

Supplementary Material

Synthesis of 8-aminoquinoline chelating moieties for chemosensor molecules

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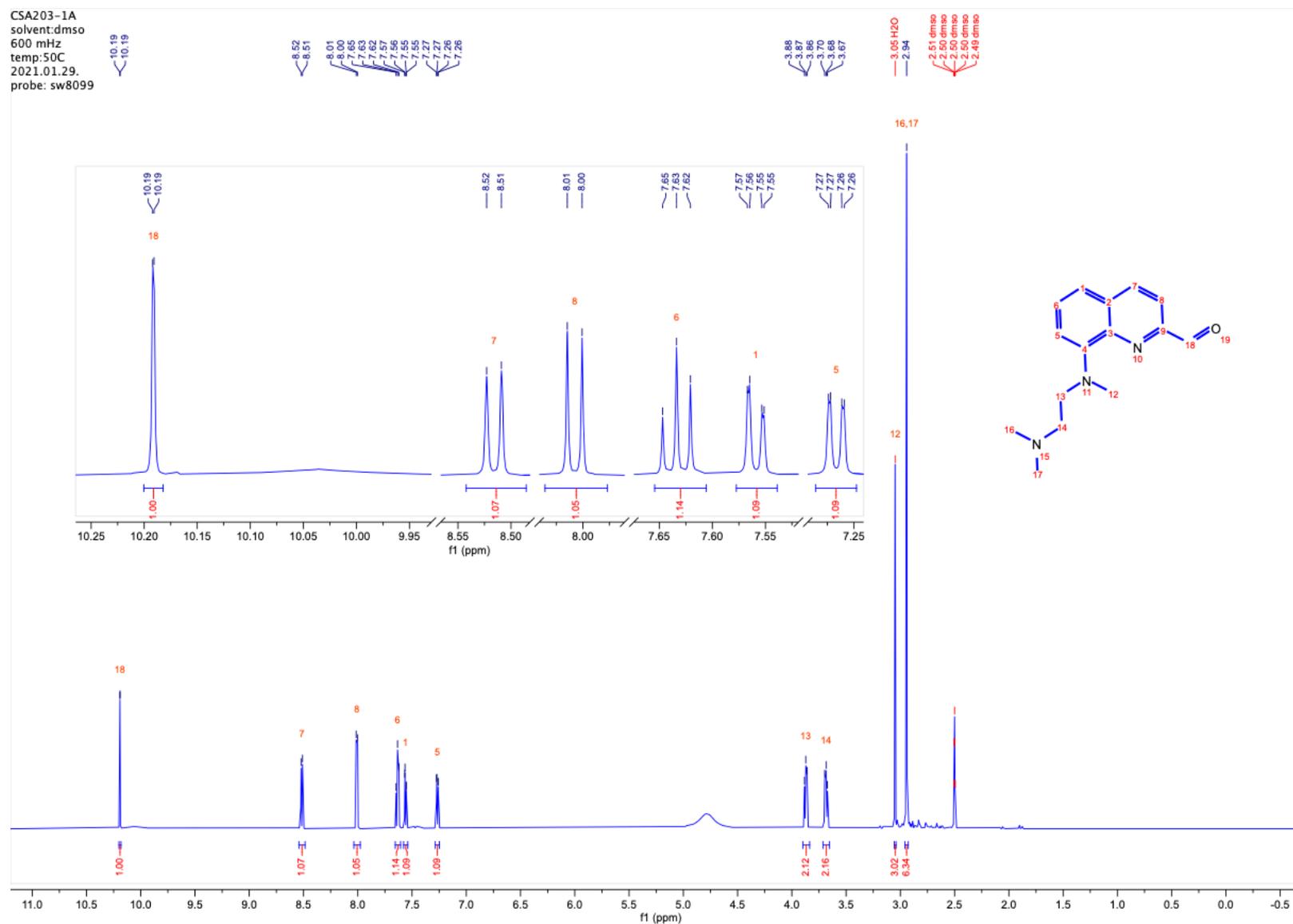


Figure S1.: ¹H NMR spectrum of compound **1b** recorded at 600 MHz in DMSO-*d*₆.

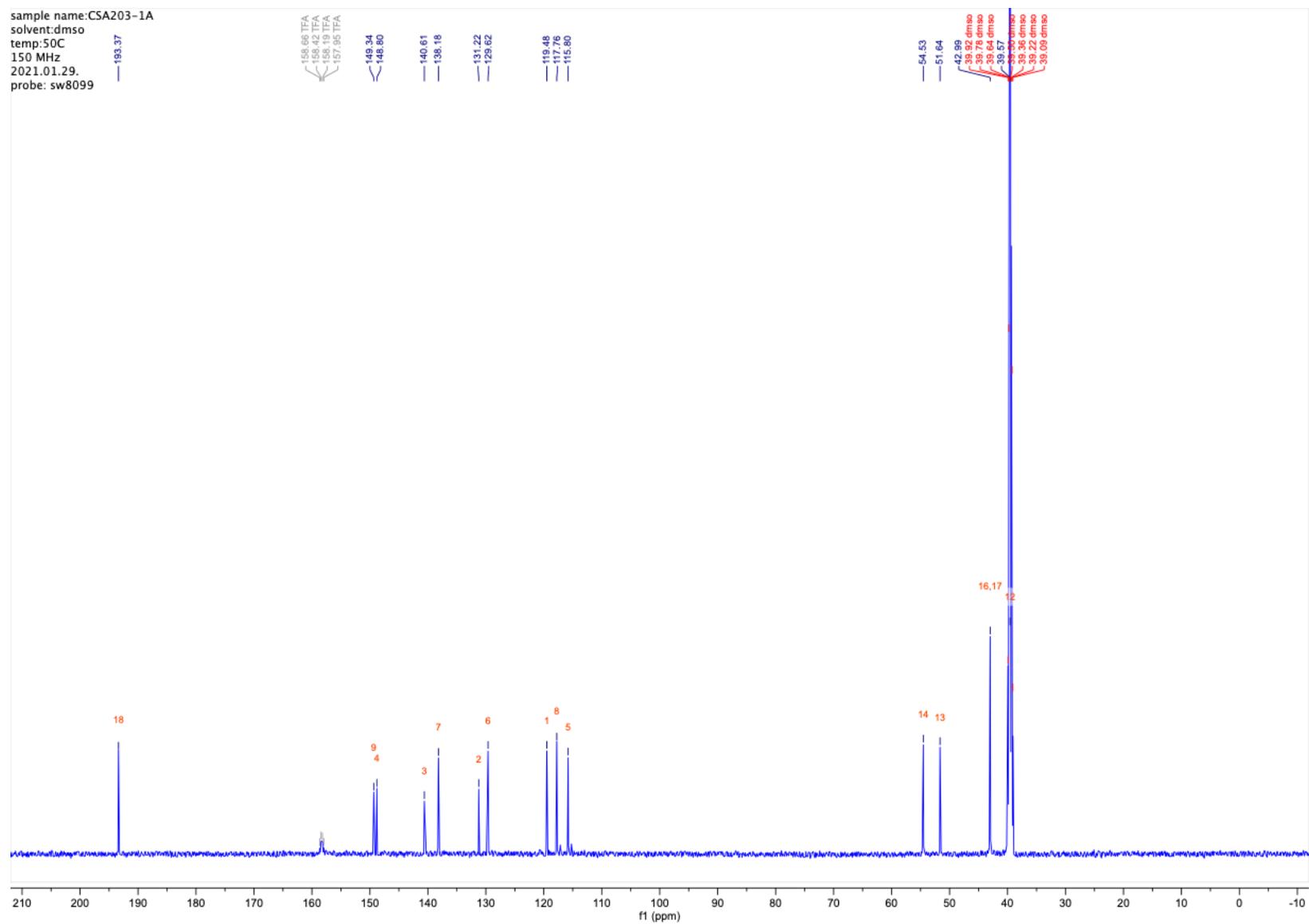


Figure S2.: ^{13}C NMR spectrum of compound **1b** recorded at 150 MHz in $\text{DMSO-}d_6$.

CSA203 #145-180 RT: 0.66-0.82 AV: 36 NL: 2.53E8
T: FTMS + p ESI Full ms [200.0000-1500.0000]

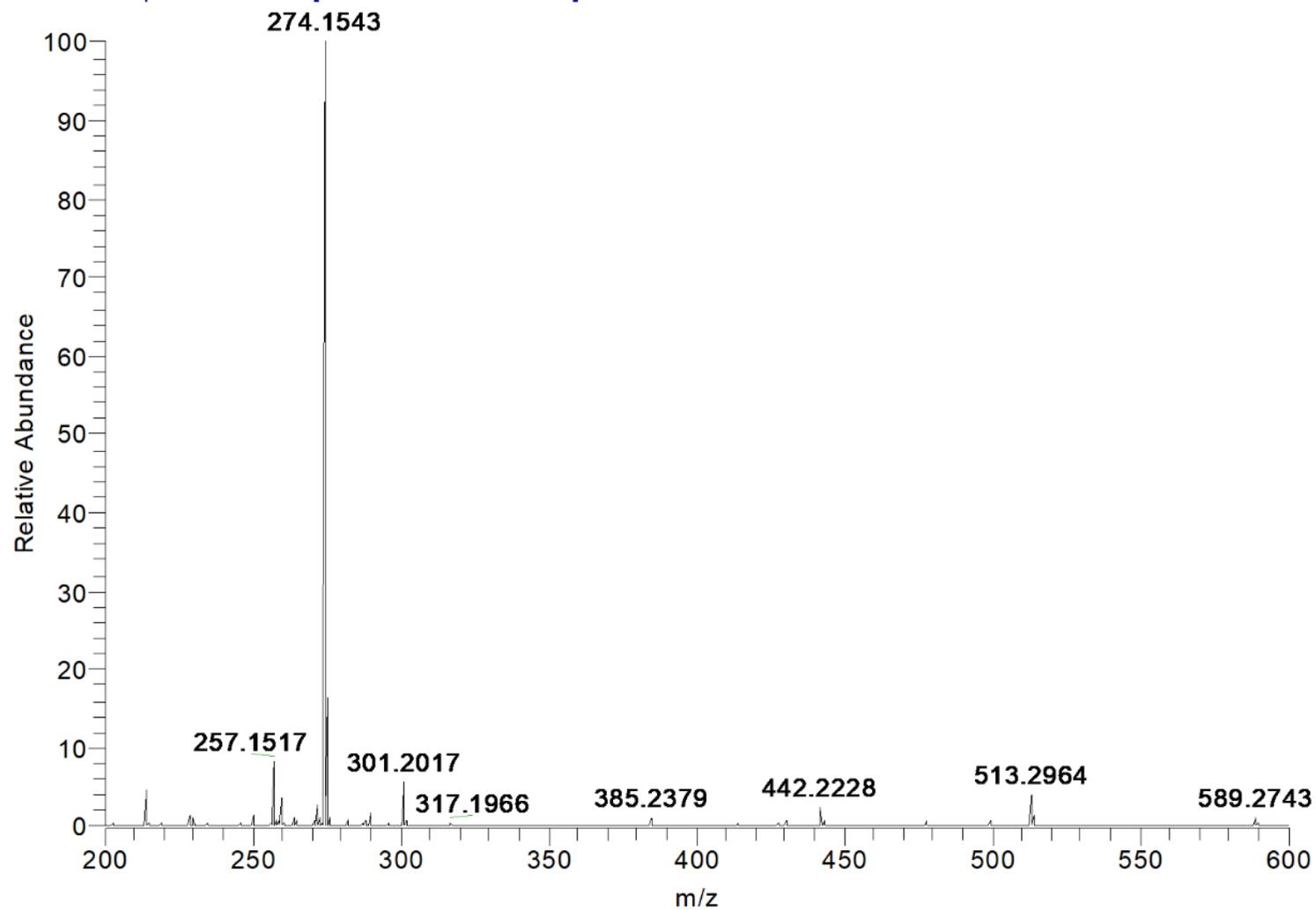


Figure S3.: HRMS spectrum of **1b**.

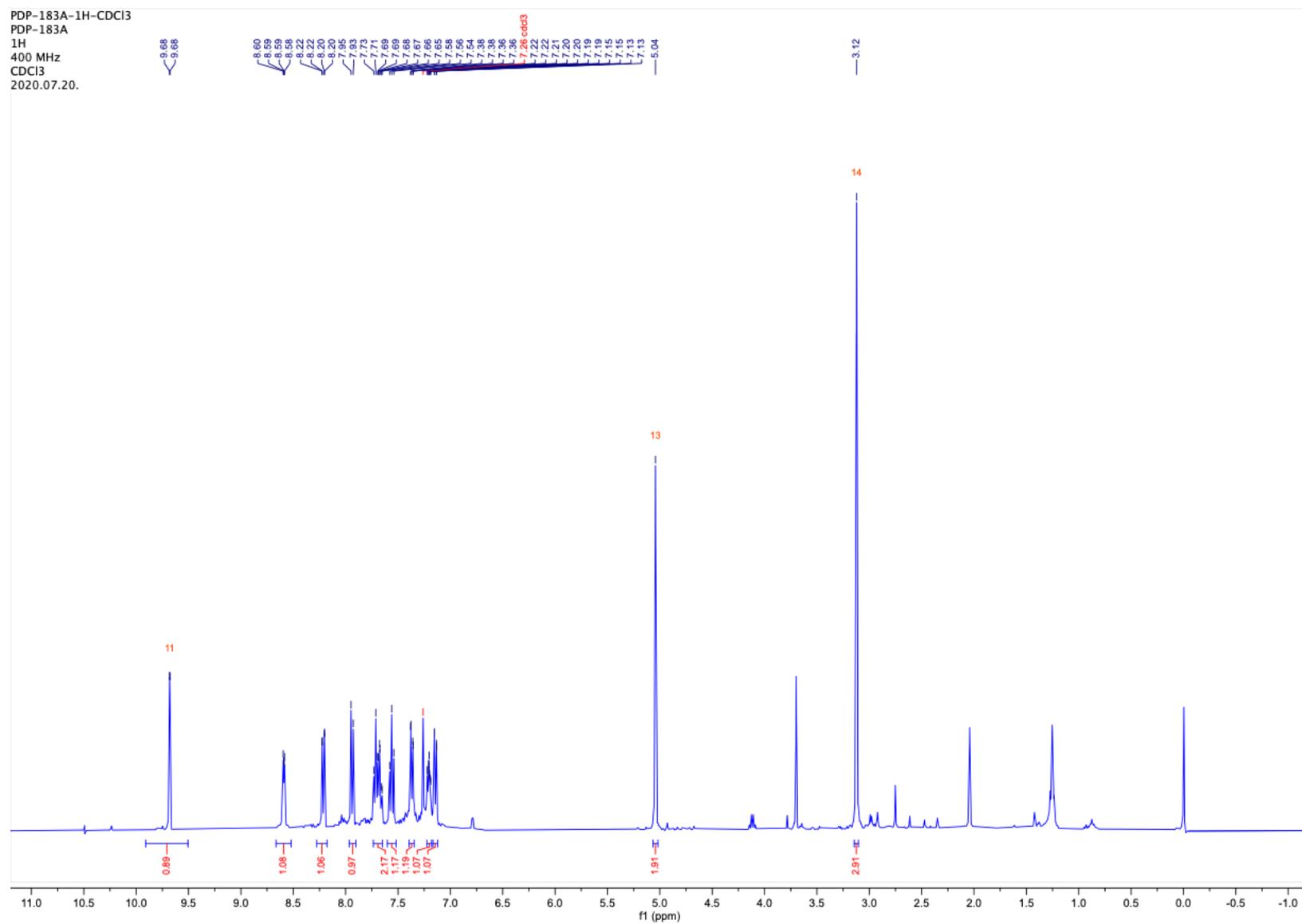


Figure S4.: ^1H NMR spectrum of compound **1c** recorded at 400 MHz in Chloroform-*d*.

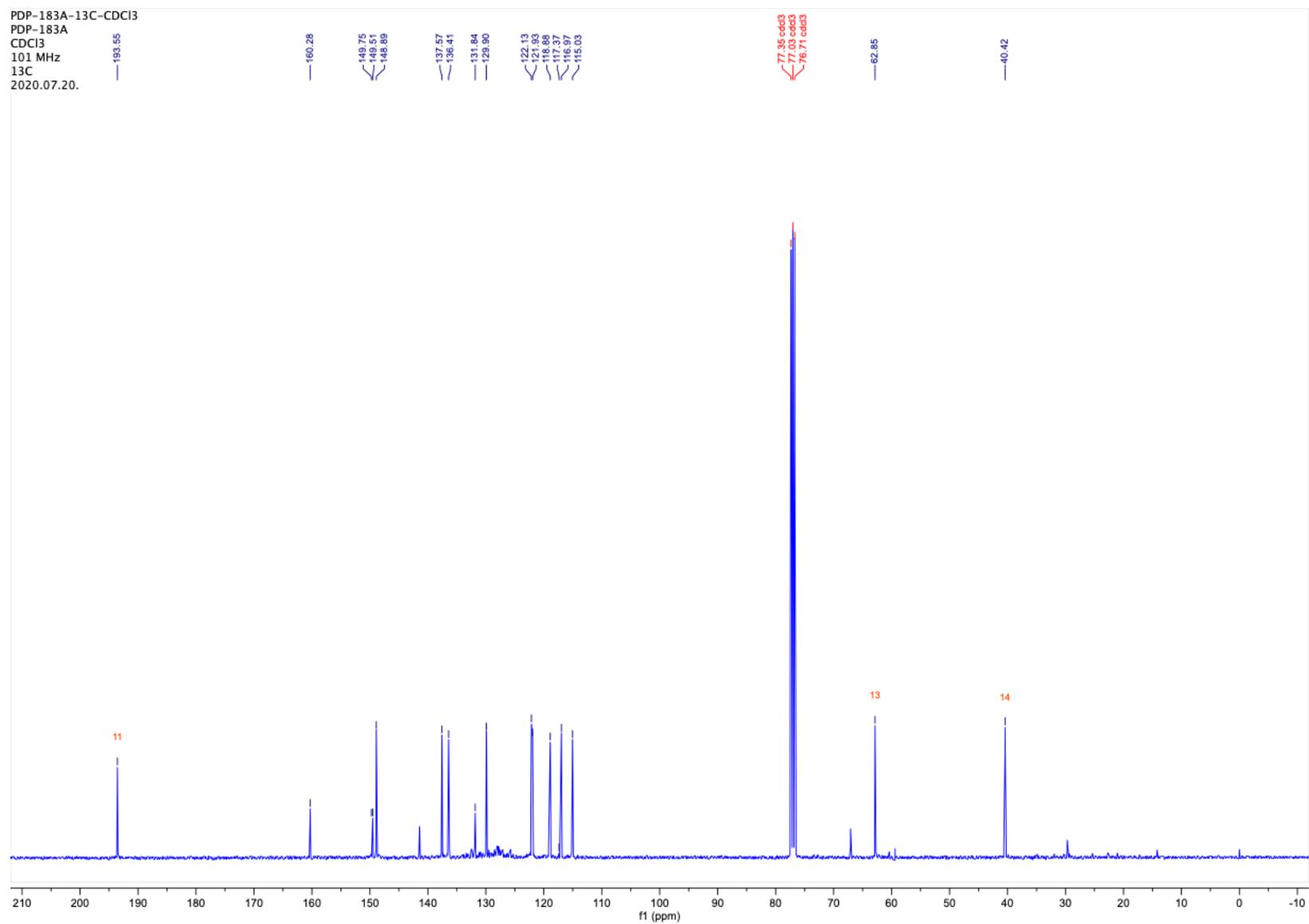


Figure S5.: ^{13}C NMR spectrum of compound **1c** recorded at 101 MHz in Chloroform-*d*.

PDP183 #117-160 RT: 0.53-0.72 AV: 44 NL: 4.42E8
T: FTMS + p ESI Full ms [200.0000-1500.0000]

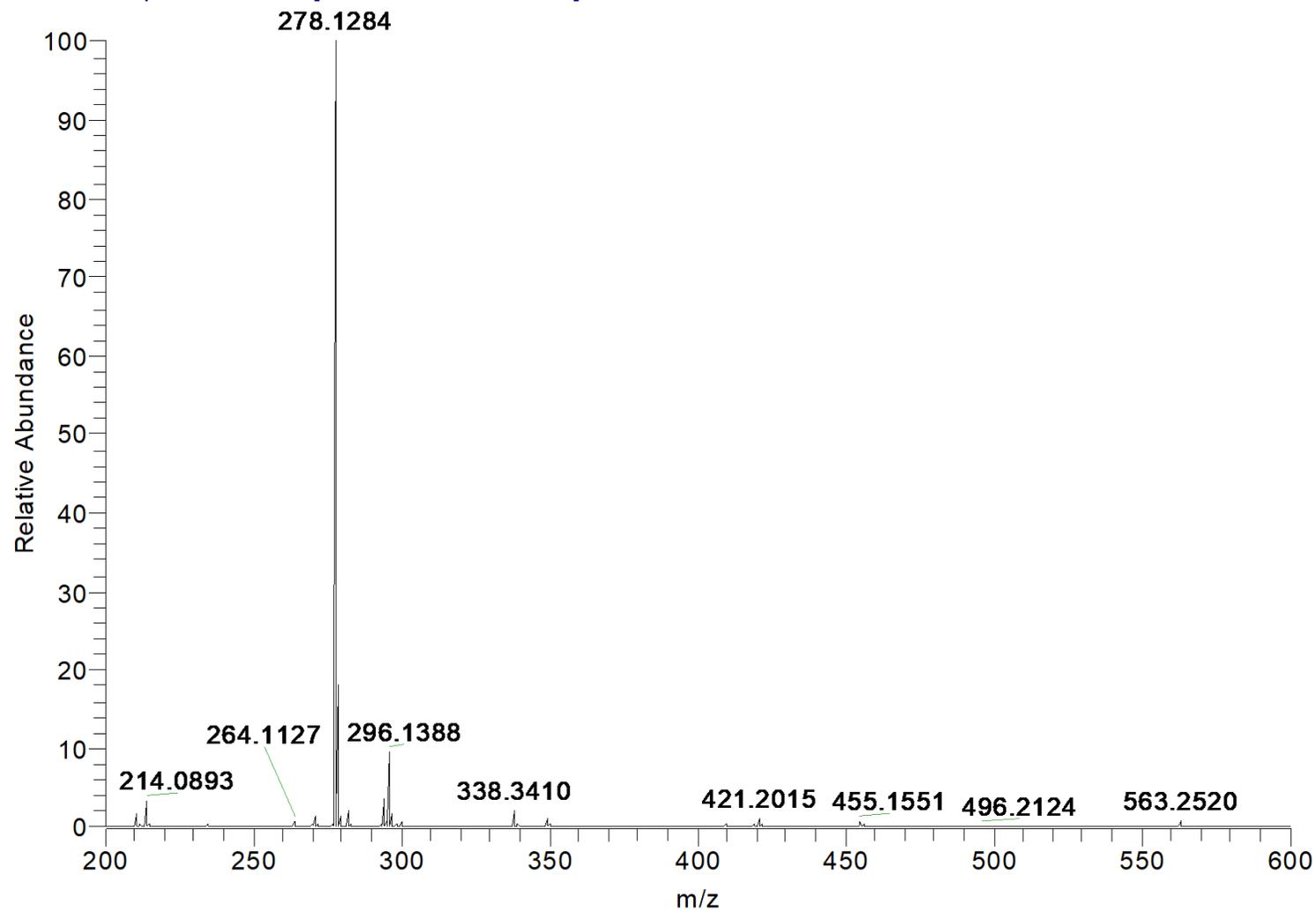


Figure S6.: HRMS spectrum of 1c.

