SUPPORTING INFORMATION

Structure-Based Design and Biological Evaluation of Triphenyl Scaffold Based Hybrid Compounds as Hydrolytically Stable Modulators of a LuxR-Type Quorum Sensing Receptor

Matthew C. O'Reilly and Helen E. Blackwell*

Department of Chemistry, University of Wisconsin–Madison, 1101 University Ave., Madison, WI 53706, USA

CONTENTS.

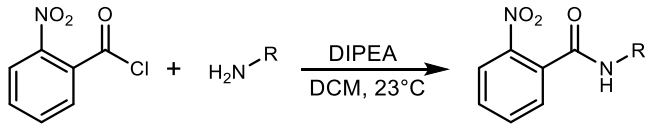
* To whom correspondence should be addressed: blackwell@chem.wisc.edu

Synthesis and characterization data for compounds 2–29.

General experimental details.

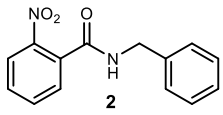
All reagents and solvents were purchased from commercial sources (Sigma-Aldrich, TCI America, or Acros Organics) and used without further purification. Analytical thin-layer chromatography (TLC) was performed on 250 μm silica plates from Silicycle. Visualization was accomplished using UV light. Flash column chromatography was performed using Silica Gel 60 (230–400 mesh) from Macherey–Nagel. All ^{1}H- and ^{13}C-NMR spectra were recorded on a Bruker Avance-400 or -500 spectrometer. Chemical shifts are reported in ppm relative to residual solvent peaks as internal standards set to δ 7.26 and δ 77.16 ($CDCl_3$) or δ 2.50 and δ 39.52 ($(CD_3)_2SO$). NMR data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, br = broad, dd = doublet of doublets, dq = doublet of quartets, td = triplet of doublets, pd = pentet of doublets, m = multiplet), coupling constant (Hz), and integration. High-resolution mass spectra (HRMS) were recorded on a Q Extractive Plus Orbitrap with an electrospray ion source.

*General procedure for synthesis of compounds **2–29**.*



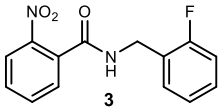
To a solution of amine (0.24 mmol, 1.2 eq.) and *N*,*N*-diisopropylamine (94 μL, 0.54 mmol, 2.5 eq.) in dichloromethane (2.2 mL, 0.1 M), 2-nitrobenzoyl chloride (28 μL, 0.22 mmol, 1.0 eq.) was added at room temperature (rt). The solution was allowed to stir for 5 min at rt, after which it was diluted with diethyl ether (15 mL). The mixture was then washed with 1 M HCl (2 x 20 mL), saturated sodium bicarbonate (2 x 20 mL), and saturated brine (20 mL). The organic layer was separated, dried over magnesium sulfate, filtered, and concentrated under reduced pressure to yield the crude product. All compounds were purified to homogeneity via flash column chromatography, with hexanes and ethyl acetate as the eluent.

*Characterization data for compounds **2–29**.*



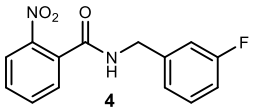
2

Compound **2** was prepared according to the general procedure and purified by flash column chromatography (30–40% ethyl acetate in hexanes, R_f = 0.1 in 30% ethyl acetate) to afford the product (46 mg, 82%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.02 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.63 (td, *J* = 7.5, 1.2 Hz, 1H), 7.55 (td, *J* = 7.8, 1.5 Hz, 1H), 7.49 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.41 – 7.32 (m, 4H), 7.32 – 7.27 (m, 1H), 6.27 (s, 1H), 4.60 (d, *J* = 5.7 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.46, 146.52, 137.54, 133.82, 132.94, 130.62, 128.93, 128.81, 128.16, 127.90, 124.70, 44.40. HRMS (TOF, ES+) $C_{14}H_{12}N_2O_3$ $[M+H]^+$ calc. mass 257.0921, found 257.0921.



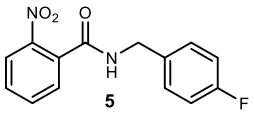
3

Compound **3** was prepared according to the general procedure and was purified by flash column chromatography (30–40% ethyl acetate in hexanes, R_f = 0.27 in 40% ethyl acetate) to afford the product (54 mg, 90%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.01 (d, *J* = 8.1 Hz, 1H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 1H), 7.50 – 7.42 (m, 2H), 7.31 – 7.25 (m, 1H), 7.14 (t, *J* = 7.5 Hz, 1H), 7.05 (t, *J* = 9.2 Hz, 1H), 6.37 (t, *J* = 6.0 Hz, 1H), 4.65 (d, *J* = 5.9 Hz, 2H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.53, 161.11 (d, *J* = 246.3 Hz), 146.52 , 133.80 , 132.78 , 130.65 , 130.62 , 129.71 (d, *J* = 8.2 Hz), 128.82 , 124.67 , 124.60 (d, *J* = 3.9 Hz), 124.47 , 115.50 (d, *J* = 21.2 Hz), 38.25 (d, *J* = 4.1 Hz). HRMS (TOF, ES+) $C_{14}H_{11}FN_2O_3$ $[M+H]^+$ calc. mass 275.0827, found 275.0826.



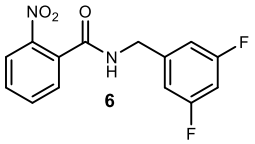
4

Compound **4** was prepared according to the general procedure and was purified by flash column chromatography (40% ethyl acetate in hexanes, R_f = 0.16 in 40% ethyl acetate) to afford the product (58 mg, 97%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.01 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.64 (td, *J* = 7.5, 1.3 Hz, 1H), 7.55 (td, *J* = 7.8, 1.5 Hz, 1H), 7.48 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.36 – 7.26 (m, 1H), 7.13 (d, *J* = 7.6 Hz, 1H), 7.05 (dt, *J* = 9.6, 2.1 Hz, 1H), 6.97 (td, *J* = 8.5, 2.6 Hz, 1H), 6.40 (t, *J* = 6.1 Hz, 1H), 4.57 (d, *J* = 5.9 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.62, 163.07 (d, *J* = 246.6 Hz), 146.50, 140.13 (d, *J* = 7.2 Hz), 133.87, 132.71, 130.73, 130.46 (d, *J* = 8.2 Hz), 128.78, 124.72, 123.59 (d, *J* = 3.0 Hz), 114.93 (d, *J* = 13.7 Hz), 114.72 (d, *J* = 13.1 Hz), 43.74 (d, *J* = 1.9 Hz). HRMS (TOF, ES+) $C_{14}H_{11}FN_2O_3$ $[M+H]^+$ calc. mass 275.0827, found 275.0826.



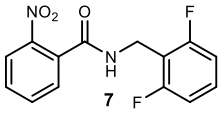
5

Compound **5** was prepared according to the general procedure and was purified by flash column chromatography (40% ethyl acetate in hexanes, R_f = 0.16 in 40% ethyl acetate) to afford the product (48 mg, 80%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.02 (d, *J* = 8.1 Hz, 1H), 7.64 (t, *J* = 7.5 Hz, 1H), 7.55 (t, *J* = 7.8 Hz, 1H), 7.47 (d, *J* = 7.5 Hz, 1H), 7.33 (dd, *J* = 8.3, 5.3 Hz, 2H), 7.02 (t, *J* = 8.4 Hz, 2H), 6.30 (s, 1H), 4.55 (d, *J* = 5.8 Hz, 2H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.50, 162.45 (d, *J* = 246.1 Hz), 146.51, 133.85, 133.40 (d, *J* = 3.3 Hz), 132.83, 130.68, 129.88 (d, *J* = 8.2 Hz), 128.79, 124.72, 115.77 (d, *J* = 21.4 Hz), 43.62. HRMS (TOF, ES+) $C_{14}H_{11}FN_2O_3$ $[M+H]^+$ calc. mass 275.0827, found 275.0826.



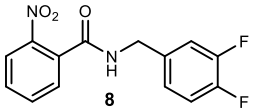
6

Compound **6** was prepared according to the general procedure and was purified by flash column chromatography (40% ethyl acetate in hexanes, R_f = 0.18 in 40% ethyl acetate) to afford the product (52 mg, 84%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.01 (d, *J* = 8.1 Hz, 1H), 7.64 (t, *J* = 7.5 Hz, 1H), 7.56 (t, *J* = 7.8 Hz, 1H), 7.47 (d, *J* = 7.5 Hz, 1H), 6.87 (d, *J* = 7.0 Hz, 2H), 6.71 (t, *J* = 8.7 Hz, 1H), 6.61 – 6.47 (m, 1H), 4.54 (d, *J* = 6.1 Hz, 2H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.76, 163.32 (dd, *J* = 249.2, 12.7 Hz), 146.54, 141.61 (t, *J* = 9.2 Hz), 133.93, 132.53, 130.90, 128.76, 124.82, 110.69 (dd, *J* = 19.5, 6.1 Hz), 103.29 (t, *J* = 25.3 Hz), 43.48. HRMS (TOF, ES+) $C_{14}H_{11}F_2N_2O_3$ $[M+H]^+$ calc. mass 293.0732, found 293.0731.



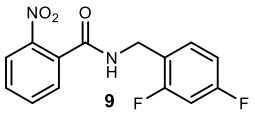
7

Compound **7** was prepared according to the general procedure and was purified by flash column chromatography (40% ethyl acetate in hexanes) to afford the product (54 mg, 87%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.02 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.63 (td, *J* = 7.5, 1.2 Hz, 1H), 7.55 (td, *J* = 7.9, 1.5 Hz, 1H), 7.47 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.32 – 7.22 (m, 1H), 6.92 (t, *J* = 7.8 Hz, 2H), 6.24 (d, *J* = 6.0 Hz, 1H), 4.73 (d, *J* = 5.7 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.19 , 161.68 (dd, *J* = 249.5, 7.9 Hz), 146.44 , 133.28 (d, *J* = 109.8 Hz), 130.64 , 129.99 (t, *J* = 10.3 Hz), 128.87 , 124.67 , 113.18 (t, *J* = 19.2 Hz), 111.88 – 111.32 (m), 32.27 (t, *J* = 3.8 Hz). HRMS (TOF, ES+) $C_{14}H_{11}F_2N_2O_3$ $[M+H]^+$ calc. mass 293.0732, found 293.0730.



8

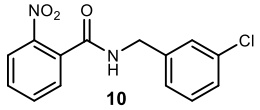
Compound **8** was prepared according to the general procedure and was purified by flash column chromatography (40–50% ethyl acetate in hexanes, R_f = 0.15 in 40% ethyl acetate) to afford the product (54 mg, 86%). ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.25 (t, *J* = 6.0 Hz, 1H), 8.05 (dd, *J* = 8.1, 1.1 Hz, 1H), 7.81 (td, *J* = 7.5, 1.2 Hz, 1H), 7.74 – 7.65 (m, 2H), 7.47 – 7.37 (m, 2H), 7.25 – 7.19 (m, 1H), 4.45 (d, *J* = 5.9 Hz, 2H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 165.63, 149.25 (dd, *J* = 245.2, 12.7 Hz), 148.43 (dd, *J* = 244.1, 12.5 Hz), 147.05, 136.74 (dd, *J* = 5.5, 3.7 Hz), 133.66, 132.18, 130.87, 129.11, 124.13, 123.99 (dd, *J* = 6.5, 3.3 Hz), 117.28 (d, *J* = 17.1 Hz), 116.23 (d, *J* = 17.4 Hz), 41.63. HRMS (TOF, ES+) $C_{14}H_{11}F_2N_2O_3$ $[M+H]^+$ calc. mass 293.0732, found 293.0730.



9

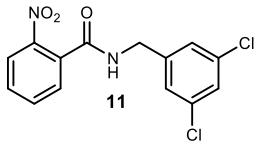
Compound **9** was prepared according to the general procedure and was purified by flash column chromatography (40% ethyl acetate in hexanes, R_f = 0.27 in 40% ethyl acetate) to afford the product (56 mg, 89%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.21 (t, *J* = 5.8 Hz, 1H), 8.04 (dd, *J* =

8.1, 1.2 Hz, 1H), 7.80 (td, *J* = 7.5, 1.2 Hz, 1H), 7.70 (td, *J* = 7.8, 1.5 Hz, 1H), 7.63 (dd, *J* = 7.5, 1.4 Hz, 1H), 7.50 (td, *J* = 8.7, 6.6 Hz, 1H), 7.25 (ddd, *J* = 10.5, 9.3, 2.6 Hz, 1H), 7.15 – 7.06 (m, 1H), 4.45 (d, *J* = 5.7 Hz, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.56, 161.49 (dd, *J* = 245.5, 12.1 Hz), 160.06 (dd, *J* = 247.5, 12.1 Hz), 147.03, 133.64, 132.14, 131.00 (dd, *J* = 9.9, 5.9 Hz), 130.87, 129.12, 124.11, 121.78 (dd, *J* = 14.9, 3.7 Hz), 111.33 (dd, *J* = 21.1, 3.7 Hz), 103.69 (t, *J* = 25.8 Hz), 36.11 (d, *J* = 4.0 Hz). HRMS (TOF, ES+) $C_{14}H_{11}F_2N_2O_3$ $[M+H]^+$ calc. mass 293.0732, found 293.0731.



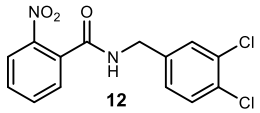
10

Compound **10** was prepared according to the general procedure and was purified by flash column chromatography (40% ethyl acetate in hexanes, R_f = 0.13 in 40% ethyl acetate) to afford the product (53 mg, 84%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96 (d, *J* = 8.1 Hz, 1H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.52 (td, *J* = 7.8, 1.5 Hz, 1H), 7.42 (dd, *J* = 7.5, 1.4 Hz, 1H), 7.28 (s, 1H), 7.27 – 7.18 (m, 3H), 6.67 (s, 1H), 4.48 (d, *J* = 5.9 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.68, 146.41, 139.68, 134.54, 133.80, 132.54, 130.65, 130.14, 128.74, 127.96, 127.89, 126.10, 124.61, 43.56. HRMS (TOF, ES+) $C_{14}H_{11}ClN_2O_3$ $[M+H]^+$ calc. mass 291.0531, found 291.0530.



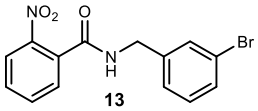
11

Compound **11** was prepared according to the general procedure and was purified by flash column chromatography (45% ethyl acetate in hexanes, R_f = 0.23 in 40% ethyl acetate) to afford the product (66 mg, 94%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.29 (t, *J* = 6.0 Hz, 1H), 8.06 (dd, *J* = 8.1, 1.1 Hz, 1H), 7.82 (td, *J* = 7.5, 1.2 Hz, 1H), 7.74 – 7.66 (m, 2H), 7.52 (t, *J* = 2.0 Hz, 1H), 7.43 (d, *J* = 1.9 Hz, 2H), 4.47 (d, *J* = 6.0 Hz, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 166.24, 147.56, 143.74, 134.42, 134.18, 132.51, 131.43, 129.56, 127.02, 126.51, 124.66, 42.14. HRMS (TOF, ES+) $C_{14}H_{10}Cl_2N_2O_3$ $[M+H]^+$ calc. mass 325.0141, found 325.0141.



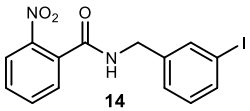
12

Compound **12** was prepared according to the general procedure and was purified by flash column chromatography (50% ethyl acetate in hexanes, R_f = 0.15 in 40% ethyl acetate) to afford the product (56 mg, 80%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.28 (t, *J* = 6.0 Hz, 1H), 8.05 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.81 (td, *J* = 7.5, 1.2 Hz, 1H), 7.75 – 7.65 (m, 2H), 7.63 (dd, *J* = 5.1, 3.1 Hz, 2H), 7.36 (dd, *J* = 8.3, 2.0 Hz, 1H), 4.46 (d, *J* = 5.9 Hz, 2H). ^{13}C NMR (100.6 MHz, $CDCl_3$) δ (ppm): ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.68, 147.07, 140.17, 133.70, 132.12, 130.93, 130.49, 129.43, 129.31, 129.09, 127.68, 124.17, 112.02, 41.55. HRMS (TOF, ES+) $C_{14}H_{10}Cl_2N_2O_3$ $[M+H]^+$ calc. mass 325.0141, found 325.0140.



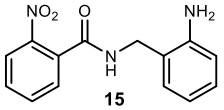
13

Compound **13** was prepared according to the general procedure and was purified by flash column chromatography (45% ethyl acetate in hexanes, R_f = 0.14 in 40% ethyl acetate) to afford the product (57 mg, 80%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.98 (d, *J* = 8.1 Hz, 1H), 7.63 (t, *J* = 7.4 Hz, 1H), 7.54 (td, *J* = 7.8, 1.5 Hz, 1H), 7.49 – 7.38 (m, 3H), 7.33 – 7.25 (m, 1H), 7.21 (t, *J* = 7.7 Hz, 1H), 6.66 (s, 1H), 4.50 (d, *J* = 5.8 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.67, 146.42, 139.94, 133.81, 132.54, 130.89, 130.84, 130.67, 130.44, 128.74, 126.60, 124.62, 122.75, 43.51. HRMS (TOF, ES+) $C_{14}H_{11}BrN_2O_3$ $[M+H]^+$ calc. mass 335.0026, found 335.0026.



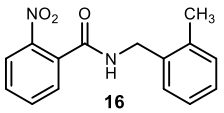
14

Compound **14** was prepared according to the general procedure and was purified by flash column chromatography (30–40% ethyl acetate in hexanes, R_f = 0.16 at 40% ethyl acetate) to afford the product (69 mg, 84%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96 (d, *J* = 8.3 Hz, 1H), 7.64 (s, 1H), 7.60 (t, *J* = 7.9 Hz, 2H), 7.52 (td, *J* = 7.8, 1.5 Hz, 1H), 7.41 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.30 (d, *J* = 7.7 Hz, 1H), 7.05 (t, *J* = 7.8 Hz, 1H), 6.63 (t, *J* = 6.0 Hz, 1H), 4.45 (d, *J* = 5.8 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.63, 146.42, 139.99, 136.80 (one set of coincident signals), 133.81, 132.53, 130.66, 130.59, 128.74, 127.26, 124.62, 94.62, 43.39. HRMS (TOF, ES+) $C_{14}H_{11}IN_2O_3$ $[M+H]^+$ calc. mass 382.9887, found 382.9885.



15

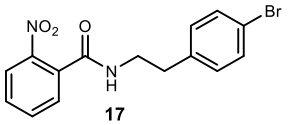
Compound **15** was prepared according to the general procedure (without the 1 M HCl wash) and was purified by flash column chromatography (50–60% ethyl acetate in hexanes, R_f = 0.20 in 60% ethyl acetate) to afford the product (50 mg, 85%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.58 (td, *J* = 7.5, 1.3 Hz, 1H), 7.51 (td, *J* = 7.8, 1.6 Hz, 1H), 7.41 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.08 (td, *J* = 7.7, 1.6 Hz, 1H), 7.03 (dd, *J* = 7.4, 1.5 Hz, 1H), 6.69 – 6.61 (m, 2H), 6.50 (t, *J* = 6.1 Hz, 1H), 4.46 (d, *J* = 5.9 Hz, 2H), 4.19 (s, 2H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.91, 146.39, 145.71, 133.78, 132.53, 130.79, 130.63, 129.51, 128.76, 124.59, 121.05, 117.99, 116.01, 41.60. HRMS (TOF, ES+) $C_{14}H_{11}N_3O_3$ $[M+H]^+$ calc. mass 272.1030, found 272.1030.



16

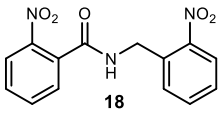
Compound **16** was prepared according to the general procedure and was purified by flash column chromatography (40% ethyl acetate in hexanes, R_f = 0.23 in 40% ethyl acetate) to afford the product (46 mg, 79%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.01 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.63 (td, *J* = 7.5, 1.3 Hz, 1H), 7.54 (td, *J* = 7.8, 1.5 Hz, 1H), 7.48 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.34 – 7.29 (m, 1H), 7.24 – 7.15 (m, 3H), 6.09 (s, 1H), 4.60 (d, *J* = 5.3 Hz, 2H), 2.39 (s, 3H). ^{13}C NMR (101

MHz, Chloroform-*d*) δ 166.30, 146.51, 136.81, 135.09, 133.79, 132.92, 130.74, 130.59, 129.03, 128.81, 128.21, 126.44, 124.68, 42.62, 19.13. HRMS (TOF, ES+) $C_{15}H_{14}N_2O_3$ $[M+H]^+$ calc. mass 271.1077, found 271.1076.



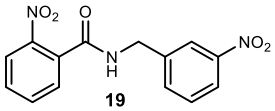
17

Compound **17** was prepared according to the general procedure and was purified by flash column chromatography (30–40% ethyl acetate in hexanes, R_f = 0.08 in 30% ethyl acetate) to afford the product (71 mg, 95%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.05 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.64 (td, *J* = 7.5, 1.2 Hz, 1H), 7.56 (td, *J* = 7.9, 1.5 Hz, 1H), 7.47 – 7.39 (m, 3H), 7.19 – 7.12 (m, 2H), 5.79 (t, *J* = 6.1 Hz, 1H), 3.71 (q, *J* = 6.6 Hz, 2H), 2.94 (t, *J* = 6.9 Hz, 2H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.63, 146.63, 137.77, 133.86, 133.06, 131.94, 130.77, 130.66, 128.72, 124.77, 120.66, 41.23, 34.92. HRMS (TOF, ES+) $C_{15}H_{13}Br\,N_2O_3$ $[M+H]^+$ calc. mass 349.0182, found 349.0182.



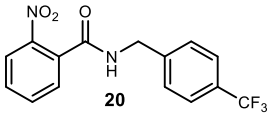
18

Compound **18** was prepared according to the general procedure and was purified by flash column chromatography (40% ethyl acetate in hexanes, R_f = 0.19 in 40% ethyl acetate) to afford the product (52 mg, 81%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.08 (d, *J* = 8.2 Hz, 1H), 8.03 (d, *J* = 8.1 Hz, 1H), 7.82 (d, *J* = 7.6 Hz, 1H), 7.67 (dt, *J* = 15.5, 7.5 Hz, 2H), 7.57 (t, *J* = 7.8 Hz, 1H), 7.54 – 7.46 (m, 2H), 6.74 (s, 1H), 4.86 (d, *J* = 6.4 Hz, 2H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.68, 148.51, 146.52, 134.49, 133.90, 133.18, 132.79, 132.67, 130.79, 129.26, 128.74, 125.28, 124.78, 42.05. HRMS (TOF, ES+) $C_{14}H_{11}\,N_3O_5$ $[M+H]^+$ calc. mass 302.0772, found 302.0770.



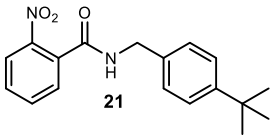
19

Compound **19** was prepared according to the general procedure and was purified by flash column chromatography (40–45% ethyl acetate in hexanes, R_f = 0.11 in 40% ethyl acetate) to afford the product (56 mg, 88%). ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.37 (t, *J* = 6.0 Hz, 1H), 8.25 (t, *J* = 2.0 Hz, 1H), 8.15 (ddd, *J* = 8.1, 2.4, 1.1 Hz, 1H), 8.06 (dd, *J* = 8.1, 1.1 Hz, 1H), 7.87 – 7.78 (m, 2H), 7.72 (td, *J* = 7.8, 1.5 Hz, 1H), 7.69 – 7.65 (m, 2H), 4.59 (d, *J* = 6.0 Hz, 2H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 165.85, 147.89, 147.10, 141.35, 134.11, 133.78, 132.13, 131.02, 129.92, 129.10, 124.25, 122.01, 121.97, 42.01. HRMS (TOF, ES+) $C_{14}H_{11}\,N_3O_5$ $[M+H]^+$ calc. mass 302.0772, found 302.0769.



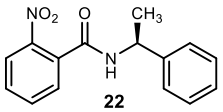
20

Compound **20** was prepared according to the general procedure and was purified by flash column chromatography (40–50% ethyl acetate in hexanes, R_f = 0.14 in 40% ethyl acetate) to afford the product (55 mg, 79%). ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.31 (t, J = 6.0 Hz, 1H), 8.05 (dd, J = 8.1, 1.1 Hz, 1H), 7.81 (td, J = 7.5, 1.2 Hz, 1H), 7.76 – 7.66 (m, 4H), 7.65 – 7.55 (m, 2H), 4.54 (d, J = 5.9 Hz, 2H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 165.68, 147.08, 143.81, 133.68, 132.18, 130.93, 129.11, 128.00, 127.63 (q, J = 31.5 Hz), 125.21 (q, J = 3.8 Hz), 124.36 (q, J = 272.1 Hz), 124.17, 42.25. HRMS (TOF, ES+) $C_{15}H_{11}F_3N_2O_3$ $[M+H]^+$ calc. mass 342.1060, found 342.1060.



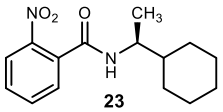
21

Compound **21** was prepared according to the general procedure and was purified by flash column chromatography (30–40% ethyl acetate in hexanes) to afford the product (60 mg, 88%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.02 (d, J = 8.1 Hz, 1H), 7.66 – 7.60 (m, 1H), 7.54 (td, J = 7.9, 1.5 Hz, 1H), 7.48 (dd, J = 7.5, 1.4 Hz, 1H), 7.38 (d, J = 8.1 Hz, 2H), 7.31 (d, J = 8.1 Hz, 2H), 6.23 (s, 1H), 4.57 (d, J = 5.5 Hz, 2H), 1.31 (s, 9H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.37, 150.93, 146.53, 134.48, 133.78, 132.99, 130.57, 128.81, 127.97, 125.85, 124.66, 44.09, 34.66, 31.44. HRMS (TOF, ES+) $C_{18}H_{20}N_2O_3$ $[M+H]^+$ calc. mass 313.1547, found 313.1545.



22

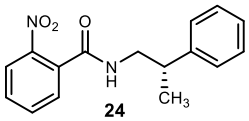
Compound **22** was prepared according to the general procedure and was purified by flash column chromatography (30–40% ethyl acetate in hexanes, R_f = 0.27 in 40% ethyl acetate) to afford the product (52 mg, 90%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.02 (dd, J = 8.2, 1.2 Hz, 1H), 7.62 (td, J = 7.5, 1.2 Hz, 1H), 7.54 (td, J = 7.8, 1.5 Hz, 1H), 7.45 (dd, J = 7.5, 1.5 Hz, 1H), 7.43 – 7.33 (m, 4H), 7.33 – 7.27 (m, 1H), 6.17 (d, J = 7.9 Hz, 1H), 5.31 (p, J = 7.1 Hz, 1H), 1.61 (d, J = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 165.68, 146.41, 142.38, 133.82, 133.11, 130.50, 128.90, 128.86, 127.78, 126.51, 124.64, 49.64, 21.17. HRMS (TOF, ES+) $C_{15}H_{14}N_2O_3$ $[M+H]^+$ calc. mass 271.1077, found 271.1076.



23

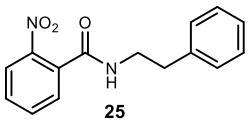
Compound **23** was prepared according to the general procedure and was purified by flash column chromatography (30–40% ethyl acetate in hexanes, R_f = 0.33 in 40% ethyl acetate) to afford the product (58 mg, 97%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.02 (dd, J = 8.2, 1.2 Hz, 1H), 7.64 (td, J = 7.5, 1.2 Hz, 1H), 7.54 (td, J = 7.9, 1.5 Hz, 1H), 7.47 (dd, J = 7.5, 1.4 Hz, 1H), 5.77 (d, J = 9.1 Hz, 1H), 4.02 (dp, J = 9.0, 6.7 Hz, 1H), 1.87 – 1.60 (m, 4H), 1.50 – 1.36 (m, 1H), 1.32 – 1.14 (m, 6H), 1.14 – 0.96 (m, 2H), 0.91 – 0.76 (m, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ

165.92, 146.44, 133.76, 133.63, 130.32, 128.84, 124.59, 50.48, 42.94, 29.22, 29.14, 26.50, 26.27, 17.66. HRMS (TOF, ES+) $C_{15}H_{20}N_2O_3$ $[M+H]^+$ calc. mass 277.1547, found 277.1547.



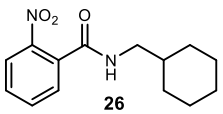
24

Compound **24** was prepared according to the general procedure and was purified by flash column chromatography (30–40% ethyl acetate in hexanes, R_f = 0.22 in 40% ethyl acetate) to afford the product (52 mg, 84%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.99 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.58 (td, *J* = 7.5, 1.3 Hz, 1H), 7.51 (td, *J* = 7.8, 1.6 Hz, 1H), 7.35 – 7.20 (m, 6H), 5.78 (s, 1H), 3.83 (ddd, *J* = 13.2, 7.1, 5.9 Hz, 1H), 3.42 (ddd, *J* = 13.6, 8.9, 5.0 Hz, 1H), 3.17 – 3.00 (m, 1H), 1.35 (d, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.49, 146.57, 143.96, 133.71, 133.15, 130.46, 128.89, 128.67, 127.42, 126.92, 124.63, 46.74, 39.76, 19.63. HRMS (TOF, ES+) $C_{16}H_{16}N_2O_3$ $[M+H]^+$ calc. mass 285.1234, found 285.1234.



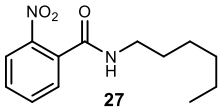
25

Compound **25** was prepared according to the general procedure and was purified by flash column chromatography (40% ethyl acetate in hexanes, R_f = 0.16 in at 40% ethyl acetate) to afford the product (50 mg, 86%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.01 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.61 (td, *J* = 7.5, 1.3 Hz, 1H), 7.53 (td, *J* = 7.9, 1.5 Hz, 1H), 7.39 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.35 – 7.29 (m, 2H), 7.28 – 7.19 (m, 3H), 5.95 (s, 1H), 3.71 (q, *J* = 6.7 Hz, 2H), 2.95 (t, *J* = 6.9 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.57, 146.56, 138.75, 133.77, 133.12, 130.51, 128.97, 128.81, 128.72, 126.71, 124.65, 41.33, 35.41. HRMS (TOF, ES+) $C_{15}H_{14}N_2O_3$ $[M+H]^+$ calc. mass 271.1077, found 271.1077.



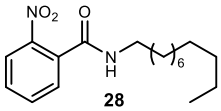
26

Compound **26** was prepared according to the general procedure and was purified by flash column chromatography (30–40% ethyl acetate in hexanes, R_f = 0.21 in 40% ethyl acetate) to afford the product (52 mg, 93%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.01 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.64 (td, *J* = 7.5, 1.2 Hz, 1H), 7.54 (td, *J* = 7.8, 1.5 Hz, 1H), 7.48 (dd, *J* = 7.5, 1.4 Hz, 1H), 6.03 (s, 1H), 3.26 (t, *J* = 6.5 Hz, 2H), 1.84 – 1.63 (m, 4H), 1.63 – 1.52 (m, 1H), 1.34 – 1.10 (m, 4H), 1.06 – 0.79 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.62, 146.56, 133.75, 133.41, 130.42, 128.85, 124.61, 46.56, 37.79, 30.95, 26.48, 25.91. HRMS (TOF, ES+) $C_{14}H_{18}N_2O_3$ $[M+H]^+$ calc. mass 263.1390, found 263.1385.



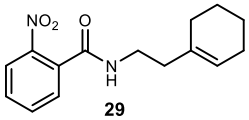
27

Compound **27** was prepared according to the general procedure and was purified by flash column chromatography (35–40% ethyl acetate in hexanes, R_f = 0.22 in 40% ethyl acetate) to afford the product (50 mg, 93%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.01 (d, *J* = 8.1 Hz, 1H), 7.64 (t, *J* = 7.5 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 1H), 7.47 (d, *J* = 7.5 Hz, 1H), 5.99 (t, *J* = 5.8 Hz, 1H), 3.41 (q, *J* = 6.8 Hz, 2H), 1.60 (p, *J* = 7.3 Hz, 2H), 1.45 – 1.17 (m, 6H), 0.97 – 0.80 (m, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.56 , 146.54 , 133.76 , 133.34 , 130.41 , 128.84 , 124.60 , 40.43 , 31.57 , 29.32 , 26.68 , 22.67 , 14.14 . HRMS (TOF, ES+) $C_{13}H_{18}N_2O_3$ $[M+H]^+$ calc. mass 251.1390, found 251.2389.



28

Compound **28** was prepared according to the general procedure and was purified by flash column chromatography (30–40% ethyl acetate in hexanes, R_f = 0.28 in 40% ethyl acetate) to afford the product (30 mg, 86%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.01 (d, *J* = 8.2 Hz, 1H), 7.63 (t, *J* = 7.4 Hz, 1H), 7.54 (t, *J* = 7.7 Hz, 1H), 7.48 (d, *J* = 7.5 Hz, 1H), 5.98 (t, *J* = 6.0 Hz, 1H), 3.41 (q, *J* = 6.8 Hz, 2H), 1.60 (p, *J* = 7.3 Hz, 2H), 1.25 (m, 16H), 0.87 (t, *J* = 6.7 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.55, 146.57, 133.74, 133.36, 130.40, 128.85, 124.60, 40.45, 32.04, 29.83, 29.73, 29.68, 29.47, 29.42, 29.38, 27.04, 22.81, 14.24. HRMS (TOF, ES+) $C_{18}H_{28}N_2O_3$ $[M+H]^+$ calc. mass 321.2173, found 321.2172.



29

Compound **29** was prepared according to the general procedure and was purified by flash column chromatography (30–40% ethyl acetate in hexanes) to afford the product (54 mg, 90%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.02 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.65 (td, *J* = 7.5, 1.2 Hz, 1H), 7.55 (td, *J* = 7.9, 1.5 Hz, 1H), 7.48 (dd, *J* = 7.5, 1.5 Hz, 1H), 5.85 (s, 1H), 5.50 (s, 1H), 3.52 (td, *J* = 6.8, 5.5 Hz, 2H), 2.25 (t, *J* = 6.8 Hz, 2H), 2.02–1.92 (m, 4H), 1.69 – 1.59 (m, 2H), 1.58–1.51 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.42, 146.65, 134.49, 133.76, 133.29, 130.47, 128.86, 124.64, 124.00, 37.88, 37.34, 27.94, 25.36, 22.90, 22.44. HRMS (TOF, ES+) $C_{15}H_{18}N_2O_3$ $[M+H]^+$ calc. mass 275.1390, found 275.1389.

Biological assay protocols and data.

Table S-1. Bacterial strains and plasmids used in this study.

Strain or plasmid	Relevant properties[a]	Ref.
E. coli		
JLD271	K-12 Δ*lacX74 sdiA271*::Cam; Cl^R	1
Plasmids		
pSC11	Broad host range *lasI'-lacZ* reporter; Ap^R	2
pJN105L	Arabinose-inducible expression vector for *lasR*; pBBRMCS backbone; Gm^R	3

[a] Abbreviations: Cl^R, chloramphenicol resistance; Ap^R, Ampicillin resistance; Gm^R, gentamicin resistance.

General considerations and conditions for E. coli LasR reporter.

All standard biological reagents were purchased from Sigma-Aldrich or Gold Biotechnology and used according to enclosed instructions. Buffers and solutions for Miller absorbance assays in *E. coli* (Z buffer, 0.1% aqueous sodium dodecyl sulfate (SDS), and phosphate buffer) were prepared as previously described.[1] Water (18 MΩ) was purified using a Millipore Feed System.

The bacterial strain and plasmids used in this study are listed in Table S-1. Freezer stocks of bacteria were maintained at -80 °C in Luria-Bertani (LB) medium and 20–50% glycerol. Bacterial overnight cultures were inoculated with single colonies that were isolated by streaking a freezer stock on an LB/agar (1.5%) plate with appropriate antibiotic supplements.

Unless otherwise noted, bacteria were grown in a standard laboratory incubator at 37 ºC with shaking (200 rpm) in LB medium (autoclave-sterilized). *E. coli* overnight cultures were grown in 13 mm x 100 mm test tubes or Erlenmeyer flasks. *E. coli* subcultures were grown in Erlenmeyer flasks. To minimize growth effects in 96-well plates, the following precautions were taken: (i) To reduce media evaporation, plates were incubated in stacks with "dummy plates" (containing sterile water in all wells) positioned on the top and bottom. Stacks of plates were placed in plastic containers to reduce air circulation. (ii) To reduce variation in ambient temperature, plates (including "dummy plates") were never stacked higher than six-fold.

E. coli LasR reporter assay protocol.

To evaluate the modulatory activities of library compounds on LasR heterologously expressed in *E. coli*, the strain JLD271 harboring plasmids pSC11 and pJN105L was grown overnight. The overnight culture was diluted 1:10 in fresh LB medium supplemented with 100 μg/mL ampicillin and 10 μg/mL gentamicin. An appropriate amount of test compound stock solution (or OdDHL stock solution for the positive control) in DMSO was added to clear 96-well microtiter plates (Costar 3370), with final DMSO concentrations not exceeding 1%. Once the subculture grew to an OD_{600} of ~0.25, arabinose was added to a final concentration of 4 mg/mL to induce LasR expression from the plasmid pJN105L. *For agonism assays*, the subculture was dispensed in 200-μL portions into each compound-treated well of the microtiter plate. *For antagonism assays*, the subculture was pre-treated with OdDHL to a final concentration of 5 nM by adding an appropriate amount from an OdDHL stock solution in DMSO. The subculture was then dispensed in 200-μL portions into each compound-treated well of the microtiter plate. Subculture containing 1% DMSO and no added OdDHL was used as a control to mimic fully inhibited LasR. The plates were incubated with shaking for 4 h.

The cultures were assayed for β-galactosidase activity following the Miller assay method, optimized for microtiter plates.[4] The OD_{600} of each well was recorded, and 50-μL aliquots from each well were transferred to the wells of a solvent-resistant 96-well microtiter plate (Costar 3879) containing 200 μL Z-buffer, 8 μL $CHCl_3$, and 4 μL 0.1% aqueous SDS. Cells were lysed by aspirating and dispensing the mixtures 30 times with a 12-channel pipettor, after which the $CHCl_3$ was allowed to settle. A 100-μL aqueous aliquot from each well was transferred to a fresh clear-bottom 96-well microtiter plate. At t = 0 min, the assay was initiated by adding 20 μL of substrate, *ortho*-nitrophenyl-β-galactoside (ONPG; 4 mg/mL in phosphate buffer), to each well.

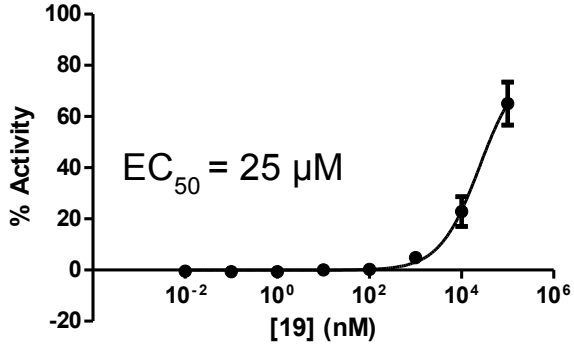
This mixture was incubated at 30 °C for 30 minutes, then 50-µL aliquots of a 1 M Na_2CO_3 solution was added to each well, terminating the reaction.

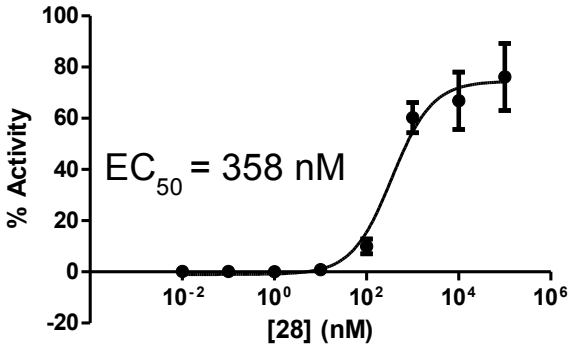
Absorbances at 420 and 550 nm were measured for each well using a plate reader. Miller units were calculated using the following formula: 1000 × (A420 – (1.75 × A550)) × ((Time ONPG incubated with lysate in minutes)$^{-1}$ × (Volume of culture lysed in mL)$^{-1}$ × OD_{600}^{-1}). In all assays, the Miller units were background-corrected relative to wells of LasR reporter subculture containing only 1% DMSO (no compound added). In agonism assays, the OD-normalized Miller units of each compound was reported relative to the OD-normalized fluorescence of a well containing enough OdDHL to fully activate LasR. In antagonism assays, percent activity was calculated by normalizing background-corrected Miller units to the control wells containing subculture treated with only OdDHL at its EC_{70} value.

All synthetic compounds were tested in triplicate, and ≥ 3 separate trials were performed using unique cultures. EC_{50} and IC_{50} values, as well as respective 95% confidence intervals, were calculated using GraphPad Prism software (v. 4.0) using a sigmoidal curve fit.

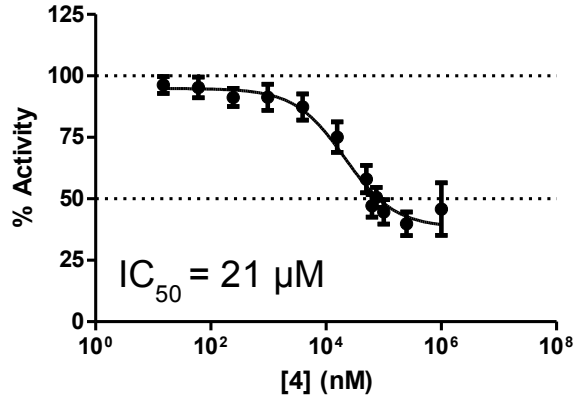
Dose response curves for hybrid compounds.

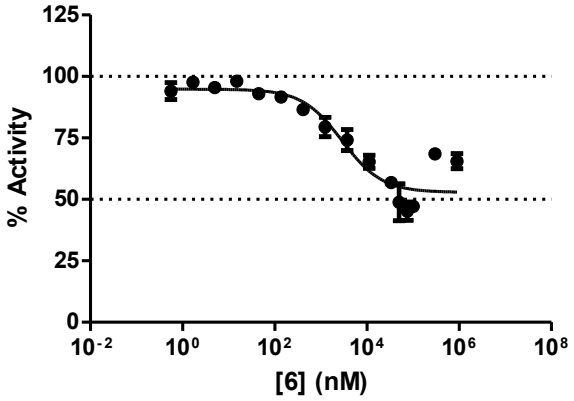
LasR agonism dose response curves and EC_{50} values for compounds **19** and **28** in the *E. coli* JLD271 reporter strain are shown below. Error bars, SEM of n ≥ 3 trials.

