Discovery of a dual SENP1 and SENP2 inhibitor

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1. Supplementary Data

1.1. Figures

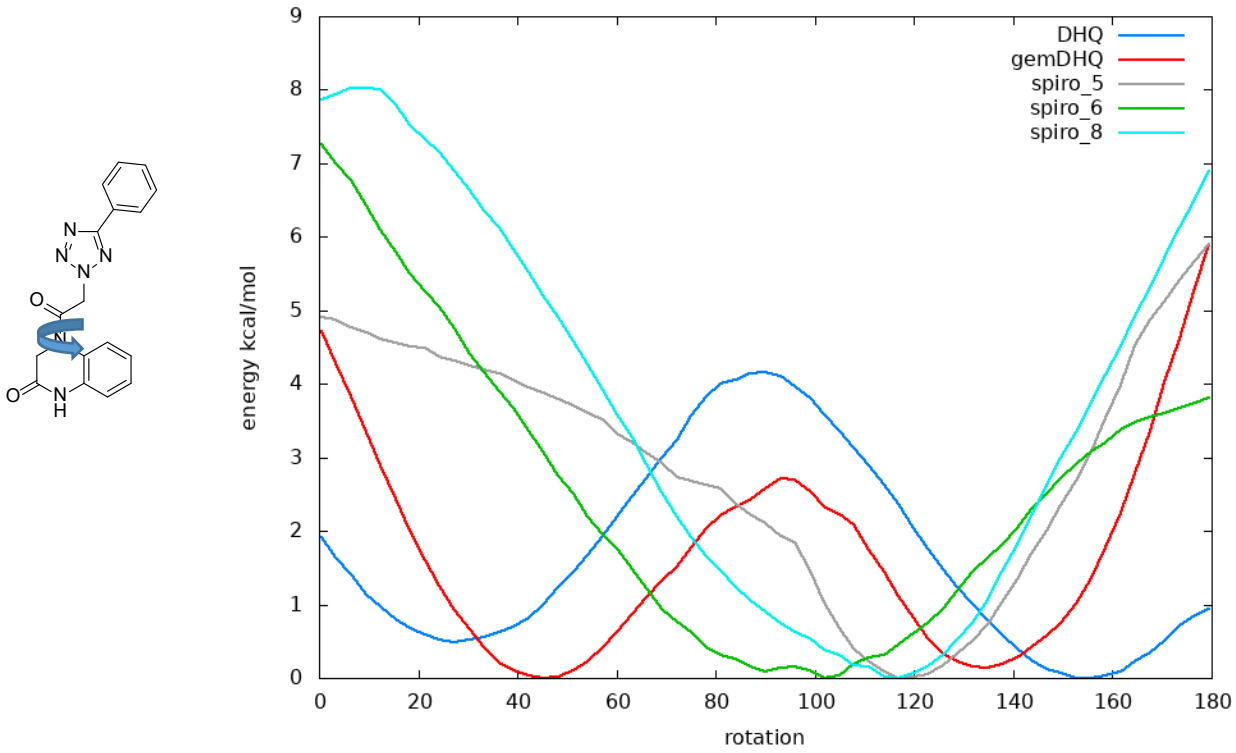
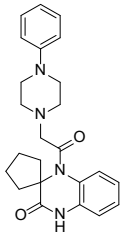
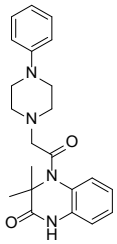
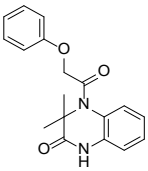
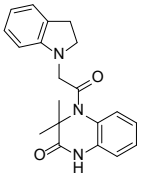
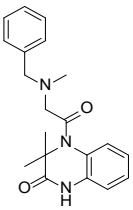
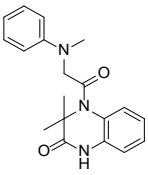
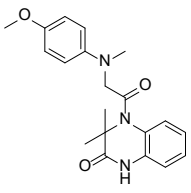
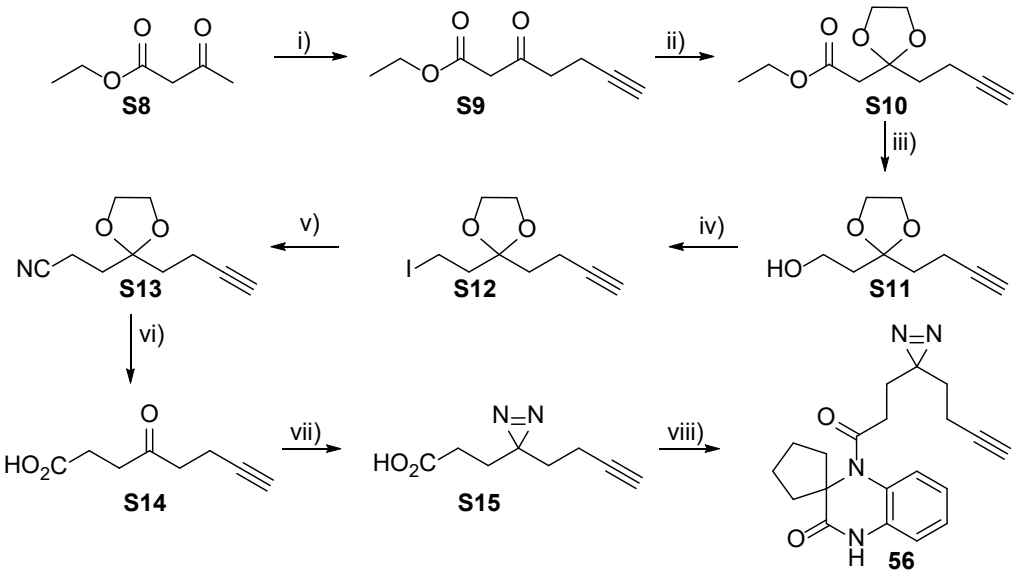


Figure S1 Calculation of the amide bond rotational barrier of **11** (spiro 5), **23** (gem-DHQ) and **24** (DHQ). Additionally the rotational barrier of the six-membered and eight membered ring DHQ is shown.

1.2. Tables

Compound	Structure	IC_{50} SENP1-SUMO1-AMC [μM] n = 2
S1		152 (74-312)[a]
S2		101 (70-146)
S3		> 200
S4		153 (132-177)
S5		> 200
S6		> 200
S7		> 200

1.3. Schemes



Scheme S1: Synthetic scheme of the photo affinity probe **56**. *Reagents & conditions*: i) 1: 2 M LDA in THF, THF, -78 °C – 0 °C, 15 minutes, 2: propargyl bromide, 1.5 h, 0 °C, 57%; ii) p-TsOH, ethylene glycol, Dean-Stark apparatus, 120 °C overnight, 85%; iii) $LiAlH_4$, THF, rt, 2 h, 90%; iv) PPh_3, I_2, imidazole, CH_2Cl_2, reflux, 1 h, v) KCN, DMF, 70 °C, 5 h, 45% over two steps; vi) 1: 5 M NaOH (aq.), reflux, 100 °C; 2: adjust pH to 1 with 5 M HCl (aq.), rt, 17 h, 89%; vii) 1: NH_3 (liq.), MeOH, -40 °C, 5 h, 2: NH_2-OSO_3H, MeOH, -40 °C – rt, overnight, 3: I_2, Et_3N, Et_2O, 0 °C – rt, 1 h, 28%; viii) 1: $SOCl_2$, CH_2Cl_2, 40 °C, 1 h, 2: **15**, CH_2Cl_2, Et_3N, rt, 1 h; 25%.

2. Experimental Section

2.1. Chemistry

2.1.1. Organic syntheses of SI compounds

1'-[2-(4-Phenylpiperazin-1-yl)acetyl]-3',4'-dihydro-1'*H*-spiro[cyclopentane-1,2'-quinoxalin]-3'-one (**S1**)

15 (55.0 mg, 0.197 mmol, 1.0 eq), 1-phenylpiperazine (37.3 µL, 38.4 mg, 0.237 mmol, 1.2 eq) and pyridine (31.9 uL, 31.2 mg, 0.395 mmol, 2.0 eq) was dissolved in DMF (3 mL) and stirred at 60 °C overnight. The reaction mixture was diluted with EtOAc (20 mL) and the organic layer was washed with brine (3 × 20 mL), 0.5 M aq. LiCl (3 × 10 mL), brine (10 mL), dried (Na_2SO_4), filtered and concentrated *in vacuo*. The residue was purifed by a SiO_2 column chromatography eluting with a gradient of 10 to 70% EtOAc in cyclohexan to afford a still impure product. A second purification by semi-prep reversed phase HPLC eluting with a gradient of 10 to 100% MeCN in H_2O with 0.2% AcOH afforded a colourless oil of **S1** (7.50 mg, 0.019 mmol, 9%). ^{1}H-NMR (500 MHz, $(CD_3)_2CO$: δ 9.38 (s, 1H), 7.67-7.63 (m, 1H), 7.29 (ddd, *J* 7.7, 7.7 1.4, 1H), 7.23-7.18 (m, 2H), 7.12-7.06 (m, 2H), 6.92-6.87 (m, 2H), 6.78 (tt, *J* 7.3, 1.1, 1H), 3.12 (s, 2H), 3.06-3.01 (m, 4H), 2.48-2.42 (m, 4H), 1.88-1.72 (m, 4H). ^{13}C-NMR (126 MHz, ($CDCl_3$): δ 172.6, 172.3, 151.6, 134.9, 130.4, 128.8, 127.4, 126.1, 122.1, 119.0, 115.7, 115.34, 115.28 54.2, 69.4, 61.3, 54.2, 48.7 35.1, 23.8. LRMS (ESI) m/z $[M+H]^+$ 405. RP-HPLC: RT 9.68 min purity: 99.6%.

4-(2-Chloroacetyl)-3,3-dimethyl-1,2,3,4-tetrahydroquinoxalin-2-one (S**16**)

16 (500 mg, 2.84 mmol, 1.0 eq), in DMF (20 mL) was cooled to 0 °C. 2-chloroacetyl chloride (462 µL, 670 mg, 4.26 mmol, 1.5 eq) was added over 15 minutes. The reaction mixture was stirred at 0 °C for 120 minutes, at which point TLC indicated complete consumption of the starting material. To the reaction mixture was added EtOAc (100 mL) and the organic layer was washed with brine (3 × 100 mL), 0.5 M aq. LiCl (3 × 50 mL), brine (100 mL), dried (Na_2SO_4), filtered and concentrated *in vacuo*. The residue was purified by a SiO_2 column eluting with a gradient of 10 to 70% EtOAc in cyclohexan to afford a yellowish solid of **S16** (665 mg, 2.63 mmol, 93%). ^{1}H NMR (500 MHz, ($CDCl_3$): δ 8.86 (s, 1H), 7.29-7.24 (m, 1H), 7.14-7.07 (m, 2H), 6.97 (dd, *J* 7.8, 1.4, 1H), 4.16 (s, 2H), 1.68 (s, 6H). ^{13}C-NMR (126 MHz, ($CDCl_3$): δ 173.0, 168.6, 129.9, 127.0, 126.5, 123.8, 123.4, 116.0, 62.6, 43.9, 22.8. LRMS (ESI) m/z $[M+H]^+$ 253.

3,3-Dimethyl-4-[2-(4-phenylpiperazin-1-yl)acetyl]-1,2,3,4-tetrahydroquinoxalin-2-one (**S2**)

S16 (50 mg, 0.198 mmol, 1.0 eq), 1-phenylpiperazine (64.2 mg, 0.396 mmol, 2.0 eq) and K_2CO_3 (54.7 mg, 0.396 mmol, 2.0 eq) was suspended in DMF (2 mL) and stirred at 120 °C in the microwave for 1 hour. The reaction mixture was diluted with EtOAc (20 mL) and the organic layer was washed with brine (3 × 20 mL), 0.5 M aq. LiCl (3 × 10 mL), brine (10 mL), dried (Na_2SO_4), filtered and concentrated *in vacuo*. The residue was purified by semi-prep reversed phase HPLC eluting with a gradient of 10 to 100% MeCN in H_2O with 0.2% AcOH to afford a colourless oil (19.2 mg, 0.051 mmol, 20%). %). MP: 160 °C dec.; ^{1}H NMR (500 MHz, $(CD_3)_2CO$: δ 9.58 (s, 1H), 7.37 (dd, *J* 7.9, 0.9, 1H), 7.23-7.18 (m, 3H), 7.11-7.04 (m, 2H), 6.92-6.86 (m, 2H), 6.78 (tt, *J* 7.4, 1.2, 1H), 3.31 (s, 2H), 3.02-2.99 (m, 4H), 2.57-2.52 (m, 1.56 (s, 6H). ^{13}C-NMR (126 MHz, ($CDCl_3$): δ 172.7, 171.7, 151.6, 131.3, 128.8, 128.1, 125.8, 123.8, 123.3, 122.3, 119.0, 115.6, 115.2, 62.2, 61.2, 52.6, 48.7, 22.7. LRMS (ESI) m/z $[M+H]^+$ 379. RP-HPLC: RT 8.79 min purity: 99.4%.

3,3-Dimethyl-4-(2-phenoxyacetyl)-1,2,3,4-tetrahydroquinoxalin-2-one (**S3**)

S16 (50 mg, 0.198 mmol, 1.0 eq), phenol (37.2 mg, 0.396 mmol, 2.0 eq), K_2CO_3 (54.7 mg, 0.396 mmol, 2.0 eq) and DMF (2 mL) was stirred at 120 °C for 1 hour under microwave irradiation, at which time the reaction showed complete consumption of the starting material by HPLC. The reaction mixture was diluted with EtOAc (20 mL) and the organic layer was washed with brine (3 × 20 mL), 0.5 M aq. LiCl (3 × 10 mL), brine (10 mL), dried (Na_2SO_4), filtered and concentrated *in vacuo*. The residue was purified by a SiO_2 column chromatography eluting with a gradient of 10 to 50% EtOAc in cyclohexan to afford a colourless solid of **S3** (47.3 mg, 0.152 mmol, 77%). Mp 140 °C dec.; ^{1}H NMR (500 MHz, $(CD_3)_2CO$: δ 9.53 (s, 1H), 7.35 (dd, *J* 8.0, 1.4 Hz, 1H), 7.27-7.20 (m, 3H), 7.12 (dd, *J* 8.0, 1.4 Hz, 1H), 7.05 (ddd, *J* 8.0, 8.0 1.4 Hz, 1H), 6.92 (tt, *J* 7.2, 1.1 Hz, 1H), 6.79-6.74 (m, 2H), 6.78 (tt, *J* 7.3, 1.1 Hz, 1H), 7.00 (dd, *J* 7.8, 1.3 Hz, 1H), 4.80 (s, 2H), 1.45 (s, 6H). ^{13}C-NMR (126 MHz, ($CDCl_3$): δ 171.3, 170.0, 158.1, 131.2, 129.3, 126.4, 123.5, 122.7, 121.1, 115.5, 114.5, 68.1, 61.4, 22.4. LRMS (ESI) m/z $[M+H]^+$ 311. RP-HPLC: RT: 12.1 min purity: 97.8%.

4-[2-(2,3-Dihydro-1*H*-indol-1-yl)acetyl]-3,3-dimethyl-1,2,3,4-tetrahydroquinoxalin-2-one (**S4**)

S16 (50 mg, 0.198 mmol, 1.0 eq), indoline (47.17 mg, 0.396 mmol, 1.2 eq), K_2CO_3 (54.7 mg, 0.396 mmol, 2.0 eq) and DMF (3 mL) and stirred at 60 °C overnight, at which point the reaction showed complete consumption of the starting material by UPLCMS. The reaction mixture was diluted with EtOAc (20 mL) and the organic layer was washed with brine (3 × 20 mL), 0.5 M aq. LiCl (3 × 10 mL), brine (10 mL), dried (Na_2SO_4), filtered and concentrated *in vacuo*. The residue was purified by a SiO_2 column chromatography eluting with a gradient of 10 to 60% EtOAc in cyclohexan to afford a colourless oil of **S4** (13.7 mg, 0.041 mmol, 21%). ^{1}H NMR (500 MHz, $(CD_3)_2CO$: δ 9.56 (s, 1H), 7.35 (dd, *J* 8.1, 1.2 Hz, 1H), 7.25 (ddd, *J* 7.9, 7.9, 1.2 Hz, 1H), 7.14-7.08 (m, 2H), 7.00-6.96 (m, 1H), 6.92-6.87 (m, 1H), 6.54 (ddd, *J* 7.6, 7.6, 0.9 Hz, 1H), 6.25 (d, *J* 7.6 Hz, 1H), 4.05 (s, 2H), 3.42 (t, *J* 8.7, 2H), 2.87 (t, *J* 8.7, 2H), 1.53 (s, 6H). ^{13}C-NMR (126 MHz, ($CDCl_3$): δ 171.73, 171.66, 151.5, 131.4, 129.3, 127.0, 126.8, 126.2, 124.1, 122.7, 117.3, 115.5, 115.4, 106.2, 61.4, 53.2, 53.1, 26.6, 22.6. LRMS (ESI) m/z $[M+H]^+$ 336. RP-HPLC: RT: 12.8 min purity: 95.4%

4-{2-[Benzyl(methyl)amino]acetyl}-3,3-dimethyl-1,2,3,4-tetrahydroquinoxalin-2-one (**S5**)

S16 (50 mg, 0.198 mmol, 1.0 eq), *N*-methylbenzylamin (48.0 mg, 0.396 mmol, 2.0 eq) and K_2CO_3 was suspended in DMF (3 mL) and heated under microwave irradiation for 1 hour at 120 °C. The reaction mixture was taken up in EtOAc (20 mL) and the organic layer was washed with sat. aq. K_2CO_3 (3 × 20 mL), brine (10 mL), dried (Na_2SO_4), filtered and concentrated *in vacuo*. The residue was purified by reversed phase column chromatography eluting with a gradient of 10 to 100% MeCN in H_2O +0.2% AcOH to afford a colourless oil of **S5** (14.5 mg, 0.043 mmol, 22%). ^{1}H NMR (500 MHz, $(CD_3)_2CO$: δ 9.58 (s, 1H), 7.29-7.15 (m, 7H), 7.10 (dd, *J* 8.0, 1.4 Hz, 1H) 6.99 (ddd, *J* 8.0, 8.0, 1.4 Hz, 1H), 3.57 (s, 2H), 3.40 (s, 2H), 2.21 (s, 3H), 1.57 (s, 6H). ^{13}C-NMR (126 MHz, ($CDCl_3$): δ 173.1, 171.8, 139.0, 131.0, 128.7, 128.0, 127.5, 126.8, 125.7, 123.7, 122.5, 115.32, 115.25, 61.2, 60.93, 60.92, 41.2, 22.6. LRMS (ESI) m/z $[M+H]^+$ 338. RP-HPLC: RT 7.16 min purity: 95.0%.

3,3-Dimethyl-4-{2-[methyl(phenyl)amino]acetyl}-1,2,3,4-tetrahydroquinoxalin-2-one (**S6**)

S16 (50 mg, 0.198 mmol, 1.0 eq), *N*-Methylanilin (42.2 mg, 0.396 mmol, 2.0 eq) and K_2CO_3 (54.7 mg, 0.396 mmol, 2.0 eq) was suspended in DMF (2 mL) and stirred at 120 °C under microwave irradiation for 5 hours. To the reaction mixture was added EtOAc (20 mL) and the organic layer was washed with brine (3 × 20 mL), 0.5 M aq. LiCl (3 × 10 mL), brine (10 mL), dried (Na_2SO_4), filtered and concentrated *in vacuo*. The residue was purified by reversed phase column chromatography eluting with a gradient of 10 to 100% MeCN in H_2O +0.2% AcOH afforded a colourless solid of **S6** (12.4 mg, 0.033 mmol, 17%). Mp 158 °C dec.; ^{1}H NMR (500 MHz, $(CD_3)_2CO$: δ9.54 (s, 1H), 7.39 (dd, *J* 7.8, 1.3 Hz, 1H), 7.28 (ddd, *J* 7.8, 7.8, 1.3 Hz, 1H), 7.17-7.07 (m, 4H), 6.61 (tt, *J* 7.3, 0.9 Hz, 1H), 6.58-6.54 (m, 2H), 4.26 (s, 2H), 2.92 (s, 3H), 1.48 (s, 6H). ^{13}C-NMR (126 MHz, ($CDCl_3$): δ 172.3, 171.8, 149.0, 131.8, 128.7, 126.6, 124.5, 122.7, 116.4, 115.6, 112.0, 61.3, 56.8, 39.0, 22.7.. LRMS (ESI) m/z $[M+H]^+$ 324. RP-HPLC: RT 12.43 min purity: 98.3%.

4-{2-[(4-Methoxyphenyl)(methyl)amino]acetyl}-3,3-dimethyl-1,2,3,4-tetrahydroquinoxalin-2-one (**S7**)

S16 (50 mg, 0.198 mmol, 1.0 eq), 4-Methoxy-*N*-methylanilin (54.3 mg, 0.396 mmol, 2.0 eq) and K_2CO_3 (54.7 mg, 0.396 mmol, 2.0 eq) was suspended in DMF (3 mL) and heated under microwave irradiation for 2 hours at 120 °C. The reaction mixture was taken up in EtOAc (20 mL) and the organic layer was washed with brine (3 × 20 mL), 0.5 M aq. LiCl (3 × 10 mL), brine (10 mL), dried (Na_2SO_4), filtered and concentrated *in vacuo*. The residue was purified on reversed phase C_{18} column eluting with a gradient of 10 to 100% MeCN in H_2O +0.2% AcOH to afford a colourless solid (8.4 mg, 0.024 mmol, 12%). Mp 131 °C dec.; ^{1}H NMR (500 MHz, $(CD_3)_2CO$): δ9.52 (s, 1H), 7.33 (dd, *J* 7.9, 1.2, 1H), 7.26 (ddd, *J* 7.9, 7.9, 1.2 Hz, 1H), 7.14 (dd, *J* 7.9, 1.2 Hz, 1H), 6.74-6.69 (m, 2H), 6.55-6.50 (m, 2H), 4.19 (s, 2H), 3.68 (s, 3H), 2.87 (s, 2H), 1.46 (s, 6H). ^{13}C-NMR (126 MHz, ($CDCl_3$): δ 172.5, 171.7, 151.8, 143.5, 131.6, 126.8, 126.4, 124.3, 122.6, 115.5, 114.3, 113.7, 61.2, 57.5, 54.8, 39.4, 22.6. LRMS (ESI) m/z $[M+H]^+$ 354. RP-HPLC: RT 12.18 min purity: 97.6%

Ethyl 3-oxohept-6-ynoate (**S9**)

Ethyl aceto acetate (**S8**) (6.00 g, 46.1 mmol, 1.0 eq) was dissolved in THF (100 mL) and cooled to -78 °C. 2 M LDA in THF (46.1 mL, 92.2 mmol, 2.0 eq) was added over 15 minutes and the solution was subsequently allowed to warm up to 0 °C and stirred for 15 minutes . The solution was cooled again to -78 °C. 80% propargyl bromide in toluene (6.86 g, 46.1 mmol, 1.0 eq) was added over 15 minutes and the reaction mixture was allowed to warm up to 0 °C and stirred for 1.5 hours at this temperature. Glacial acetic acid (5.9 mL) was carefully added to quench the reaction mixture. The suspension was concentrated *in vacuo*, and the residue was dissolved in EtOAc (150 mL) and H_2O (100 mL). The organic extracts were washed with brine (2 × 100 mL), dried (Na_2SO_4), filtered, and concentrated *in vacuo* to afford a 3 to 1 mixture of product and starting material. The residual oil was purified by a Kugelrohr vacuum distillation to afford a pale yellow oil of **S9** (4.42 g, 26.3 mmol, 57%). ^{1}H NMR (500 MHz, $CDCl_3$): δ4.22 (q, *J* 7.2 Hz, 2H), 3.49 (s, 2H), 2.83 (t, *J* 7.2 Hz, 2H), 2.50 (td, *J* 7.2, 2.5 Hz, 2H), 1.98 (t, *J* 2.5 Hz, 1H), 1.30 (t, *J* 7.2 Hz, 3H). ^{13}C-NMR (126 MHz, $CDCl_3$): δ 200.6, 166.9, 82.5, 69.0, 61.5, 49.2, 41.6, 14.1, 12.8.

Ethyl 2-[2-(but-3-yn-1-yl)-1,3-dioxolan-2-yl]acetate (**S10**)

Ethyl 3-oxohept-6-ynoate (**S9**) (4.30 g, 25.6 mmol, 1.0 eq) was dissolved in toluene (150 mL). To this solution ethylene glycol (1.75 g, 28.1 mmol, 1.1 eq) and 4-toluenesulfonic acid monohydrate (0.24 g, 1.3 mmol, 0.05 eq) was added and stirred at reflux in a Dean-Stark apparatus overnight. After cooling to ambient temperature the organic layer were washed with 1 M aq. Na_2CO_3 (3 × 100 mL), brine (100 mL), dried (Na_2SO_4), filtered and concentrated *in vacuo* to afford a pale yellow oil of **S10** (4.62 g, 21.8 mmol, 85%), which was used without further purification. ^{1}H NMR (500 MHz, $CDCl_3$): δ 4.18 (q, *J* 7.3 Hz, 2H), 4.05-3.97 (m, 4H), 2.67 (s, 2H), 2.36-2.30 (m, 2H), 2.19-2.11 (m, 2H), 1.95 (t, *J* 2.5, 1H), 1.29 (t, *J* 7.3 Hz, 3H).

2-[2-(But-3-yn-1-yl)-1,3-dioxolan-2-yl]ethan-1-ol (**S11**)

S10 (6.80 g, 32.0 mmol, 1.0 eq) was dissolved in THF and cooled to 0 °C. 2 M $LiAlH_4$ in THF (17.0 mL, 34.0 mmol, 1.05 eq) was carefully added over 15 minutes. The yellow solution was warmed up to ambient temperature and stirred for 2 hours, at which point the reduction was completed. The yellow solution was cooled to 0 °C. EtOAc (5 mL) was slowly added followed by careful addition of H_2O (10 mL). The THF was evaporated *in vacuo*. To the residue EtOAc (150 mL) and sat. rochelle solution (100 mL) was added and dissolved. The organic layer was washed with brine (2 × 100 mL), dried (Na_2SO_4), filtered and concentrated *in vacuo* to afford a yellow oil of **S11** (4.90 g, 28.8 mmol, 90%), which was used without further purification. ^{1}H-NMR (500 MHz, CDCl3): δ 4.06-3.98 (m, 4H), 3.78 (q, *J* = 7.7 Hz, 2H), 2.70-2.63 (m, 1H), 2.33-2.27 (m, 2H), 2.01-1.92 (m, 5H). ^{13}C-NMR (126 MHz, $CDCl_3$): δ 111.1, 83.9, 68.3, 65.0, 58.7, 38.2, 35.9, 13.2.

3-[2-(But-3-yn-1-yl)-1,3-dioxolan-2-yl]propanenitrile (**S13**)

PPh_3 (8.31 g, 31.7 mmol, 1.1 eq) and 1*H*-imidazole (5.88 g, 86.3 mmol, 3.0 eq) were dissolved in CH_2Cl_2 (300 mL). Iodine (8.77 g, 34.5 mmol, 1.2 eq) was added portion wise and stirred for 15 min at ambient temperature. MIB-4-274 (4.90 g, 28.8 mmol, 1.0 eq) in CH_2Cl_2 (50 mL) was added over 15 minutes. The reaction mixture was heated at reflux for 1 hour, at which point the reaction was completed. The brown solution was cooled to ambient temperature and quenched with 10% w/v aq. $Na_2S_2O_3$ (150 mL).The organic layer was washed with brine (2 × 150 mL), dried (Na_2SO_4), filtered and concentrated *in vacuo*. The residual solid was stirred in cyclohexan (170 mL) and TBME (20 mL) for 5 minutes, filtered and concentrated *in vacuo* to afford a yellow oil (**S12**, 6.90 g), which contains around 30% PPh_3, which was used without further purification. This crude mixture was taken up in DMF (25 mL) and KCN (0.85 g, 13.0 mmol, 1.1 eq) was added. This reaction mixture was stirred for 5 hours at 70 °C. Upon cooling to ambient temperature the suspension was dissolved with 10% aq. $NaHCO_3$ (50 mL) and EtOAc (100 mL). The organic layer was washed with with 0.5 M aq. LiCl (2 × 10 mL), brine (10 mL), dried (Na_2SO_4), filtered, and concentrated *in vacuo*. The residue was purified by a SiO_2 column eluting with a gradient of 0% to 20% EtOAc in cyclohexane to afford a colourless oil of **S13** (2.20 g, 12.9 mmol, 45% over two steps). ^{1}H NMR (500 MHz, $CDCl_3$): δ 4.01 (s, 4H),2.43 (t, *J* 7.7 Hz, 2H), 2.32-2.27 (m, 2H), 2.07 (t, *J* 7.5 Hz, 2H), 1.98 (t, *J* 2.7 Hz, 1H), 1.90 (t, *J* 7.7 Hz, 2H); ^{13}C-NMR (126 MHz, $CDCl_3$): δ 119.7, 108.9, 83.6, 68.6, 65.3, 35.9, 32.5, 13.2, 11.6.

