

4-(5-Benzyl-3-((4-fluorophenyl)sulfonyl)-5-methyl-4,5-dihydrofuran-2-yl)-2-nitrobenzamide

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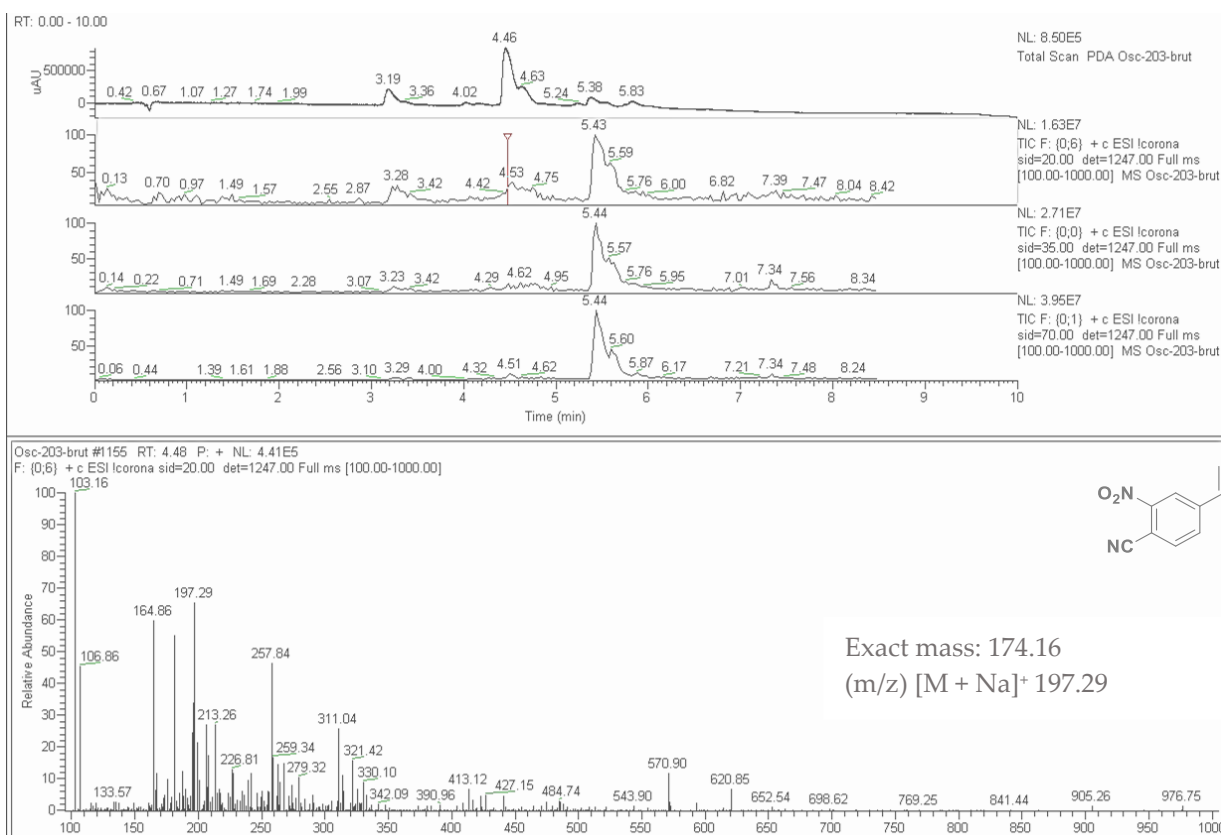


Figure S1: LC-MS spectra of compound 1

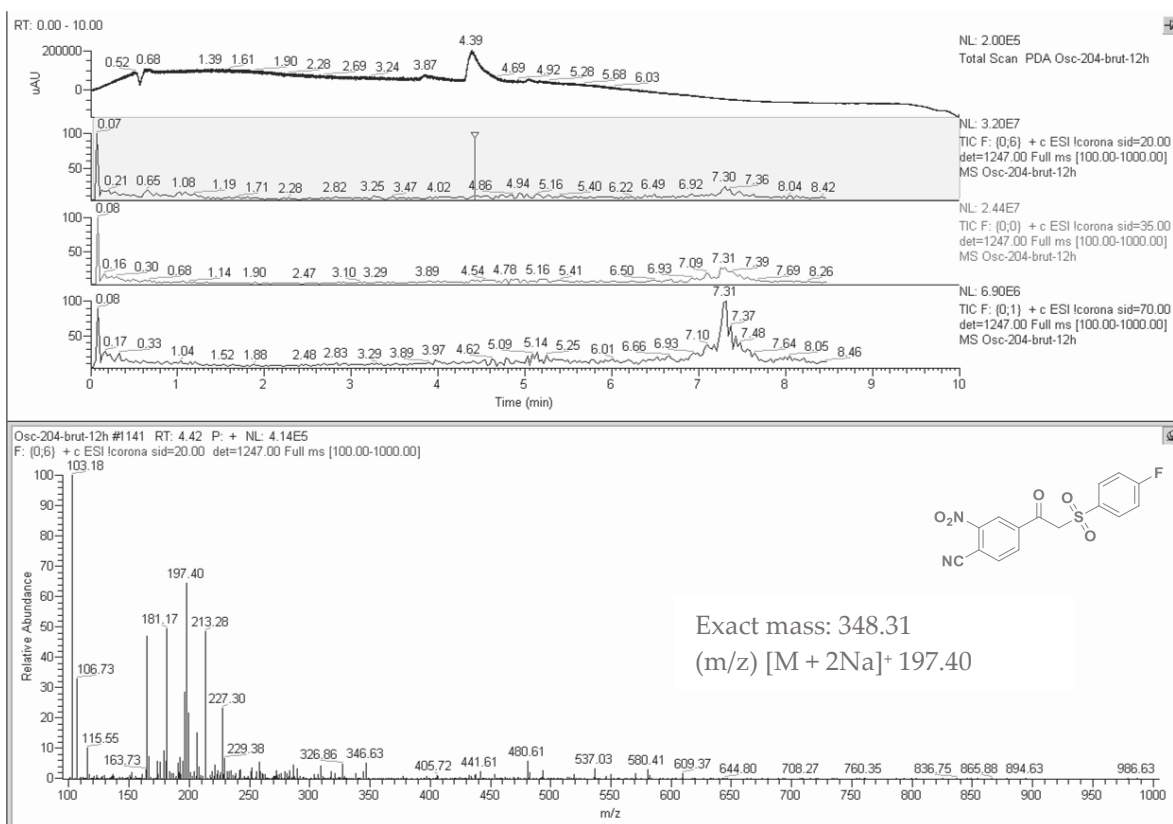


Figure S2: LC-MS spectra of compound 2

Osc-212_Mex1 6 (0.157) AM2 (Ar,18000.0,0.00,0.00); Cm (1:20)