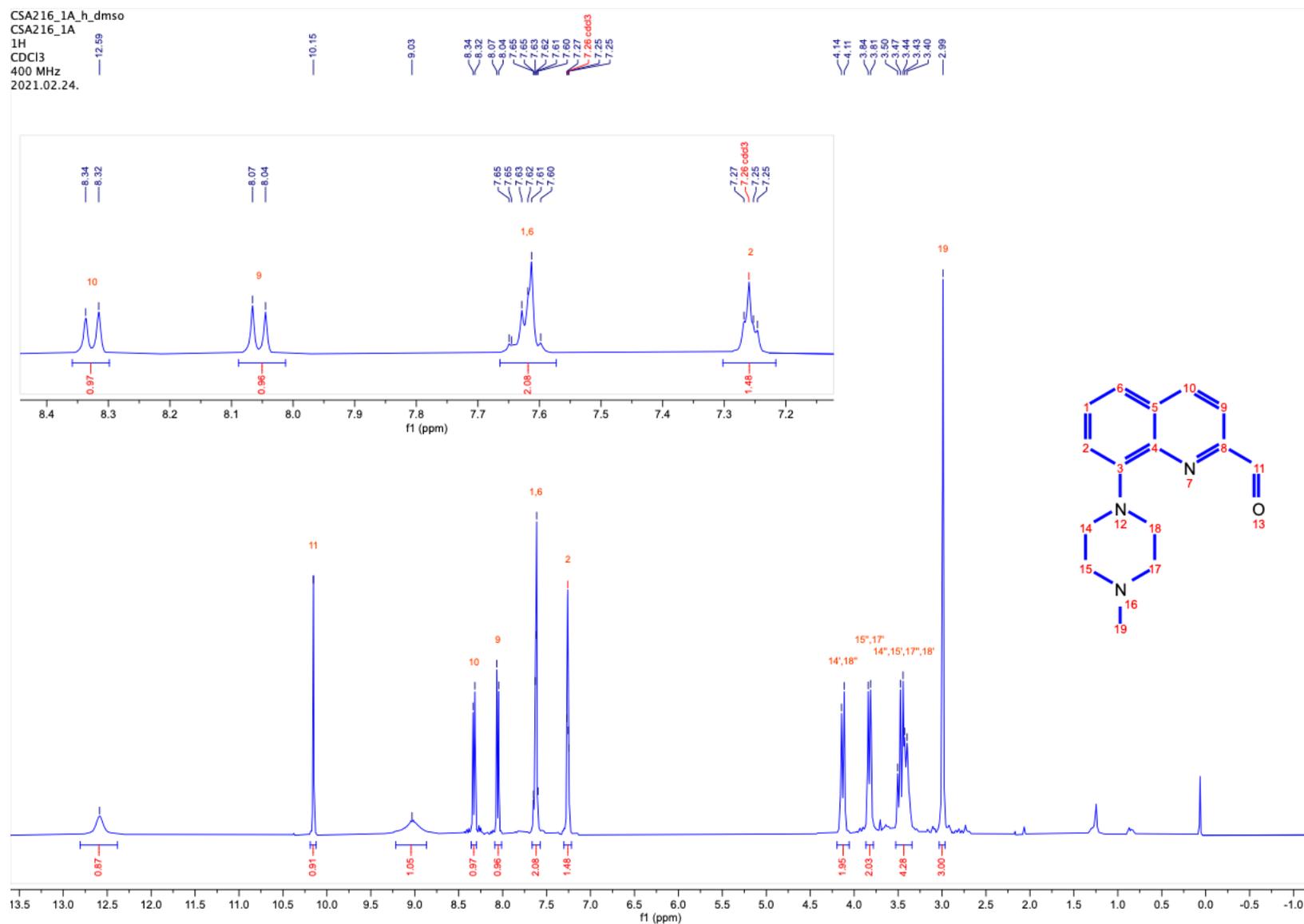


Figure S7.: ^1H NMR spectrum of compound **1d** recorded at 400 MHz in Chloroform-*d*.

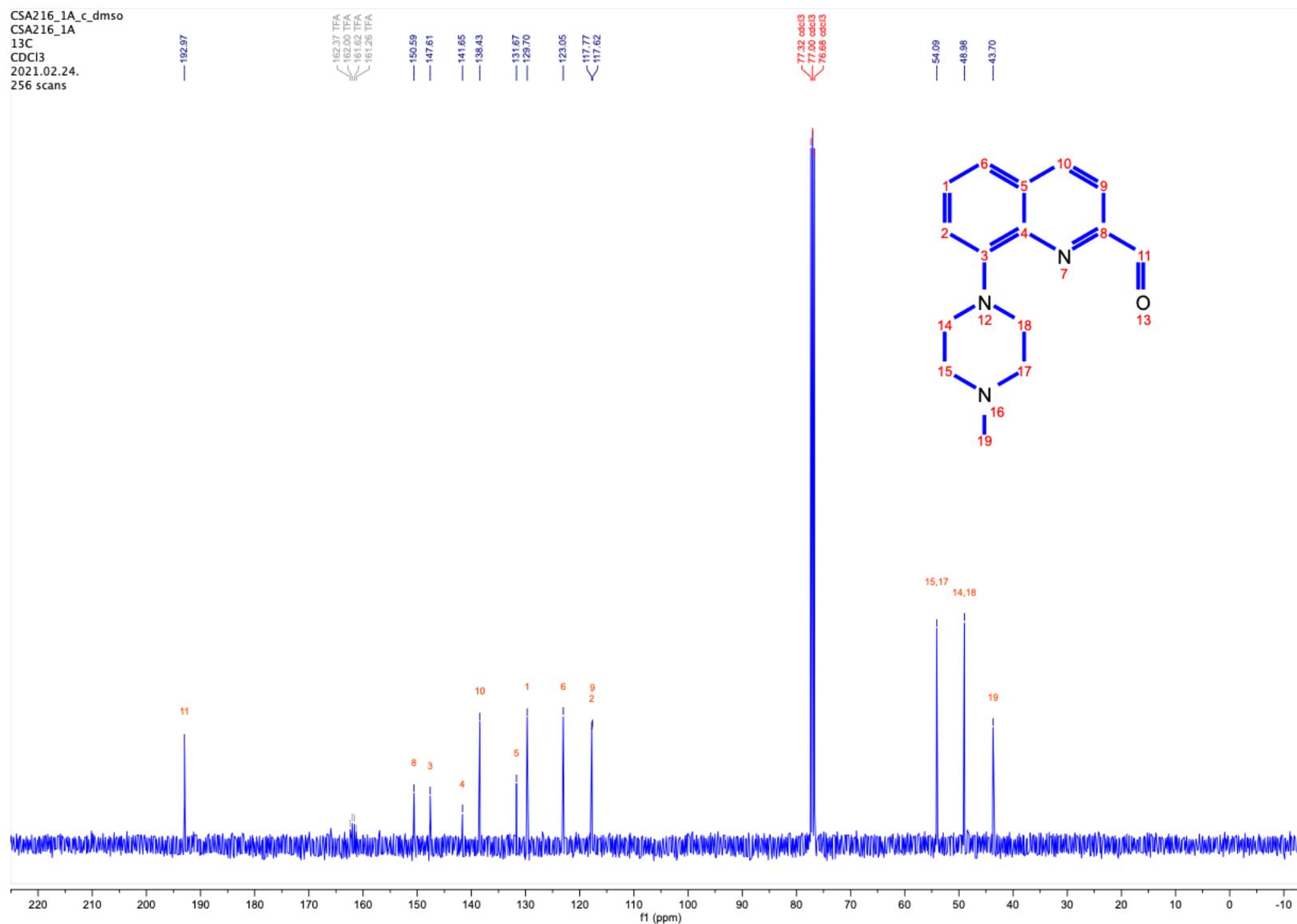


Figure S8.: ^{13}C NMR spectrum of compound **1d** recorded at 101 MHz in Chloroform-*d*.

CSA216 #108-141 RT: 0.49-0.64 AV: 34 NL: 8.46E7
T: FTMS + p ESI Full ms [200.0000-1500.0000]

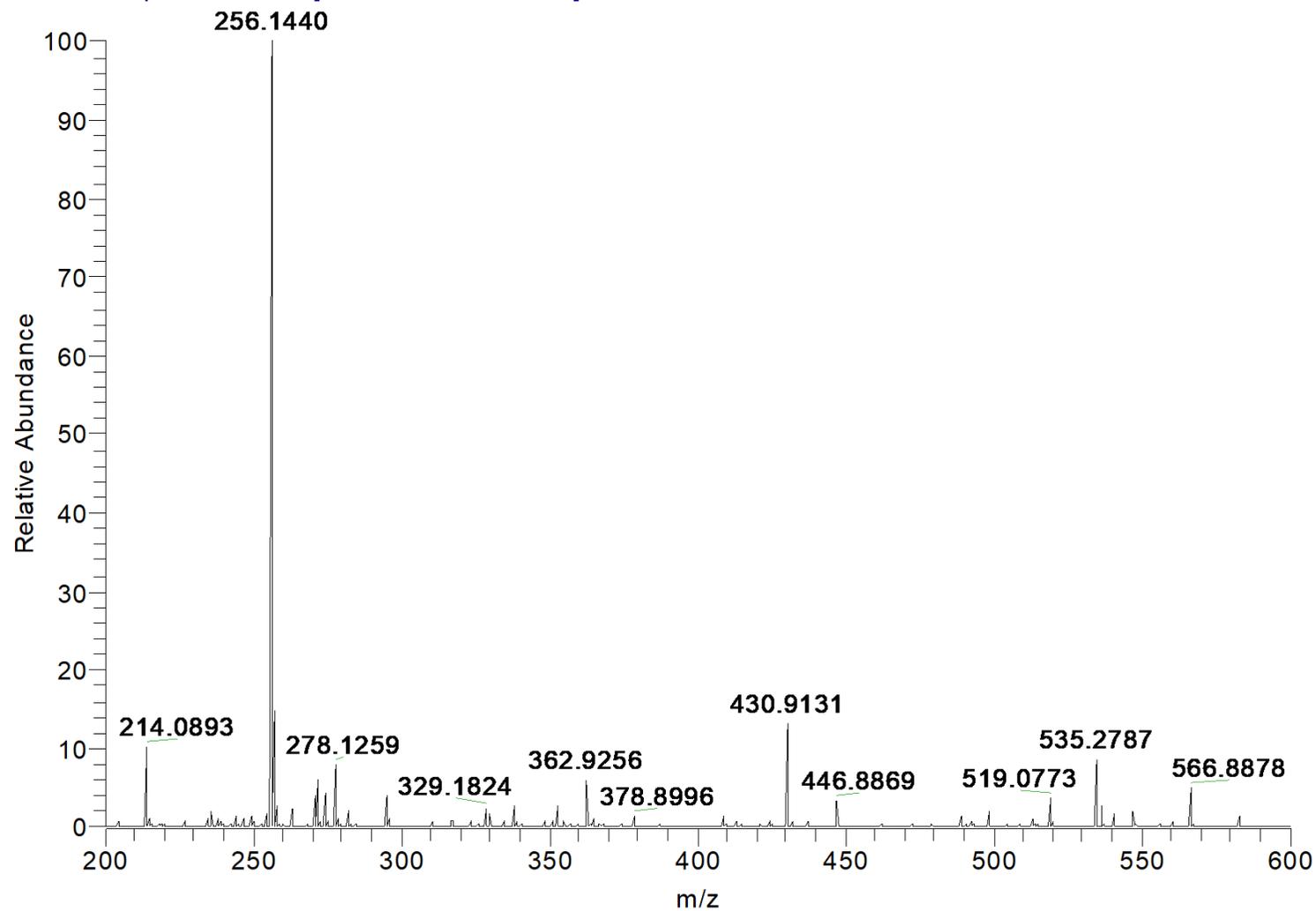


Figure S9.: HRMS spectrum of 1d.

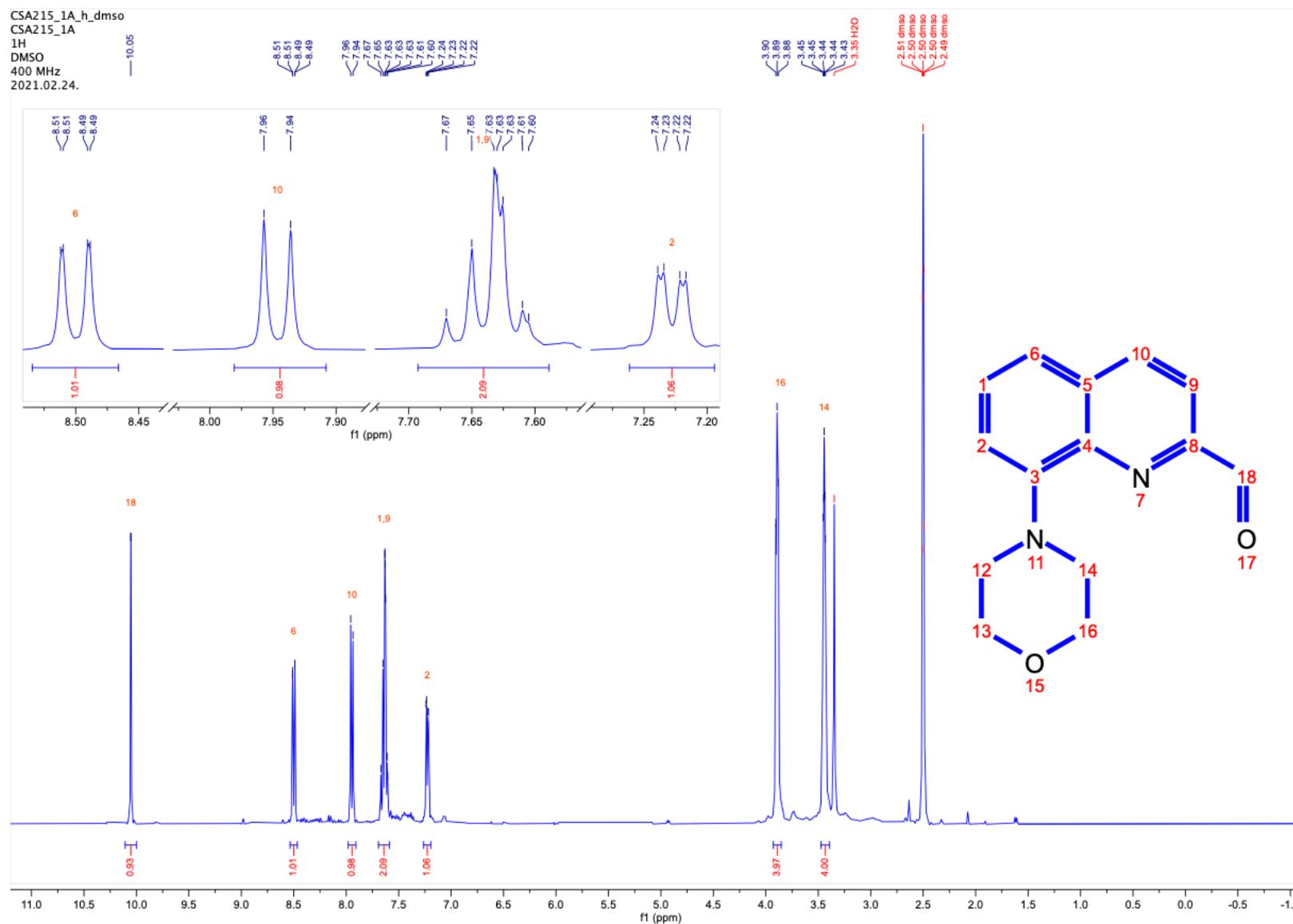


Figure S10.: ¹H NMR spectrum of compound **1e** recorded at 400 MHz in DMSO-*d*₆.

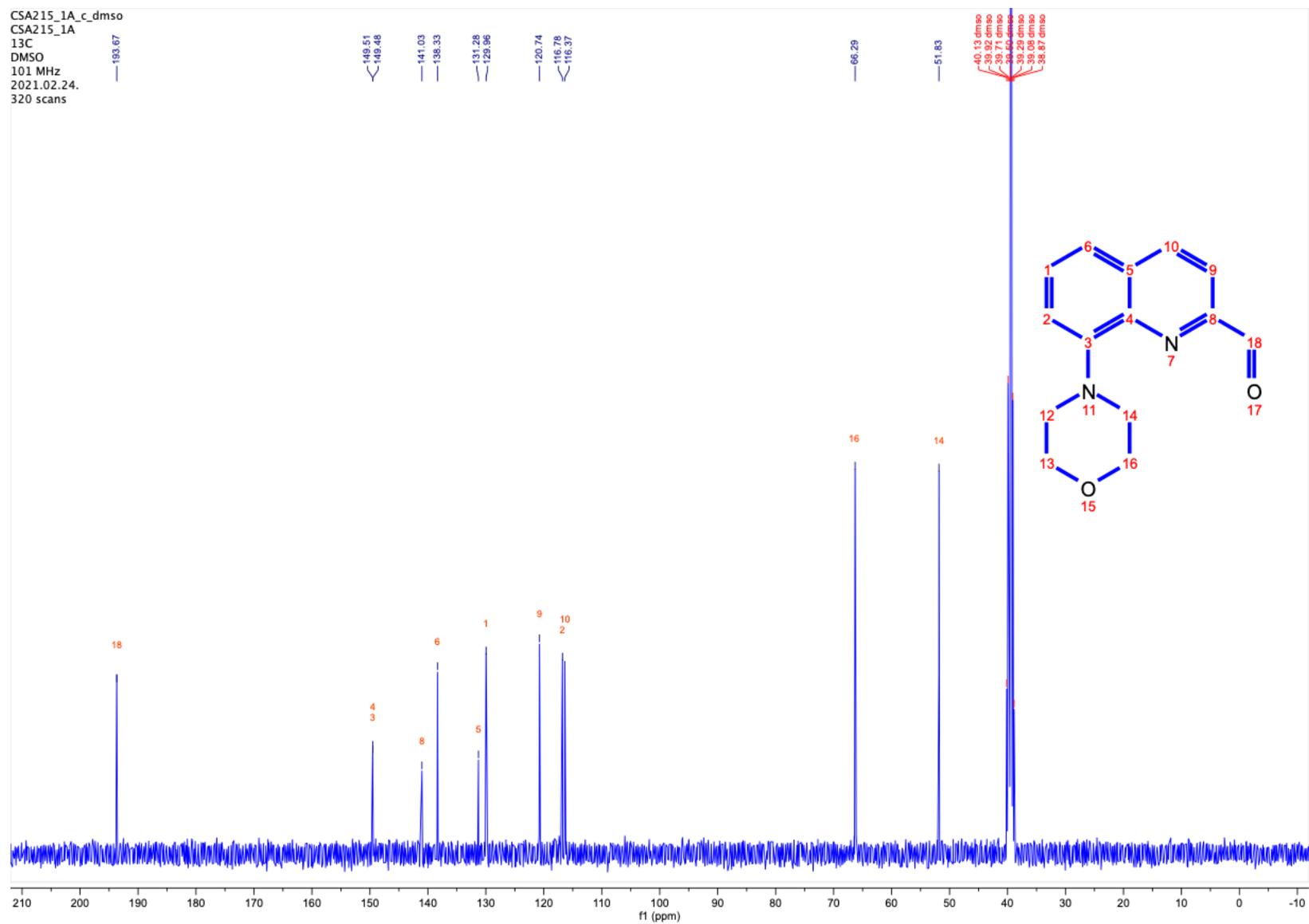


Figure S11.: ^{13}C NMR spectrum of compound **1e** recorded at 101 MHz in $\text{DMSO-}d_6$.