4-Oxooct-7-ynoic acid (**S14**)

S13 (2.15 g, 12.0 mmol, 1.0 eq) and 10% aq. NaOH (10 mL) was stirred at reflux for 5 hours. Upon cooling the pH of the aq. layer was adjusted with 5 M aq. HCl to 1 and stirred at ambient temperature overnight. The organic extracts of aq. layer were extracted with EtOAc (5 × 50 mL). The combined organic layers were dried (Na_2SO_4), filtered and concentrated *in vacuo*. The residue was purified by a SiO_2 column eluting with a gradient of 50% to 100% of EtOAc in cyclohexane containing 2% of AcOH to afford a pale yellow solid (1.64 g, 10.6 mmol, 89%). ^{1}H NMR (500 MHz, $CDCl_3$): δ 2.80-2.71 (m, 4H), 2.71-2.66 (m, 2H), 2.52-2.46 (m, 2H), 1.97 (t, *J* 7.5 Hz, 1H). ^{13}C-NMR (126 MHz, $CDCl_3$): δ 206.4, 178.3, 82.9, 68.8, 41.3, 36.8, 27.7, 12.9.

3-[3-(But-3-yn-1-yl)-3*H*-diazirin-3-yl]propanoic acid (**S15**)

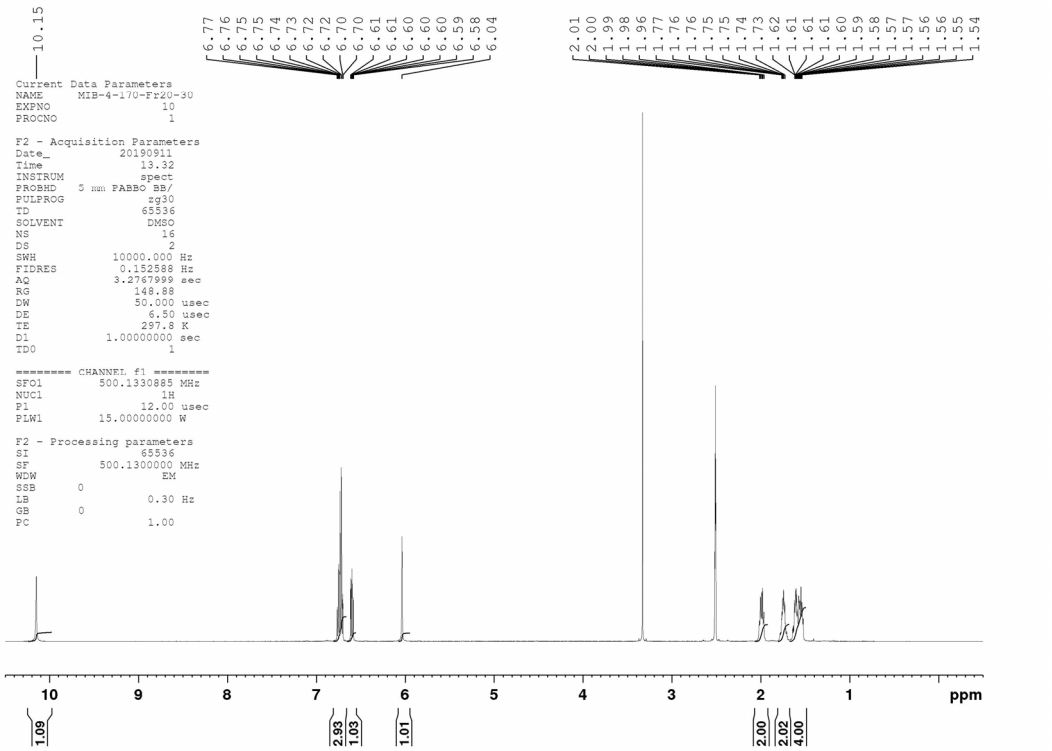
S14 (1000 mg, 6.49 mmol, 1.0 eq) was dissolved in dry MeOH (5 mL) and liquid ammonia (20 mL) was condensed into the apparatus. This solution was stirred at -40 °C for 5 h. A solution of hydroxylamine O-sulfonic acid (676 mg, 10.4 mmol, 1.6 eq) in dry MeOH (8 mL) was added dropwise. After one hour at −40 °C the suspension was allowed to warm up to ambient temperature overnight. The suspension was diluted with MeOH (5 mL), filtered, rinsed with MeOH (10 mL), and concentrated *in vacuo*. The residual oil was dissolved in Et_2O (10 mL) and triethylamine (2 mL), and cooled to 0 °C. I_2 (2.5 g) was added in 5 portions until the brown colour persist. After 1 hour at ambient temperature the solution was diluted with EtOAc (50 mL). The pH was adjusted to 2 with 1 M aq. HCl (10 mL) and the organic layer was washed with 10% aq. $Na_2S_2O_3$ (50 mL), 1 M aq. HCl (50 mL), dried (Na_2SO_4), filtered and concentrated *in vacuo*. The residue was purified by a SiO_2 column eluting with a gradient of 10% to 50% petroleum ether in EtOAc containing 1% AcOH, to afford a yellow oil (304 mg, 1.83 mmol, 28%). ^{1}H NMR (500 MHz, $CDCl_3$): δ 2.18 (t, *J* 7.6 Hz, 2H), 2.05-1.98 (m, 3H), 1.82 (t, *J* 7.5 Hz, 2H), 1.67 (t, *J* 7.5 Hz, 2H). ^{13}C-NMR (126 MHz, $CDCl_3$): δ 178.0, 82.5, 69.3, 32.2, 28.1, 27.8, 27.5, 13.2.

3. Supplementary Data

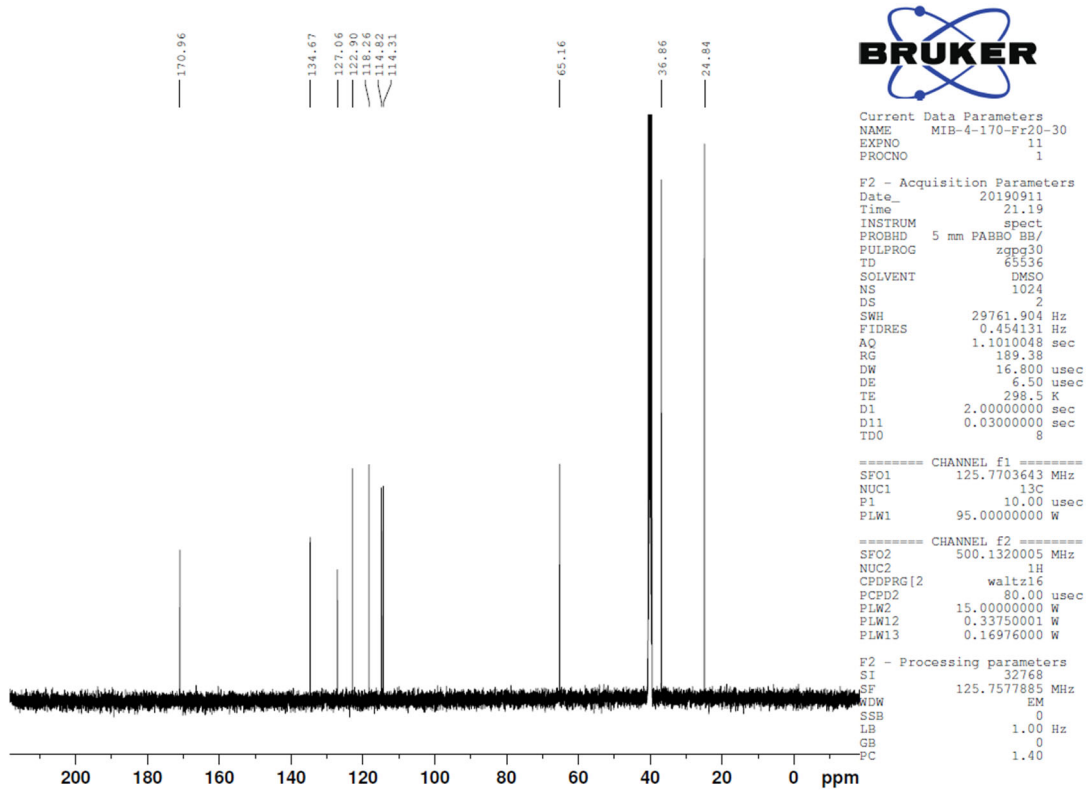
3.1. NMR and HPLC spectra

Compound 15

^{1}H-NMR



^{13}C-NMR



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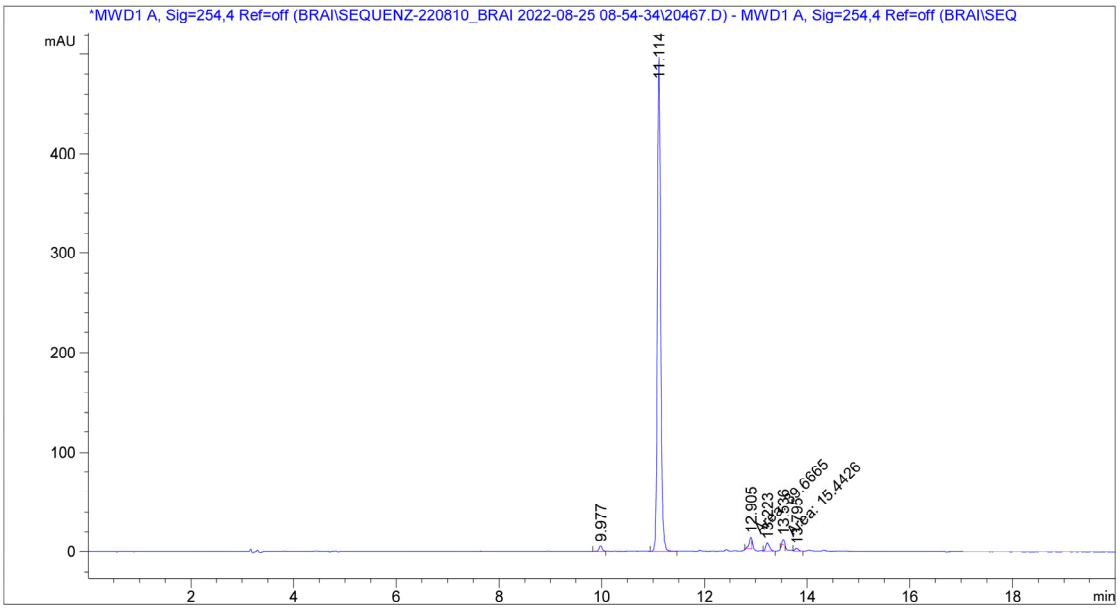


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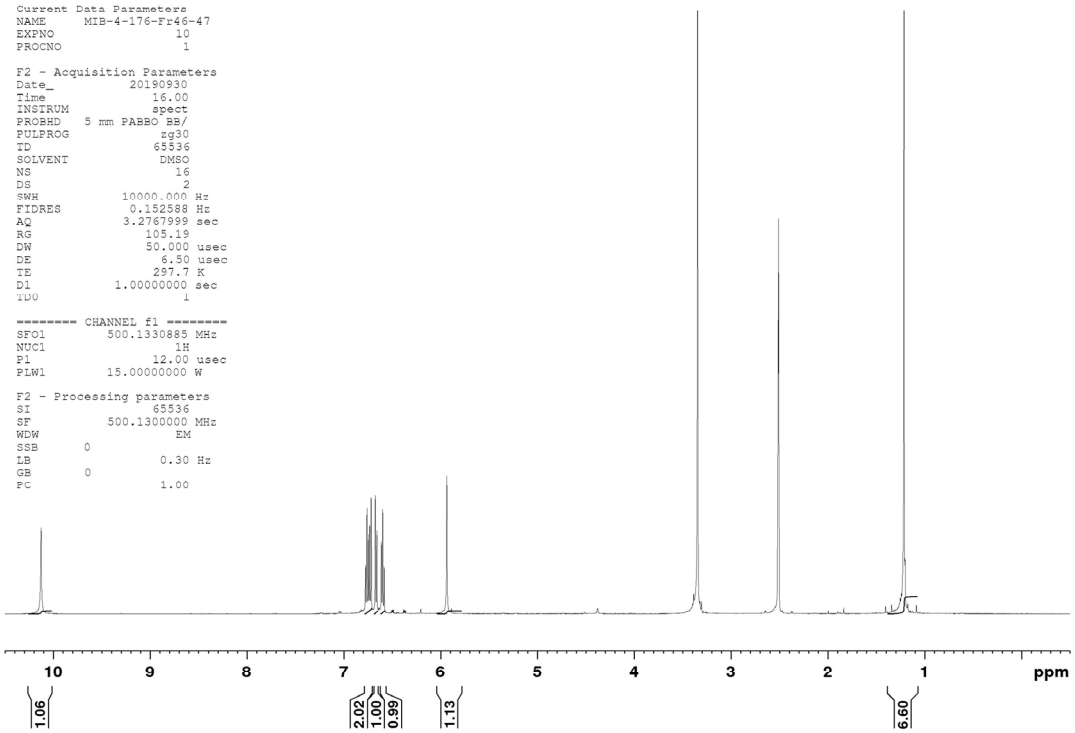
Compound 16

^{1}H-NMR



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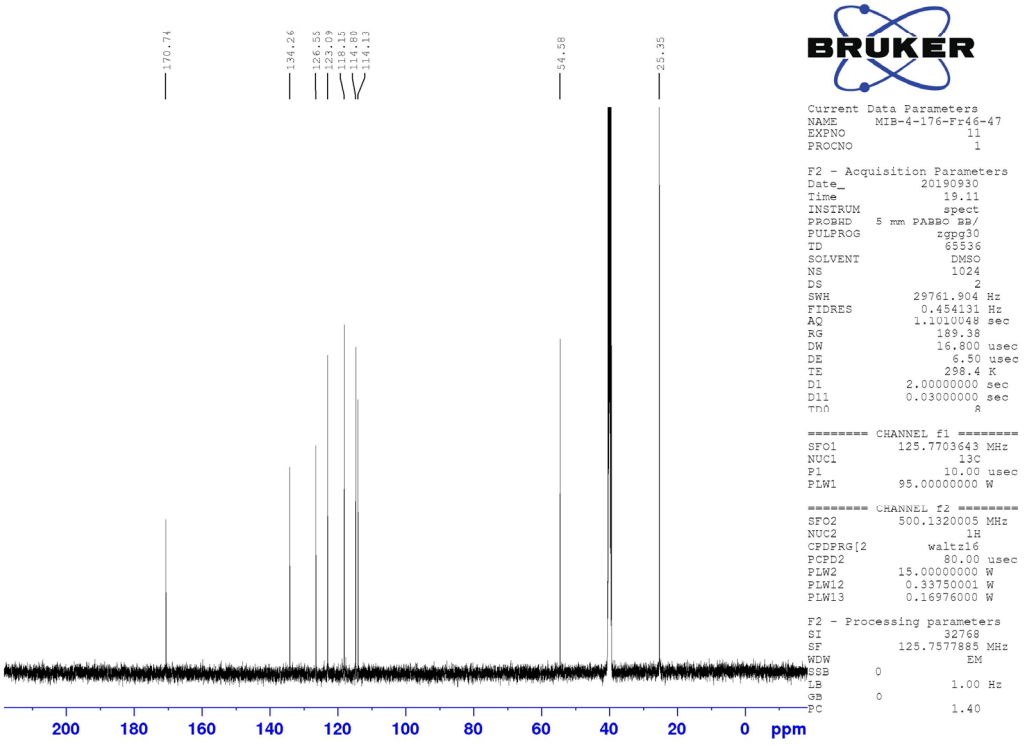

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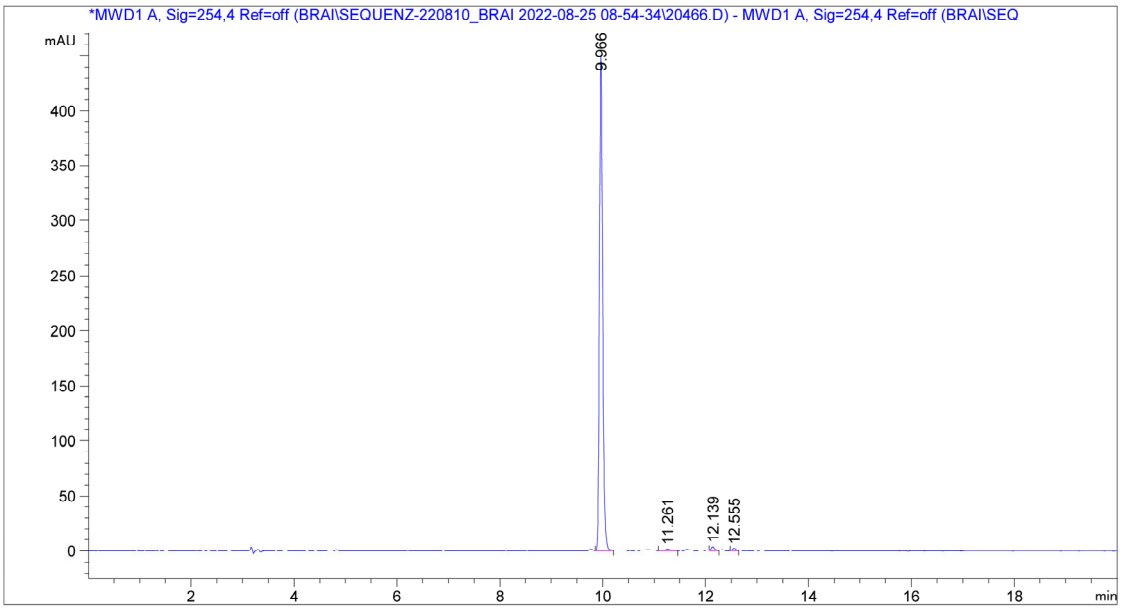


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Compound 18

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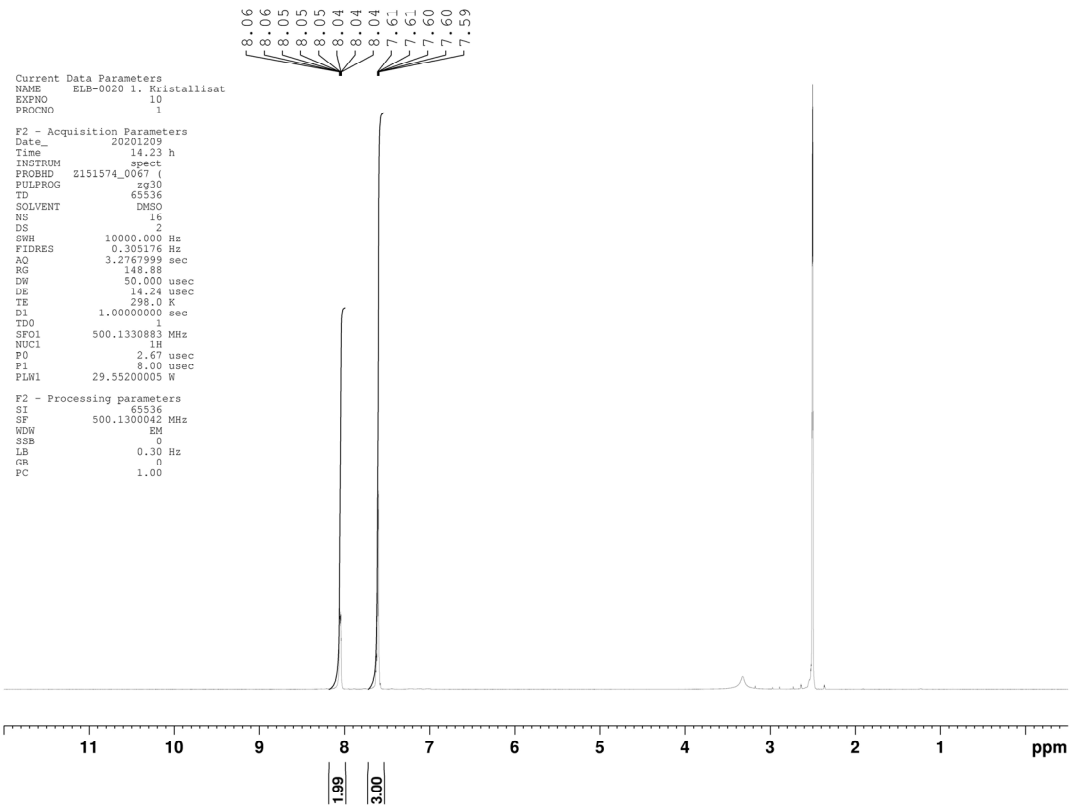

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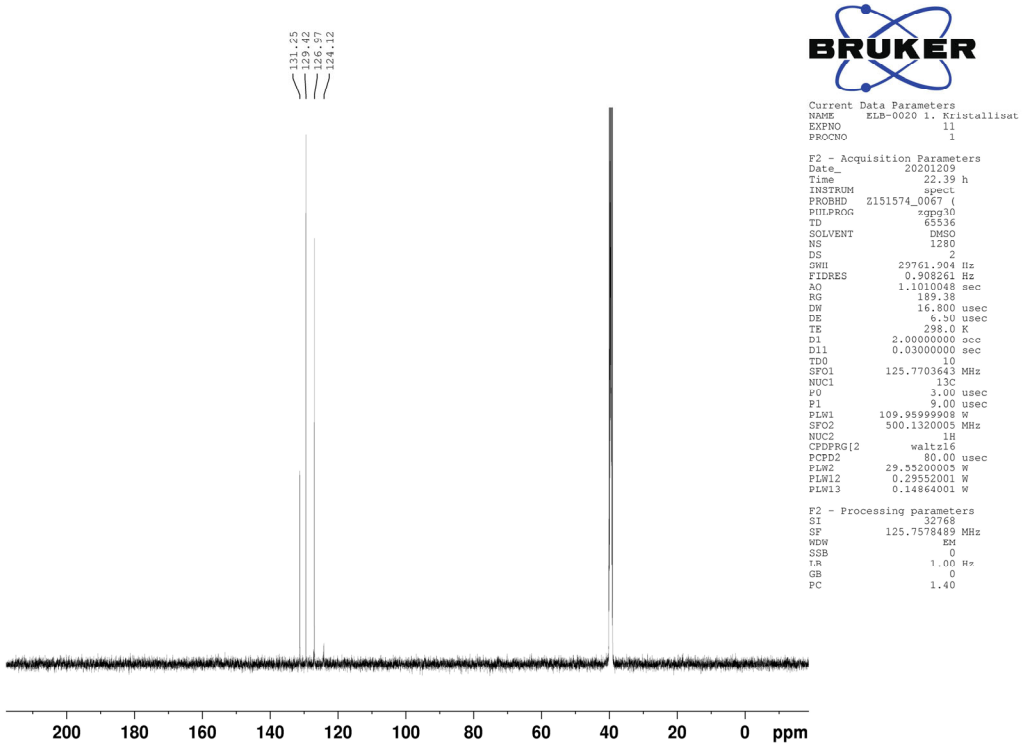

Compound 19

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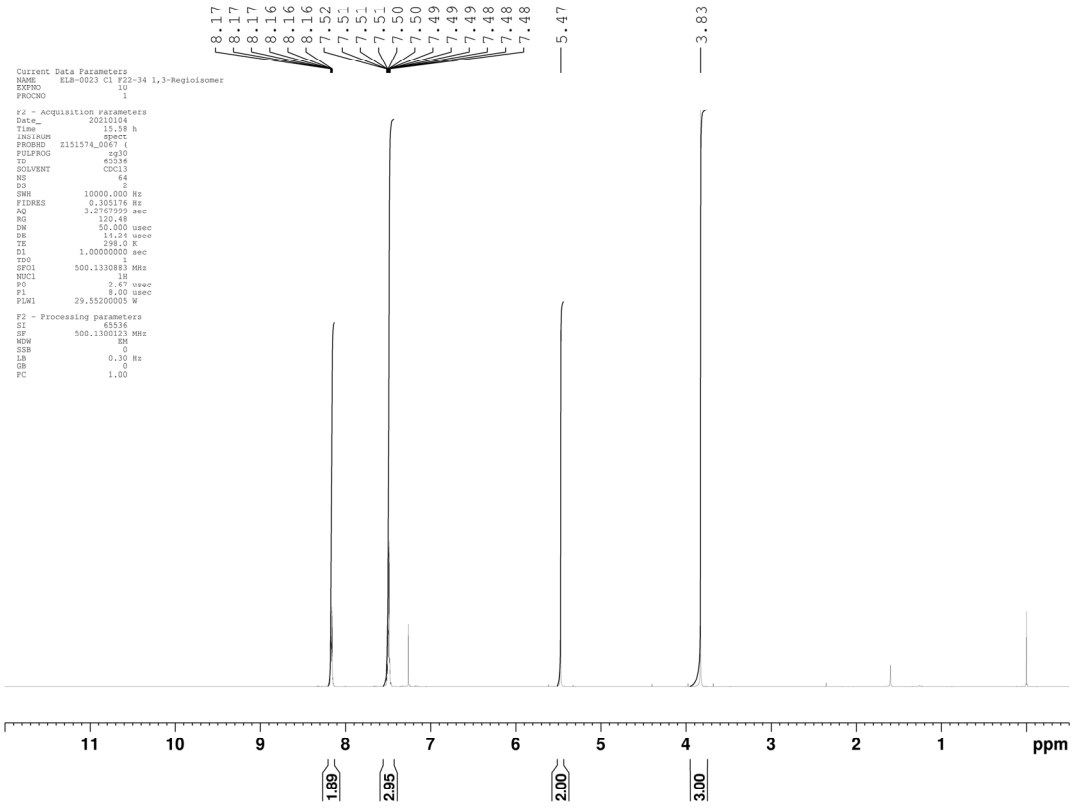

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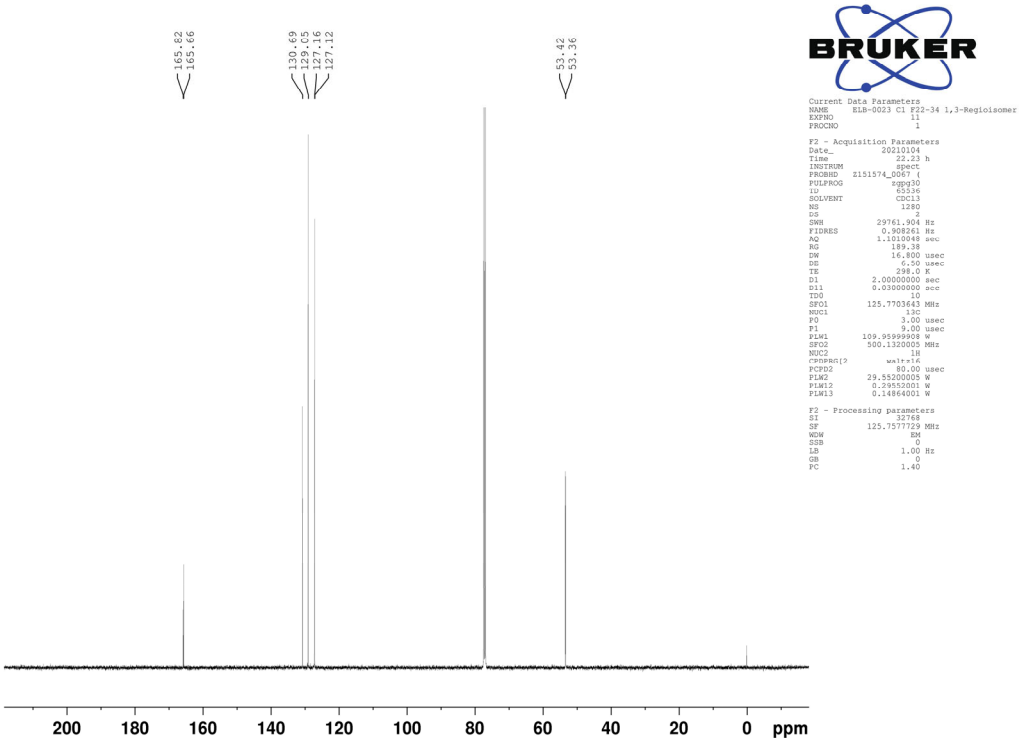

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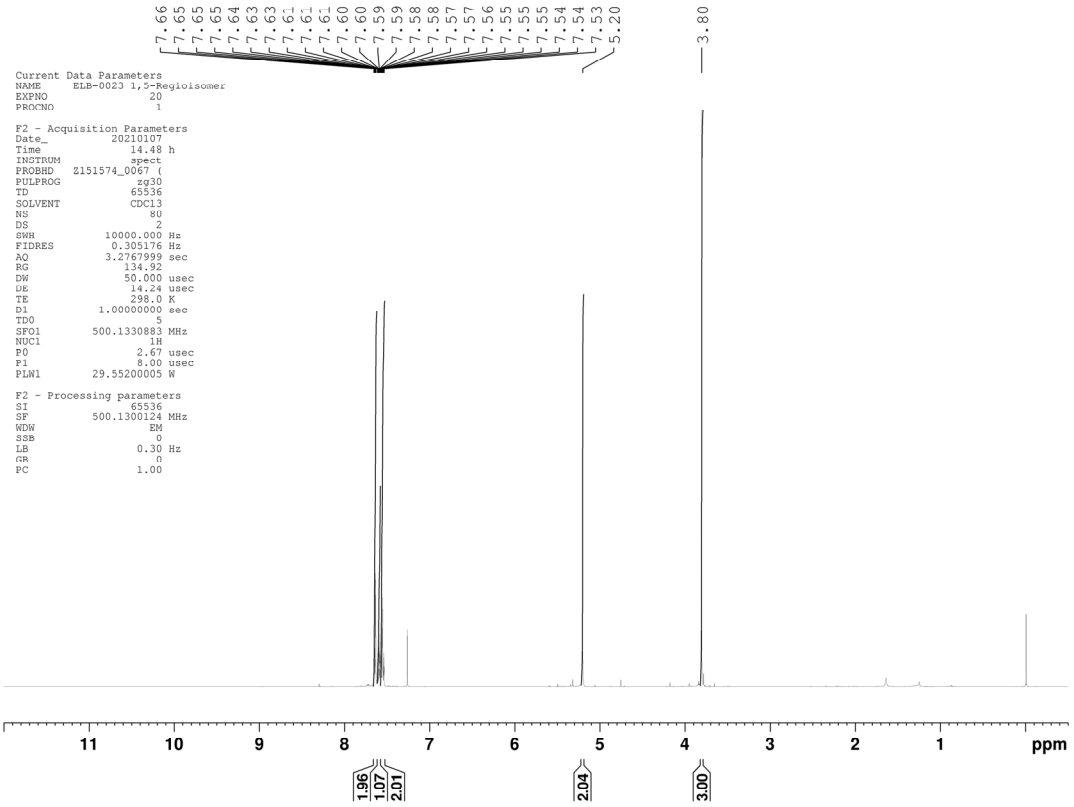