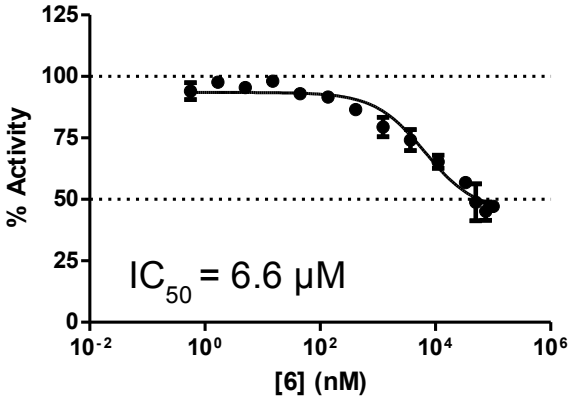


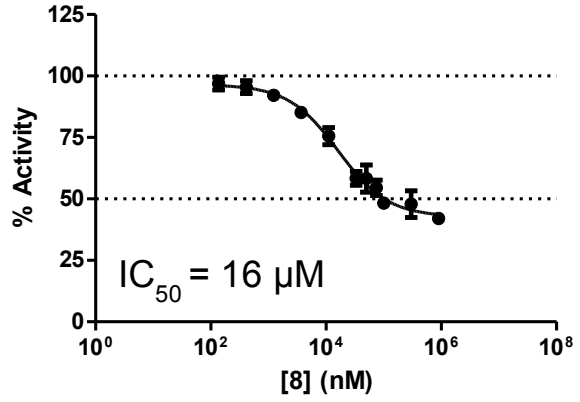


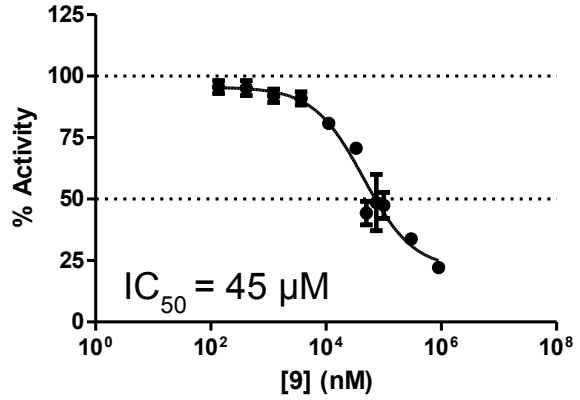
LasR antagonism dose response curves and IC_{50} values for active hybrid compounds in the *E. coli* JLD271 reporter strain are shown below. In the case where non-monotonic behavior was observed, two curves are shown; the left curve incorporates all data points measured, while the right curve incorporates only data points where LasR inhibition was noted. Compounds were screened against 5 nM OdDHL. IC_{50} values were calculated from the plots on right. Error bars, SEM of n ≥ 3 trials.

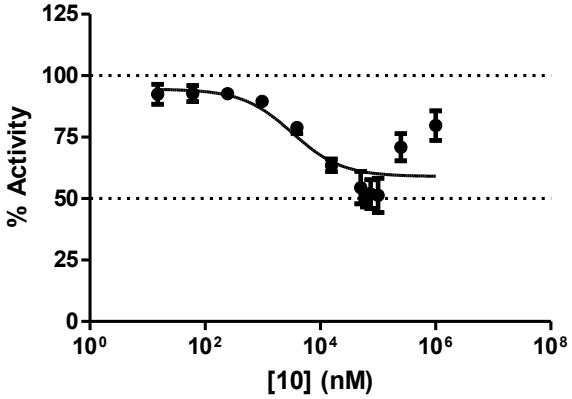


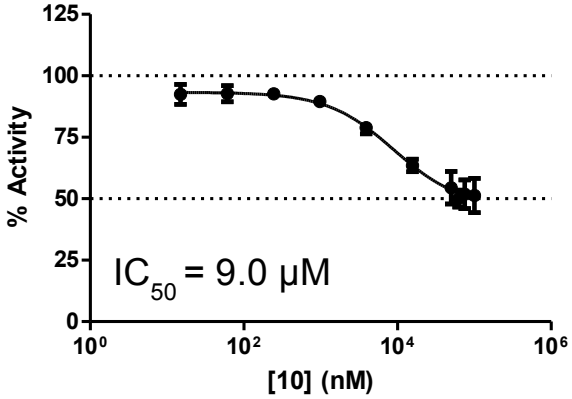


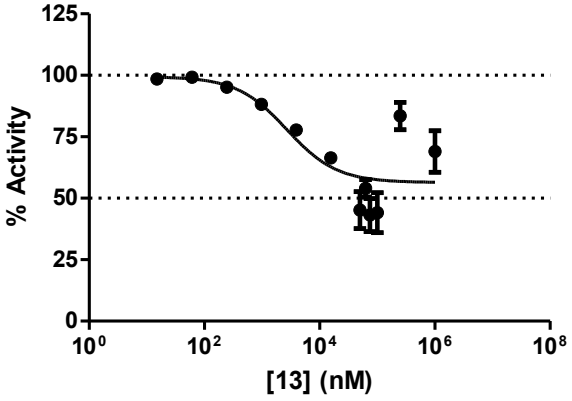


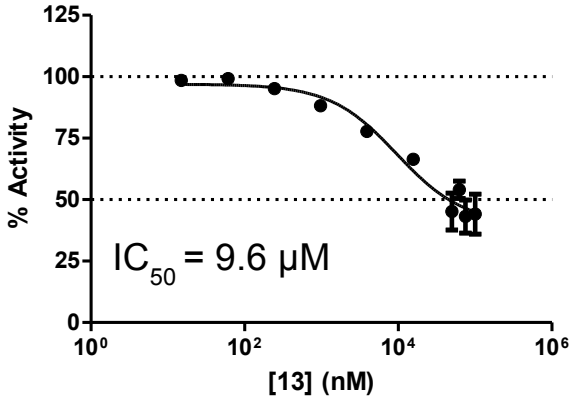


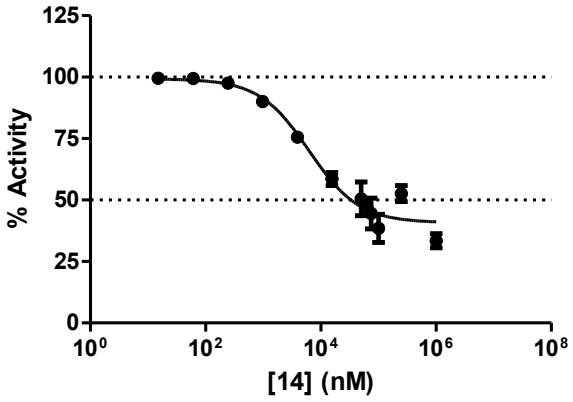

% Activity
125
100
75
50
25
0
IC50 = 45 µM
10^0
10^2
10^4
10^6
10^8
[9] (nM)

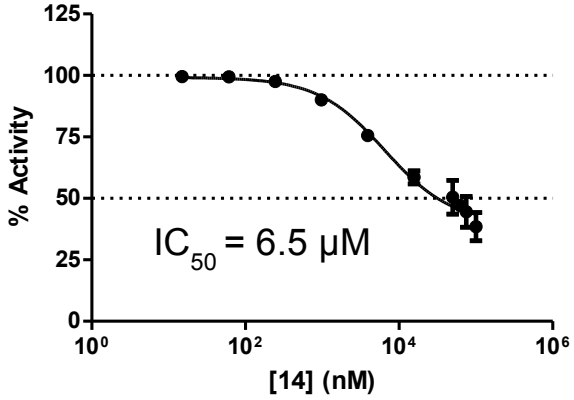

% Activity
125
100
75
50
25
0
10^0
10^2
10^4
10^6
10^8
[10] (nM)

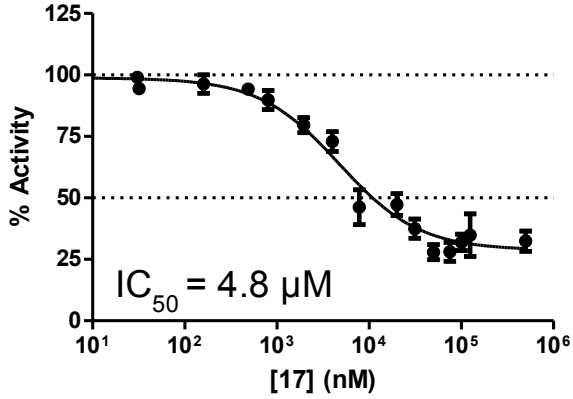

% Activity
125
100
75
50
25
0
IC50 = 9.0 µM
10^0
10^2
10^4
10^6
[10] (nM)

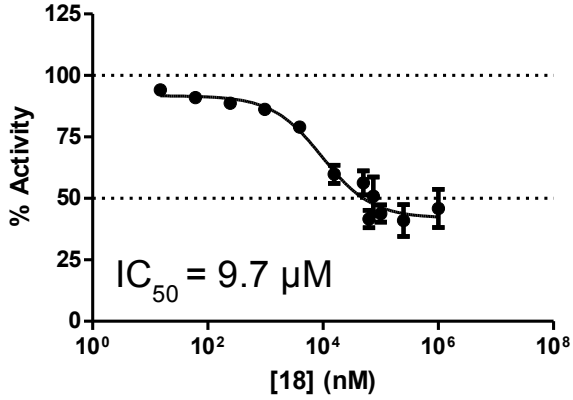

% Activity
125
100
75
50
25
0
10^0
10^2
10^4
10^6
10^8
[13] (nM)

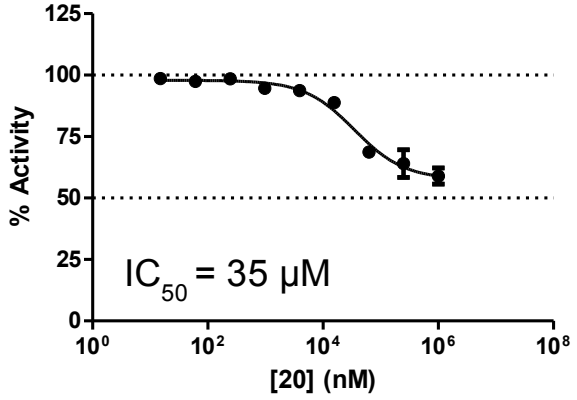

% Activity
125
100
75
50
25
0
IC50 = 9.6 µM
10^0
10^2
10^4
10^6
[13] (nM)

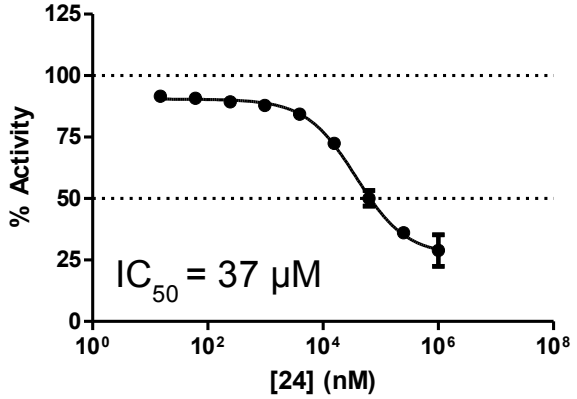

125
100
75
50
25
0
% Activity
10^0
10^2
10^4
10^6
10^8
[14] (nM)

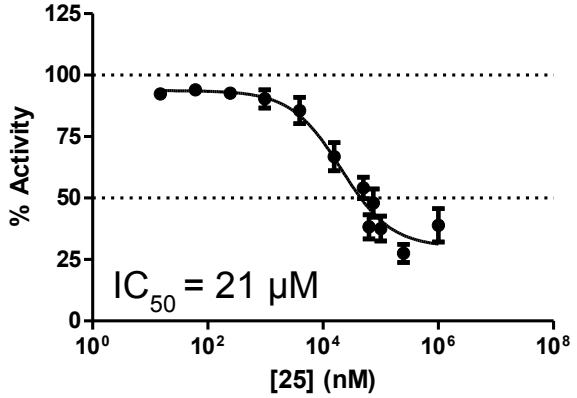

125
100
75
50
25
0
% Activity
IC_{50} = 6.5 µM
10^0
10^2
10^4
10^6
[14] (nM)

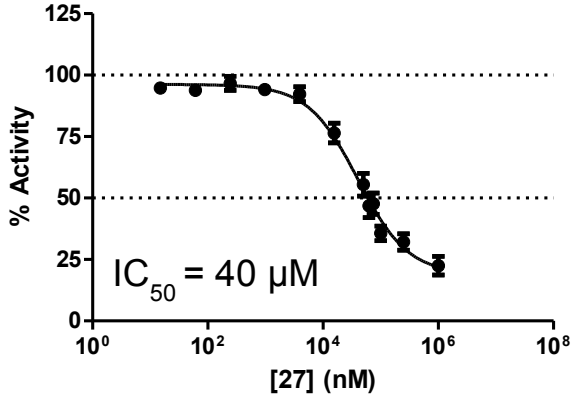

125
100
75
50
25
0
% Activity
IC_{50} = 4.8 µM
10^1
10^2
10^3
10^4
10^5
10^6
[17] (nM)

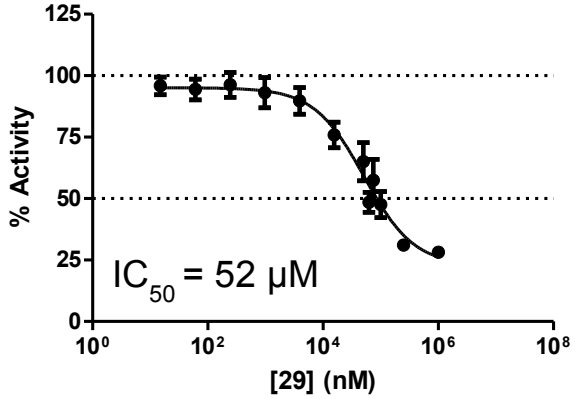

125
100
75
50
25
0
% Activity
IC_{50} = 9.7 µM
10^0
10^2
10^4
10^6
10^8
[18] (nM)


125
100
75
50
25
0
% Activity
IC50 = 35 μM
10^0
10^2
10^4
10^6
10^8
[20] (nM)


125
100
75
50
25
0
% Activity
IC50 = 37 μM
10^0
10^2
10^4
10^6
10^8
[24] (nM)

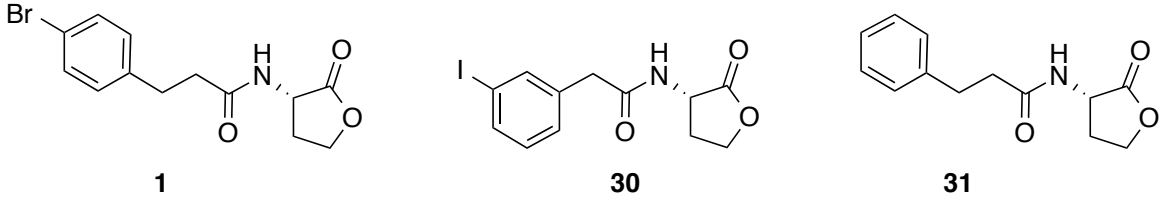

125
100
75
50
25
0
% Activity
IC50 = 21 μM
10^0
10^2
10^4
10^6
10^8
[25] (nM)


125
100
75
50
25
0
% Activity
IC50 = 40 µM
10^0
10^2
10^4
10^6
10^8
[27] (nM)

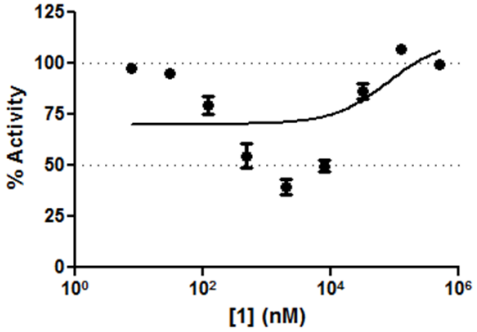

125
100
75
50
25
0
% Activity
IC50 = 52 µM
10^0
10^2
10^4
10^6
10^8
[29] (nM)

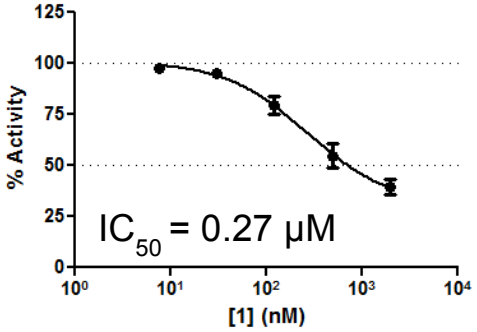
Dose response curves for AHL congeners.

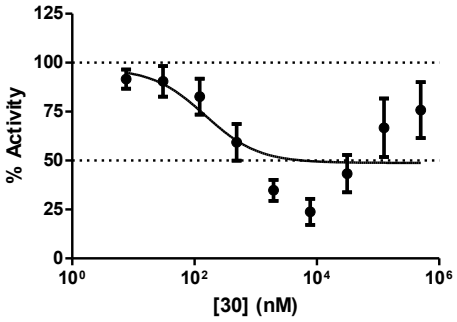
LasR antagonism dose response curves for AHLs **1**, **30**, and **31** are provided below. Methods to obtain these dose curves and IC_{50} values are analogous to those for the hybrid compounds above. Two curves are shown for each AHL; the left curve incorporates all data points measured, while the right curve incorporates only data points where LasR inhibition was noted.

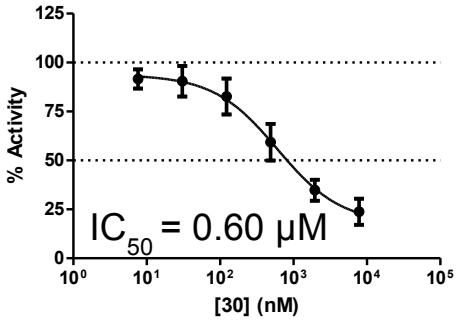


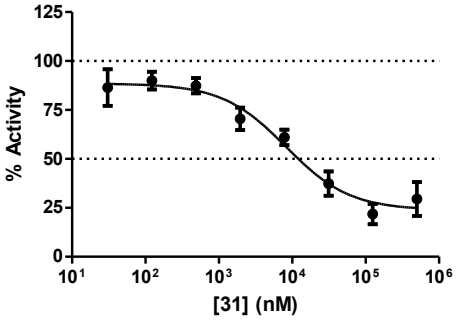
1 **30** **31**

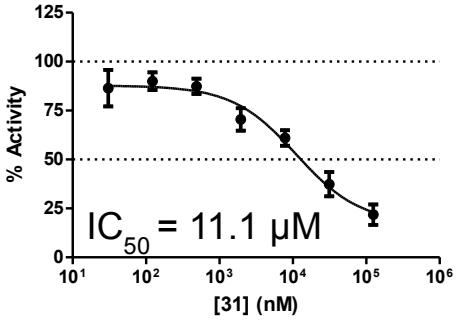












Compound stability studies.

HPLC instrumentation and method.

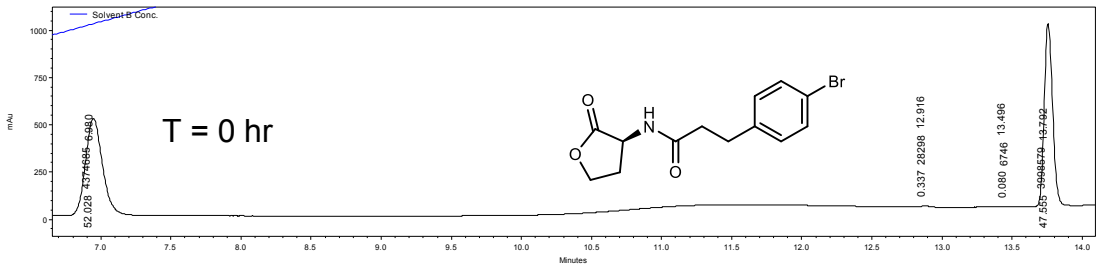
A Shimadzu high performance liquid chromatograph (HPLC) equipped with an analytical Gemini C18 column (5 μm, 4.6 mm x 250 mm, 110 Å) and a UV-vis diode array detector was used to study compound decomposition. Standard HPLC conditions were as follows: flow rate = 1 mL/min; mobile phase A = 18 MΩ water + 0.1% trifluoroacetic acid; mobile phase B = acetonitrile + 0.1% TFA. For all compounds, the method was as follows: (i) start with isocratic 15% B (3 minutes), (ii) followed by a linear gradient from 15% to 95% B (6 minutes), and (iii) end with isocratic 95% B (6 minutes).

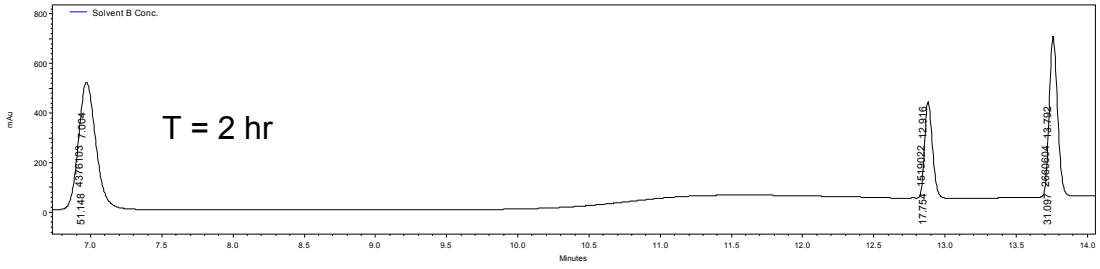
Protocol for determining compound stability.

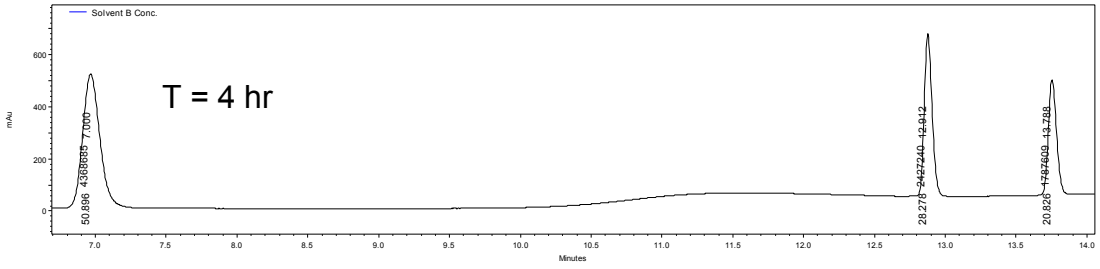
To evaluate the aqueous stabilities of the AHL-based and hybrid LasR modulators, compounds **1**, **14**, **17**, and **30** were dissolved in 2-(*N*-morpholino)ethanesulfonic acid (MES) buffer at pH 6, tris(hydroxymethyl)aminomethane (TRIS) buffer at pH 7, or TRIS buffer at pH 8 to a concentration of 50 μM (0.5% DMSO). These solutions were placed in a 37 °C incubator with shaking, and 150 μL aliquots were taken at time = 0 and (approximately) every two hours thereafter. The aliquots were immediately injected onto an HPLC, and the area under the curve (AUC) at 220 nm was compared at each time-point to measure compound decomposition. Caffeine (50 μM) was added to the samples at time = 0. This compound served as an internal standard that maintained the same AUC throughout the assay (error ≤ 1–5%). The chromatograms below show each compound at each time-point at the three different pH values. Throughout all trials, the peak at 7 minutes corresponds to caffeine, while the peak at 13.5–15 minutes at time = 0 corresponds to the compound of interest. At pH 8, caffeine's AUC varied less than 1%. At pH 7, caffeine's AUC varied less than 3%. At pH 6, caffeine's AUC varied less than 5%.

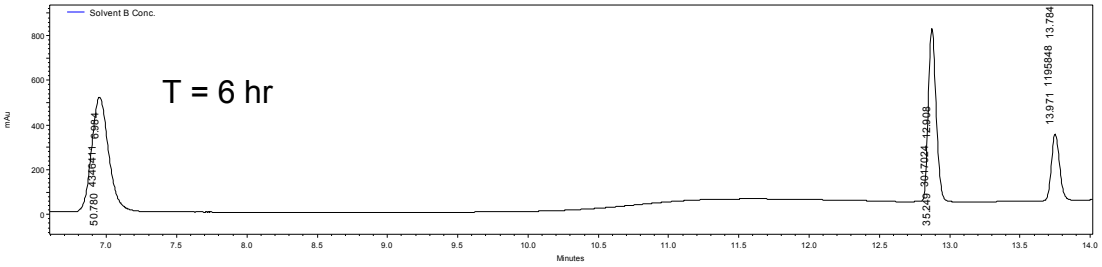
HPLC traces indicating compound stability.

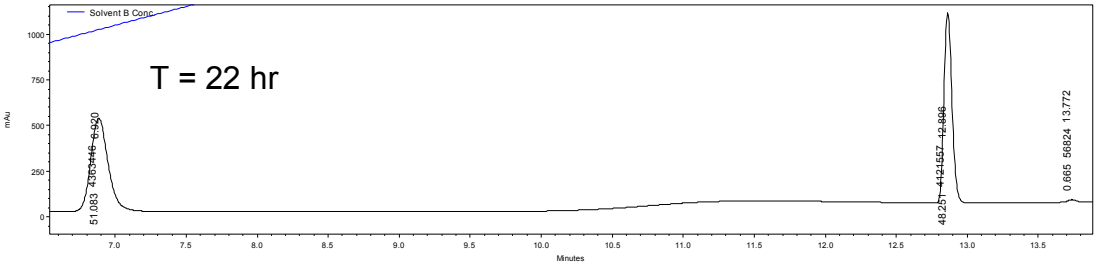
Compound **1** at pH 8.





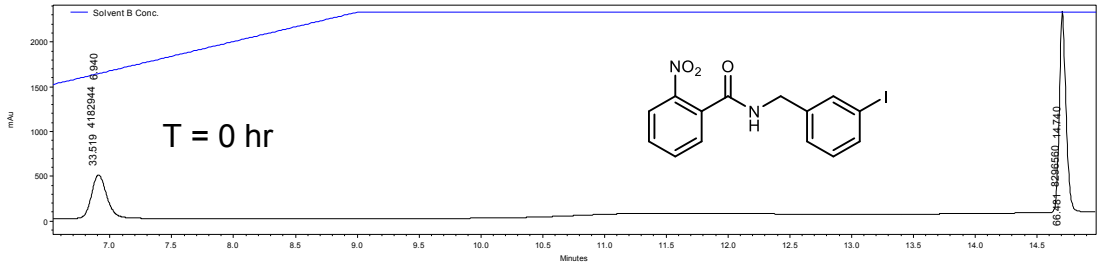


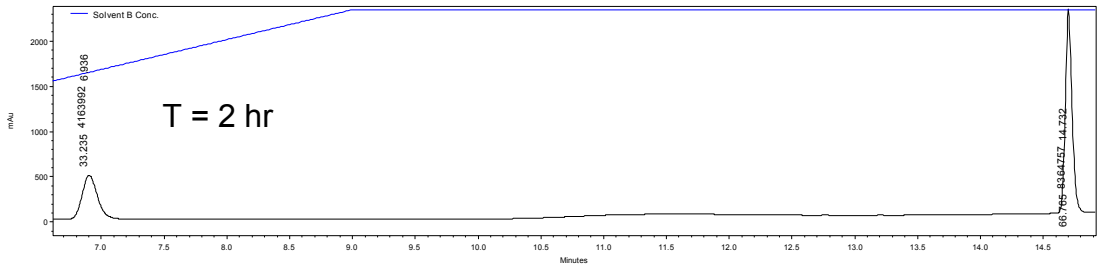


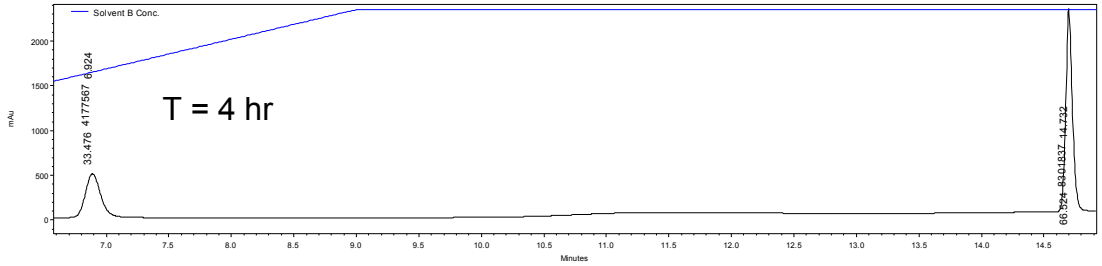


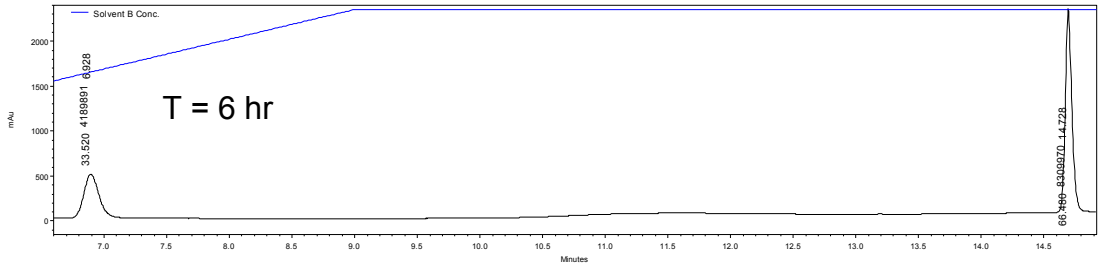
0 hours	2 hours	4 hours	6 hours	22 hours
100%	67%	45%	40%	1%

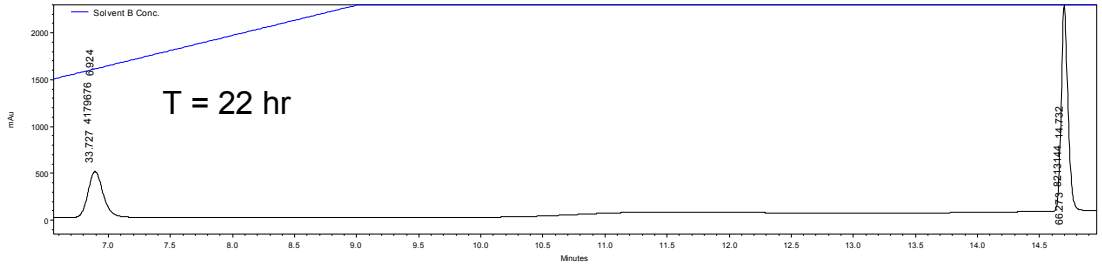
Compound **14** at pH 8.





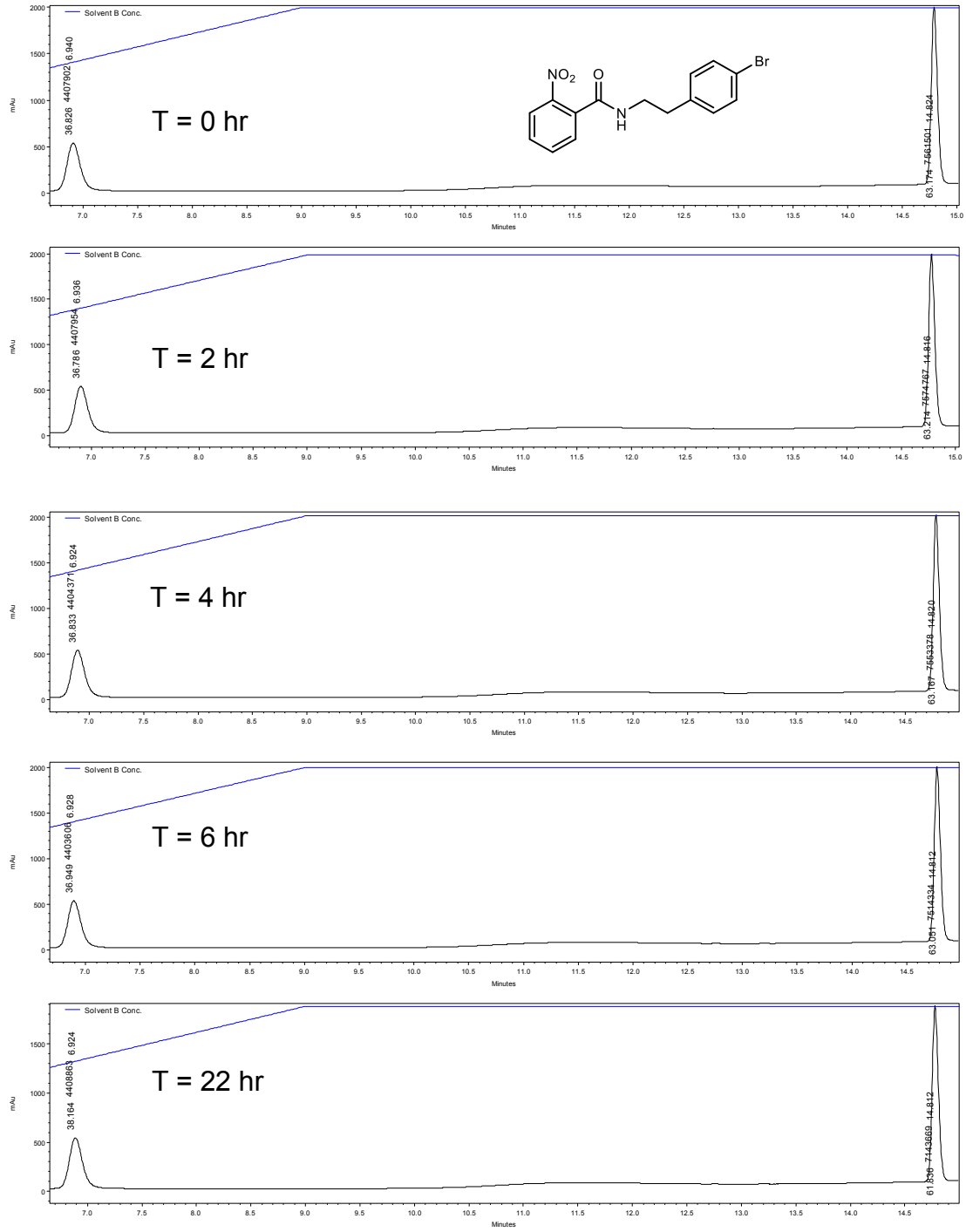






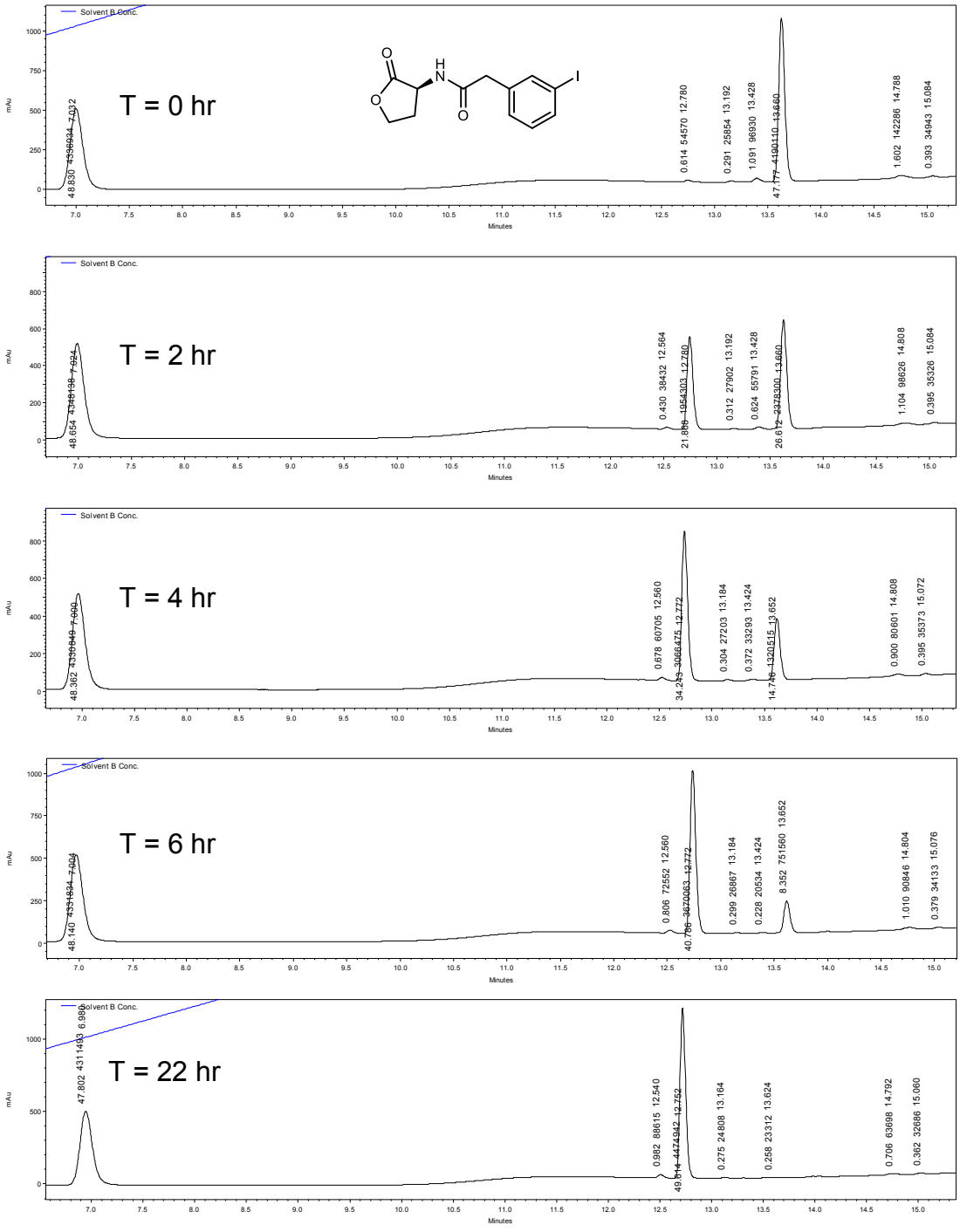
0 hours	2 hours	4 hours	6 hours	22 hours
100%	100%	100%	100%	99%

Compound **17** at pH 8.



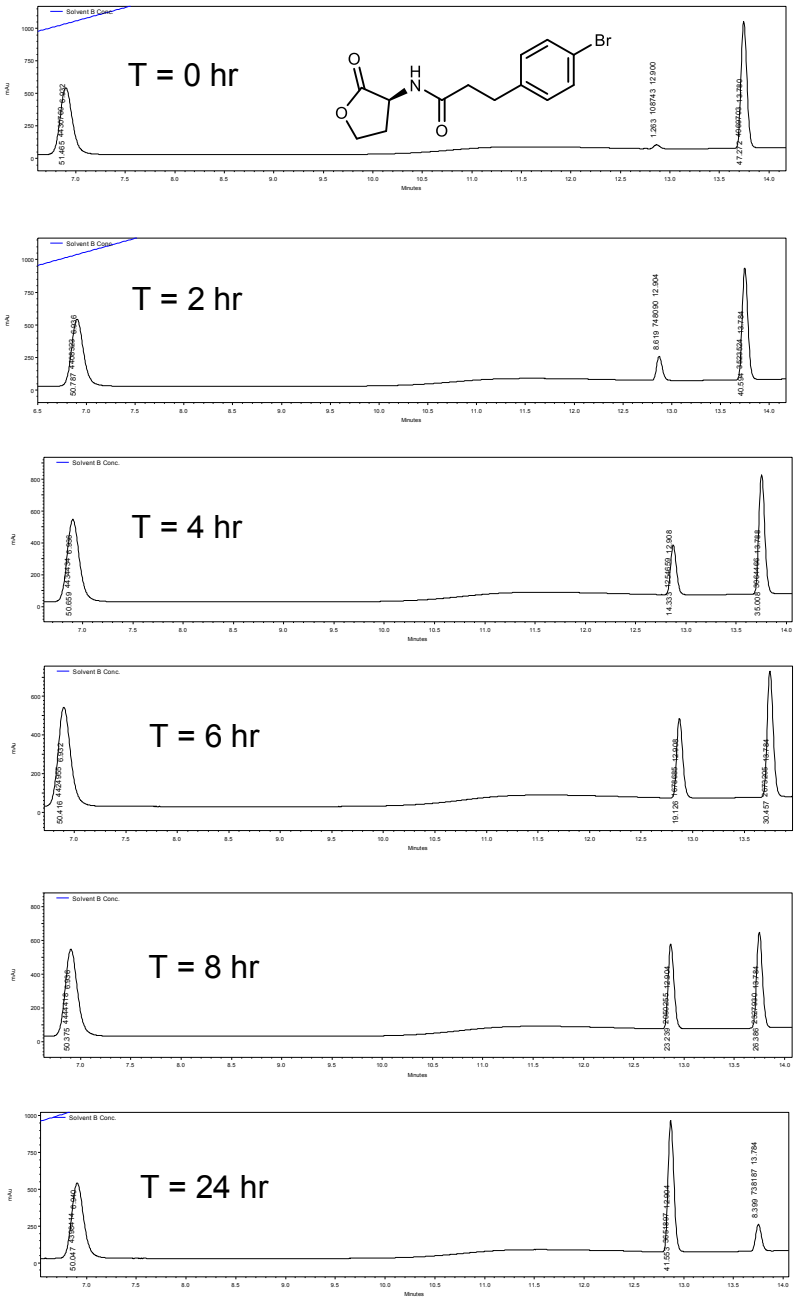
0 hours	2 hours	4 hours	6 hours	22 hours
100%	100%	100%	99%	94%

Compound **30** at pH 8.



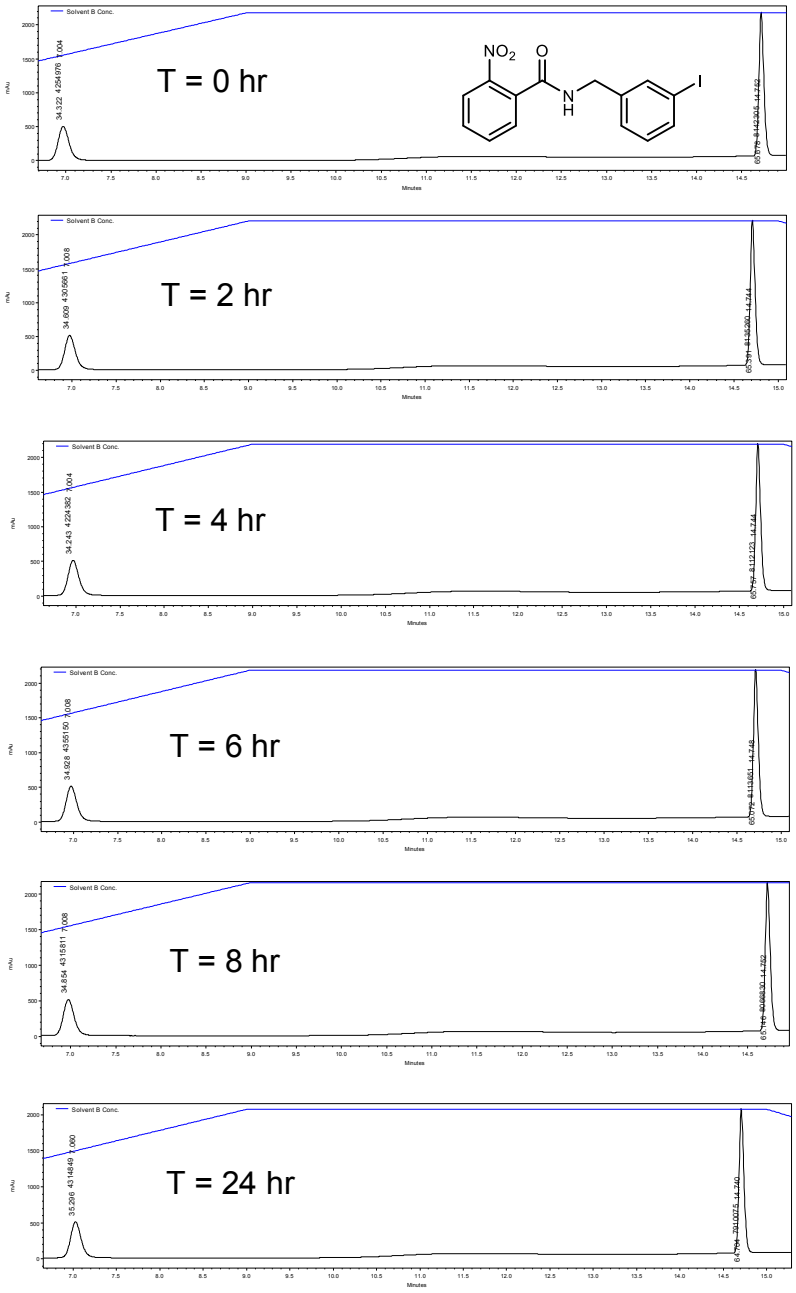
0 hours	2 hours	4 hours	6 hours	22 hours
100%	57%	32%	18%	0%

Compound **1** at pH 7.