1: TOF MS ES+
9.34e5

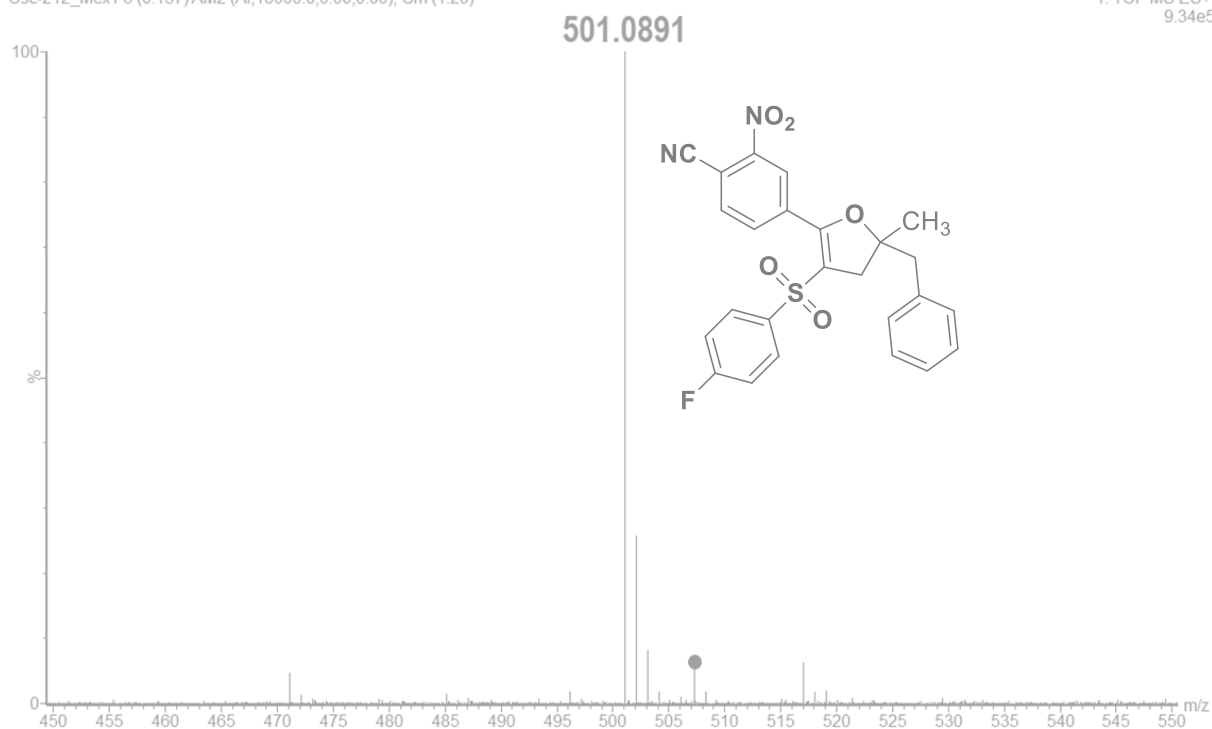


Figure S3: HRMS spectra of compound 3

Osc-260_2_Mex1 4 (0.123) AM2 (Ar,18000.0,0.00,0.00); Cm (1:20)

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1.11e6

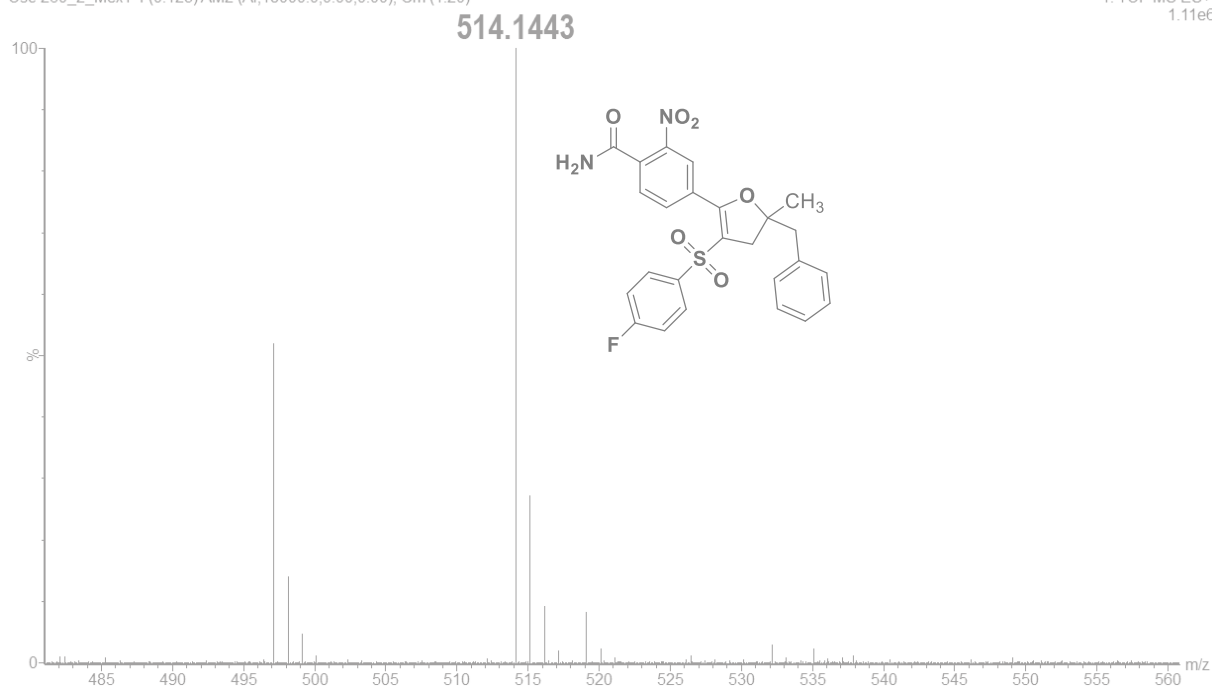


Figure S4: HRMS spectra of compound 4

Osc-275_Mex3 12 (0.299) AM2 (Ar,18000.0,0.

1: TOF MS ES+
1.12e6

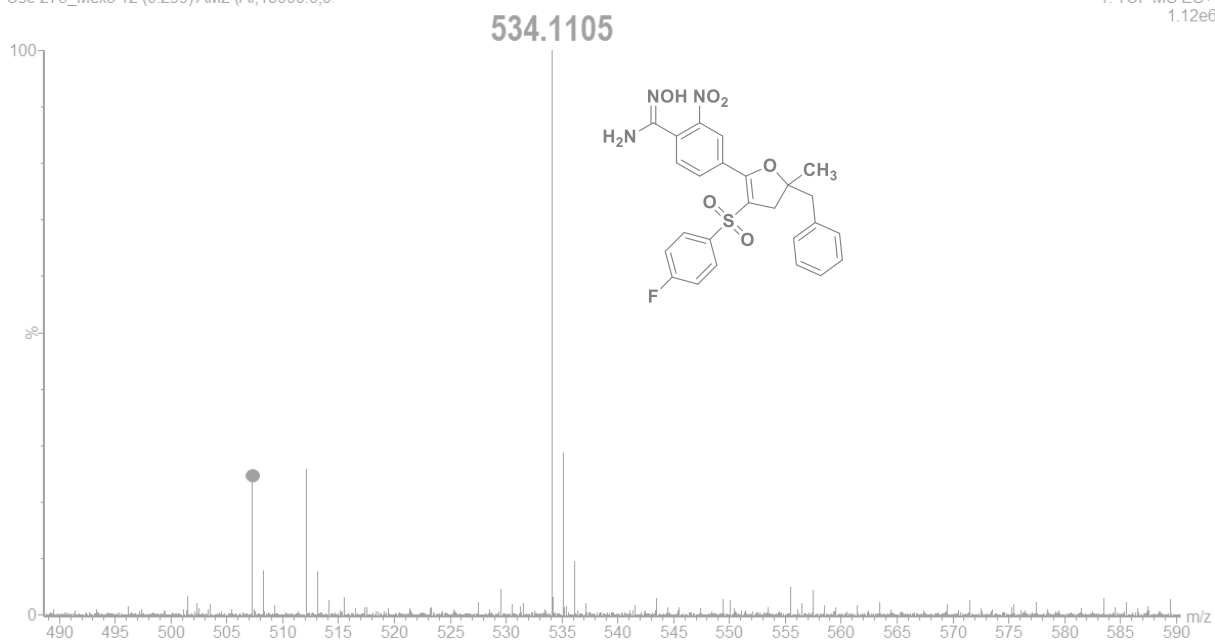


Figure S5: HRMS spectra of compound 5

2-Nitro-4-vinylbenzonitrile (**1**) - C₉H₆N₂O₂

¹H NMR (400 MHz, CDCl₃): δ (ppm) 8.32 (s, 1H, CH_{Ar}), 7.86 (d, ³J_{H-H} = 8.0 Hz, 1H, CH_{Ar}), 7.78 (d, ³J_{H-H} = 8.0 Hz, 1H, CH_{Ar}), 6.80 (dd, ³J_{H-H} = 10.9 Hz, ³J_{H-H} = 17.6 Hz, 1H, CH), 6.05 (d, ³J_{H-H} = 17.6 Hz, 1H, H-CH₂), 5.66 (d, ³J_{H-H} = 10.9 Hz, 1H, H-CH₂).