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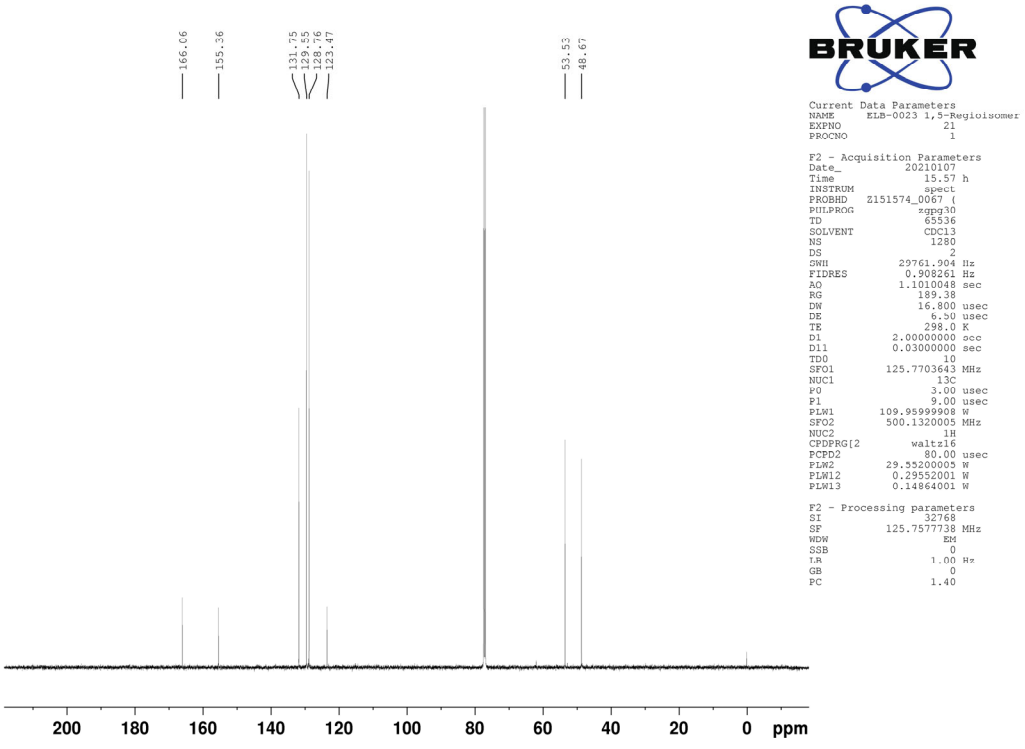

Compound 21

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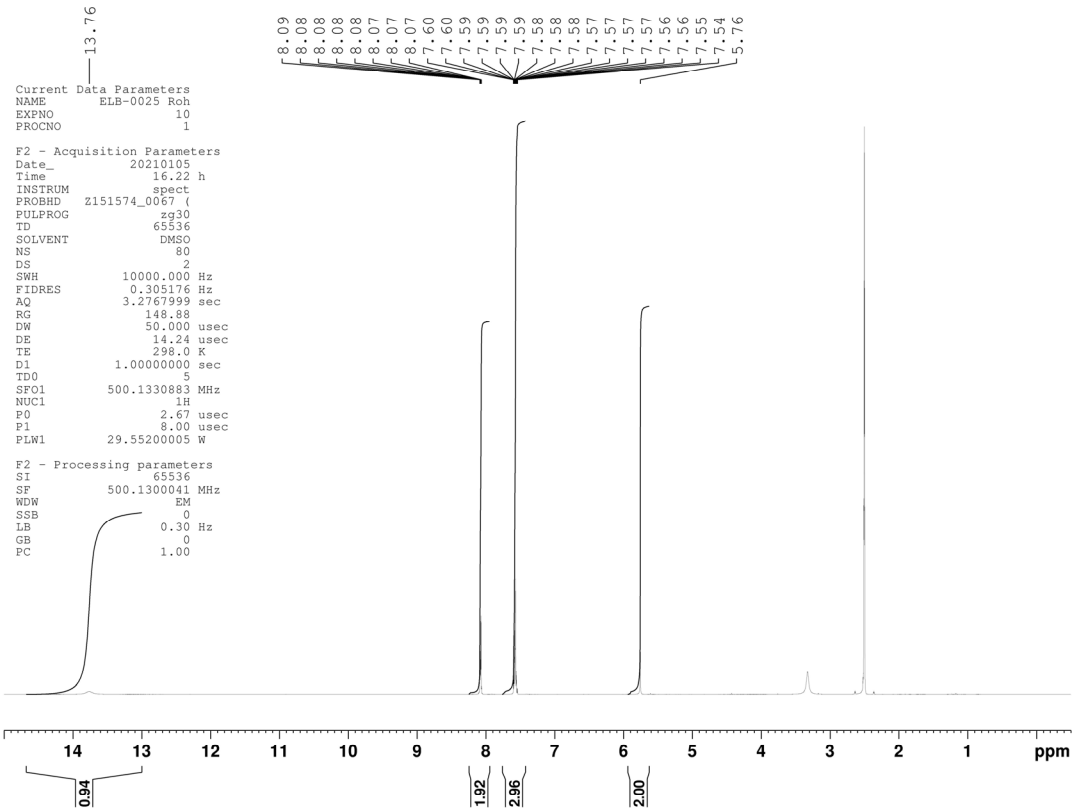

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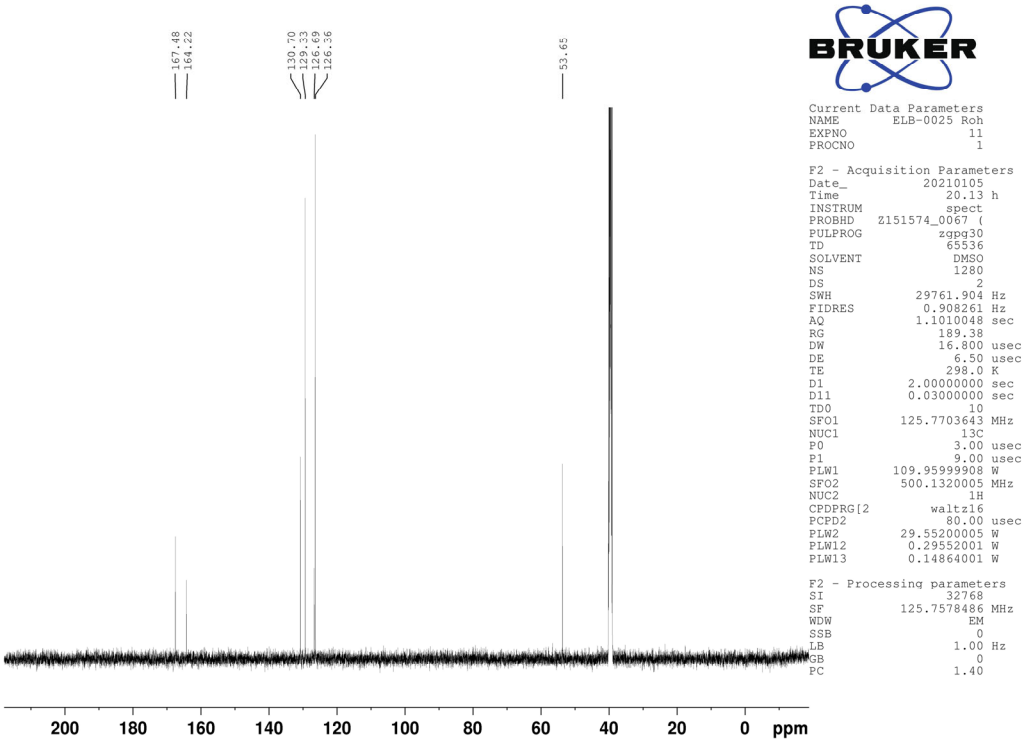

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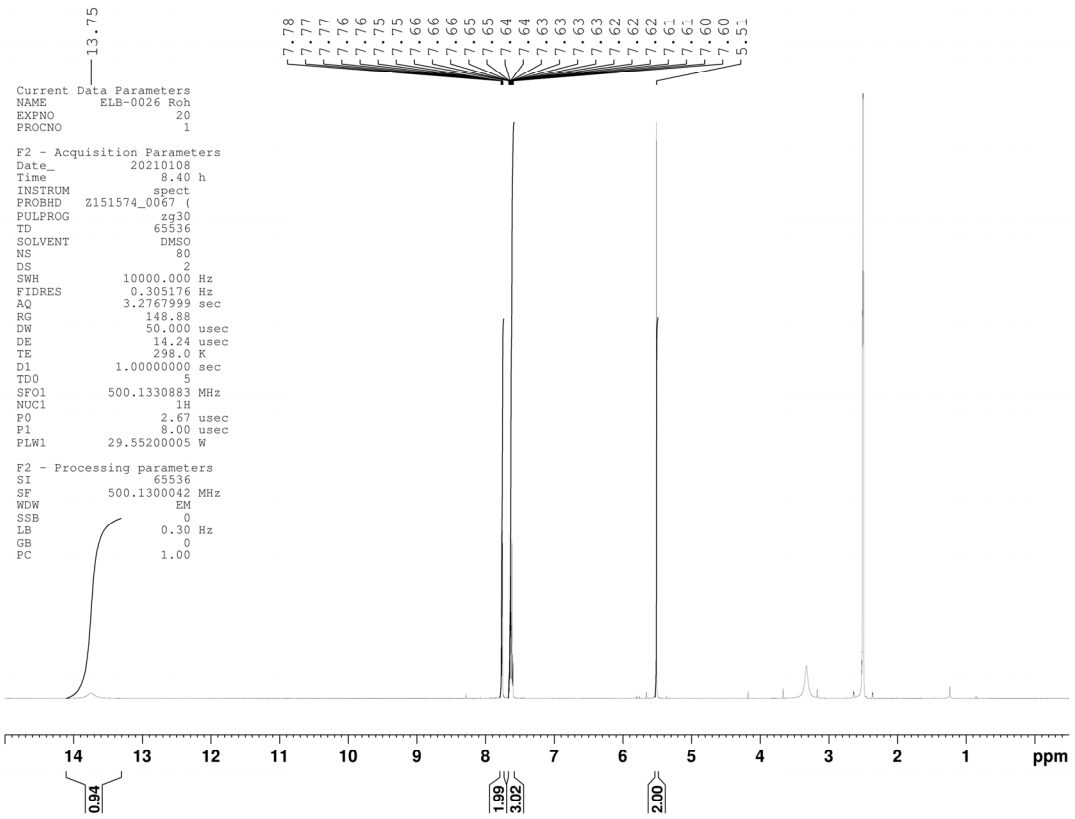

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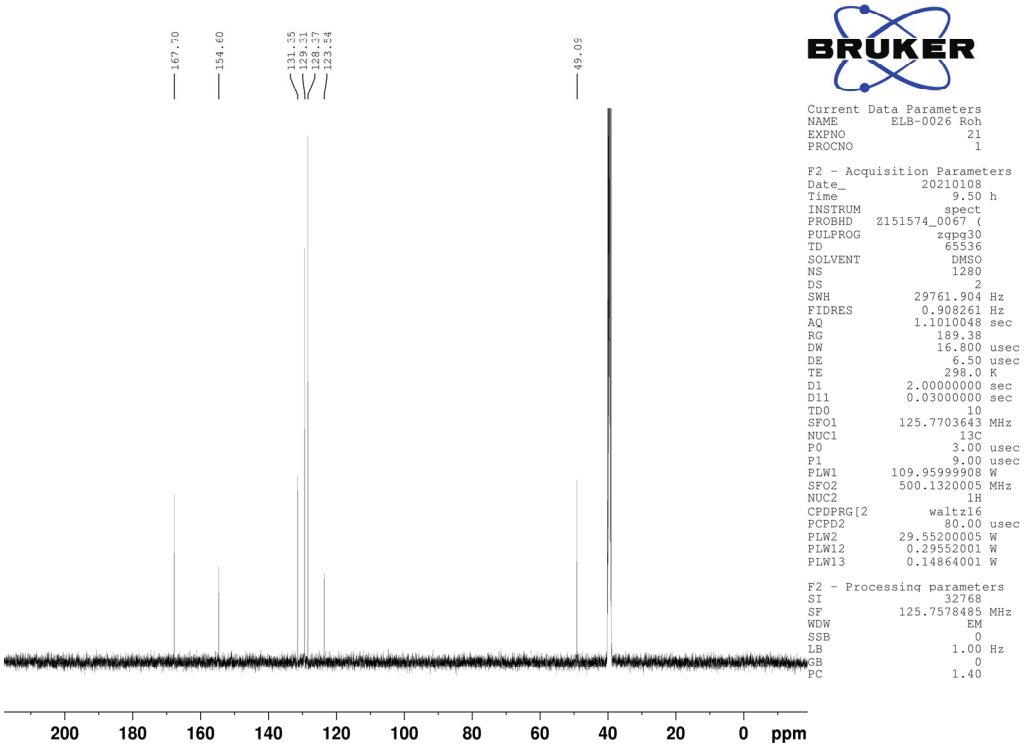

Compound 11

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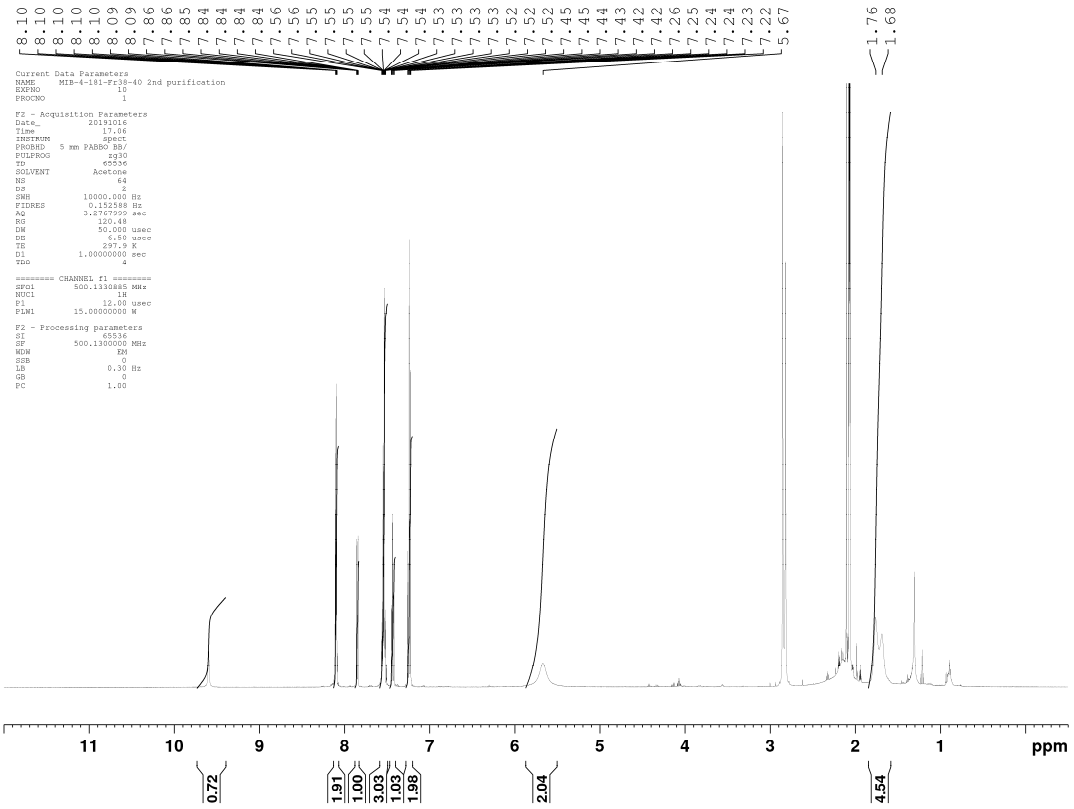

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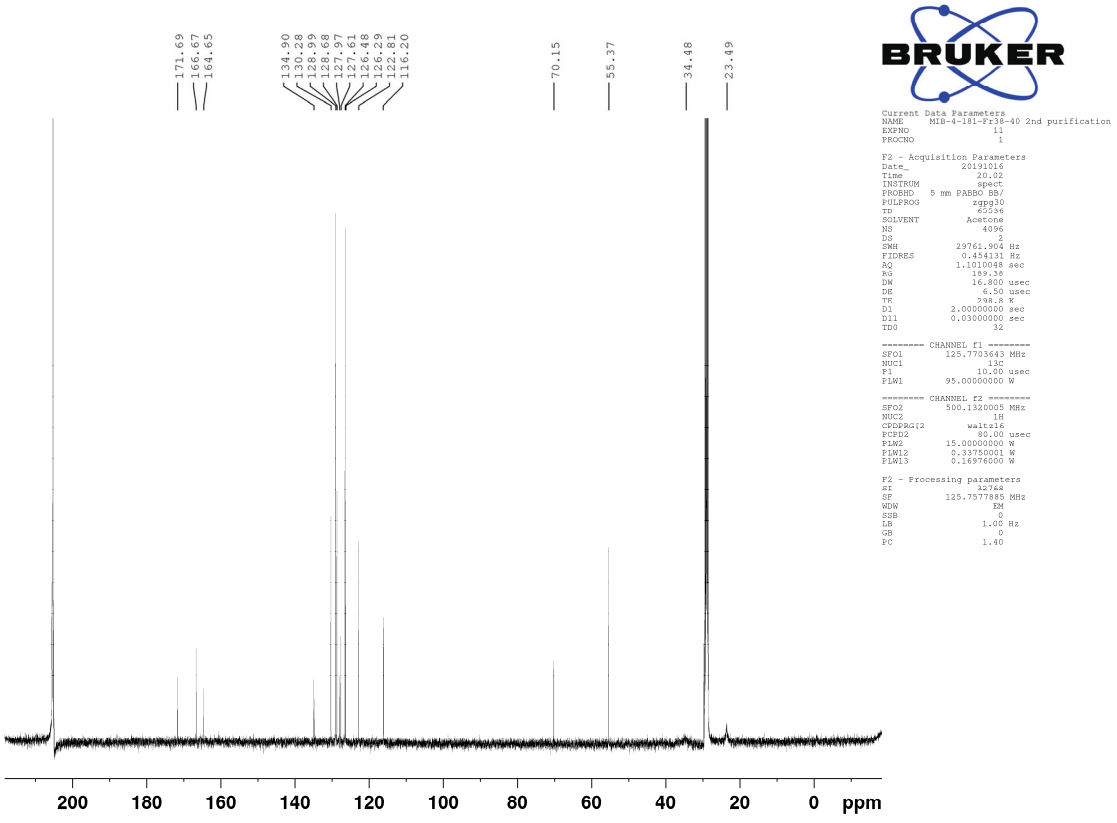

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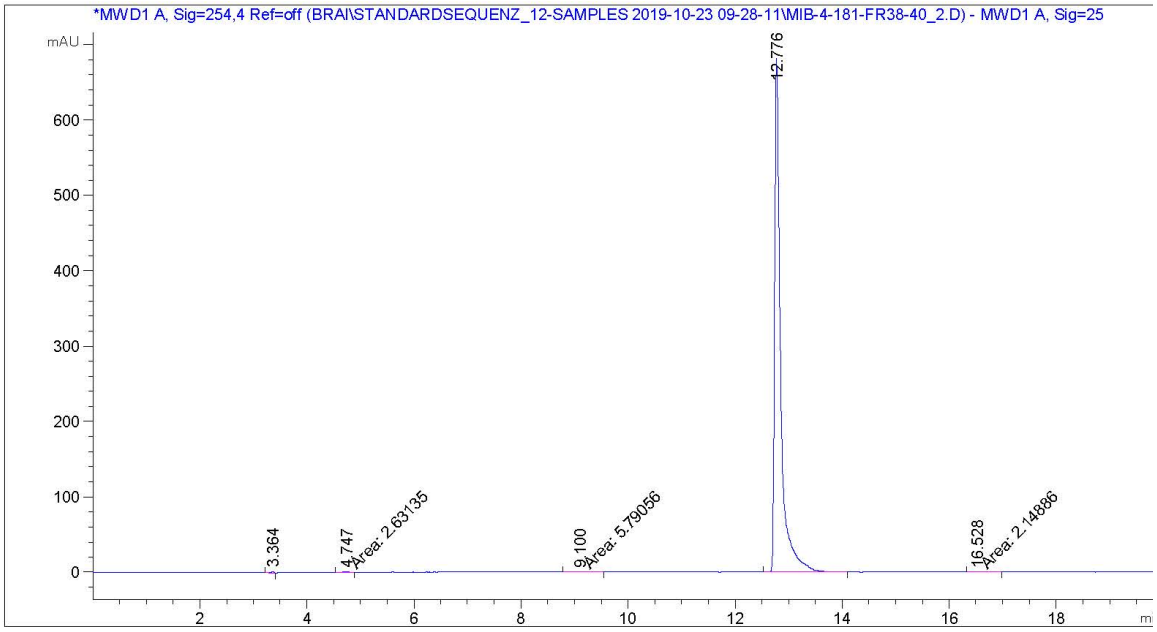


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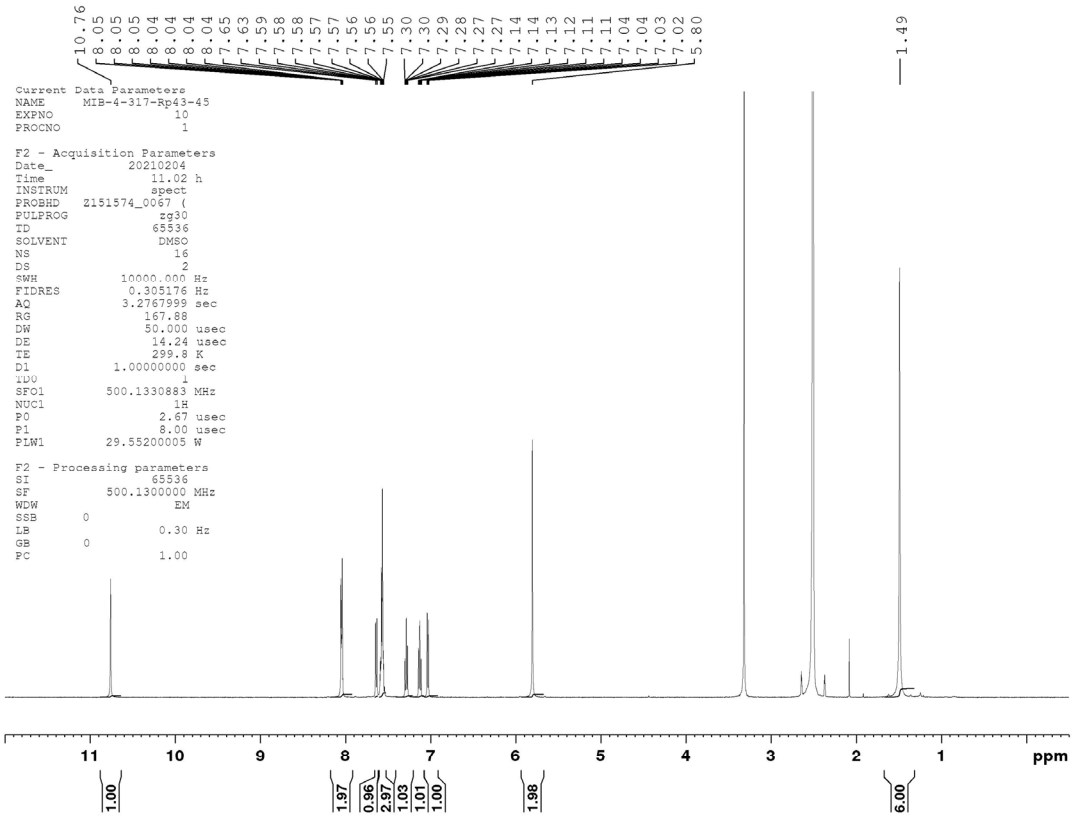

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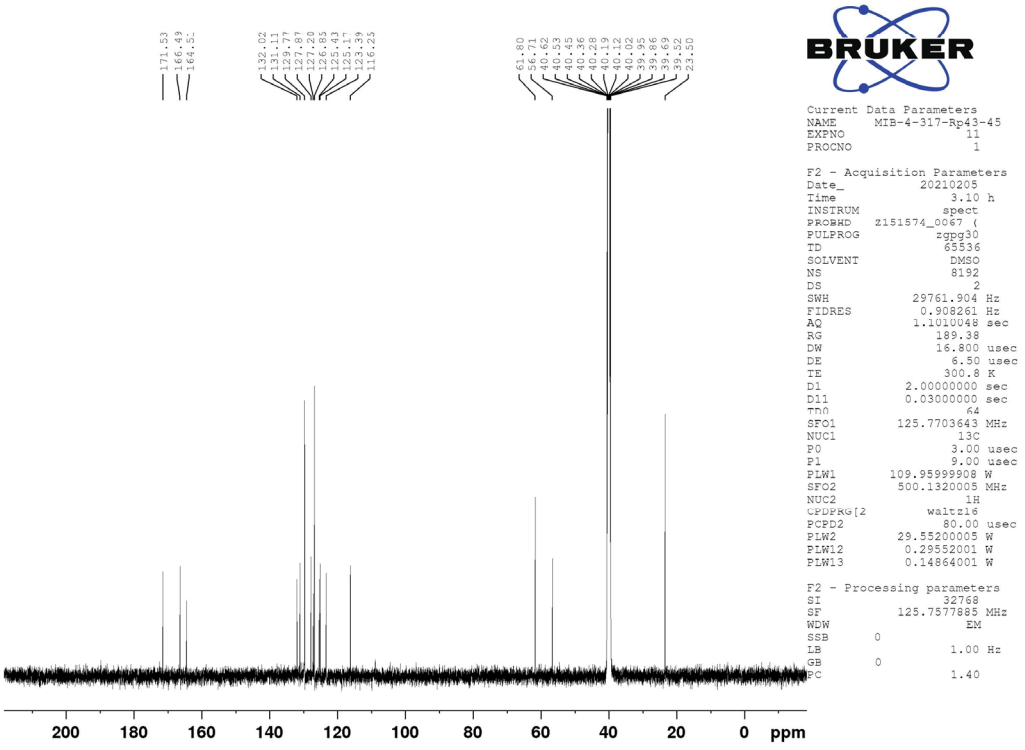

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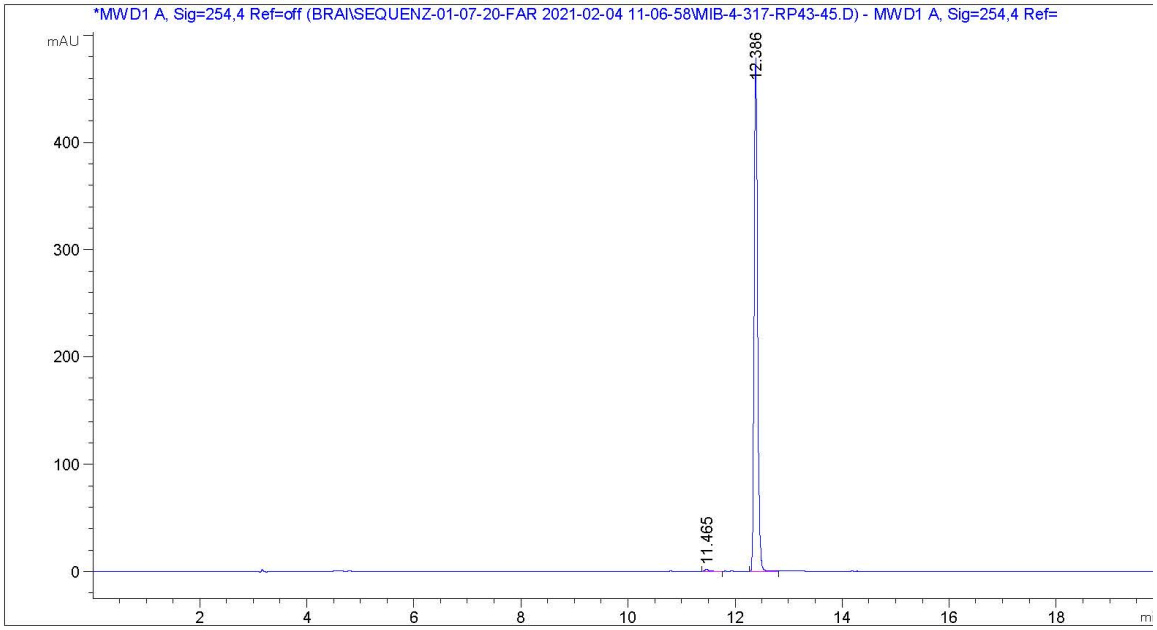


