

# Regioselective Cyclic Iminium Formation of Ugi Advanced Intermediates: Rapid Access to 3,4-Dihydropyrazin-2(1*H*)-ones and Other Diverse Nitrogen-Containing Heterocycles

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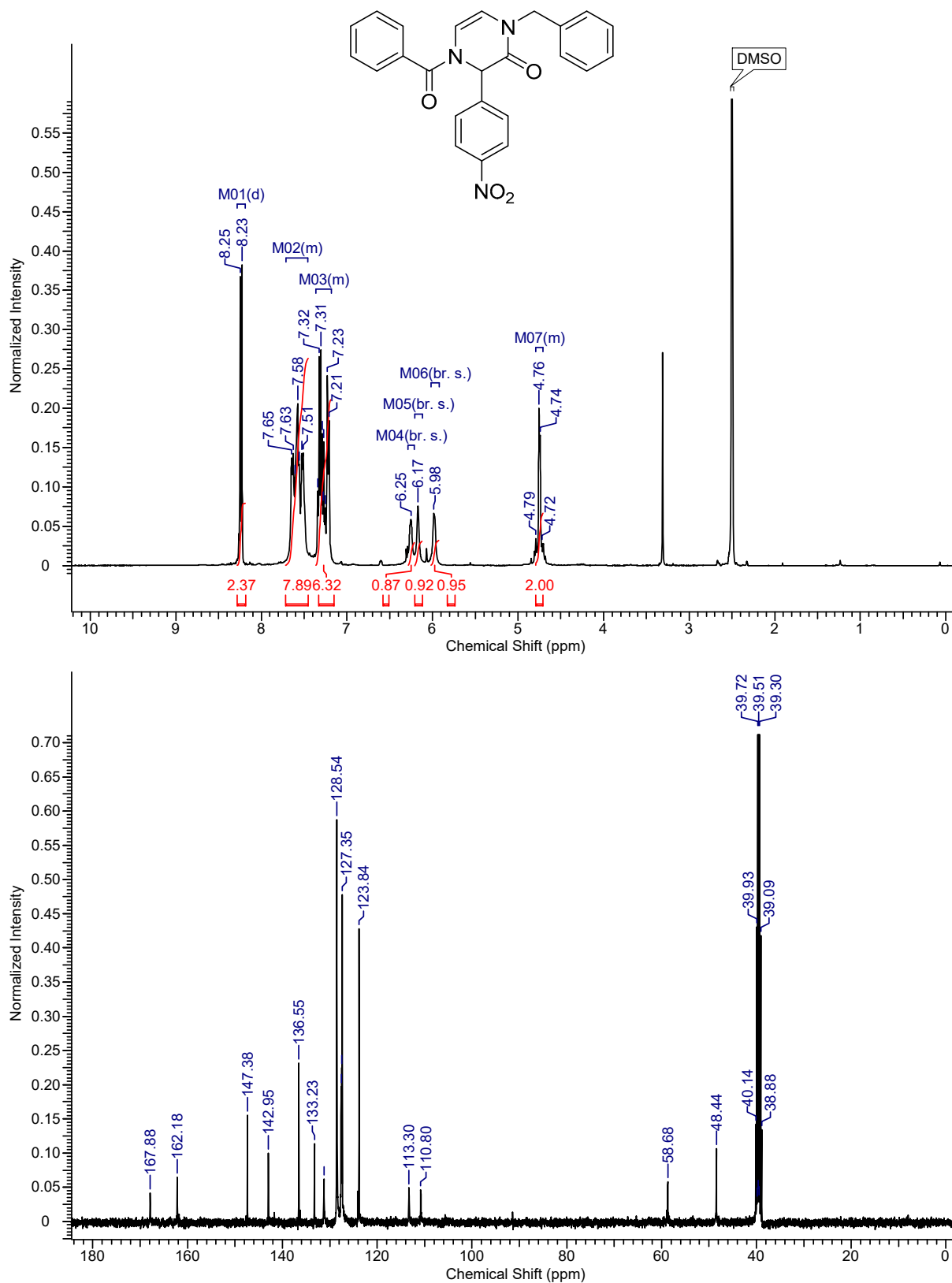
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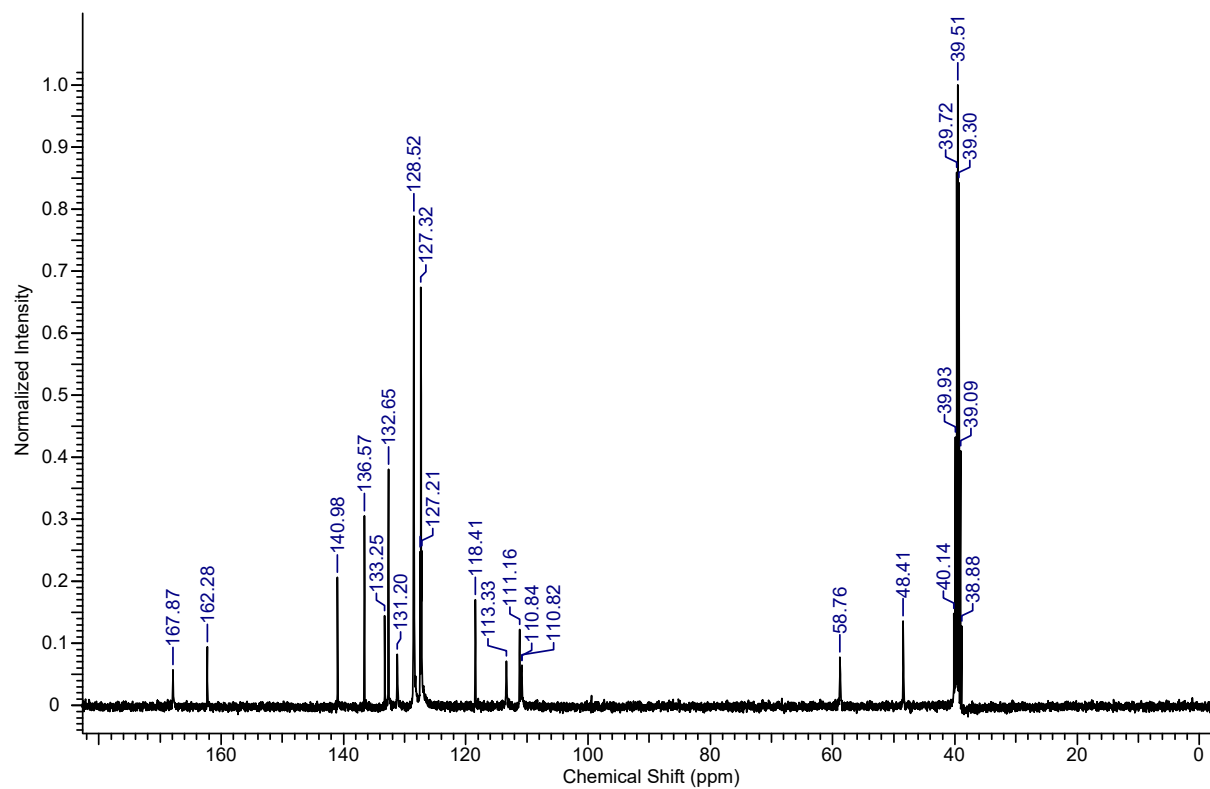
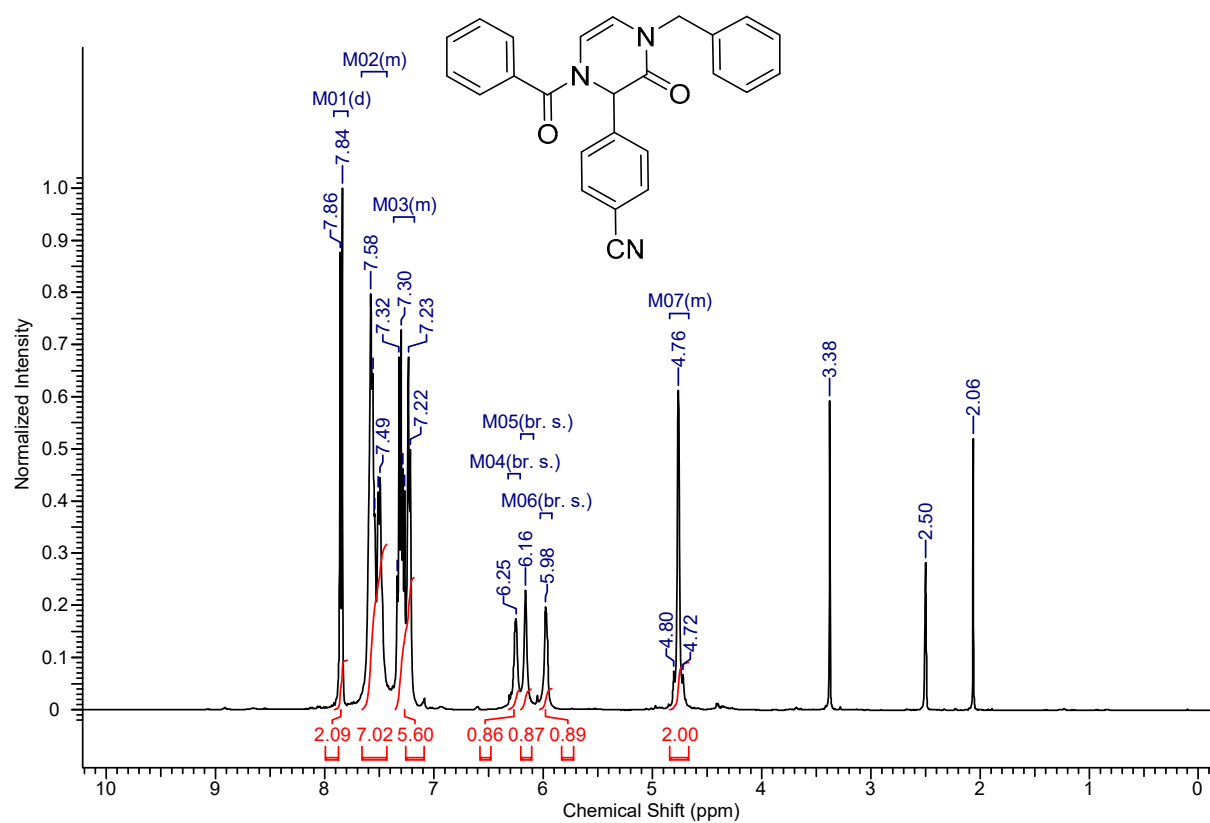
1. <sup>1</sup> H and <sup>13</sup> C NMR Spectra .....	S2
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## 1. $^1\text{H}$ and $^{13}\text{C}$ NMR Spectra