CSA215 #108-150 RT: 0.49-0.68 AV: 43 NL: 5.93E8
T: FTMS + p ESI Full ms [200.0000-1500.0000]

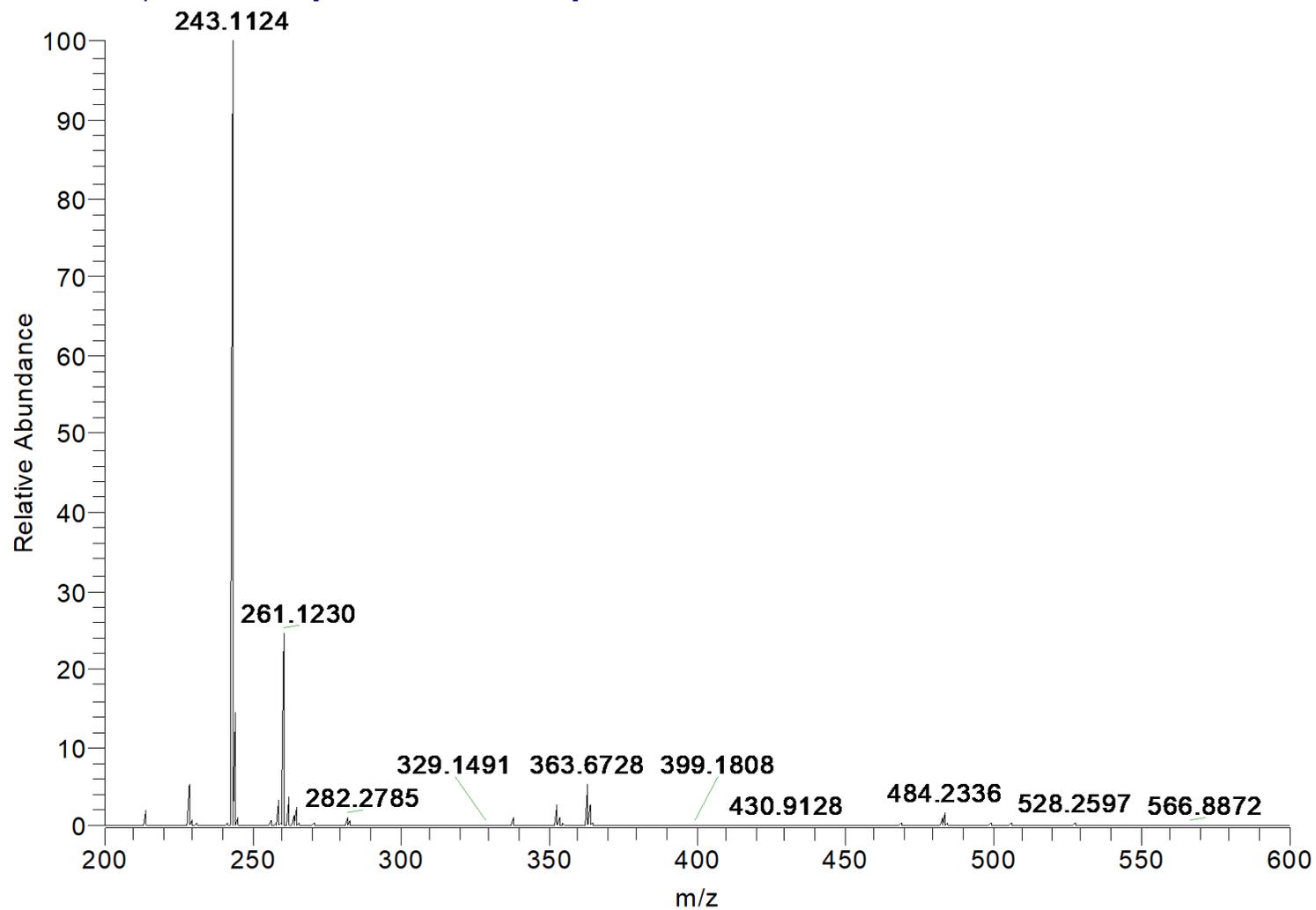


Figure S12.: HRMS spectrum of 1e.

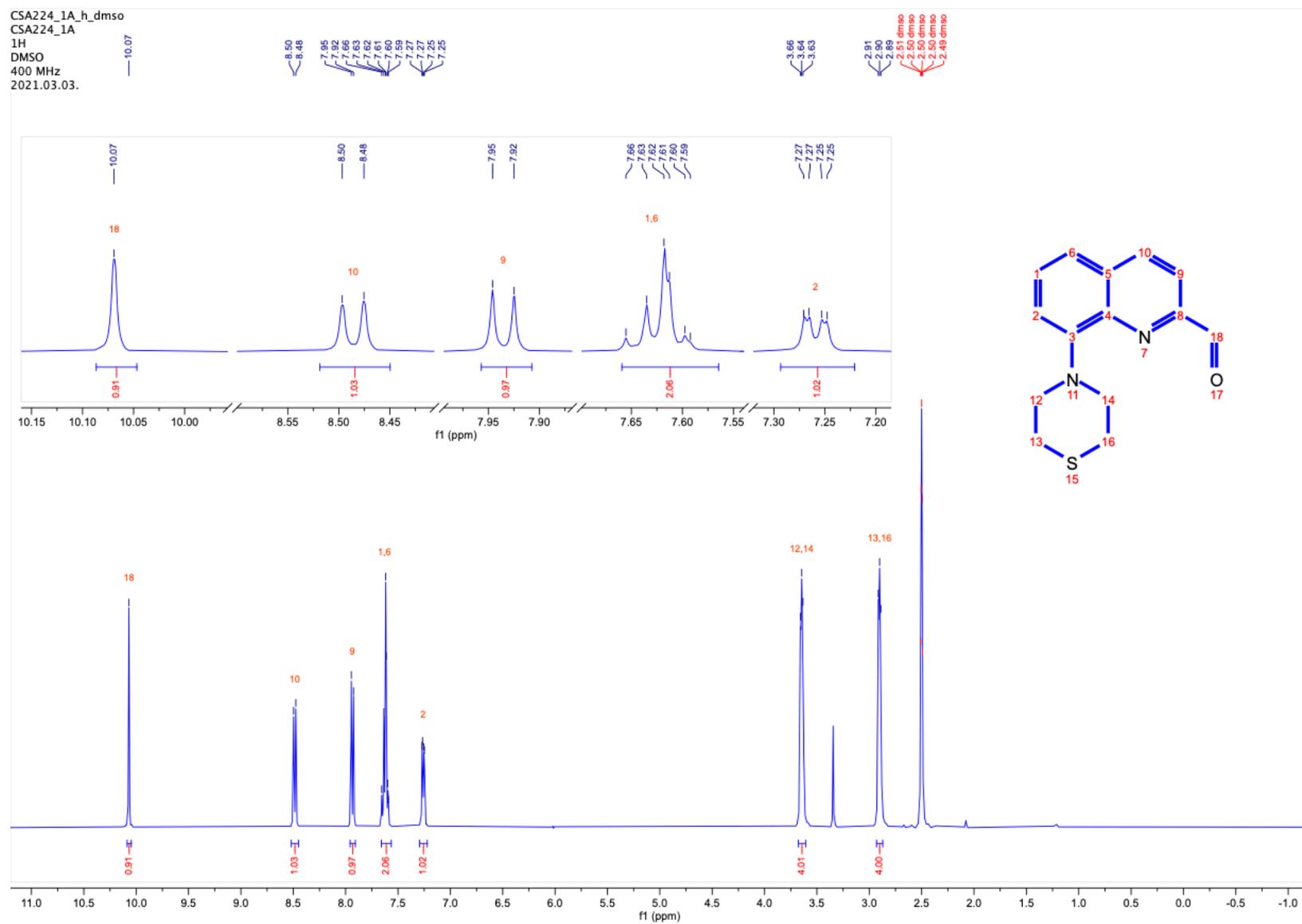


Figure S13.: ^1H NMR spectrum of compound **1f** recorded at 400 MHz in $\text{DMSO}-d_6$.

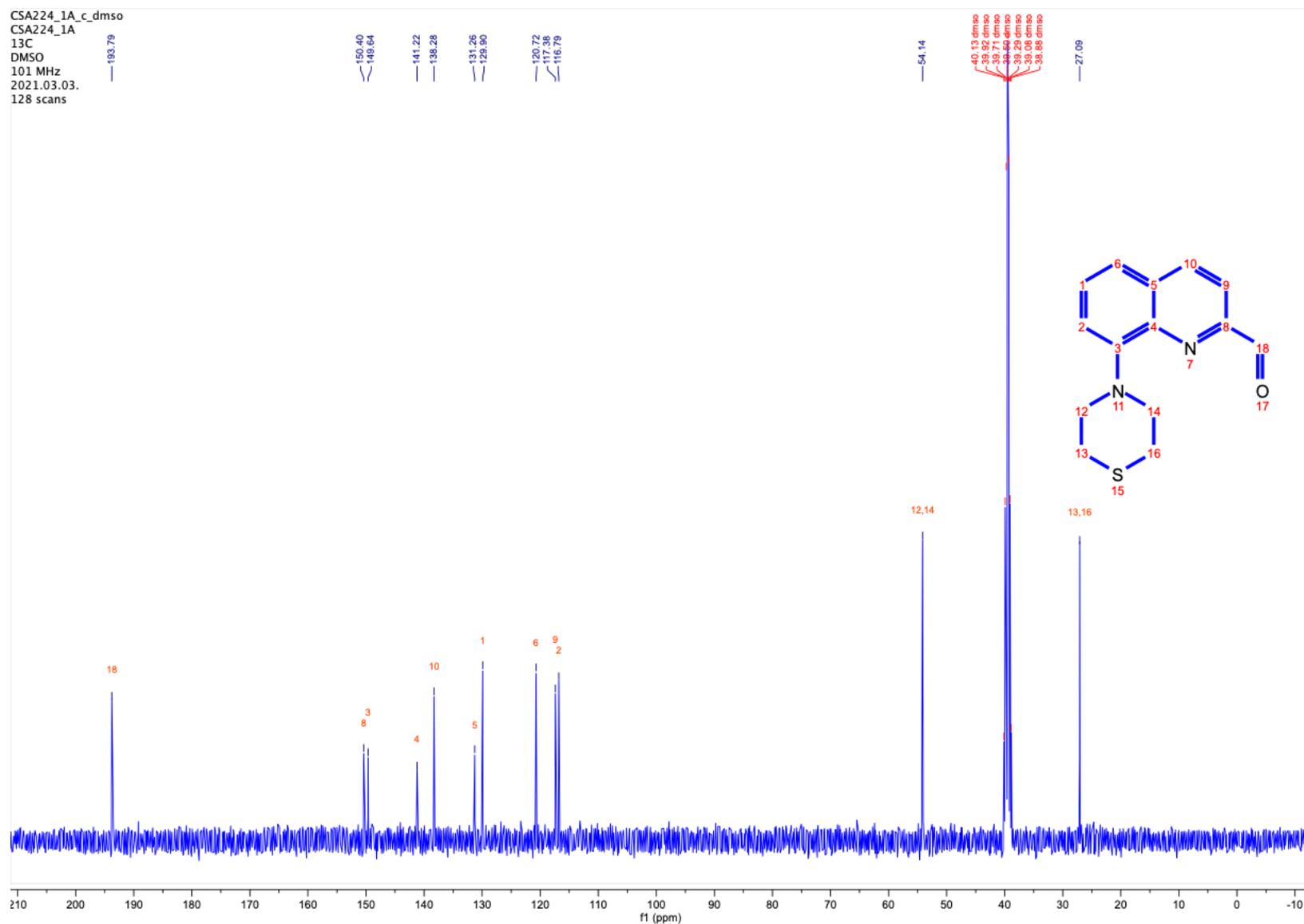


Figure S14.: ^{13}C NMR spectrum of compound **1f** recorded at 101 MHz in $\text{DMSO-}d_6$.

CSA224_1A #111-146 RT: 0.50-0.66 AV: 36 NL: 2.98E8
T: FTMS + p ESI Full ms [200.0000-1500.0000]

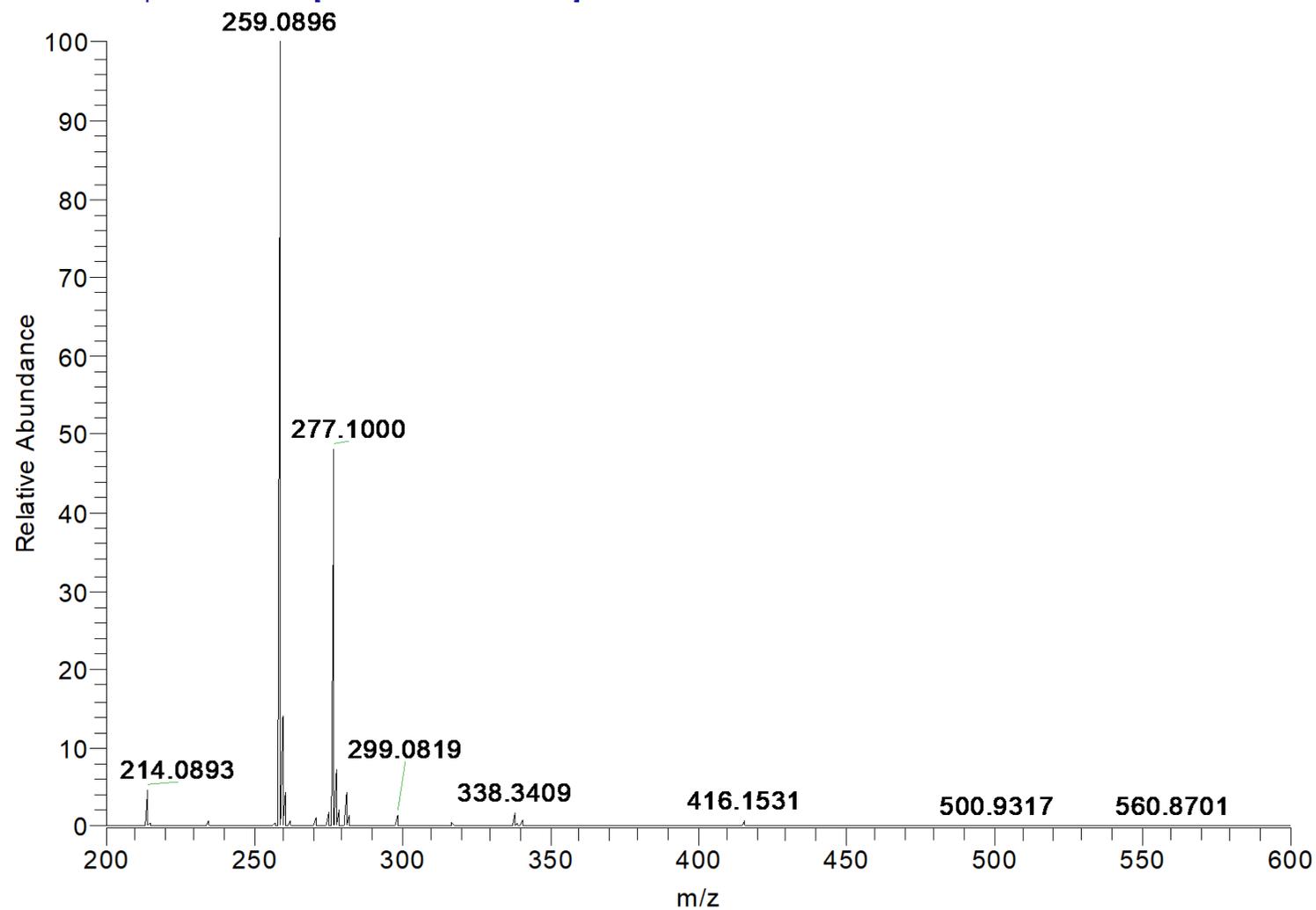


Figure S15.: HRMS spectrum of 1f.

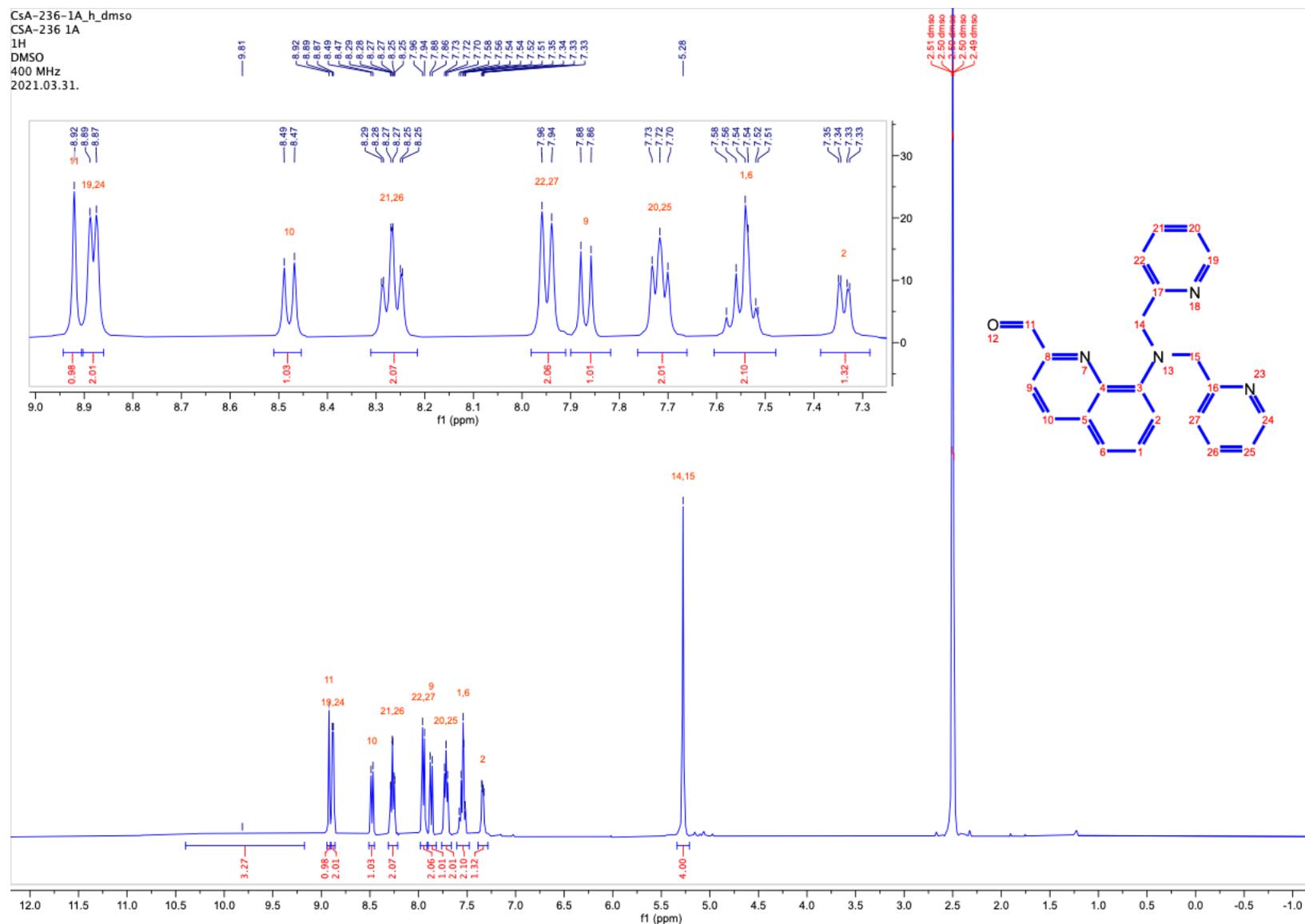


Figure S16.: ^1H NMR spectrum of compound **1g** recorded at 400 MHz in $\text{DMSO}-d_6$.

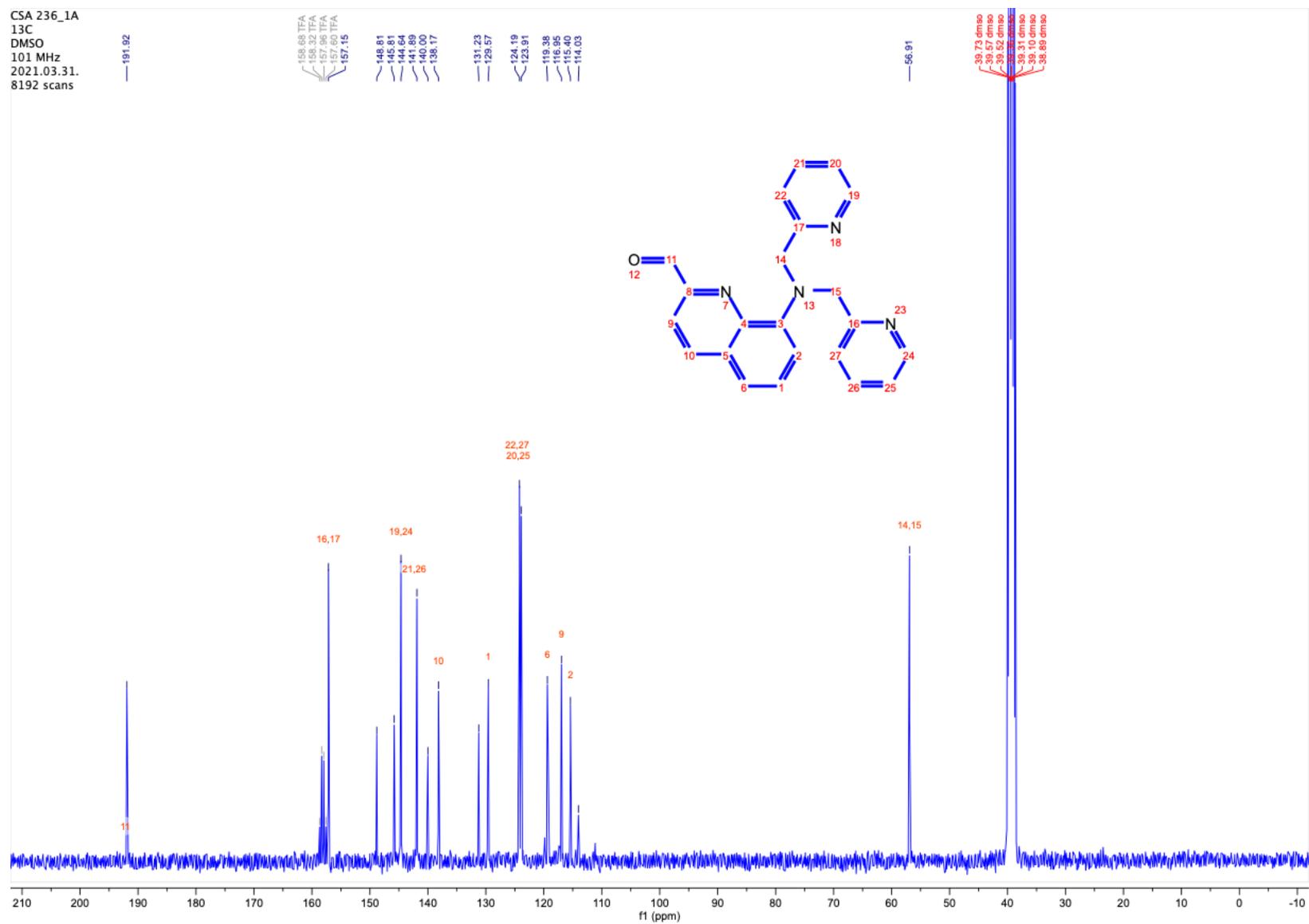


Figure S17.: ^{13}C NMR spectrum of compound **1g** recorded at 101 MHz in $\text{DMSO-}d_6$.