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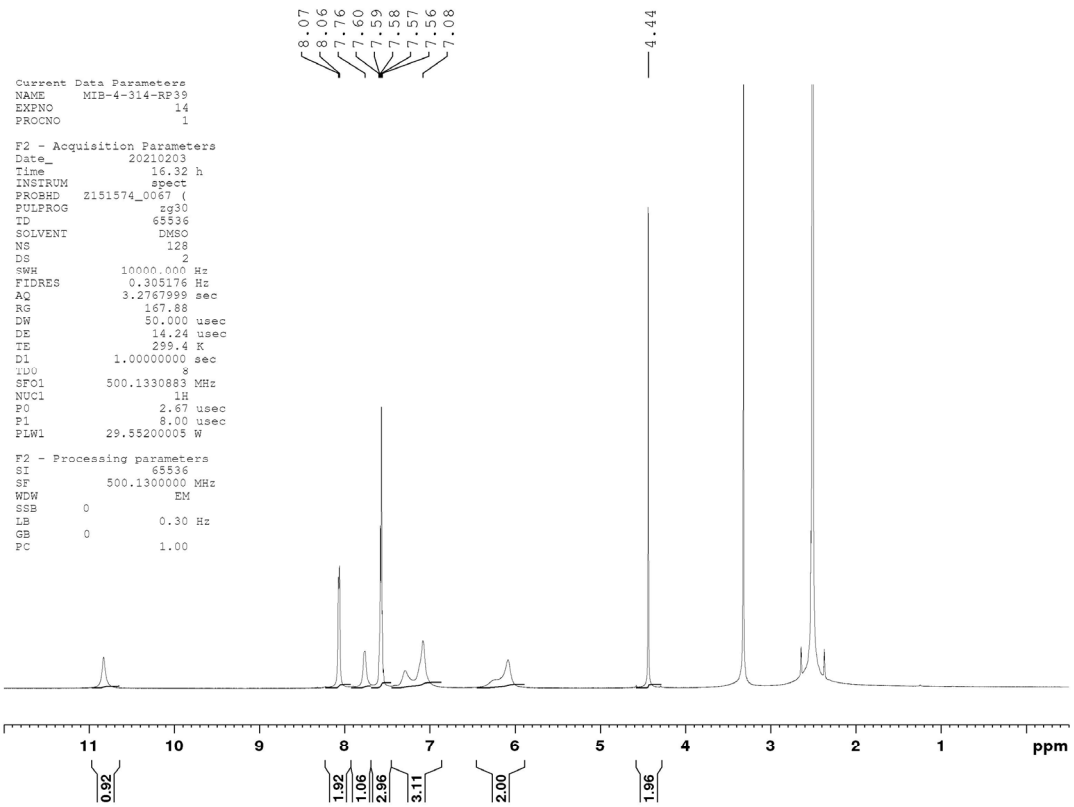

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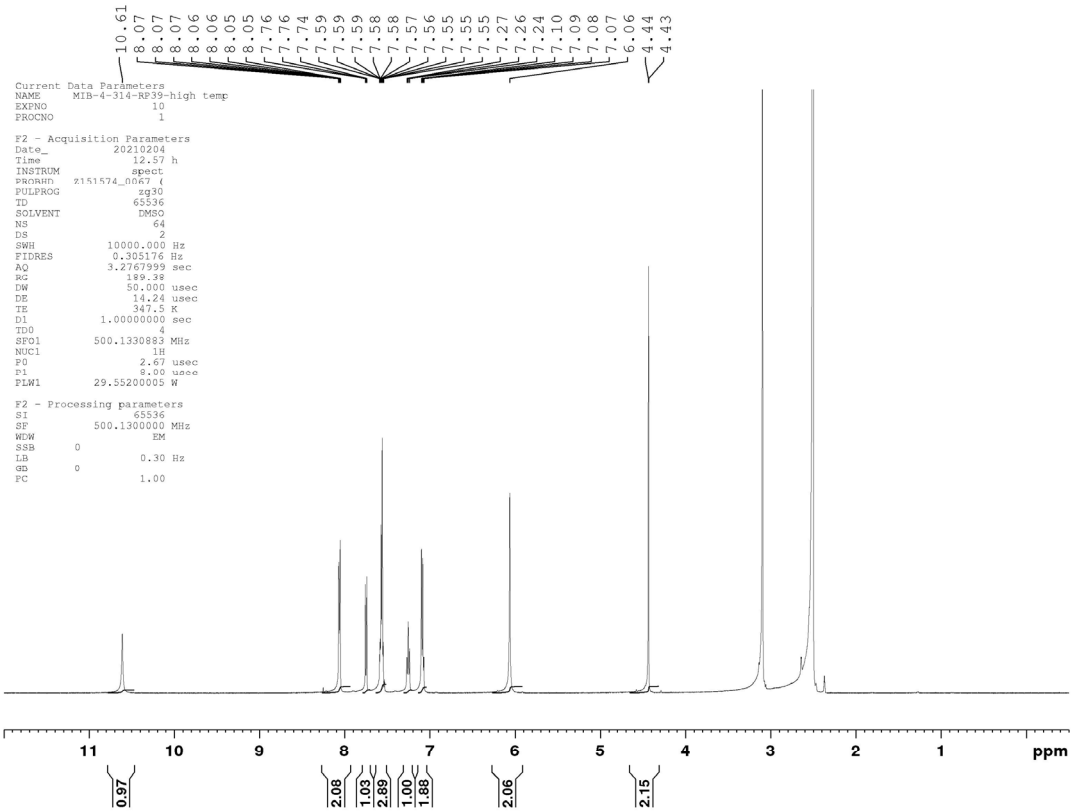
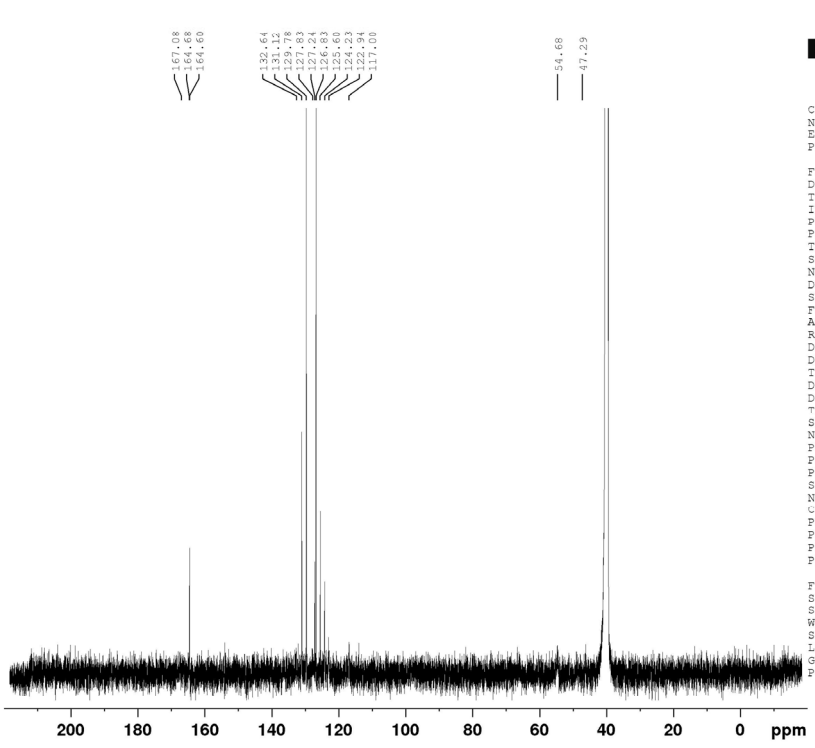


^{13}C-NMR

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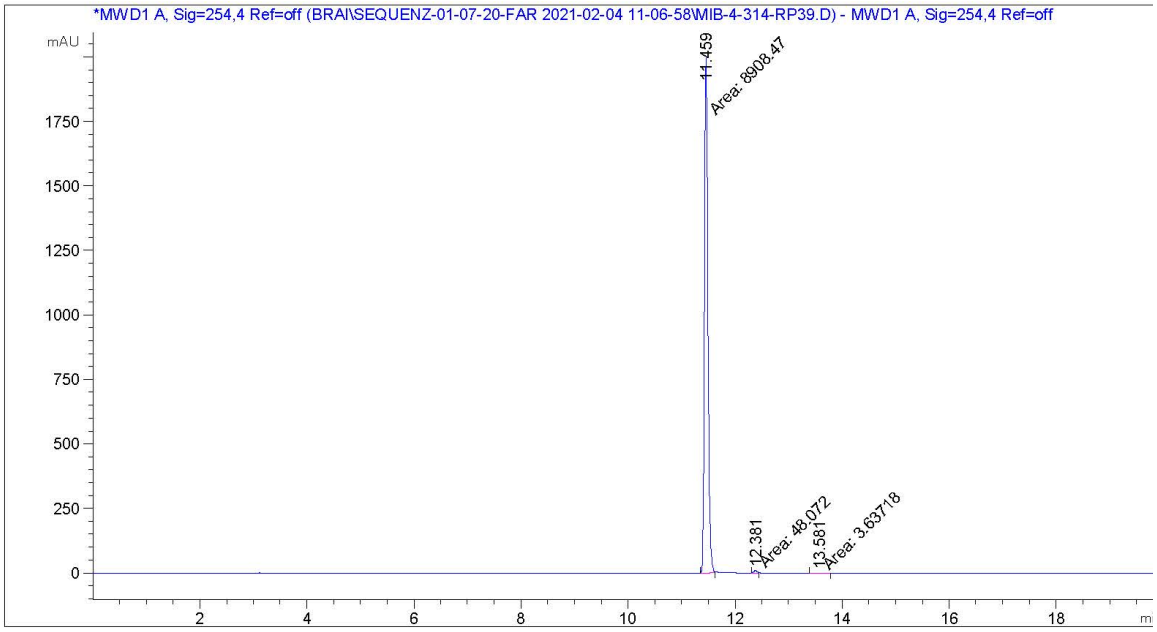


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Compound 26

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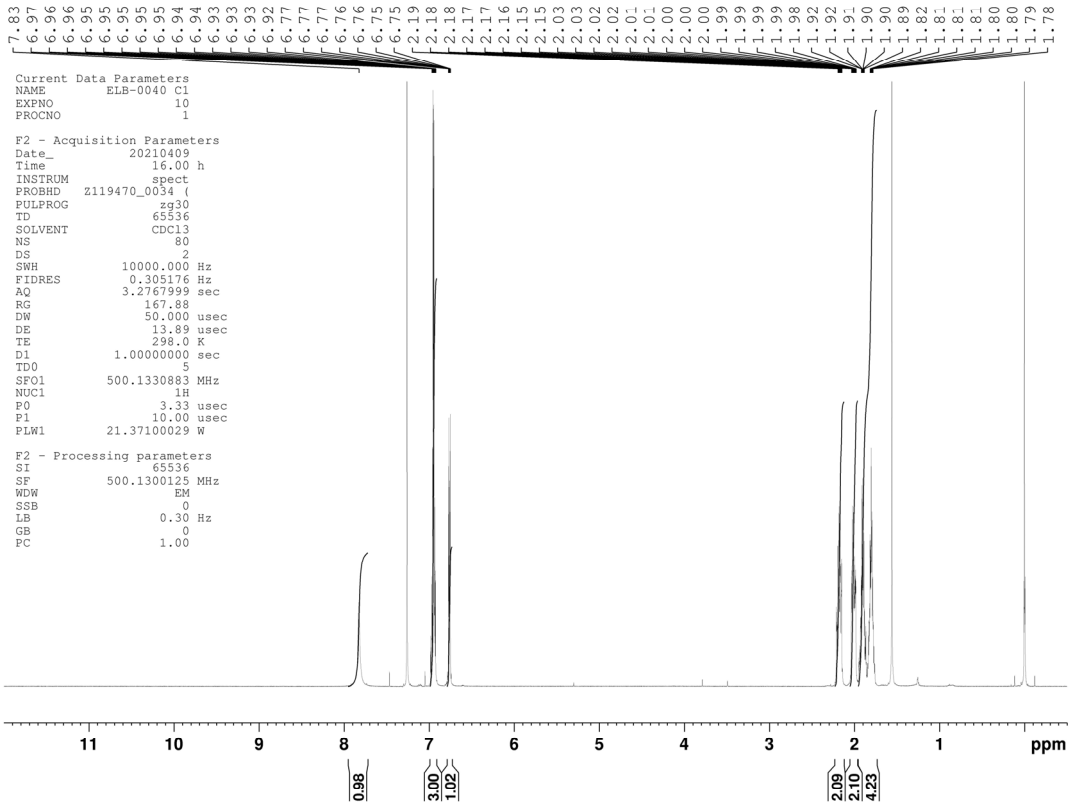

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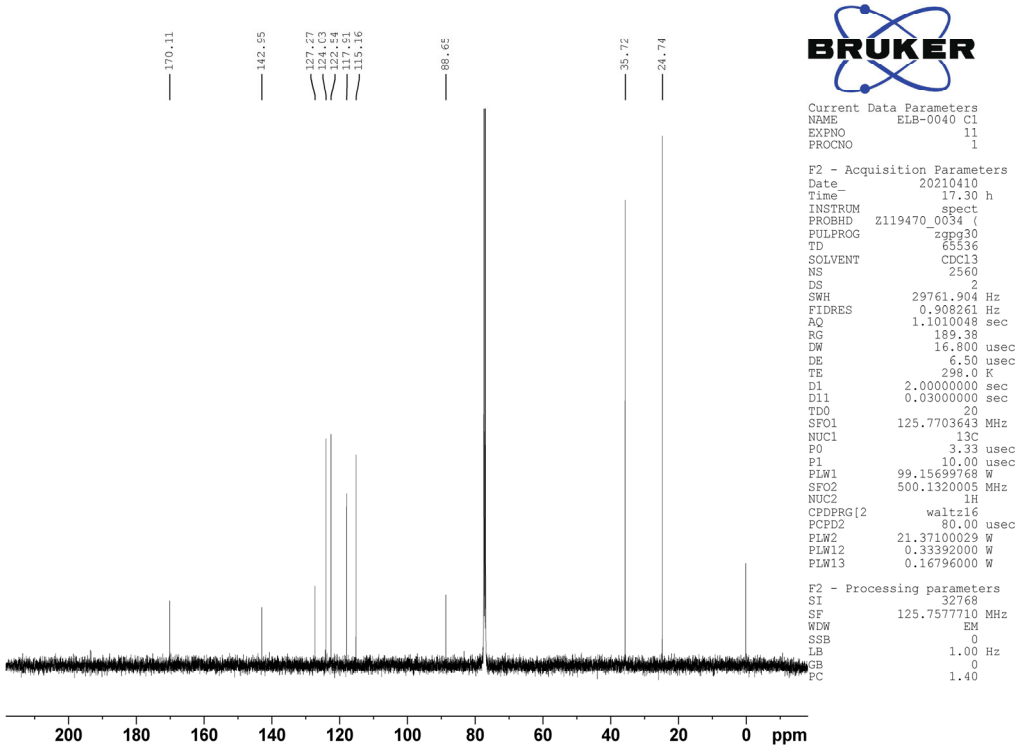

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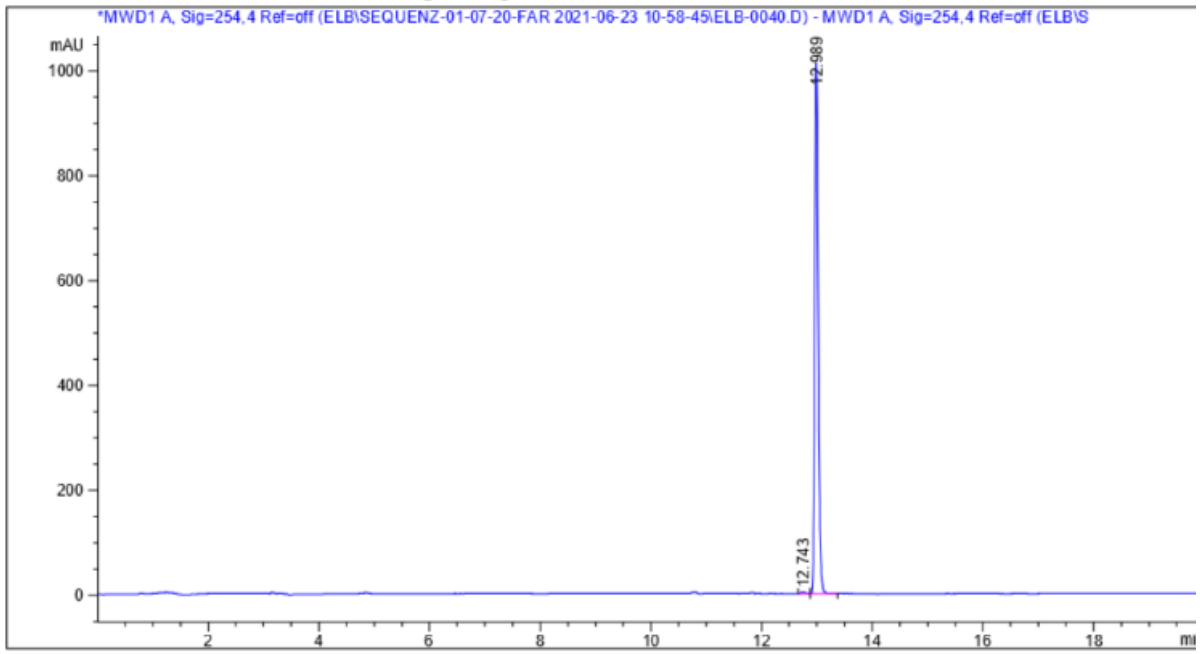


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Compound 27

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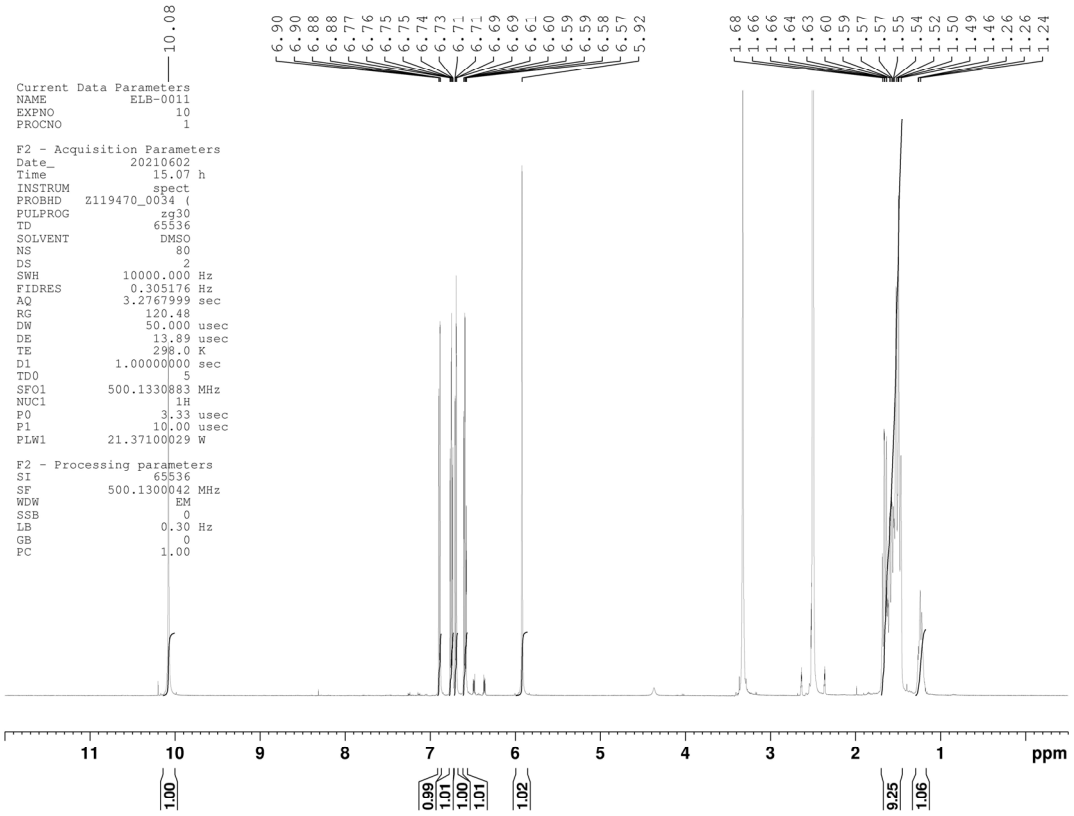

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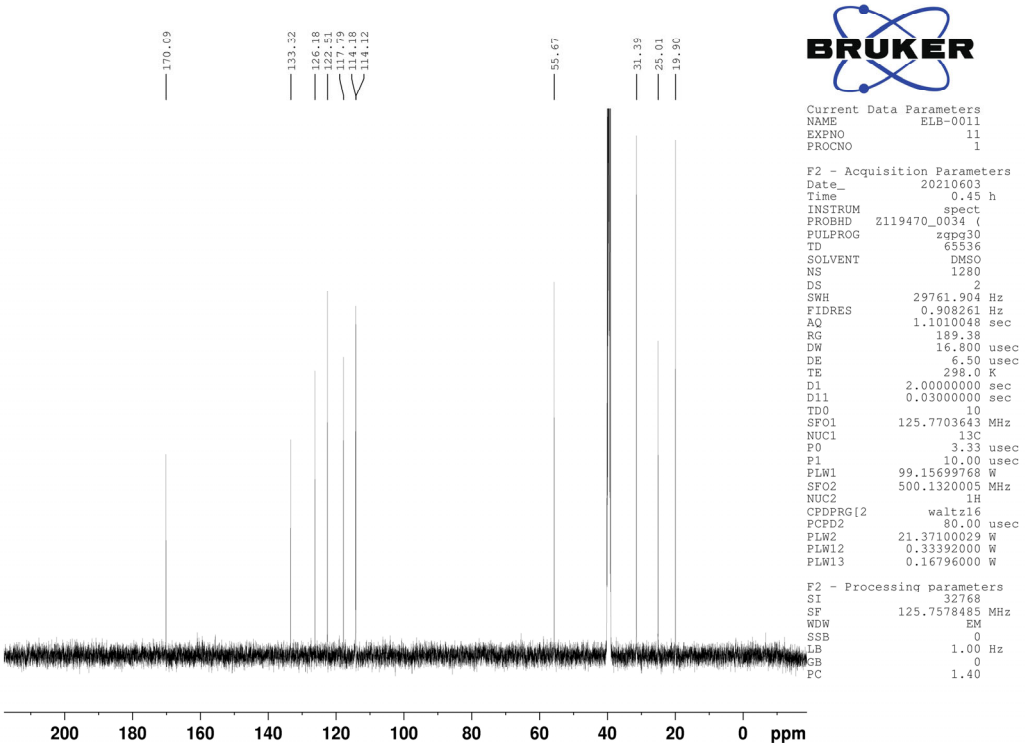

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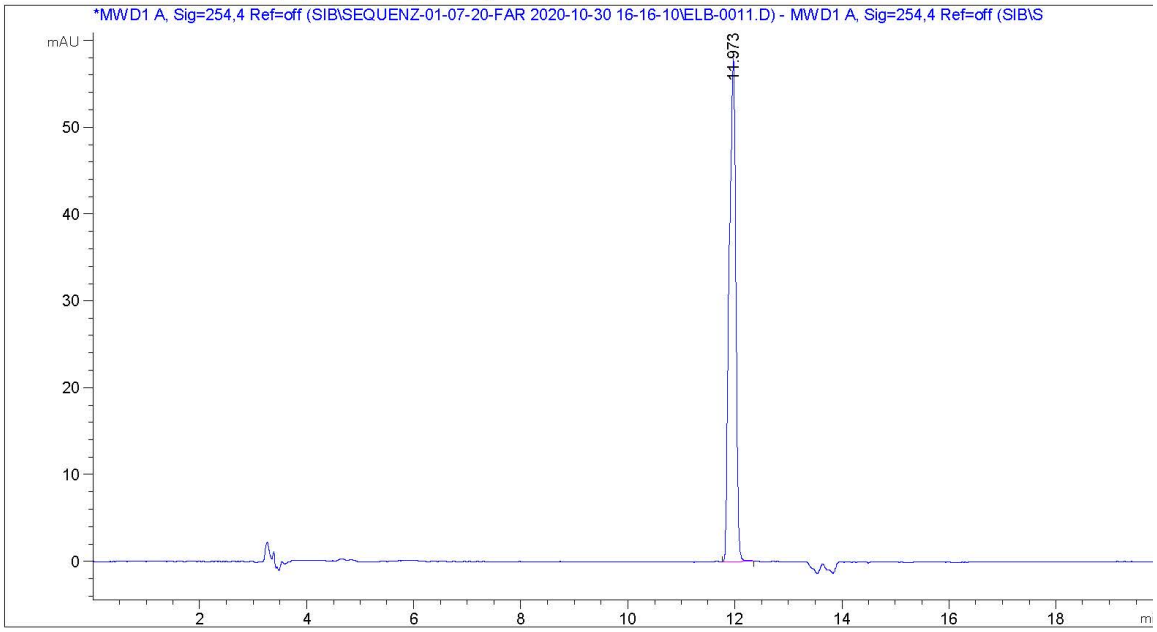


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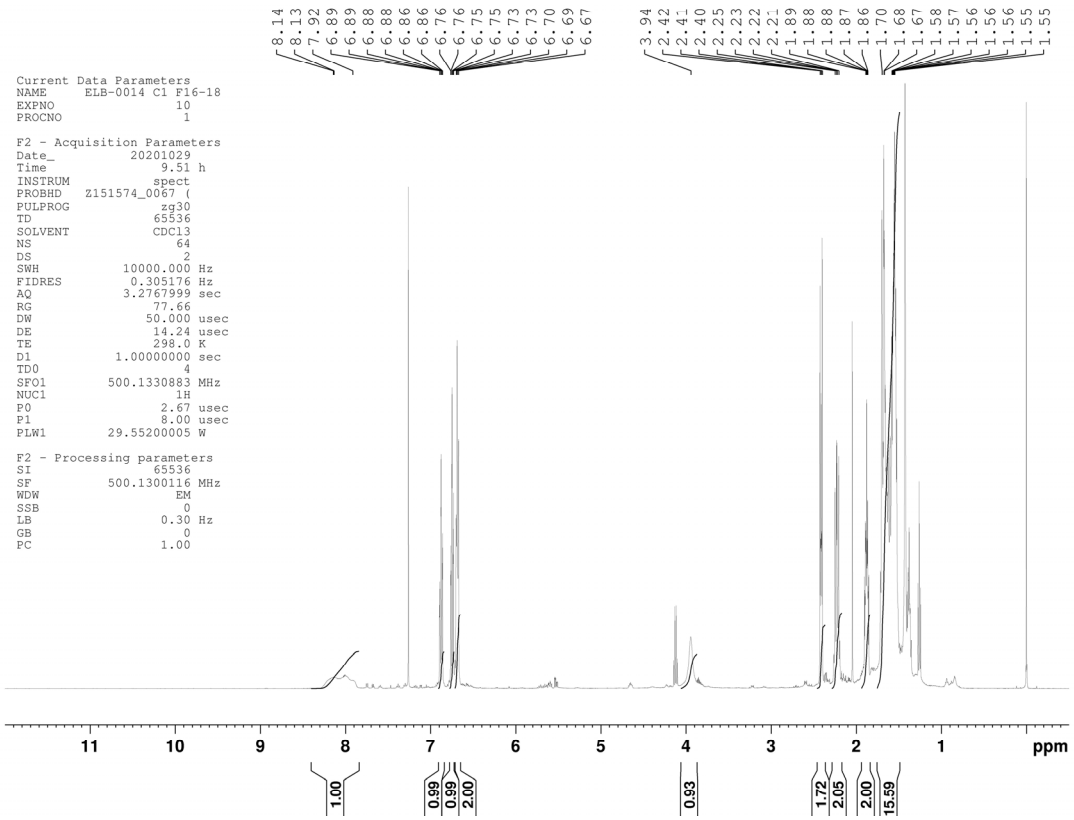
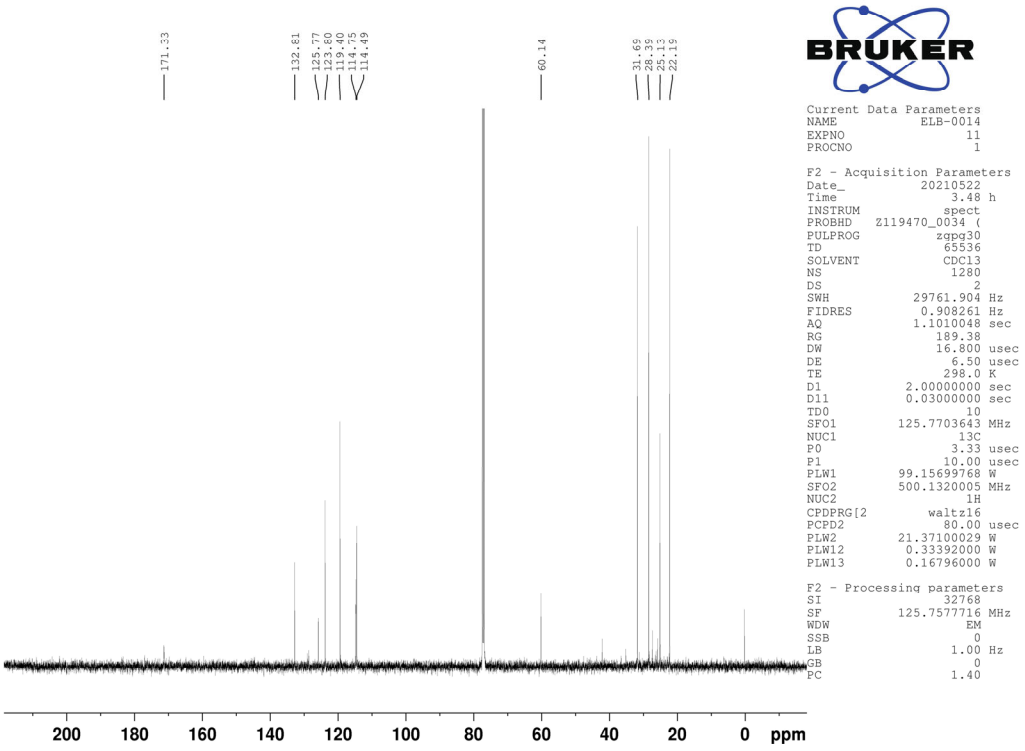
Compound 28