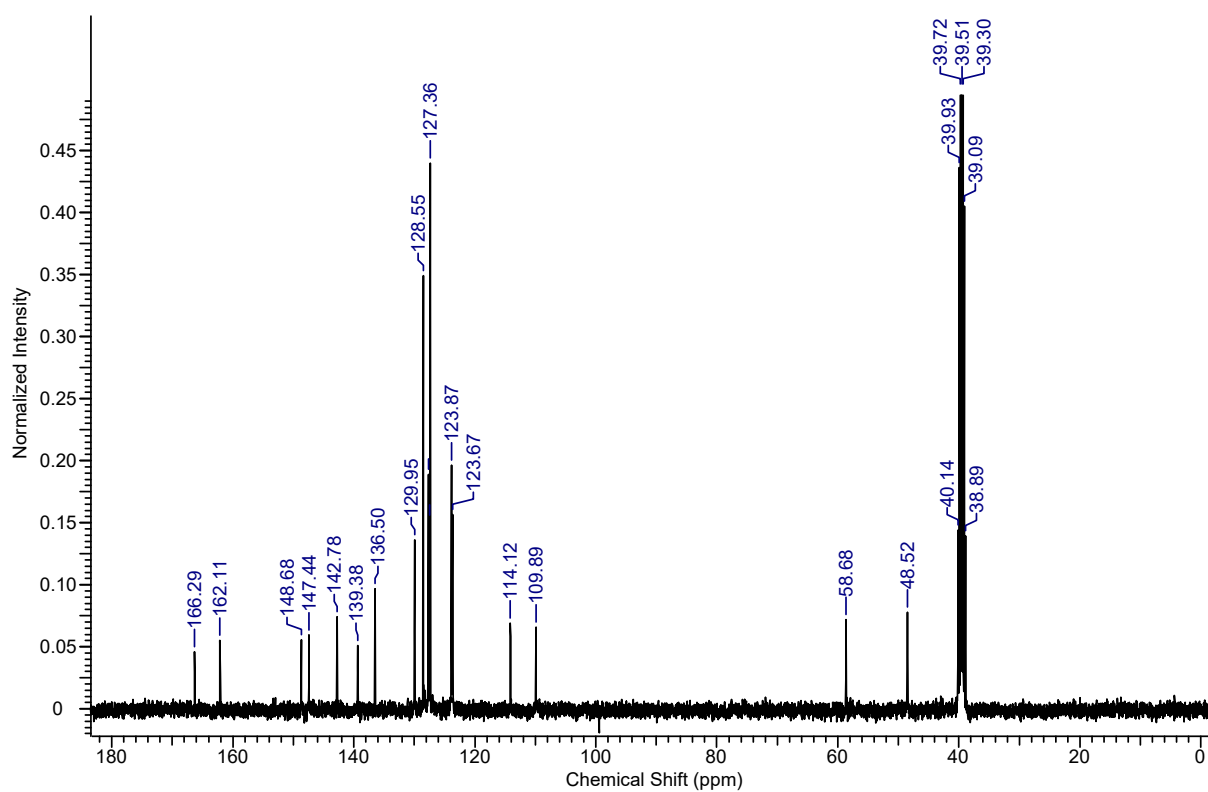
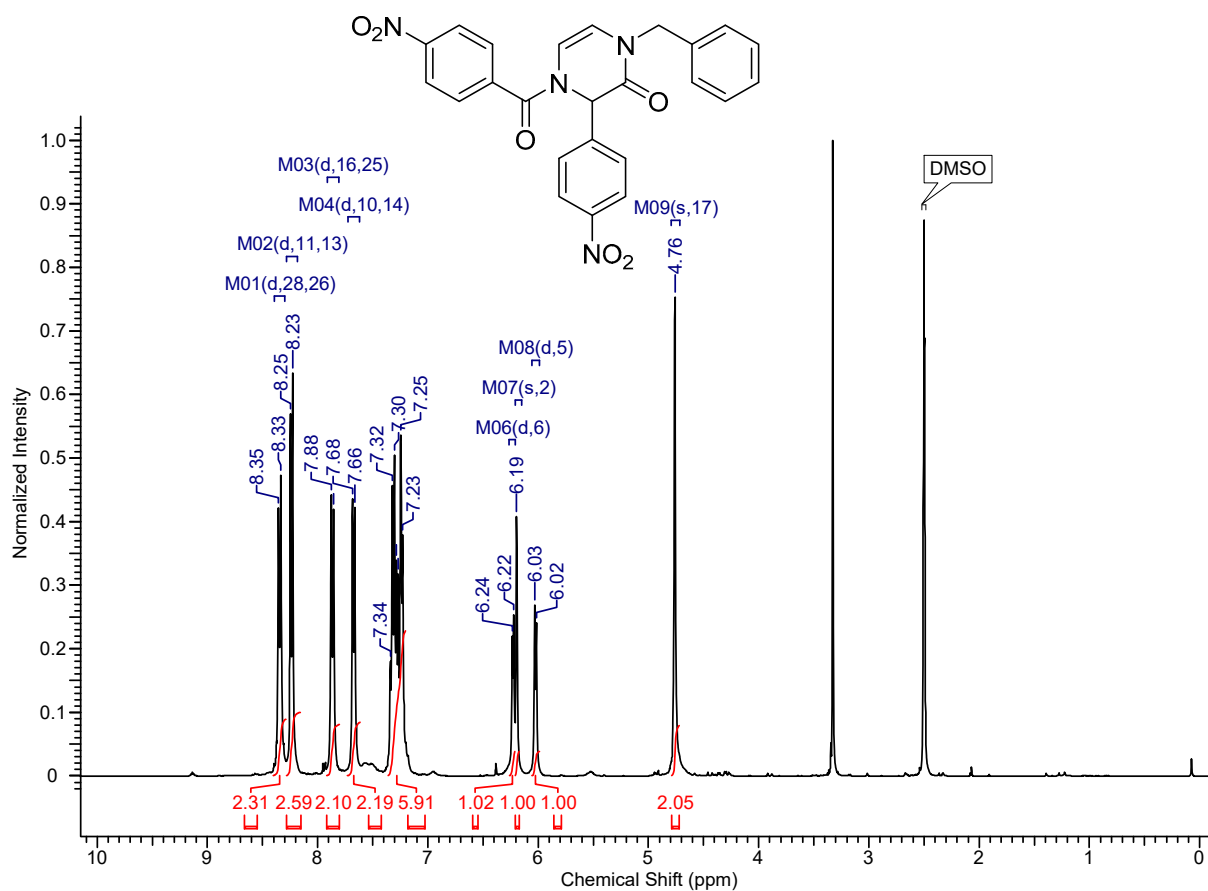
$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra ( $d_6$ -DMSO) for compound 2a



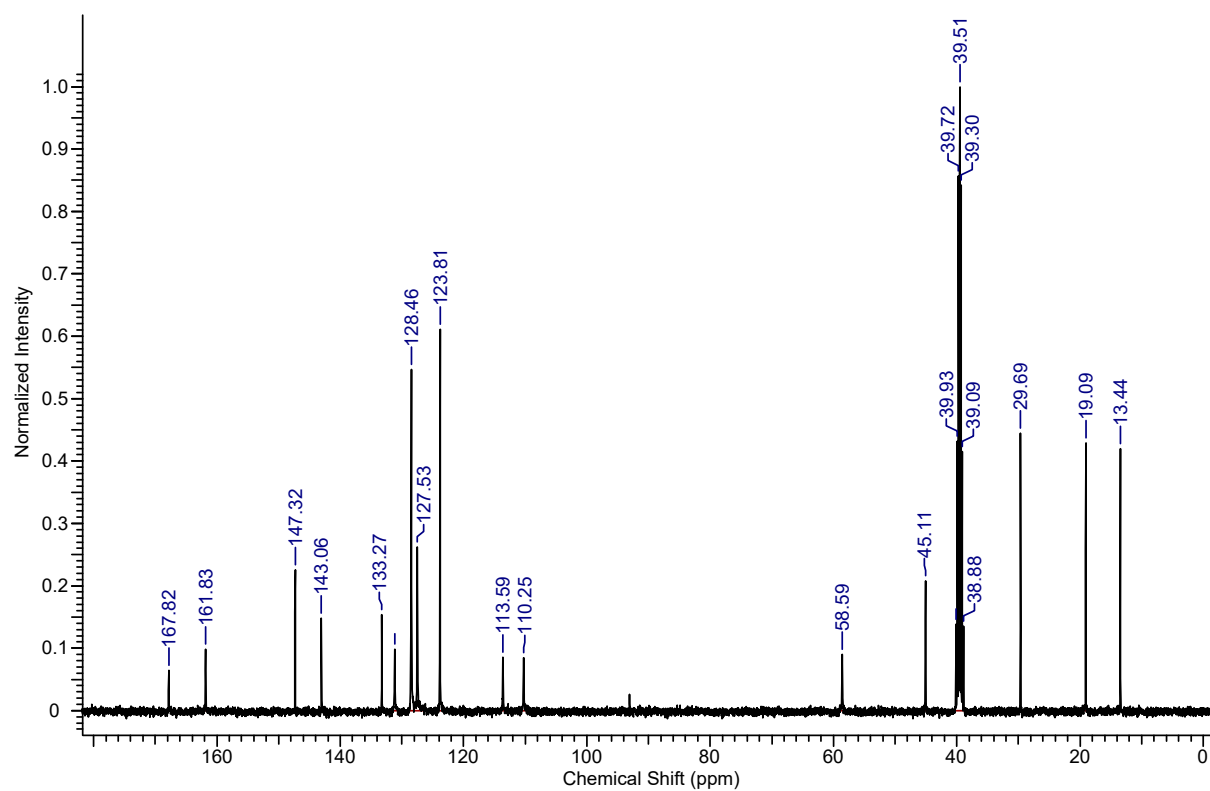
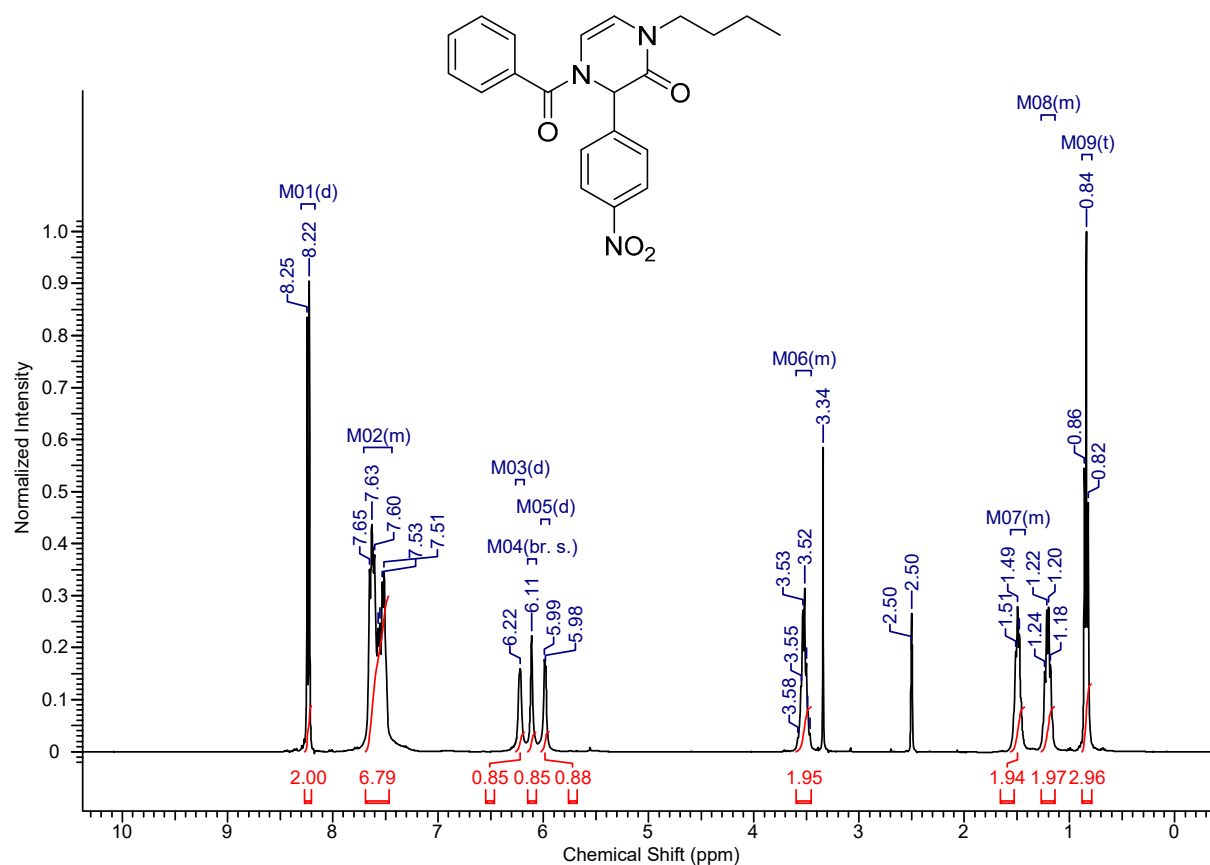
$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra ( $d_6$ -DMSO) for compound 2b