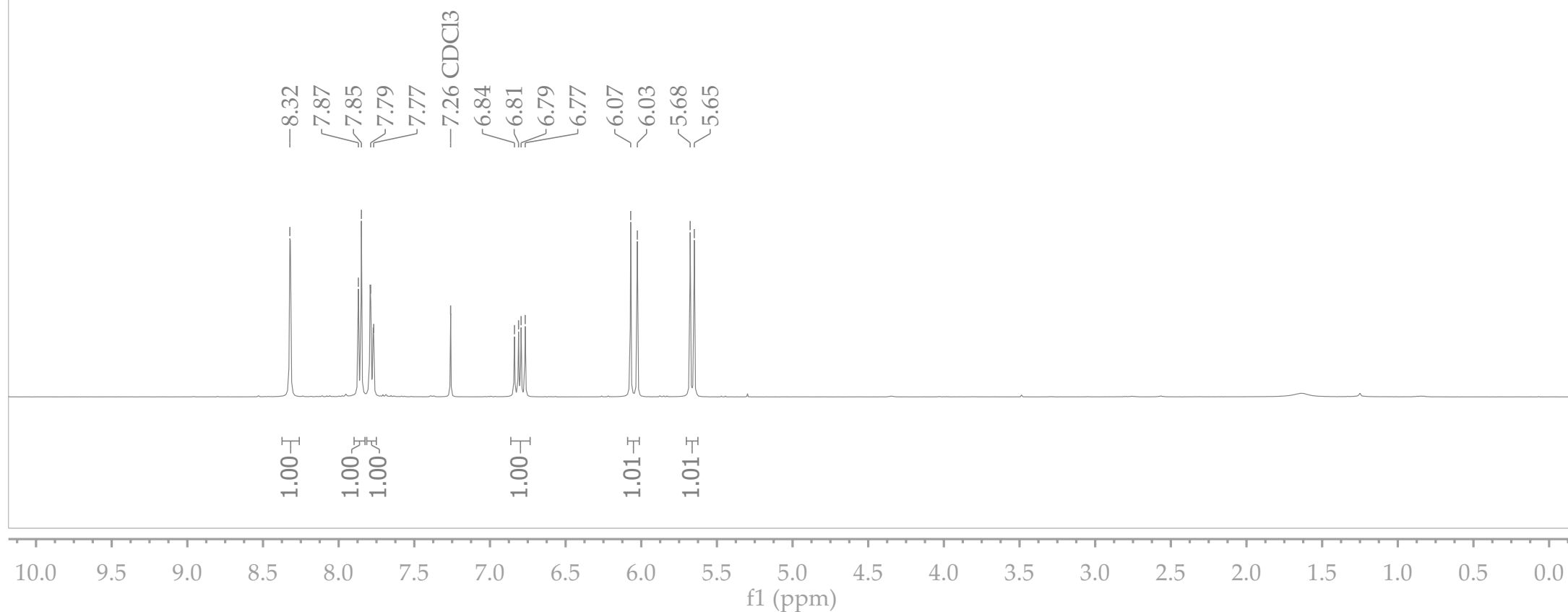
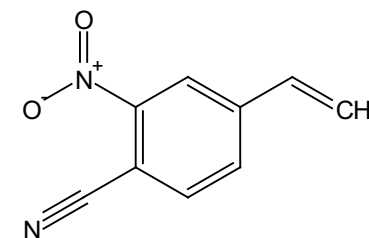


Figure S6: ¹H NMR spectra of compound 1

2-Nitro-4-vinylbenzonitrile (**1**) - C₉H₆N₂O₂

¹³C NMR (100 MHz, CDCl₃): δ (ppm) 143.6 (C), 135.9 (CH_{Ar}), 133.6 (CH_{Ar}), 131.4 (CH_{Ar}), 122.9 (CH_{Ar}), 121.1 (2C), 115.2 (C), 106.4 (C).

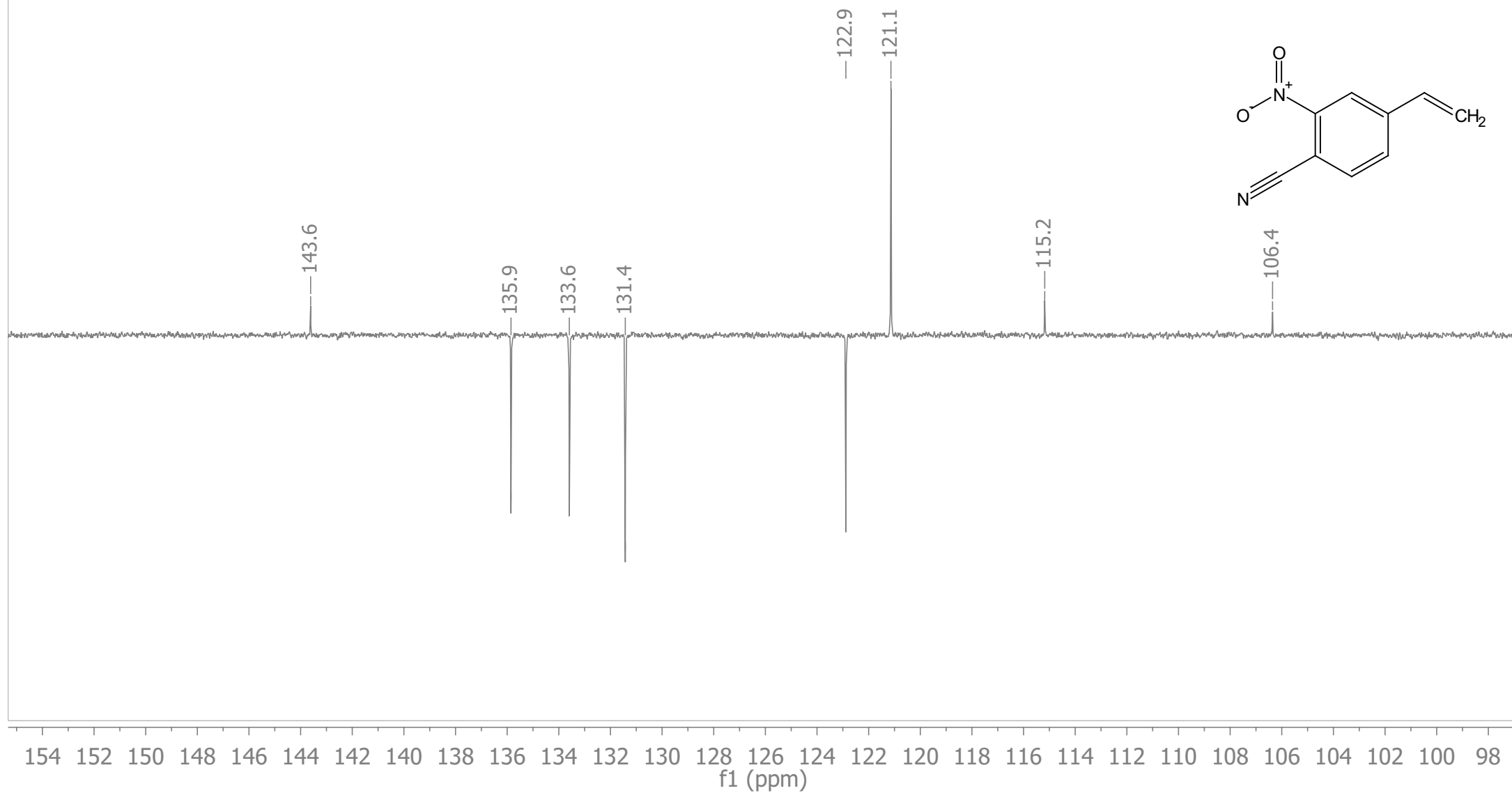


Figure S7: ¹³C NMR spectra of compound 1

4-(2-((4-Fluorophenyl)sulfonyl)acetyl)-2-nitrobenzonitrile (**2**) - C₁₅H₉FN₂O₅S

¹H NMR (400 MHz, CDCl₃): δ (ppm) 8.88 (s, 1H, CH_{Ar}), 8.45 (d, ³J_{H-H} = 8.1 Hz, 1H, CH_{Ar}), 8.12 (d, ³J_{H-H} = 8.1 Hz, 1H, CH_{Ar}), 7.92-7.89 (m, 2H, CH_{Ar}), 7.34-7.29 (m, 2H, CH_{Ar}), 4.79 (s, 2H, CH₂).