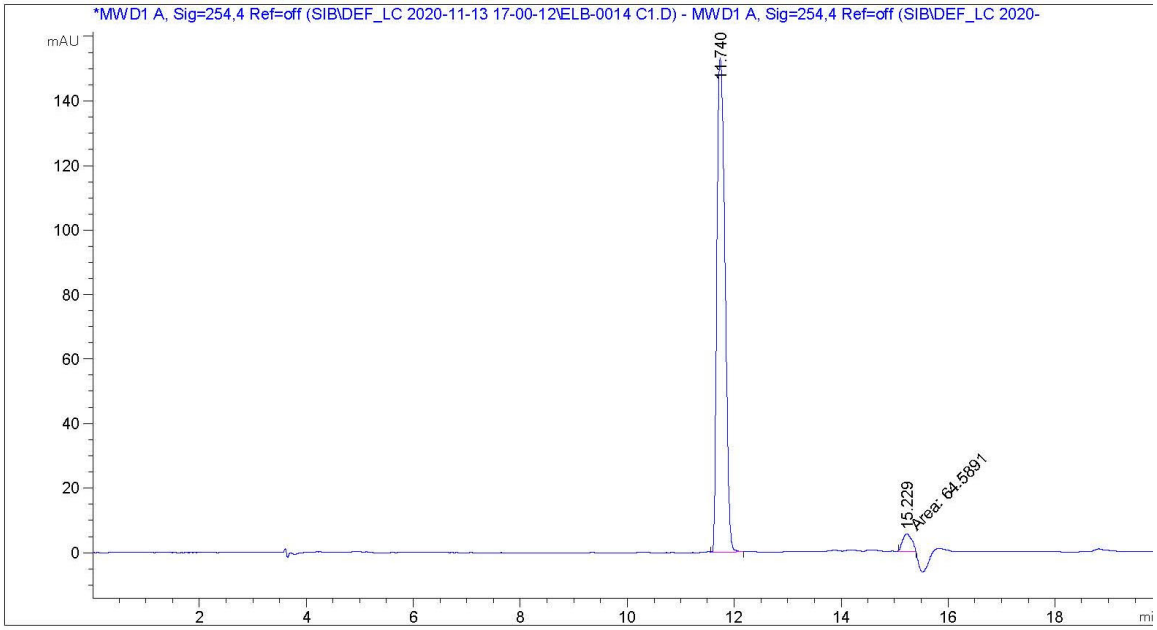
^{1}H-NMR



^{13}C-NMR



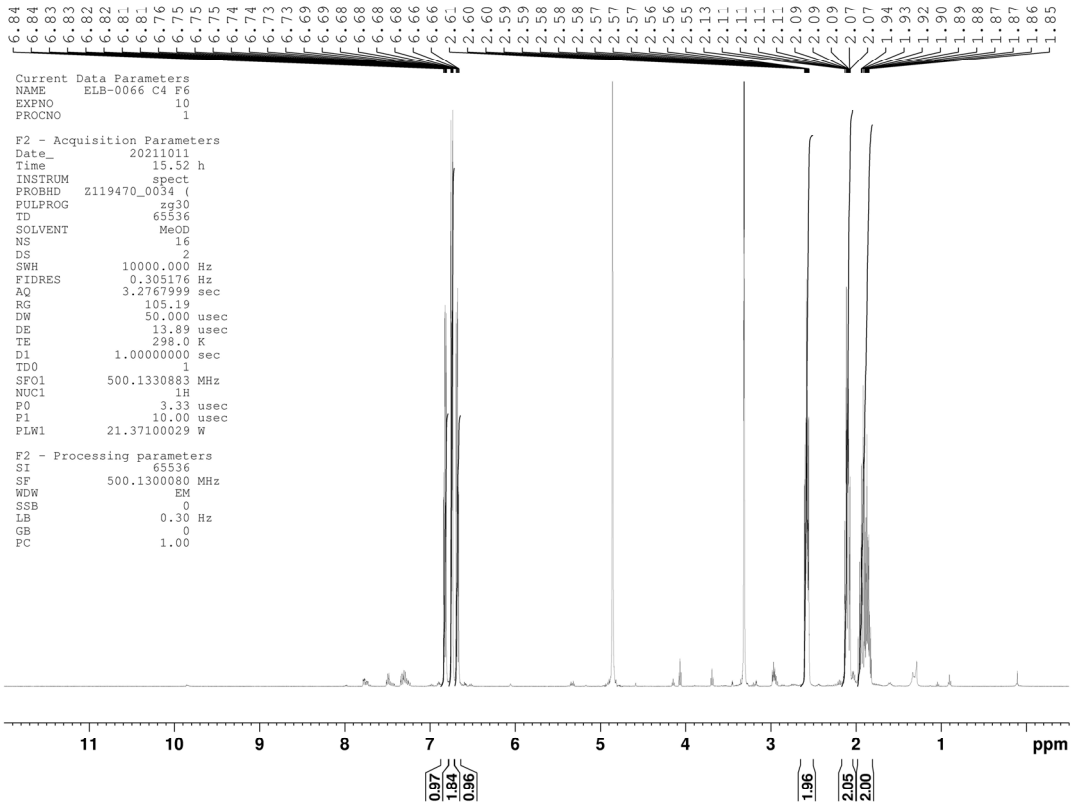
LC



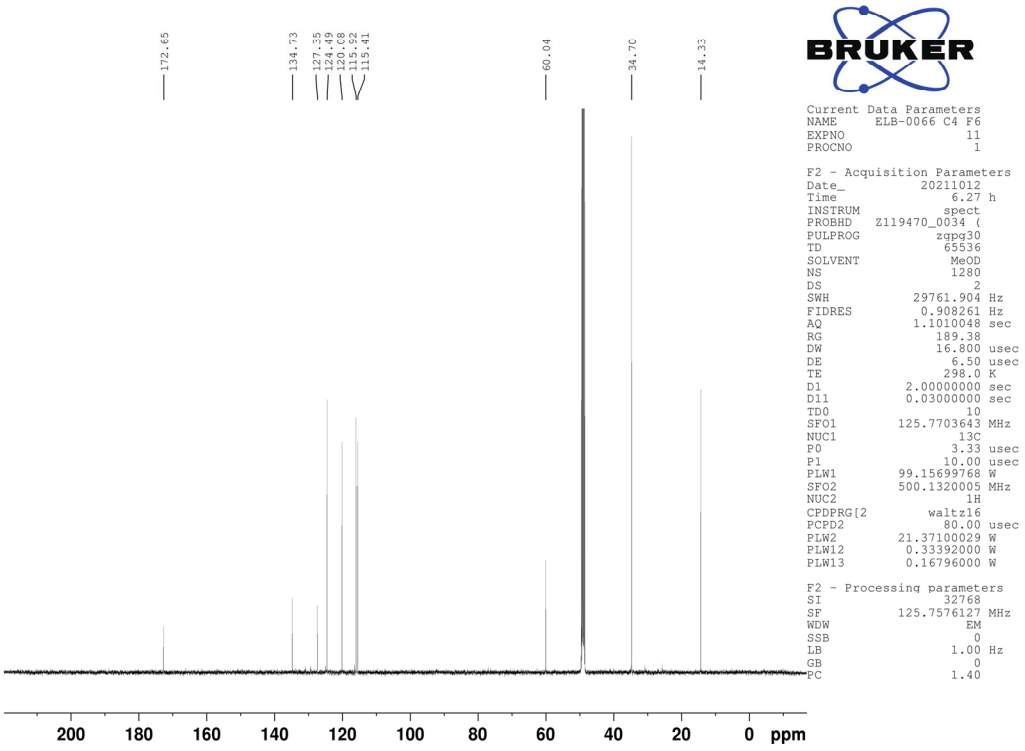

```
=====================================================================
                    Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.740 VB    0.1715 1595.30127  153.24013  96.1088
   2  15.229 MM    0.1993   64.58913    5.40105   3.8912

Totals :                  1659.89040  158.64118
```

Compound 29

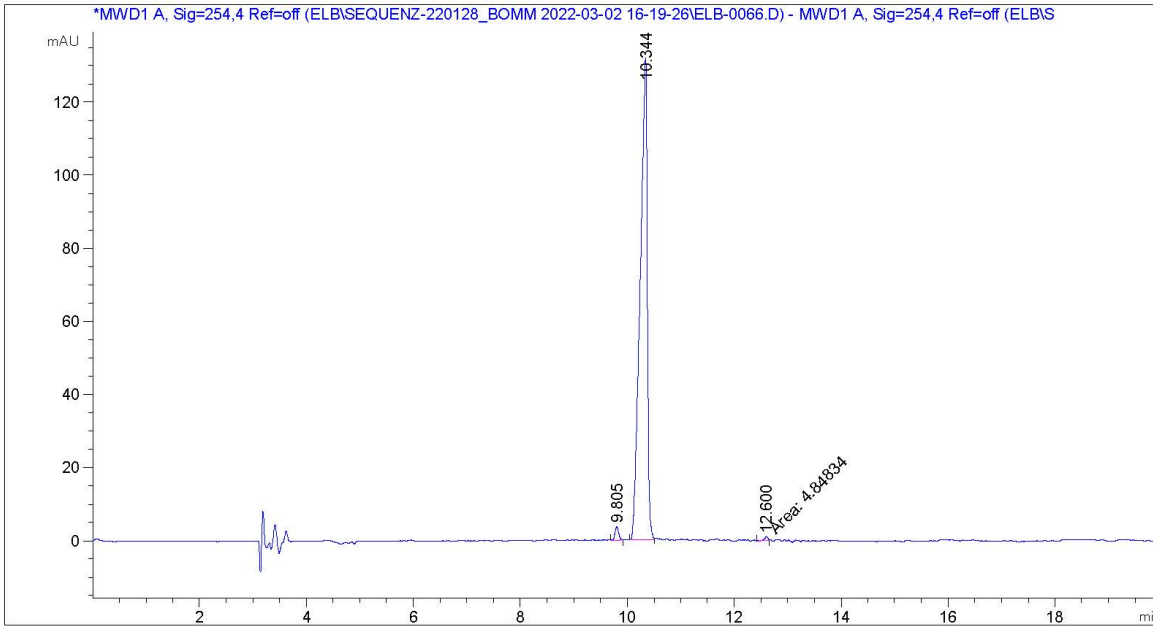
^{1}H-NMR



^{13}C-NMR



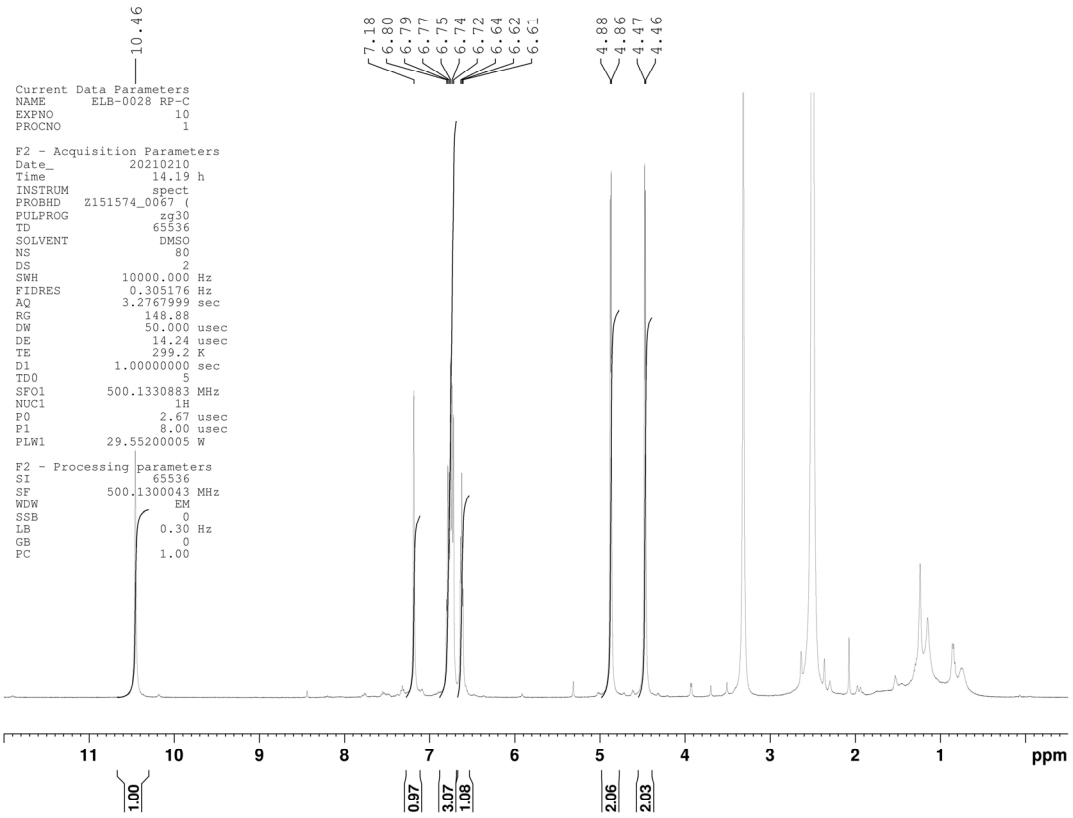
LC



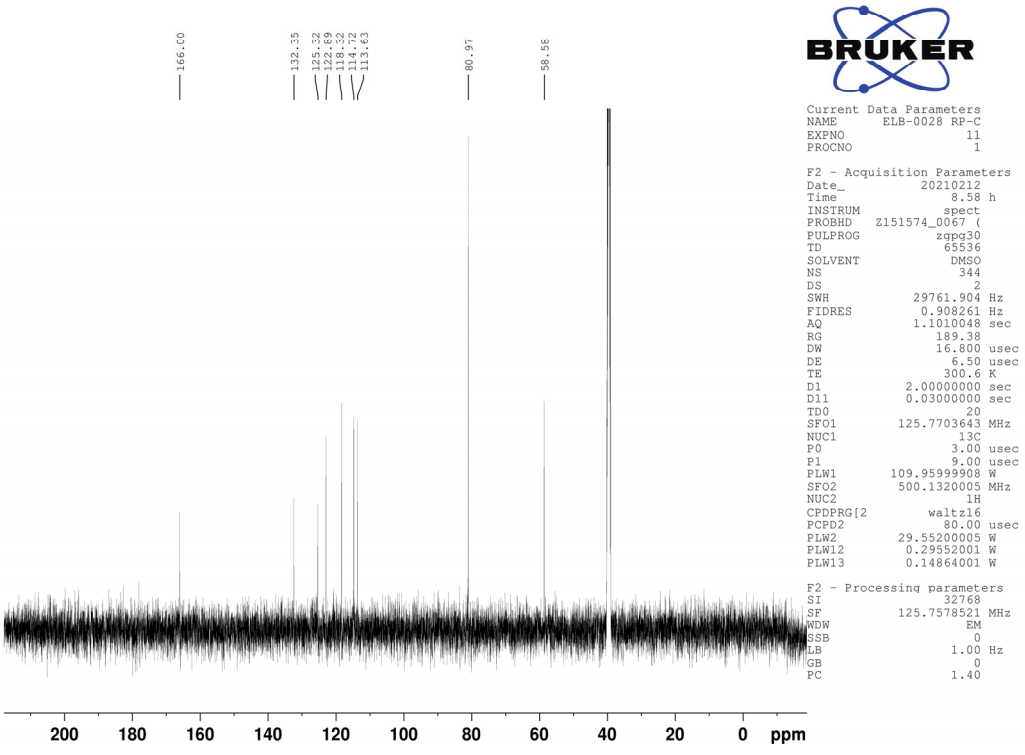

```
=====================================================================
                    Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1   9.805 VV    0.0733   18.23354    3.71084   1.4620
   2  10.344 VV    0.1241 1224.05200  132.16112  98.1492
   3  12.600 MM    0.0820    4.84834 9.85984e-1   0.3888

Totals :                  1247.13388  136.85794
```

Compound 30

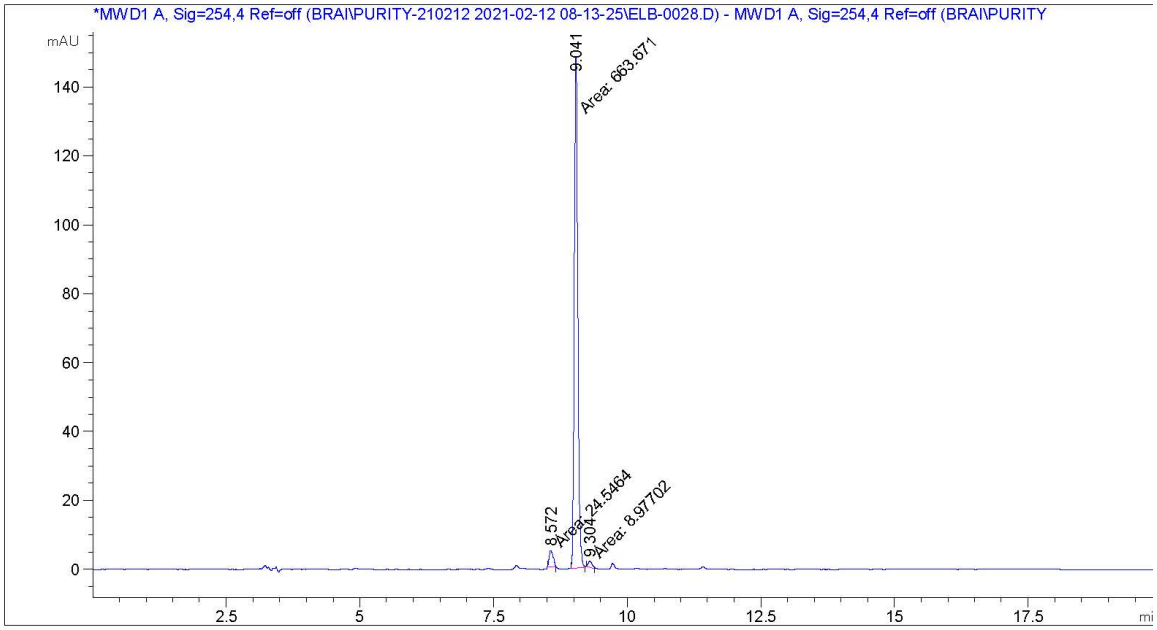
^{1}H-NMR



^{13}C-NMR



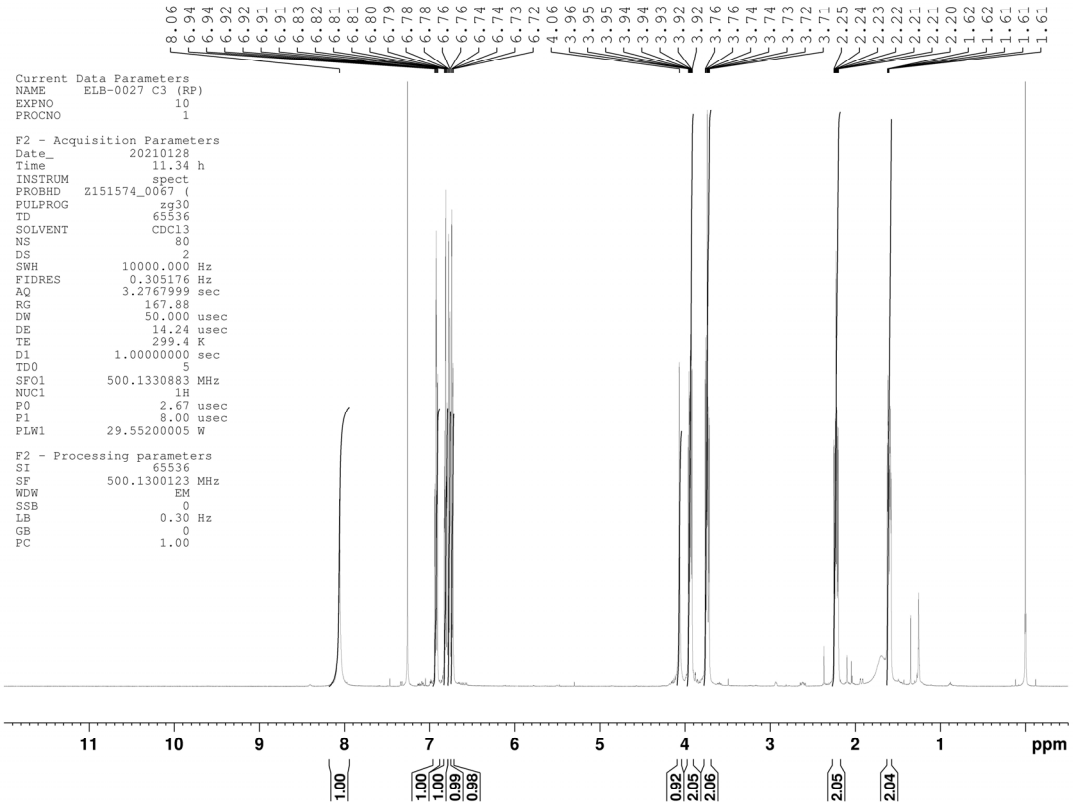
LC



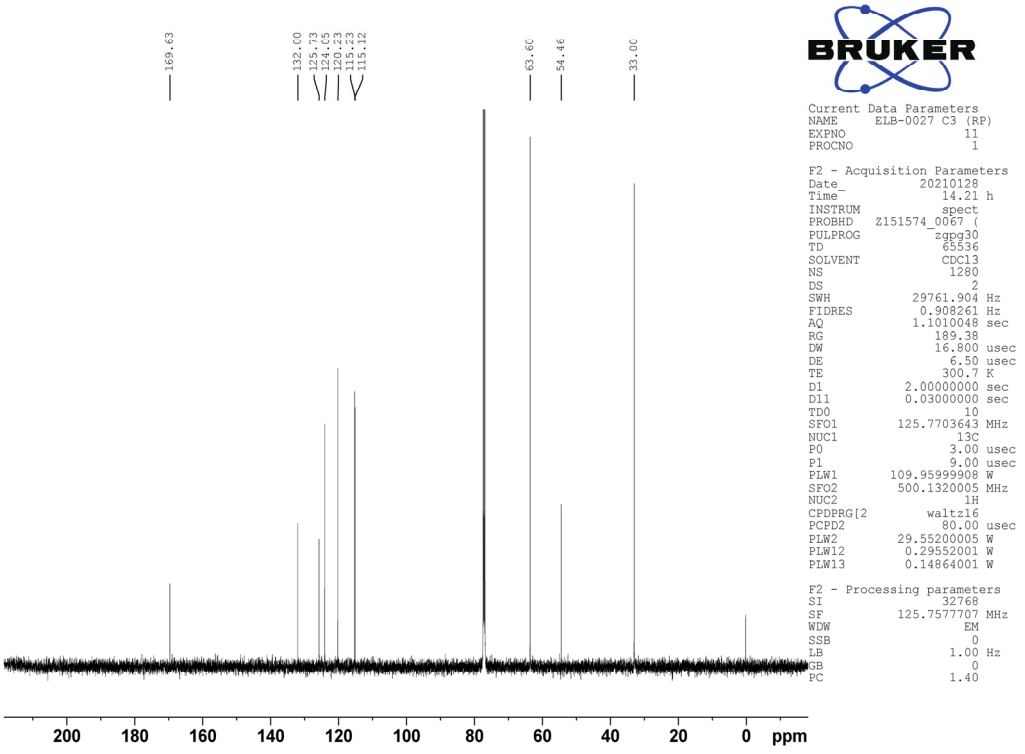

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.572 MM    0.0860   24.54641    4.75823   3.5207
   2   9.041 MM    0.0741  663.67084  149.22447  95.1917
   3   9.304 MM    0.0904    8.97702    1.65500   1.2876
```

Compound 31

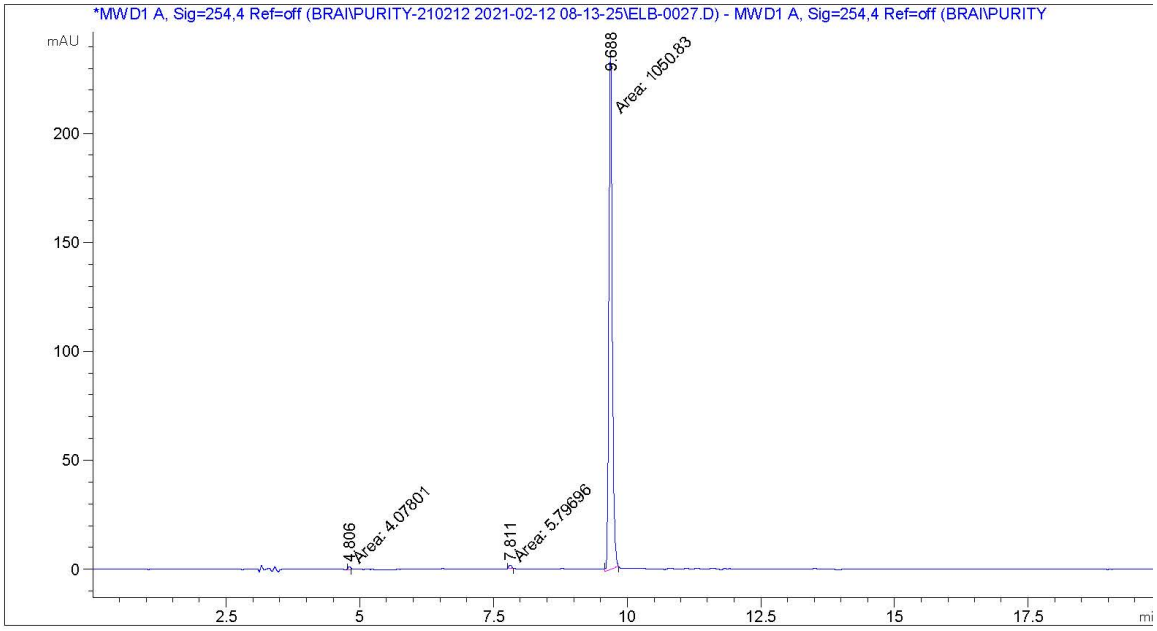
^{1}H-NMR



^{13}C-NMR



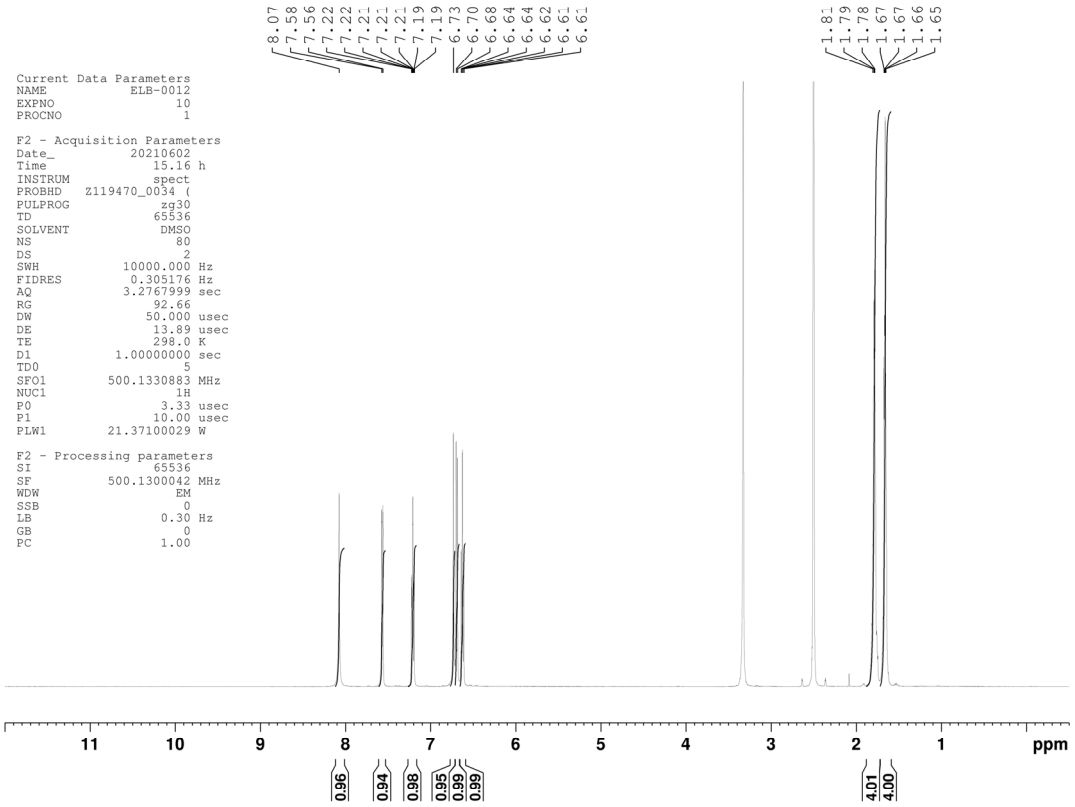
LC



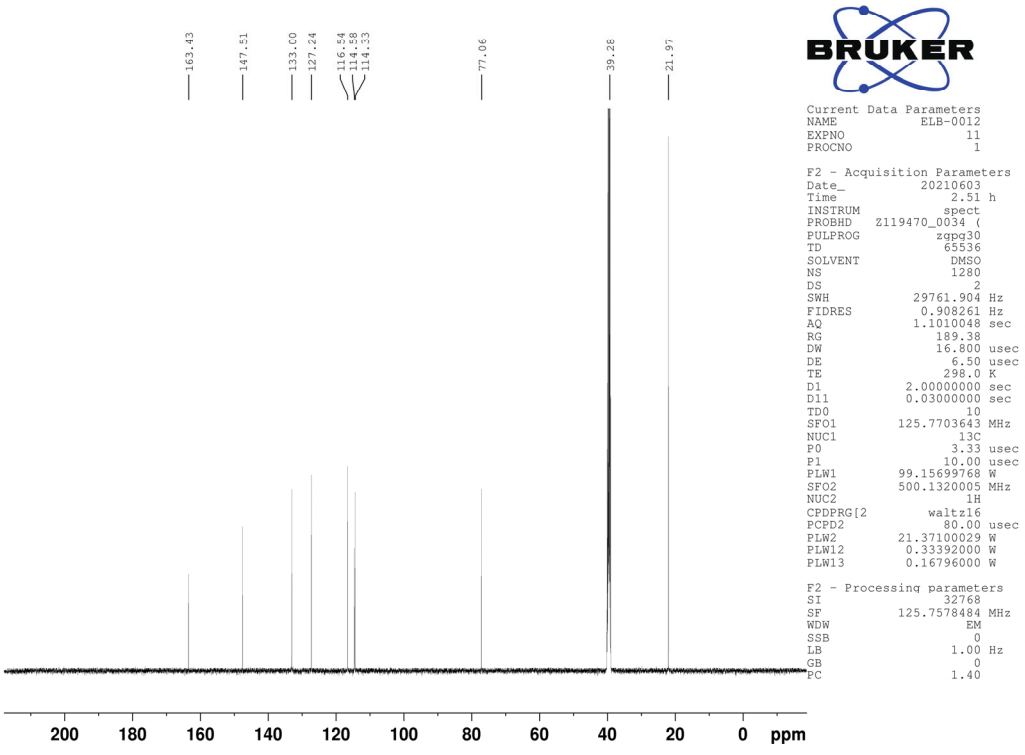