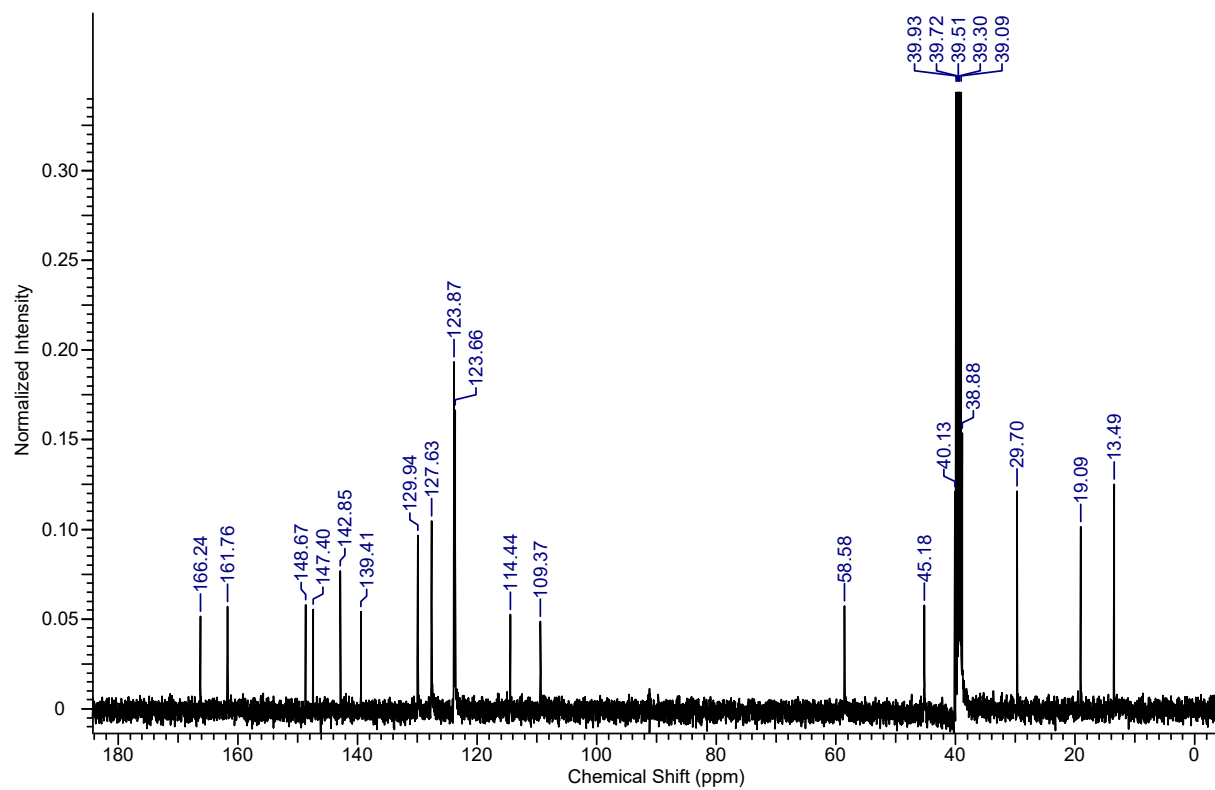
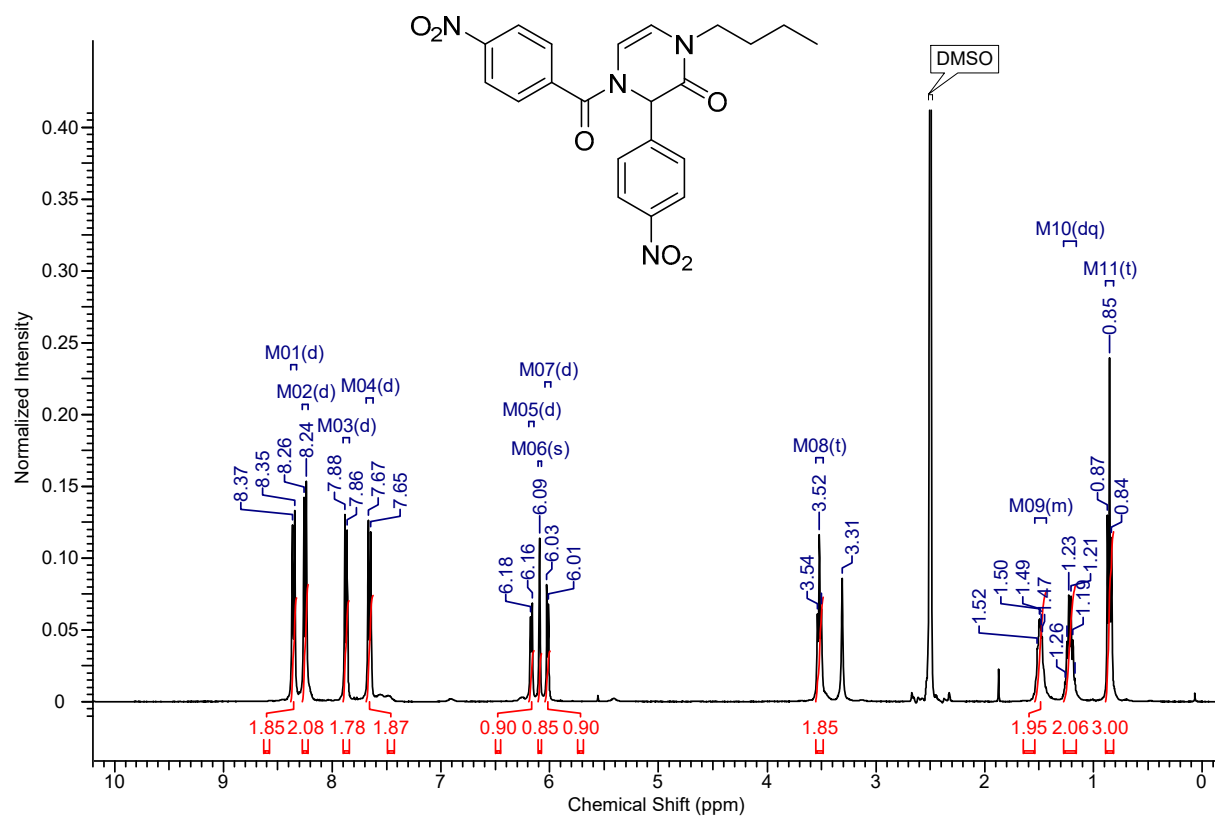
<sup>1</sup>H and <sup>13</sup>C NMR spectra (*d*<sub>6</sub>-DMSO) for compound 2c



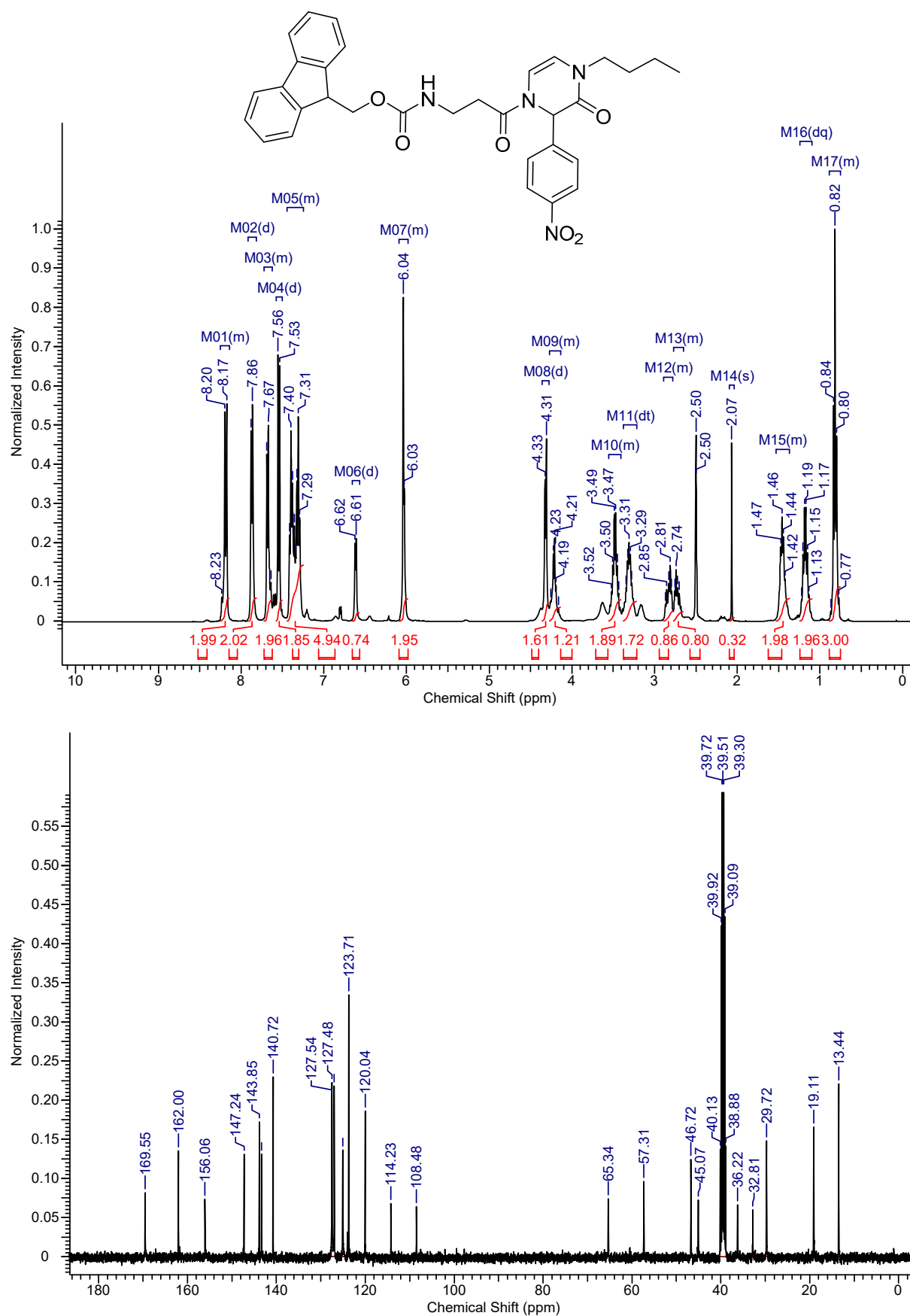
<sup>1</sup>H and <sup>13</sup>C NMR spectra (*d*<sub>6</sub>-DMSO) for compound 2d