CSA236 #119-148 RT: 0.54-0.67 AV: 30 NL: 1.00E7
T: FTMS + p ESI Full ms [200.0000-1500.0000]

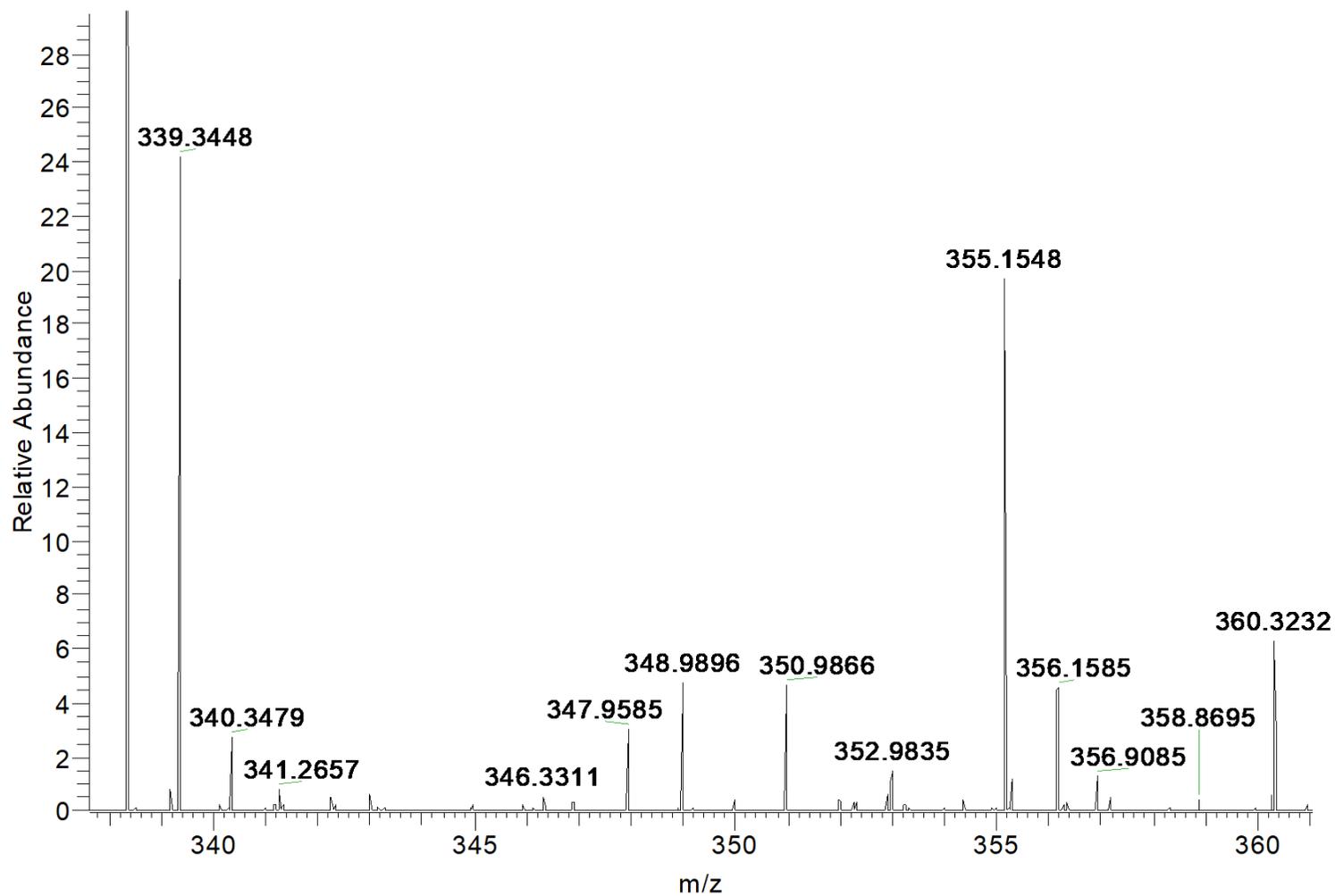


Figure S18.: HRMS spectrum of 1g.

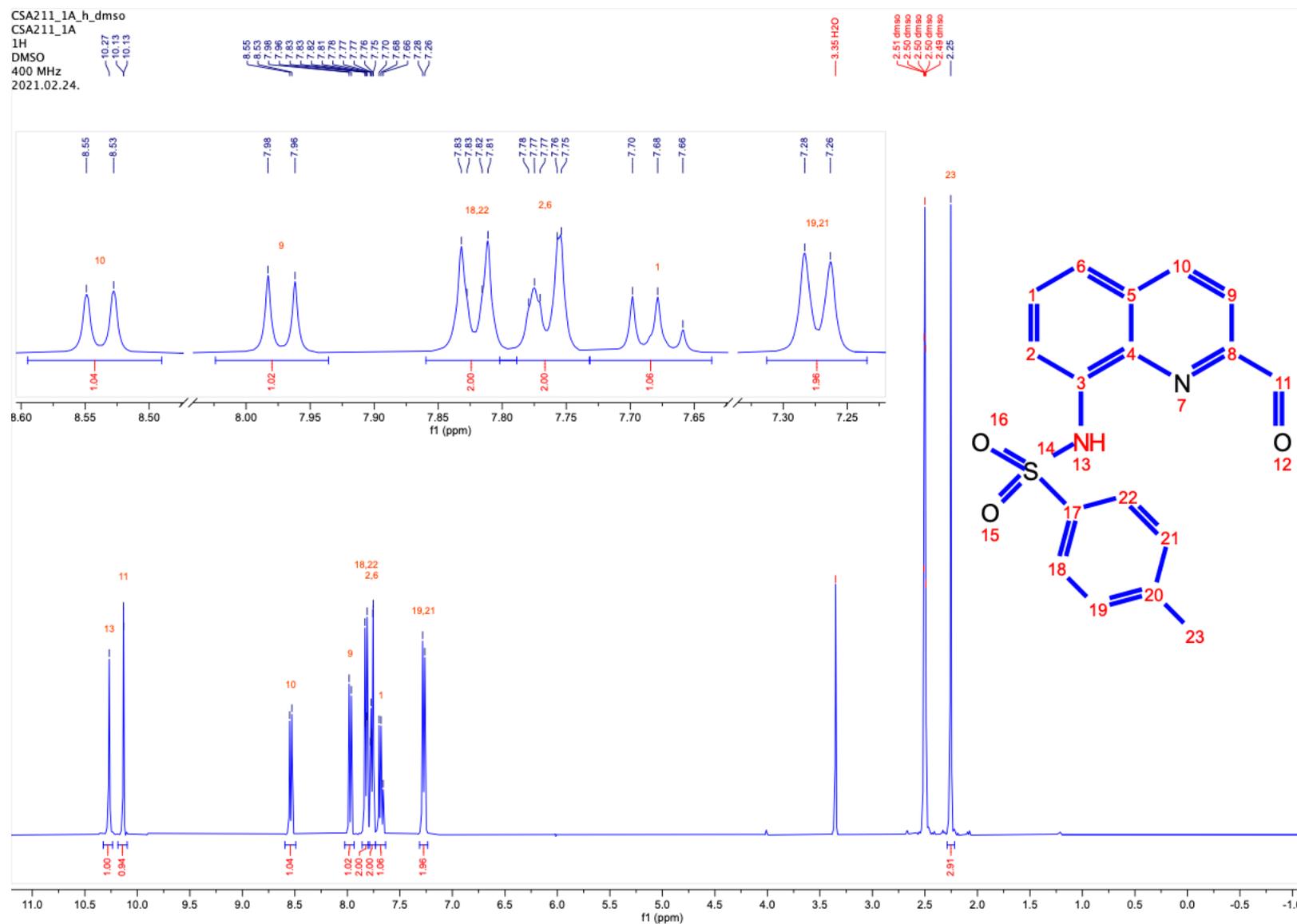


Figure S19.: ¹H NMR spectrum of compound **1h** recorded at 400 MHz in DMSO-*d*₆.

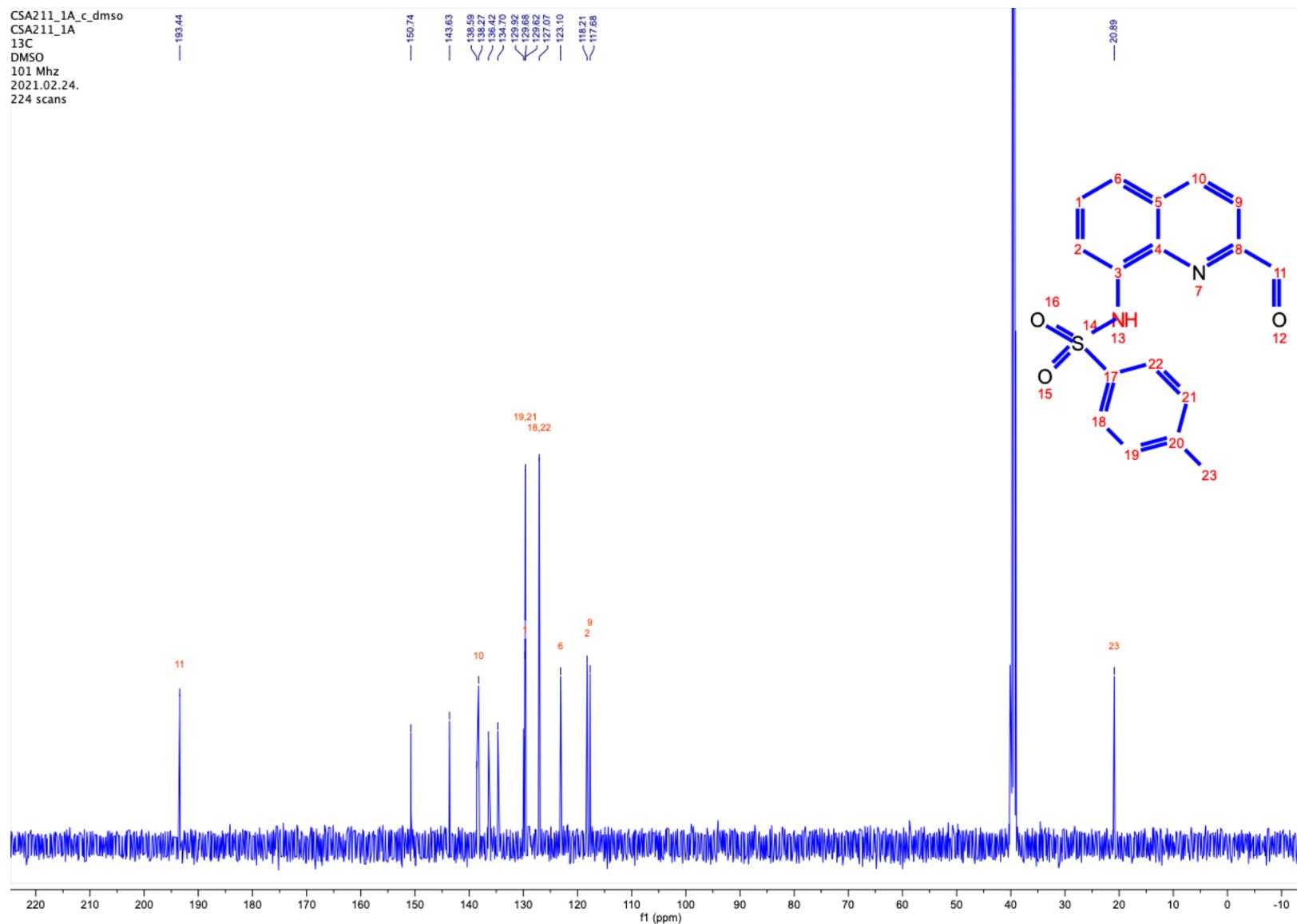


Figure S20.: ^{13}C NMR spectrum of compound **1h** recorded at 101 MHz in $\text{DMSO-}d_6$.

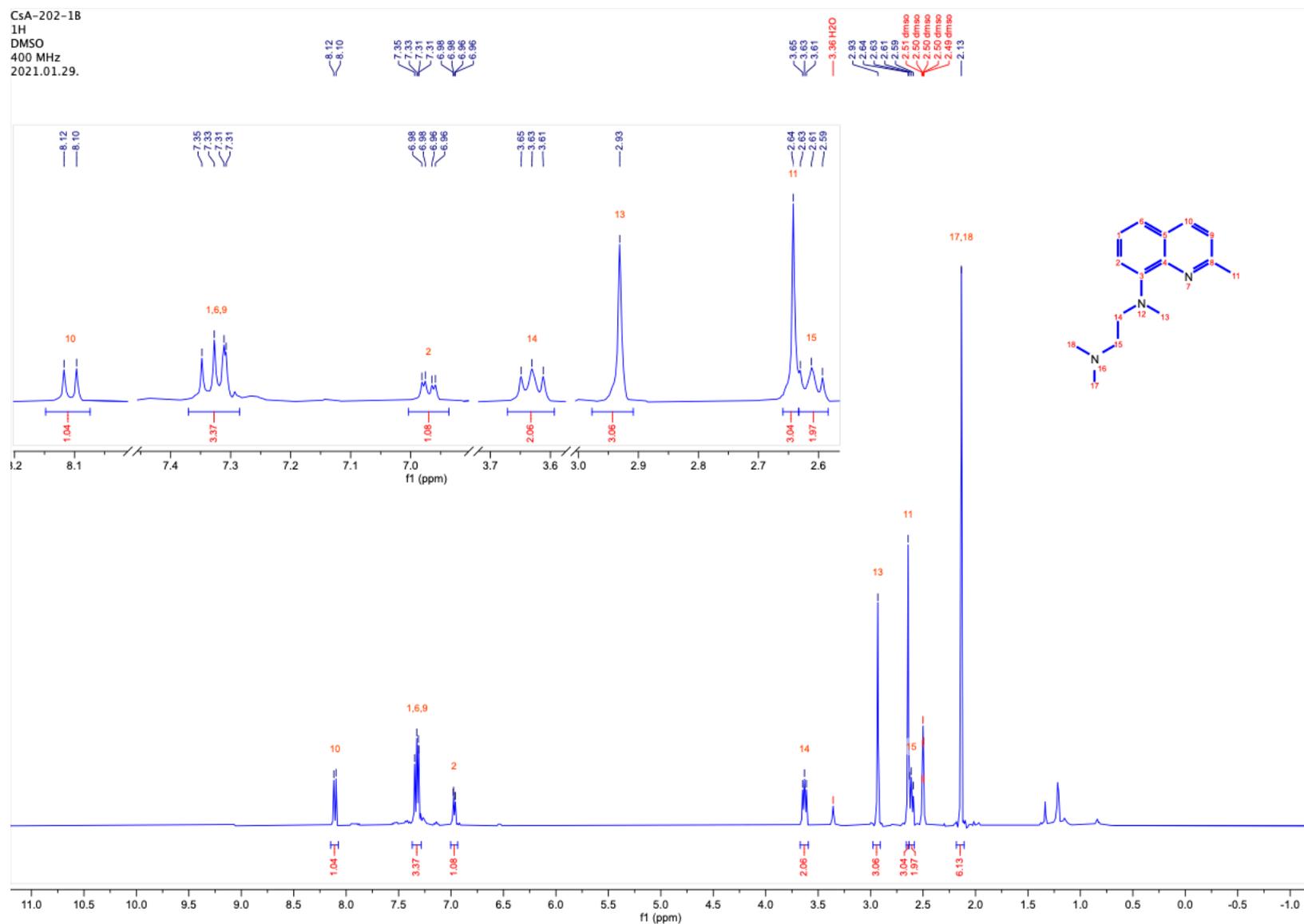


Figure S21.: ^1H NMR spectrum of compound **4b** recorded at 400 MHz in $\text{DMSO-}d_6$.

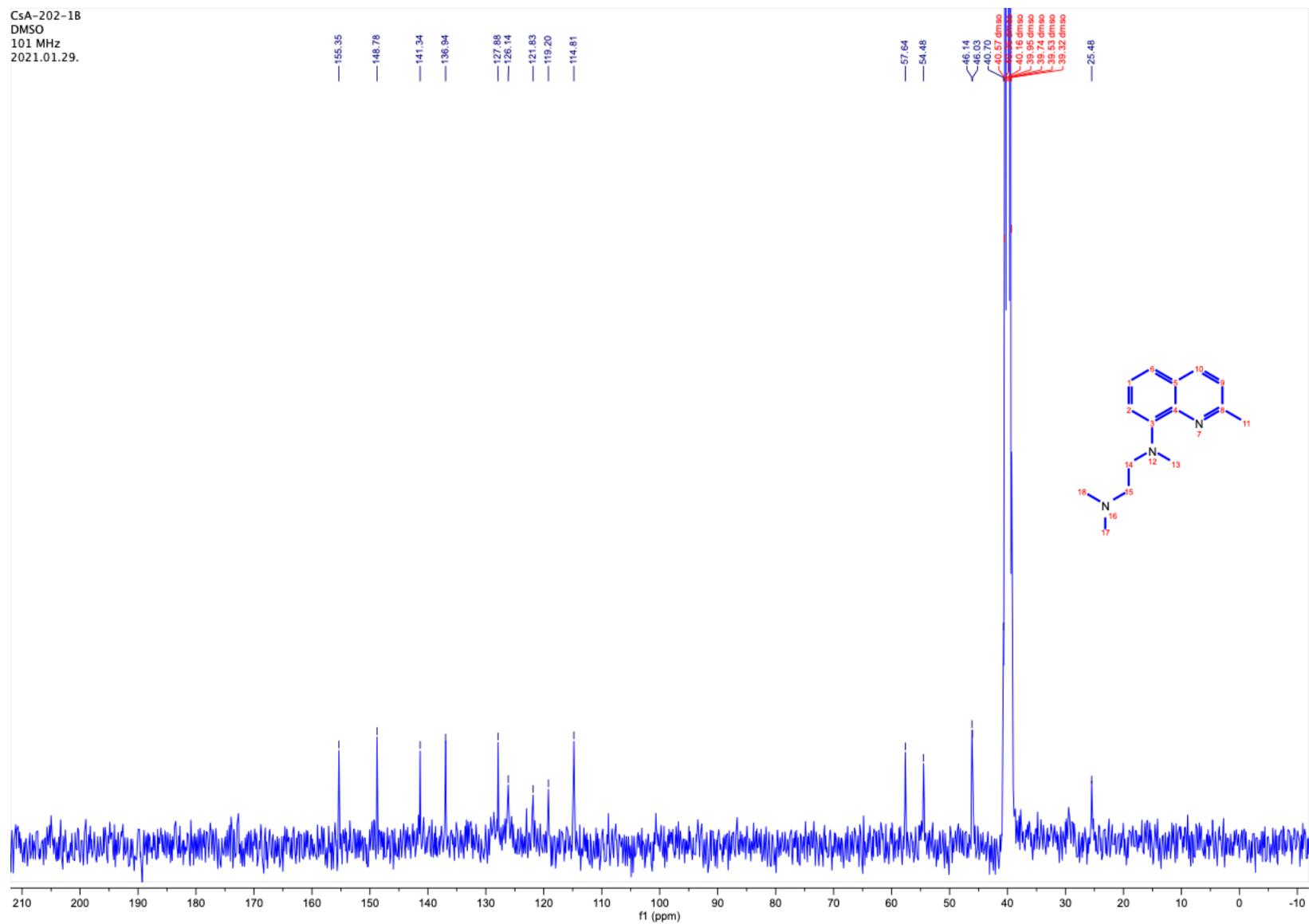


Figure S22.: ^{13}C NMR spectrum of compound **4b** recorded at 101 MHz in $\text{DMSO-}d_6$.