```
=====================================================================
                    Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.806 MM    0.0548    4.07801    1.24037   0.3845
   2   7.811 MM    0.0585    5.79696    1.65210   0.5465
   3   9.688 MM    0.0741 1050.83008  236.41370  99.0690

Totals :                  1060.70505  239.30617
```

Compound 32

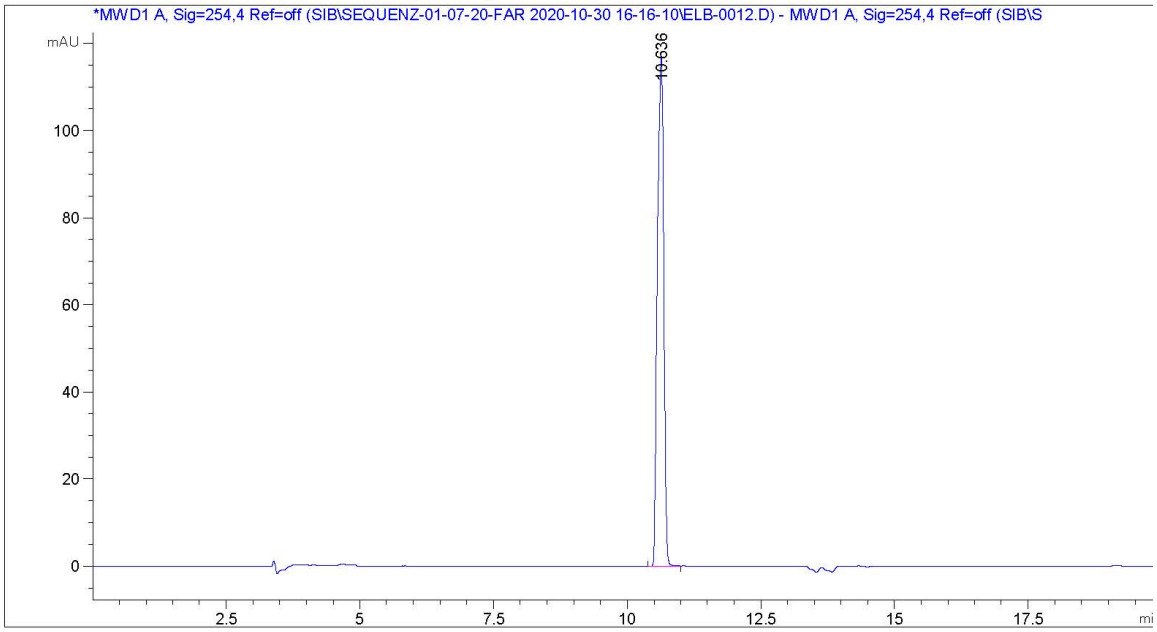
^{1}H-NMR



^{13}C-NMR



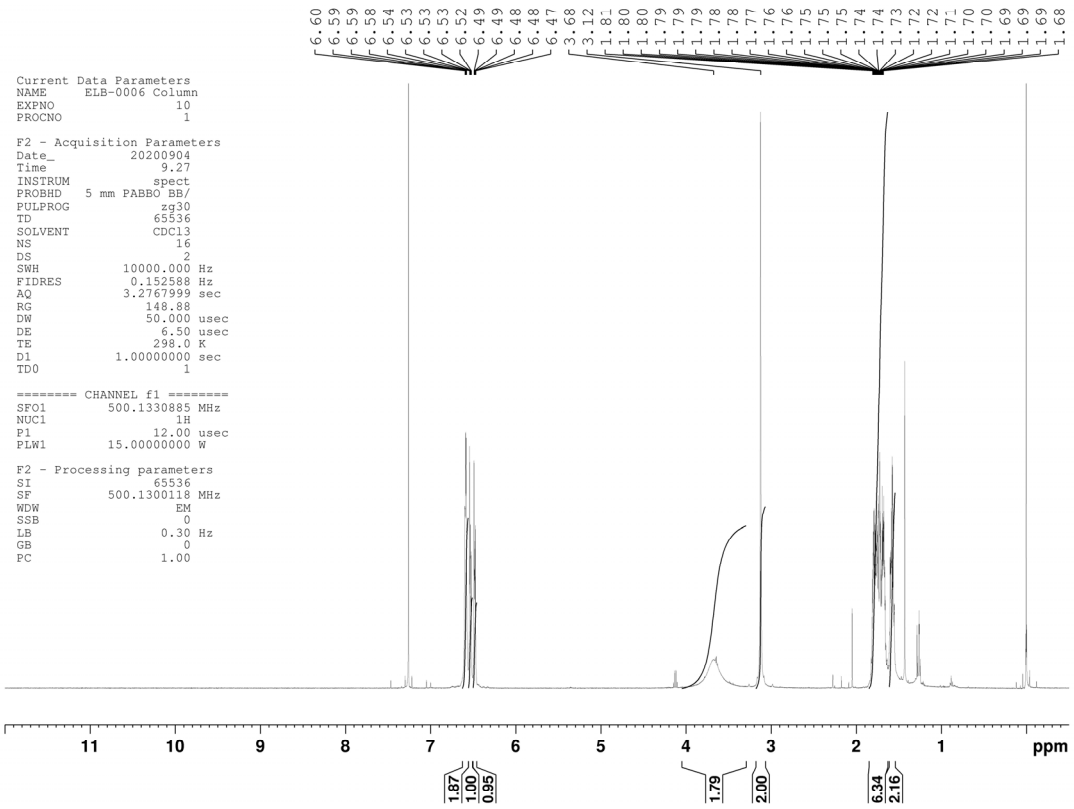
LC



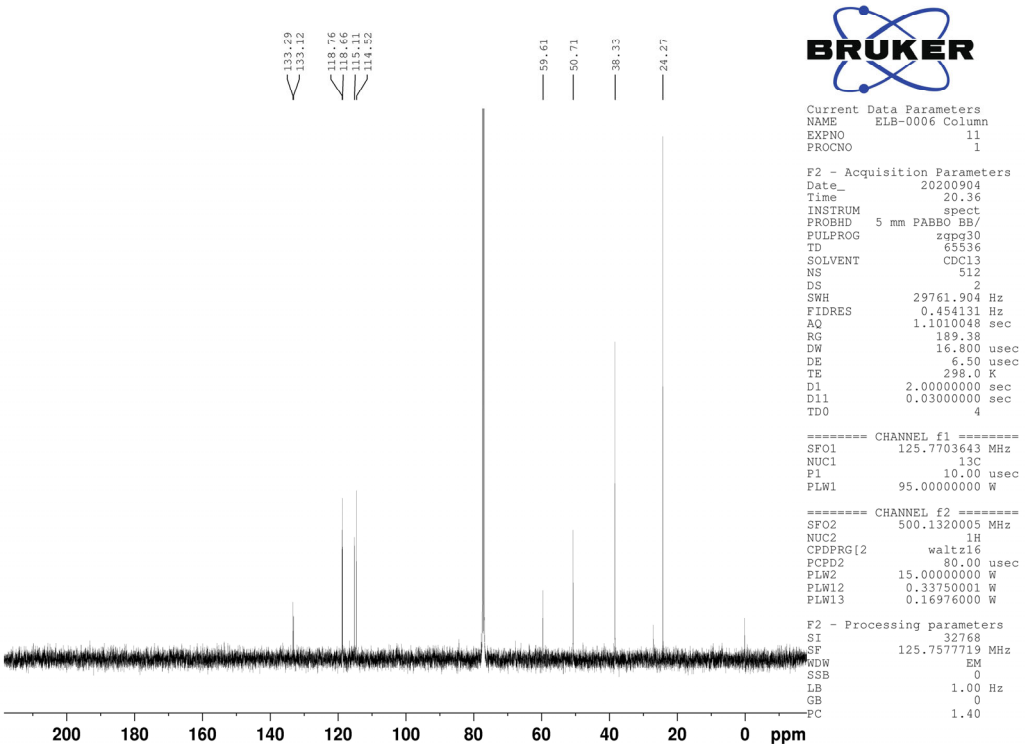

```
=====================================================================
                    Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.636 BB    0.1378  957.72064  116.57840 100.0000

Totals :                   957.72064  116.57840
```

Compound 33

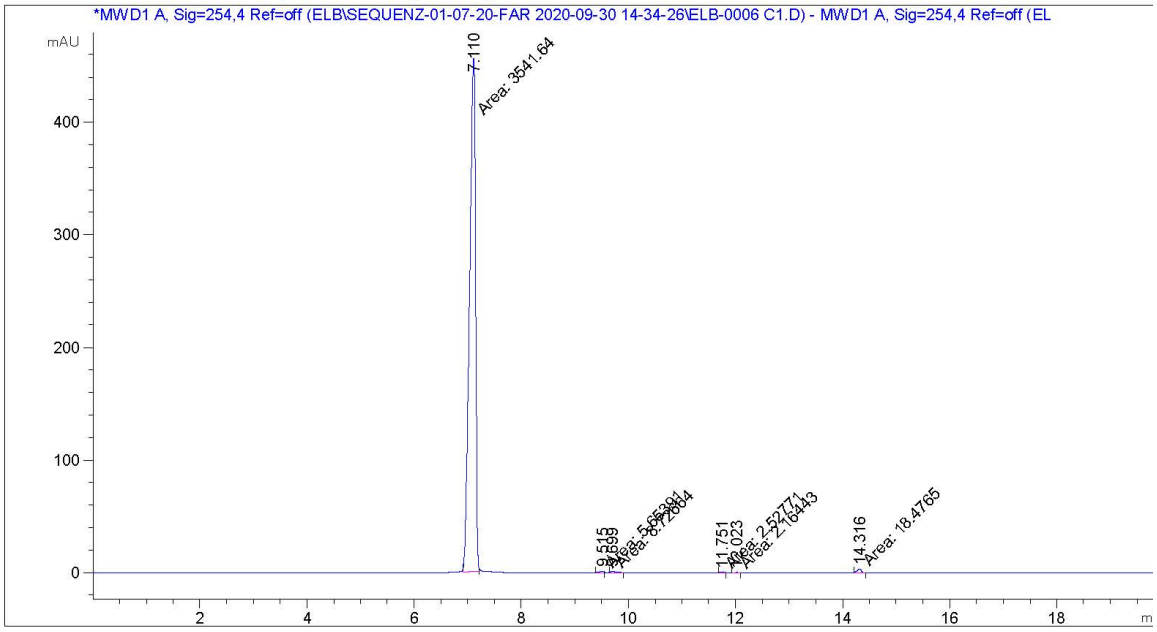
^{1}H-NMR



^{13}C-NMR



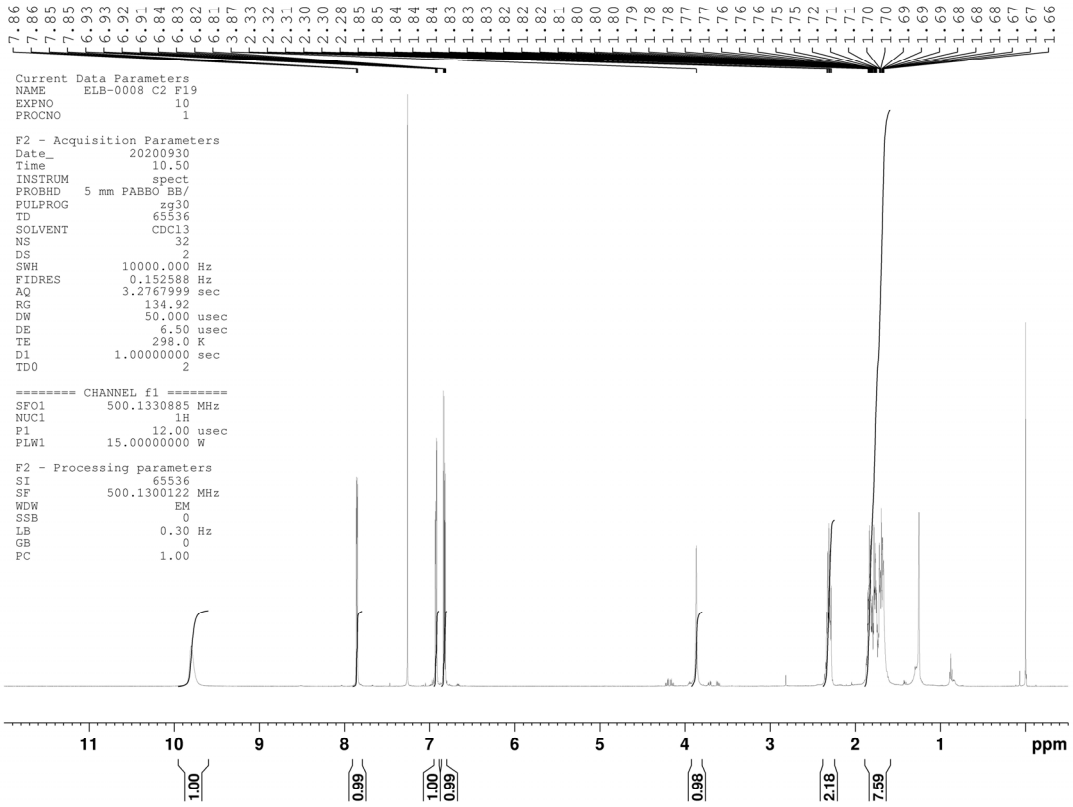
LC



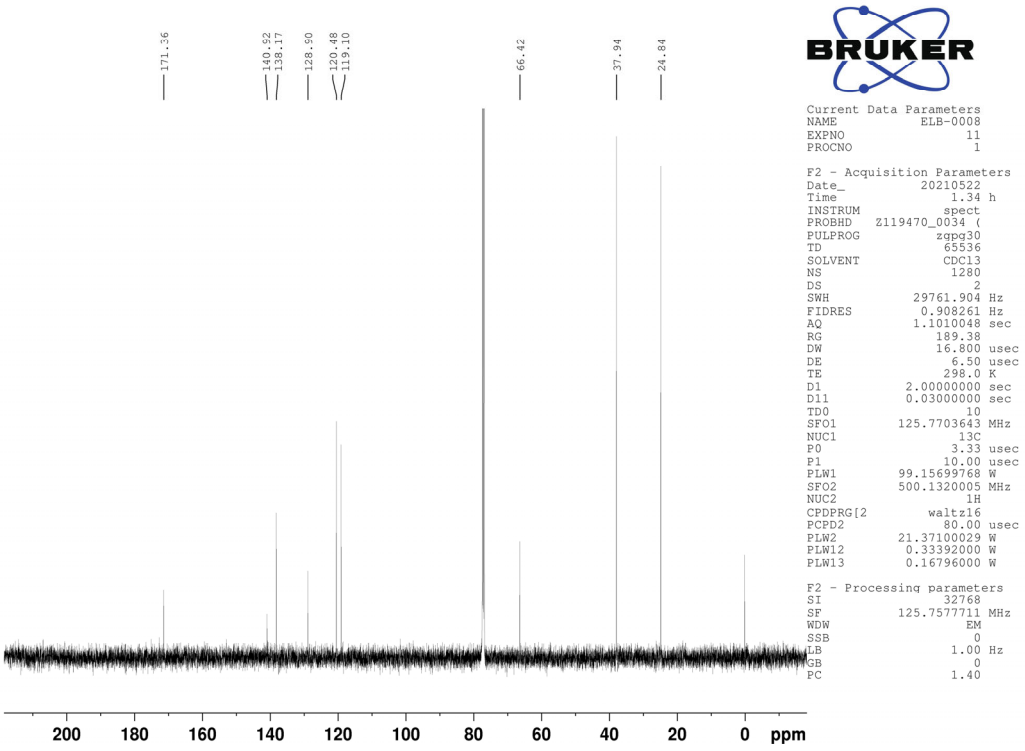

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.110 MM T  0.1294 3541.63672  456.25479  98.9509
   2   9.515 MM T  0.0947    5.65391 9.95205e-1   0.1580
   3   9.699 MM T  0.1257    8.72664    1.15742   0.2438
   4  11.751 MM T  0.0934    2.52771 4.51045e-1   0.0706
   5  12.023 MM T  0.1099    2.16443 3.28346e-1   0.0605
   6  14.316 MM T  0.0921   18.47653    3.34177   0.5162
```

Compound 34

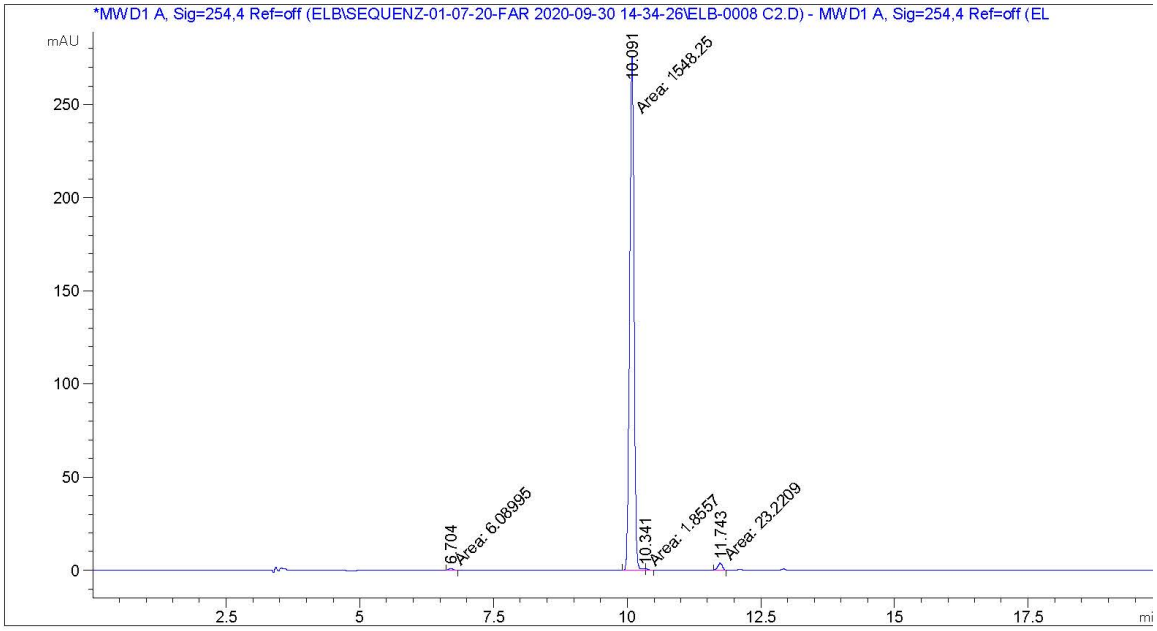
^{1}H-NMR



^{13}C-NMR



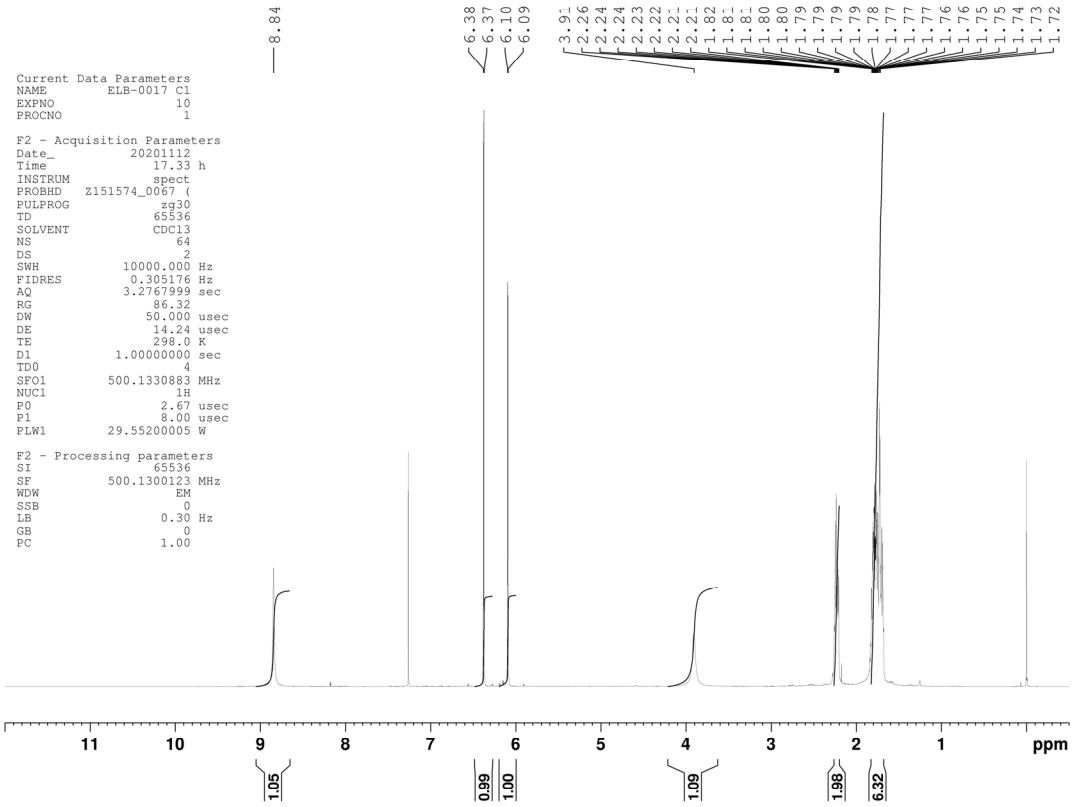
LC



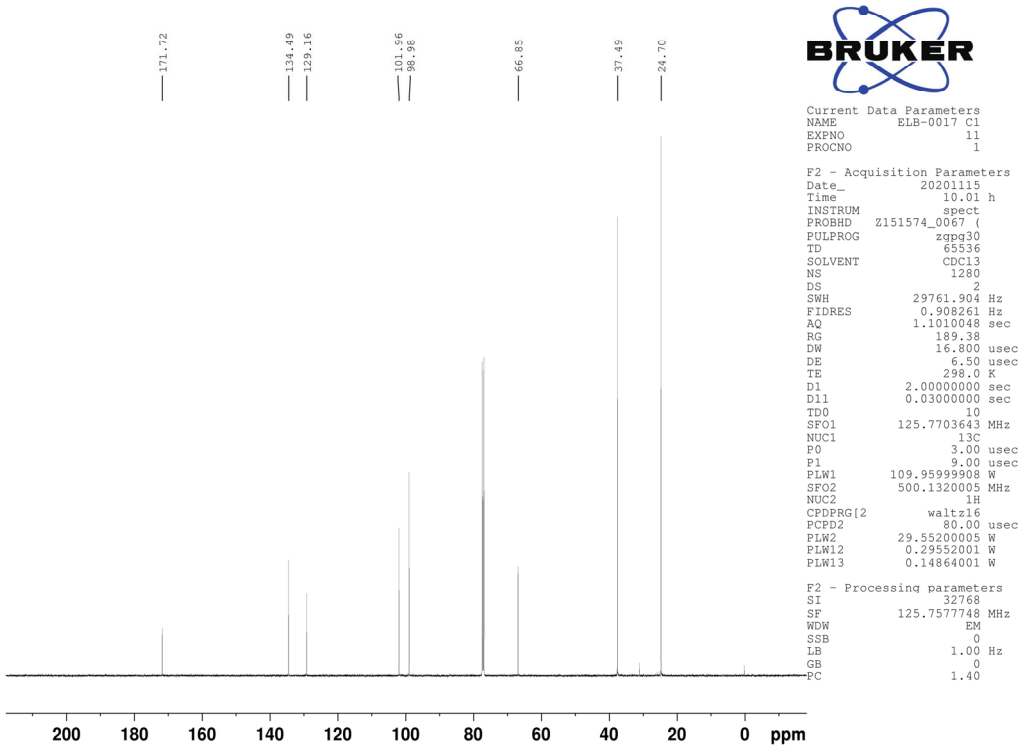

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.704 MM T  0.0994    6.08995    1.02136   0.3856
   2  10.091 MF T  0.0936 1548.24792  275.67526  98.0267
   3  10.341 FM T  0.0590    1.85570 5.24229e-1   0.1175
   4  11.743 MM T  0.1006   23.22087    3.84733   1.4702