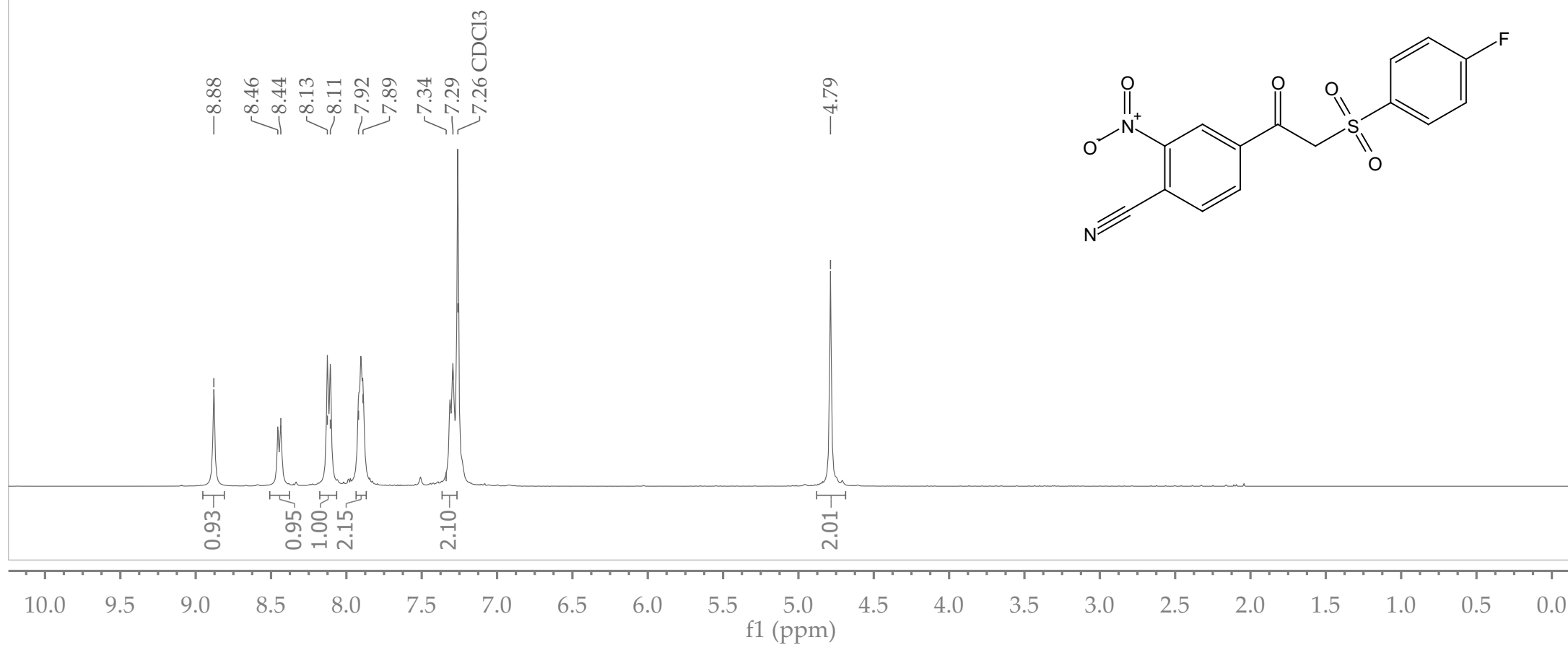


Figure S8: ¹H NMR spectra of compound **2**

4-(2-((4-Fluorophenyl)sulfonyl)acetyl)-2-nitrobenzonitrile (**2**) - C₁₅H₉FN₂O₅S

¹³C NMR (100 MHz, CDCl₃): δ (ppm) 185.4 (C), 166.7 (d, J_{C-F} = 258.9 Hz, C), 149.2 (C), 139.4 (C), 136.6 (CH_{Ar}), 134.3 (CH_{Ar}), 134.0 (C), 131.7 (d, J_{C-F} = 9.8 Hz, 2CH_{Ar}), 126.0 (CH_{Ar}), 117.1 (d, J_{C-F} = 23.0 Hz, 2CH_{Ar}), 114.1 (C), 112.6 (C), 64.1 (CH₂).

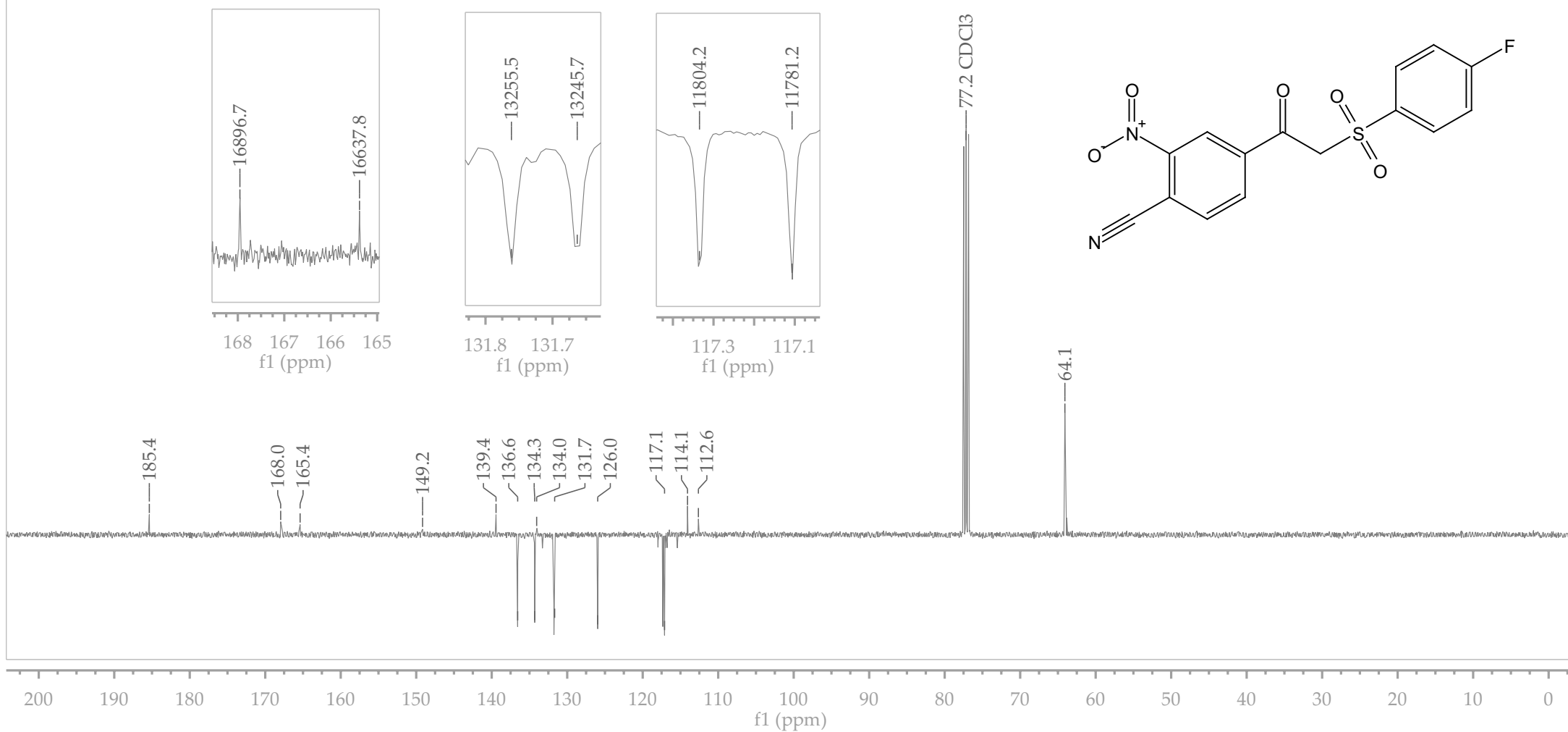


Figure S9: ¹³C NMR spectra of compound **2**

4-(5-Benzyl-3-((4-fluorophenyl)sulfonyl)-5-methyl-4,5-dihydrofuran-2-yl)-2-nitrobenzonitrile (**3**) - C₂₅H₁₉FN₂O₅S