CSA202 #146-155 RT: 0.66-0.70 AV: 10 NL: 4.33E8
T: FTMS + p ESI Full ms [200.0000-1500.0000]

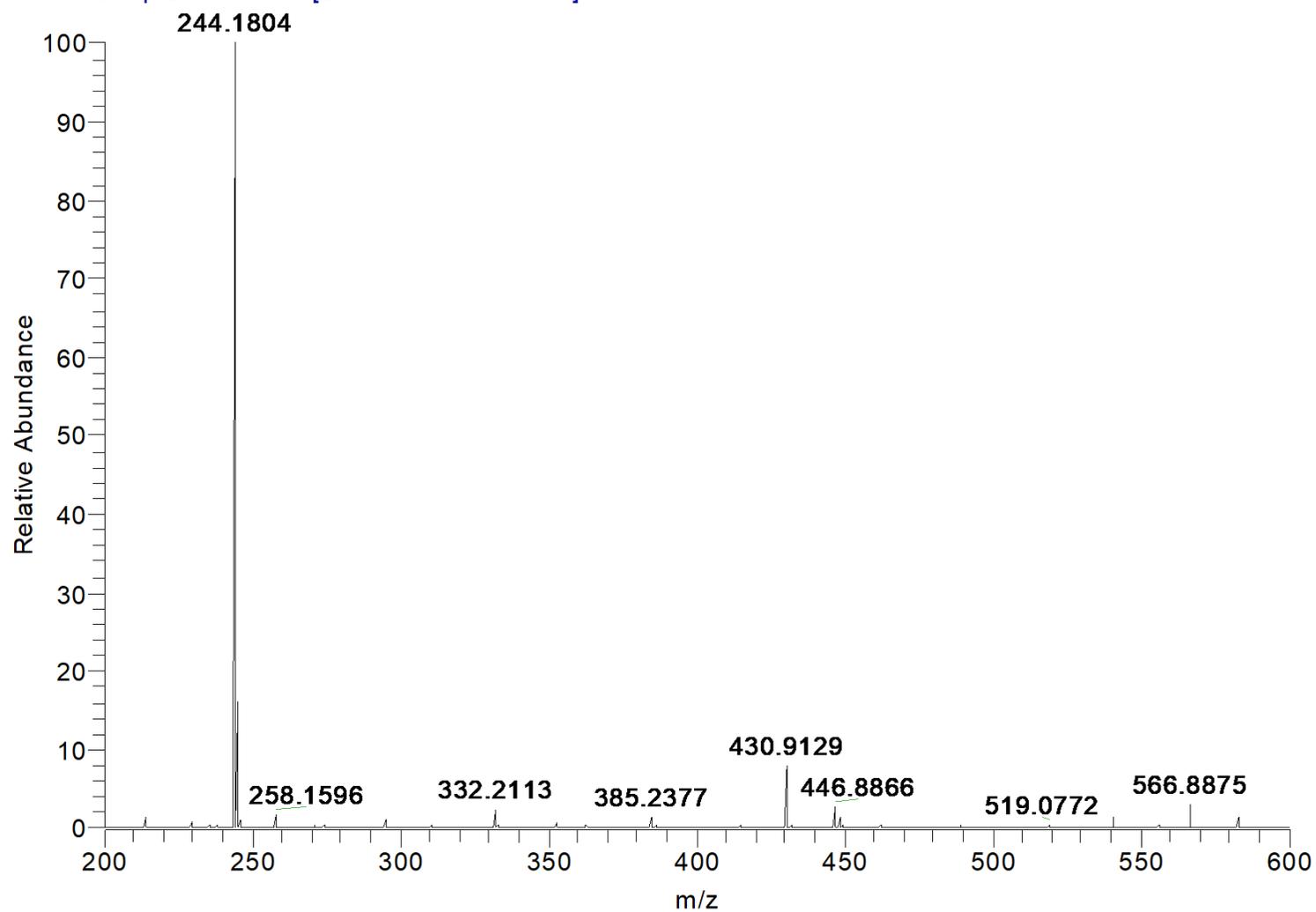


Figure S23.: HRMS spectrum of 4b.

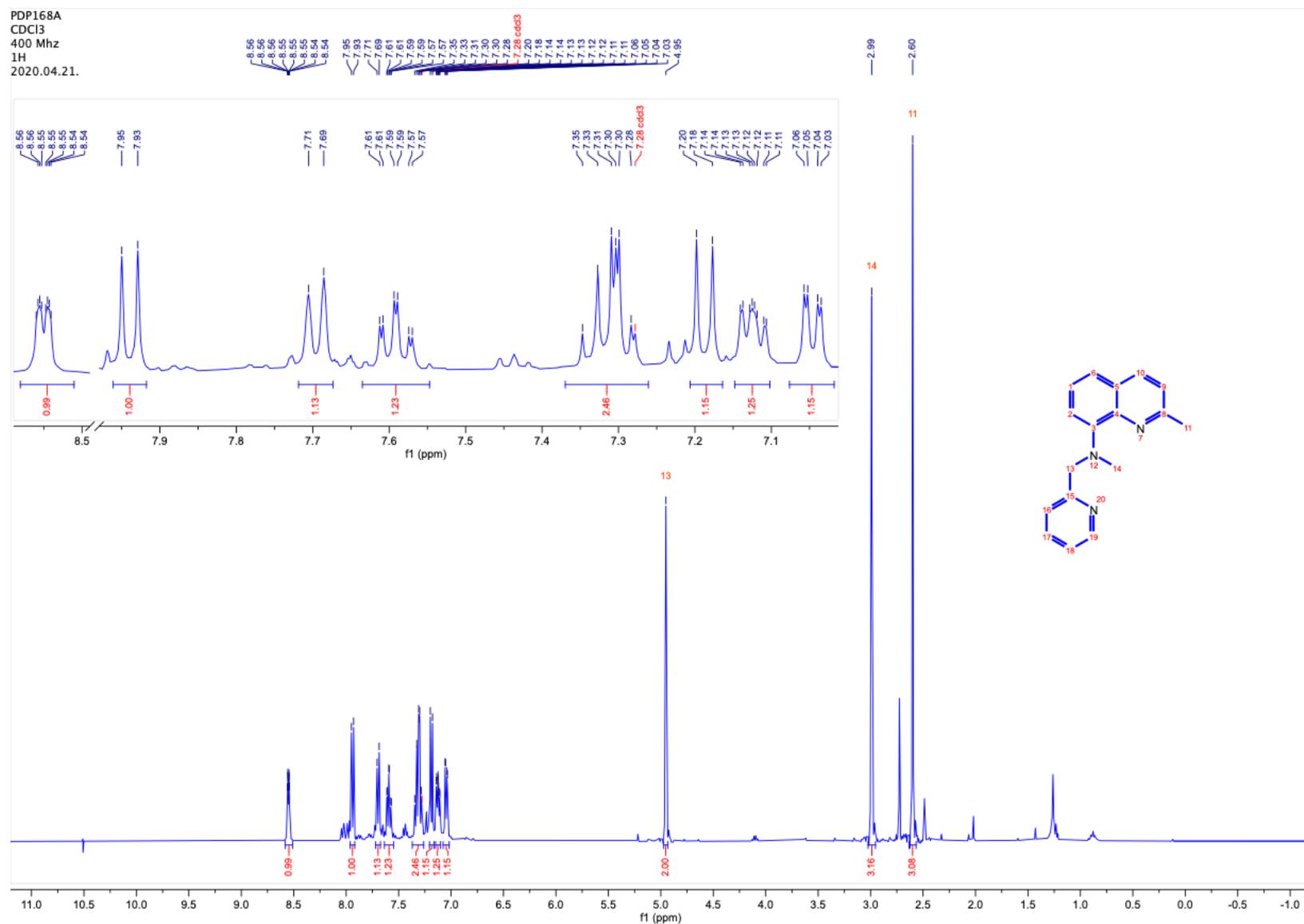


Figure S24.: ¹H NMR spectrum of compound **4c** recorded at 400 MHz in Chloroform-*d*.

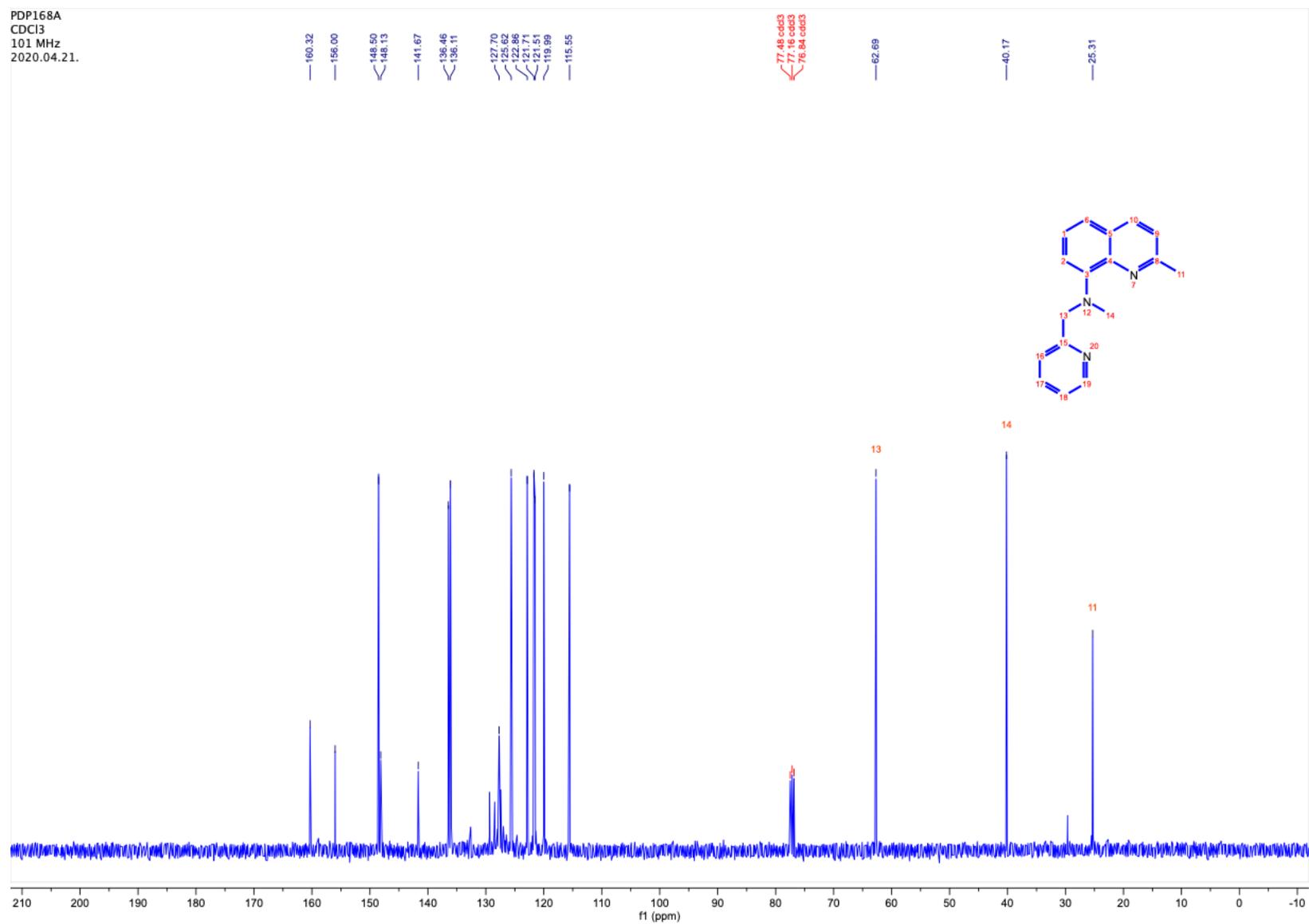


Figure S25.: ¹³C NMR spectrum of compound **4c** recorded at 101 MHz in Chloroform-*d*.

PDP168 #113-135 RT: 0.51-0.61 AV: 23 NL: 6.77E8
T: FTMS + p ESI Full ms [200.0000-1500.0000]

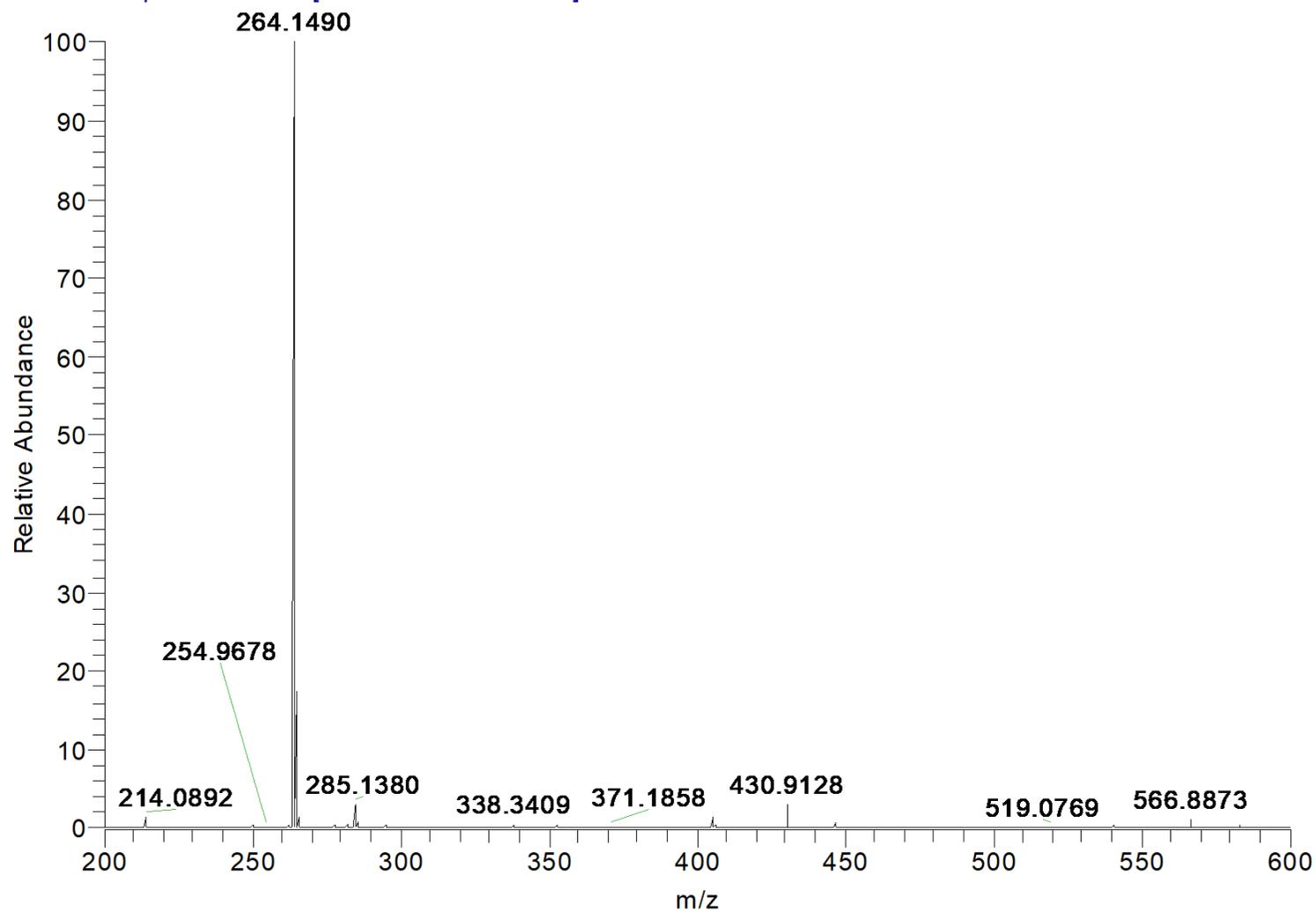


Figure S26.: HRMS spectrum of 4c.

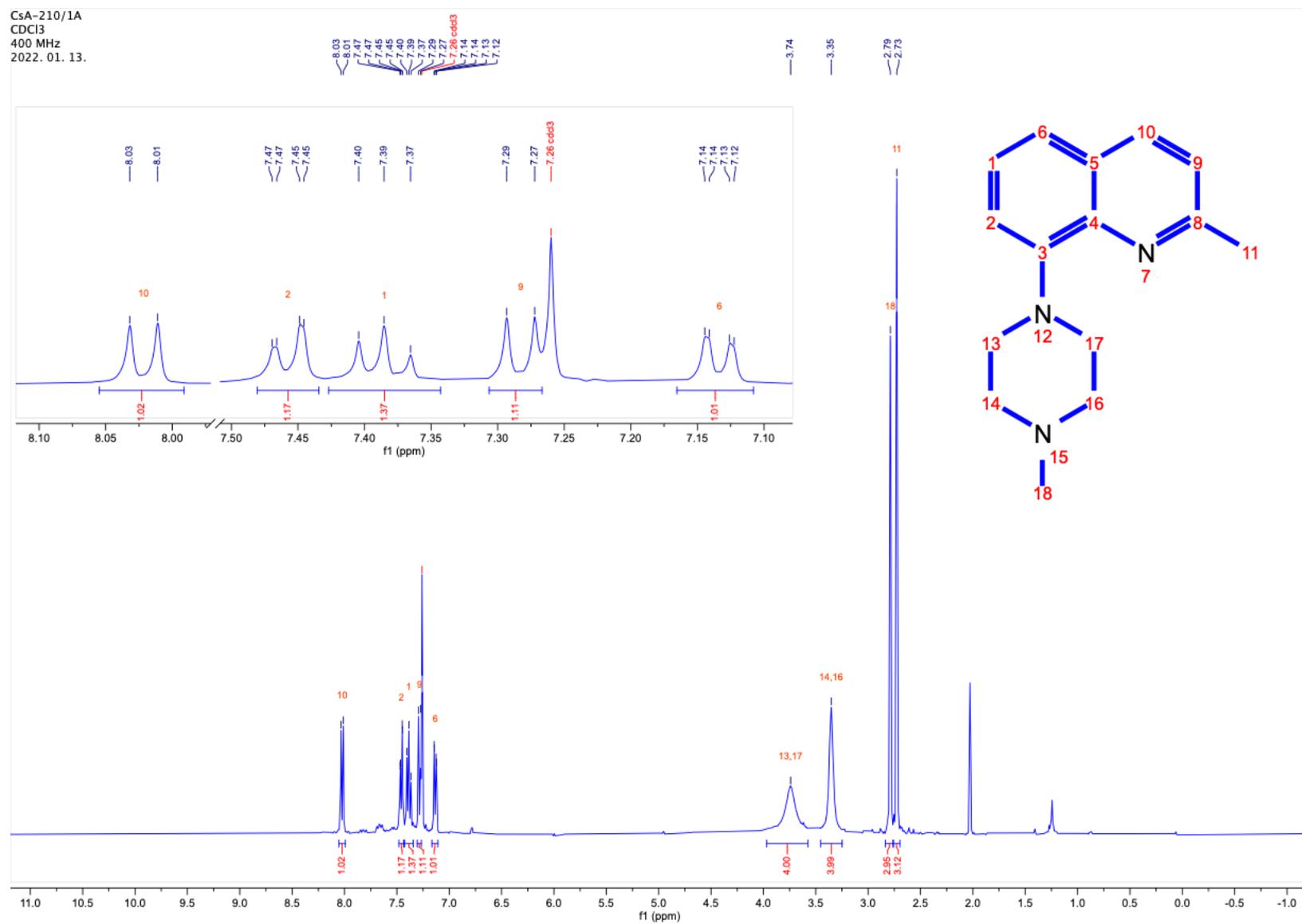


Figure S27.: ¹H NMR spectrum of compound **4d** recorded at 400 MHz in DMSO-*d*₆.

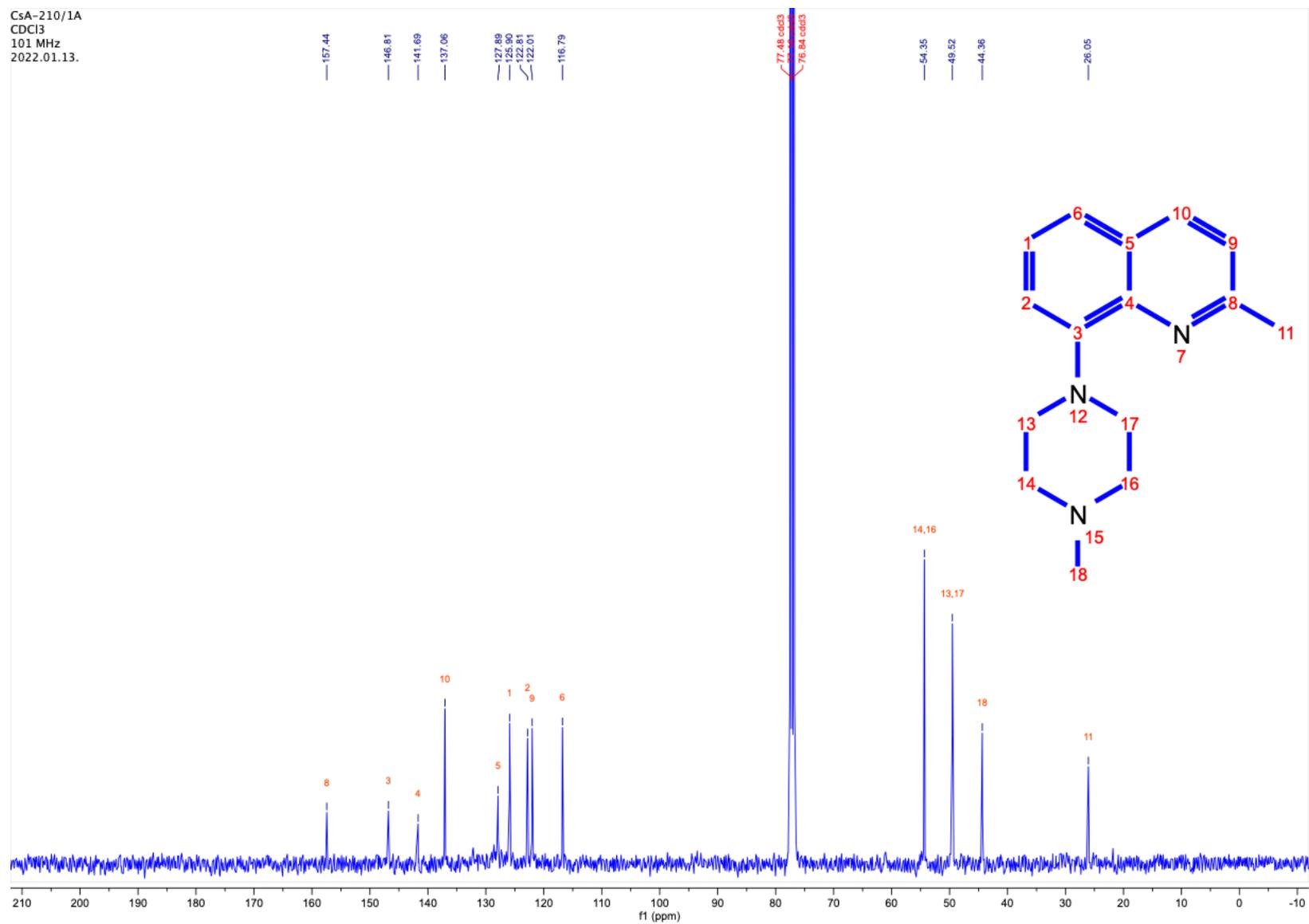


Figure S28.: ¹³C NMR spectrum of compound **4d** recorded at 101 MHz in DMSO-*d*₆.