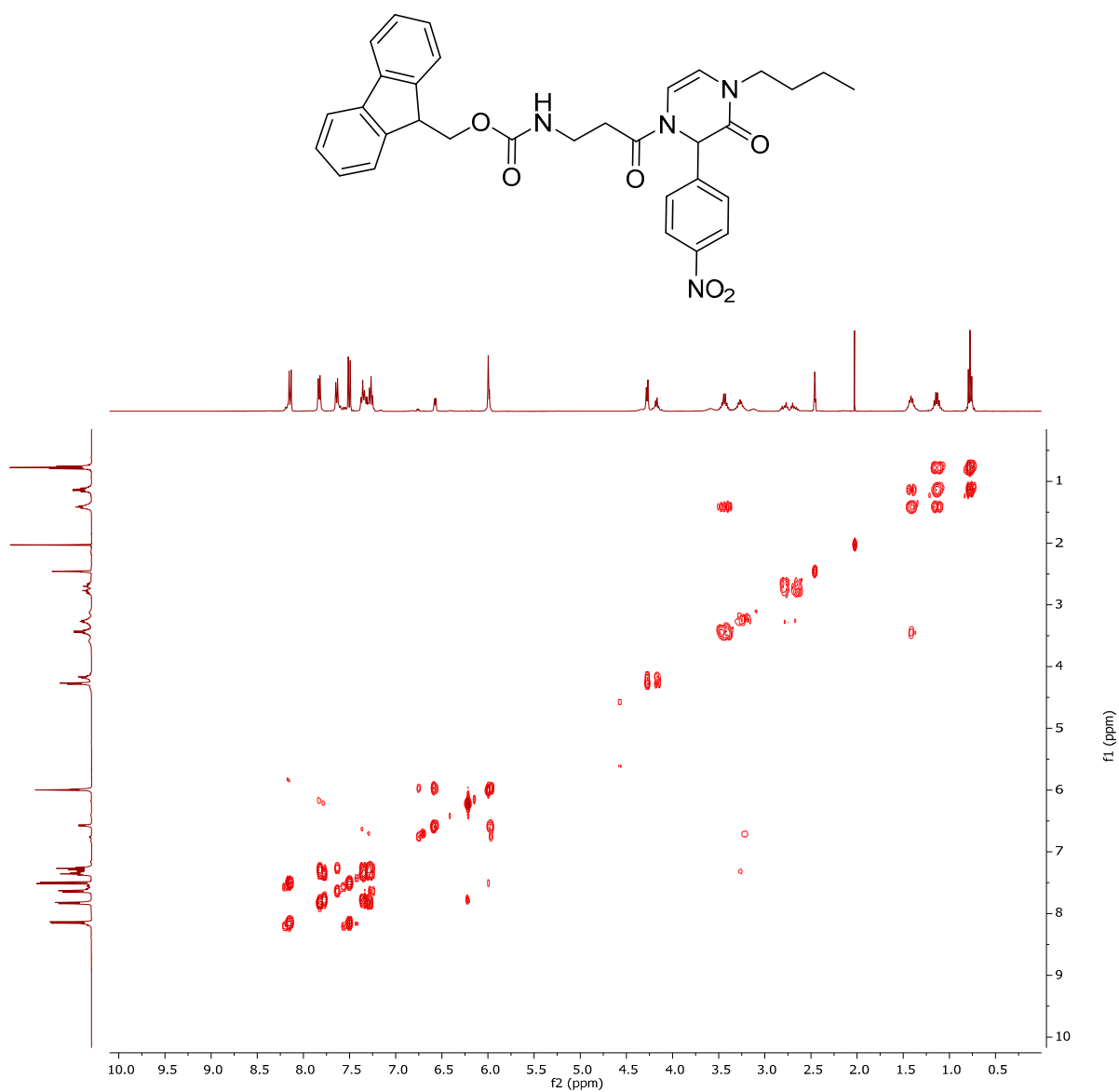
$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra ( $d_6$ -DMSO) for compound 2e



$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra ( $d_6$ -DMSO) for compound 2f

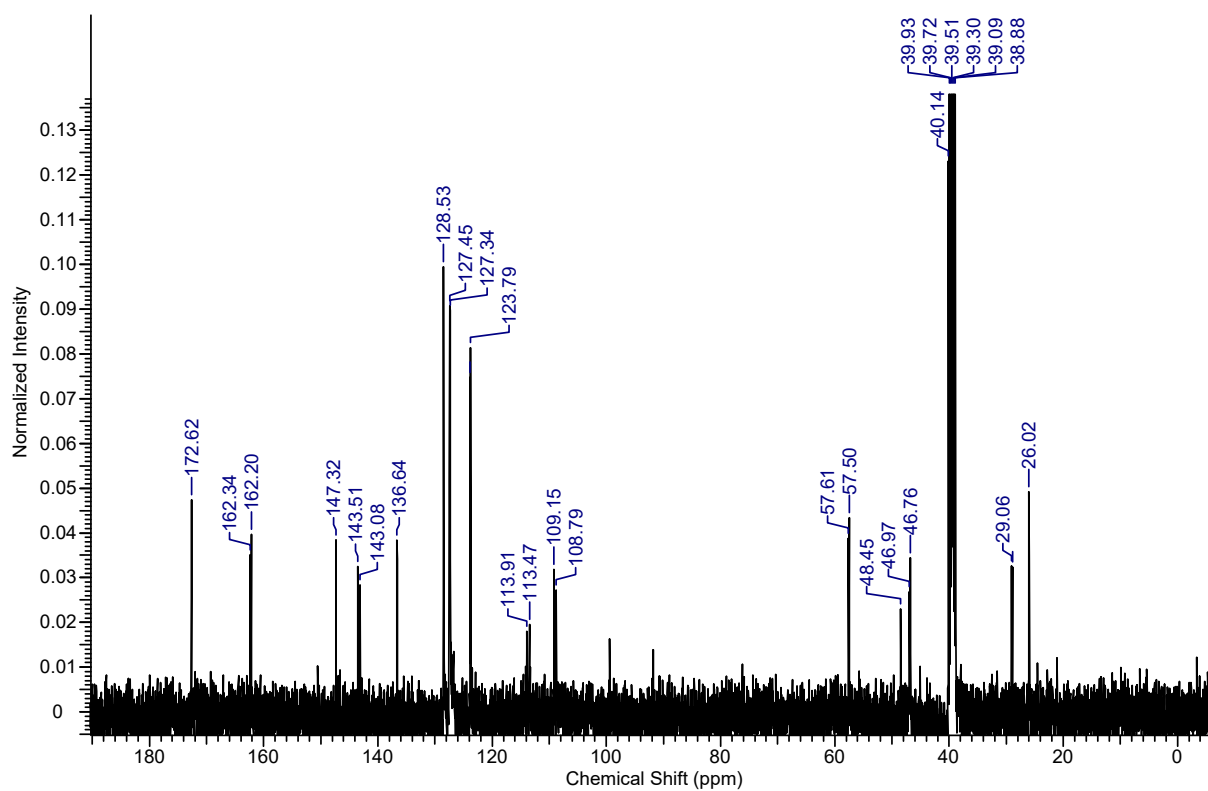
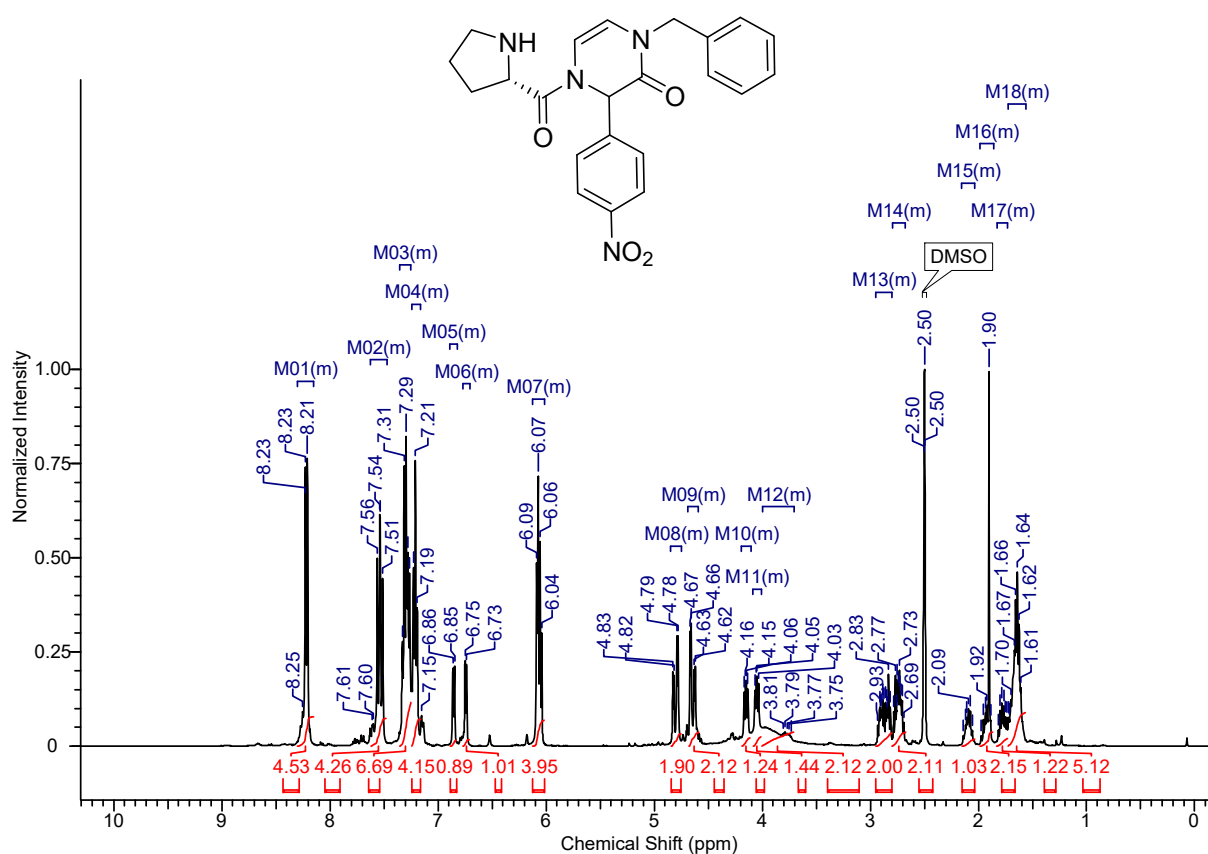


