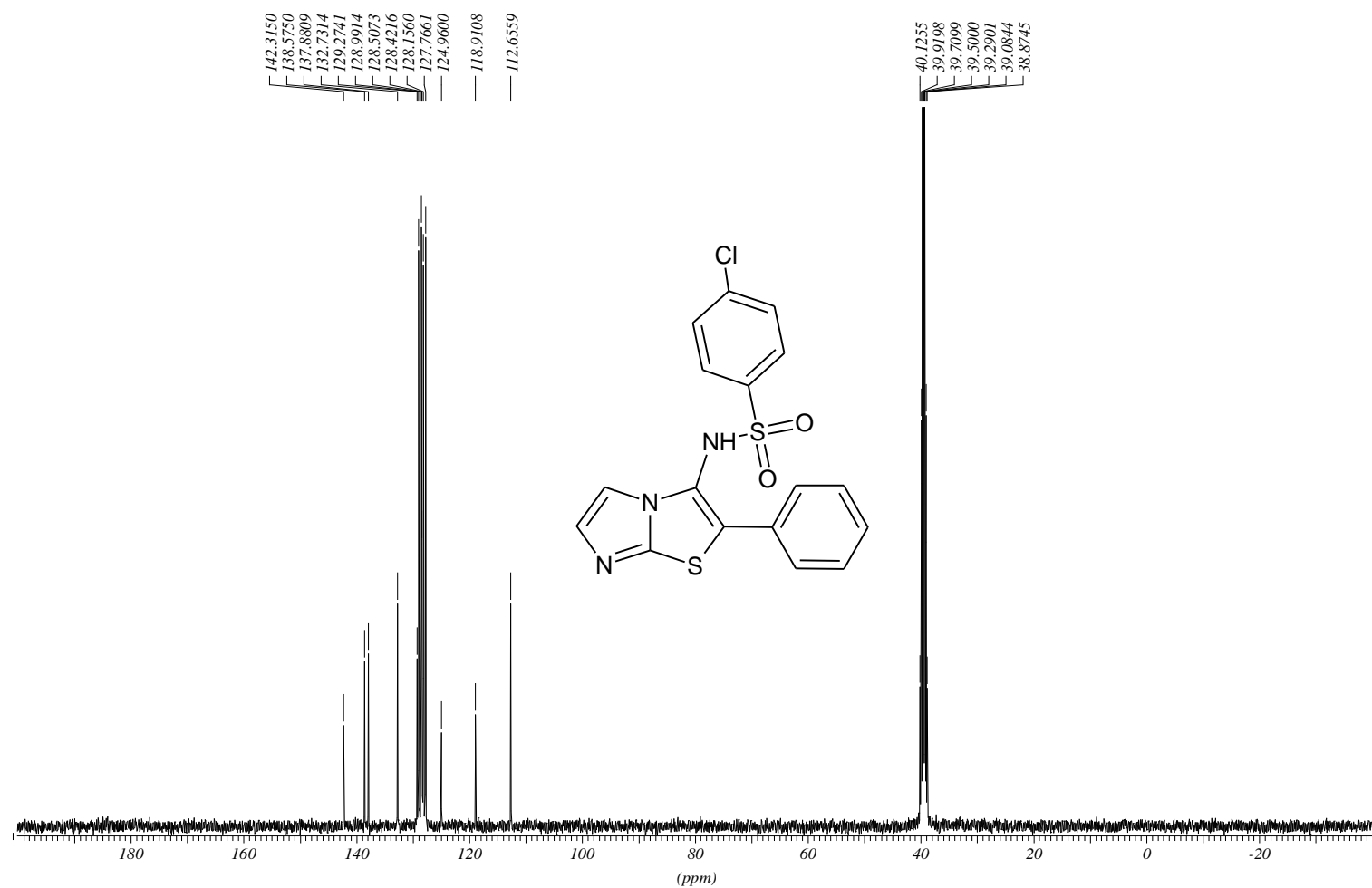
¹H NMR spectrum of **4bd** (400.13 MHz, DMSO-*d*₆)



¹³C NMR spectrum of **4bd** (100.61 MHz, DMSO-*d*₆)



¹H NMR spectrum of **4cd** (400.13 MHz, DMSO-*d*₆)



¹³C NMR spectrum of **4cd** (100.61 MHz, DMSO-*d*₆)