CSA210 #103-153 RT: 0.47-0.69 AV: 51 NL: 3.36E8
T: FTMS + p ESI Full ms [200.0000-1500.0000]

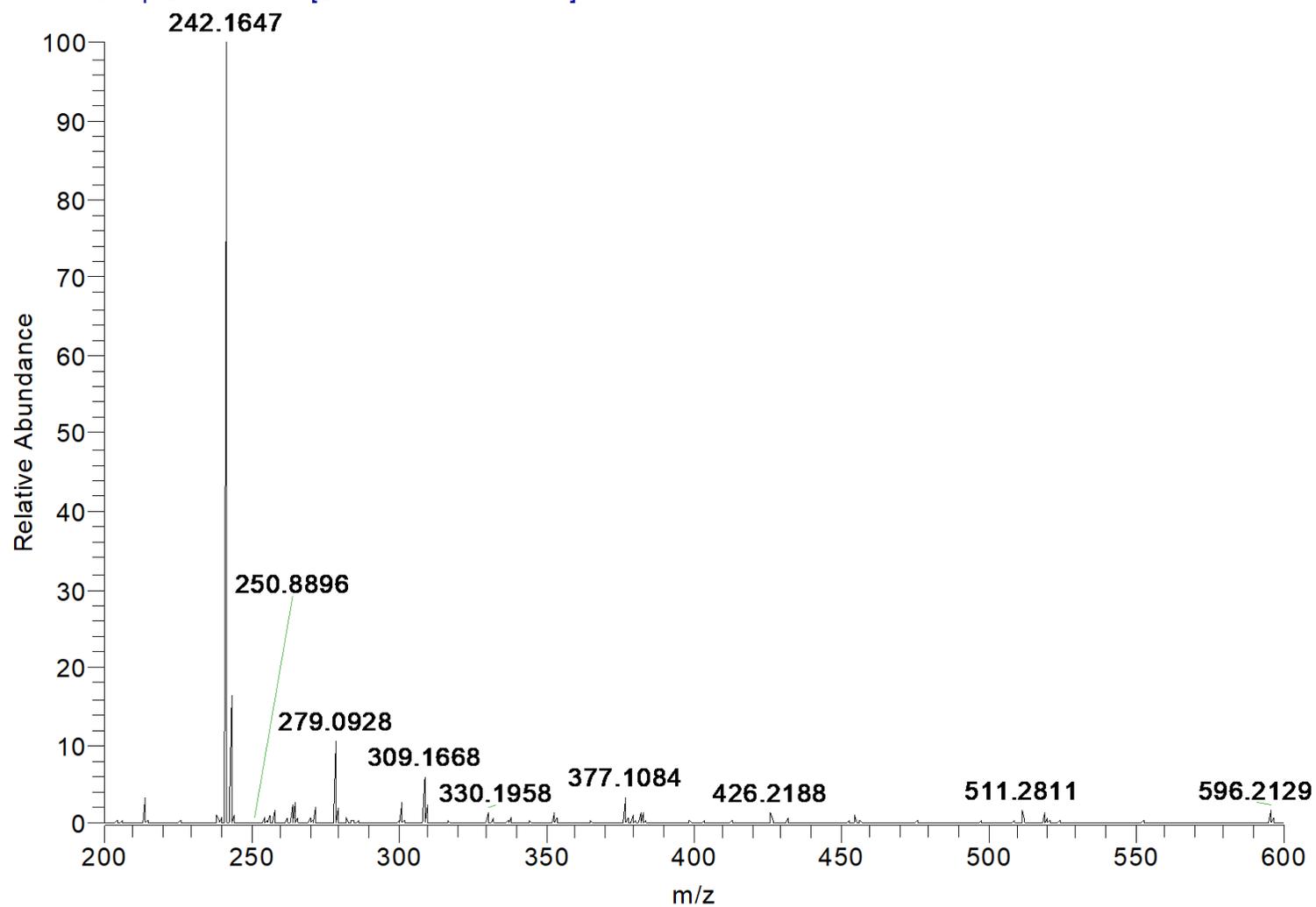


Figure S29.: HRMS spectrum of 4d.

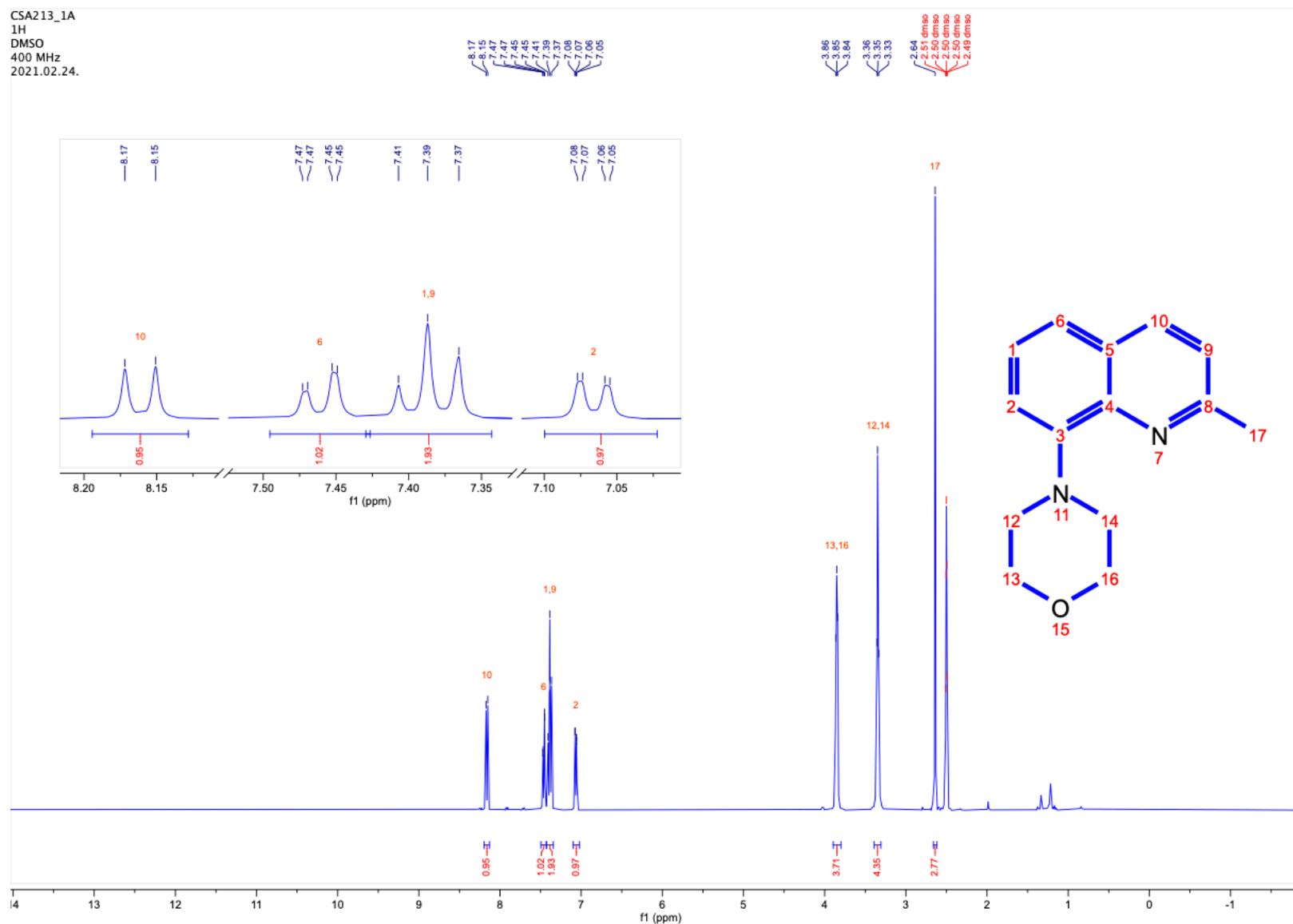


Figure S30.: ^1H NMR spectrum of compound **4e** recorded at 400 MHz in $\text{DMSO}-d_6$.

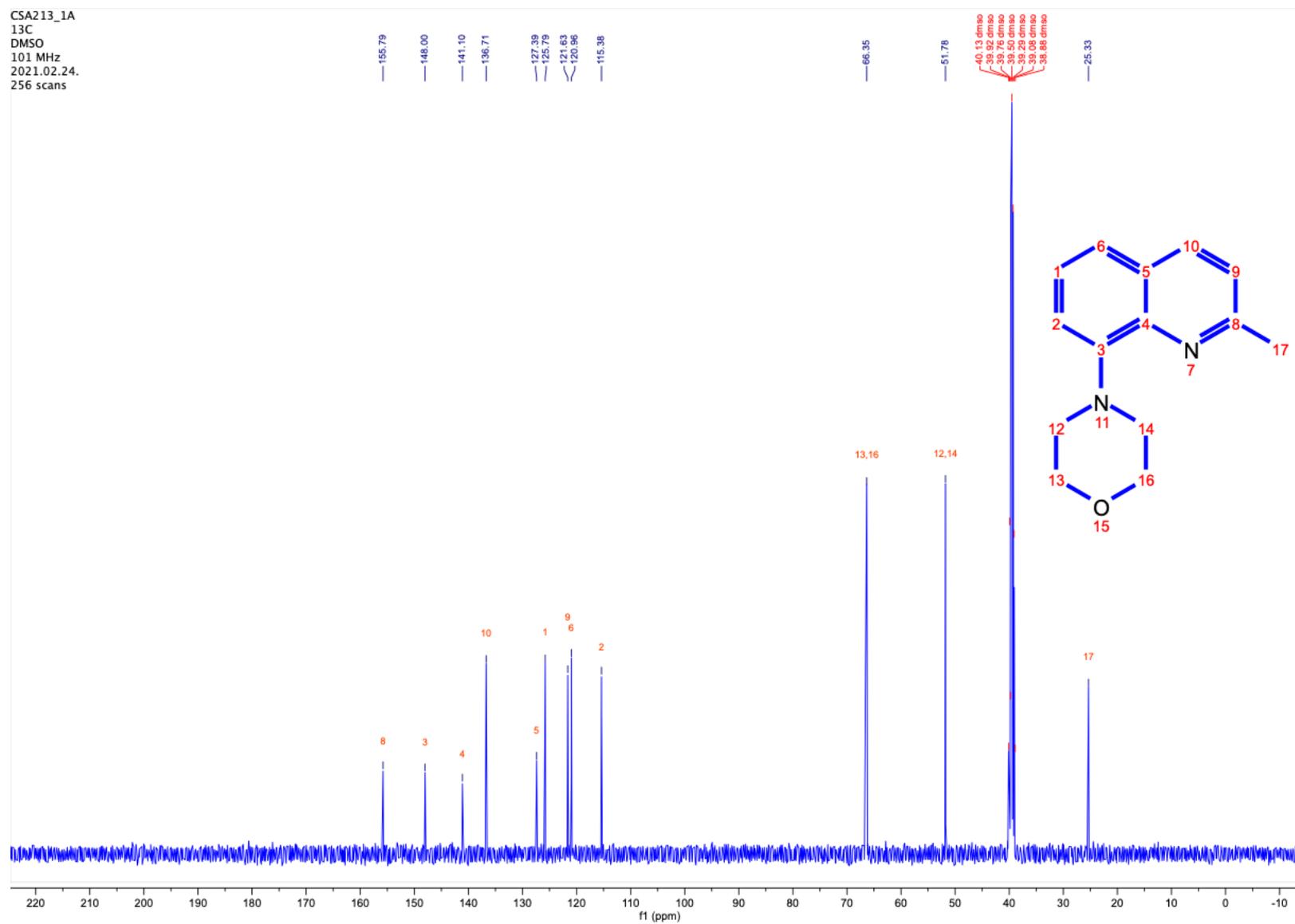


Figure S31.: ^{13}C NMR spectrum of compound **4e** recorded at 101 MHz in $\text{DMSO}-d_6$.

CSA213 #115-135 RT: 0.52-0.61 AV: 21 NL: 3.59E9
T: FTMS + p ESI Full ms [200.0000-1500.0000]

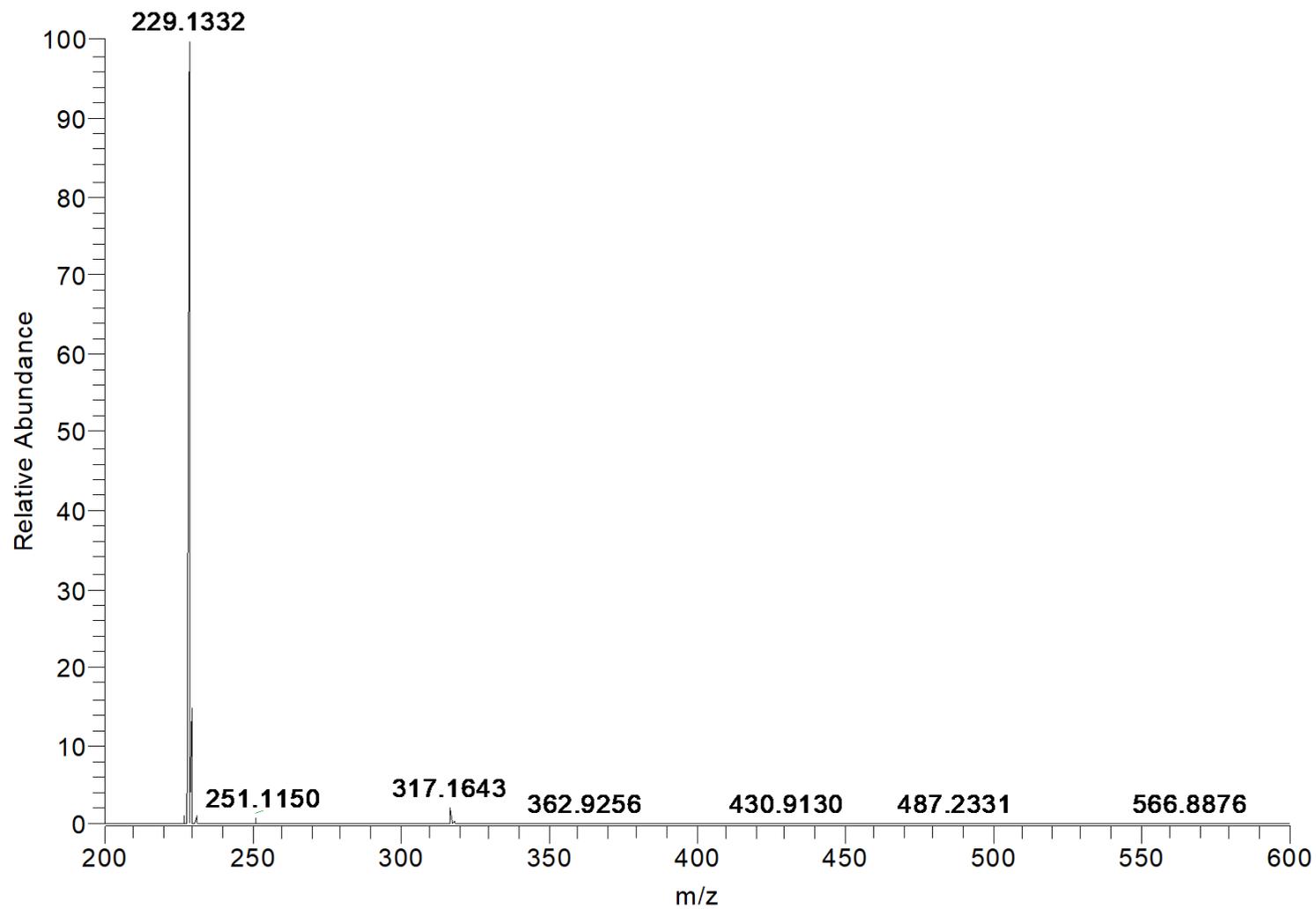


Figure S32.: HRMS spectrum of 4e.

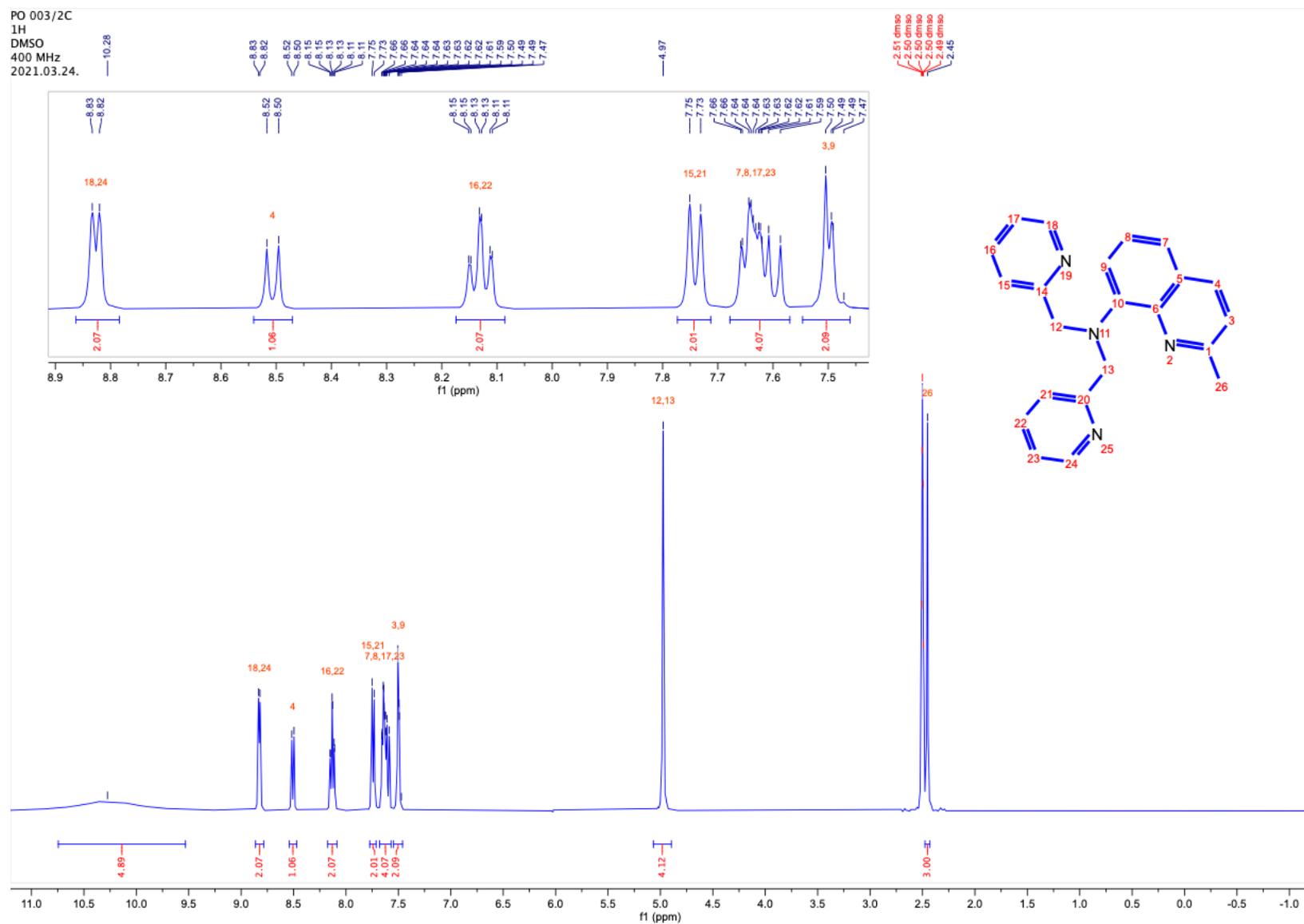


Figure S33.: ^1H NMR spectrum of compound **4g** recorded at 400 MHz in $\text{DMSO-}d_6$.

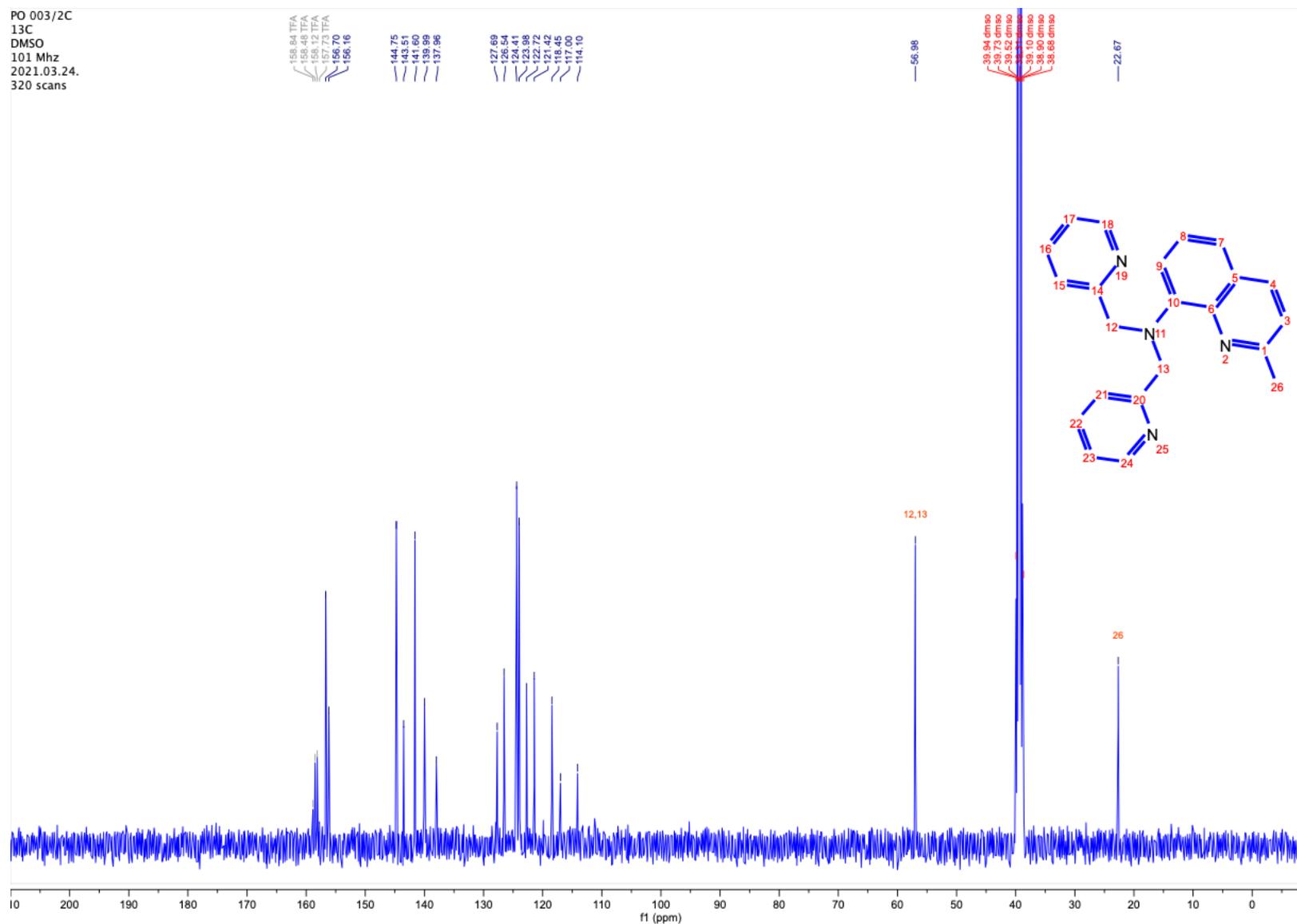


Figure S34.: ^{13}C NMR spectrum of compound **4g** recorded at 101 MHz in $\text{DMSO}-d_6$.