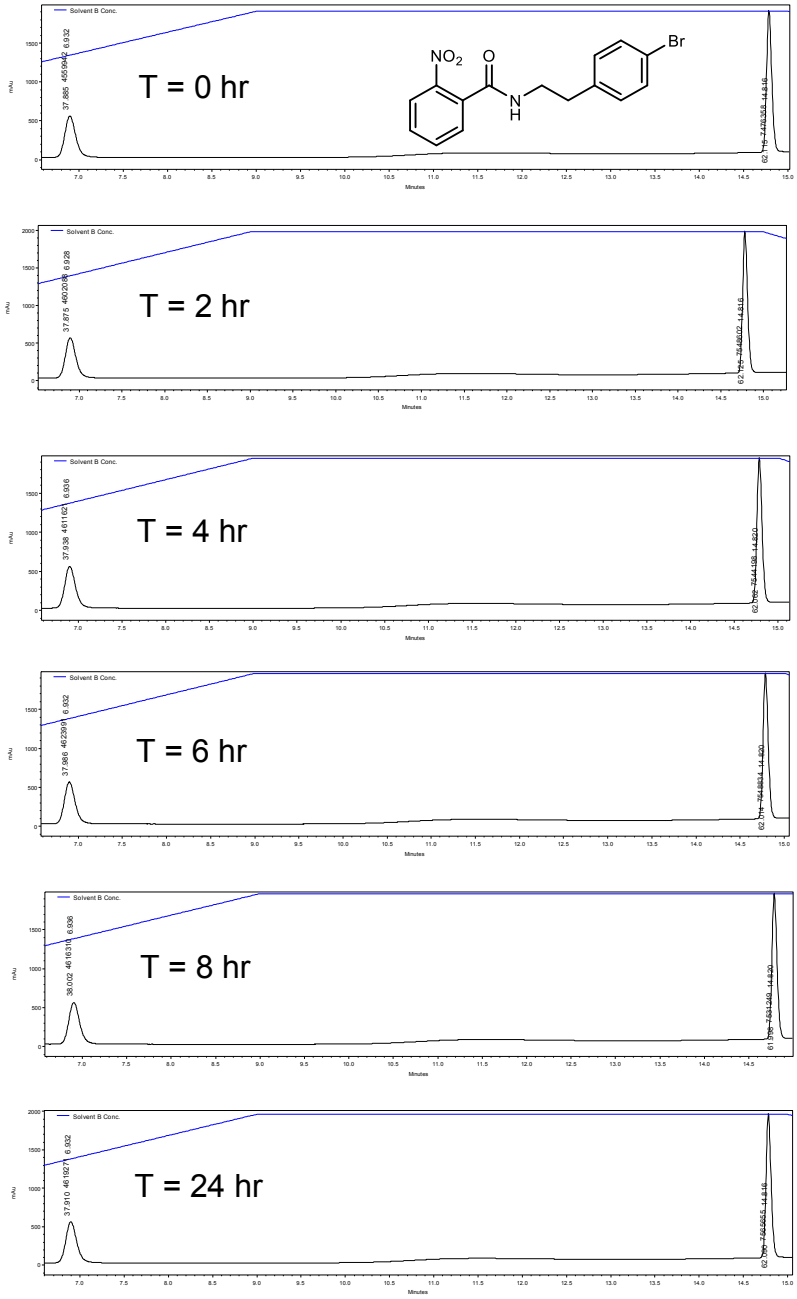
0 hours	2 hours	4 hours	6 hours	8 hours	24 hours
100%	86%	75%	66%	57%	18%

Compound **14** at pH 7.



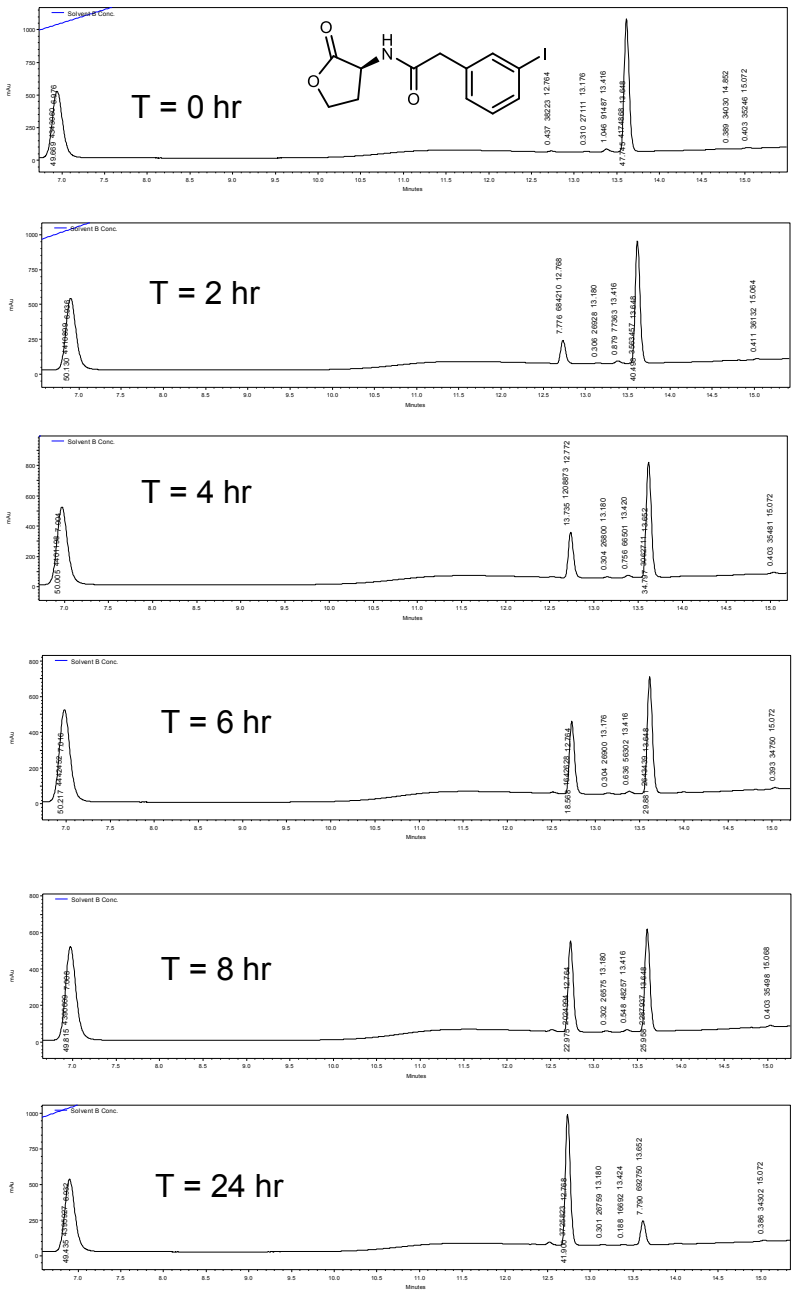
0 hours	2 hours	4 hours	6 hours	8 hours	24 hours
100%	100%	100%	100%	99%	97%

Compound **17** at pH 7.



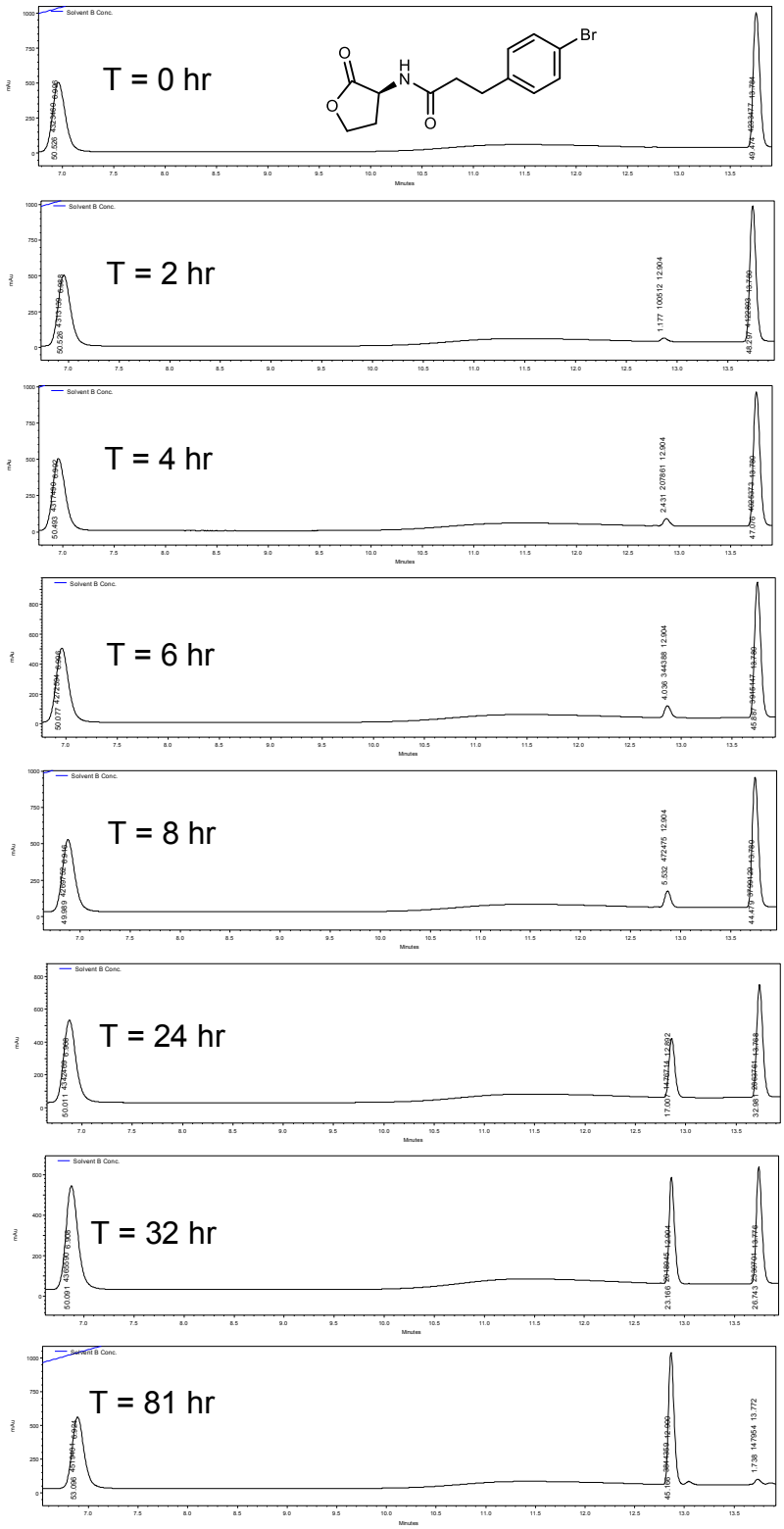
0 hours	2 hours	4 hours	6 hours	8 hours	24 hours
100%	100%	100%	100%	100%	100%

Compound **30** at pH 7.



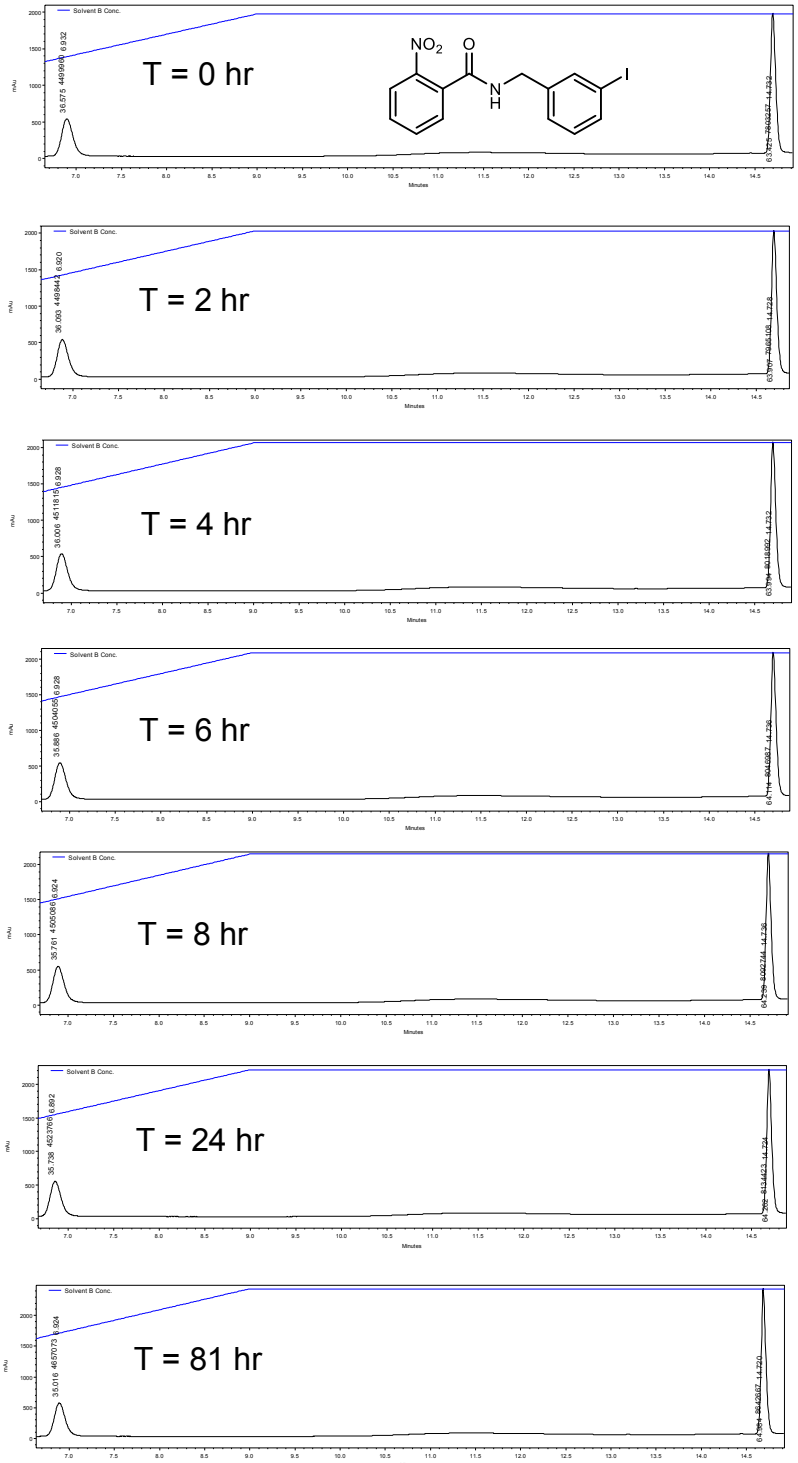
0 hours	2 hours	4 hours	6 hours	8 hours	24 hours
100%	85%	73%	63%	54%	17%

Compound **1** at pH 6.



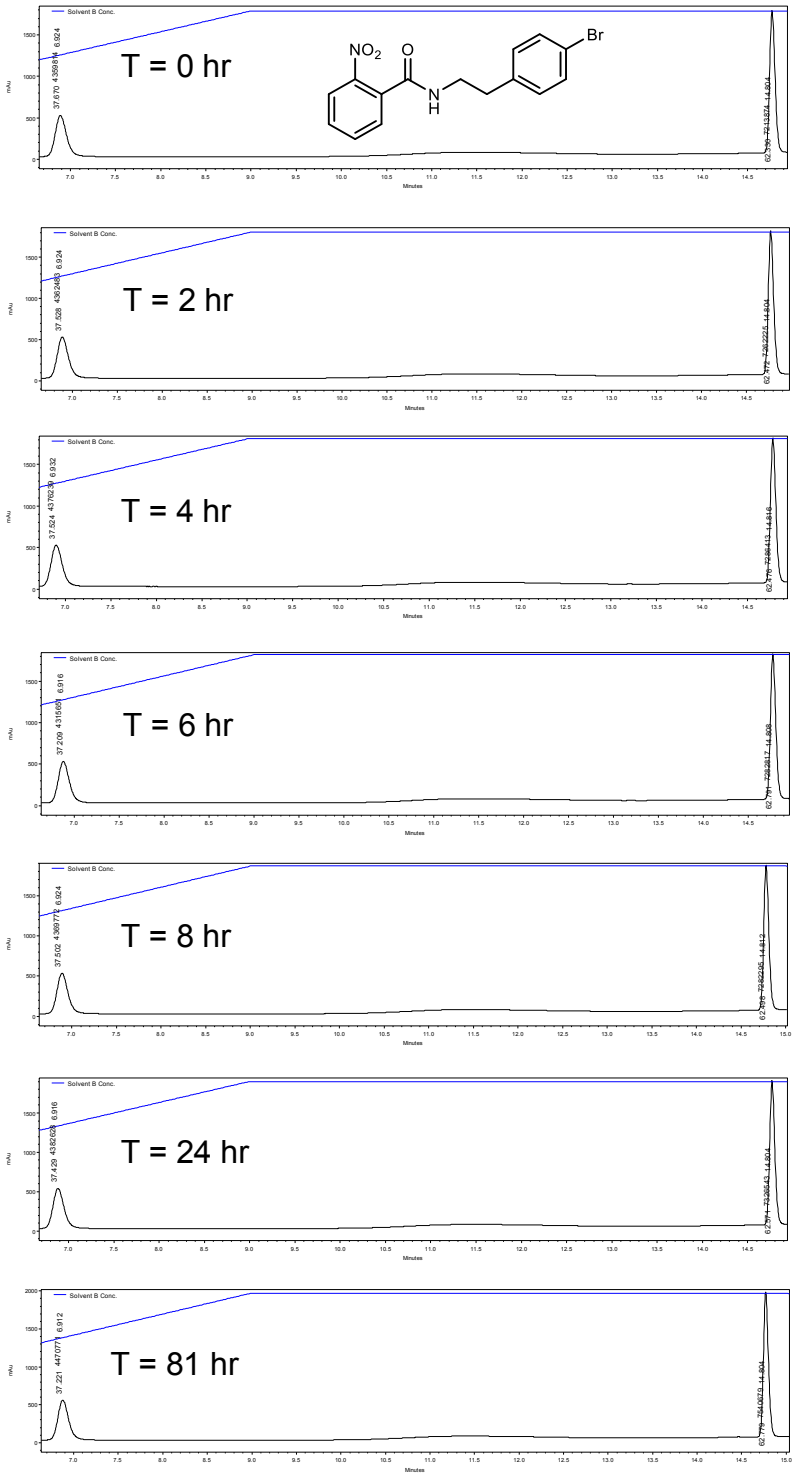
0 hours	2 hours	4 hours	6 hours	8 hours	24 hours	32 hours	81 hours
100%	97%	95%	92%	90%	67%	55%	3%

Compound **14** at pH 6.



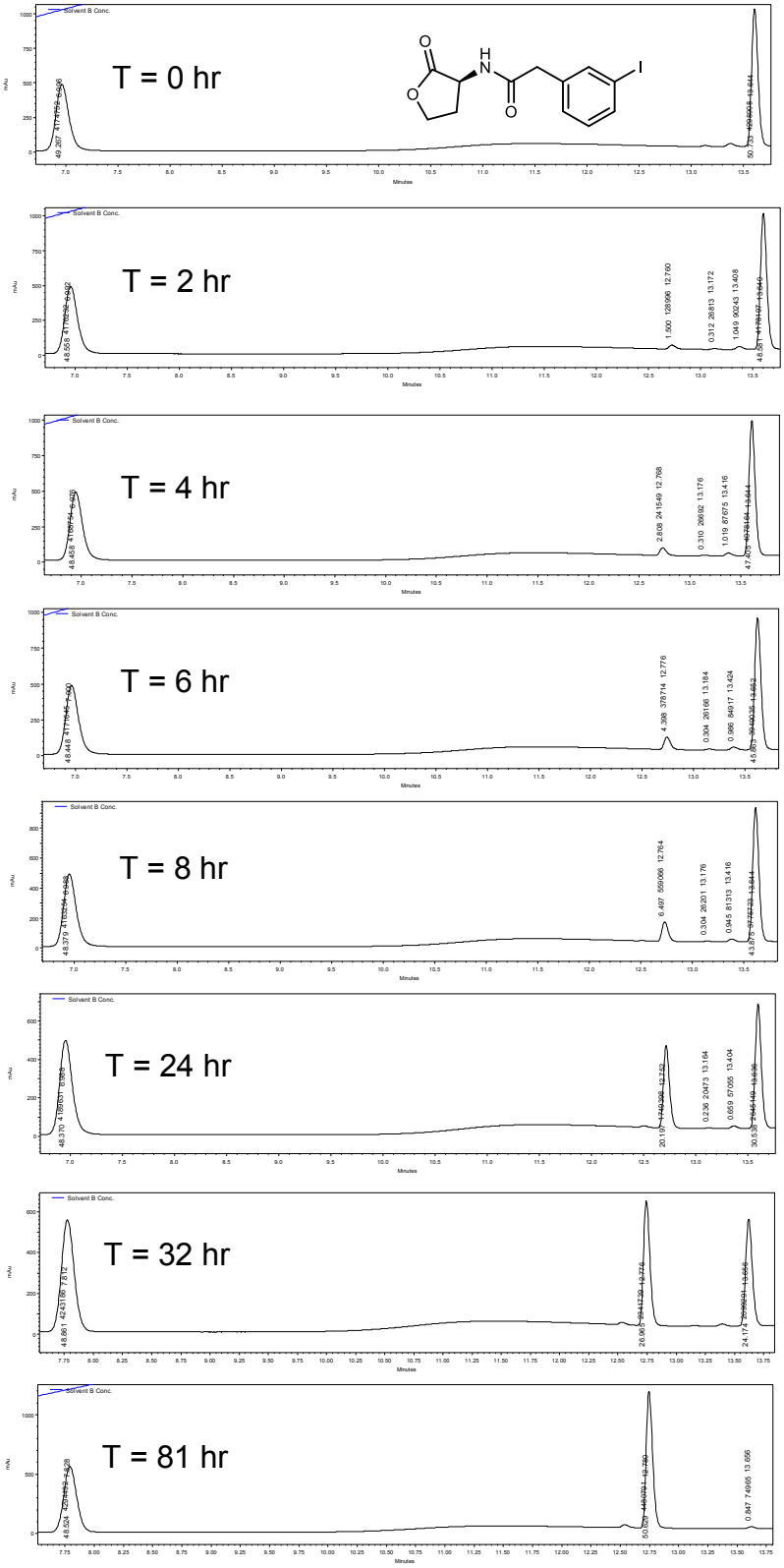
0 hours	2 hours	4 hours	6 hours	8 hours	24 hours	81 hours
100%	100%	100%	100%	100%	100%	100%

Compound **17** at pH 6.



0 hours	2 hours	4 hours	6 hours	8 hours	24 hours	81 hours
100%	100%	100%	100%	100%	100%	100%

Compound **30** at pH 6.



0 hours	2 hours	4 hours	6 hours	8 hours	24 hours	32 hours	81 hours
100%	97%	95%	92%	88%	61%	49%	2%

References.

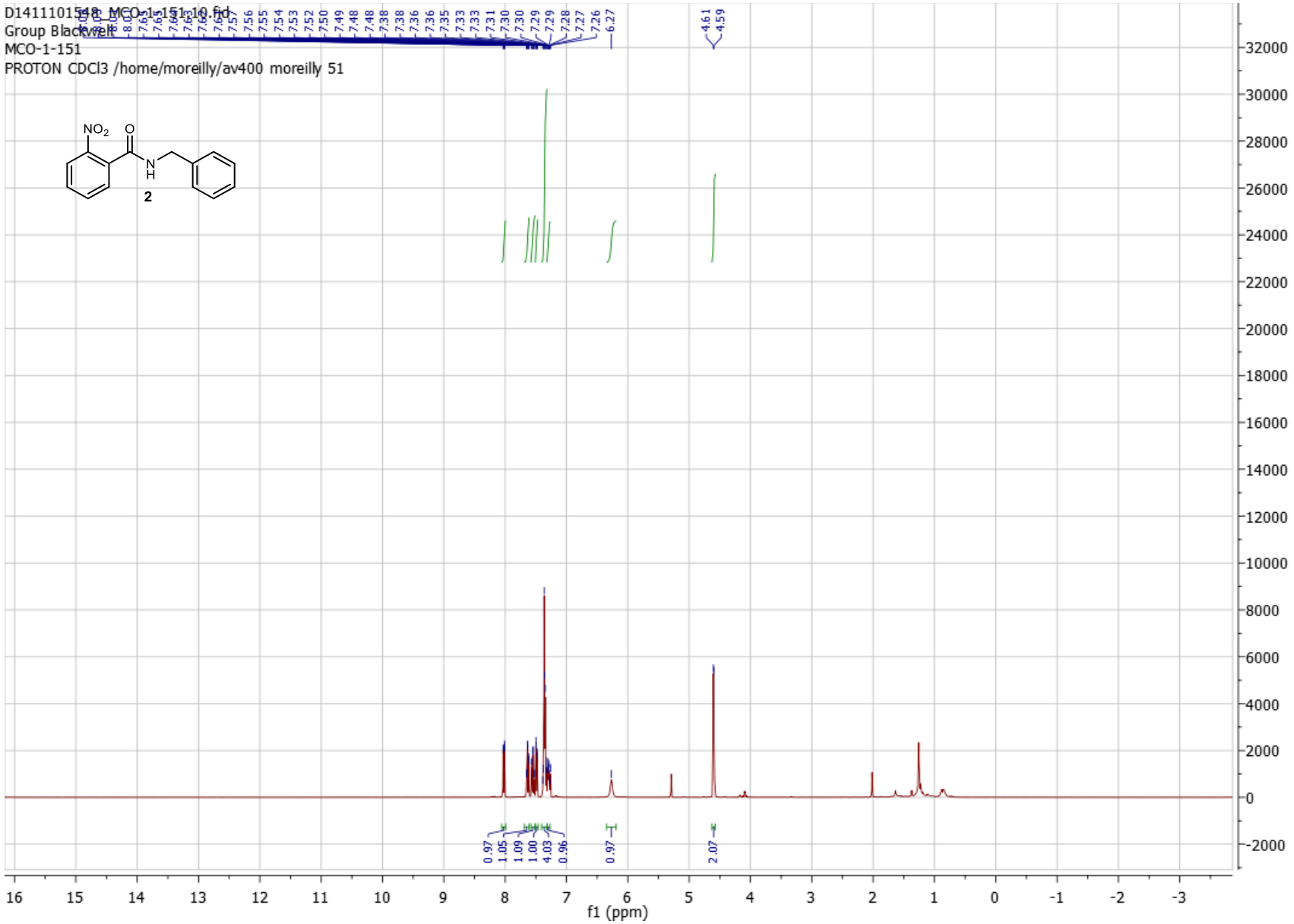
(1) Lindsay, A.; Ahmer, B. M. M. *J. Bacteriol.* **2005**, *187*, 5054–5058.

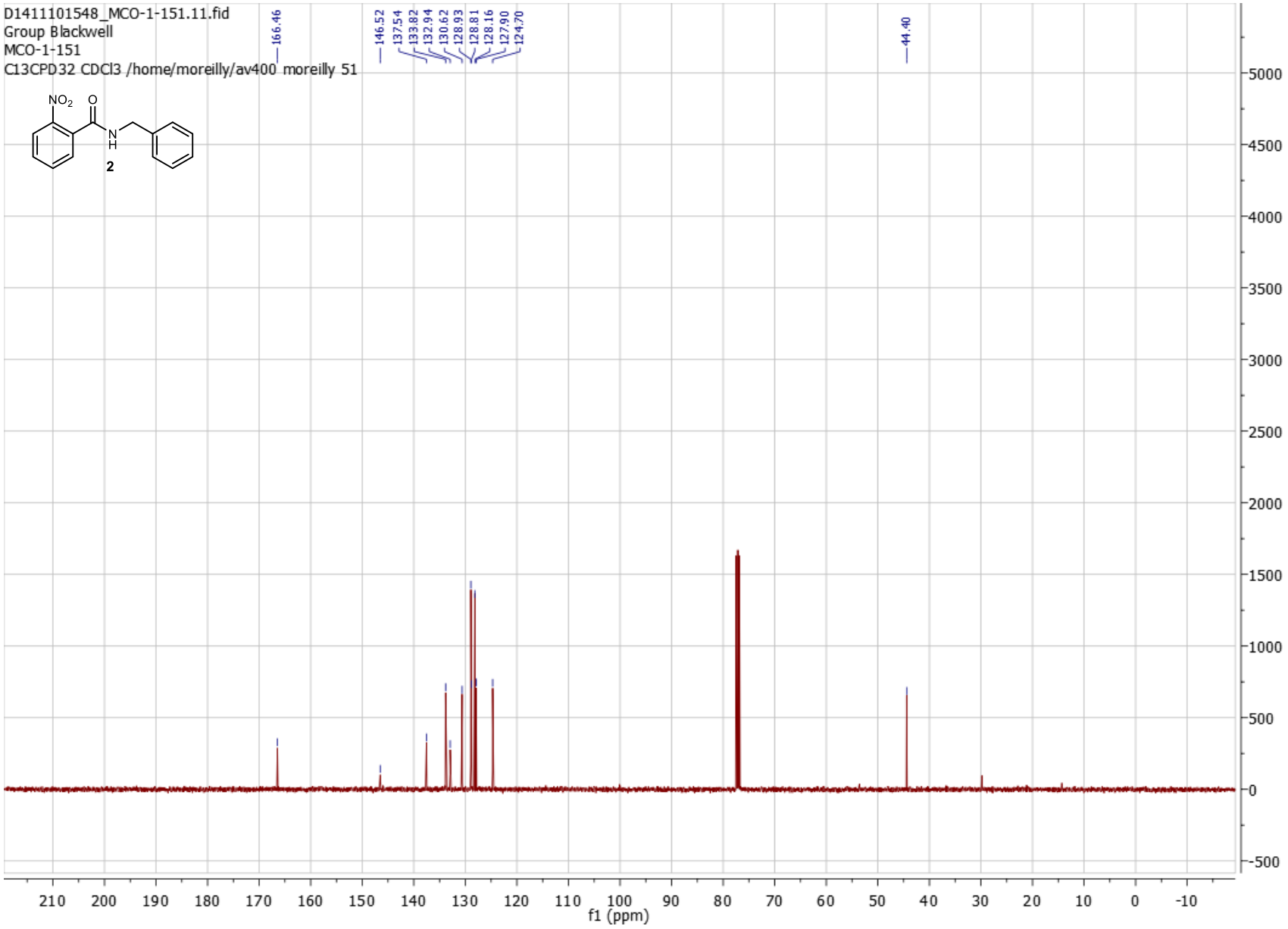
(2) Chugani, S. A; Whiteley, M.; Lee, K. M.; D'Argenio, D.; Manoil, C.; Greenberg, E. P. *Proc. Natl. Acad. Sci. U. S. A.* **2001**, *98*, 2752–2757.

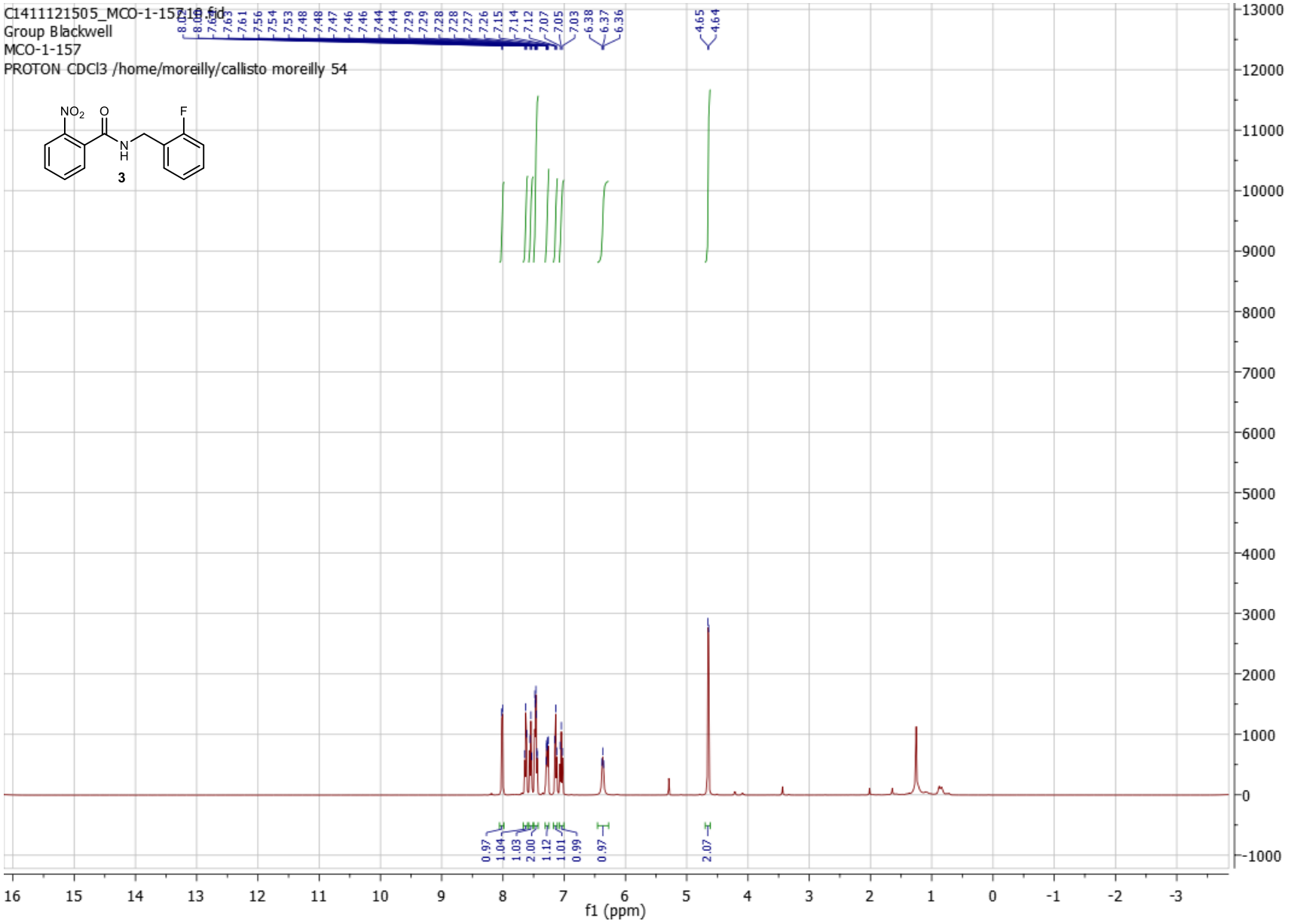
(3) Lee, J.-H.; Lequette, Y.; Greenberg, E. P. *Mol. Microbiol.* **2006**, *59*, 602–609.

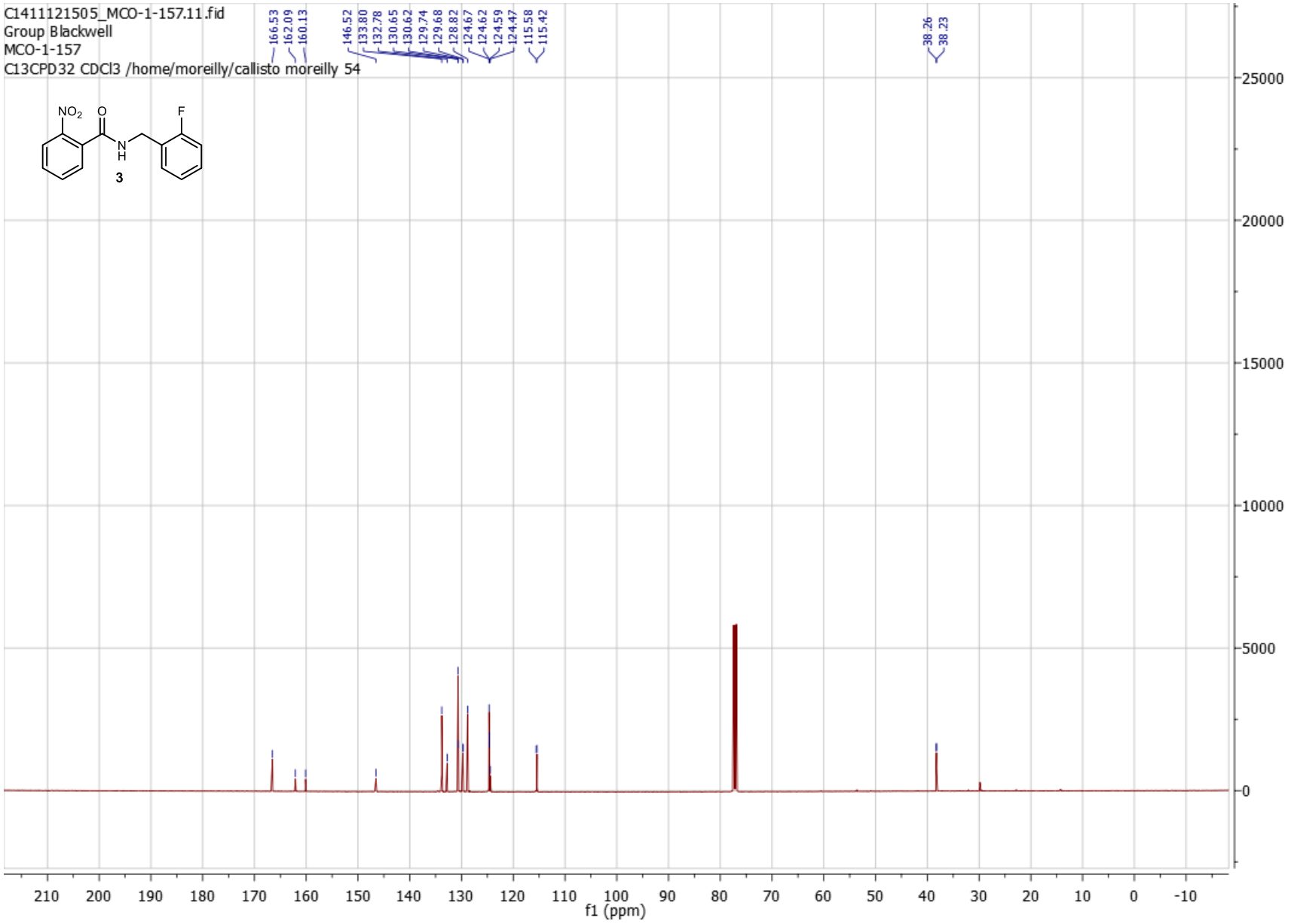
(4) Griffith, K. L.; Wolf, R. E. *Biochem. Biophys. Res. Commun.* **2002**, *290*, 397–402.