$^1\text{H} - ^1\text{H}$  COSY spectrum ( $d_6$ -DMSO) for compound 2f

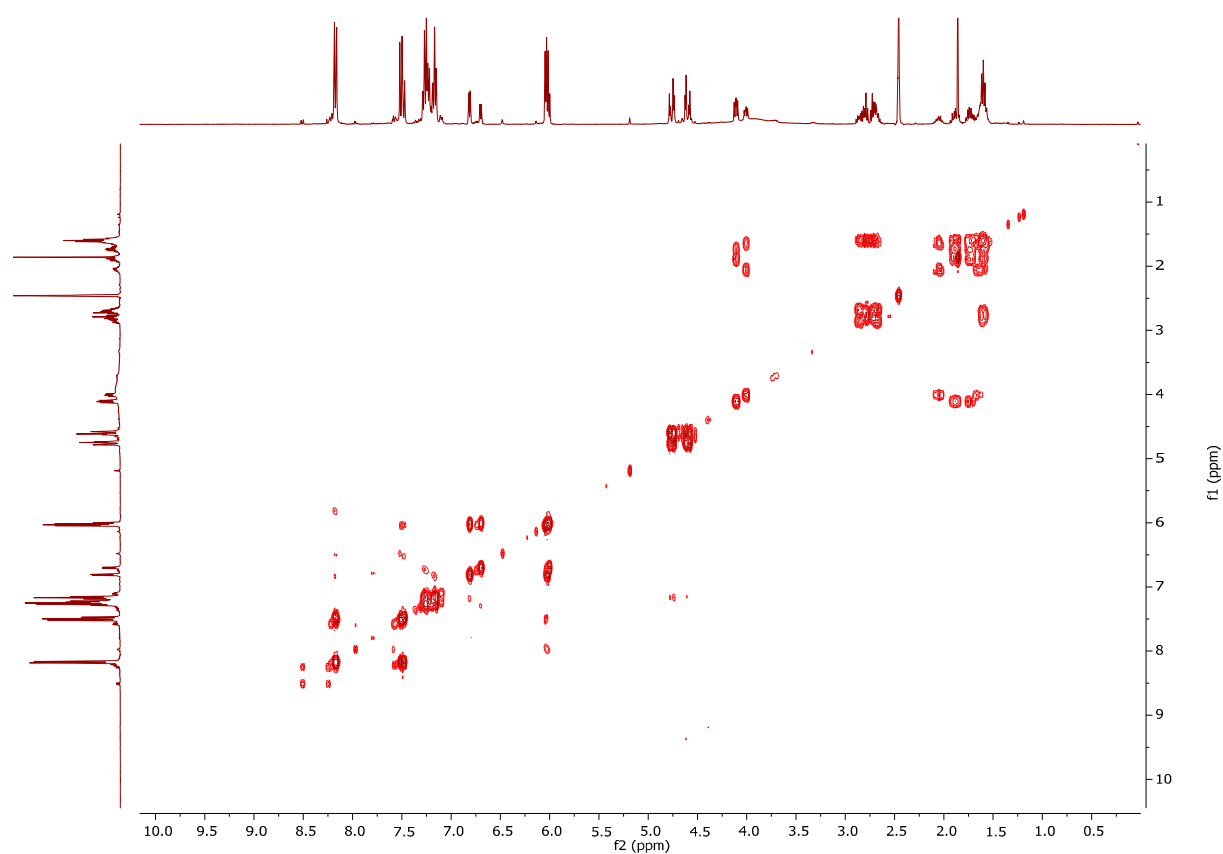




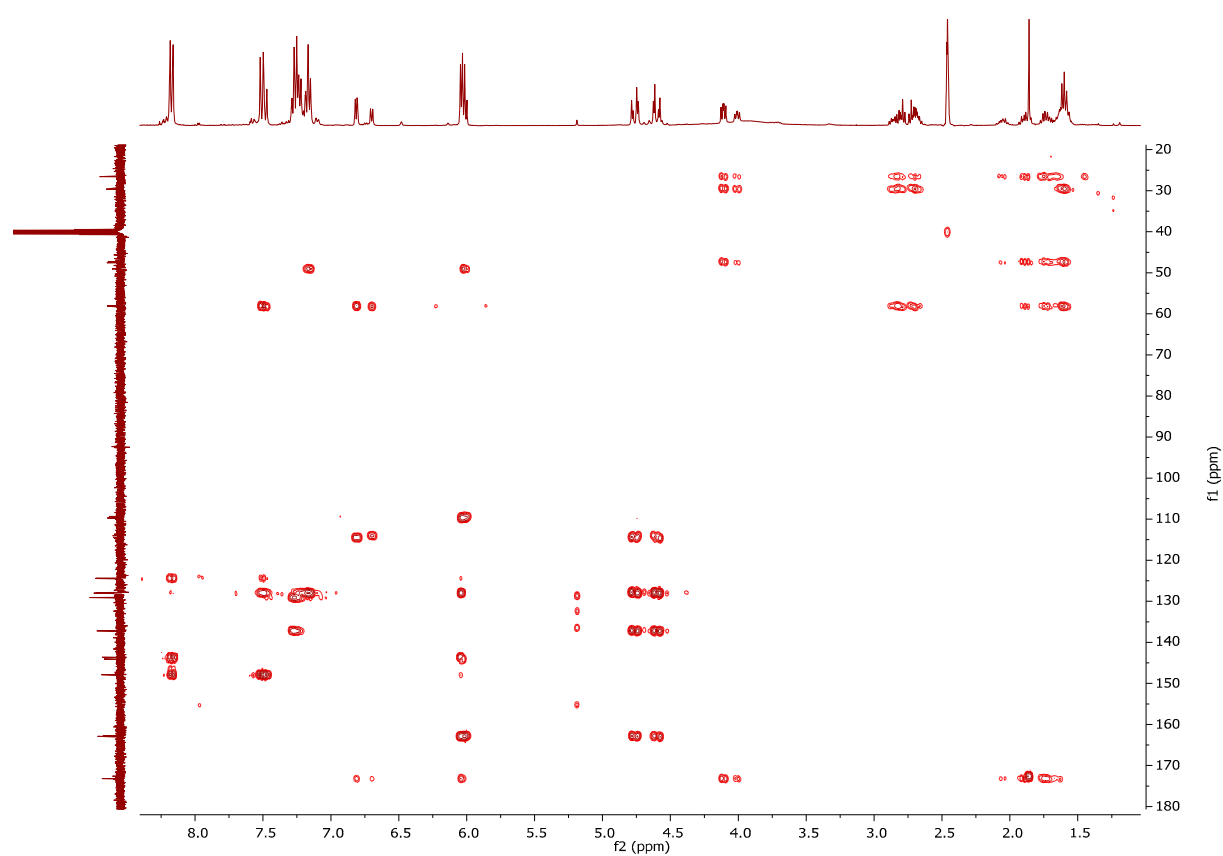
$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra ( $d_6$ -DMSO) for compound 2g



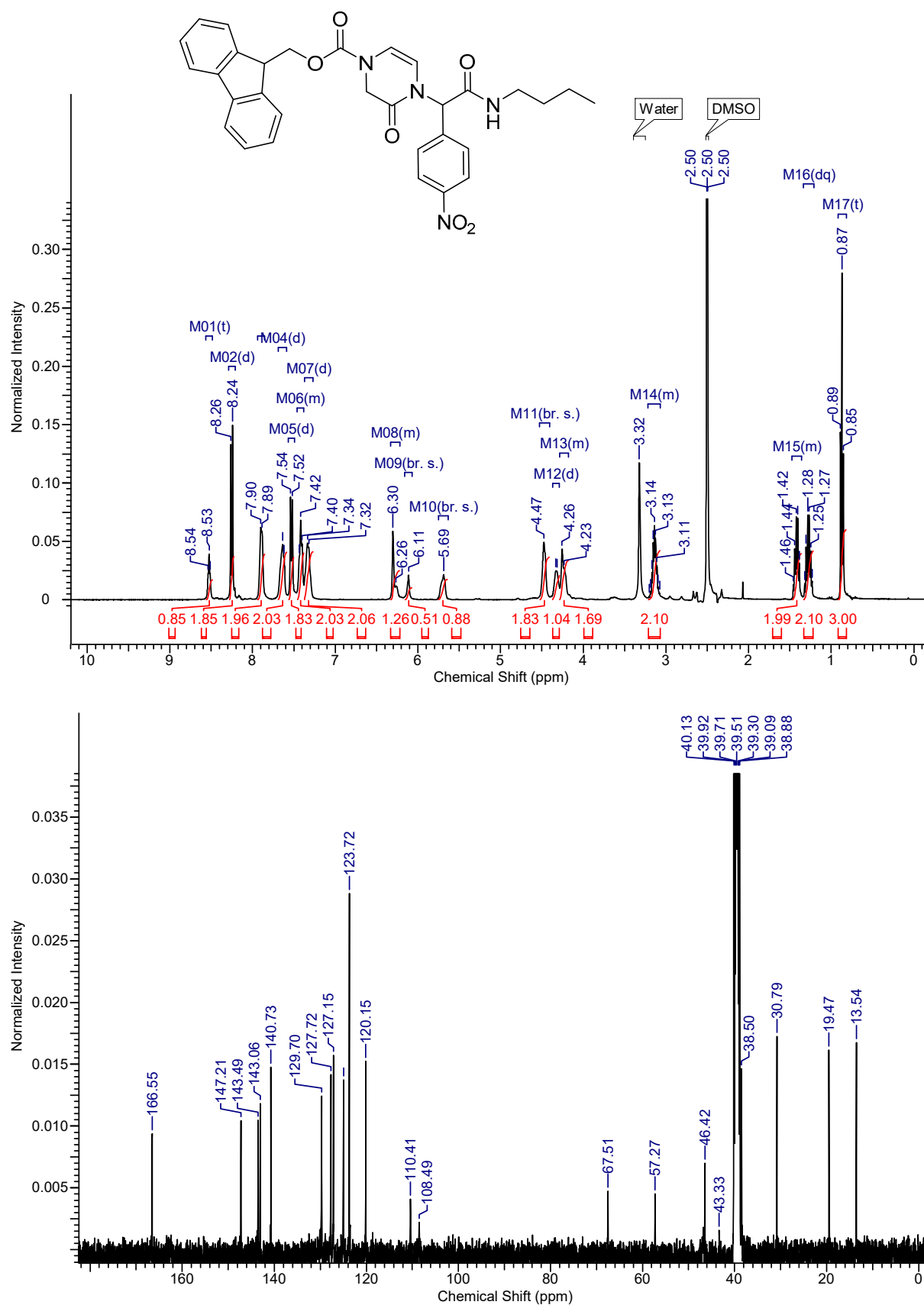
$^1\text{H} - ^1\text{H}$  COSY spectrum ( $d_6$ -DMSO) for compound 2g