¹H NMR (400 MHz, CDCl₃): δ (ppm) 8.45 (d, ⁴J_{H-H} = 1.6 Hz, 1H, CH_{Ar}), 8.06 (dd, ⁴J_{H-H} = 1.6 Hz, ³J_{H-H} = 8.1 Hz, 1H, CH_{Ar}), 7.94 (d, ³J_{H-H} = 8.2 Hz, 1H, CH_{Ar}), 7.58-7.54 (m, 2H, 2CH_{Ar}), 7.24-7.12 (m, 5H, 5CH_{Ar}), 7.05 (d, ³J_{H-H} = 8.2 Hz, 2H, 2CH_{Ar}), 3.04 (d, ²J_{H-H} = 14.7 Hz, 2H, CH₂), 2.92-2.82 (m, 2H, CH₂), 1.43 (s, 3H, CH₃).

HRMS: *m/z* [M + NH₄]⁺ calculated 501.0891; found 501.0891.

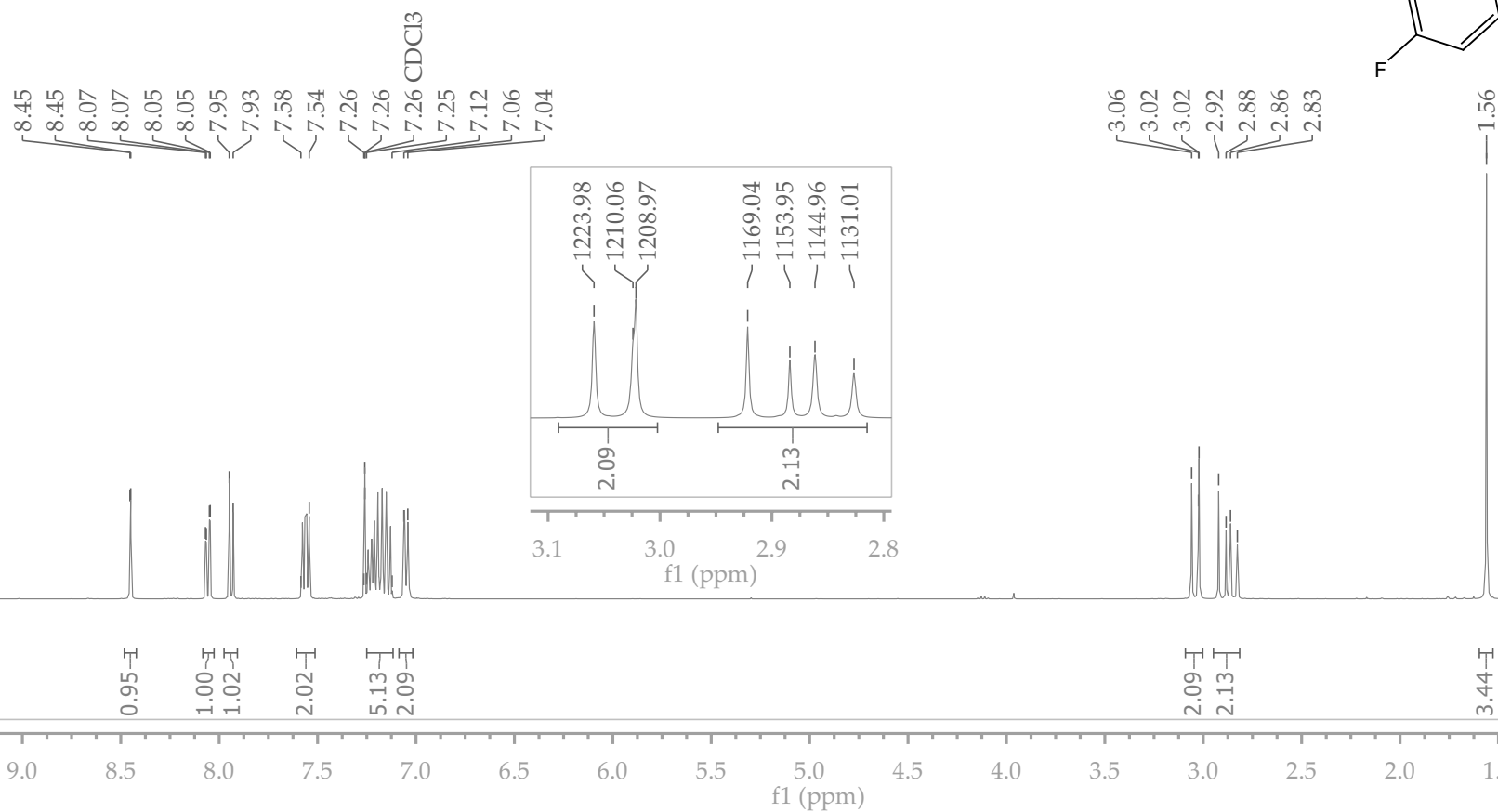
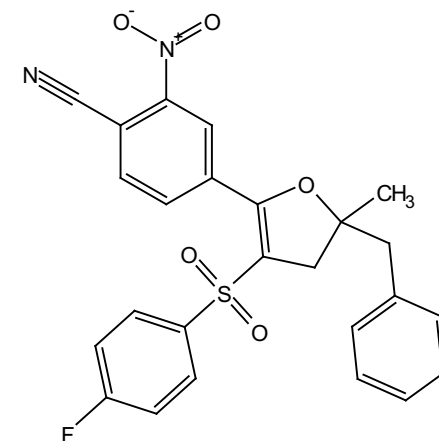


Figure S10: ¹H NMR spectra of compound 3

4-(5-Benzyl-3-((4-fluorophenyl)sulfonyl)-5-methyl-4,5-dihydrofuran-2-yl)-2-nitrobenzonitrile (**3**) - C₂₅H₁₉FN₂O₅S

¹³C NMR (100 MHz, CDCl₃) δ (ppm) 166.6 (d, *J*_{C-F} = 255.9 Hz, C), 164.3 (C), 157.5 (C), 136.7 (d, *J*_{C-F} = 3.5 Hz, C), 135.2 (CH_{Ar}), 135.1 (CH_{Ar}), 135.0 (2C), 134.4 (C), 130.3 (2CH_{Ar}), 129.8 (d, *J*_{C-F} = 10.1 Hz, 2CH_{Ar}), 128.5 (2CH_{Ar}), 127.4 (CH_{Ar}), 126.4 (CH_{Ar}), 116.8 (d, *J*_{C-F} = 22.5 Hz, 2CH_{Ar}), 114.6 (C), 113.7 (C), 109.5 (C), 89.9 (C), 46.7 (CH₂), 41.7 (CH₂), 27.7 (CH₃).