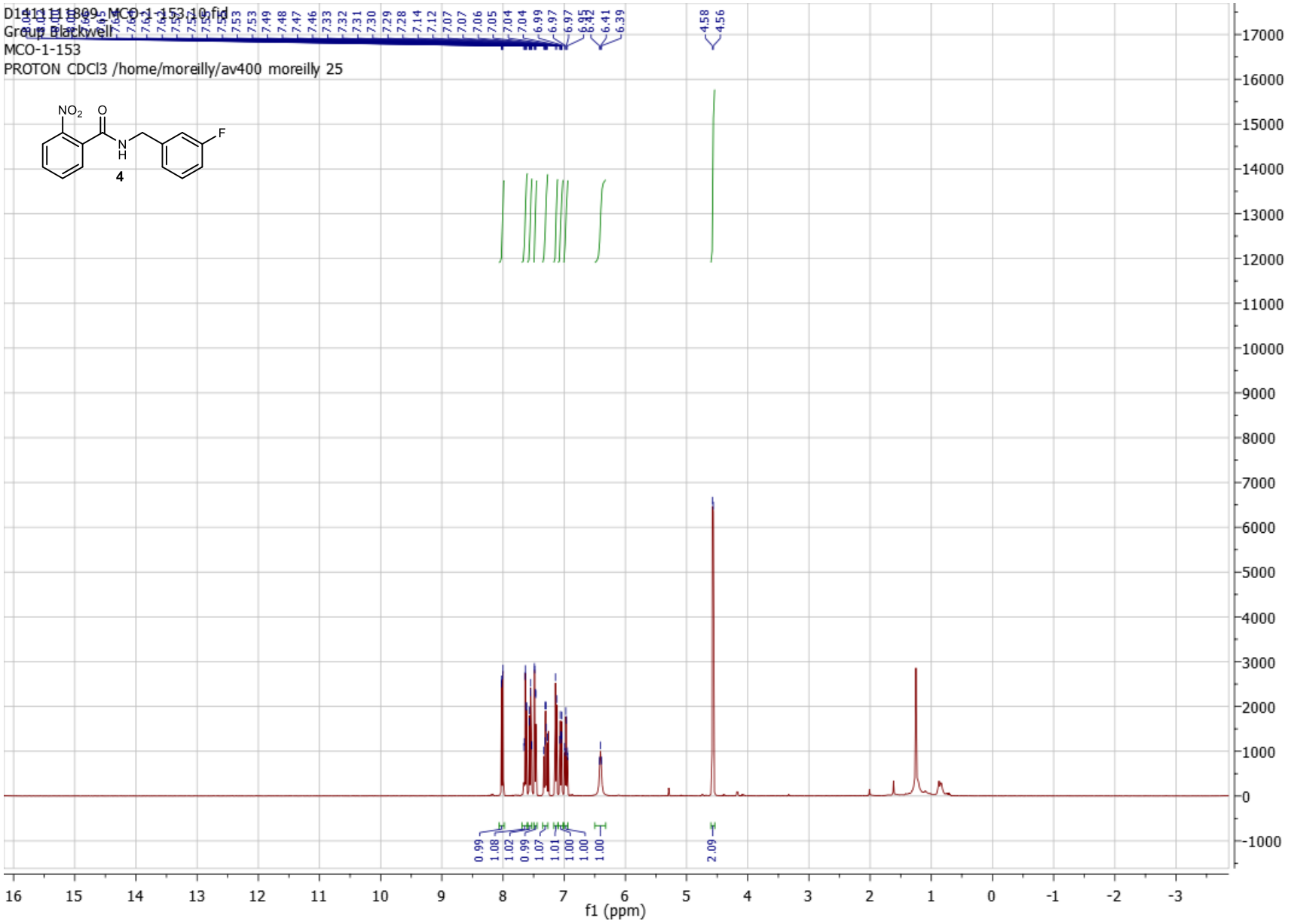
NMR SPECTRA

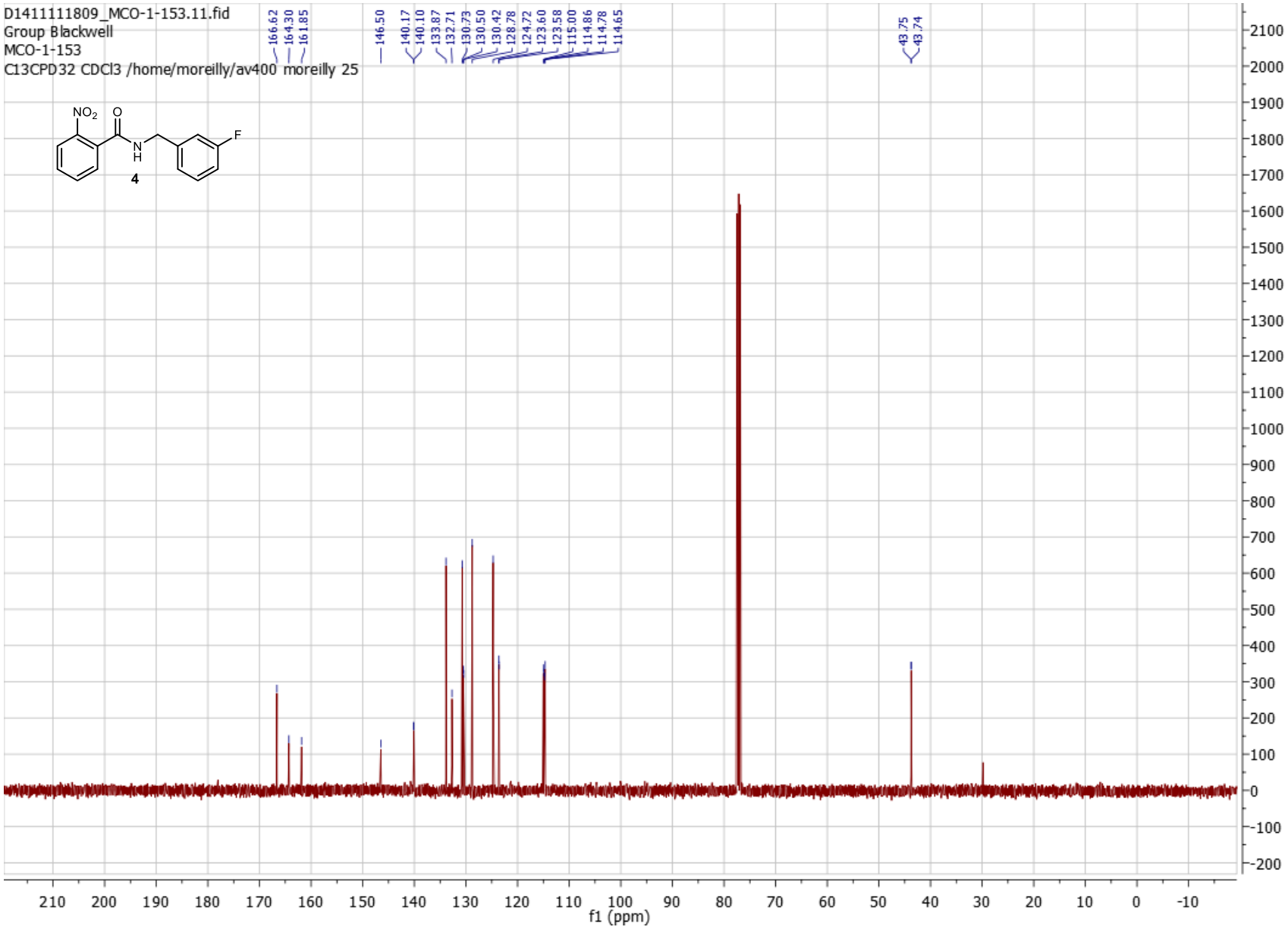

D1411101548 MCO-1-151-10.fid
Group Blackwell
MCO-1-151
PROTON CDCl3 /home/moreilly/av400 moreilly 51
NO2
O
N
H
2
f1 (ppm)

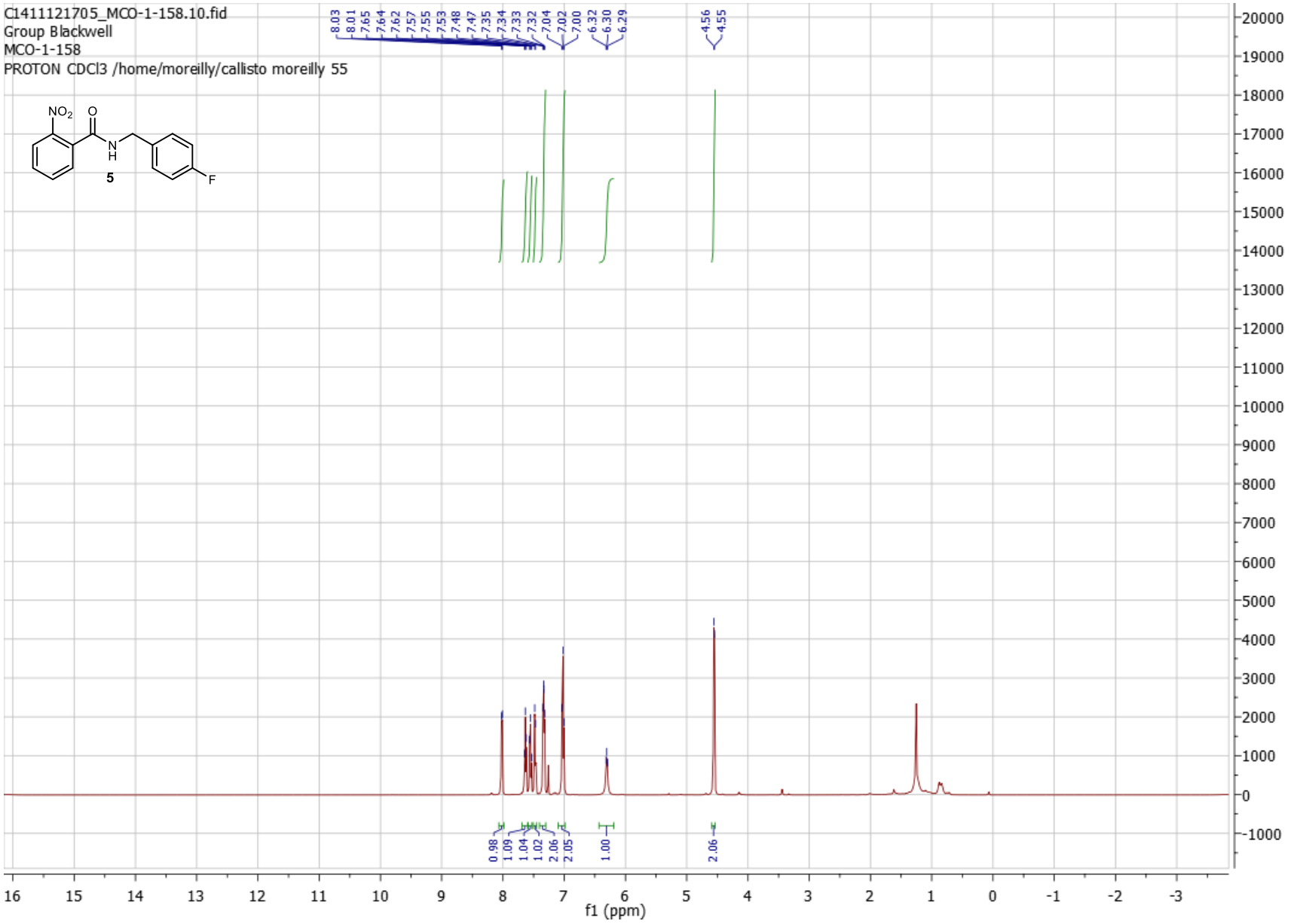

D1411101548_MCO-1-151.11.fid
Group Blackwell
MCO-1-151
C13CPD32 CDCl3 /home/moreilly/av400 moreilly 51
166.46
146.52
137.54
133.82
132.94
130.62
128.93
128.81
128.16
127.90
124.70
44.40
NO2
O
N
H
2
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

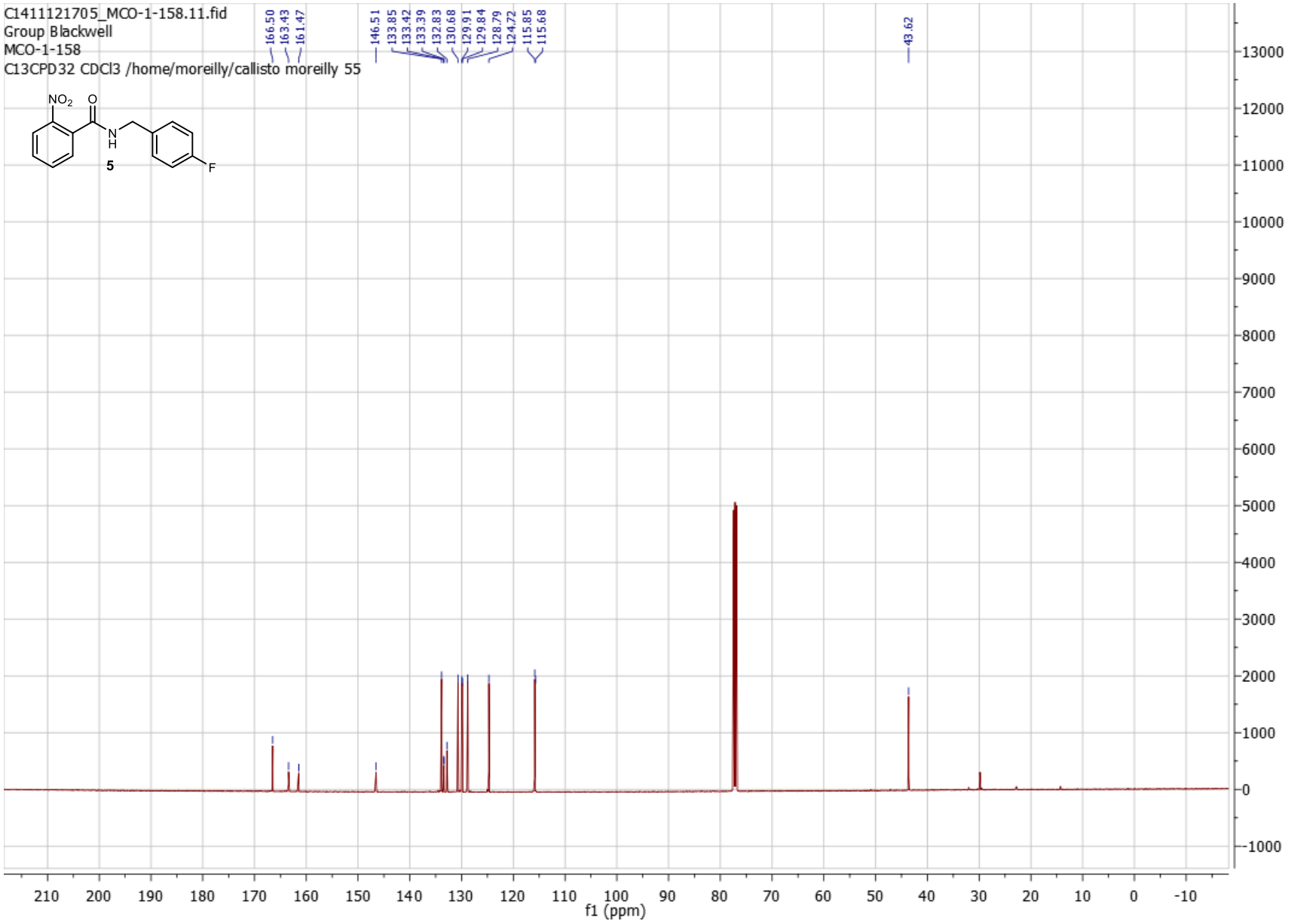

C1411121505_MCO-1-157_1H.fid
Group Blackwell
MCO-1-157
PROTON CDCl3 /home/moreilly/callisto moreilly 54
NO2
O
F
N
H
3
8.02
8.00
7.63
7.61
7.56
7.54
7.53
7.48
7.48
7.47
7.46
7.46
7.44
7.44
7.29
7.29
7.28
7.28
7.27
7.26
7.15
7.14
7.12
7.07
7.05
7.03
6.38
6.37
6.36
4.65
4.64
0.97
1.04
1.03
2.00
1.12
1.01
0.99
0.97
2.07
f1 (ppm)

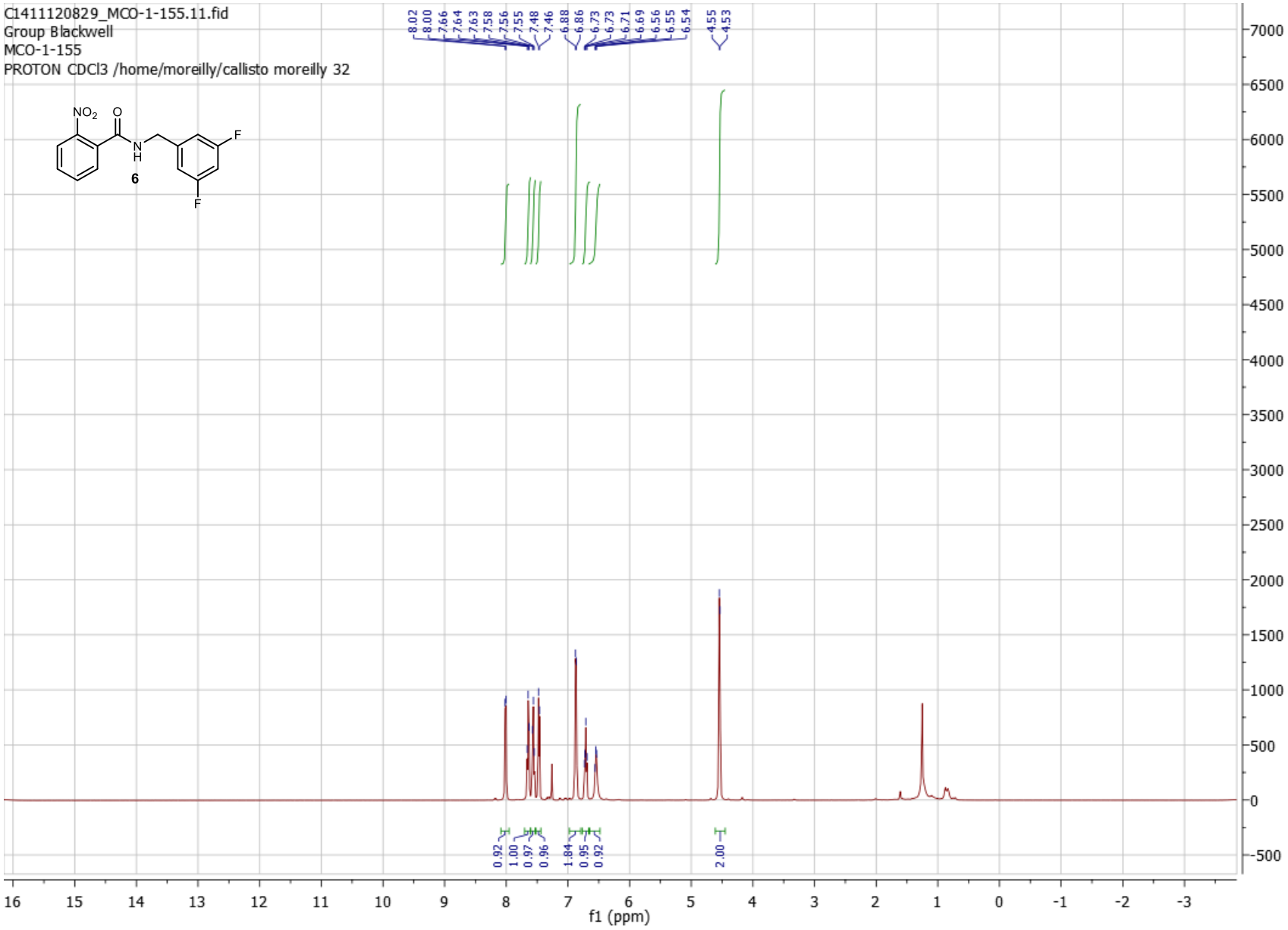

C1411121505_MCO-1-157.11.fid
Group Blackwell
MCO-1-157
C13CPD32 CDCl3 /home/moreilly/callisto moreilly 54
166.53
162.09
160.13
146.52
133.80
132.78
130.65
130.62
129.74
129.68
128.82
124.67
124.62
124.59
124.47
115.58
115.42
38.26
38.23
NO2
O
F
N
H
3
25000
20000
15000
10000
5000
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

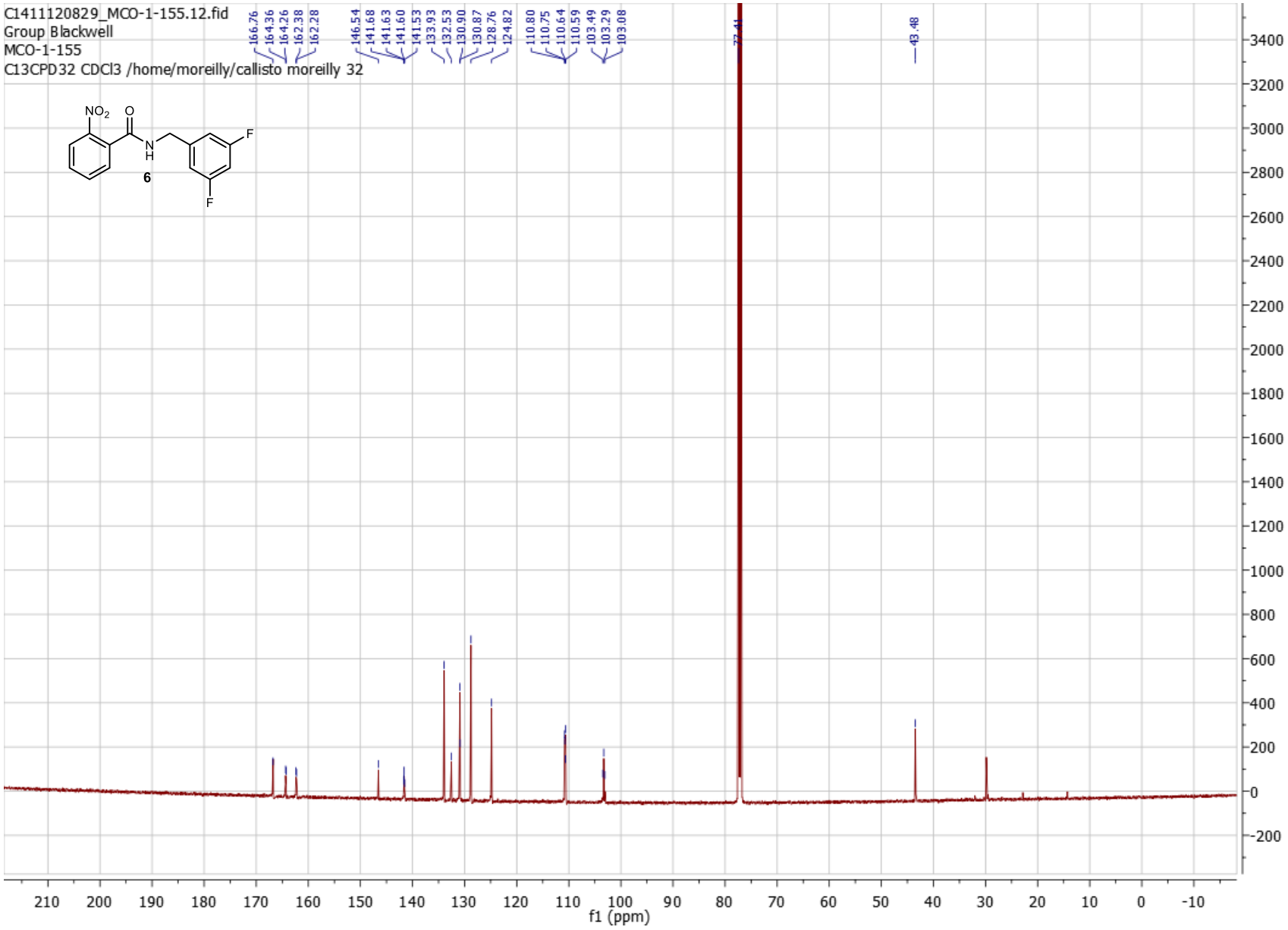

D141111809_MCO-1-153-10.fid
Group Blackwell
MCO-1-153
PROTON CDCl3 /home/moreilly/av400 moreilly 25
NO2
O
N
H
F
4
f1 (ppm)

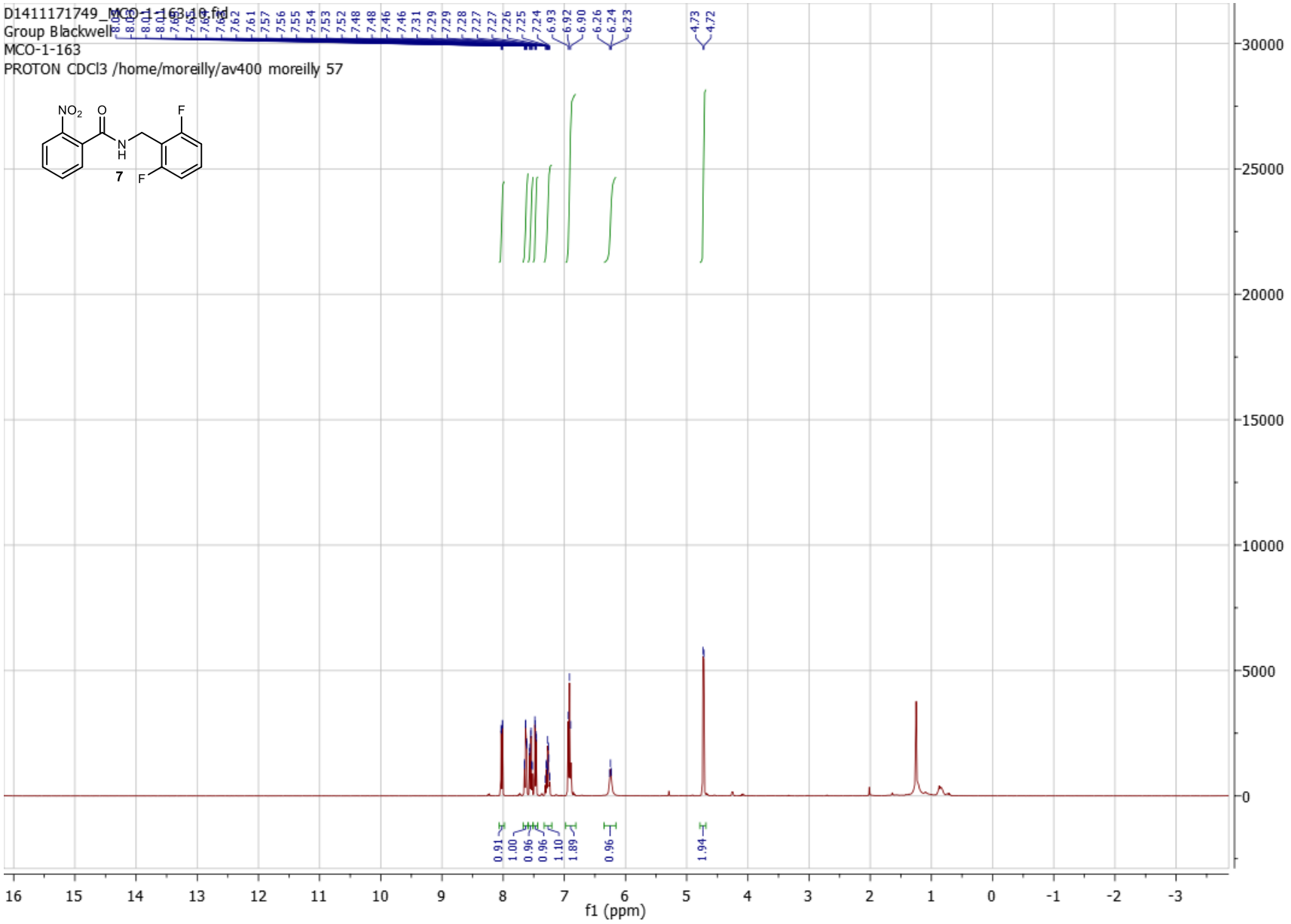

D1411111809_MCO-1-153.11.fid
Group Blackwell
MCO-1-153
C13CPD32 CDCl3 /home/moreilly/av400 moreilly 25
166.62
164.30
161.85
146.50
140.17
140.10
133.87
132.71
130.73
130.50
130.42
128.78
124.72
123.60
123.58
115.00
114.86
114.78
114.65
43.75
43.74
NO2
O
N
H
F
4
f1 (ppm)

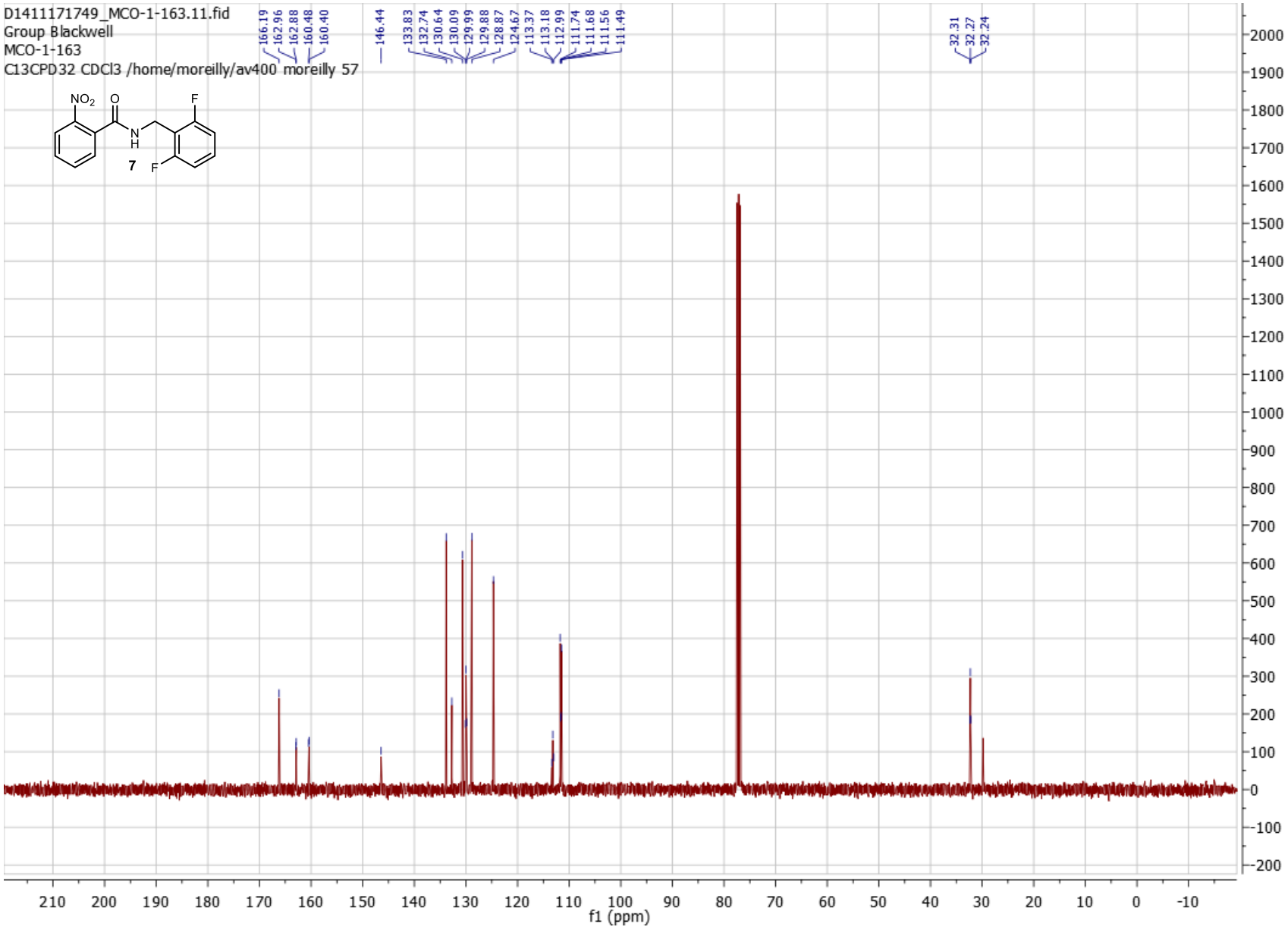

C1411121705_MCO-1-158.10.fid
Group Blackwell
MCO-1-158
PROTON CDCl3 /home/moreilly/callisto moreilly 55
8.03
8.01
7.65
7.64
7.62
7.57
7.55
7.53
7.48
7.47
7.35
7.34
7.33
7.32
7.04
7.02
7.00
6.32
6.30
6.29
4.56
4.55
NO2
O
N
H
F
5
0.98
1.09
1.04
1.02
2.06
2.05
1.00
2.06
f1 (ppm)

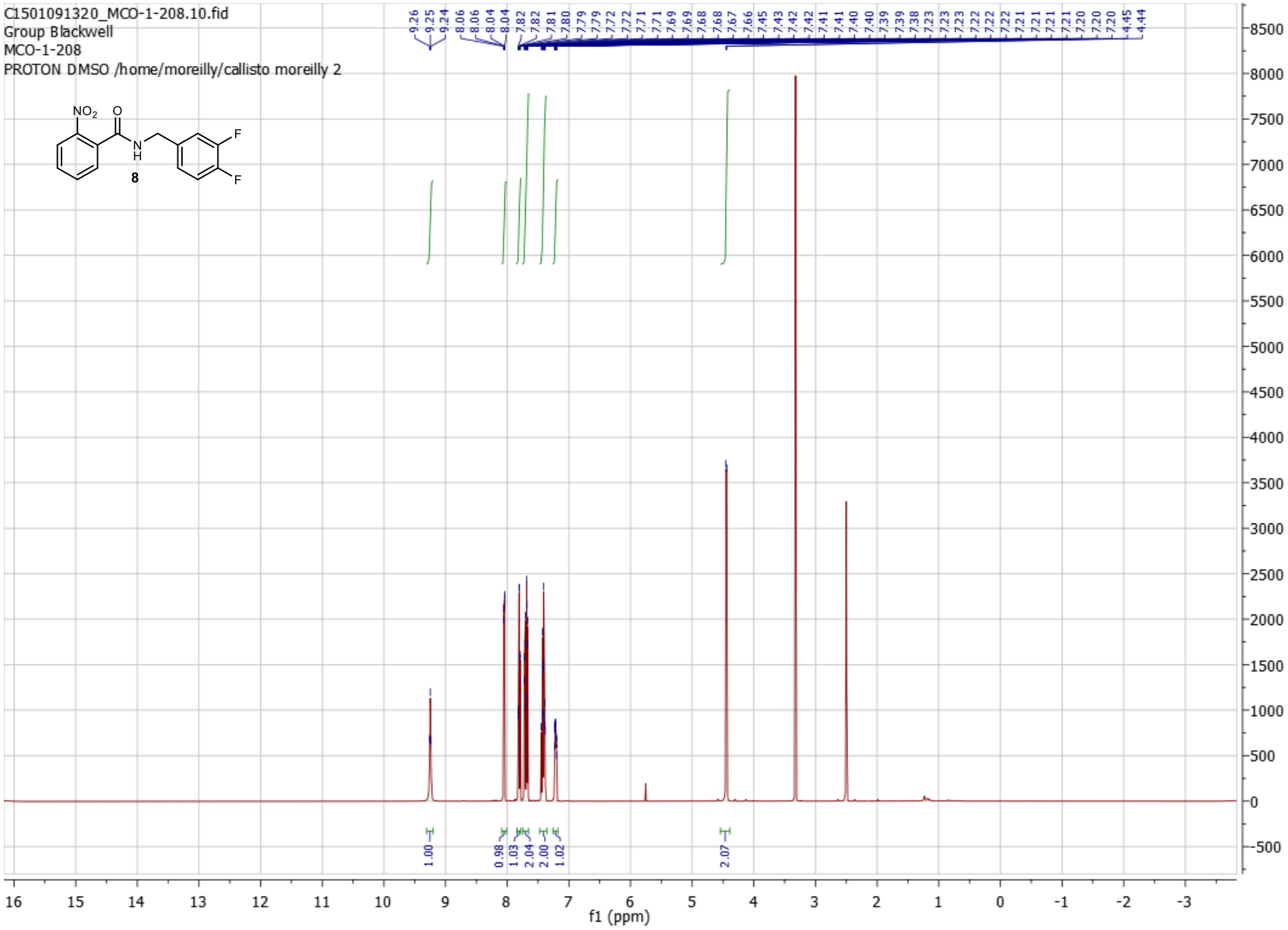

C1411121705_MCO-1-158.11.fid
Group Blackwell
MCO-1-158
C13CPD32 CDCl3 /home/moreilly/callisto moreilly 55
166.50
163.43
161.47
146.51
133.85
133.42
133.39
132.83
130.68
129.91
129.84
128.79
124.72
115.85
115.68
43.62
NO2
O
N
H
F
5
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

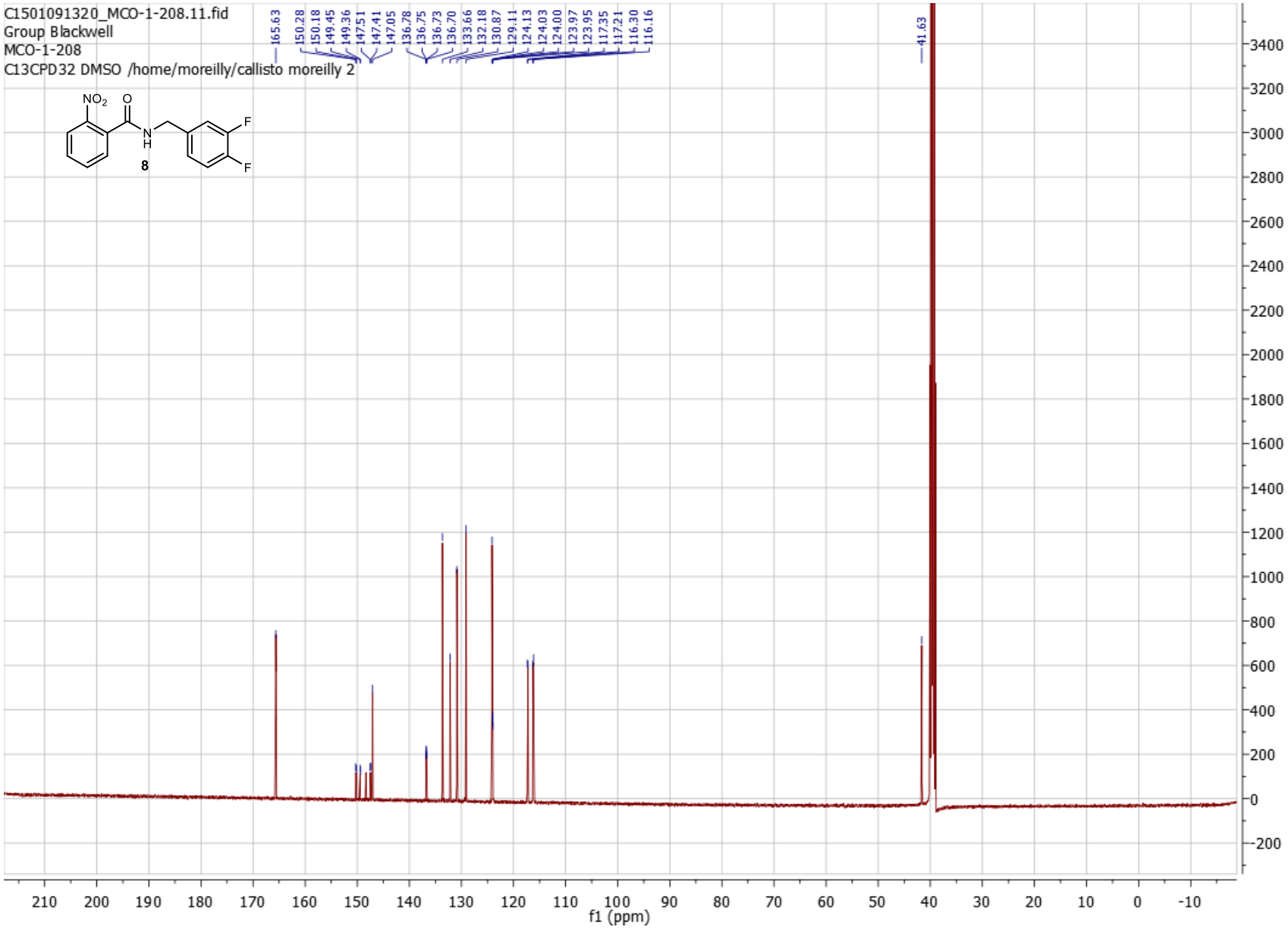

C1411120829_MCO-1-155.11.fid
Group Blackwell
MCO-1-155
PROTON CDCl3 /home/moreilly/callisto moreilly 32
NO2
O
N
H
F
F
6
8.02
8.00
7.66
7.64
7.63
7.58
7.56
7.55
7.48
7.46
6.88
6.86
6.73
6.73
6.71
6.69
6.56
6.55
6.54
4.55
4.53
0.92
1.00
0.97
0.96
1.84
0.95
0.92
2.00
f1 (ppm)

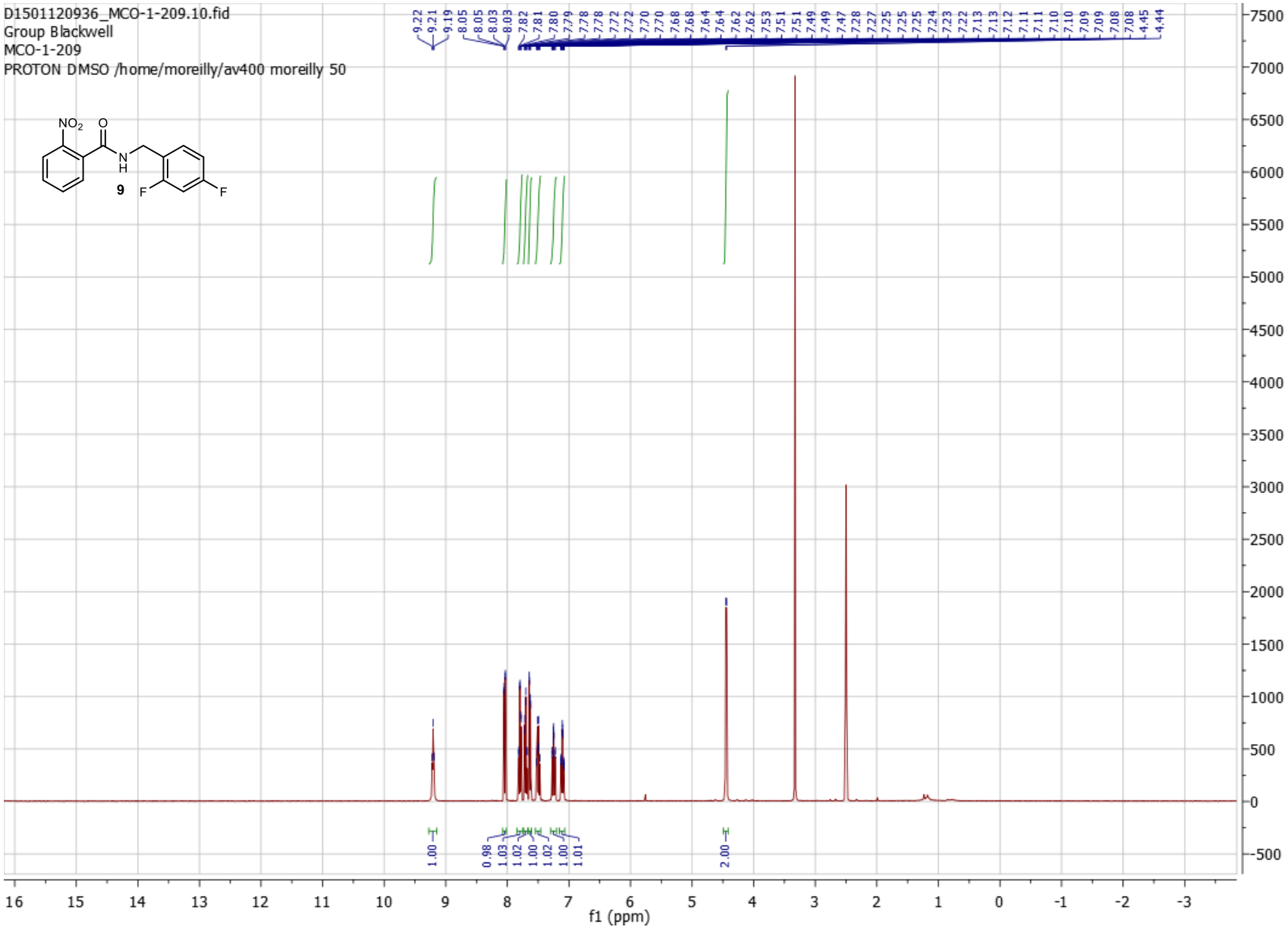

C1411120829_MCO-1-155.12.fid
Group Blackwell
MCO-1-155
C13CPD32 CDCl3 /home/moreilly/callisto moreilly 32
166.76
164.36
164.26
162.38
162.28
146.54
141.68
141.63
141.60
141.53
133.93
132.53
130.90
130.87
128.76
124.82
110.80
110.75
110.64
110.59
103.49
103.29
103.08
77.41
43.48
NO2
O
N
H
F
F
6
f1 (ppm)