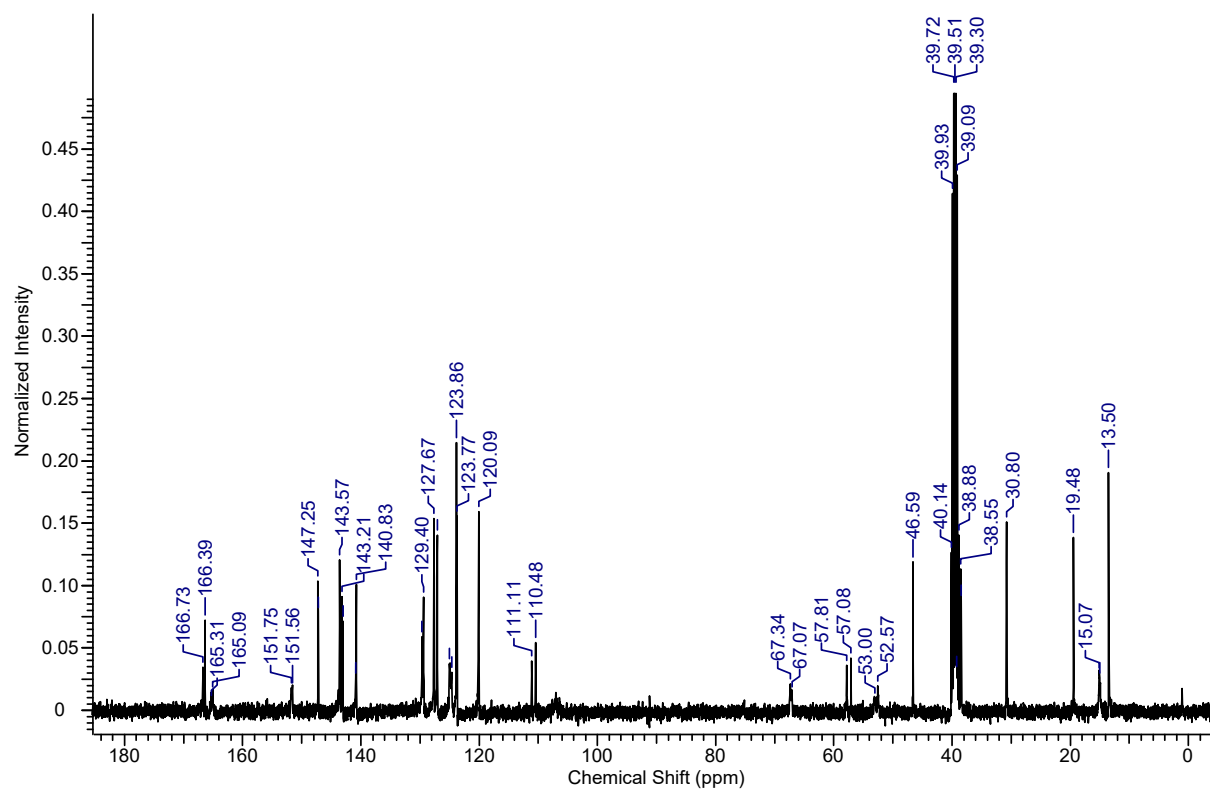
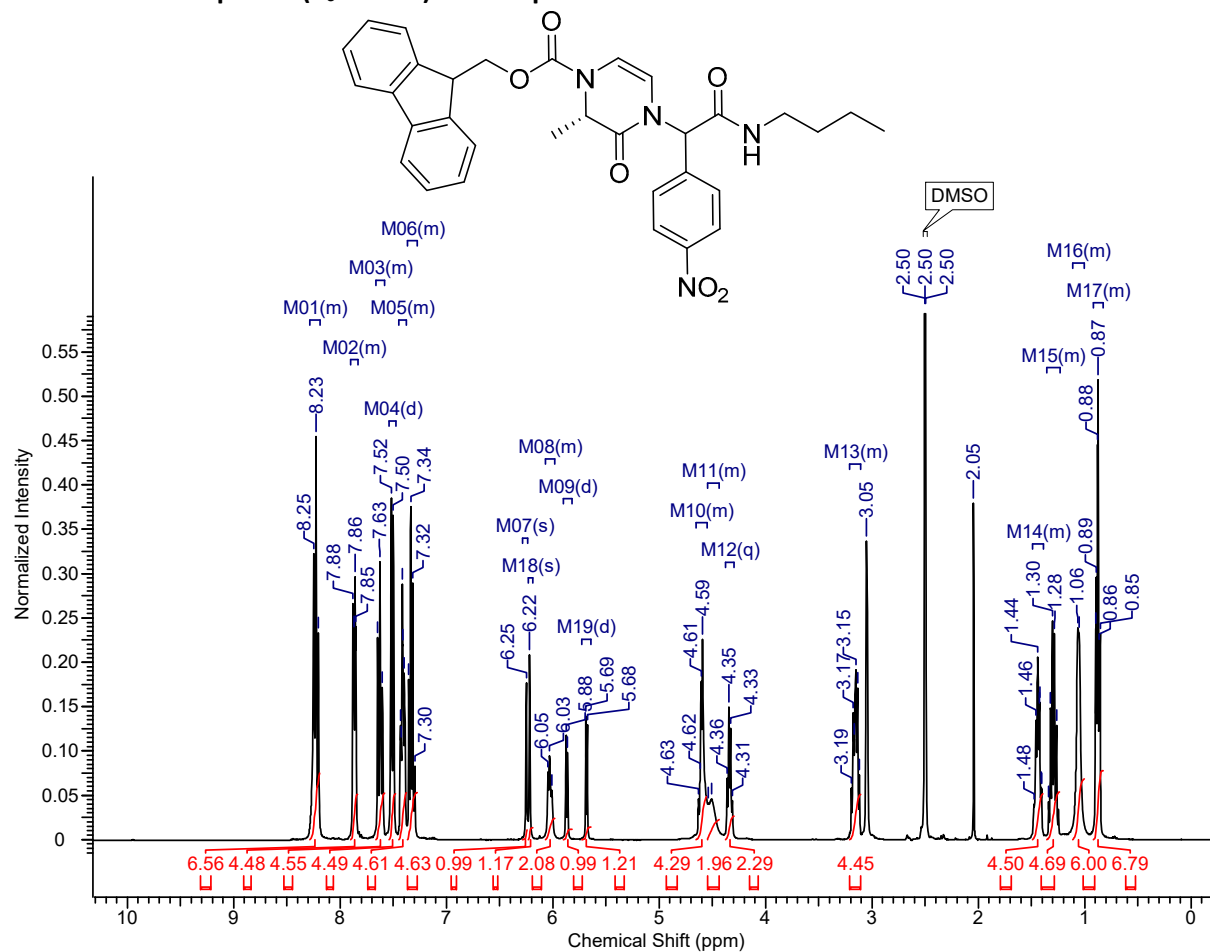
$^1\text{H} - ^{13}\text{C}$  HMBC spectrum ( $d_6$ -DMSO) for compound 2g



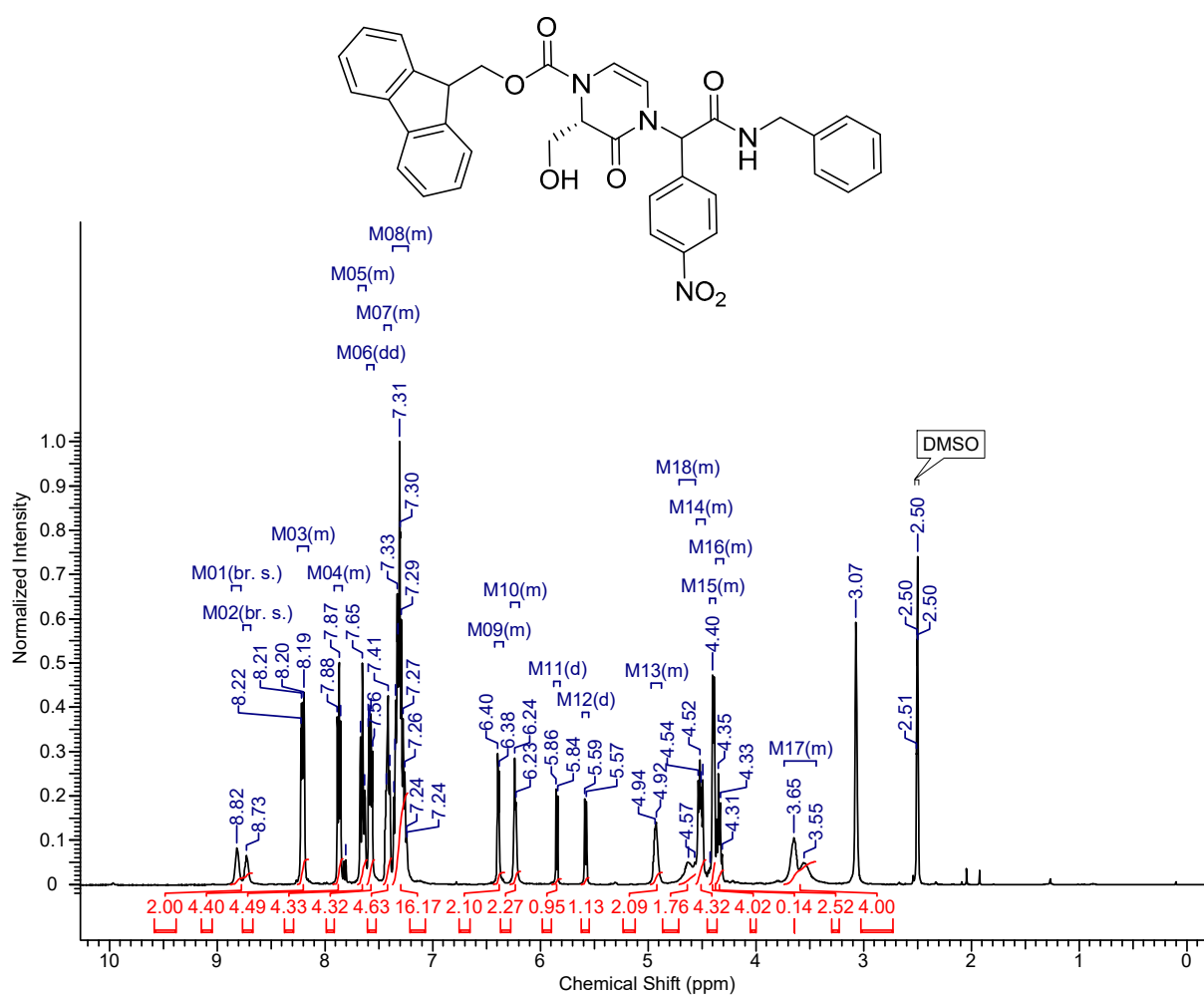
$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra ( $d_6$ -DMSO) for compound 3a