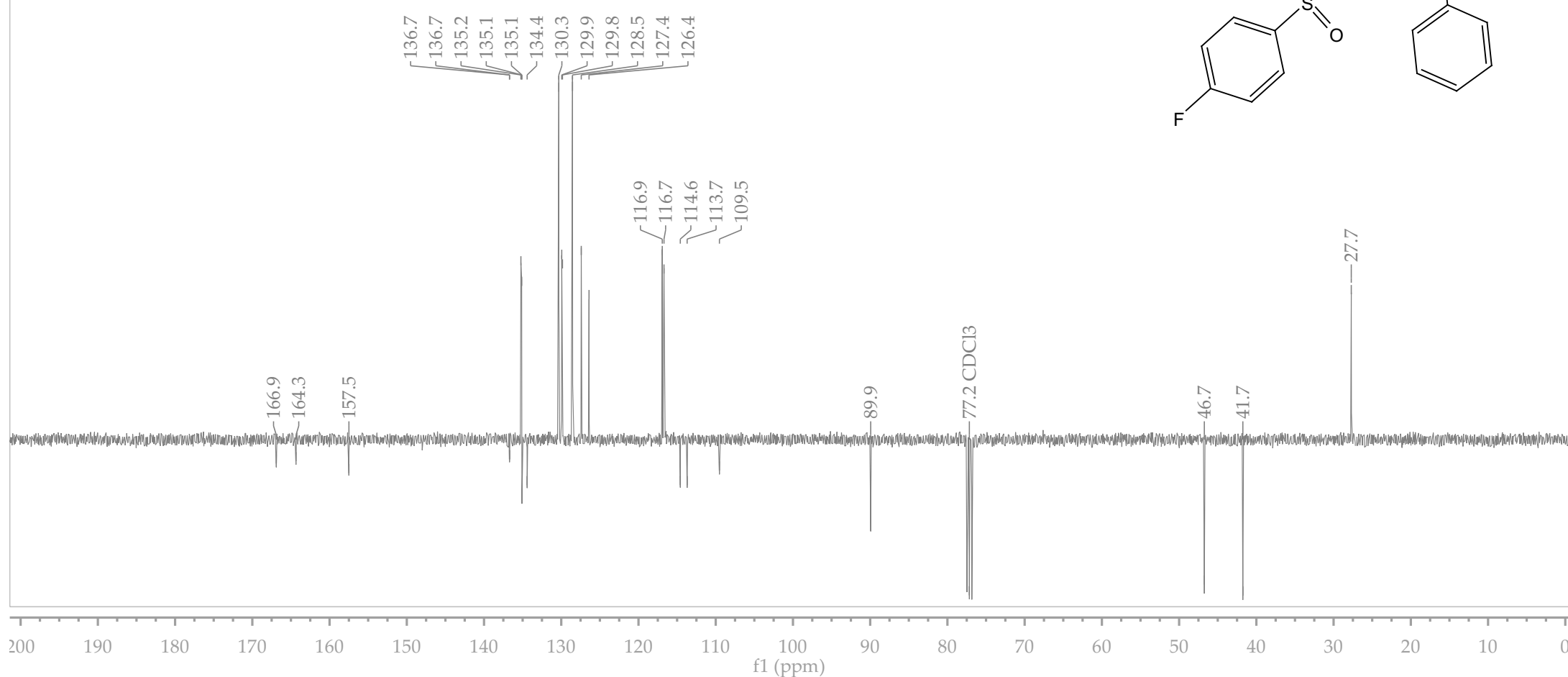
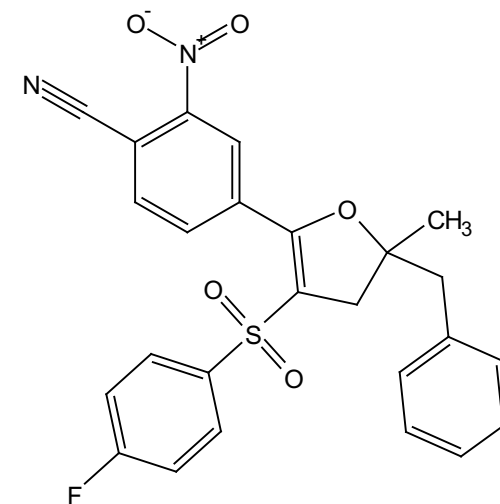


Figure S11: ¹³C NMR spectra of compound 3

4-(5-Benzyl-3-((4-fluorophenyl)sulfonyl)-5-methyl-4,5-dihydrofuran-2-yl)-2-nitrobenzamide (**4**) - C₂₅H₂₁FN₂O₆S

¹H NMR (400 MHz, CDCl₃): δ (ppm) 8.17 (d, ⁴J_{H-H} = 1.6 Hz, 1H, CH_{Ar}), 7.91 (dd, ⁴J_{H-H} = 1.6 Hz, ²J_{H-H} = 8.0 Hz, 1H, CH_{Ar}), 7.60 (d, ³J_{H-H} = 8.1 Hz, 1H, CH_{Ar}), 7.57-7.52 (m, 2H, 2CH_{Ar}), 7.24-7.10 (m, 5H, 5CH_{Ar}), 7.05 (d, ³J_{H-H} = 7.7 Hz, 2H, 2CH_{Ar}), 6.09 (br s, 2H, NH₂), 3.03 (d, ²J_{H-H} = 13.9 Hz, 1H, CH₂), 3.02 (d, ²J_{H-H} = 14.8 Hz, 1H, CH₂), 2.88 (d, ²J_{H-H} = 14.8 Hz, 1H, CH₂), 2.83 (d, ²J_{H-H} = 13.9 Hz, 1H, CH₂), 1.54 (s, 3H, CH₃).

HRMS: *m/z* [M + NH₄]⁺ calculated 514.1443; found 514.1443.

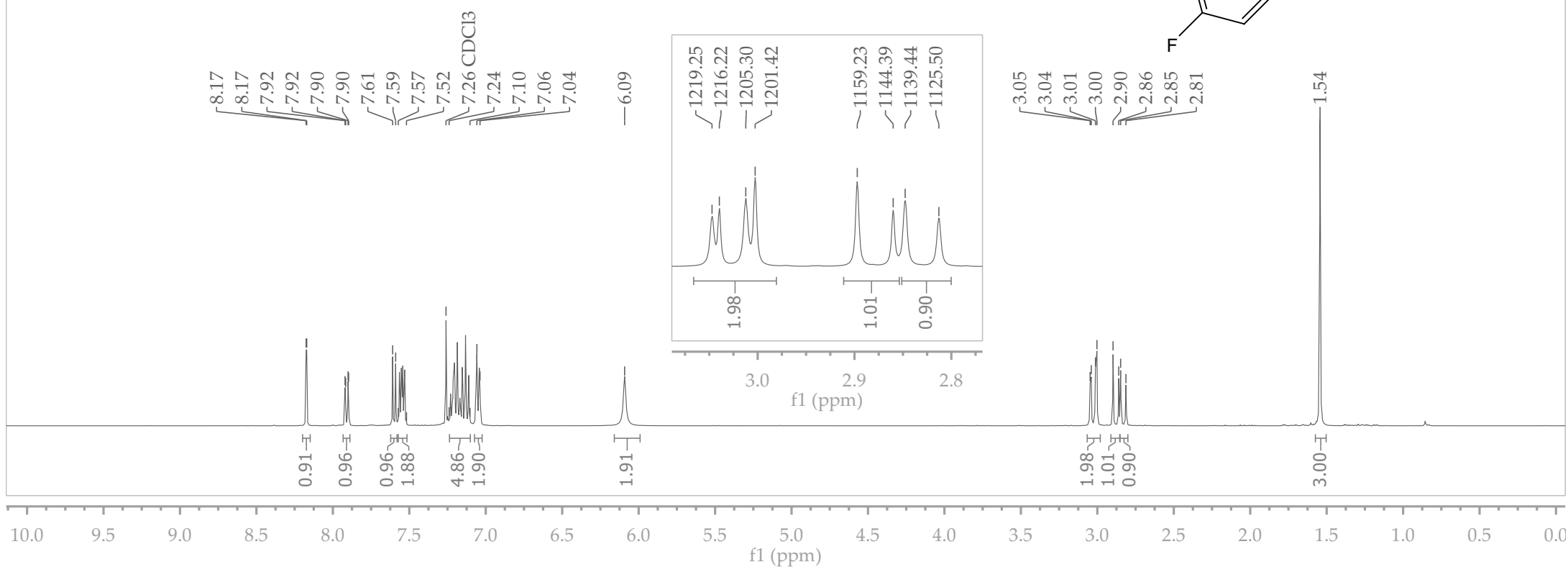
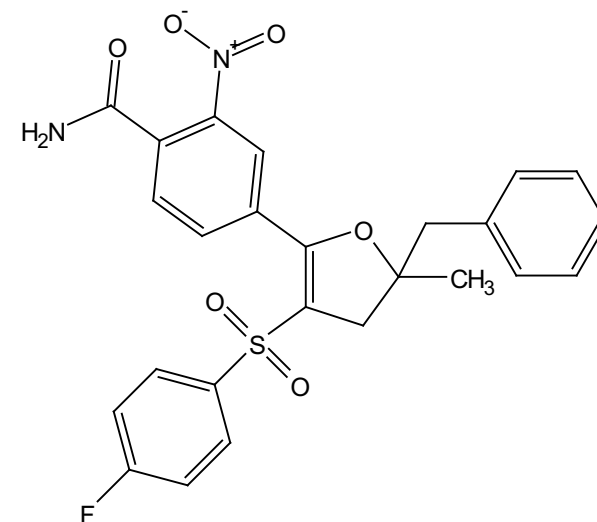