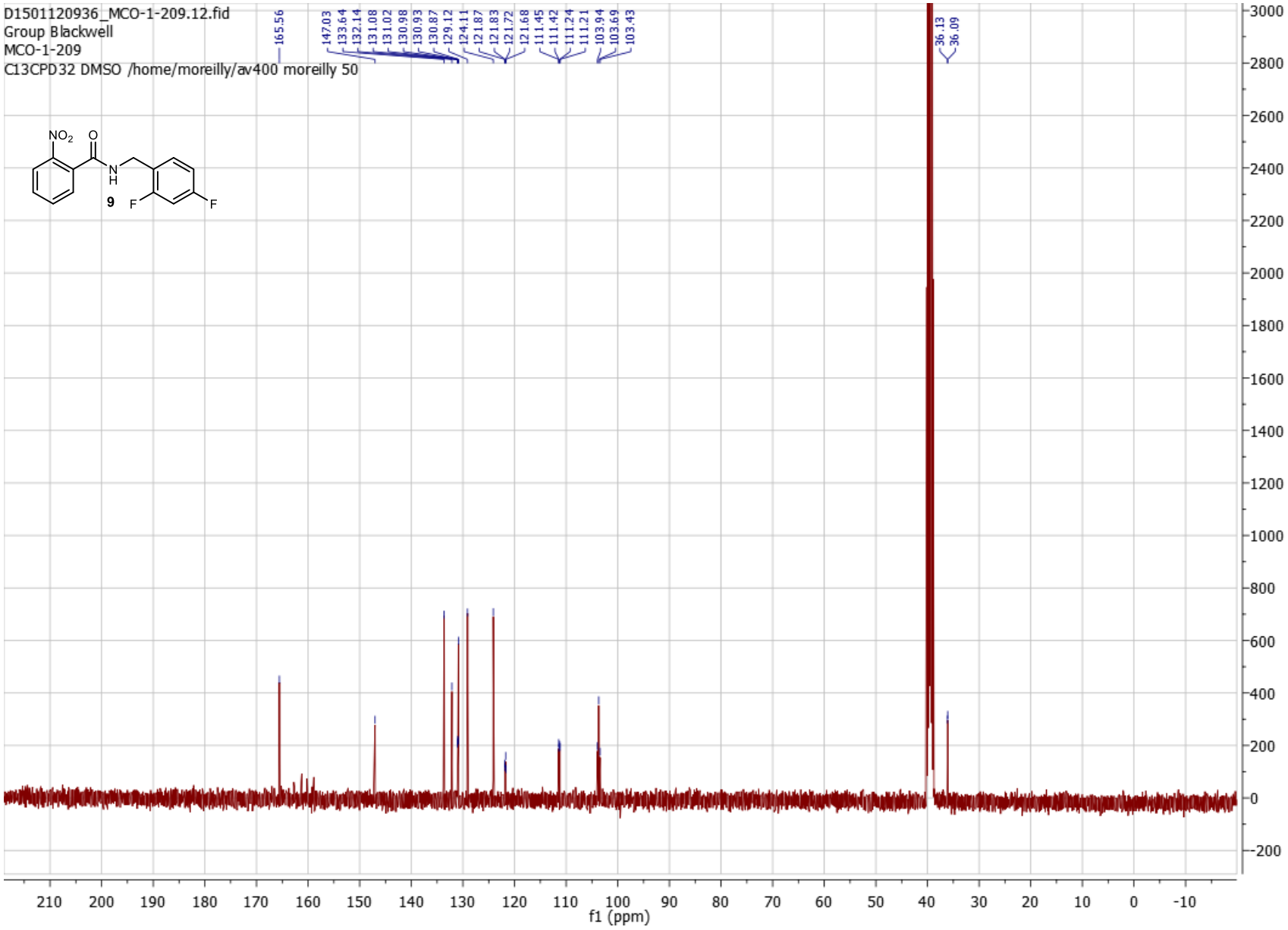

D1411171749_MCO-1-163-1H.fid
Group Blackwell
MCO-1-163
PROTON CDCl3 /home/moreilly/av400 moreilly 57
NO2
O
N
H
F
F
7
8.04
8.03
8.02
8.01
7.69
7.68
7.67
7.66
7.63
7.62
7.61
7.57
7.56
7.55
7.54
7.53
7.52
7.48
7.48
7.46
7.46
7.31
7.29
7.29
7.28
7.27
7.27
7.26
7.25
7.24
6.93
6.92
6.90
6.26
6.24
6.23
4.73
4.72
0.91
1.00
0.96
0.96
1.10
1.89
0.96
1.94
30000
25000
20000
15000
10000
5000
0
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

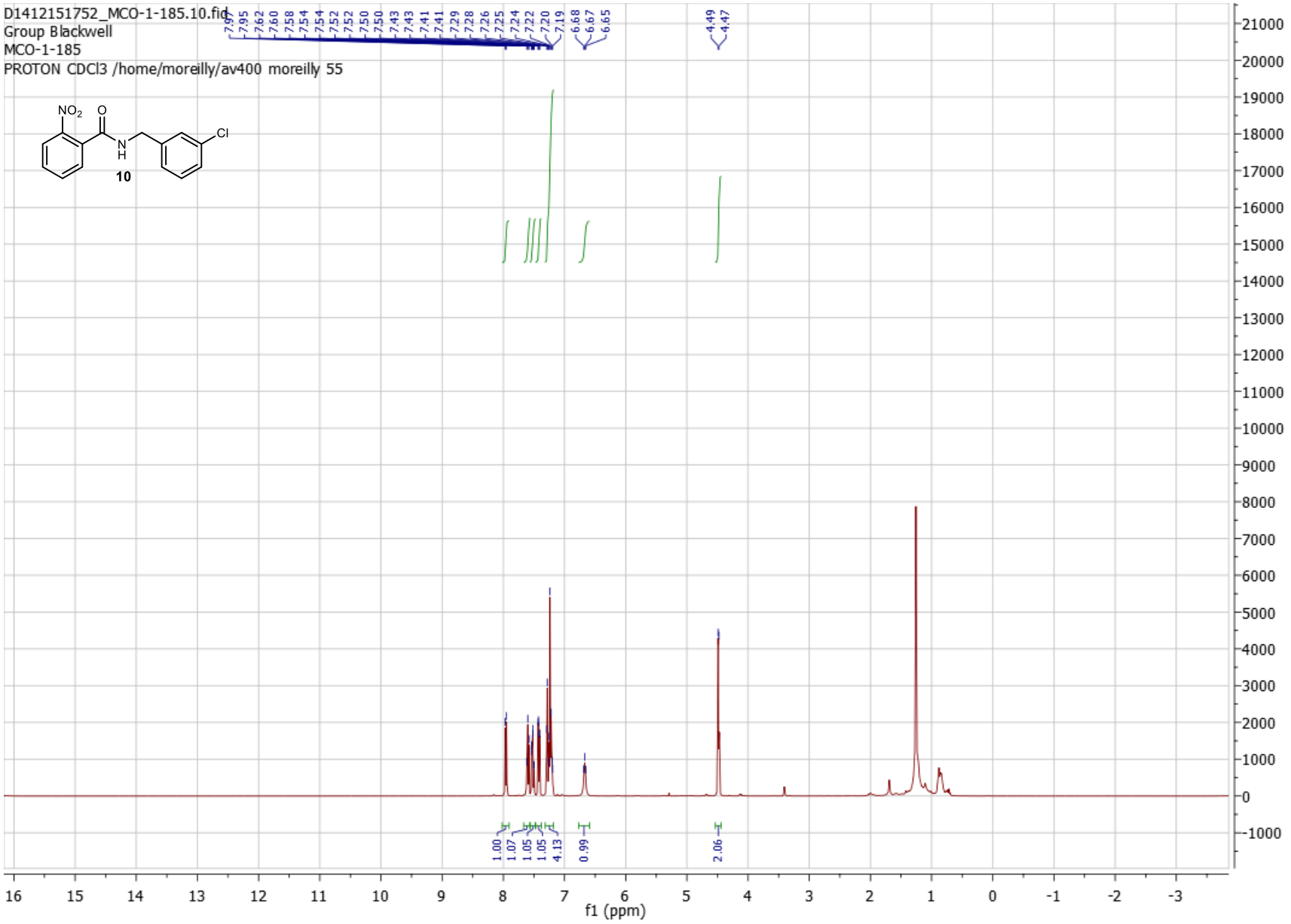

D1411171749_MCO-1-163.11.fid
Group Blackwell
MCO-1-163
C13CPD32 CDCl3 /home/moreilly/av400 moreilly 57
166.19
162.96
162.88
160.48
160.40
146.44
133.83
132.74
130.64
130.09
129.99
129.88
128.87
124.67
113.37
113.18
112.99
111.74
111.68
111.56
111.49
32.31
32.27
32.24
NO2
O
F
N
H
7
F
f1 (ppm)

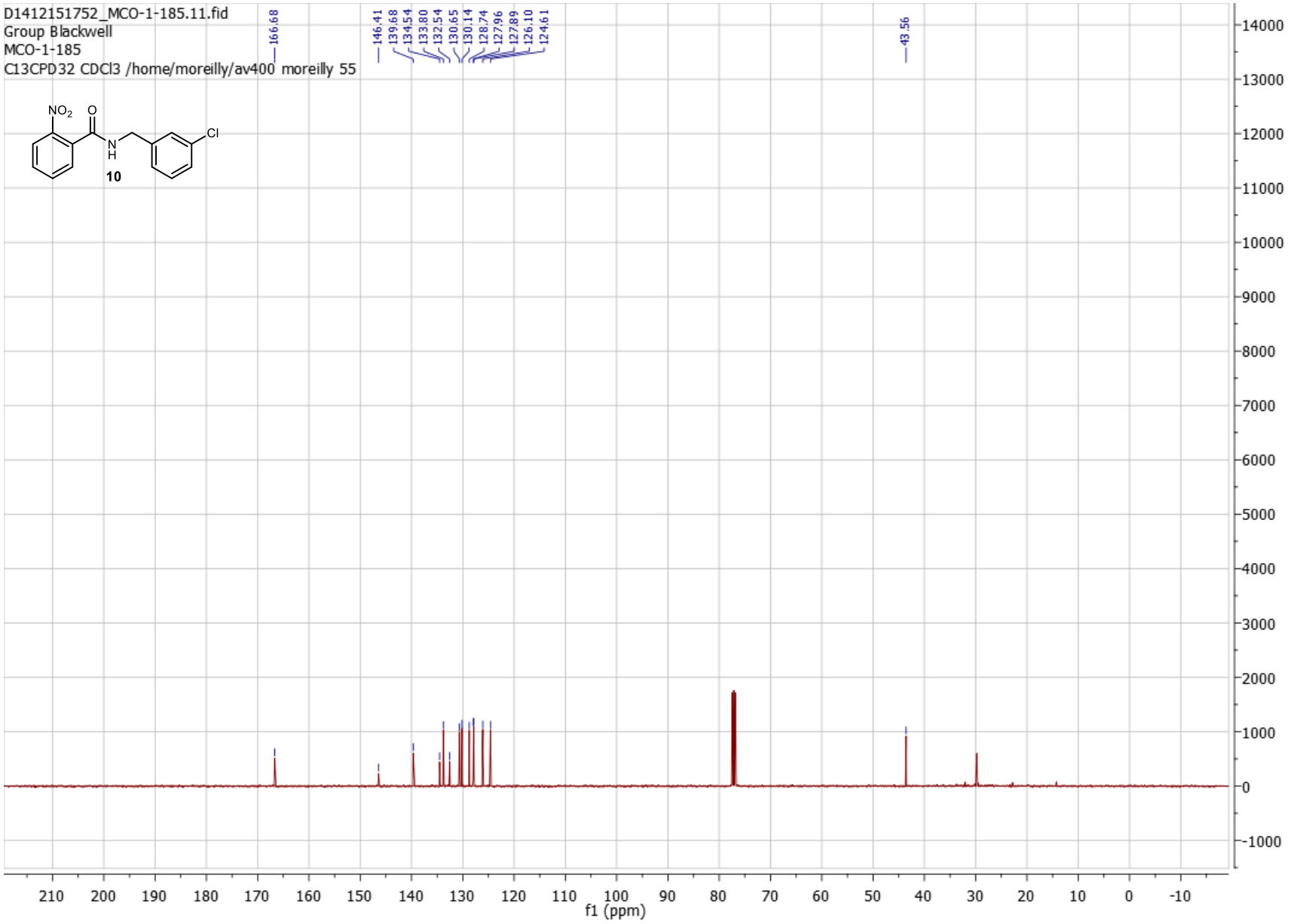

C1501091320_MCO-1-208.10.fid
Group Blackwell
MCO-1-208
PROTON DMSO /home/moreilly/callisto moreilly 2
NO2
O
N
H
F
F
8
f1 (ppm)

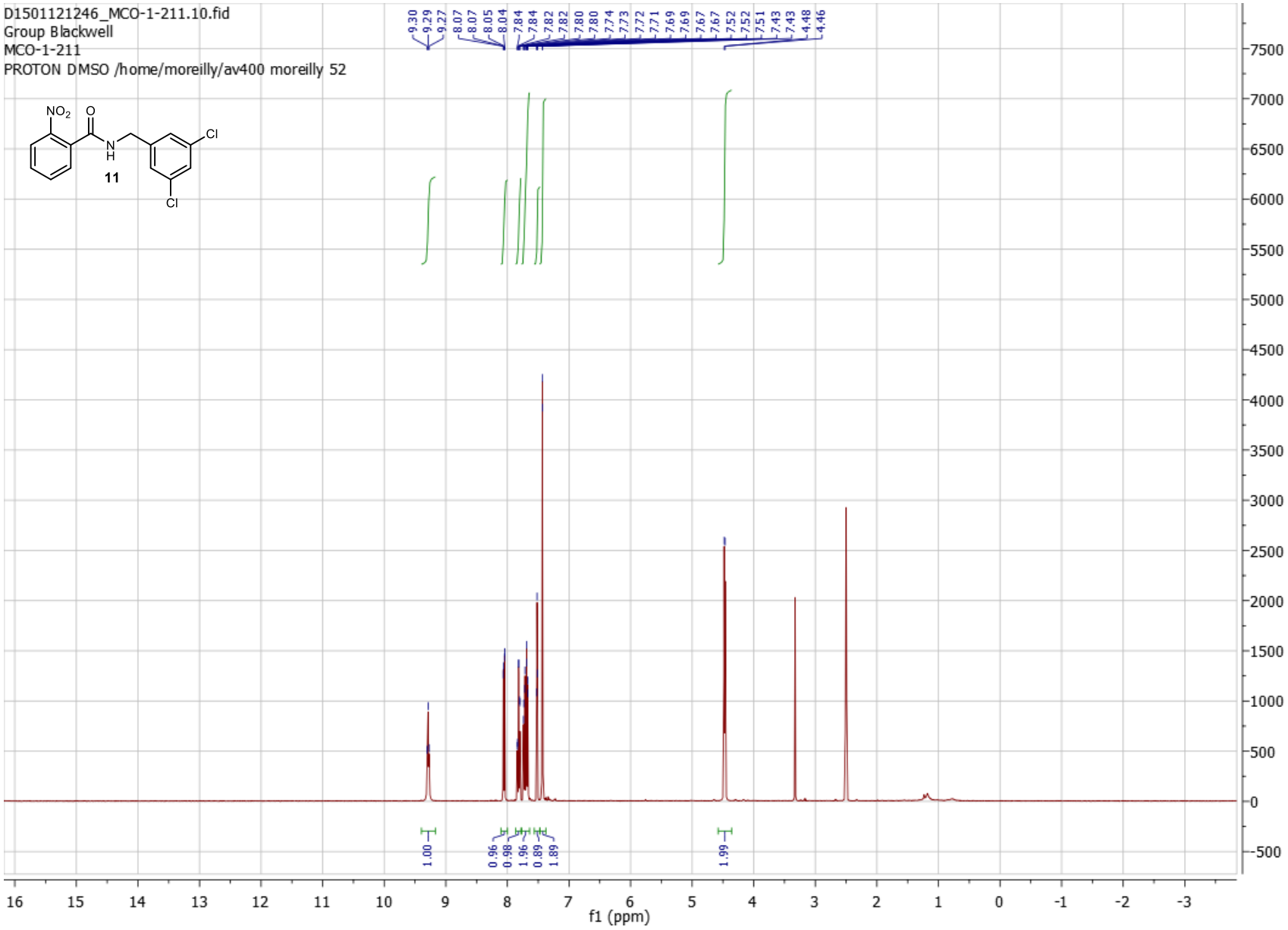

C1501091320_MCO-1-208.11.fid
Group Blackwell
MCO-1-208
C13CPD32 DMSO /home/moreilly/callisto moreilly 2
165.63
150.28
150.18
149.45
149.36
147.51
147.41
147.05
136.78
136.75
136.73
136.70
133.66
132.18
130.87
129.11
124.13
124.03
124.00
123.97
123.95
117.35
117.21
116.30
116.16
41.63
NO2
O
N
H
F
F
8
f1 (ppm)

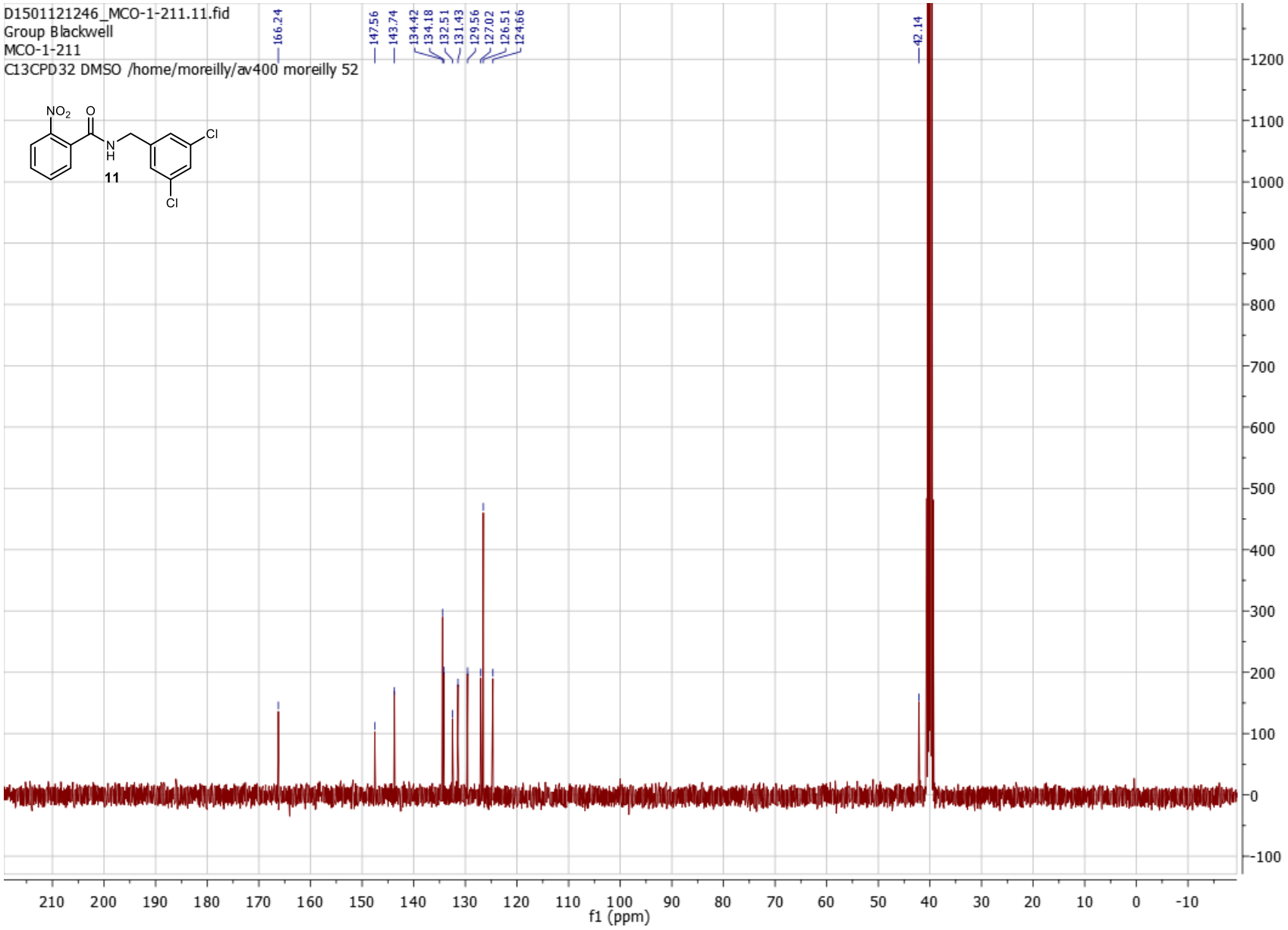

D1501120936_MCO-1-209.10.fid
Group Blackwell
MCO-1-209
PROTON DMSO /home/moreilly/av400 moreilly 50
NO2
O
N
H
F
F
9
f1 (ppm)

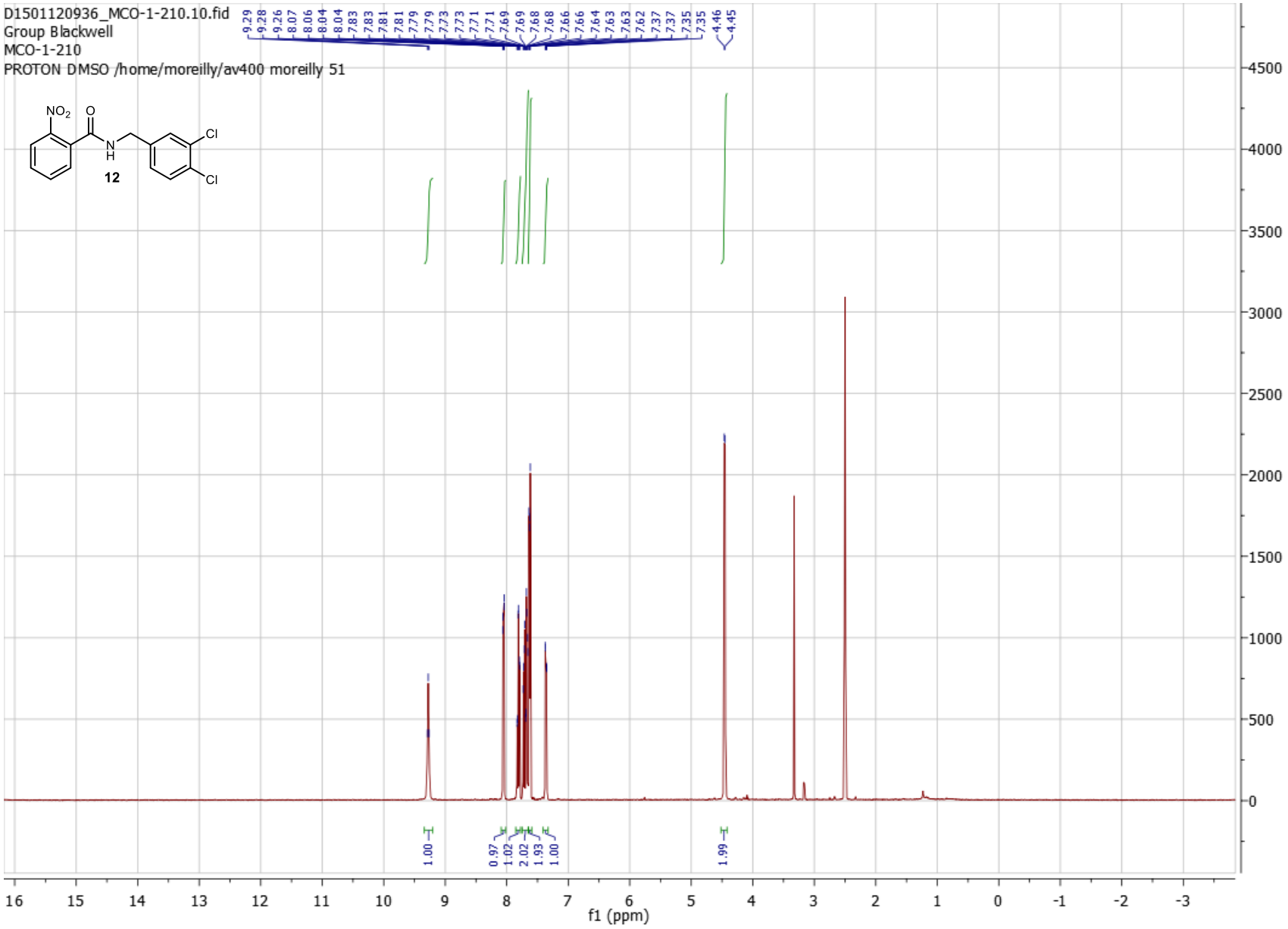

D1501120936_MCO-1-209.12.fid
Group Blackwell
MCO-1-209
C13CPD32 DMSO /home/moreilly/av400 moreilly 50
165.56
147.03
133.64
132.14
131.08
131.02
130.98
130.93
130.87
129.12
124.11
121.87
121.83
121.72
121.68
111.45
111.42
111.24
111.21
103.94
103.69
103.43
36.13
36.09
NO2
O
N
H
F
F
9
f1 (ppm)

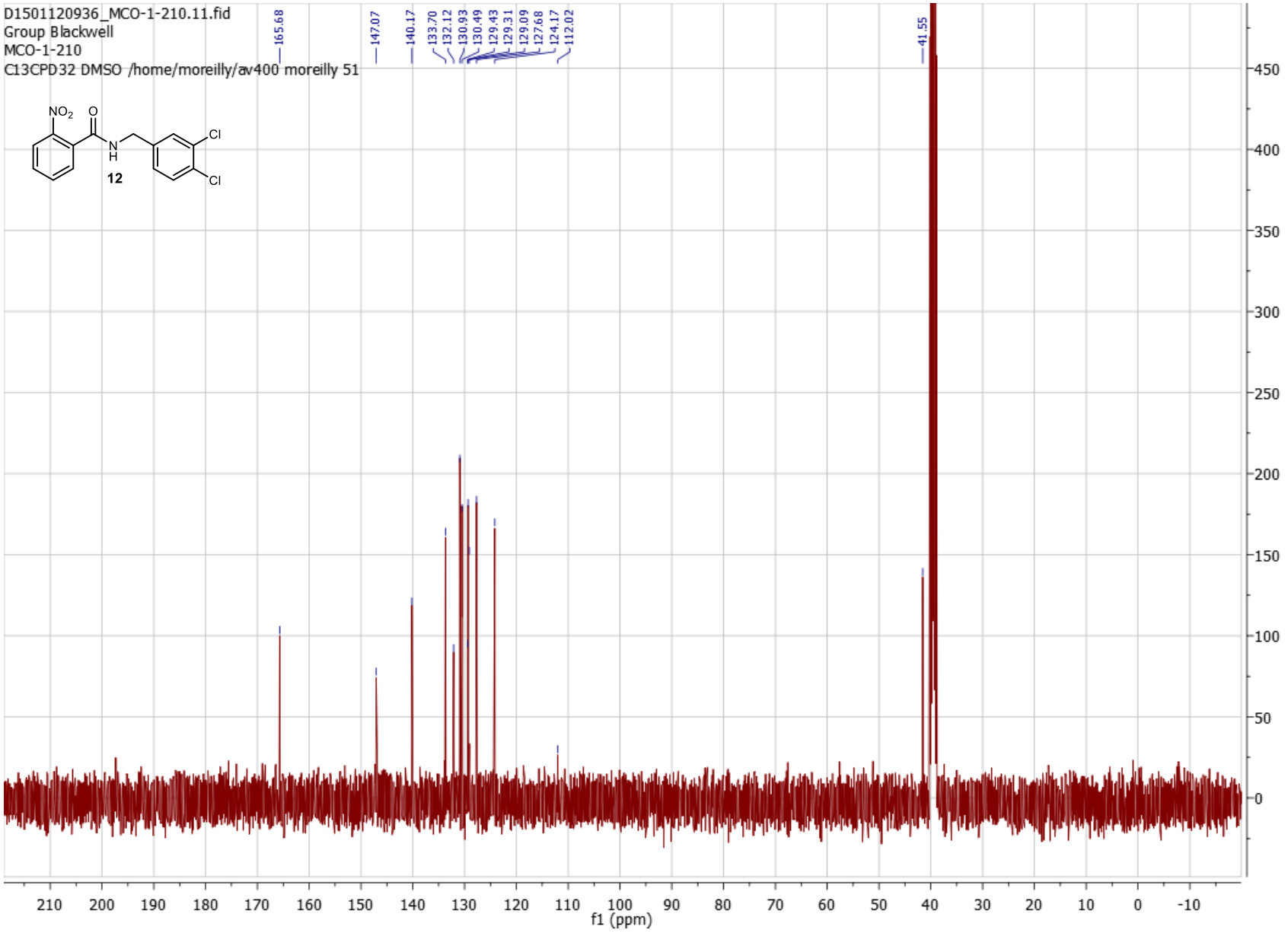

D1412151752_MCO-1-185.10.fid
Group Blackwell
MCO-1-185
PROTON CDCl3 /home/moreilly/av400 moreilly 55
NO2
O
N
H
Cl
10
7.97
7.95
7.62
7.60
7.58
7.54
7.54
7.52
7.52
7.50
7.50
7.43
7.43
7.41
7.41
7.29
7.28
7.26
7.25
7.24
7.22
7.20
7.19
6.68
6.67
6.65
4.49
4.47
1.00
1.07
1.05
1.05
4.13
0.99
2.06
f1 (ppm)

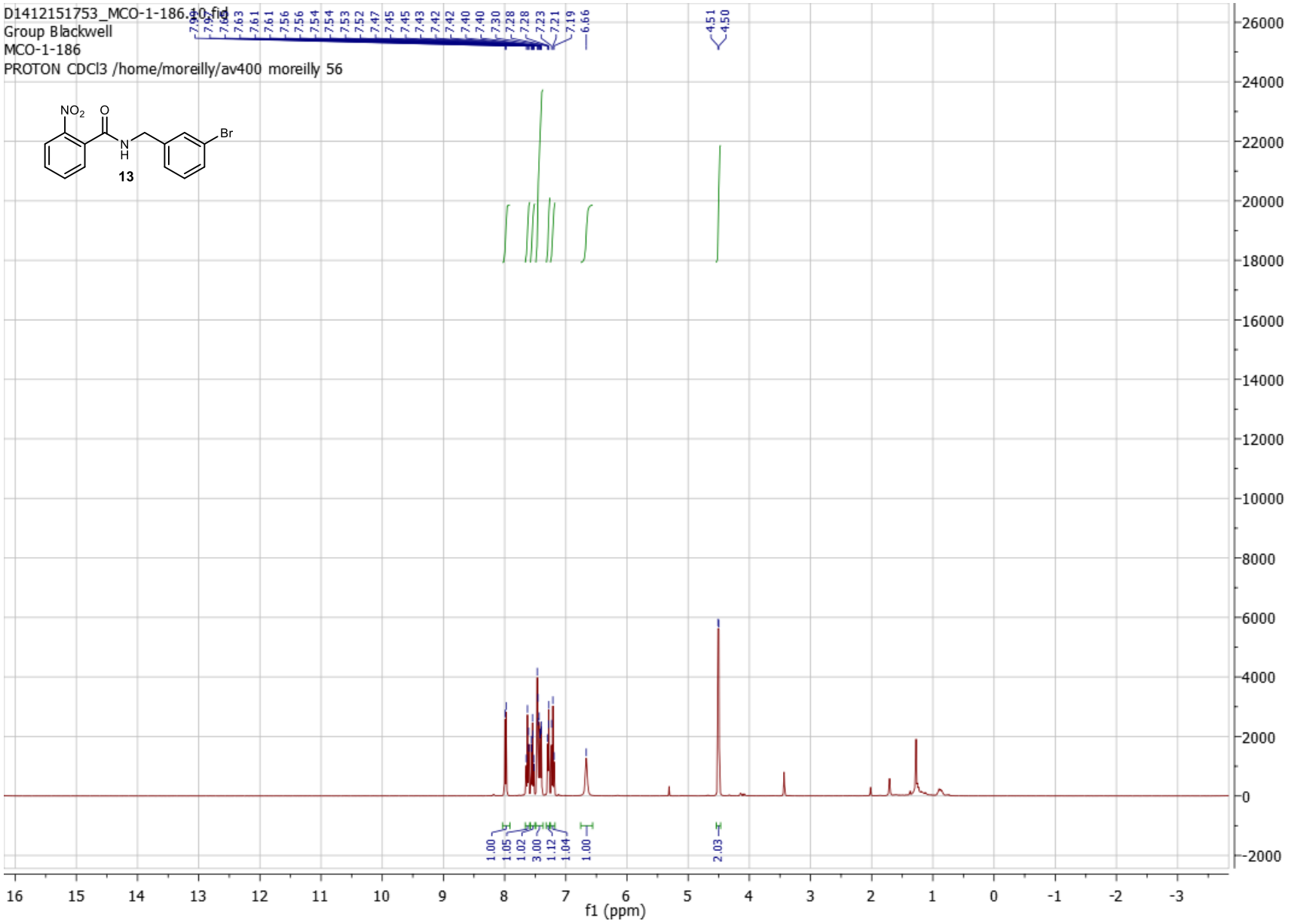

D1412151752_MCO-1-185.11.fid
Group Blackwell
MCO-1-185
C13CPD32 CDCl3 /home/moreilly/av400 moreilly 55
166.68
146.41
139.68
134.54
133.80
132.54
130.65
130.14
128.74
127.96
127.89
126.10
124.61
43.56
NO2
O
N
H
Cl
10
f1 (ppm)

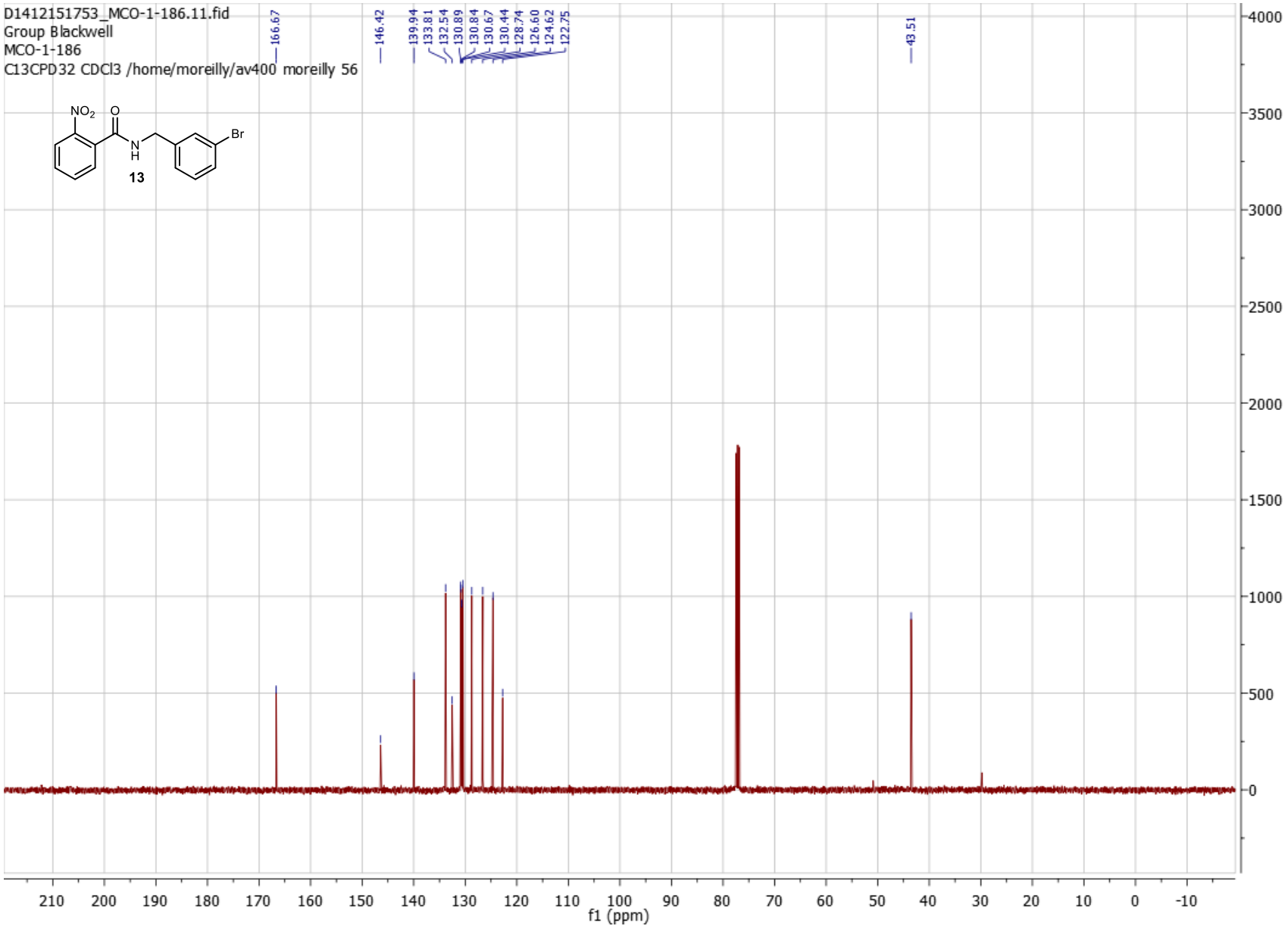

D1501121246_MCO-1-211.10.fid
Group Blackwell
MCO-1-211
PROTON DMSO /home/moreilly/av400 moreilly 52
NO2
O
N
H
Cl
Cl
11
9.30
9.29
9.27
8.07
8.07
8.05
8.04
7.84
7.84
7.82
7.82
7.80
7.80
7.74
7.73
7.72
7.71
7.69
7.69
7.67
7.67
7.52
7.52
7.51
7.43
7.43
4.48
4.46
1.00
0.96
0.98
1.96
0.89
1.89
1.99
f1 (ppm)

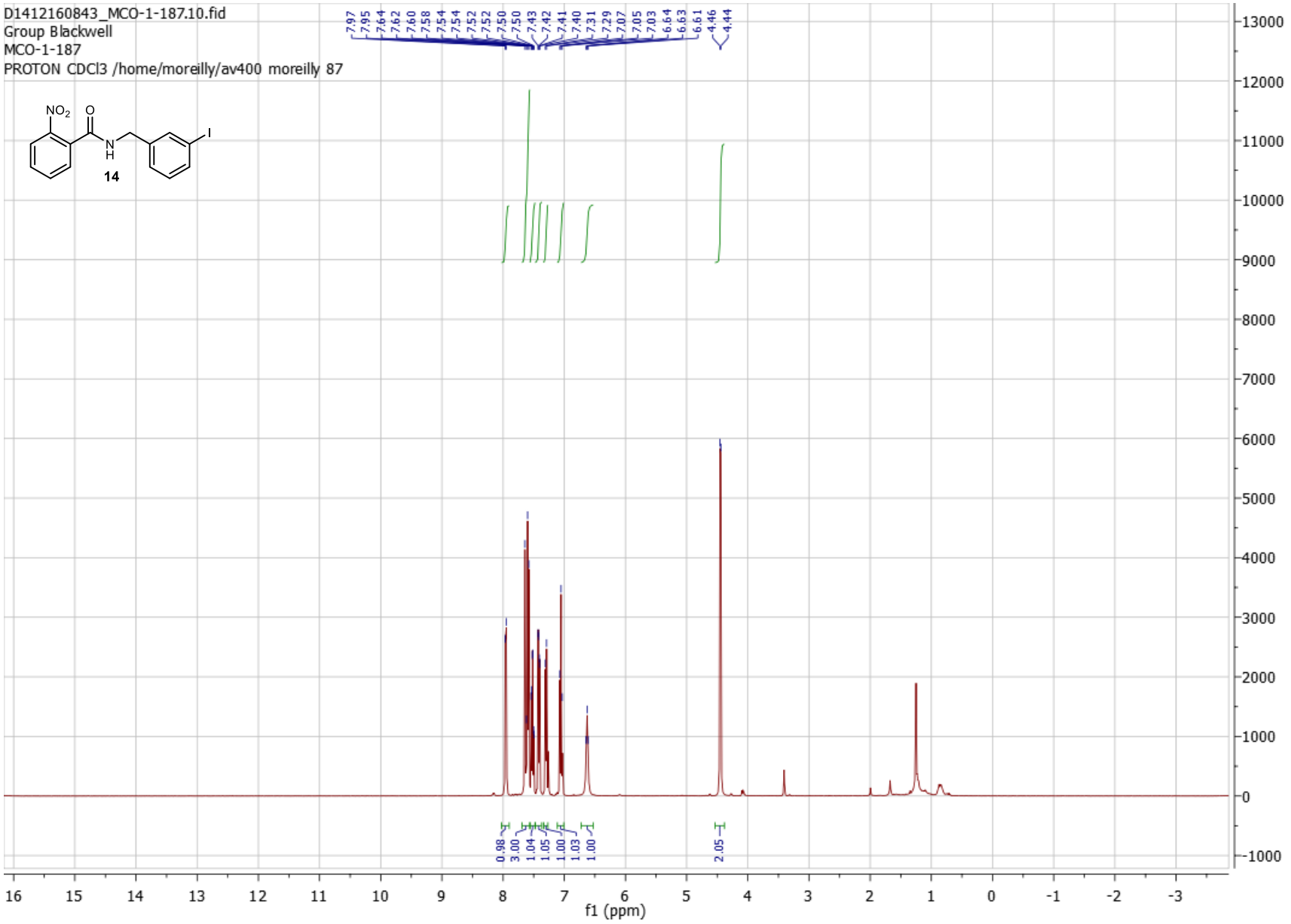

D1501121246_MCO-1-211.11.fid
Group Blackwell
MCO-1-211
C13CPD32 DMSO /home/moreilly/av400 moreilly 52
166.24
147.56
143.74
134.42
134.18
132.51
131.43
129.56
127.02
126.51
124.66
42.14
NO2
O
N
H
Cl
Cl
11
f1 (ppm)