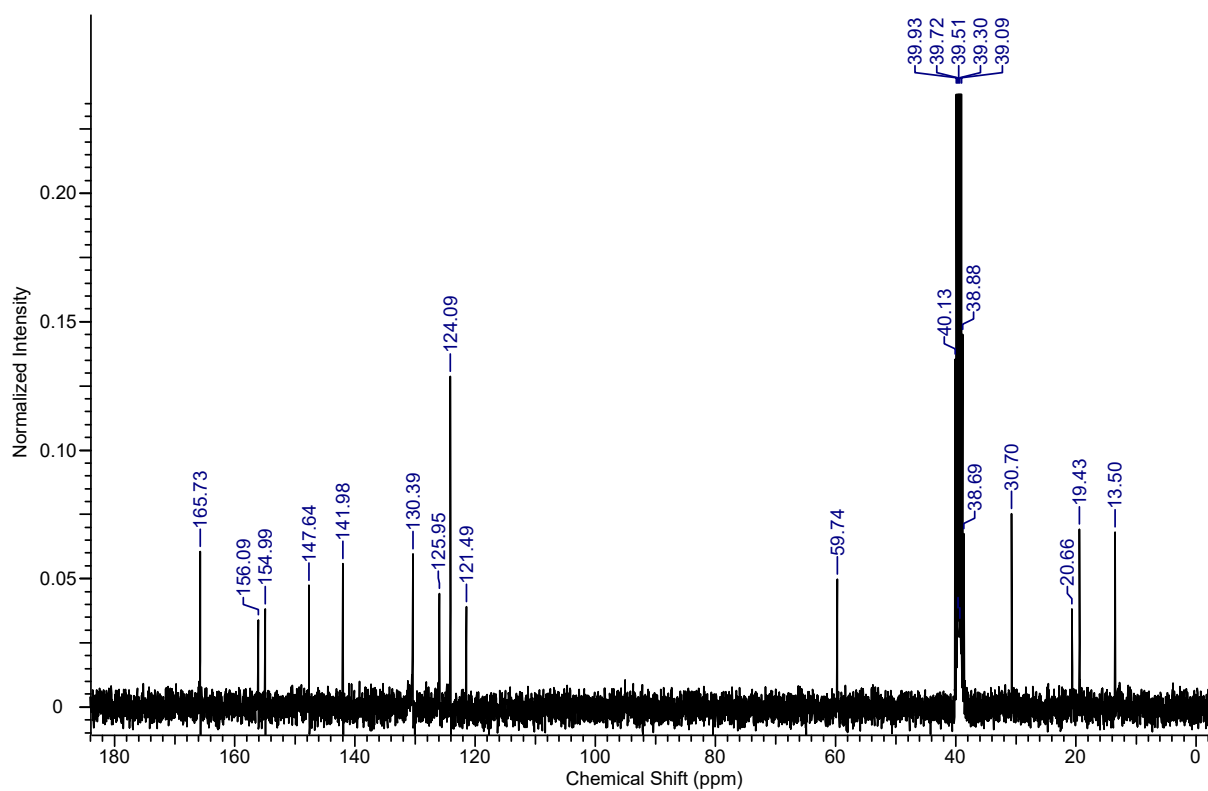
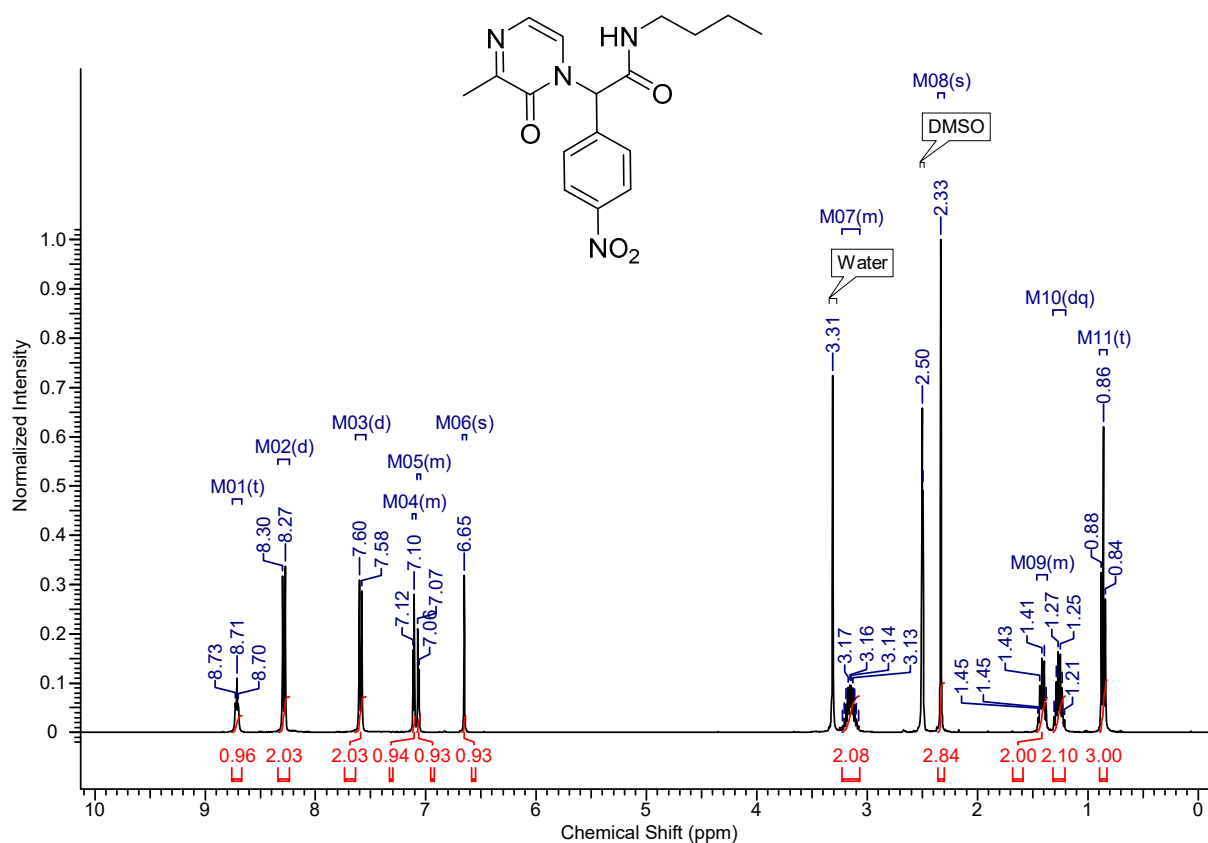
$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra ( $d_6$ -DMSO) for compound 3b



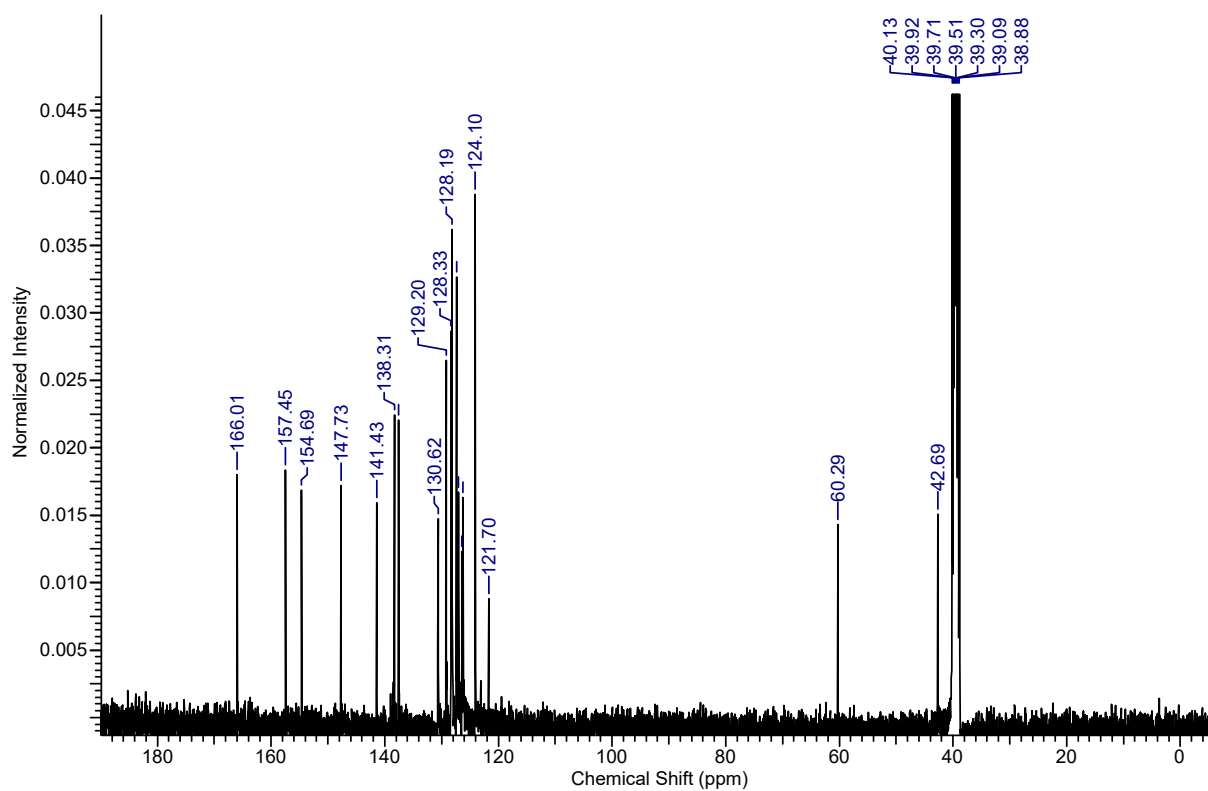
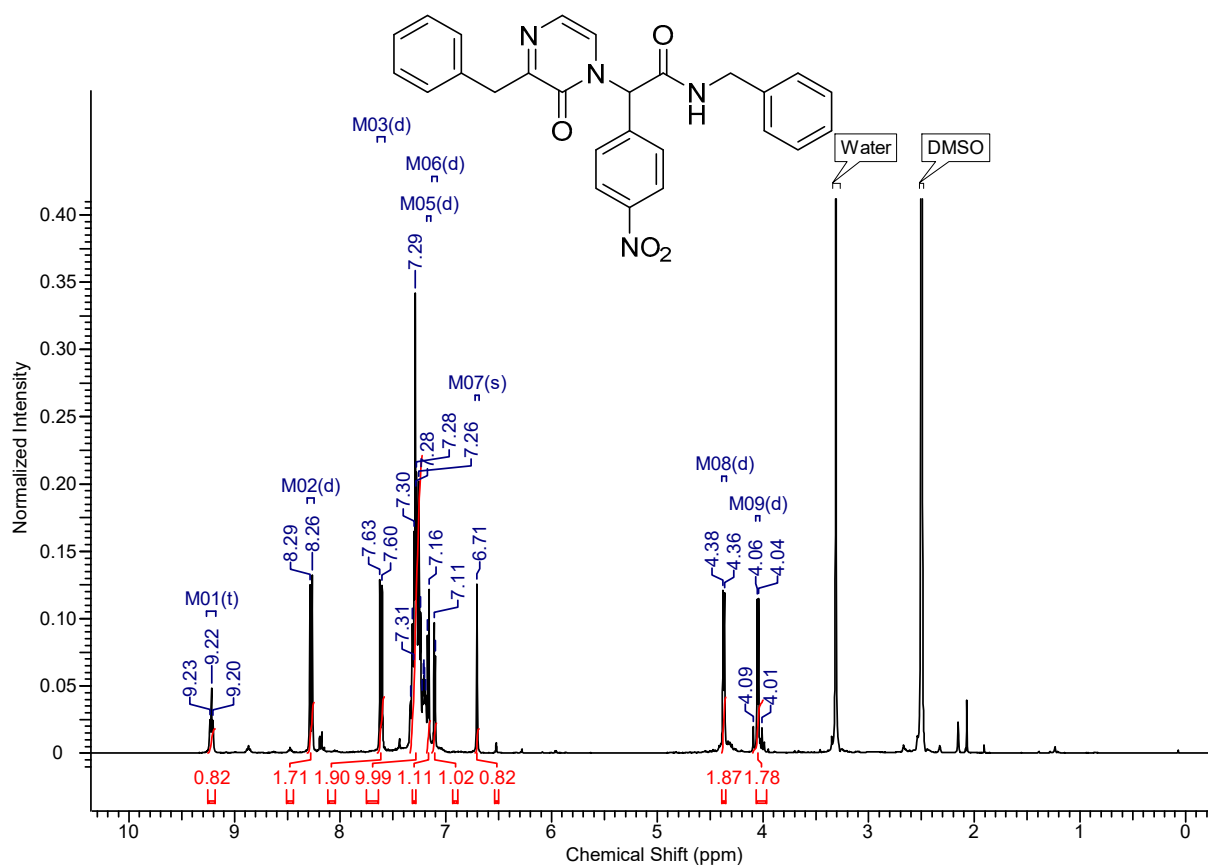
$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra ( $d_6$ -DMSO) for compound 3c



$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra ( $d_6$ -DMSO) for compound 4a



$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra ( $d_6$ -DMSO) for compound 4b