Figure S12: ¹H NMR spectra of compound **4**

4-(5-Benzyl-3-((4-fluorophenyl)sulfonyl)-5-methyl-4,5-dihydrofuran-2-yl)-2-nitrobenzamide (**4**) - C₂₅H₂₁FN₂O₆S

¹³C NMR (100 MHz, CDCl₃) δ (ppm) 167.8 (C), 165.6 (d, *J*_{C-F} = 255.5 Hz, C), 159.0 (C), 145.9 (C), 137.1 (C), 135.2 (C), 134.9 (CH_{Ar}), 133.8 (C), 131.6 (C), 130.4 (2CH_{Ar}), 129.8 (d, *J*_{C-F} = 9.6 Hz, 2CH_{Ar}), 128.5 (2CH_{Ar}), 128.3 (CH_{Ar}), 127.3 (CH_{Ar}), 125.5 (CH_{Ar}), 116.7 (d, *J*_{C-F} = 23.5 Hz, 2CH_{Ar}), 112.1 (C), 89.5 (C), 46.7 (CH₂), 41.6 (CH₂), 27.7 (CH₃).

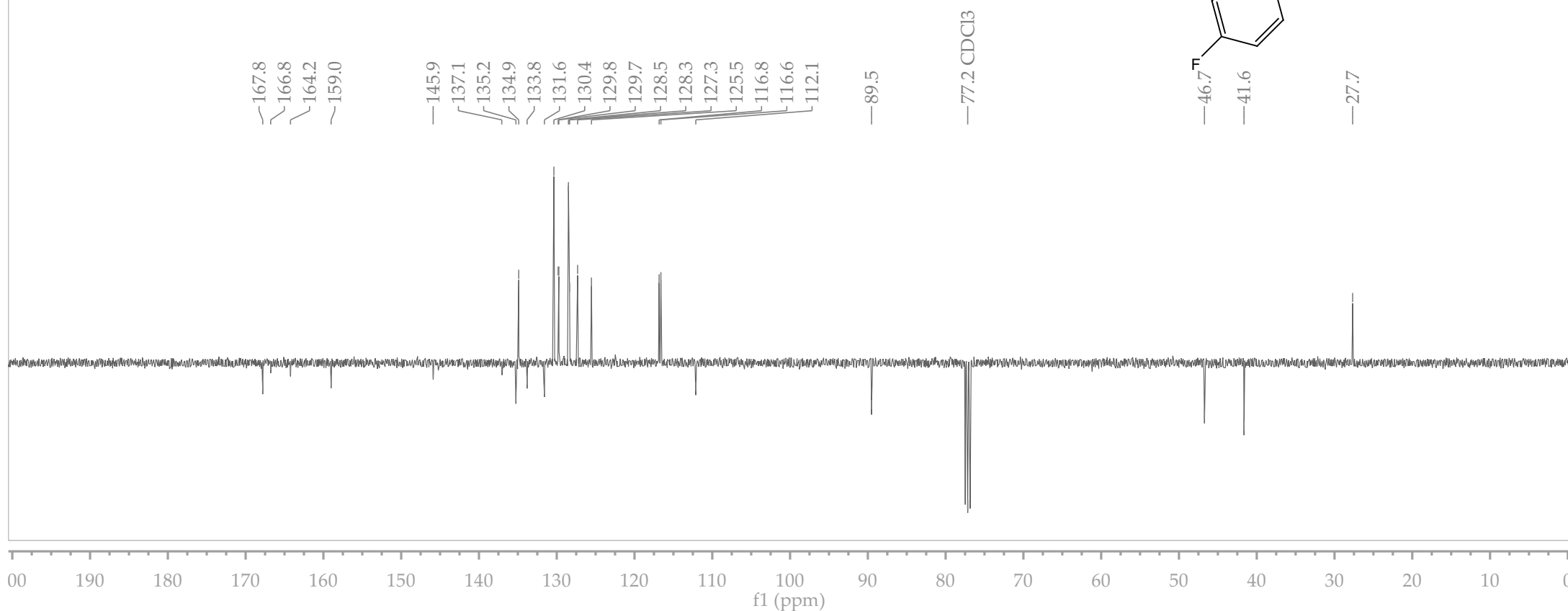
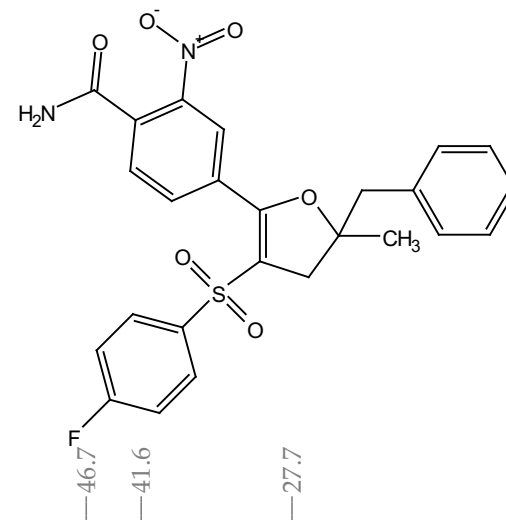


Figure S13: ¹³C NMR spectra of compound 4

4-(5-Benzyl-3-((4-fluorophenyl)sulfonyl)-5-methyl-4,5-dihydrofuran-2-yl)-*N'*-hydroxy-2-nitrobenzimidamide (**5**) - C₂₅H₂₂FN₃O₆S

¹H NMR (400 MHz, CDCl₃): δ (ppm) 8.05 (s, 1H, CH_{Ar}), 7.89 (d, ³J_{H-H} = 8.6 Hz, 1H, CH_{Ar}), 7.66 (d, ³J_{H-H} = 8.5 Hz, 1H, CH_{Ar}), 7.57-7.52 (m, 2H, CH_{Ar}), 7.23-7.03 (m, 7H, 7CH_{Ar}), 5.12 (br s, 2H, NH₂), 3.03 (d, ²J_{H-H} = 14.5 Hz, 2H, CH₂), 2.89-2.82 (m, 2H, CH₂), 1.53 (s, 3H, CH₃). OH not observed.

HRMS: *m/z* [M + Na]⁺ calculated 534.1106; found 534.1105.