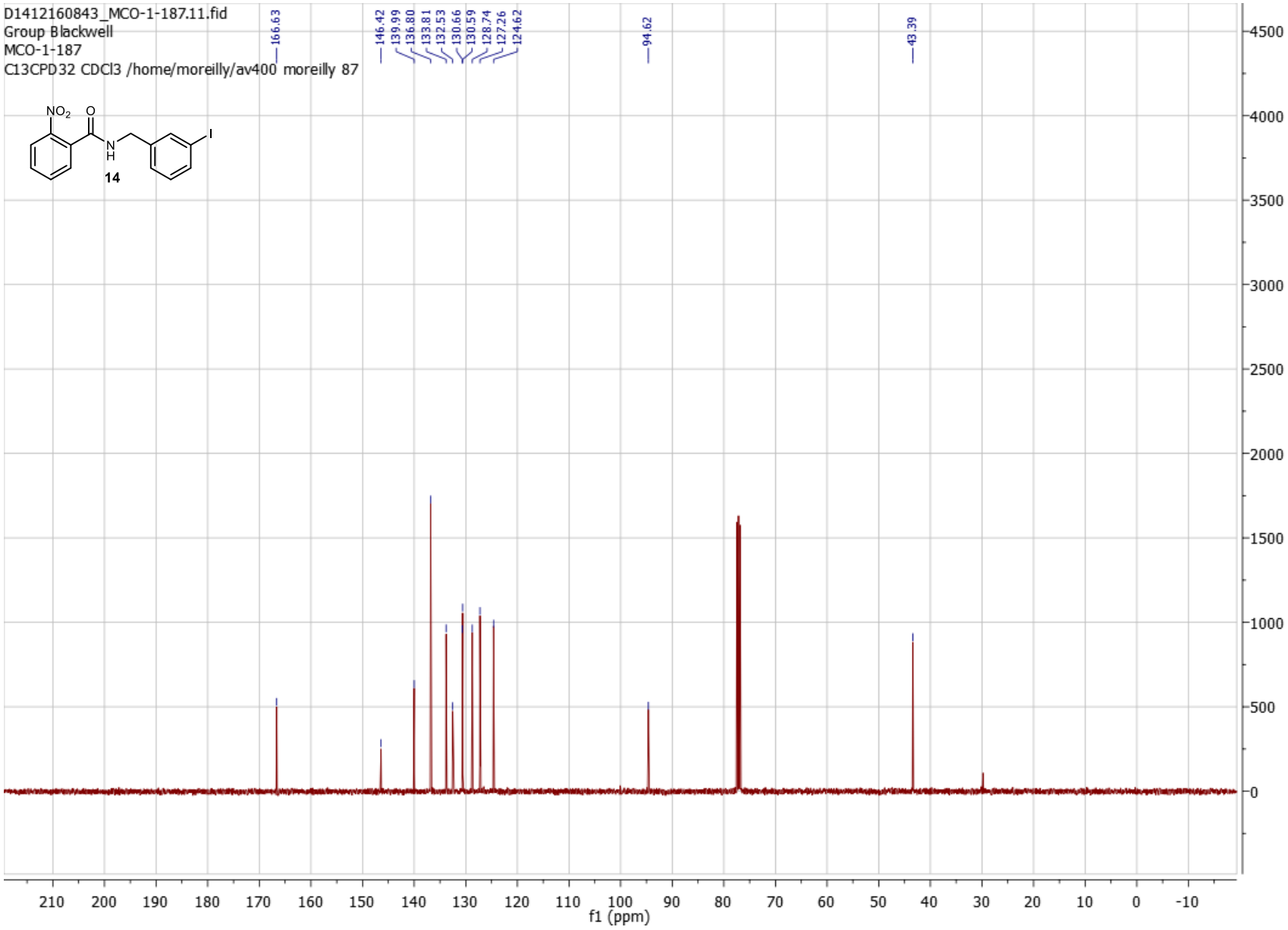

D1501120936_MCO-1-210.10.fid
Group Blackwell
MCO-1-210
PROTON DMSO /home/moreilly/av400 moreilly 51
9.29
9.28
9.26
8.07
8.06
8.04
8.04
7.83
7.81
7.81
7.79
7.79
7.73
7.73
7.71
7.71
7.69
7.69
7.68
7.68
7.66
7.66
7.64
7.63
7.63
7.62
7.37
7.37
7.35
7.35
4.46
4.45
NO2
O
N
H
Cl
Cl
12
4500
4000
3500
3000
2500
2000
1500
1000
500
0
1.00
0.97
1.02
2.02
1.93
1.00
1.99
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

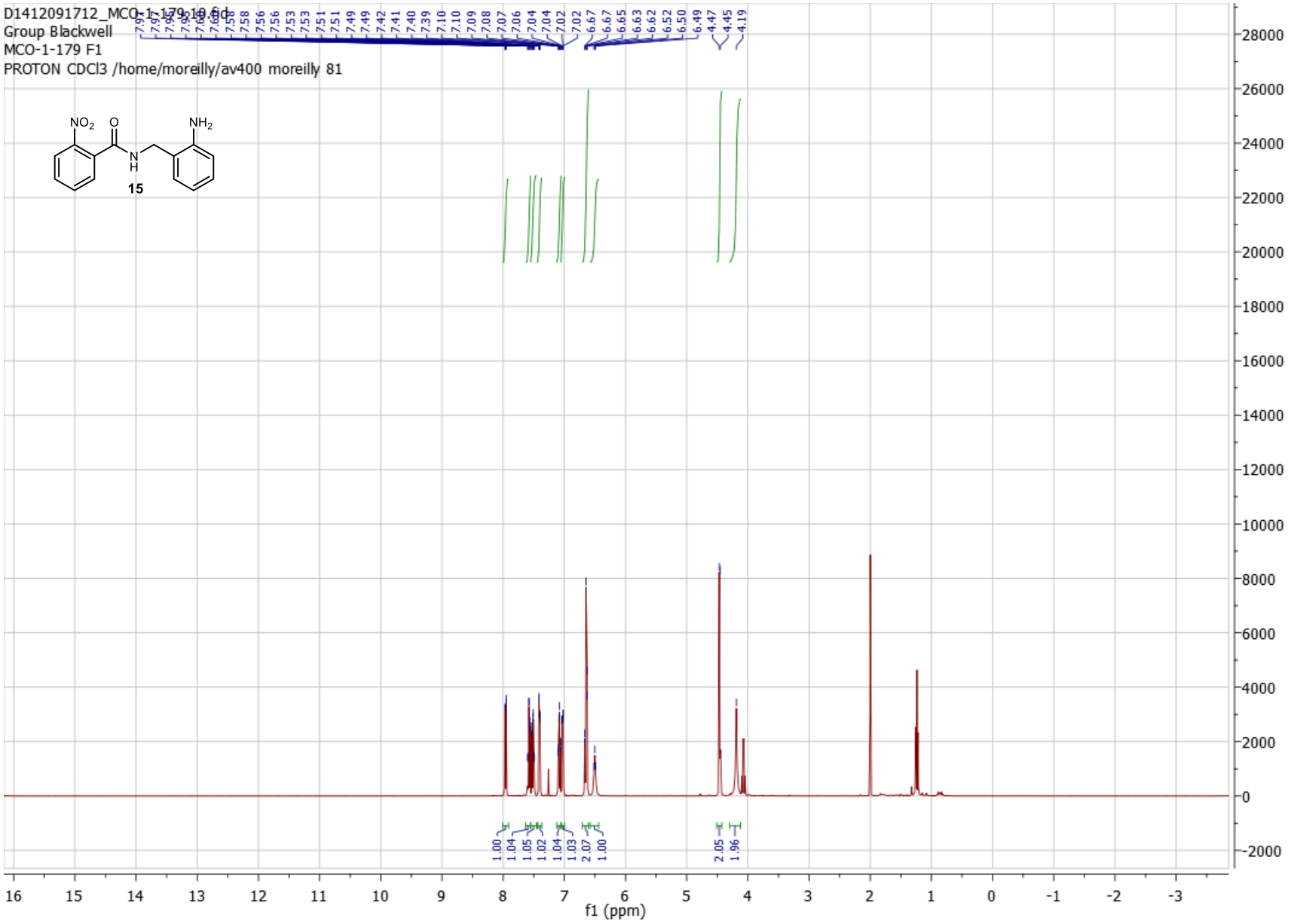

D1501120936_MCO-1-210.11.fid
Group Blackwell
MCO-1-210
C13CPD32 DMSO /home/moreilly/av400 moreilly 51
165.68
147.07
140.17
133.70
132.12
130.93
130.49
129.43
129.31
129.09
127.68
124.17
112.02
41.55
NO2
O
N
H
Cl
Cl
12
f1 (ppm)

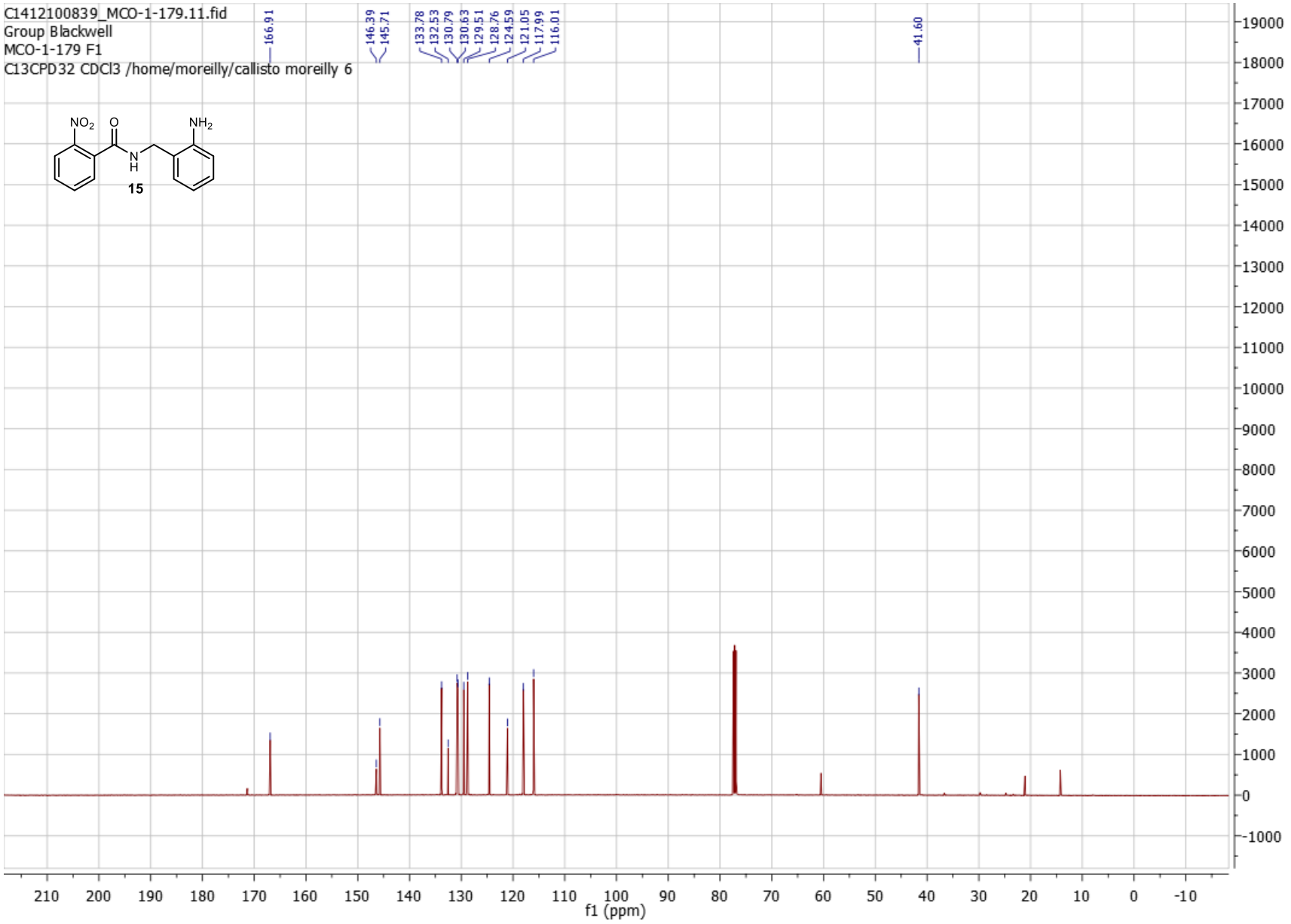

D1412151753_MCO-1-186.10.fid
Group Blackwell
MCO-1-186
PROTON CDCl3 /home/moreilly/av400 moreilly 56
NO2
O
N
H
Br
13
f1 (ppm)

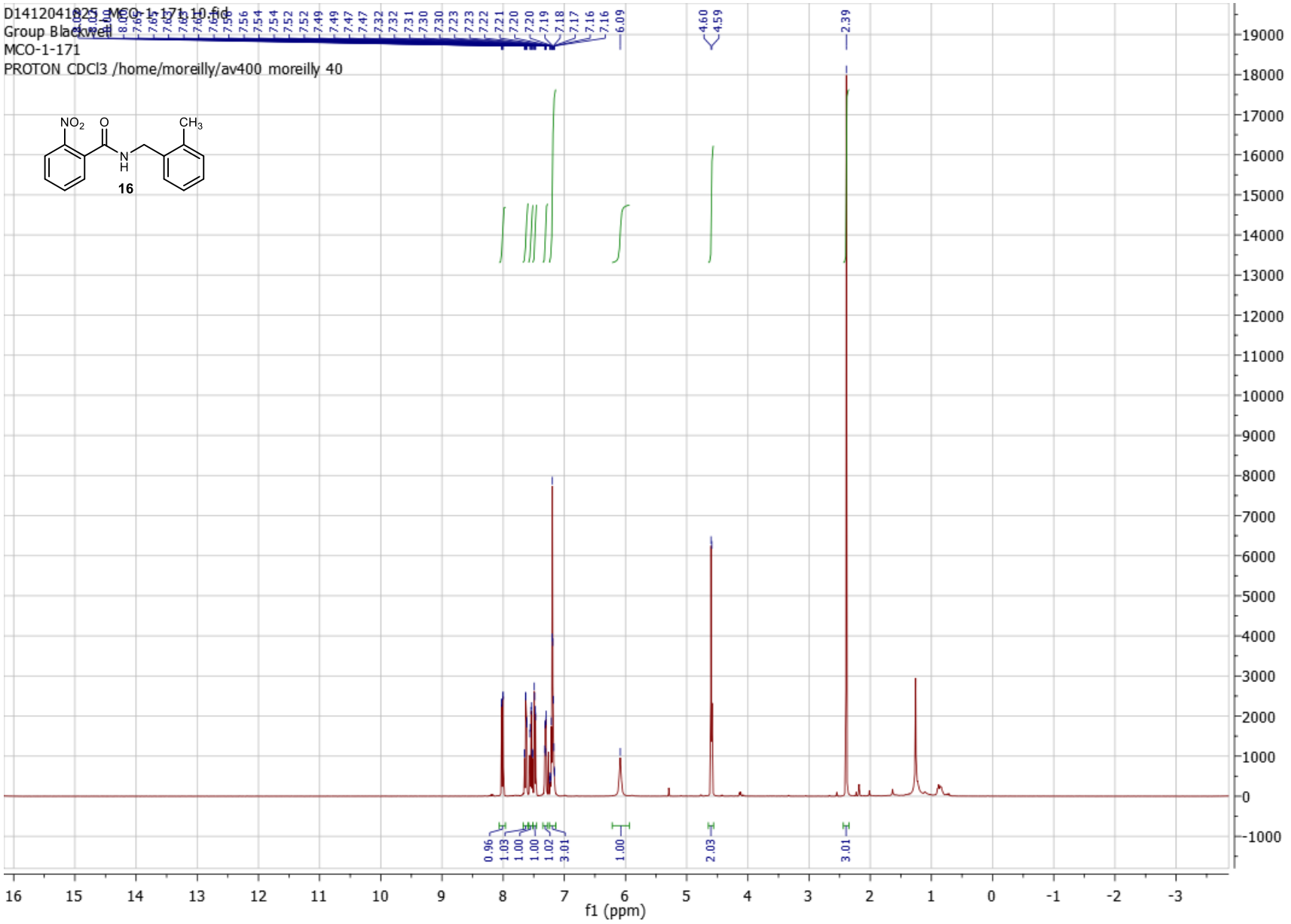

D1412151753_MCO-1-186.11.fid
Group Blackwell
MCO-1-186
C13CPD32 CDCl3 /home/moreilly/av400 moreilly 56
166.67
146.42
139.94
133.81
132.54
130.89
130.84
130.67
130.44
128.74
126.60
124.62
122.75
43.51
NO2
O
N
H
Br
13
4000
3500
3000
2500
2000
1500
1000
500
0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

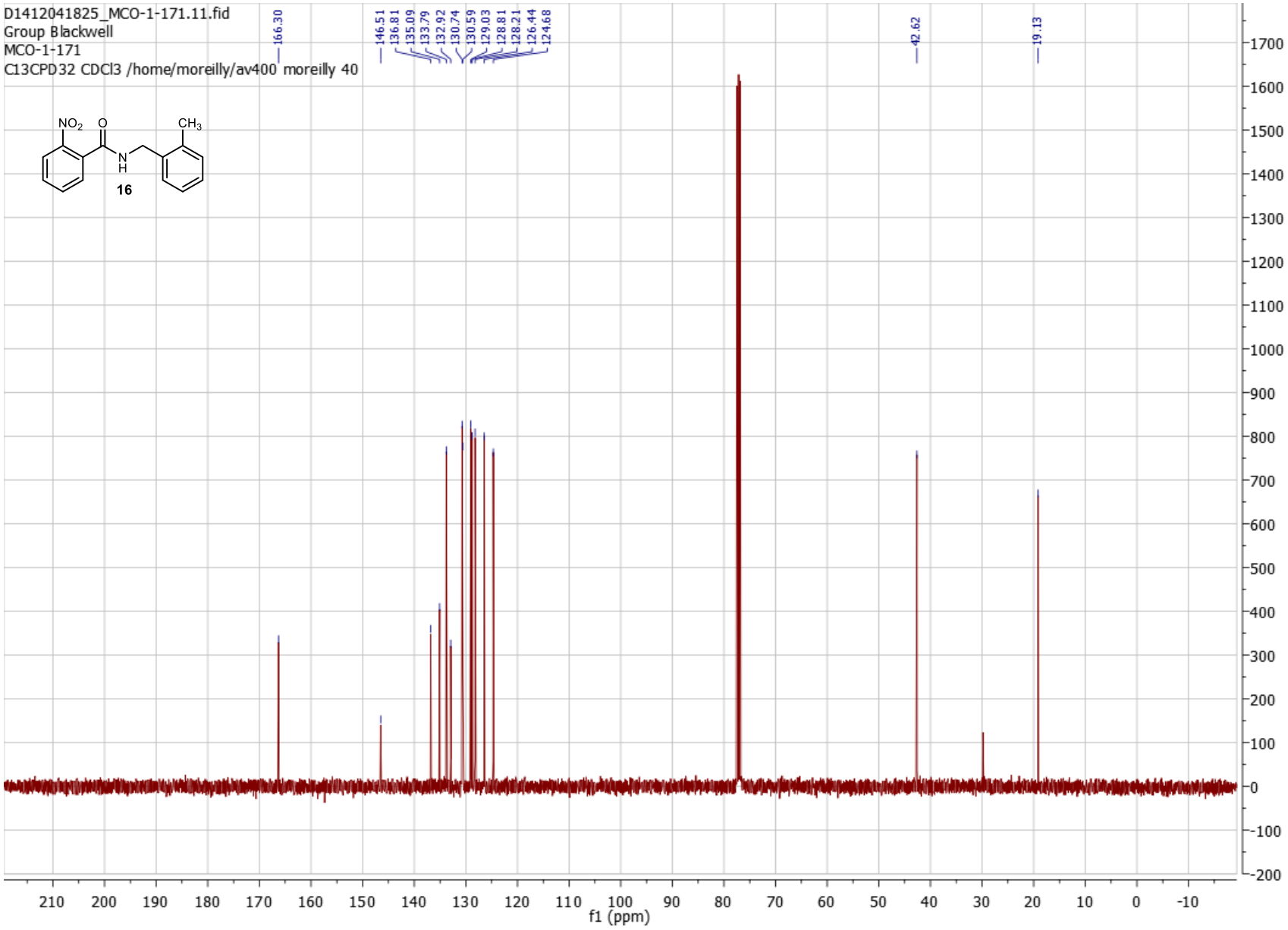

D1412160843_MCO-1-187.10.fid
Group Blackwell
MCO-1-187
PROTON CDCl3 /home/moreilly/av400 moreilly 87
NO2
O
N
H
I
14
7.97
7.95
7.64
7.62
7.60
7.58
7.54
7.54
7.52
7.52
7.50
7.50
7.43
7.42
7.41
7.40
7.31
7.29
7.07
7.05
7.03
6.64
6.63
6.61
4.46
4.44
0.98
3.00
1.04
1.05
1.00
1.03
1.00
2.05
f1 (ppm)

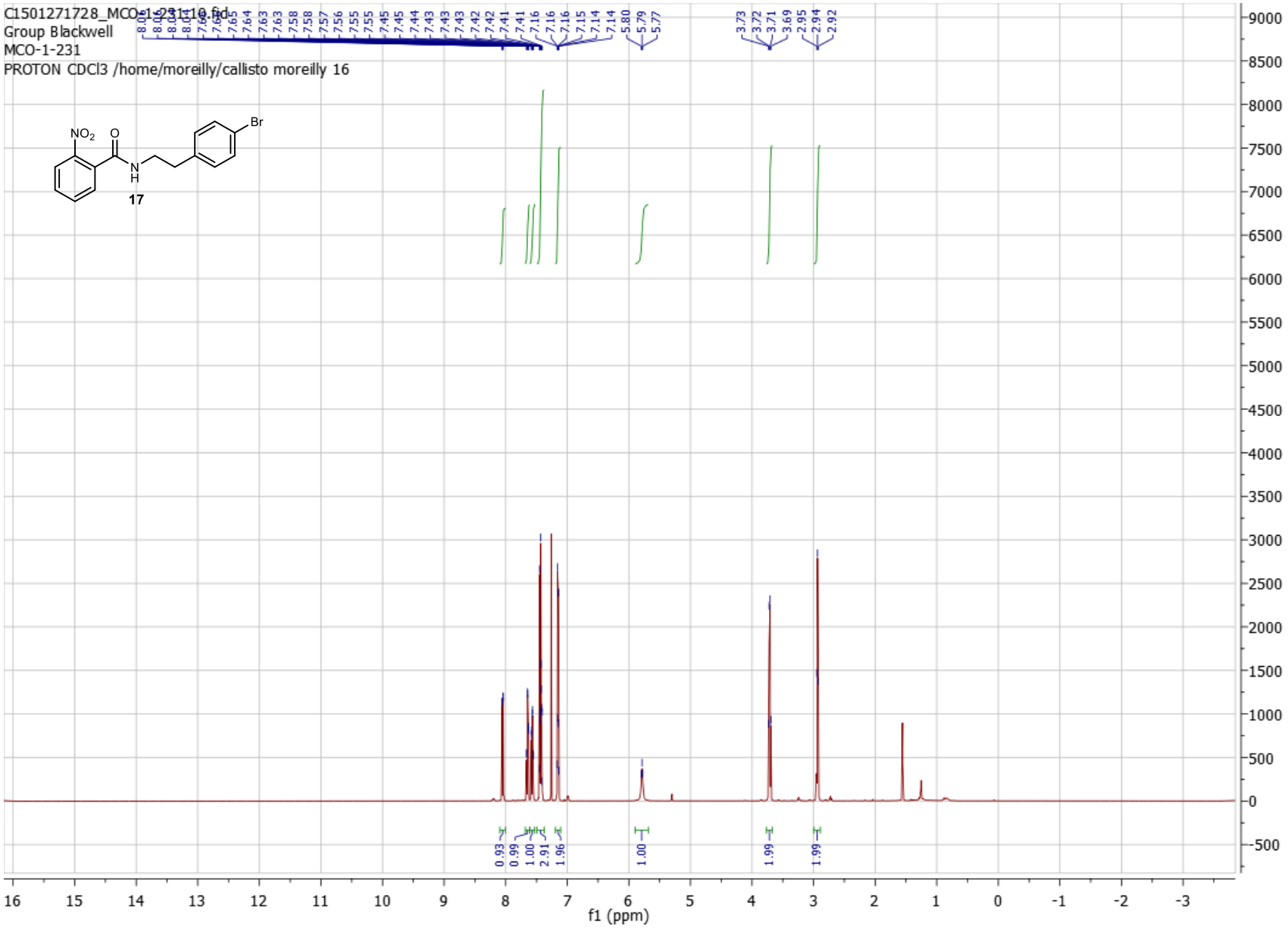

D1412160843_MCO-1-187.11.fid
Group Blackwell
MCO-1-187
C13CPD32 CDCl3 /home/moreilly/av400 moreilly 87
166.63
146.42
139.99
136.80
133.81
132.53
130.66
130.59
128.74
127.26
124.62
94.62
43.39
NO2
O
N
H
I
14
4500
4000
3500
3000
2500
2000
1500
1000
500
0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

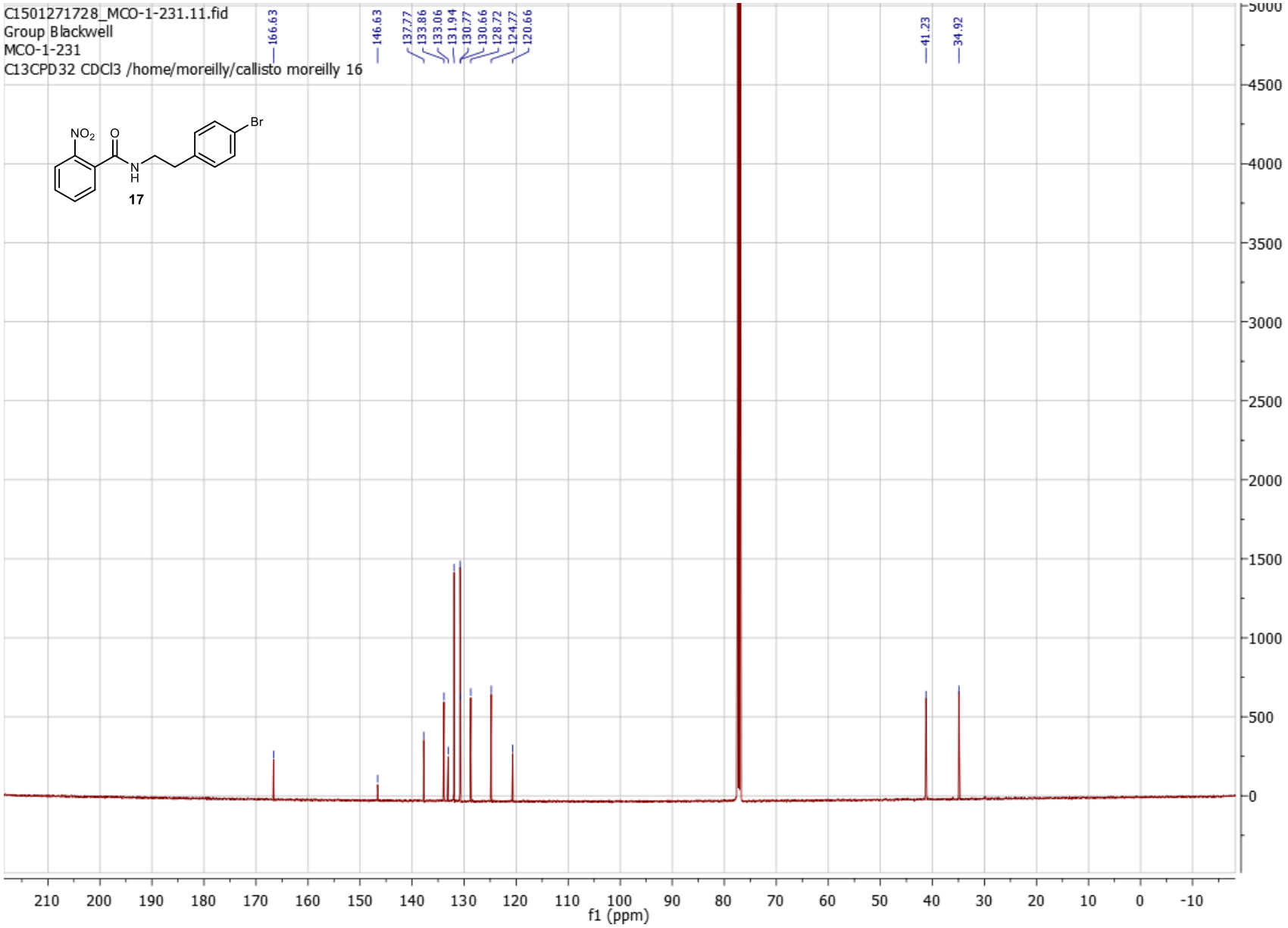

D1412091712_MCO-1-179-1H.fid
Group Blackwell
MCO-1-179 F1
PROTON CDCl3 /home/moreilly/av400 moreilly 81
NO2
O
NH2
H
N
15
f1 (ppm)

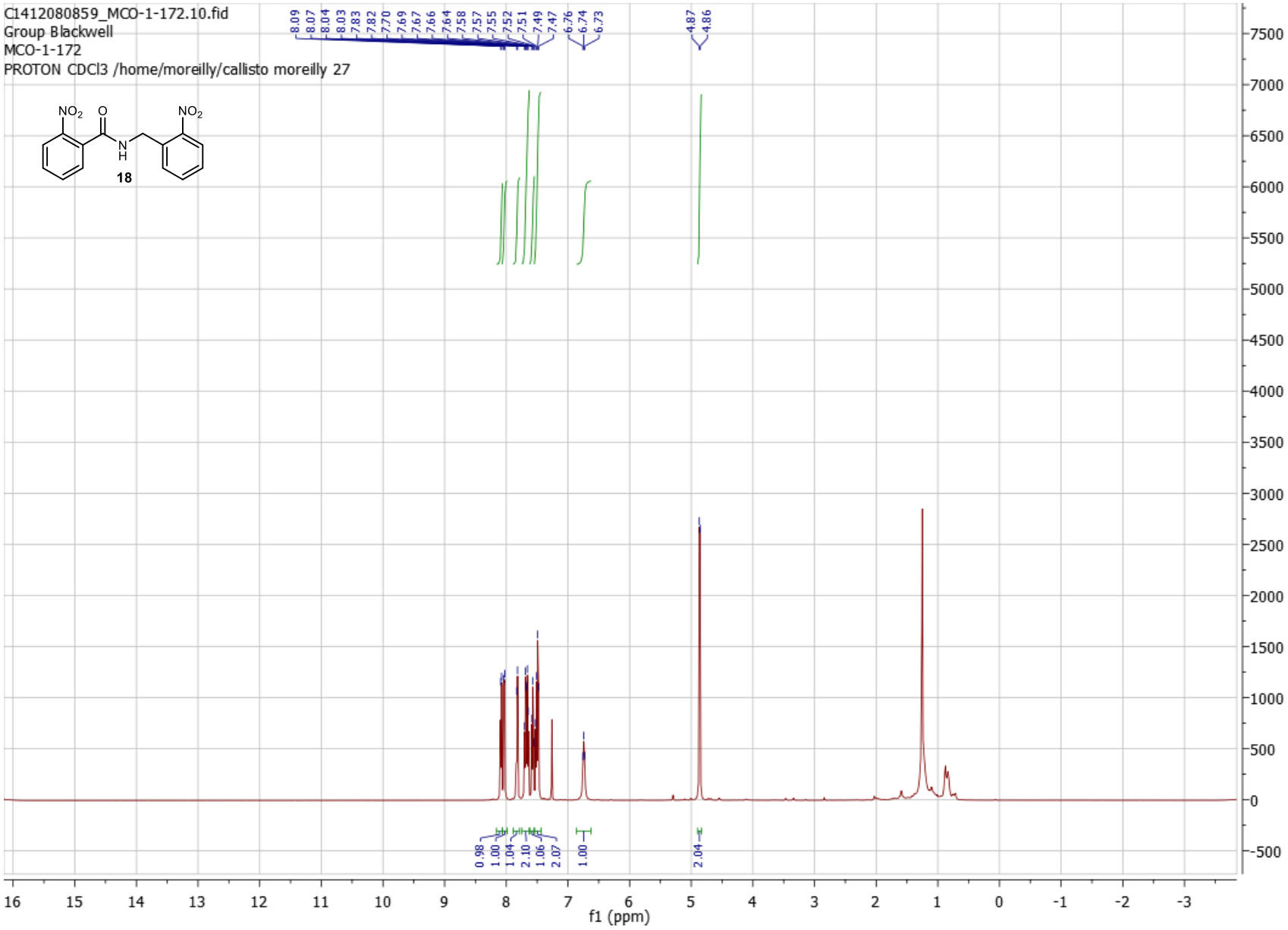

C1412100839_MCO-1-179.11.fid
Group Blackwell
MCO-1-179 F1
C13CPD32 CDCl3 /home/moreilly/callisto moreilly 6
166.91
146.39
145.71
133.78
132.53
130.79
130.63
129.51
128.76
124.59
121.05
117.99
116.01
41.60
NO2
O
NH2
N
H
15
f1 (ppm)

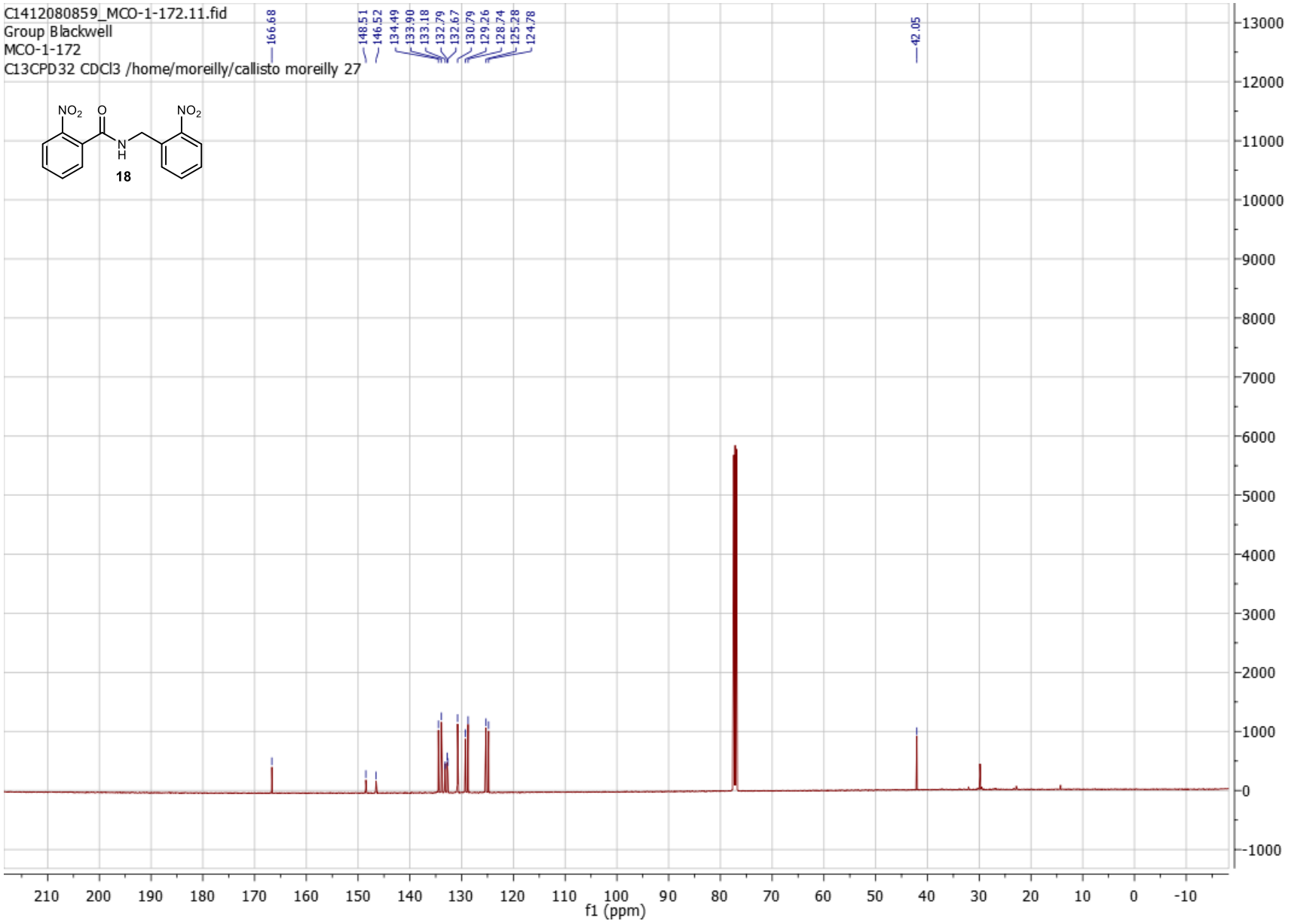

D1412041825 MCO-1-171-10.fid
Group Blackwell
MCO-1-171
PROTON CDCl3 /home/moreilly/av400 moreilly 40
NO2
O
CH3
N
H
16
7.67
7.65
7.63
7.62
7.56
7.54
7.52
7.49
7.47
7.32
7.31
7.30
7.23
7.22
7.21
7.20
7.19
7.18
7.17
7.16
6.09
4.60
4.59
2.39
0.96
1.03
1.00
1.00
1.02
3.01
1.00
2.03
3.01
f1 (ppm)

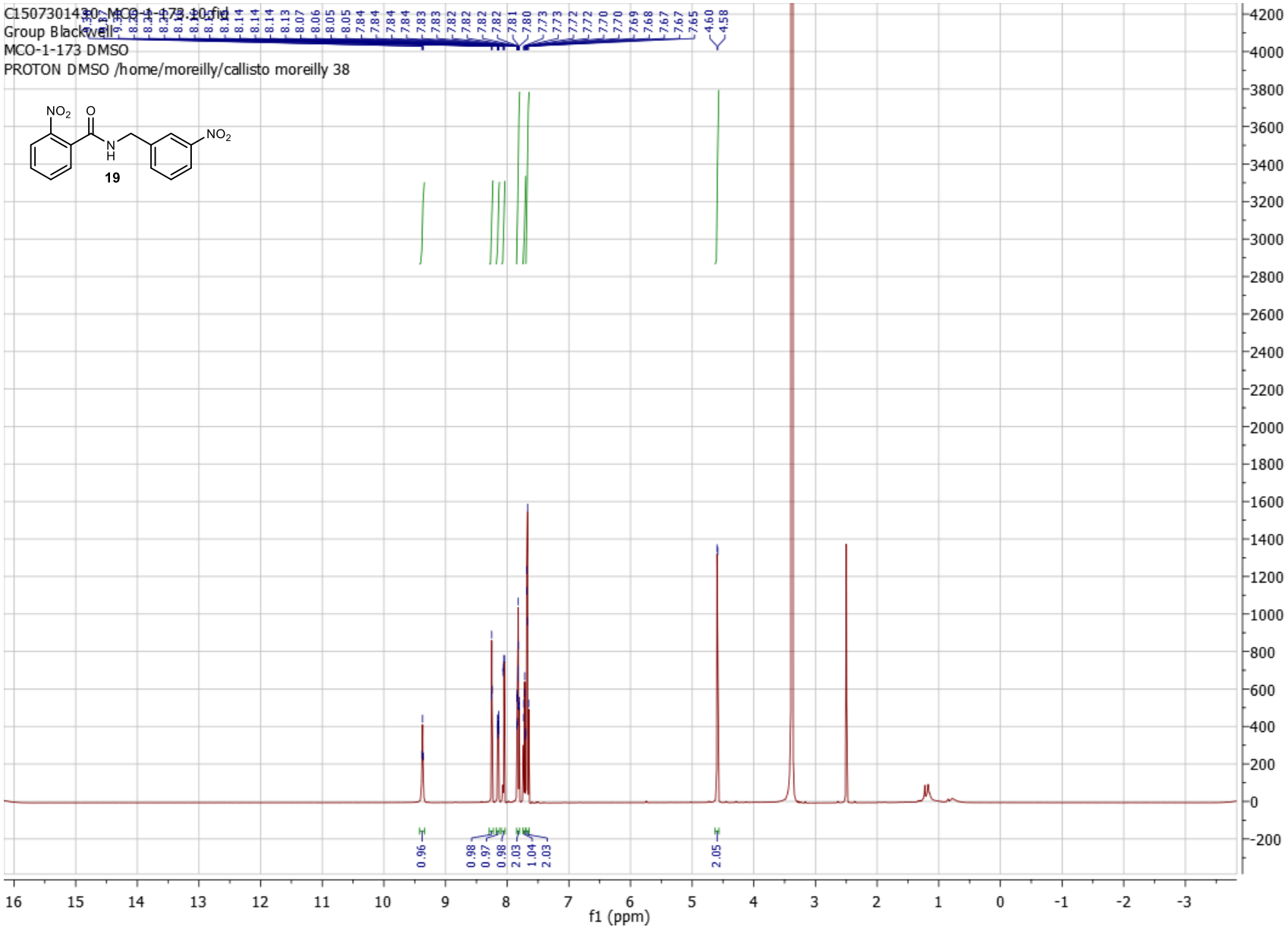

D1412041825_MCO-1-171.11.fid
Group Blackwell
MCO-1-171
C13CPD32 CDCl3 /home/moreilly/av400 moreilly 40
166.30
146.51
136.81
135.09
133.79
132.92
130.74
130.59
129.03
128.81
128.21
126.44
124.68
42.62
19.13
NO2
O
N
H
CH3
16
f1 (ppm)

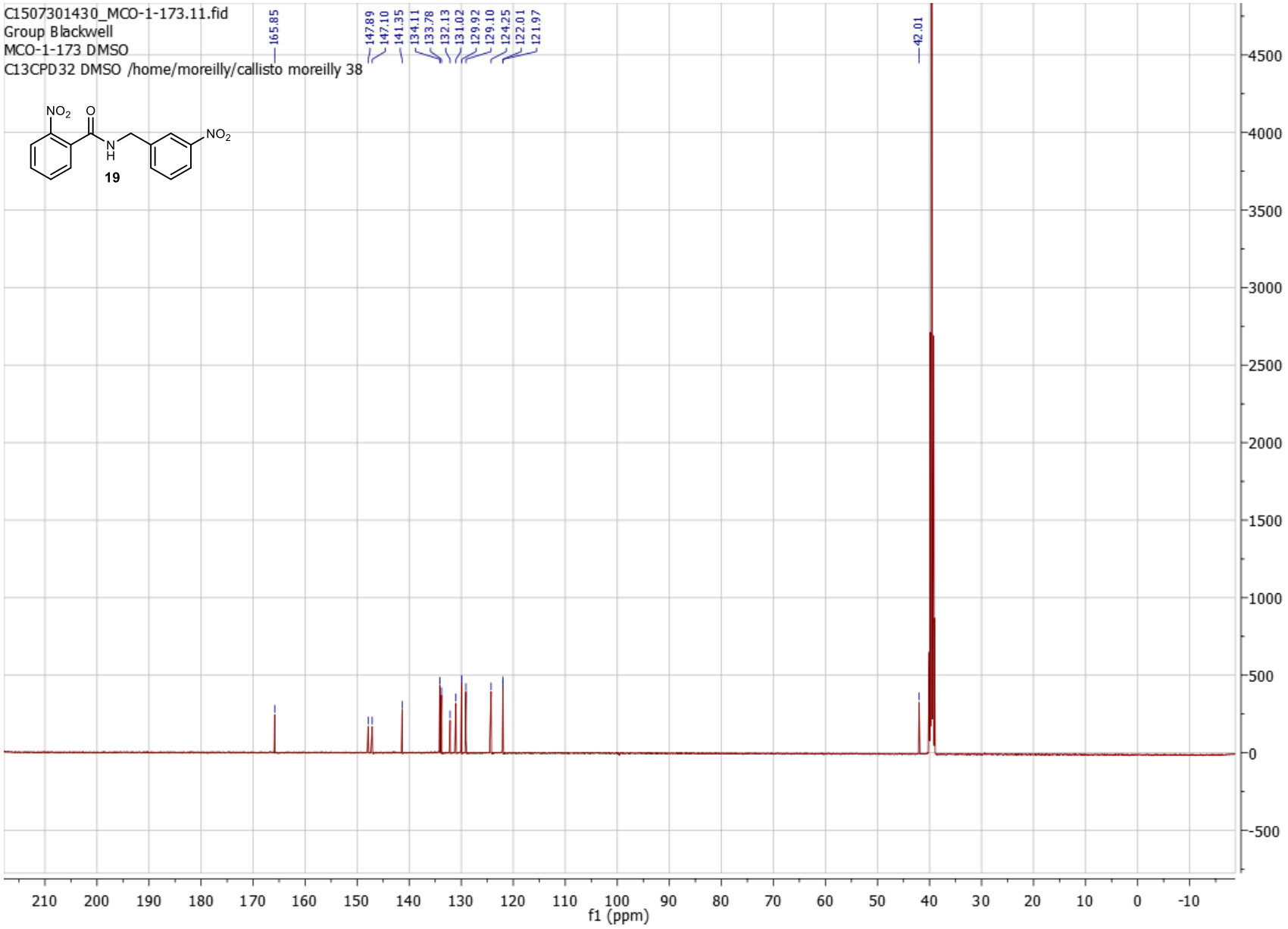

C1501271728_MCO-1-231-1H.fid
Group Blackwell
MCO-1-231
PROTON CDCl3 /home/moreilly/callisto moreilly 16
NO2
O
N
H
Br
17
f1 (ppm)