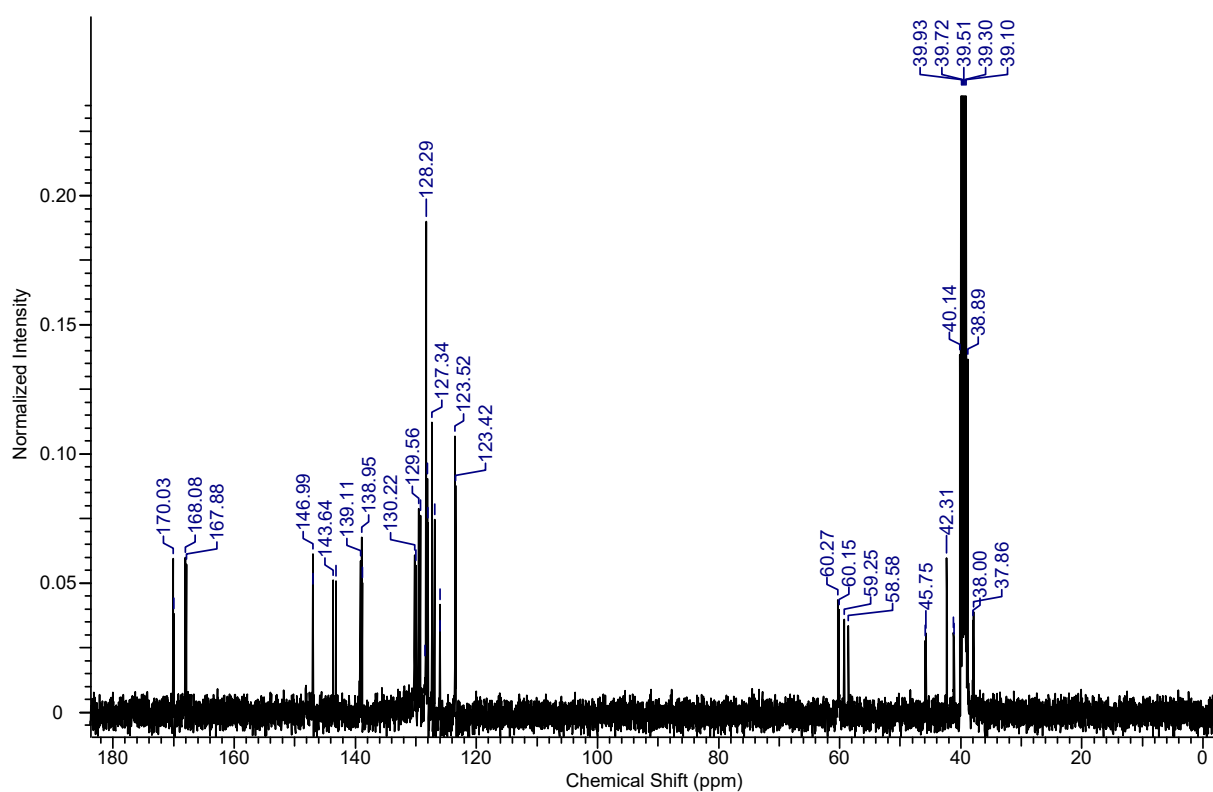


Chemical structure of compound 10: O=C(NCc1ccccc1)C(c2ccc([N+](=O)[O-])cc2)N3CC[C@H](Cc4ccccc4)C3=O

<sup>1</sup>H NMR spectrum (DMSO-d<sub>6</sub>) of compound 10. The x-axis represents the chemical shift in ppm, ranging from 10 to 0. The y-axis represents the normalized intensity, ranging from 0 to 1.0. The spectrum shows several peaks, with integration values provided below the baseline.

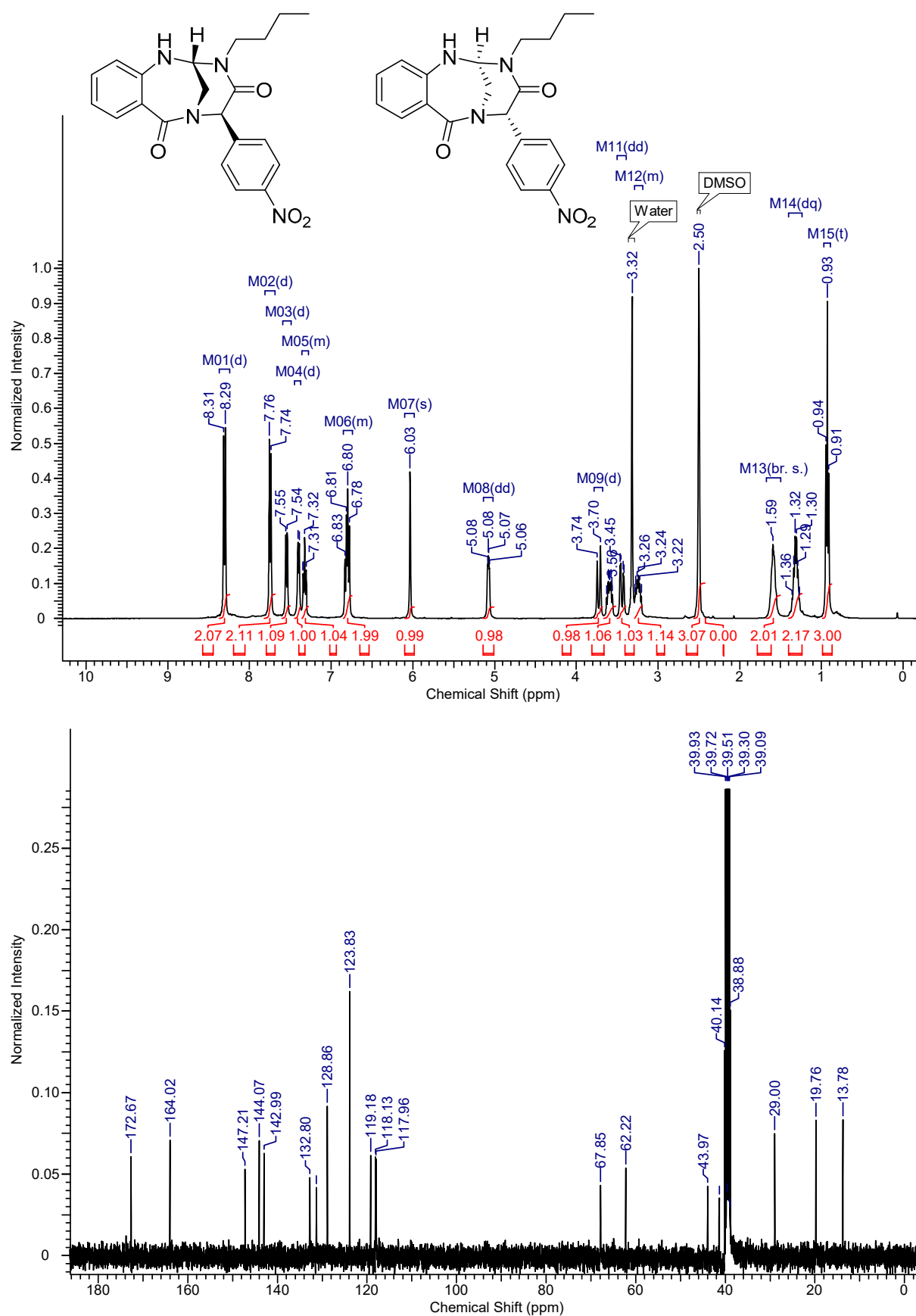
Peak assignments and integration values:

- 8.88 (t, 2.00)
- 8.87 (t, 2.13)
- 8.85 (t, 2.05)
- 8.84 (t, 2.12)
- 8.82 (t, 23.87)
- 8.24 (t, 1.01)
- 8.22 (t, 0.98)
- 8.20 (t, 4.21)
- 8.18 (t, 0.97)
- 8.16 (t, 1.04)
- 8.14 (t, 1.06)
- 8.12 (t, 1.78)
- 8.10 (t, 1.07)
- 8.08 (t, 1.05)
- 8.06 (t, 9.00)
- 7.26 (t, 4.36)
- 7.25 (t, 4.42)
- 7.24 (t, 4.40)
- 7.23 (t, 3.48)
- 7.22 (t, 3.35)
- 7.21 (t, 3.32)
- 7.20 (t, 2.93)
- 7.19 (t, 2.91)
- 7.18 (t, 2.87)
- 7.17 (t, 2.86)
- 7.16 (t, 2.85)
- 7.15 (t, 2.83)
- 7.14 (t, 2.82)
- 7.13 (t, 2.80)
- 7.12 (t, 2.67)
- 7.11 (t, 2.67)
- 7.10 (t, 2.67)
- 7.09 (t, 2.67)
- 7.08 (t, 2.67)
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- 7.05 (t, 2.67)
- 7.04 (t, 2.67)
- 7.03 (t, 2.67)
- 7.02 (t, 2.67)
- 7.01 (t, 2.67)
- 7.00 (t, 2.67)
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- 6.34 (t, 4.42)
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- 6.32 (t, 3.48)
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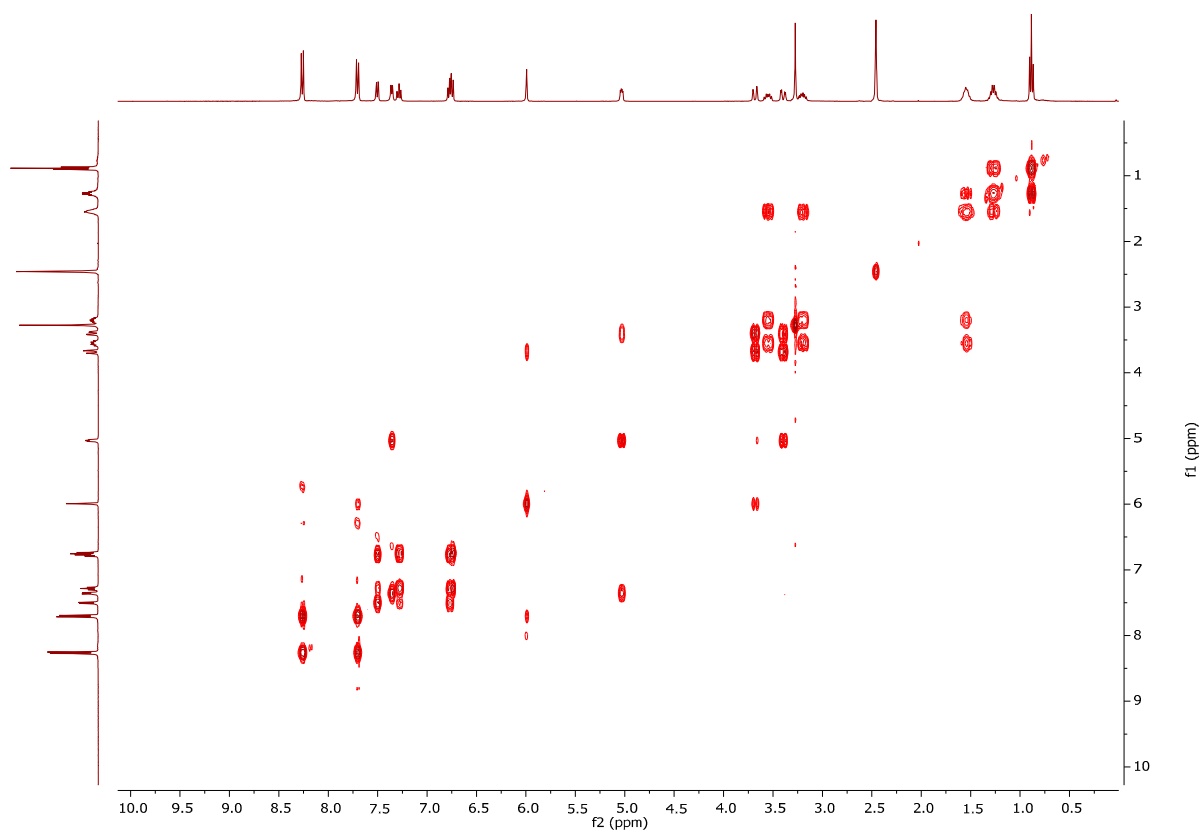




$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra ( $d_6$ -DMSO) for compound 6a



$^1\text{H} - ^1\text{H}$  COSY spectrum ( $d_6$ -DMSO) for compound 6a



$^1\text{H} - ^{13}\text{C}$  HMBC spectrum ( $d_6$ -DMSO) for compound 6a