PO003_2C #115-155 RT: 0.52-0.70 AV: 41 NL: 1.77E9
T: FTMS + p ESI Full ms [200.0000-1500.0000]

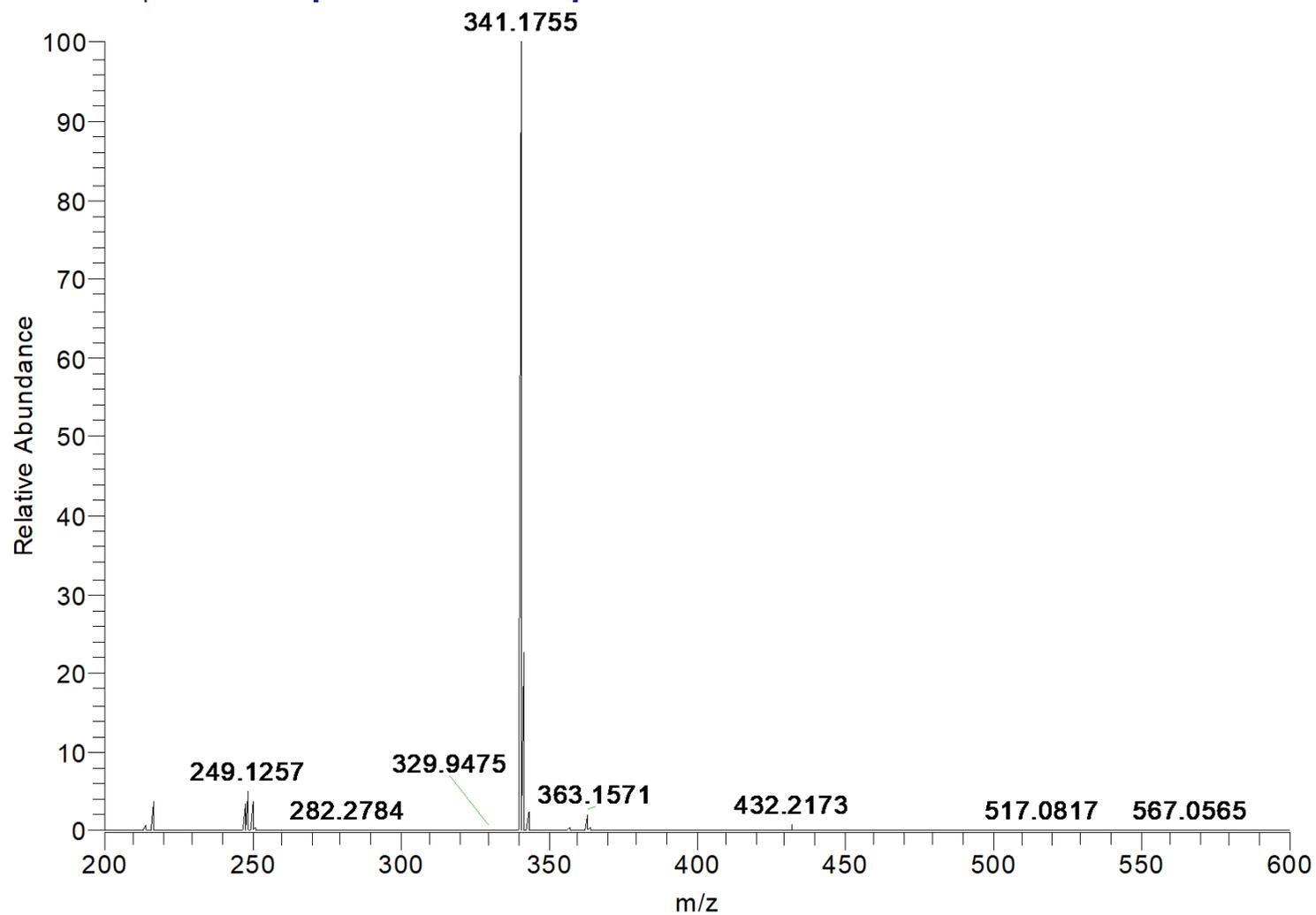


Figure S35.: HRMS spectrum of 4g.

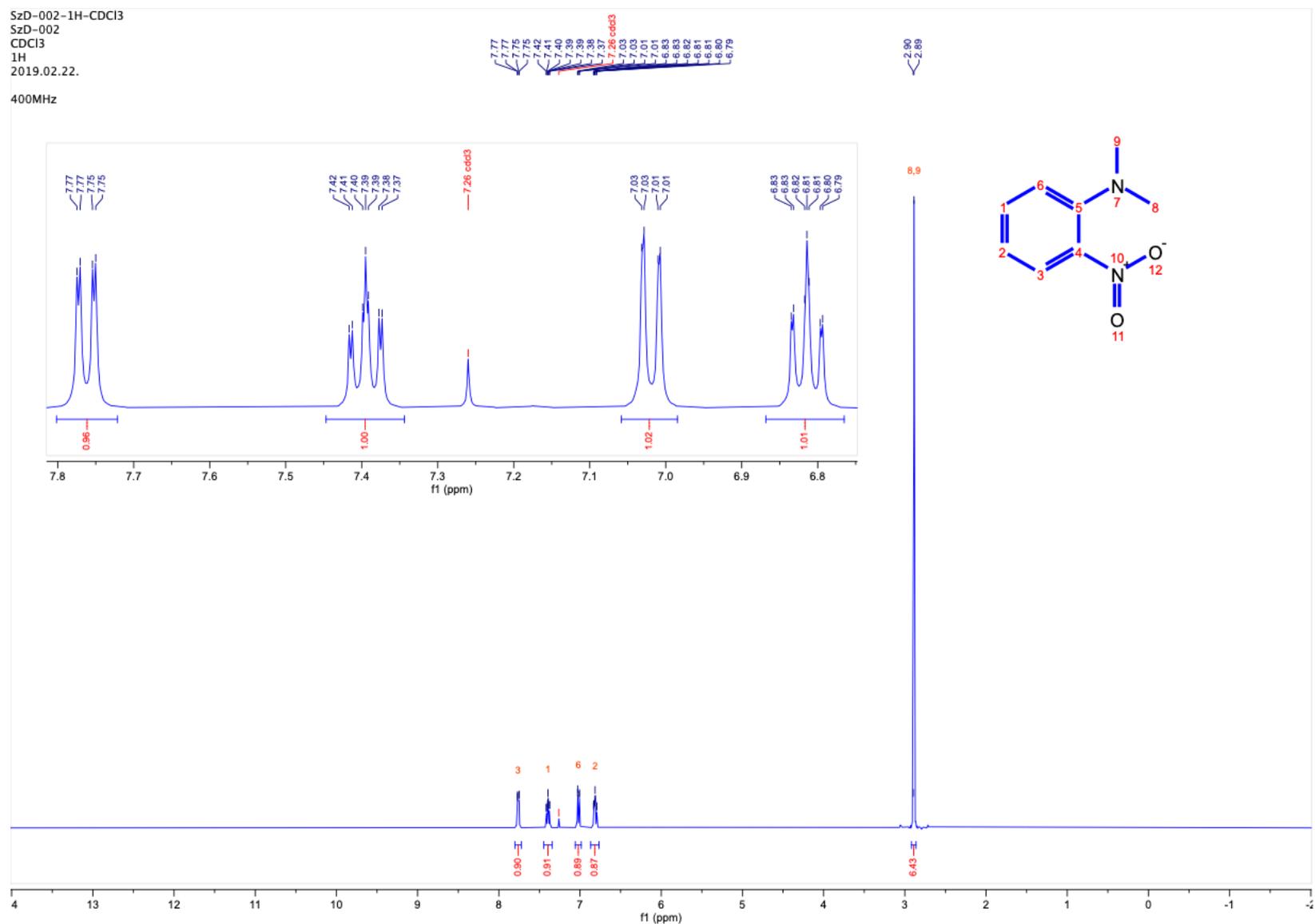


Figure S36.: ^1H NMR spectrum of known compound **6** recorded at 400 MHz in Chloroform-*d*.

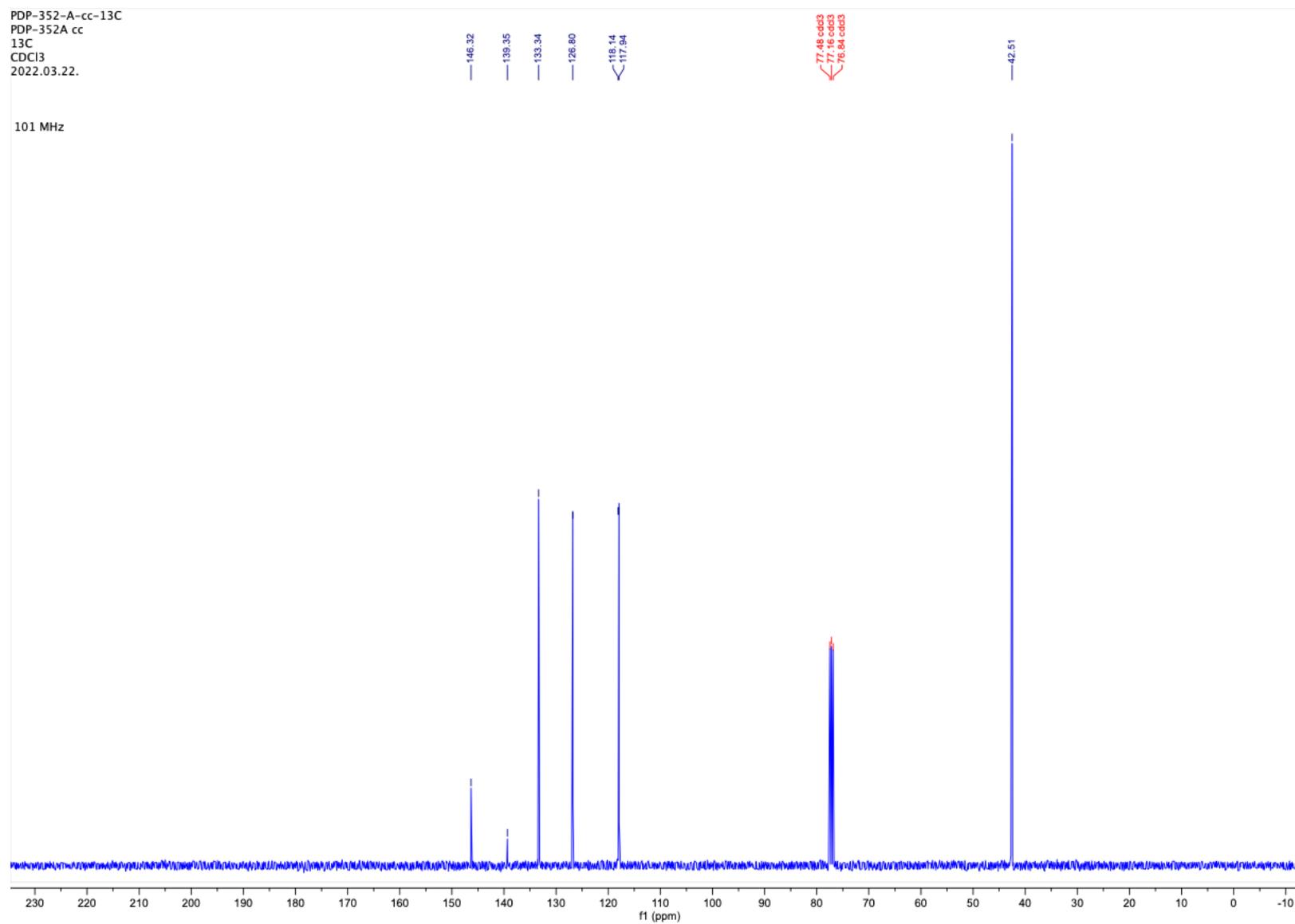


Figure S37.: ^{13}C NMR spectrum of known compound **6** recorded at 101 MHz in Chloroform-*d*.

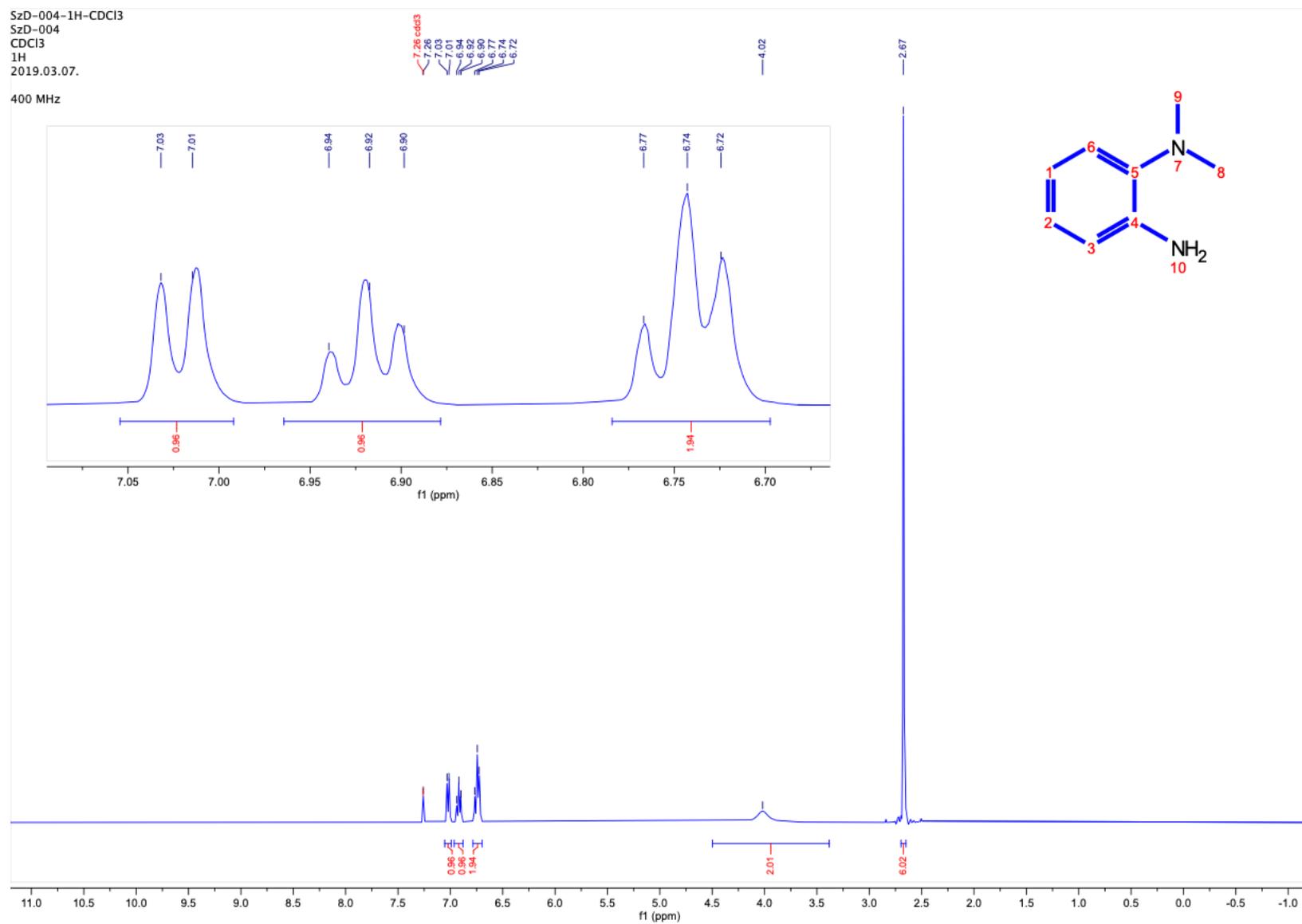


Figure S38.: ^1H NMR spectrum of known compound **7** recorded at 400 MHz in Chloroform-*d*.

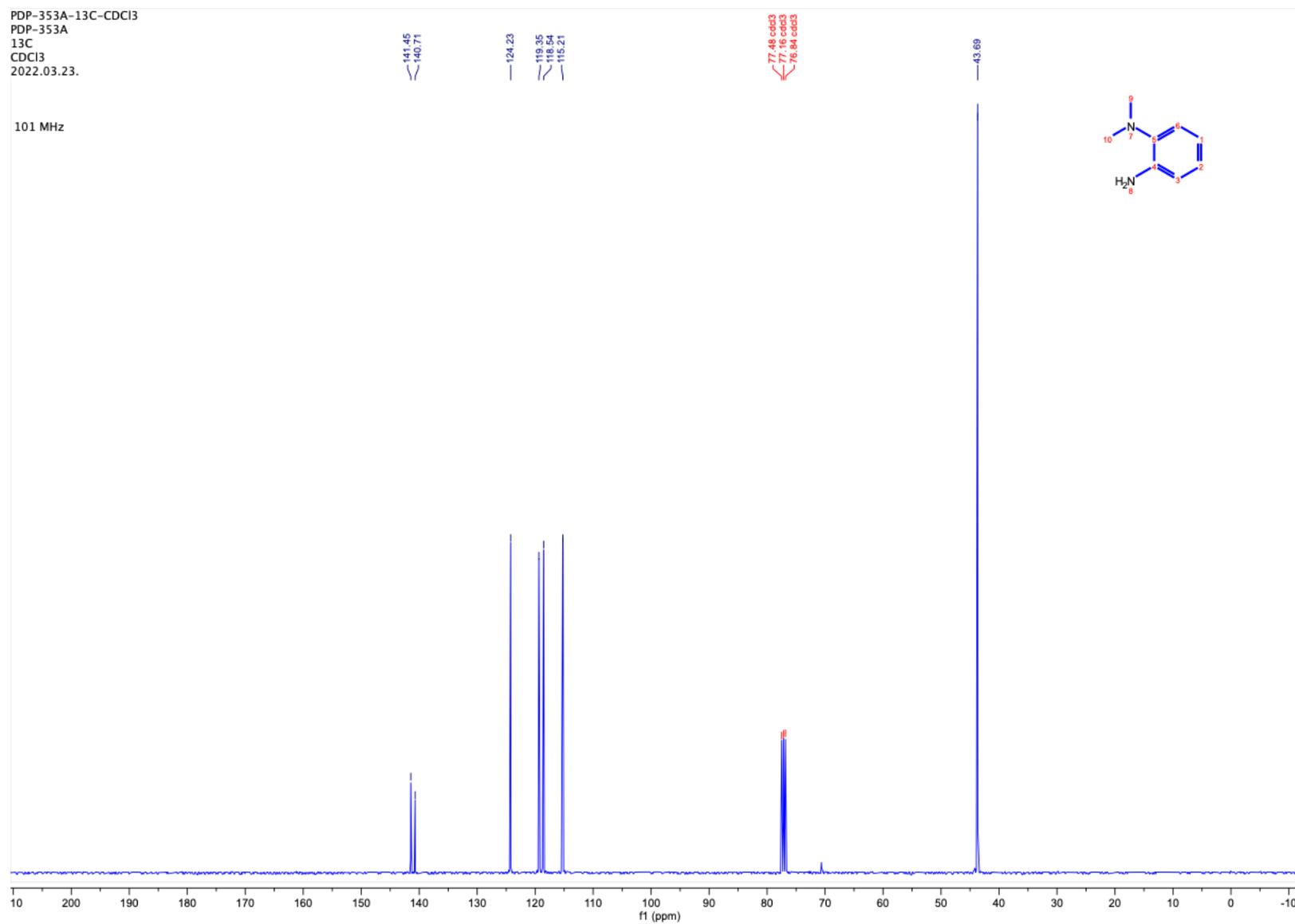


Figure S39.: ¹³C NMR spectrum of known compound **7** recorded at 101 MHz in Chloroform-*d*.