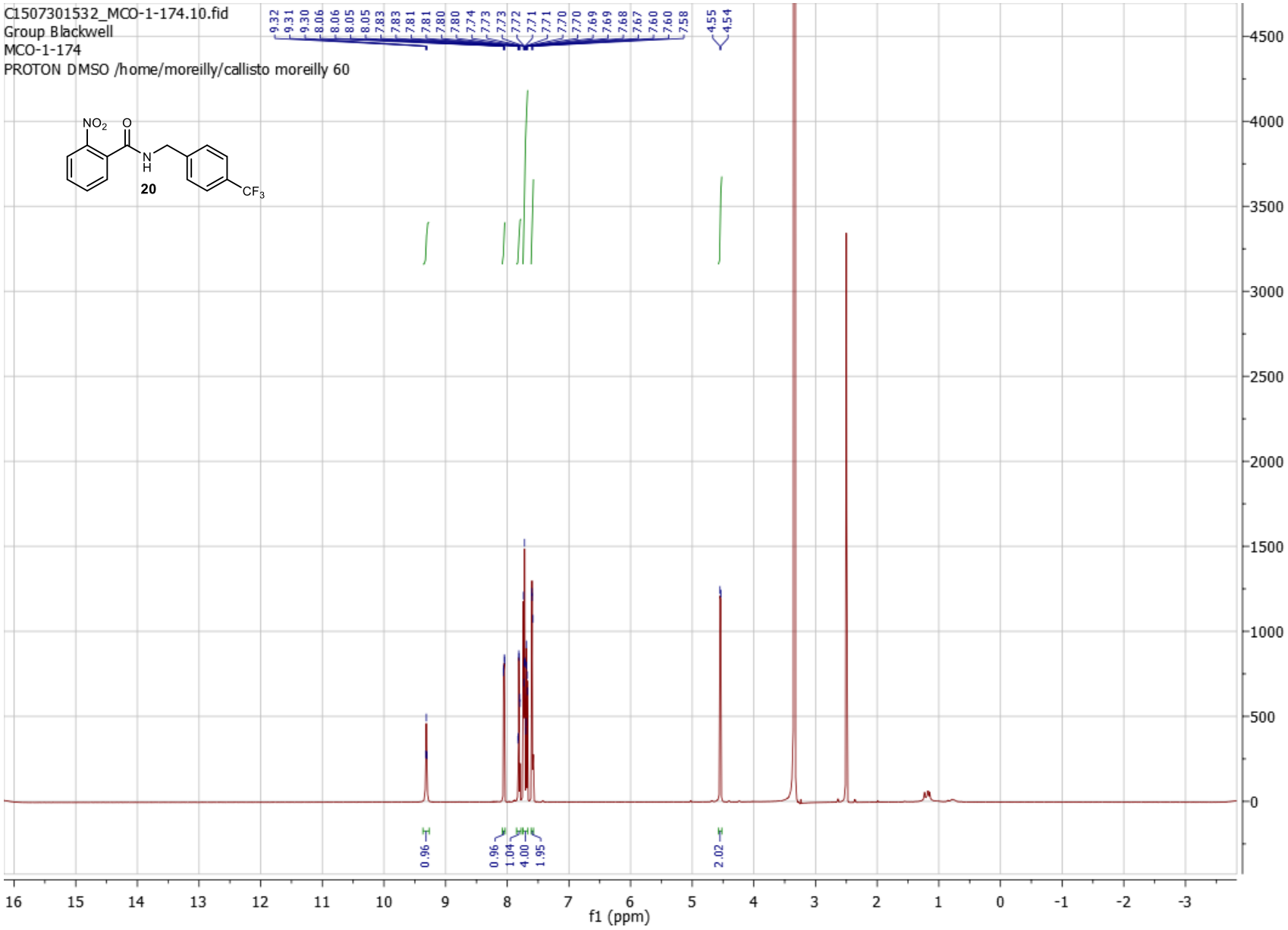

C1501271728_MCO-1-231.11.fid
Group Blackwell
MCO-1-231
C13CPD32 CDCl3 /home/moreilly/callisto moreilly 16
166.63
146.63
137.77
133.86
133.06
131.94
130.77
130.66
128.72
124.77
120.66
41.23
34.92
NO2
O
N
H
Br
17
f1 (ppm)

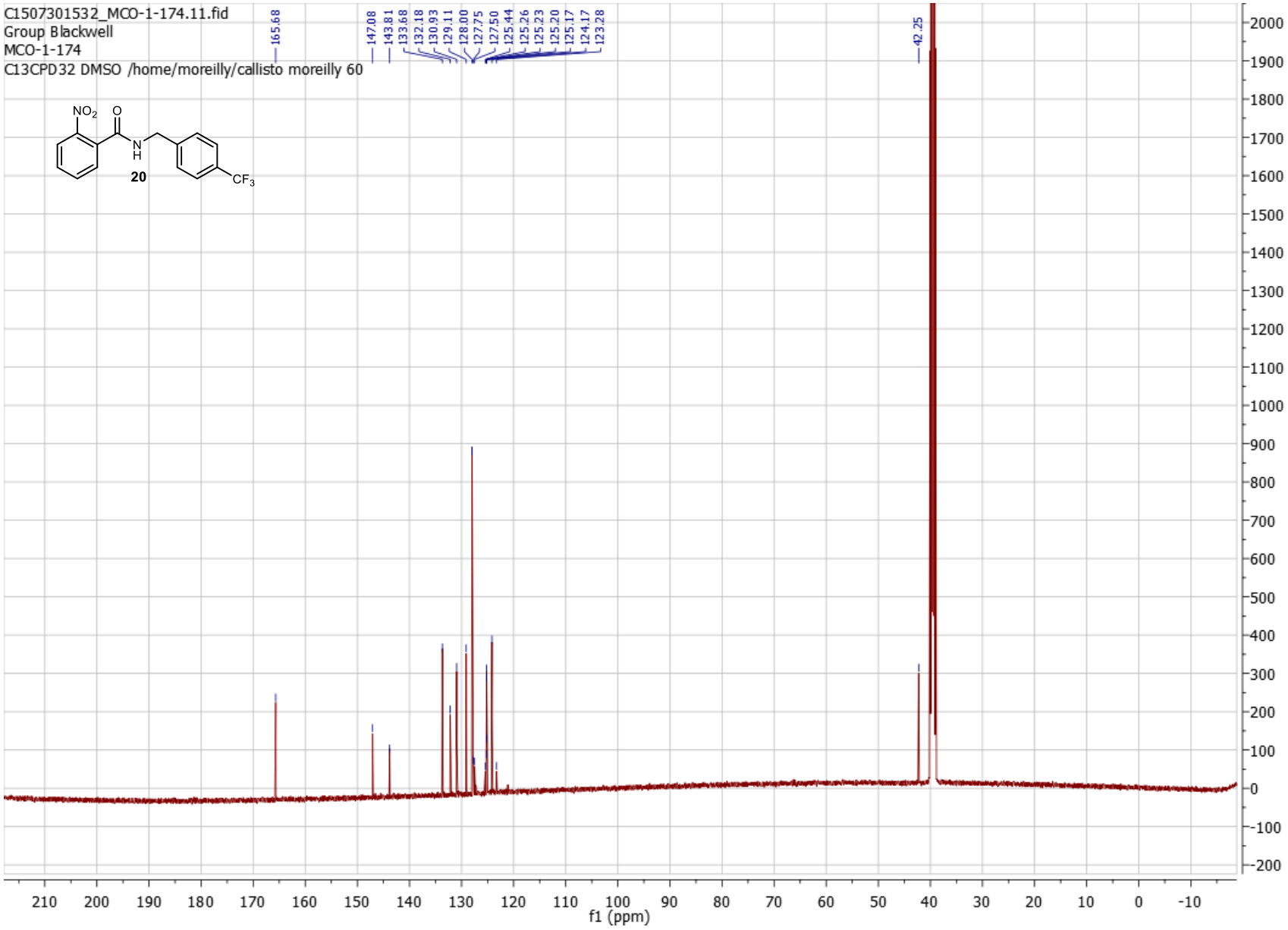

C1412080859_MCO-1-172.10.fid
Group Blackwell
MCO-1-172
PROTON CDCl3 /home/moreilly/callisto moreilly 27
8.09
8.07
8.04
8.03
7.83
7.82
7.70
7.69
7.67
7.66
7.64
7.58
7.57
7.55
7.52
7.51
7.49
7.47
6.76
6.74
6.73
4.87
4.86
NO2
O
N
H
NO2
18
0.98
1.00
1.04
2.10
1.06
2.07
1.00
2.04
f1 (ppm)

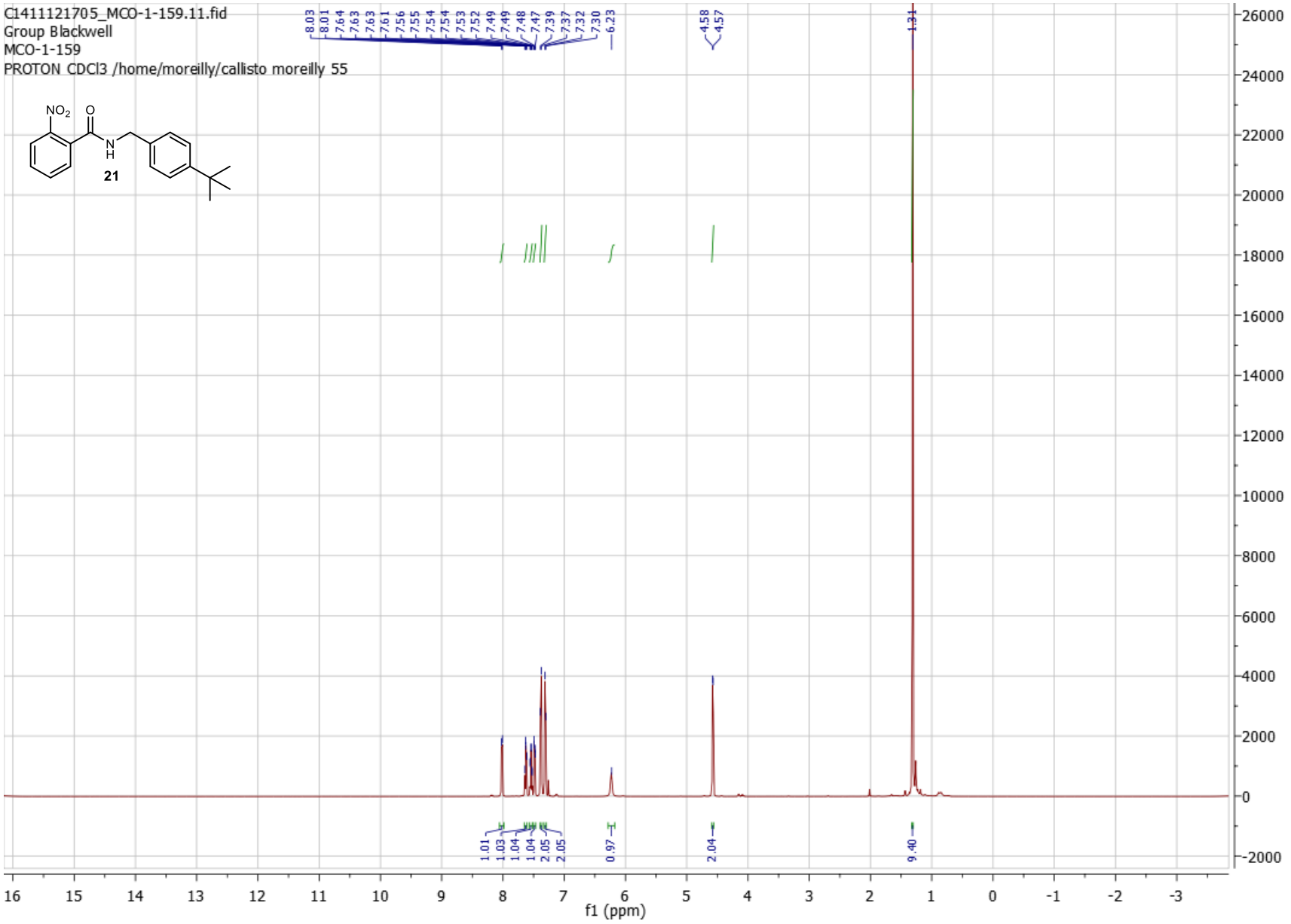

C1412080859_MCO-1-172.11.fid
Group Blackwell
MCO-1-172
C13CPD32 CDCl3 /home/moreilly/callisto moreilly 27
166.68
148.51
146.52
134.49
133.90
133.18
132.79
132.67
130.79
129.26
128.74
125.28
124.78
42.05
NO2
O
NO2
N
H
18
f1 (ppm)

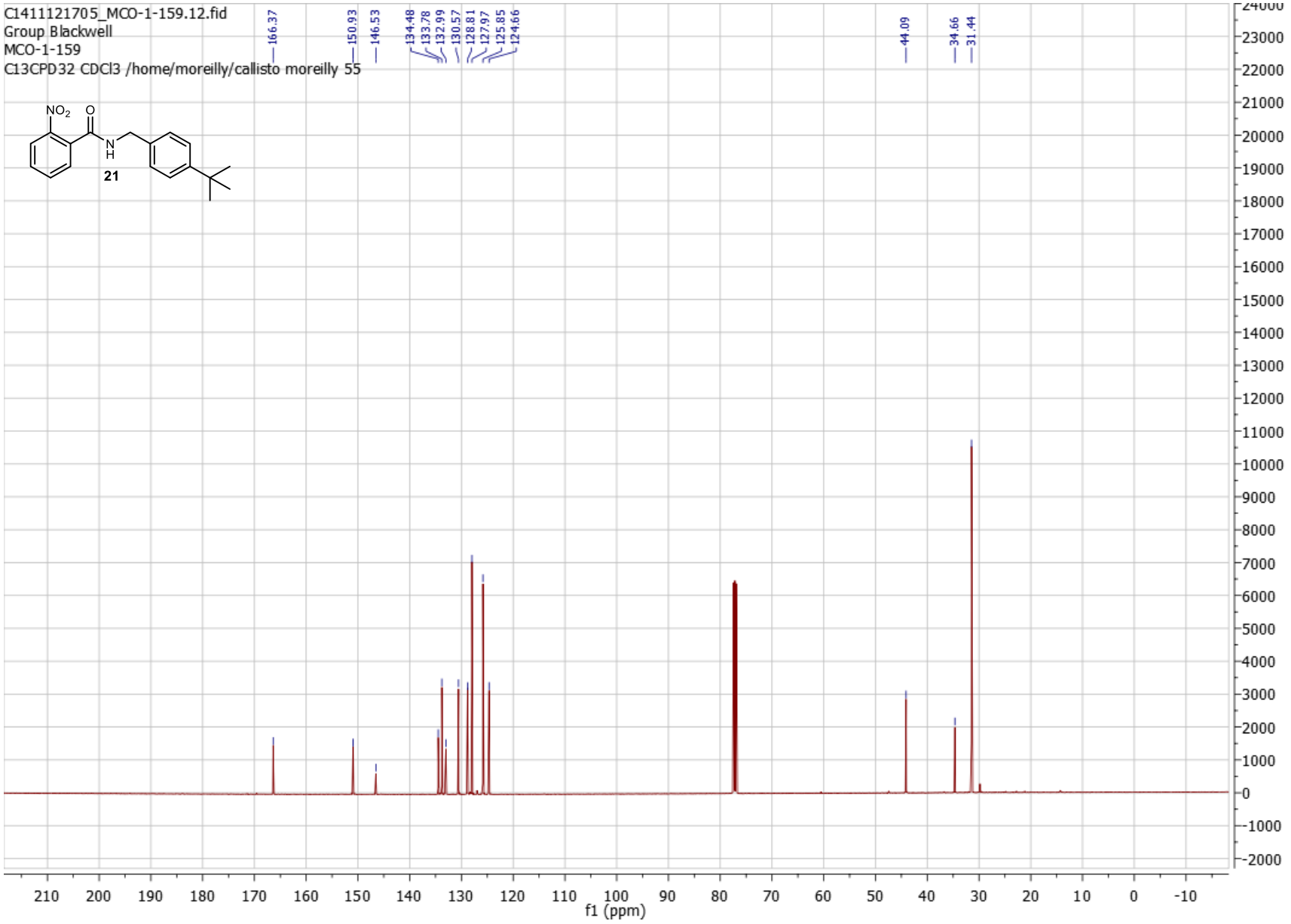

C150730143O_MCO-1-173_10.fid
Group Blackwell
MCO-1-173 DMSO
PROTON DMSO /home/moreilly/callisto moreilly 38
NO2
O
N
H
NO2
19
f1 (ppm)

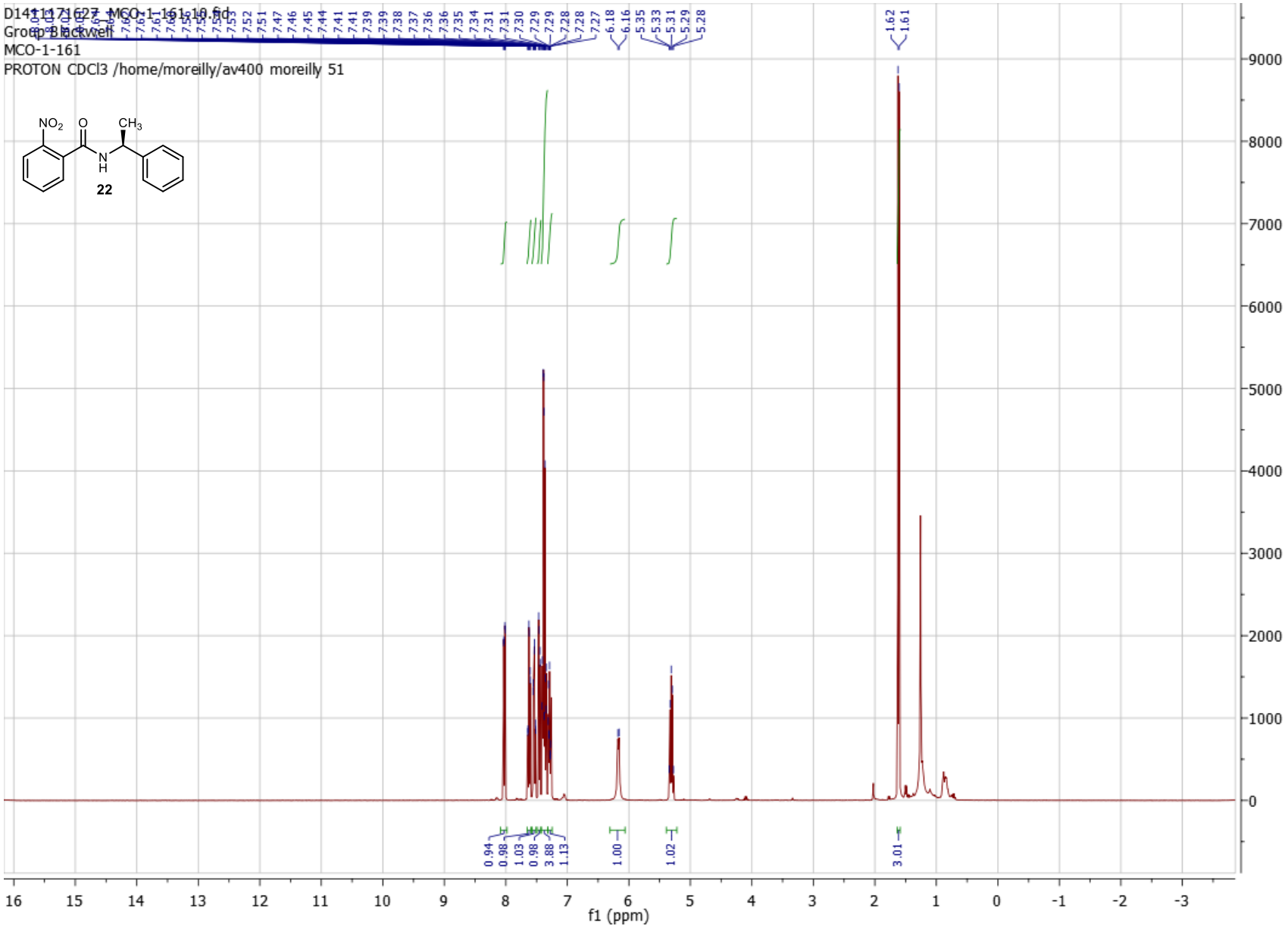

C1507301430_MCO-1-173.11.fid
Group Blackwell
MCO-1-173 DMSO
C13CPD32 DMSO /home/moreilly/callisto moreilly 38
165.85
147.89
147.10
141.35
134.11
133.78
132.13
131.02
129.92
129.10
124.25
122.01
121.97
42.01
NO2
O
N
H
NO2
19
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

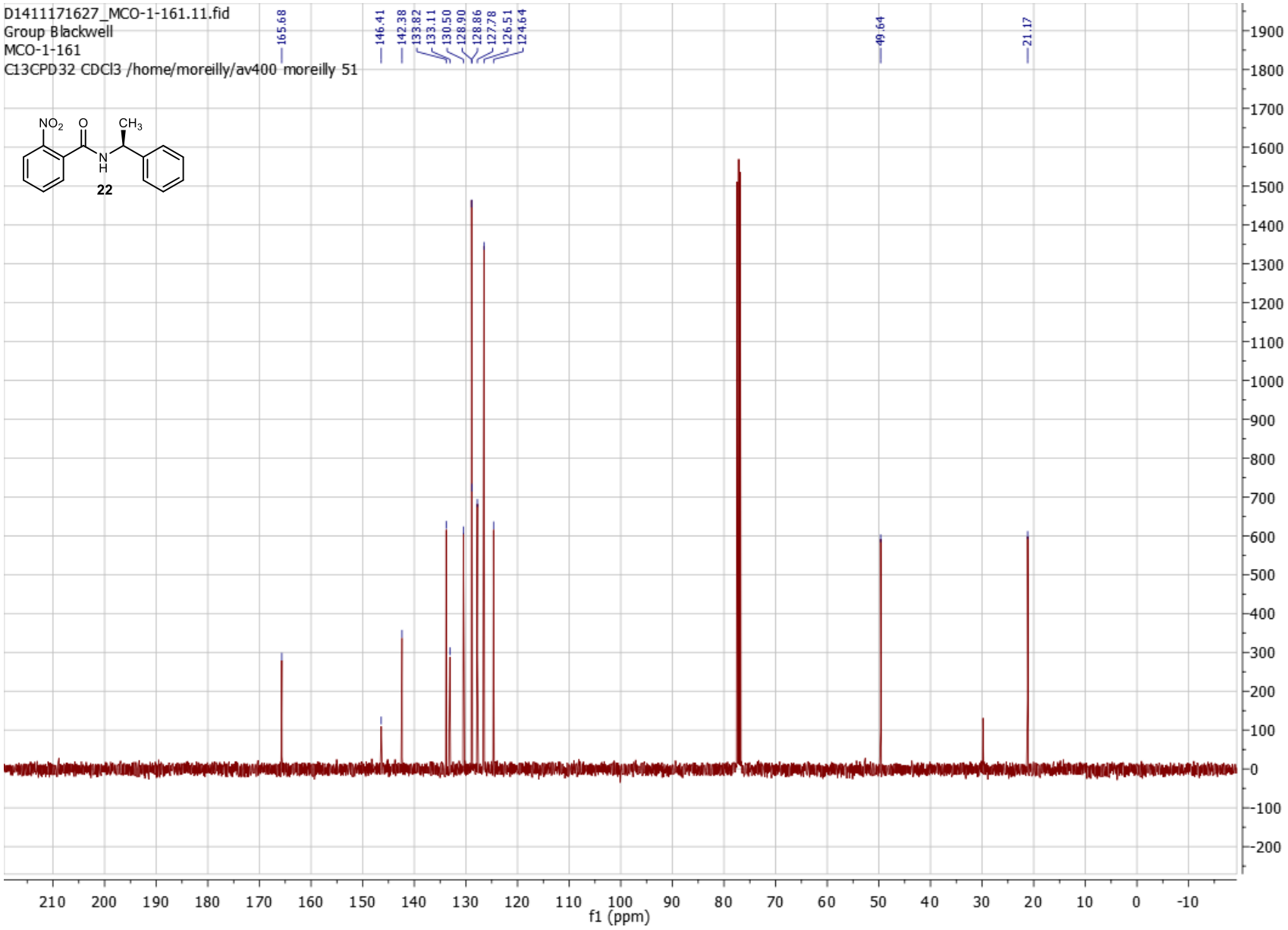

C1507301532_MCO-1-174.10.fid
Group Blackwell
MCO-1-174
PROTON DMSO /home/moreilly/callisto moreilly 60
NO2
O
N
H
CF3
20
9.32
9.31
9.30
8.06
8.06
8.05
8.05
7.83
7.83
7.81
7.81
7.80
7.80
7.74
7.73
7.73
7.72
7.71
7.71
7.70
7.70
7.69
7.69
7.68
7.67
7.60
7.60
7.58
4.55
4.54
0.96
0.96
1.04
4.00
1.95
2.02
f1 (ppm)

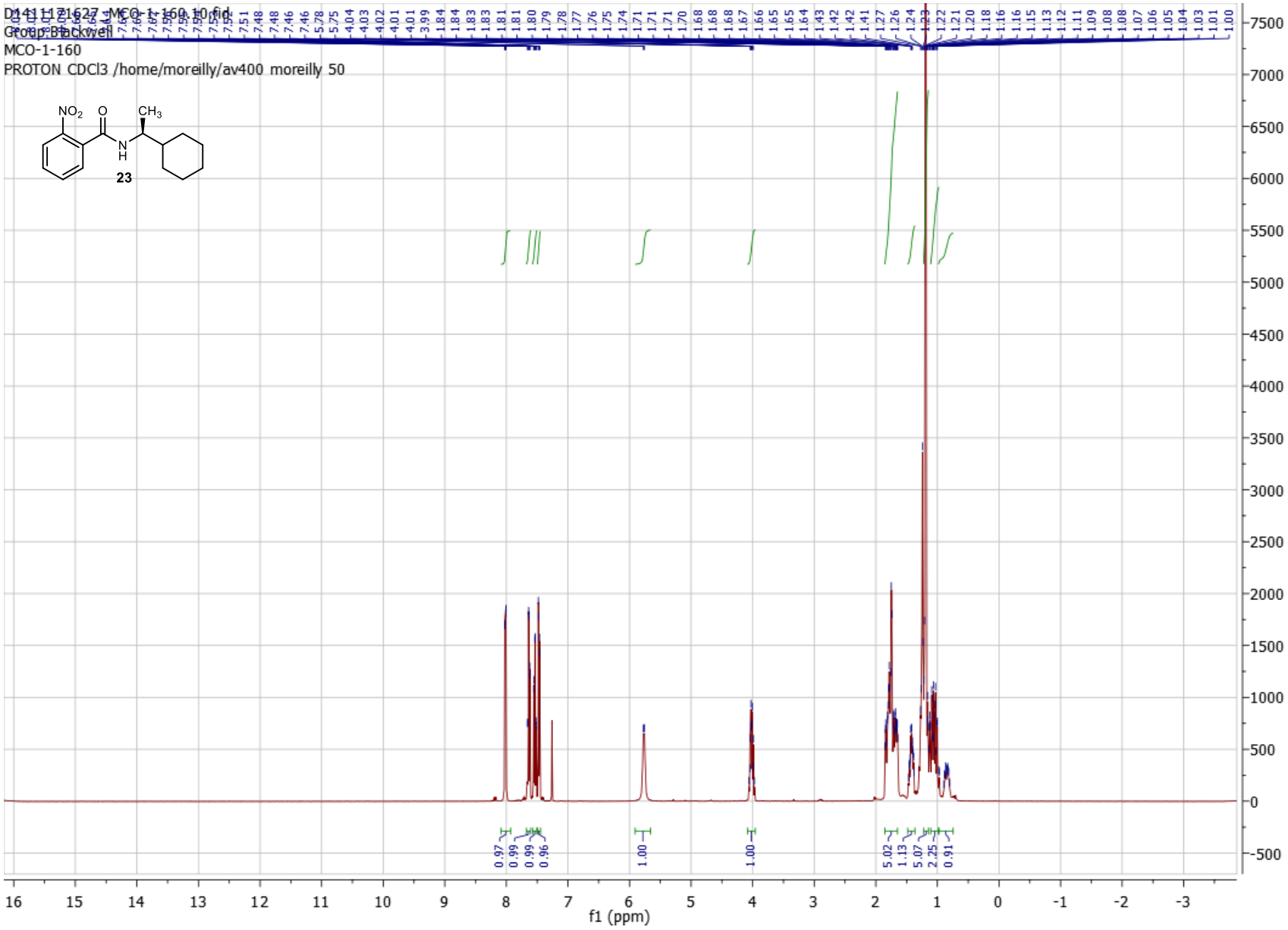

C1507301532_MCO-1-174.11.fid
Group Blackwell
MCO-1-174
C13CPD32 DMSO /home/moreilly/callisto moreilly 60
165.68
147.08
143.81
133.68
132.18
130.93
129.11
128.00
127.75
127.50
125.44
125.26
125.23
125.20
125.17
124.17
123.28
42.25
NO2
O
N
H
CF3
20
f1 (ppm)

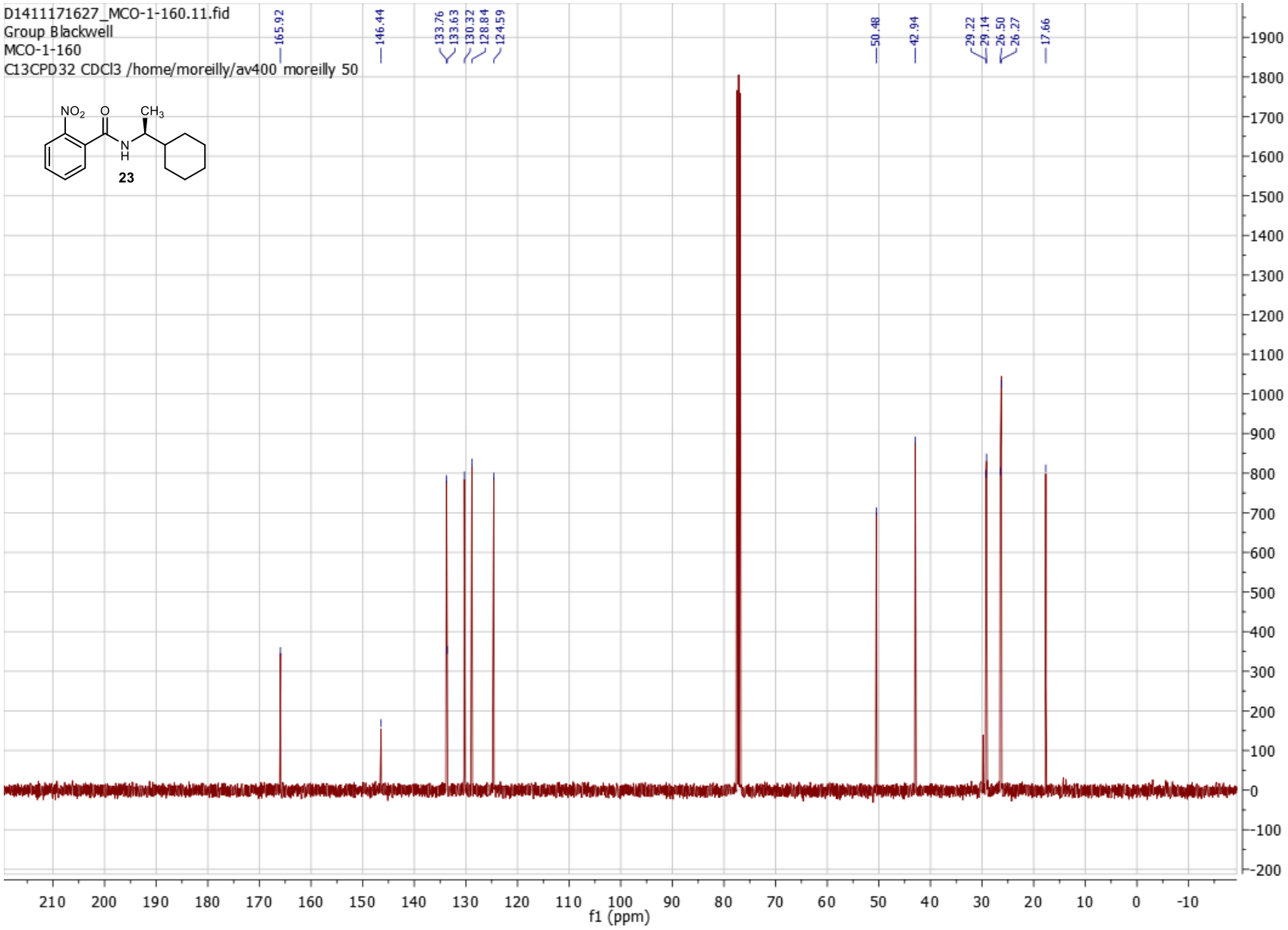

C1411121705_MCO-1-159.11.fid
Group Blackwell
MCO-1-159
PROTON CDCl3 /home/moreilly/callisto moreilly 55
NO2
O
N
H
21
8.03
8.01
7.64
7.63
7.63
7.61
7.56
7.55
7.54
7.54
7.53
7.52
7.49
7.49
7.48
7.47
7.39
7.37
7.32
7.30
6.23
4.58
4.57
1.31
1.01
1.03
1.04
1.04
2.05
2.05
0.97
2.04
9.40
f1 (ppm)

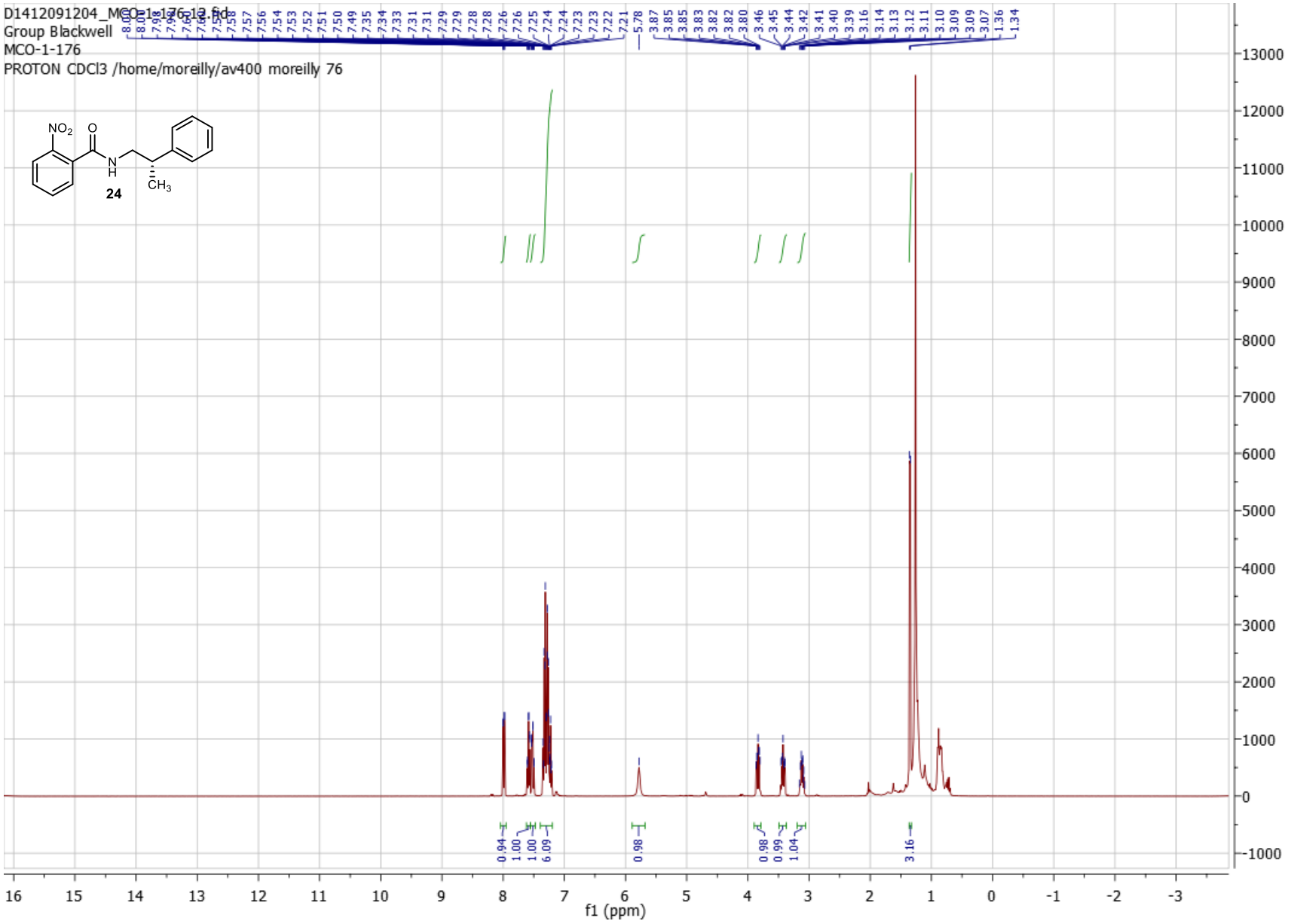

C1411121705_MCO-1-159.12.fid
Group Blackwell
MCO-1-159
C13CPD32 CDCl3 /home/moreilly/callisto moreilly 55
166.37
150.93
146.53
134.48
133.78
132.99
130.57
128.81
127.97
125.85
124.66
44.09
34.66
31.44
NO2
O
N
H
21
f1 (ppm)

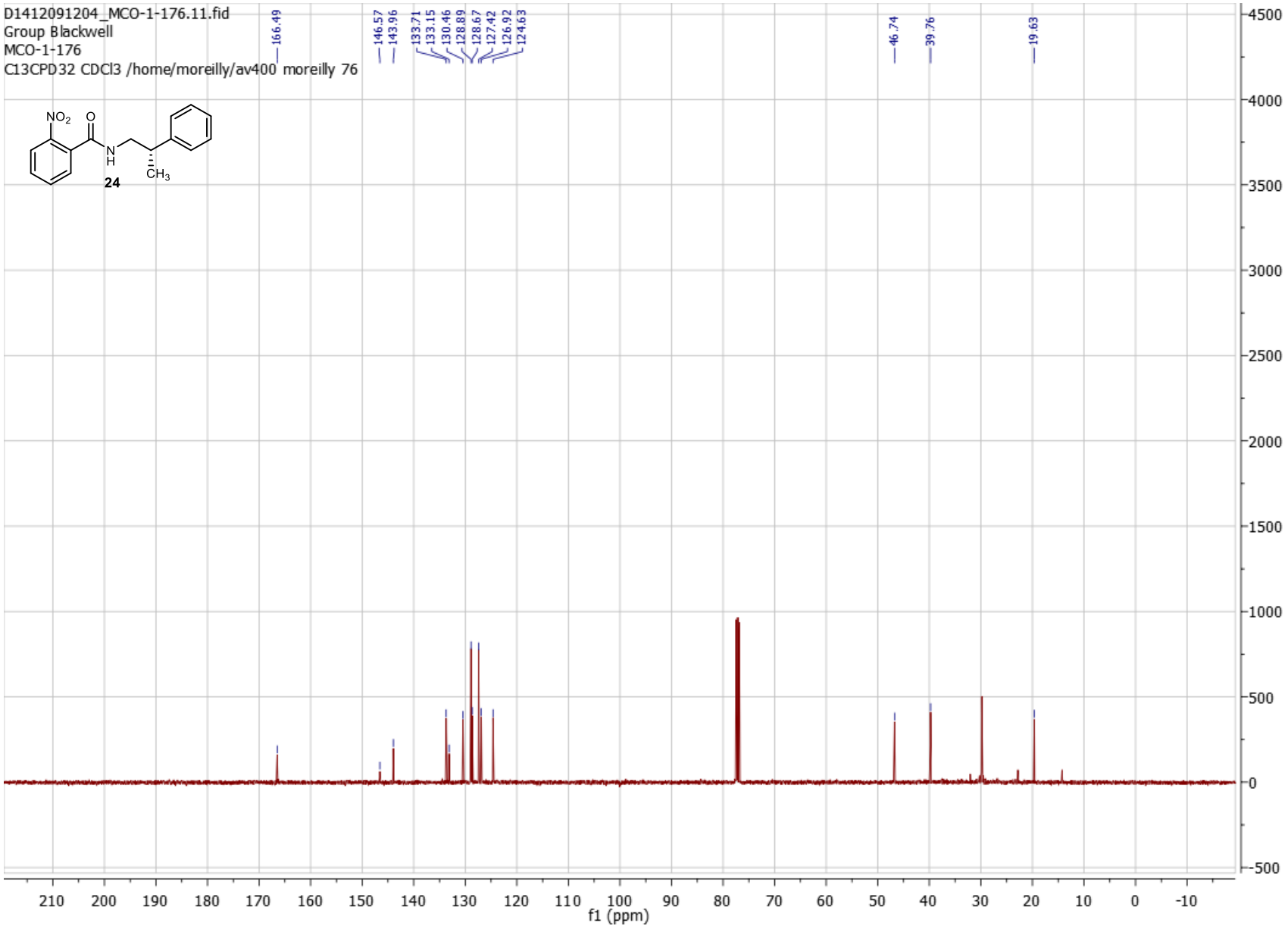

D141117627 MCO-1-161-10.fid
Group Blackwell
MCO-1-161
PROTON CDCl3 /home/moreilly/av400 moreilly 51
NO2
O
CH3
N
H
22
7.66
7.61
7.55
7.53
7.52
7.51
7.47
7.46
7.45
7.44
7.41
7.41
7.39
7.39
7.38
7.37
7.36
7.36
7.35
7.34
7.31
7.31
7.30
7.29
7.29
7.28
7.27
6.18
6.16
5.35
5.33
5.31
5.29
5.28
1.62
1.61
0.94
0.98
1.03
0.98
3.88
1.13
1.00
1.02
3.01
f1 (ppm)