Totals :                  1579.41445  281.06818
```

Compound 35

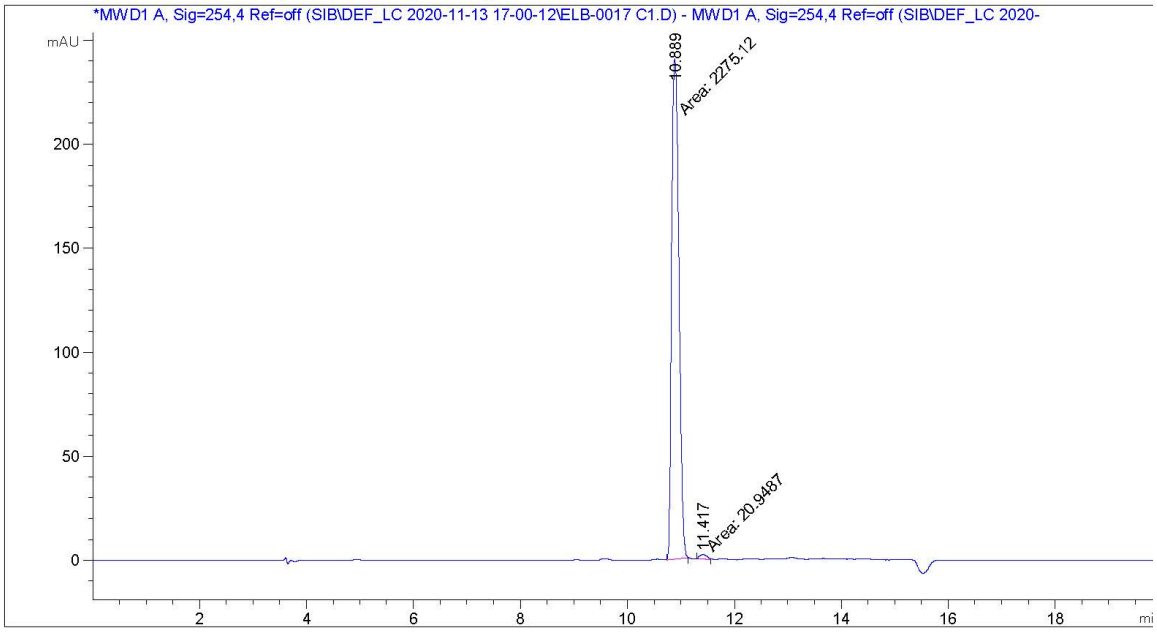
^{1}H-NMR



^{13}C-NMR



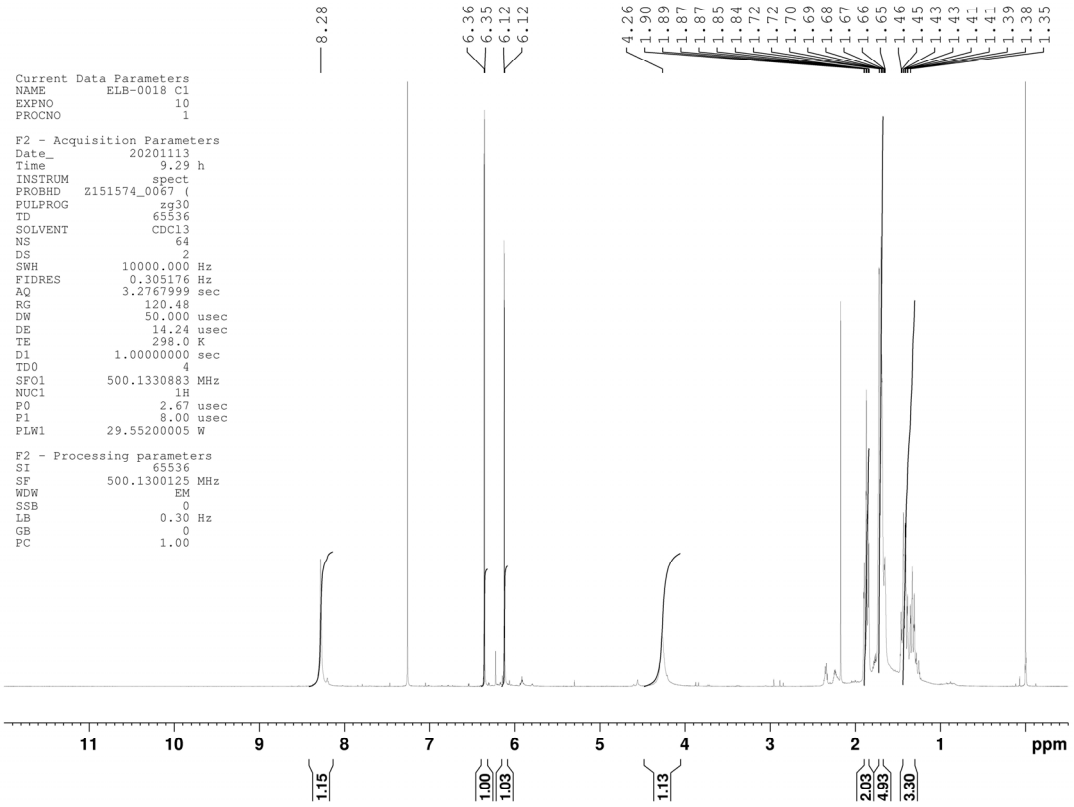
LC



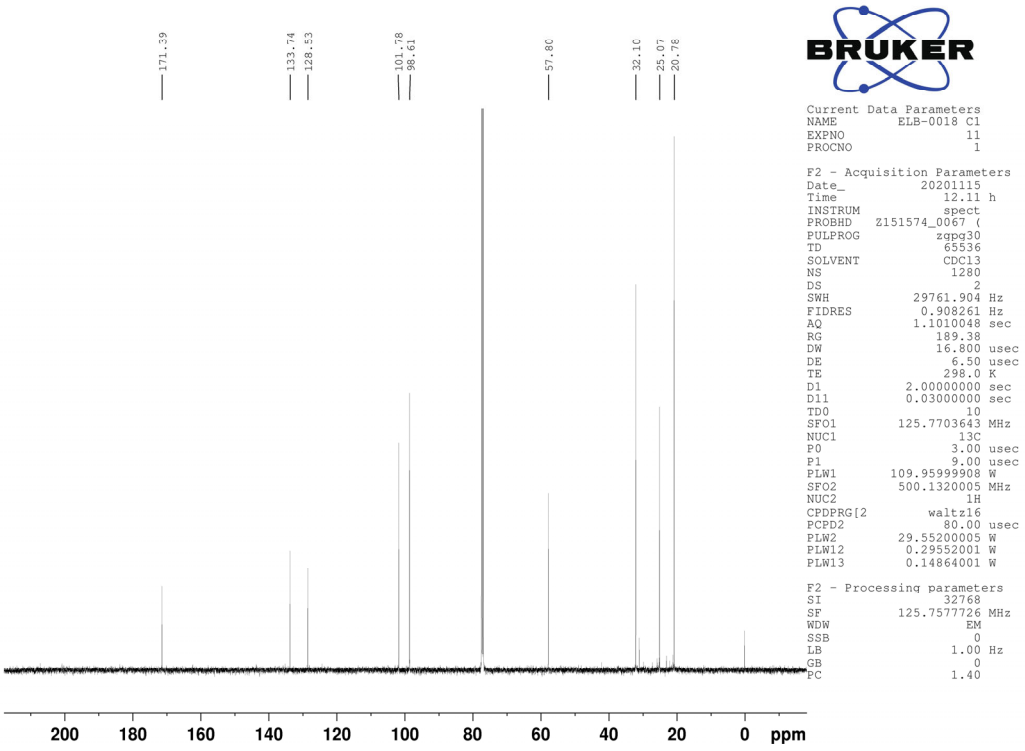

```
=====================================================================
                    Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.889 MM    0.1576 2275.11841  240.67653  99.0876
   2  11.417 MM    0.1658   20.94868    2.10626   0.9124

Totals :                  2296.06709  242.78279
```

Compound 36

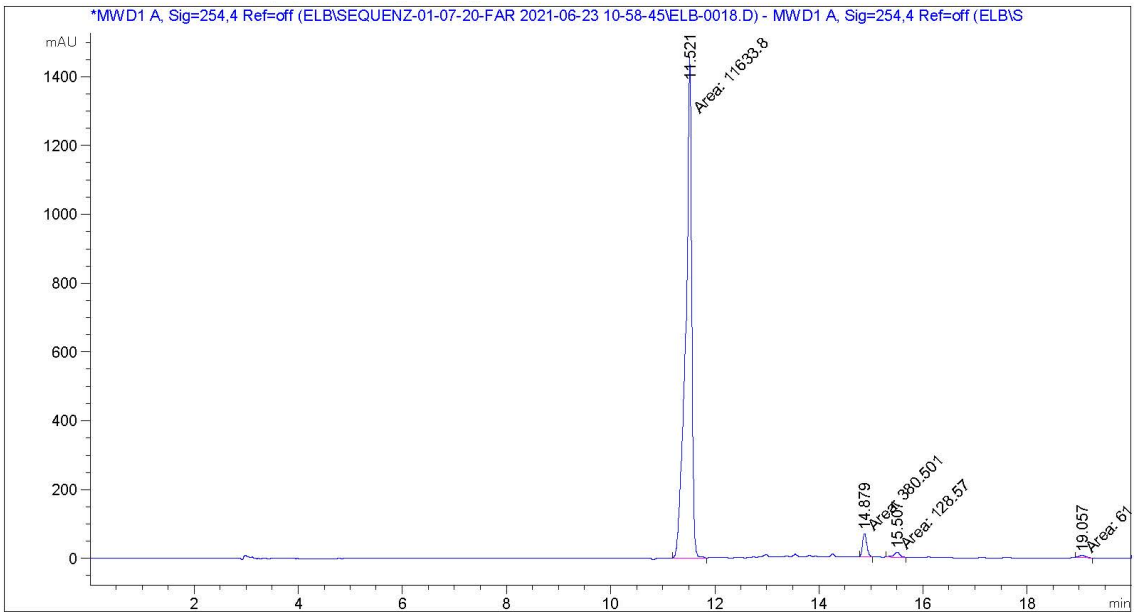
^{1}H-NMR



^{13}C-NMR



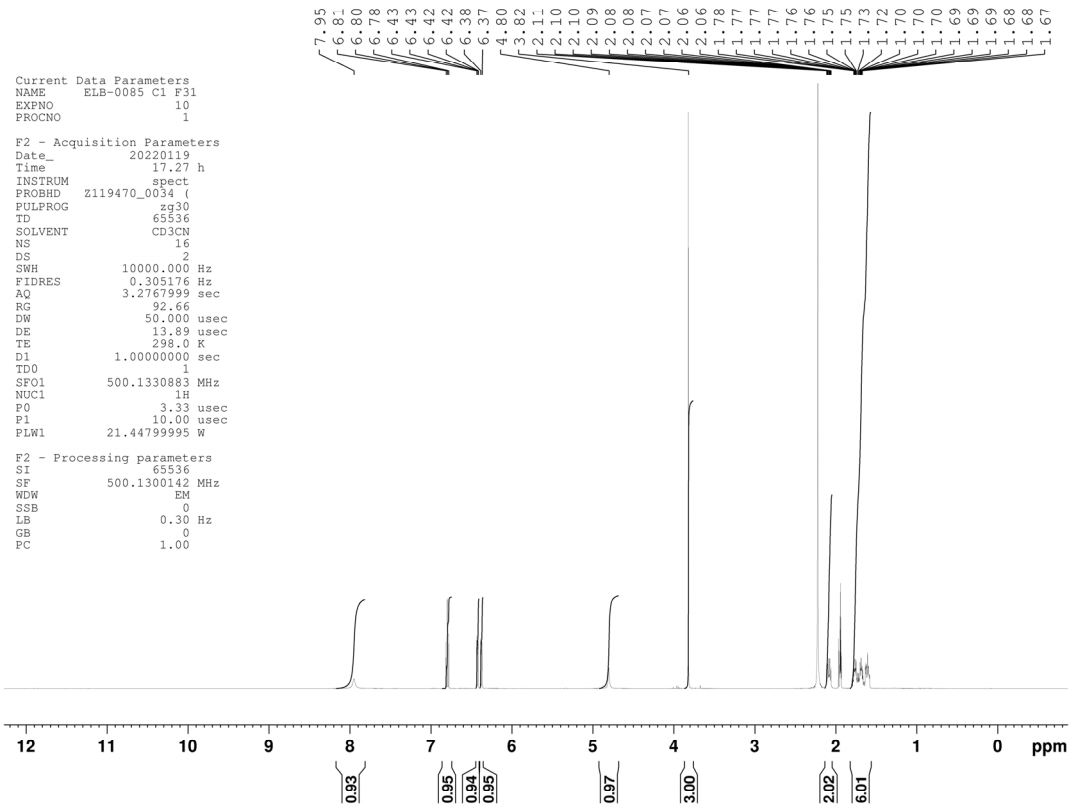
LC



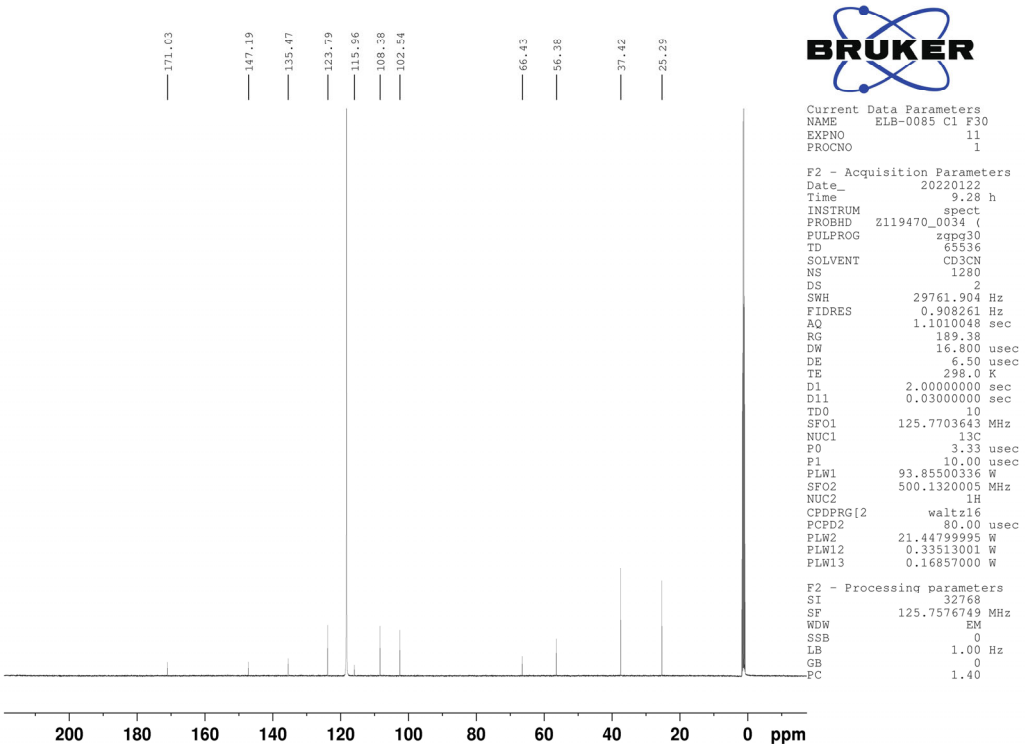

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.521 MM    0.1329 1.16338e4  1459.25366  95.3272
   2  14.879 MM    0.0937  380.50146   67.65564   3.1178
   3  15.507 MM    0.1446  128.57019   14.82338   1.0535
   4  19.057 MM    0.1630   61.19766    6.25837   0.5015

Totals :                  1.22041e4  1547.99105
```

Compound 37

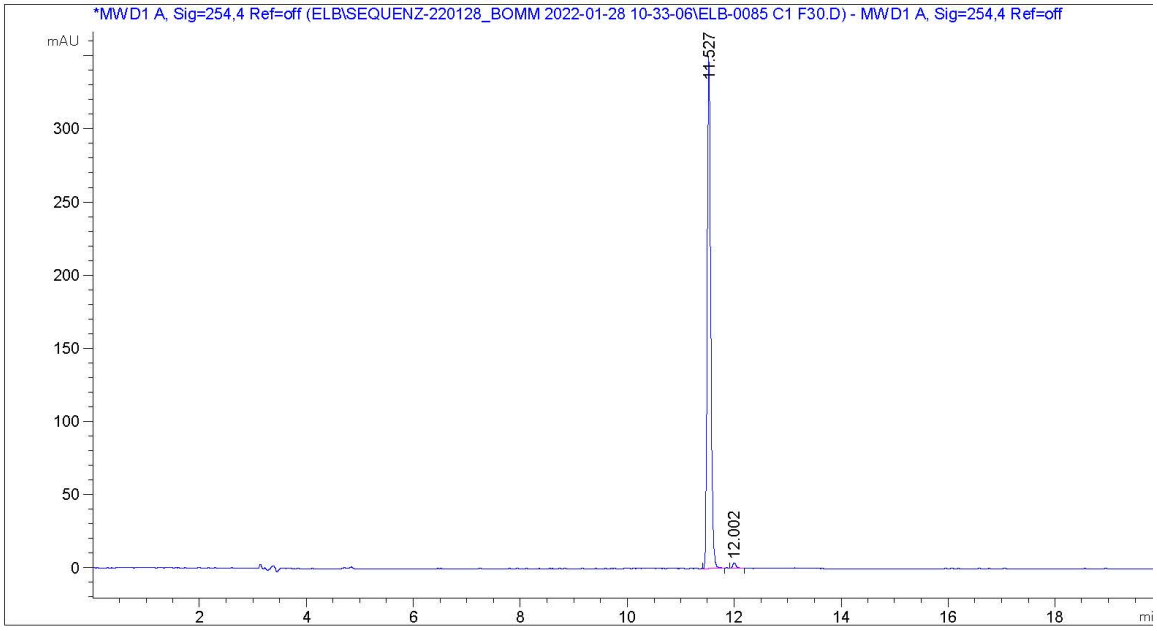
^{1}H-NMR



^{13}C-NMR



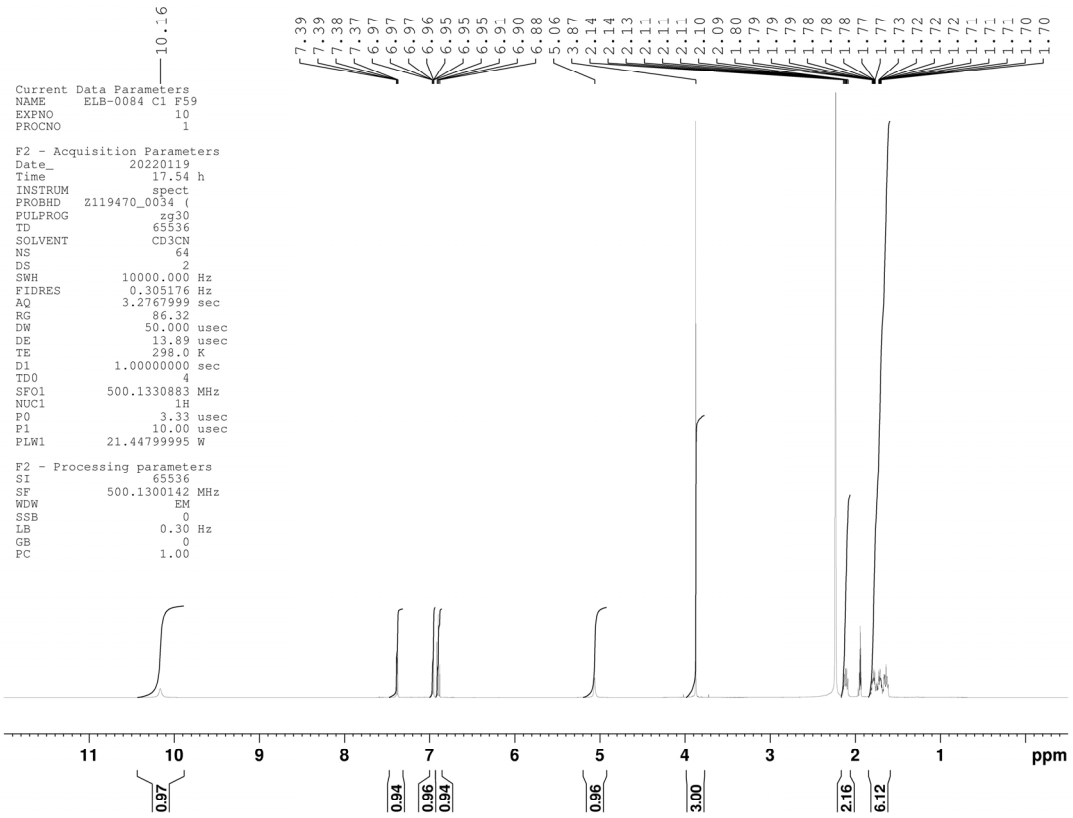
LC



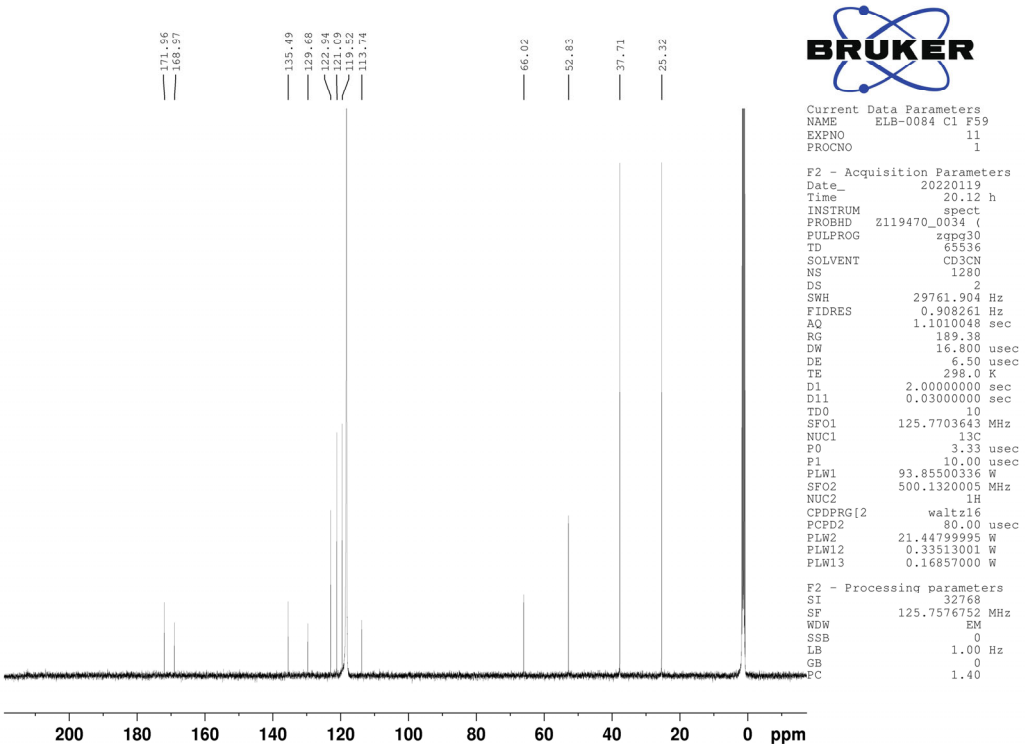

```
=====================================================================
                    Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.527 VV    0.0701 1559.25256  349.38745  98.9104
   2  12.002 VB    0.0718   17.17689    3.58976   1.0896

Totals :                  1576.42945  352.97722
```

Compound 38

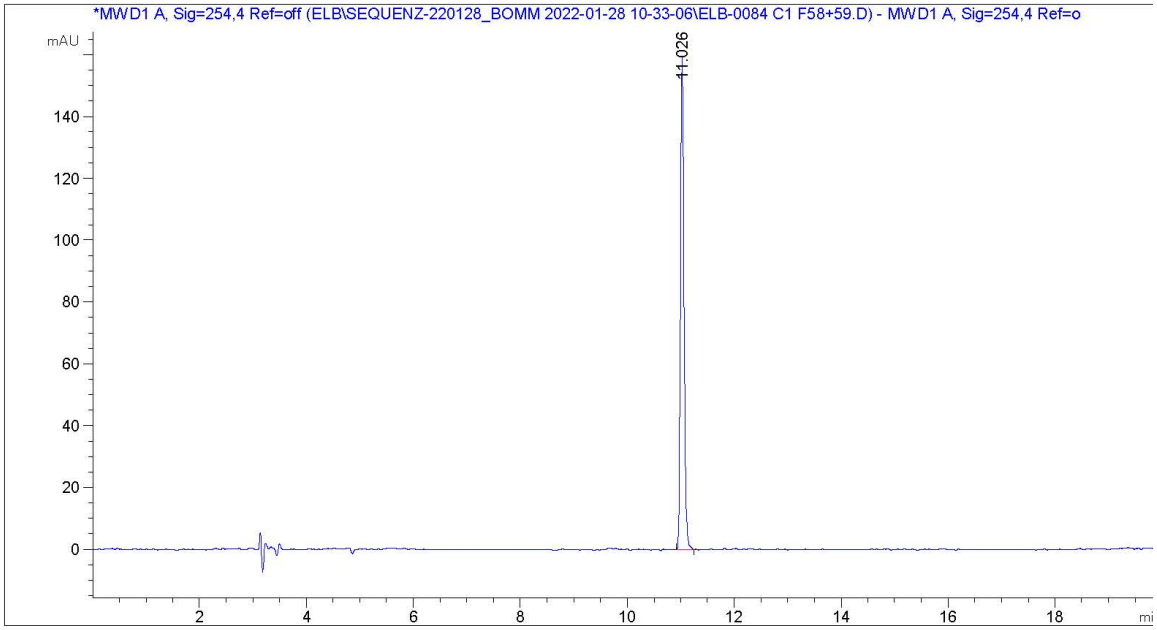
^{1}H-NMR



^{13}C-NMR



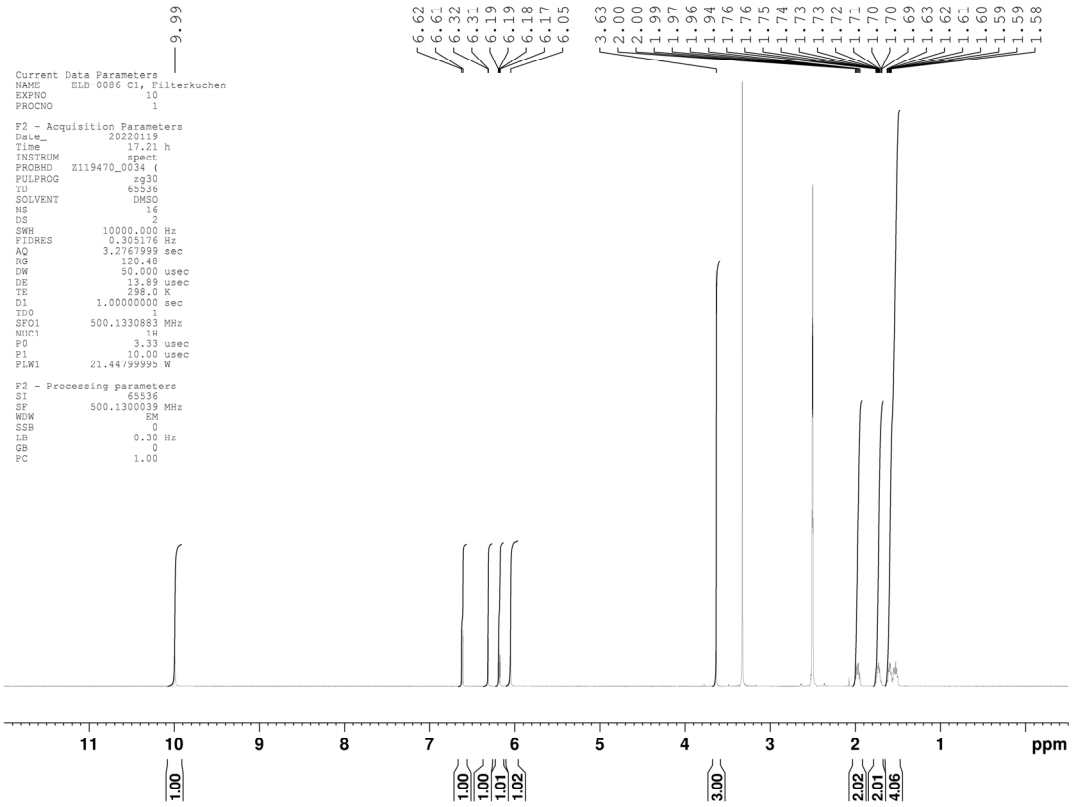
LC



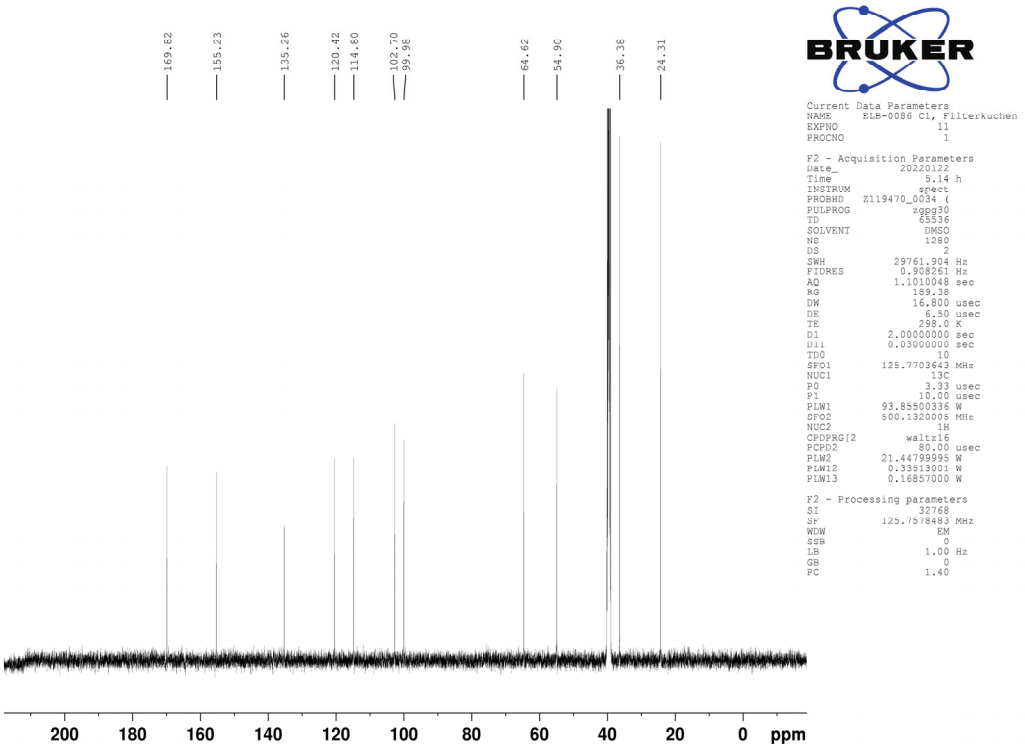

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.026 VV    0.0705  717.39008  159.36082 100.0000