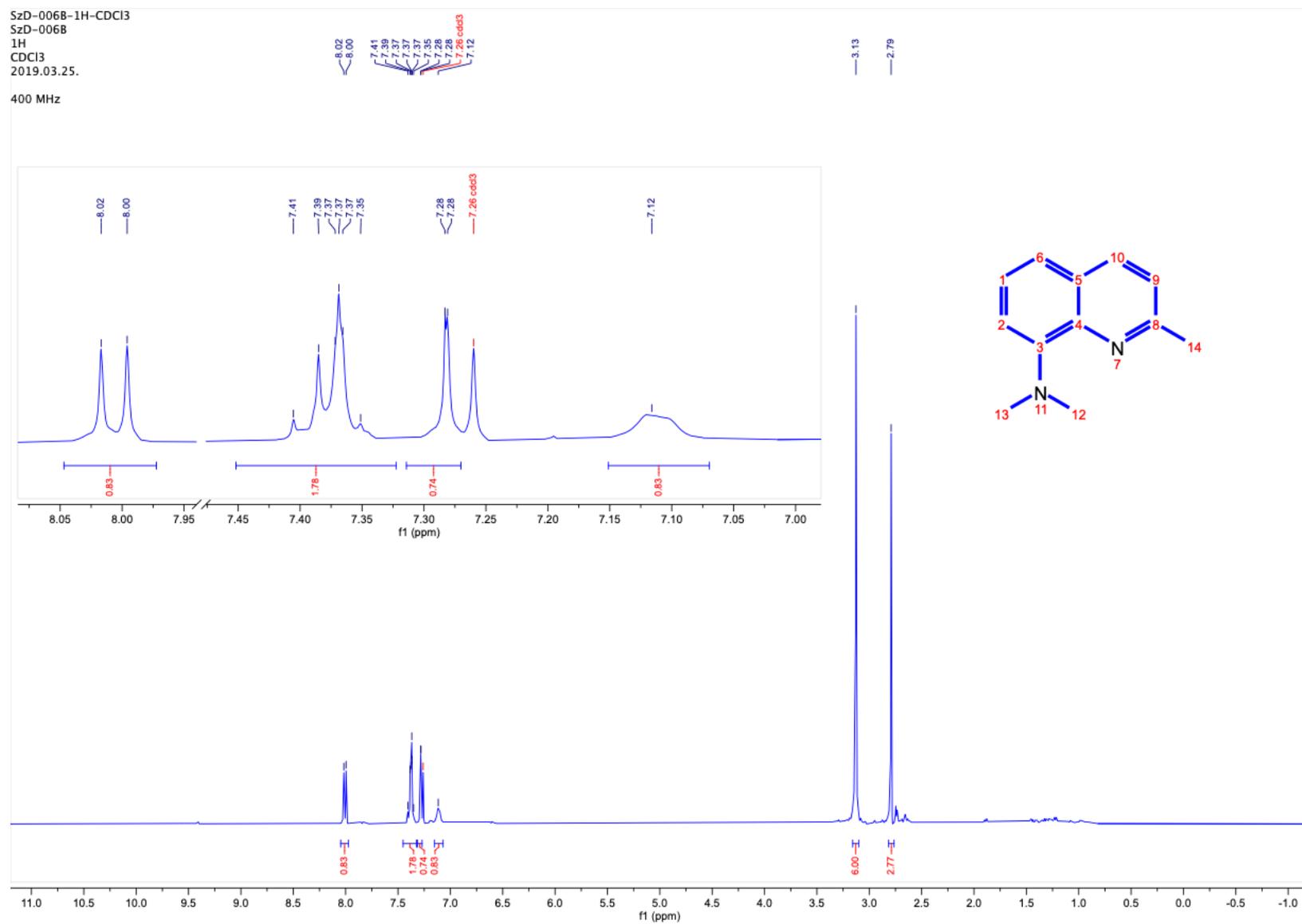


Figure S40.: ^1H NMR spectrum of known compound **4a** recorded at 400 MHz in Chloroform-*d*.

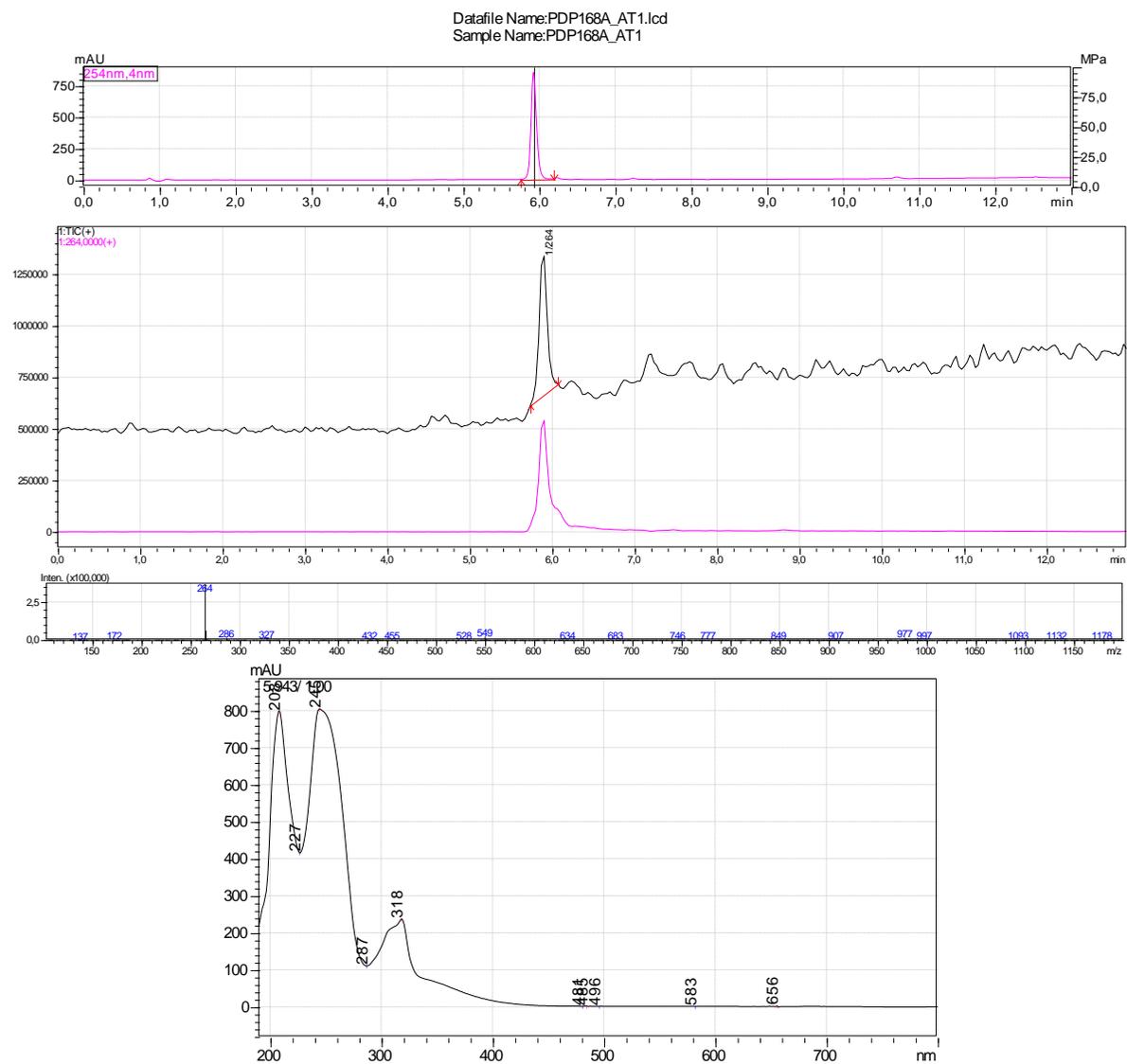


Figure S41.: HPLC UV and MS chromatograms, mass spectrum and UV-VIS spectrum of known compound 4a.

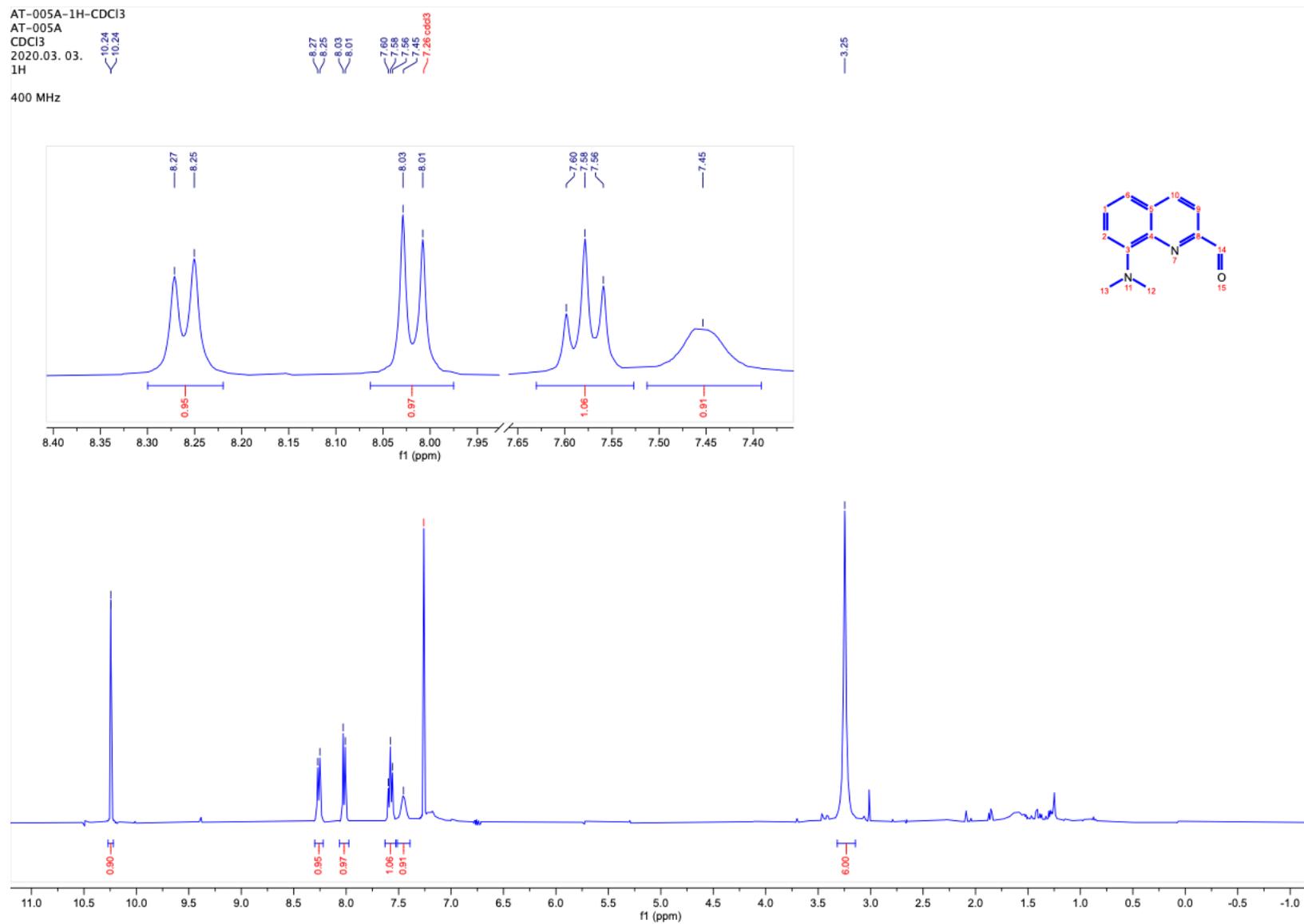


Figure S42.: ^1H NMR spectrum of known compound **1a** recorded at 400 MHz in Chloroform-*d*.

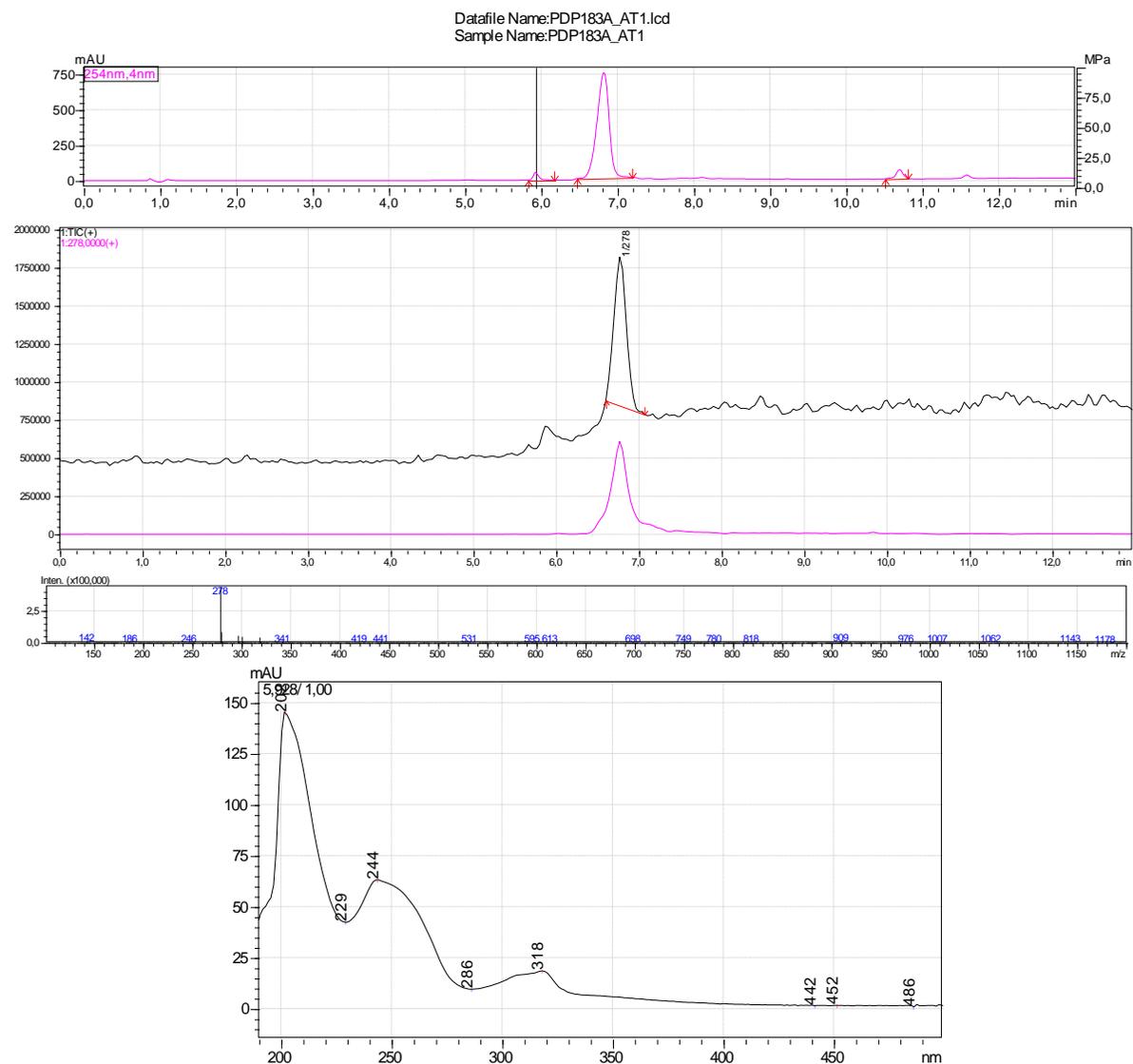


Figure S43.: HPLC UV and MS chromatograms, mass spectrum and UV-VIS spectrum of known compound 1a.

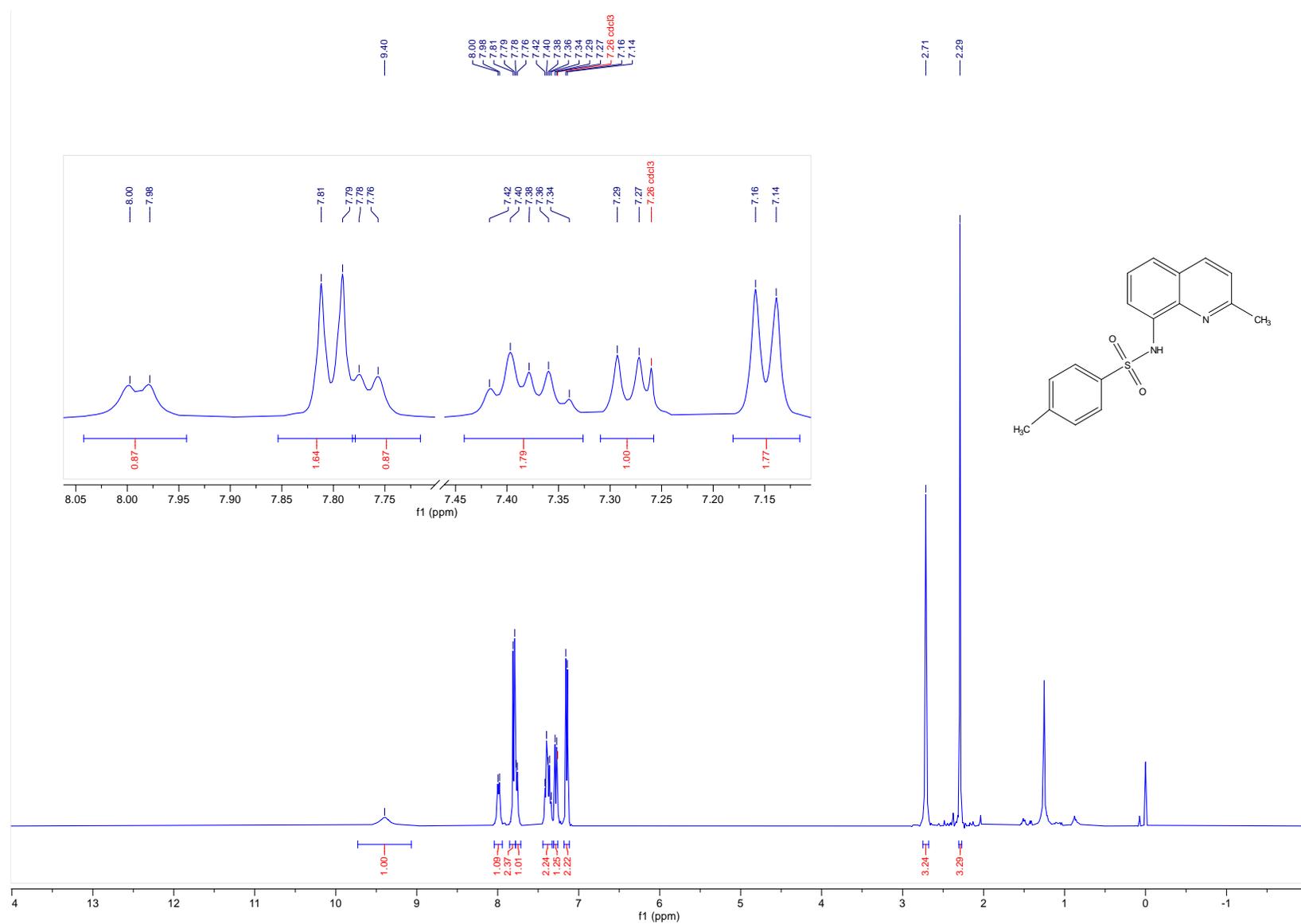


Figure S44.: ^1H NMR spectrum of known compound **4h** recorded at 400 MHz in Chloroform-*d*.

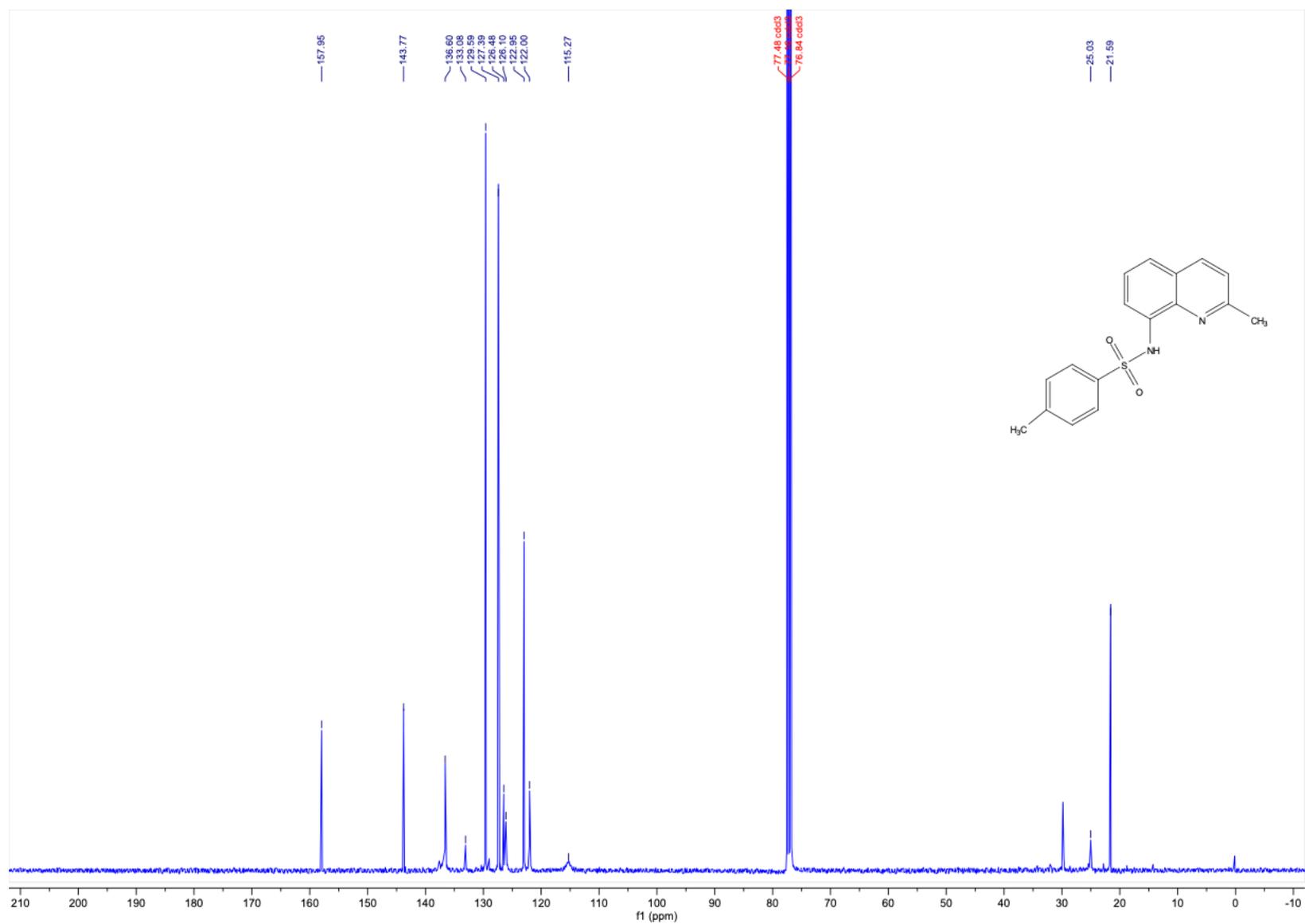


Figure S45.: ^{13}C NMR spectrum of known compound **4h** recorded at 101 MHz in Chloroform-*d*.