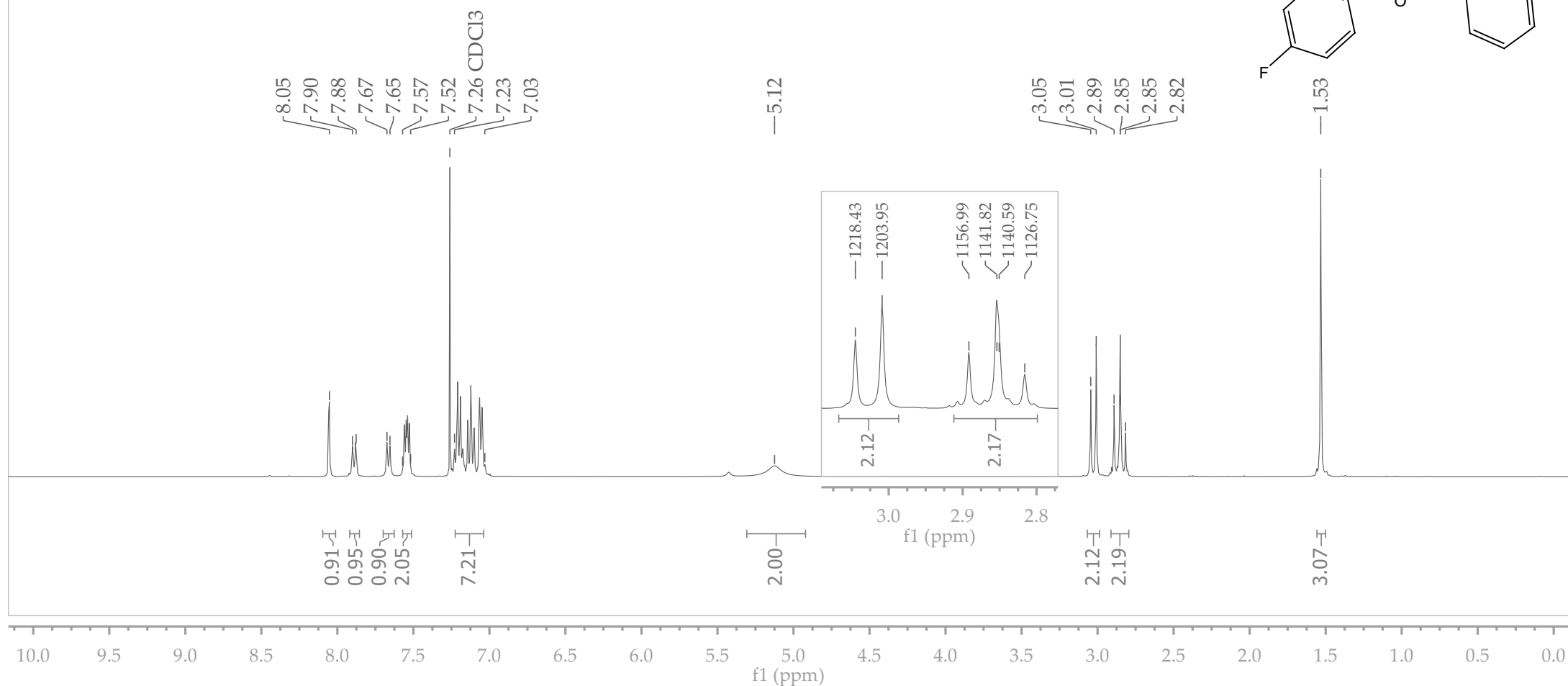
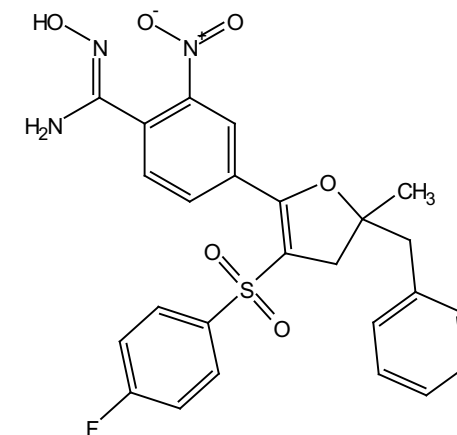


Figure S14: ¹H NMR spectra of compound **5**

4-(5-Benzyl-3-((4-fluorophenyl)sulfonyl)-5-methyl-4,5-dihydrofuran-2-yl)-*N'*-hydroxy-2-nitrobenzimidamide (**5**) - C₂₅H₂₂FN₃O₆S

¹³C NMR (100 MHz, CDCl₃) δ (ppm) 165.5 (d, *J*_{C-F} = 255.9 Hz, C), 159.1 (C), 150.4 (C), 148.0 (C), 137.1 (C), 135.3 (C), 134.1 (CH_{Ar}), 131.7 (C), 130.9 (CH_{Ar}), 130.4 (2CH_{Ar}), 129.8 (d, *J*_{C-F} = 9.7 Hz, 2CH_{Ar}), 128.8 (C), 128.5 (2CH_{Ar}), 127.3 (CH_{Ar}), 125.3 (CH_{Ar}), 116.7 (d, *J*_{C-F} = 22.8 Hz, 2CH_{Ar}), 112.2 (C), 89.5 (C), 46.7 (CH₂), 41.7 (CH₂), 27.6 (CH₃).

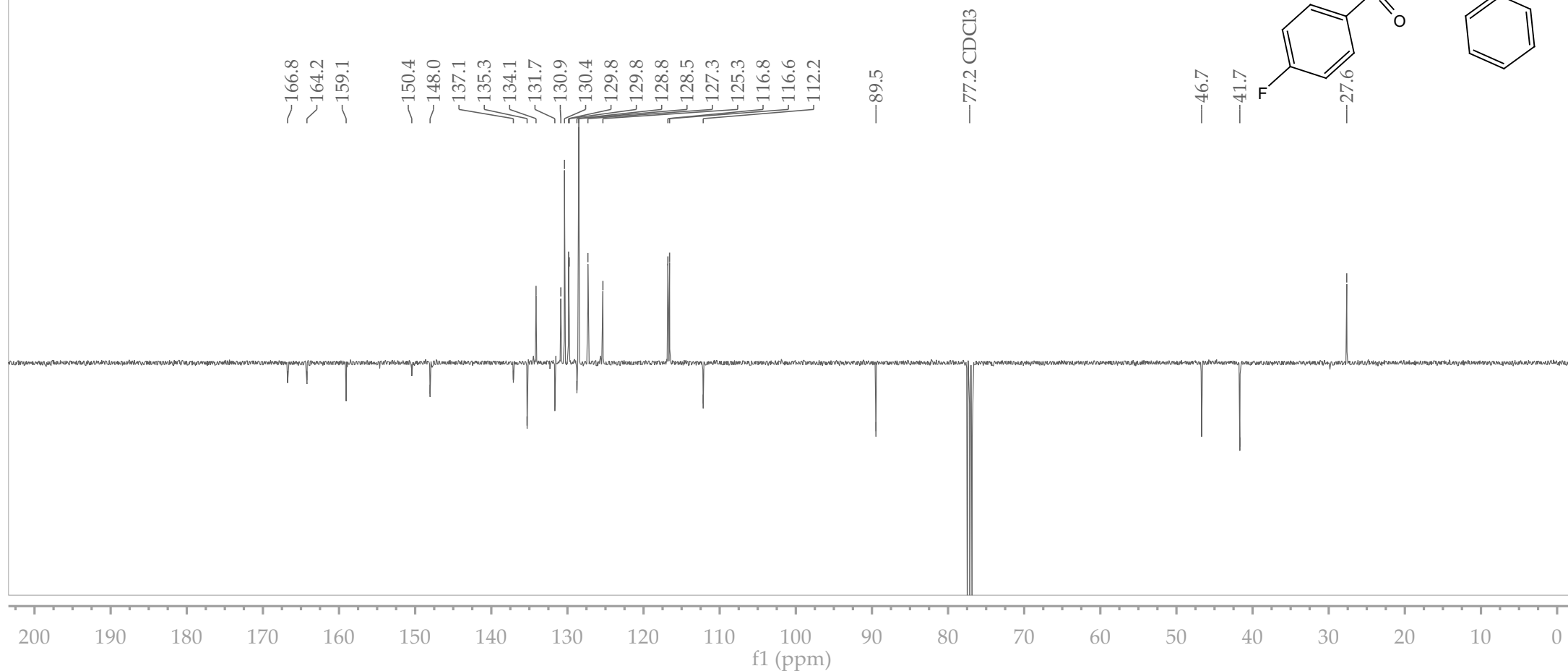


Figure S15: ¹³C NMR spectra of compound **5**