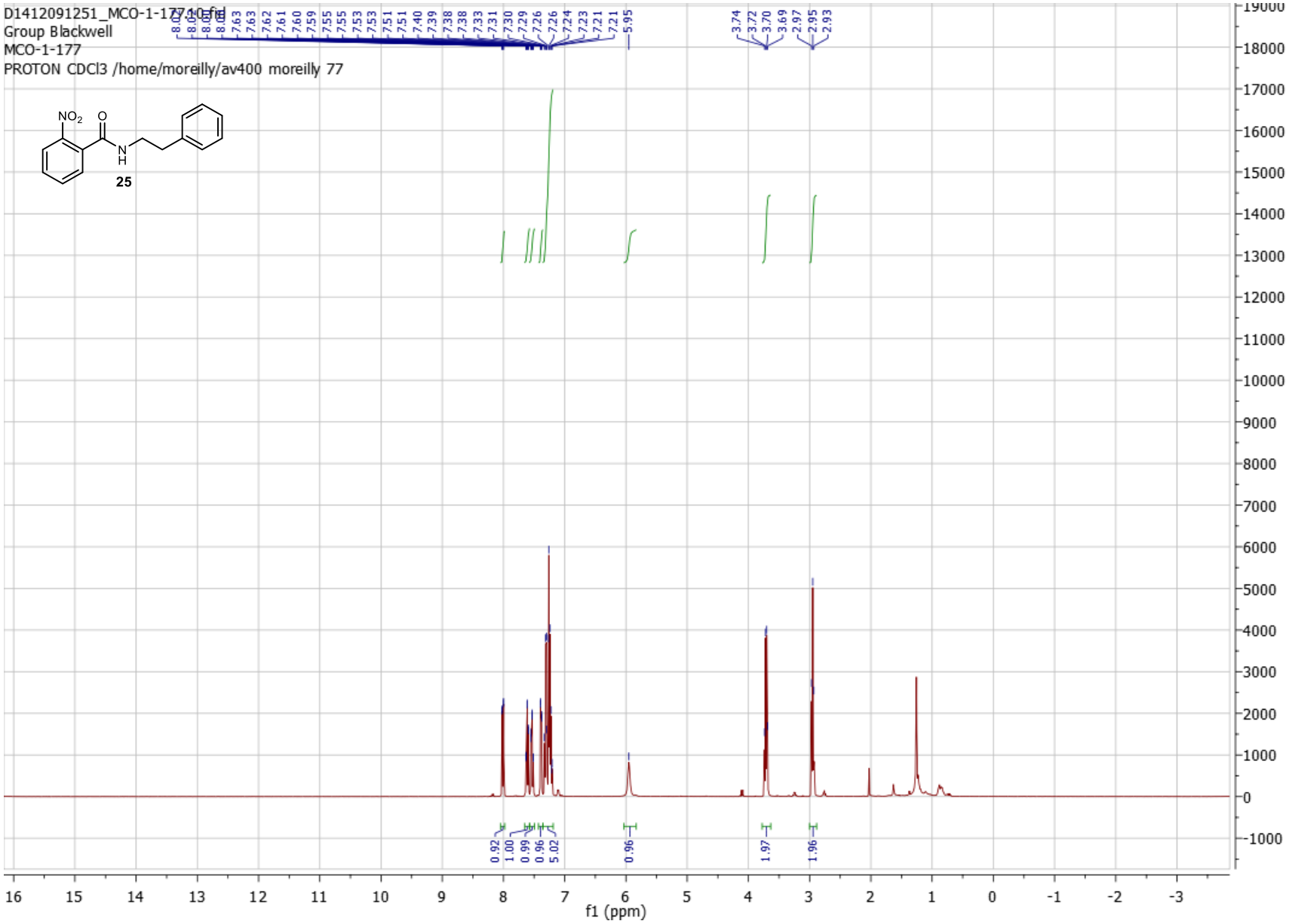

D1411171627_MCO-1-161.11.fid
Group Blackwell
MCO-1-161
C13CPD32 CDCl3 /home/moreilly/av400 moreilly 51
165.68
146.41
142.38
133.82
133.11
130.50
128.90
128.86
127.78
126.51
124.64
49.64
21.17
NO2
O
CH3
N
H
22
f1 (ppm)

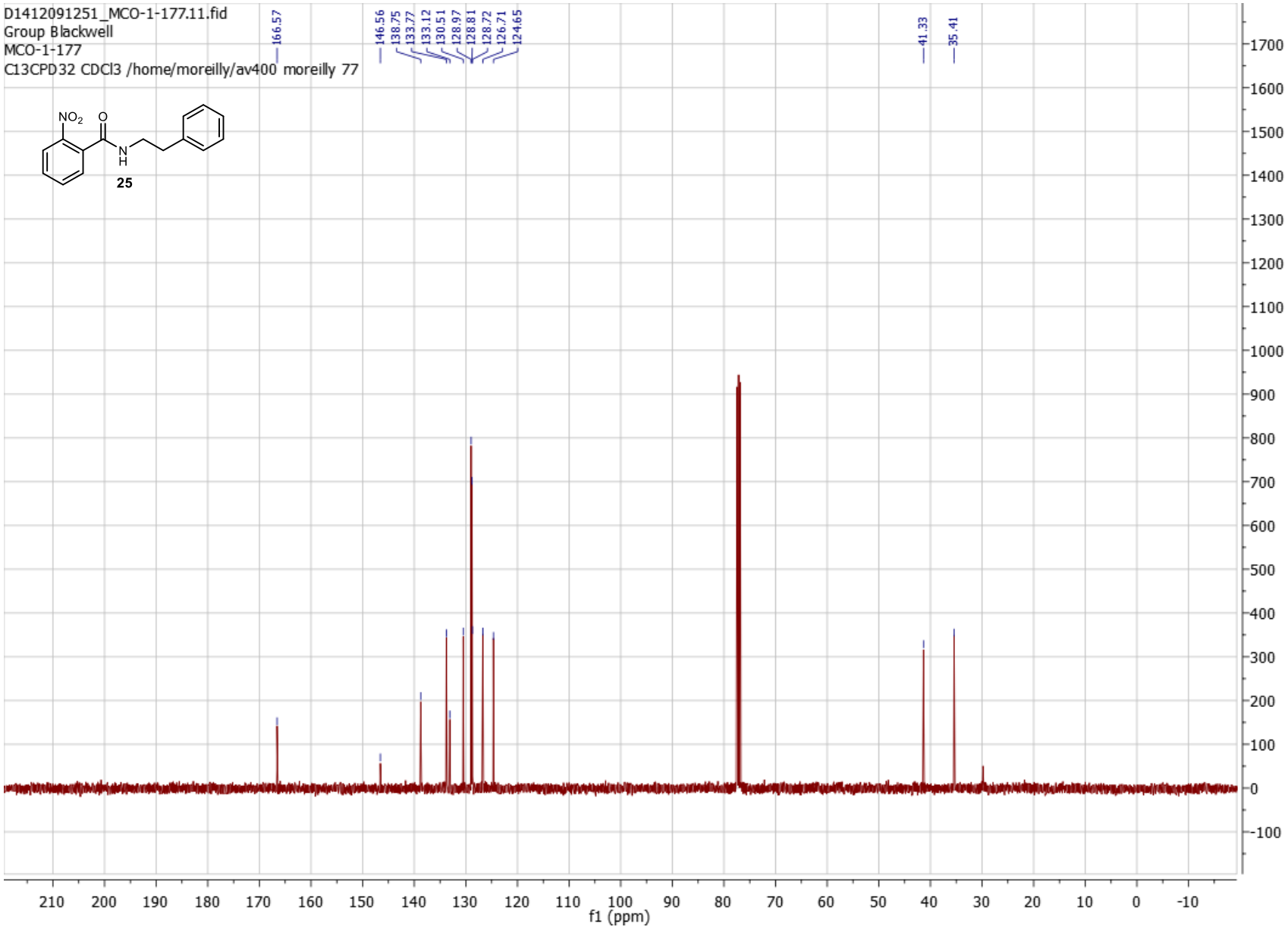

D141117627 MCO-1-160 10.fid
Group Blackwell
MCO-1-160
PROTON CDCl3 /home/moreilly/av400 moreilly 50
NO2
O
CH3
N
H
23
f1 (ppm)

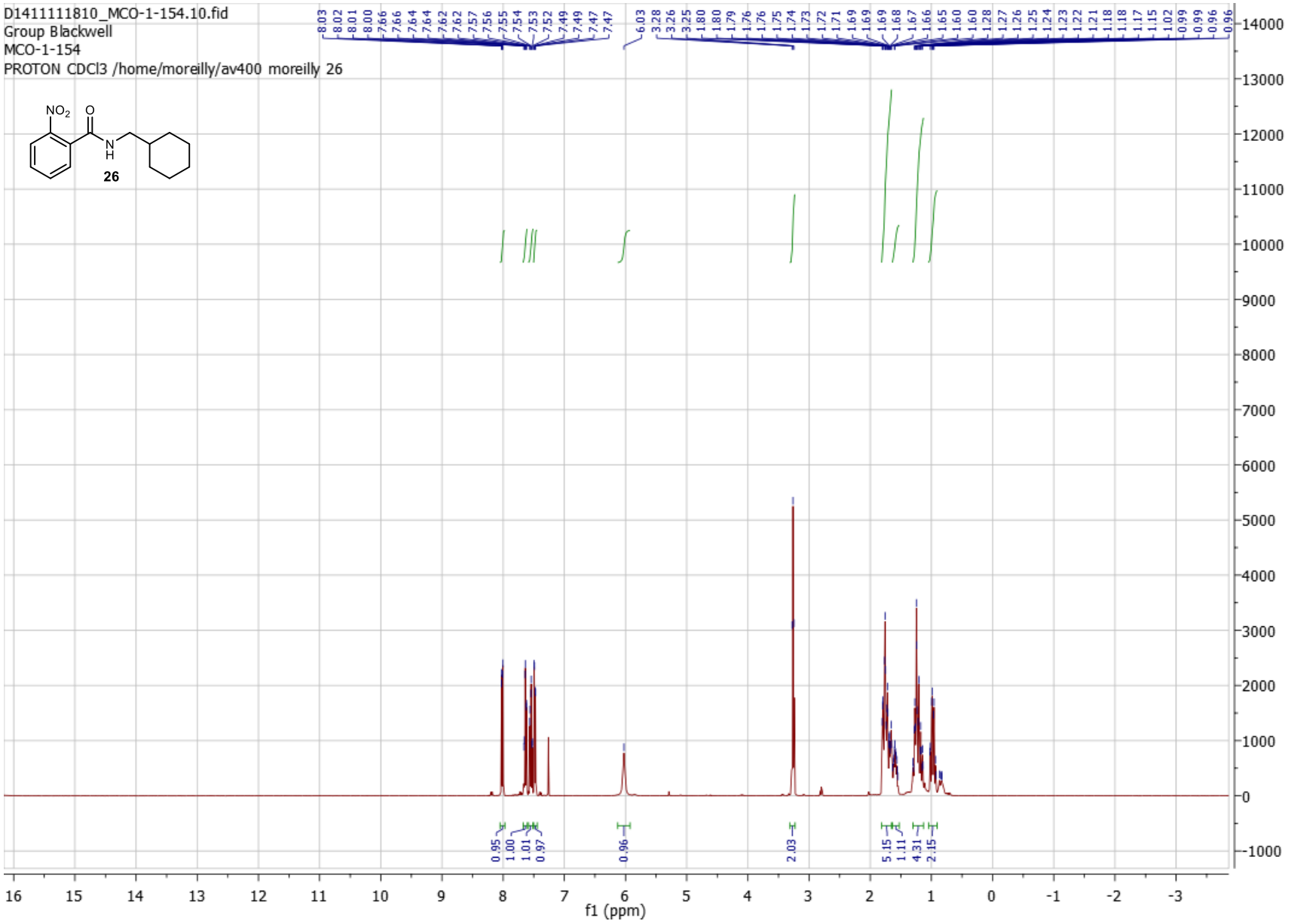

D1411171627_MCO-1-160.11.fid
Group Blackwell
MCO-1-160
C13CPD32 CDCl3 /home/moreilly/av400 moreilly 50
165.92
146.44
133.76
133.63
130.32
128.84
124.59
50.48
42.94
29.22
29.14
26.50
26.27
17.66
NO2
O
CH3
N
H
23
f1 (ppm)

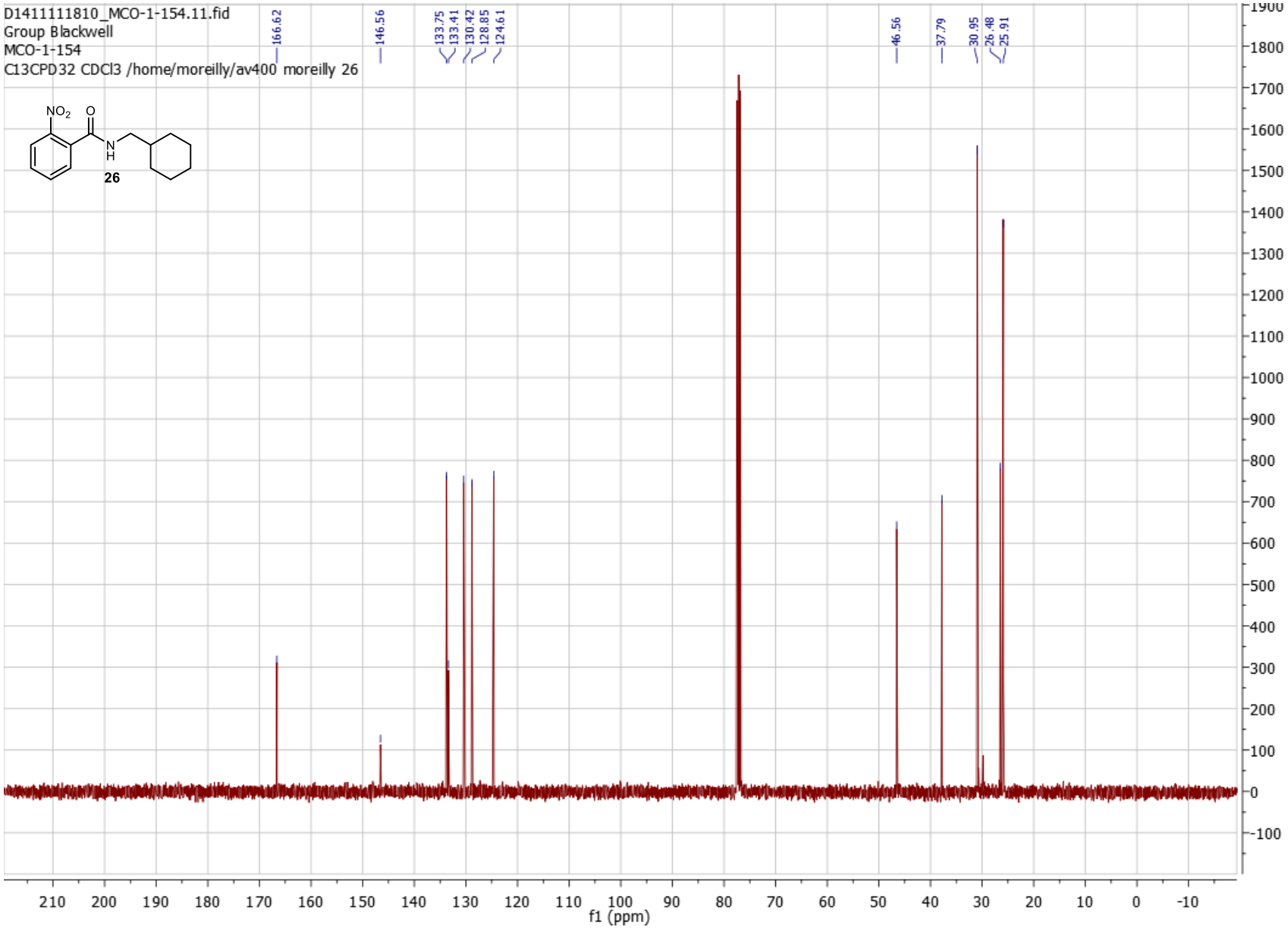

D1412091204_MCO-1-176-13.fid
Group Blackwell
MCO-1-176
PROTON CDCl3 /home/moreilly/av400 moreilly 76
NO2
O
N
H
CH3
24
f1 (ppm)

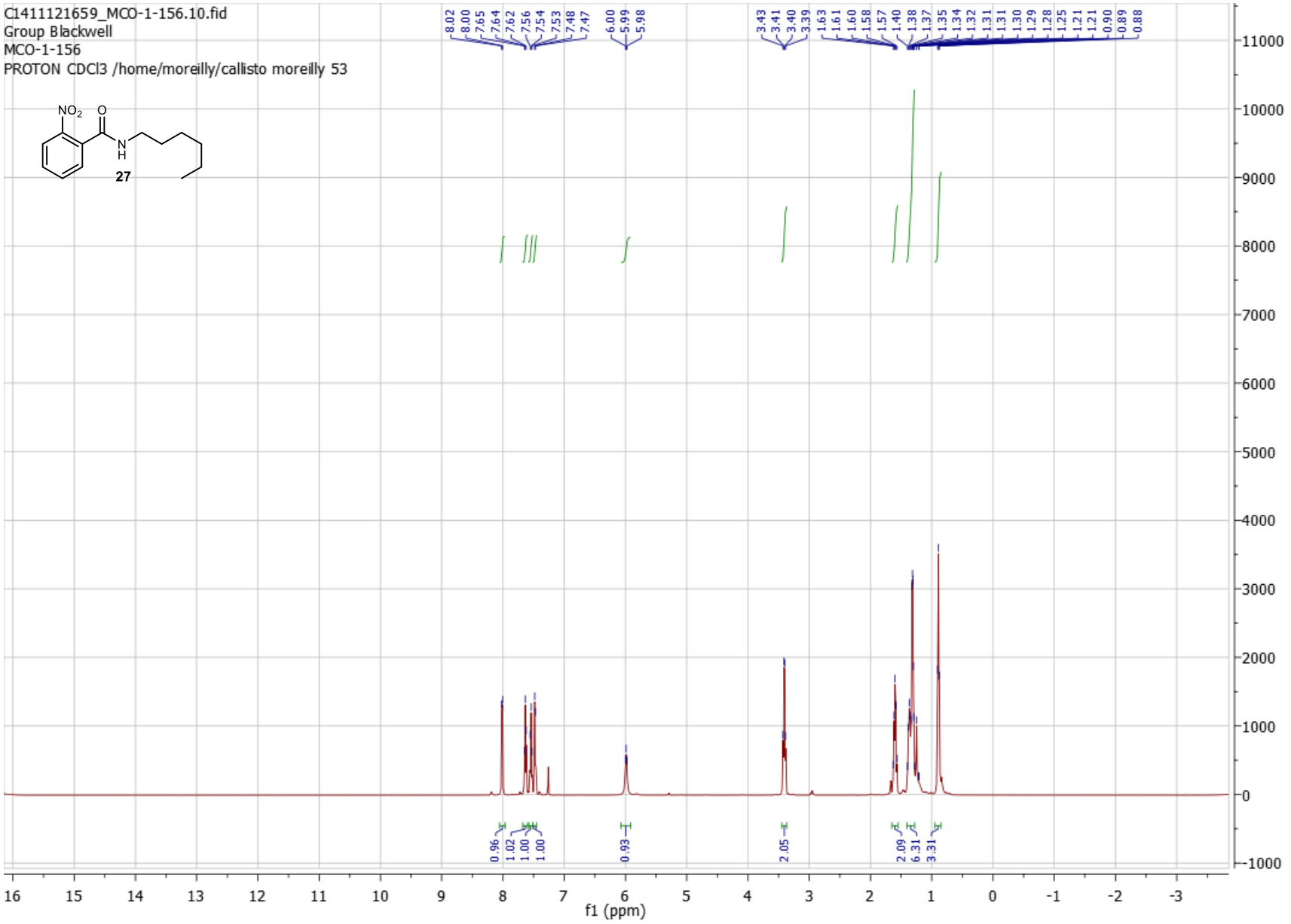

D1412091204_MCO-1-176.11.fid
Group Blackwell
MCO-1-176
C13CPD32 CDCl3 /home/moreilly/av400 moreilly 76
166.49
146.57
143.96
133.71
133.15
130.46
128.89
128.67
127.42
126.92
124.63
46.74
39.76
19.63
NO2
O
N
H
CH3
24
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

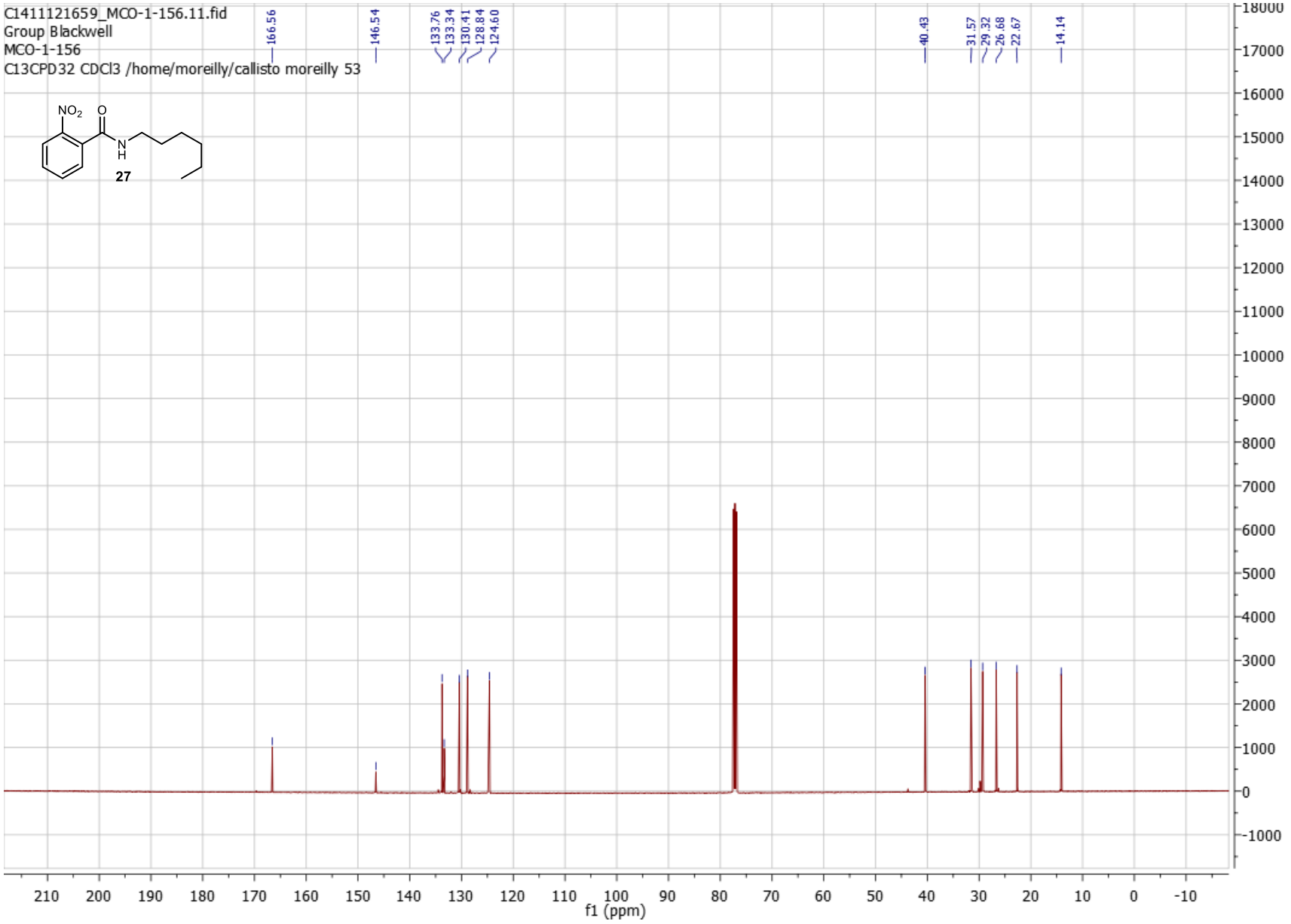

D1412091251_MCO-1-177-10.fid
Group Blackwell
MCO-1-177
PROTON CDCl3 /home/moreilly/av400 moreilly 77
NO2
O
N
H
25
f1 (ppm)

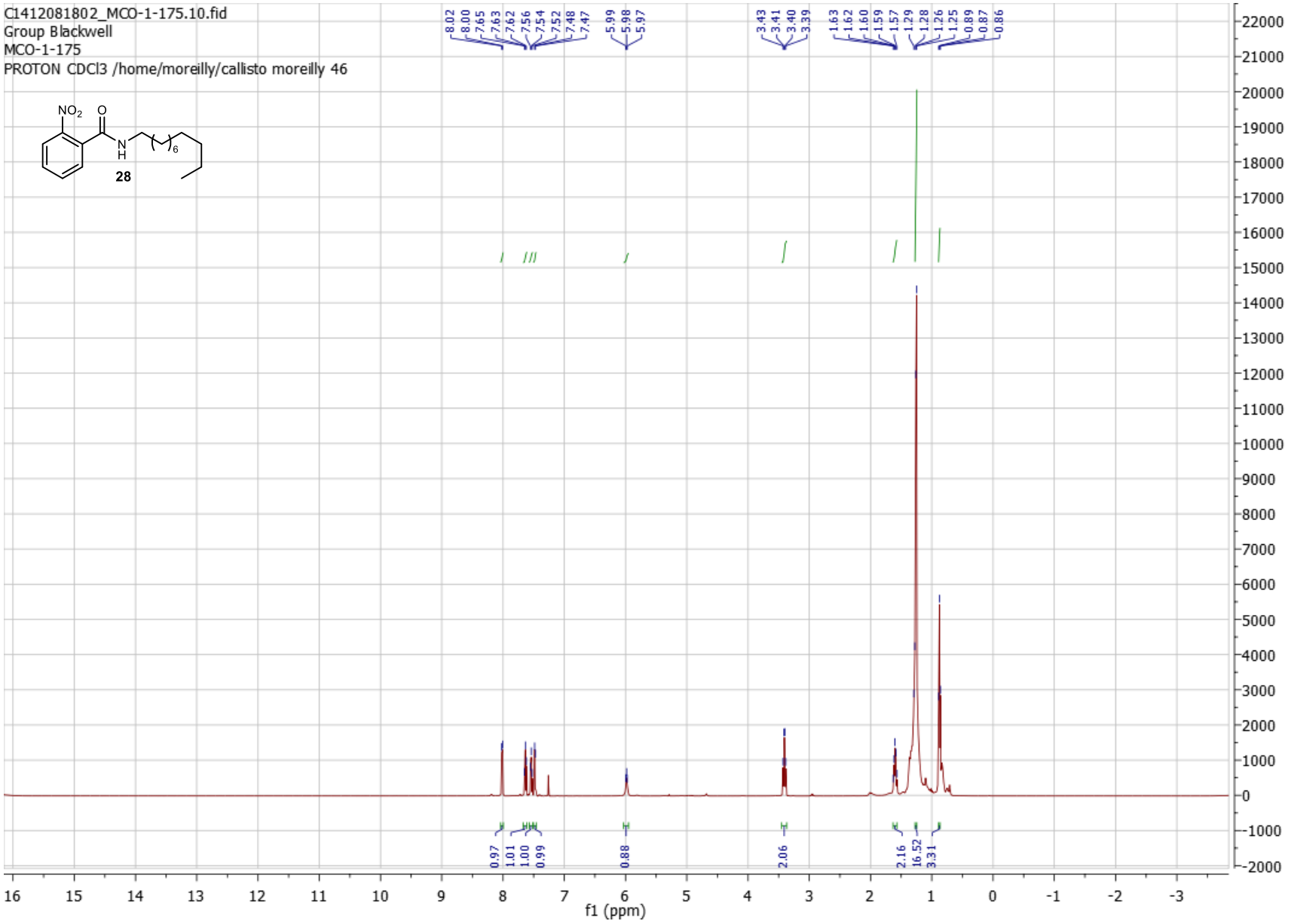

D1412091251_MCO-1-177.11.fid
Group Blackwell
MCO-1-177
C13CPD32 CDCl3 /home/moreilly/av400 moreilly 77
166.57
146.56
138.75
133.77
133.12
130.51
128.97
128.81
128.72
126.71
124.65
41.33
35.41
NO2
O
N
H
25
f1 (ppm)

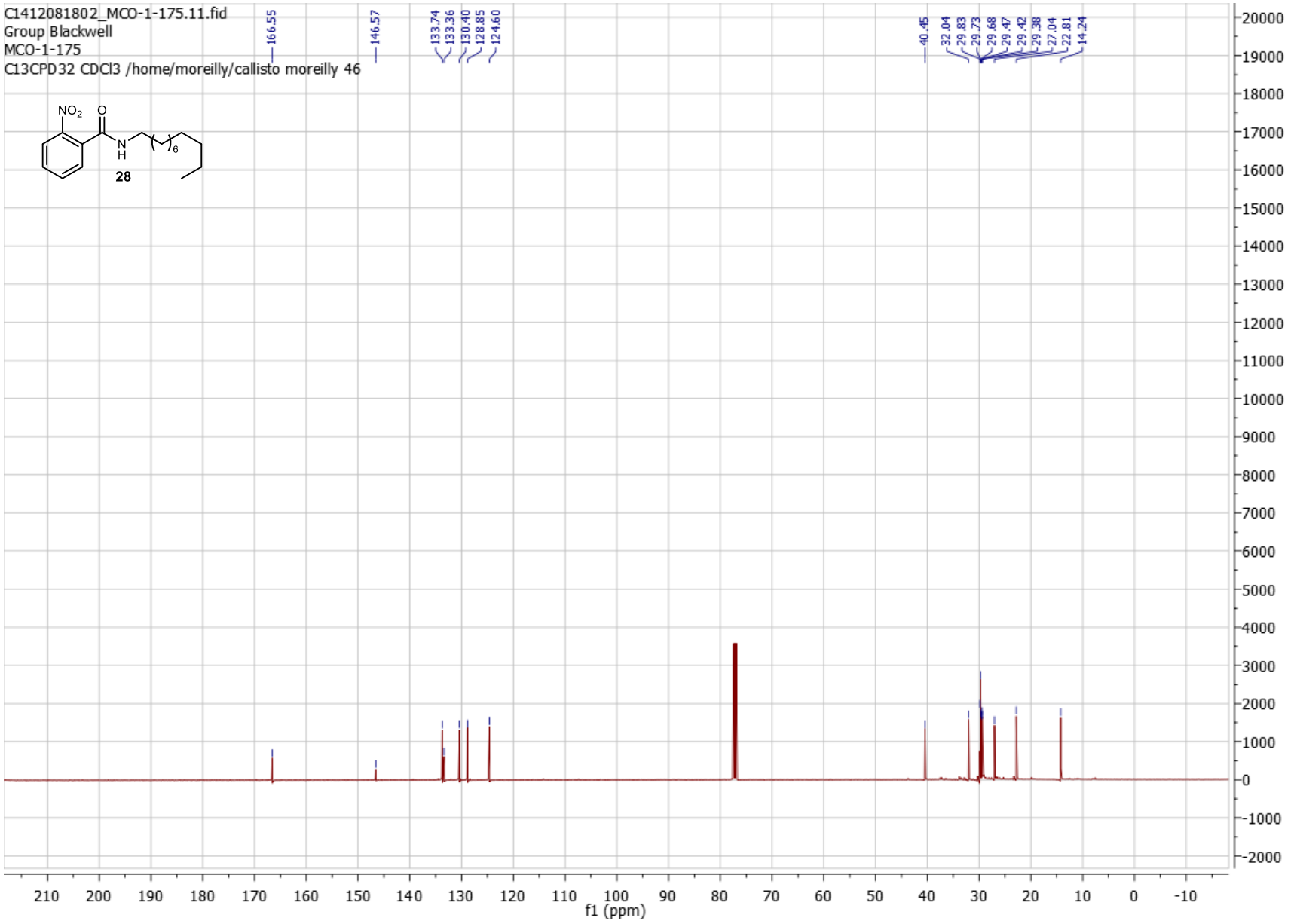

D1411111810_MCO-1-154.10.fid
Group Blackwell
MCO-1-154
PROTON CDCl3 /home/moreilly/av400 moreilly 26
NO2
O
N
H
26
f1 (ppm)

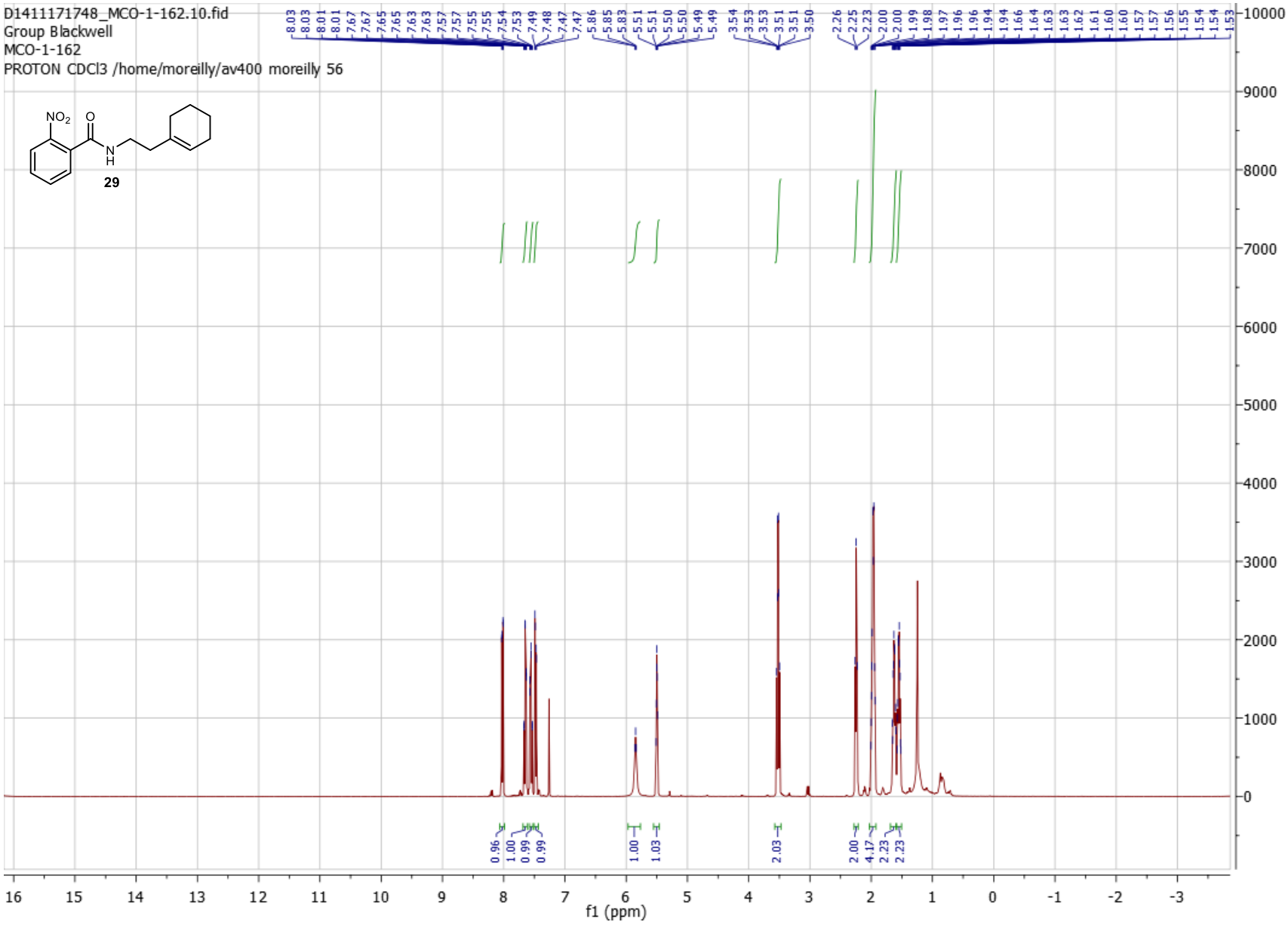

D1411111810_MCO-1-154.11.fid
Group Blackwell
MCO-1-154
C13CPD32 CDCl3 /home/moreilly/av400 moreilly 26
166.62
146.56
133.75
133.41
130.42
128.85
124.61
46.56
37.79
30.95
26.48
25.91
NO2
O
N
H
26
f1 (ppm)

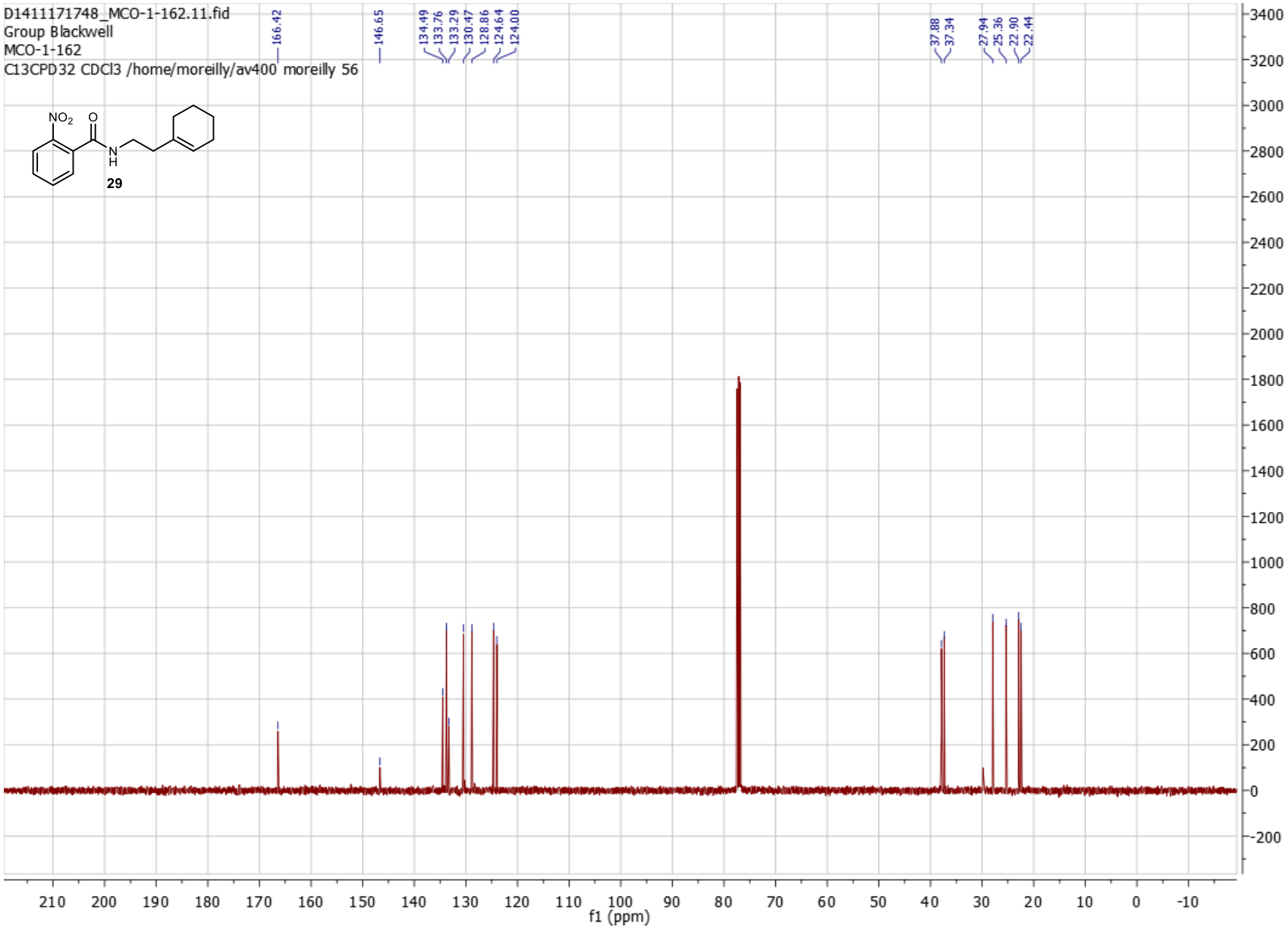

C1411121659_MCO-1-156.10.fid
Group Blackwell
MCO-1-156
PROTON CDCl3 /home/moreilly/callisto moreilly 53
NO2
O
N
H
27
8.02
8.00
7.65
7.64
7.62
7.56
7.54
7.53
7.48
7.47
6.00
5.99
5.98
3.43
3.41
3.40
3.39
1.63
1.61
1.60
1.58
1.57
1.40
1.38
1.37
1.35
1.34
1.32
1.31
1.31
1.30
1.29
1.28
1.25
1.21
1.21
0.90
0.89
0.88
0.96
1.02
1.00
1.00
0.93
2.05
2.09
6.31
3.31
f1 (ppm)


C1411121659_MCO-1-156.11.fid
Group Blackwell
MCO-1-156
C13CPD32 CDCl3 /home/moreilly/callisto moreilly 53
166.56
146.54
133.76
133.34
130.41
128.84
124.60
40.43
31.57
29.32
26.68
22.67
14.14
NO2
O
N
H
27
f1 (ppm)


C1412081802_MCO-1-175.10.fid
Group Blackwell
MCO-1-175
PROTON CDCl3 /home/moreilly/callisto moreilly 46
NO2
O
N
H
6
28
8.02
8.00
7.65
7.63
7.62
7.56
7.54
7.52
7.48
7.47
5.99
5.98
5.97
3.43
3.41
3.40
3.39
1.63
1.62
1.60
1.59
1.57
1.29
1.28
1.26
1.25
0.89
0.87
0.86
0.97
1.01
1.00
0.99
0.88
2.06
2.16
16.52
3.31
f1 (ppm)


C1412081802_MCO-1-175.11.fid
Group Blackwell
MCO-1-175
C13CPD32 CDCl3 /home/moreilly/callisto moreilly 46
166.55
146.57
133.74
133.36
130.40
128.85
124.60
40.45
32.04
29.83
29.73
29.68
29.47
29.42
29.38
27.04
22.81
14.24
NO2
O
N
H
6
28
f1 (ppm)


D1411171748_MCO-1-162.10.fid
Group Blackwell
MCO-1-162
PROTON CDCl3 /home/moreilly/av400 moreilly 56
NO2
O
N
H
29
f1 (ppm)


D1411171748_MCO-1-162.11.fid
Group Blackwell
MCO-1-162
C13CPD32 CDCl3 /home/moreilly/av400 moreilly 56
166.42
146.65
134.49
133.76
133.29
130.47
128.86
124.64
124.00
37.88
37.34
27.94
25.36
22.90
22.44
NO2
O
N
H
29
f1 (ppm)