Totals :                   717.39008  159.36082
```

Compound 39

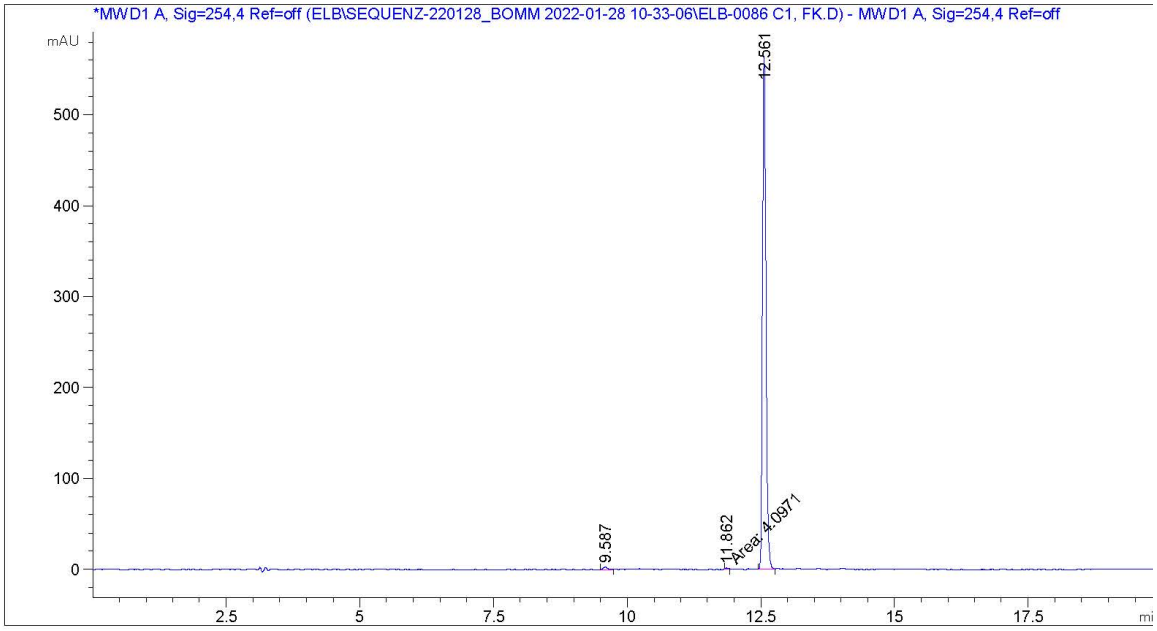
^{1}H-NMR



^{13}C-NMR



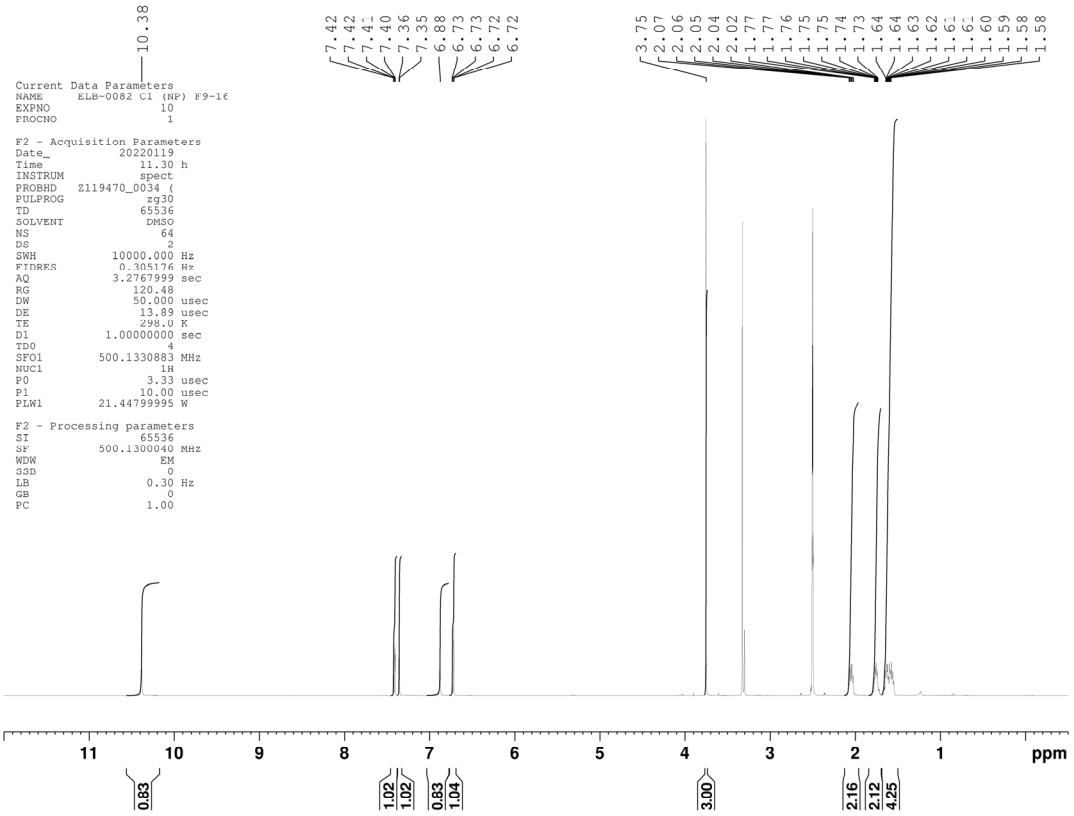
LC



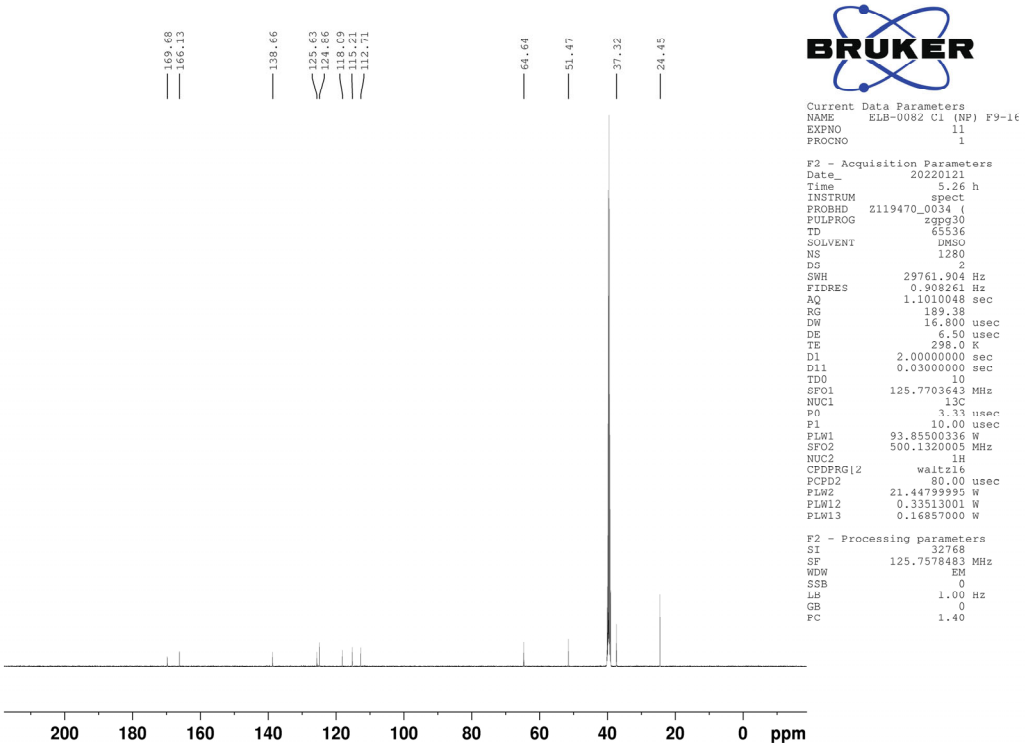

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.587 BV    0.0752   12.16766    2.39638   0.4755
   2  11.862 MM    0.0569    4.09710    1.19958   0.1601
   3  12.561 BV    0.0686 2542.89893  564.26318  99.3645

Totals :                  2559.16368  567.85914
```

Compound 40

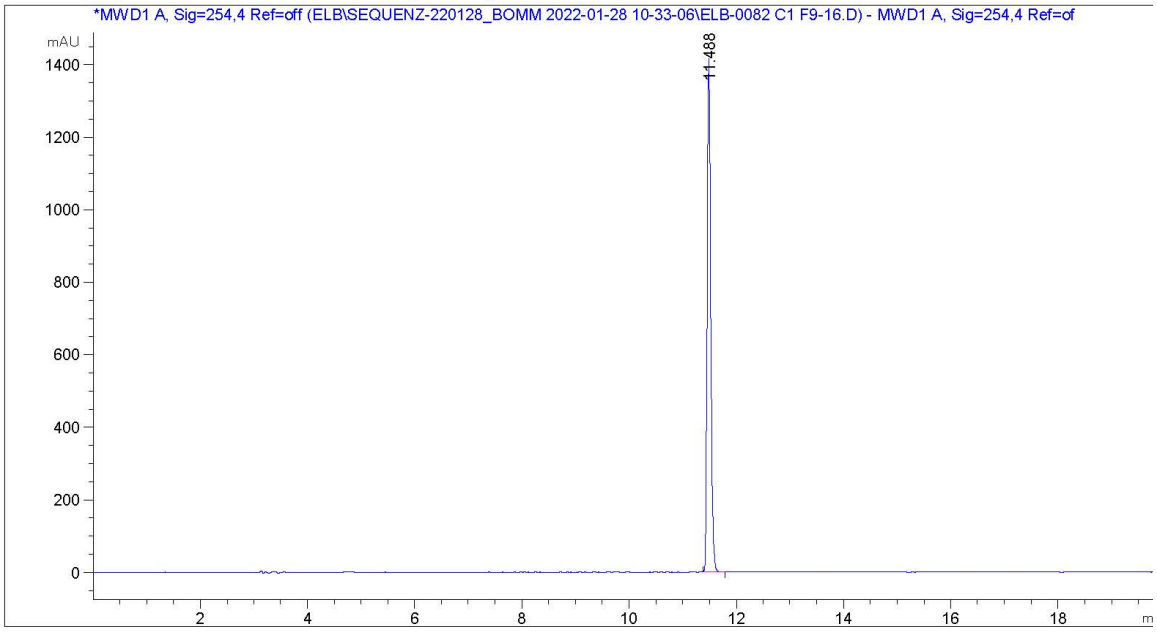
^{1}H-NMR



^{13}C-NMR



LC

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=====================================================================
                      Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

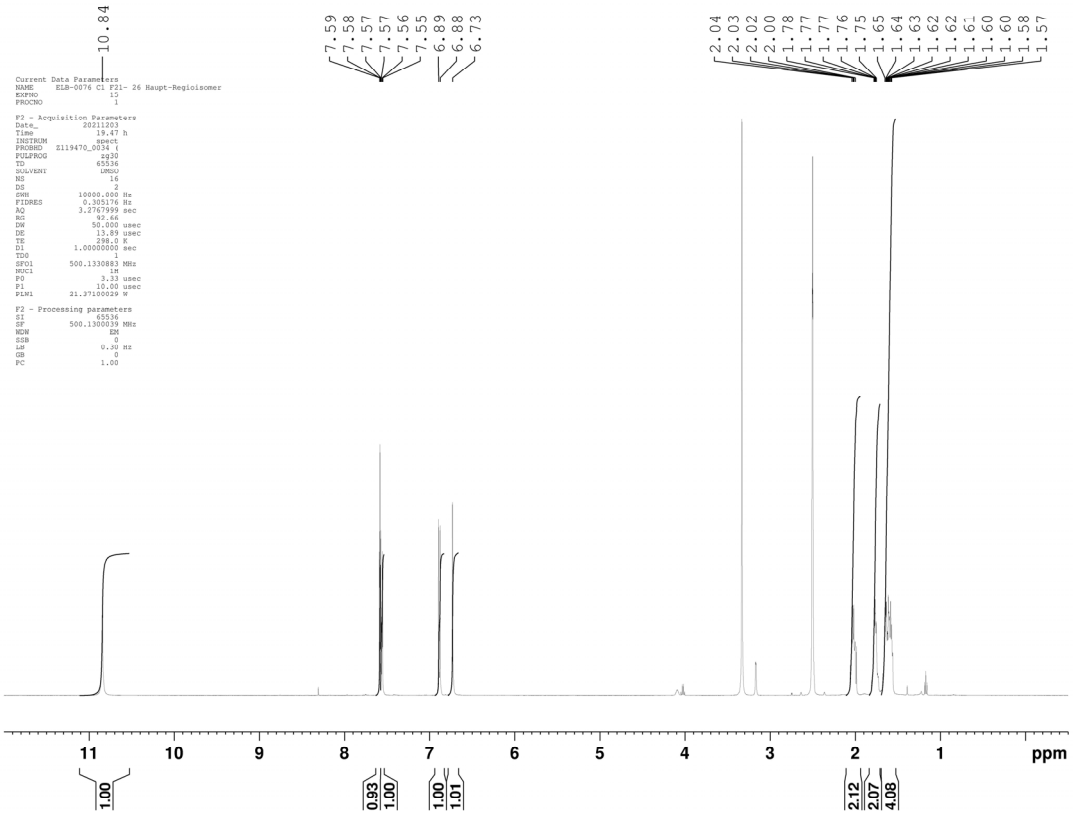

Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.488 BV    0.0705 6371.96045 1417.23743 100.0000

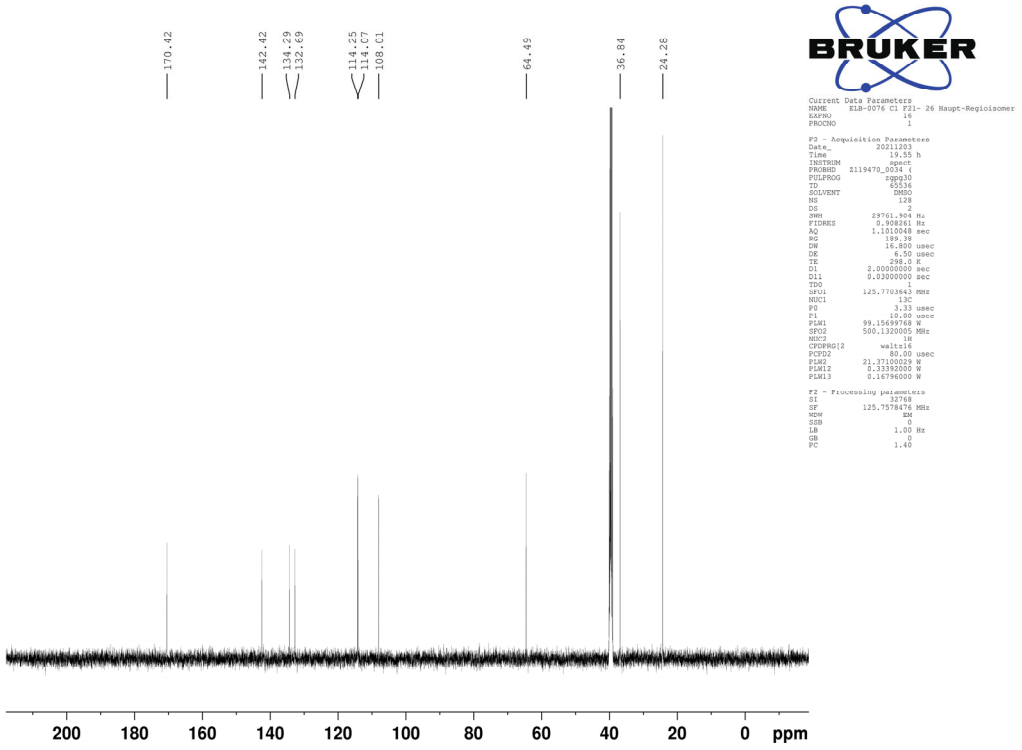
Totals :                  6371.96045 1417.23743
```

Compound 41

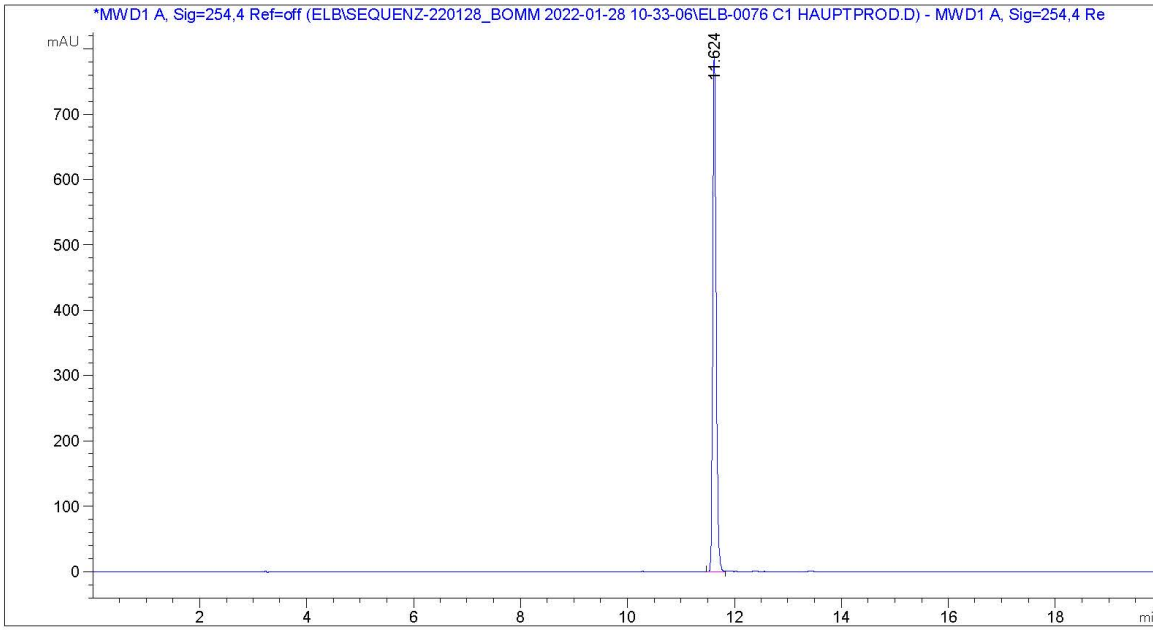
^{1}H-NMR



^{13}C-NMR



LC

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=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.624 BV    0.0679 3507.93848  788.64679 100.0000

Totals :                  3507.93848  788.64679
```
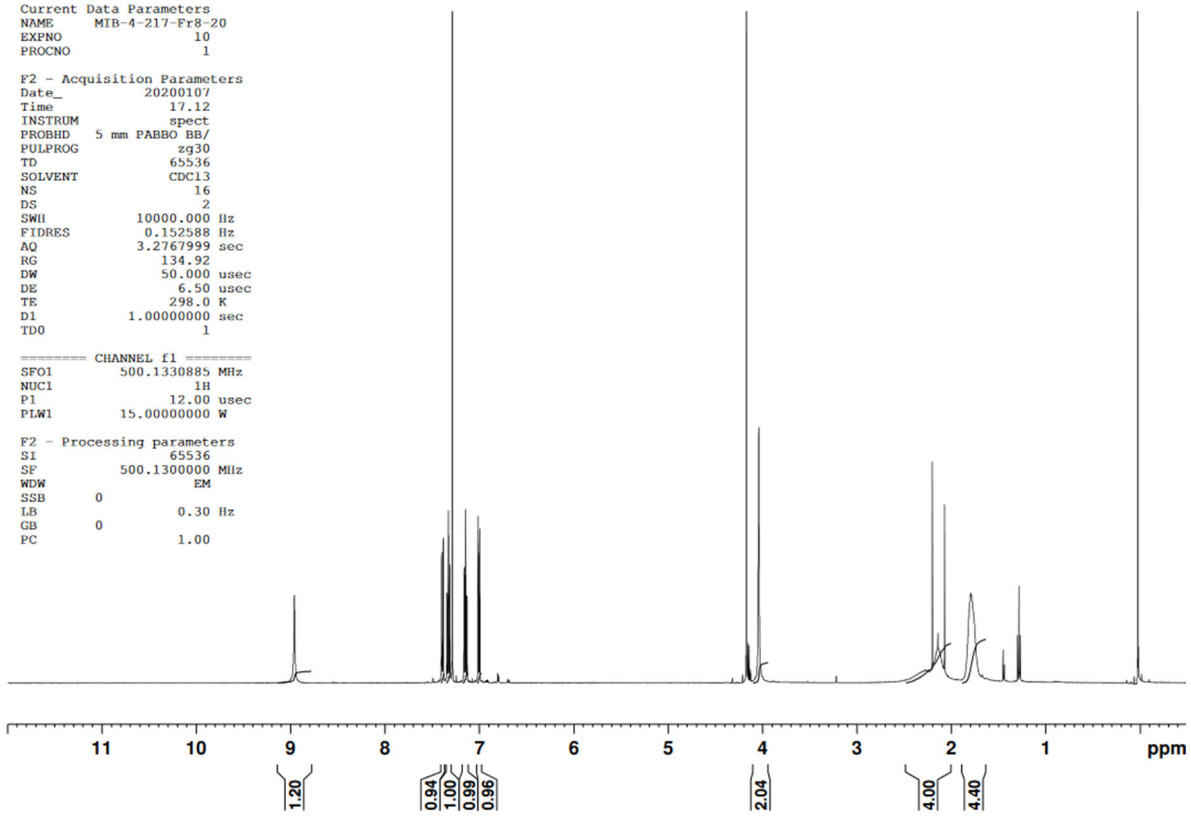
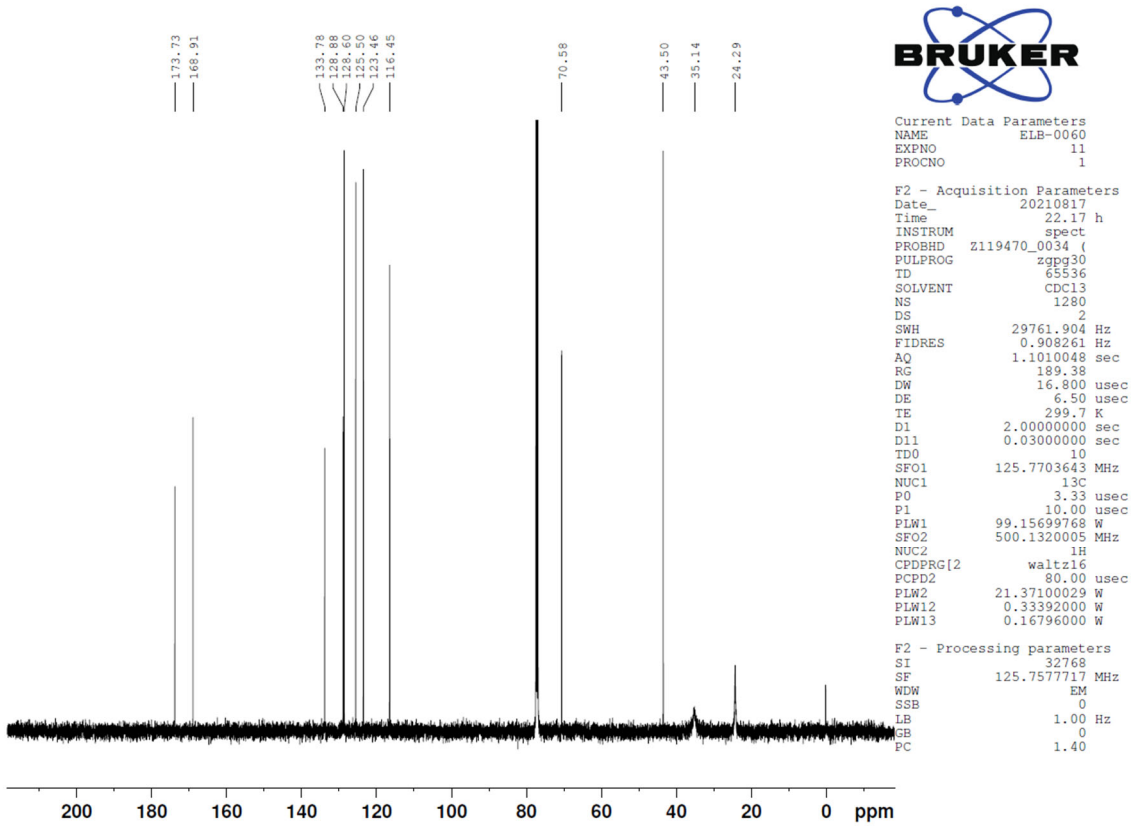

Compound 42

^{1}H-NMR

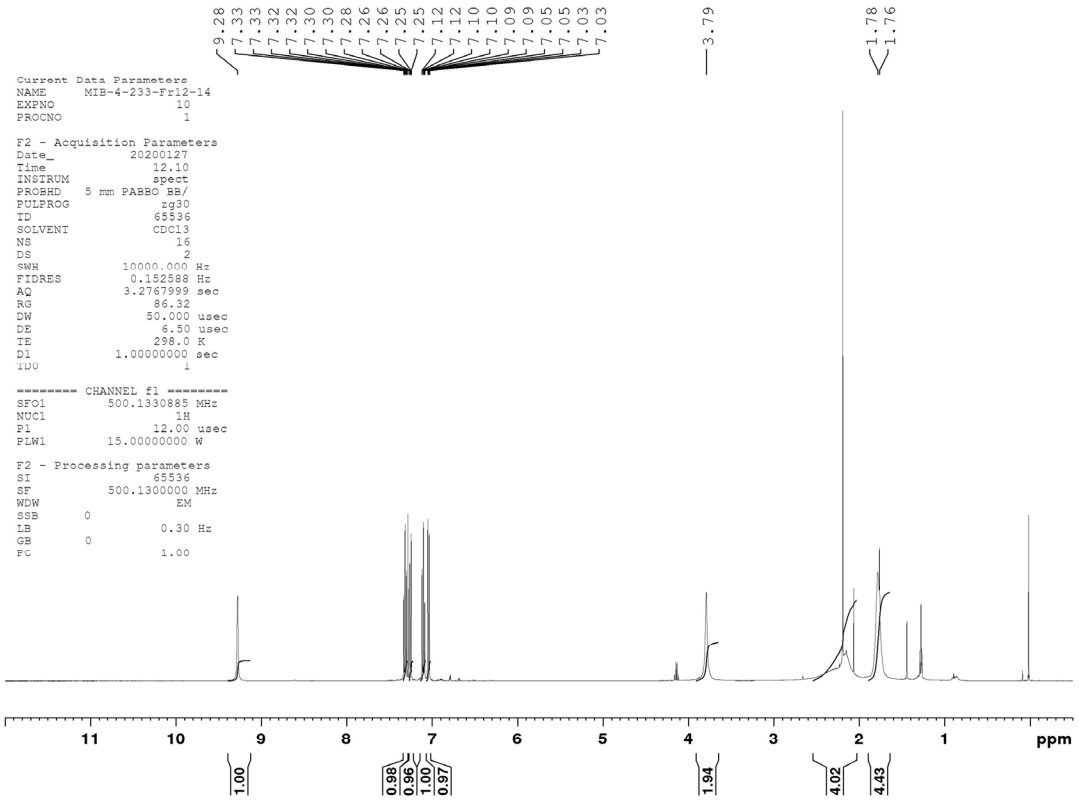


^{13}C-NMR

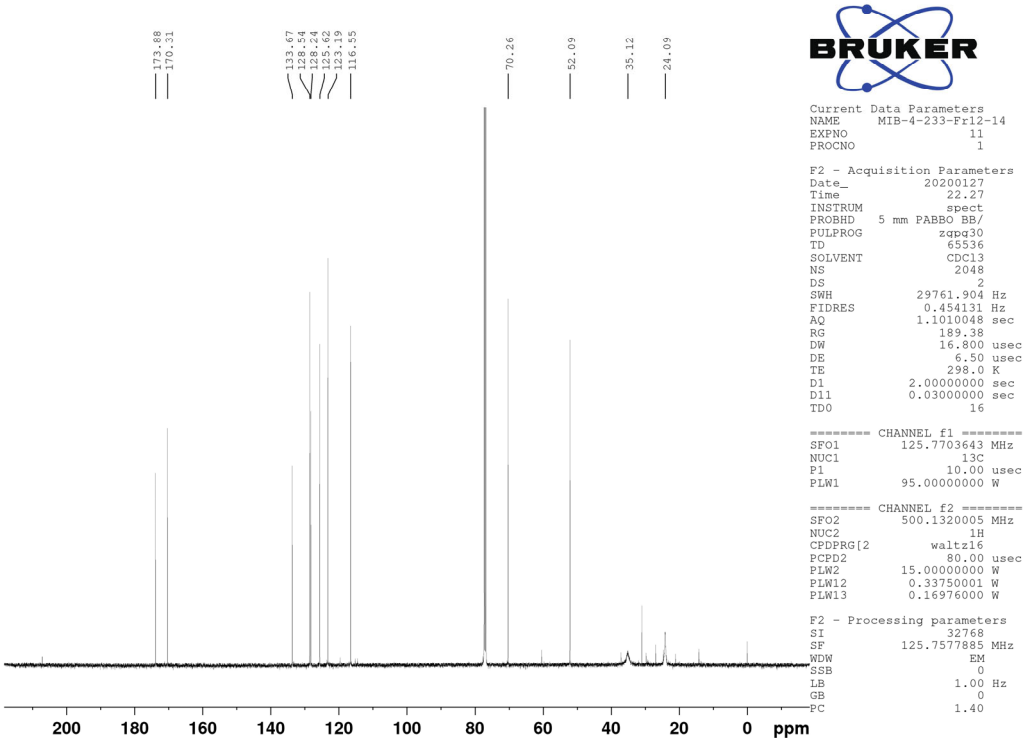


Compound 43

^{1}H-NMR

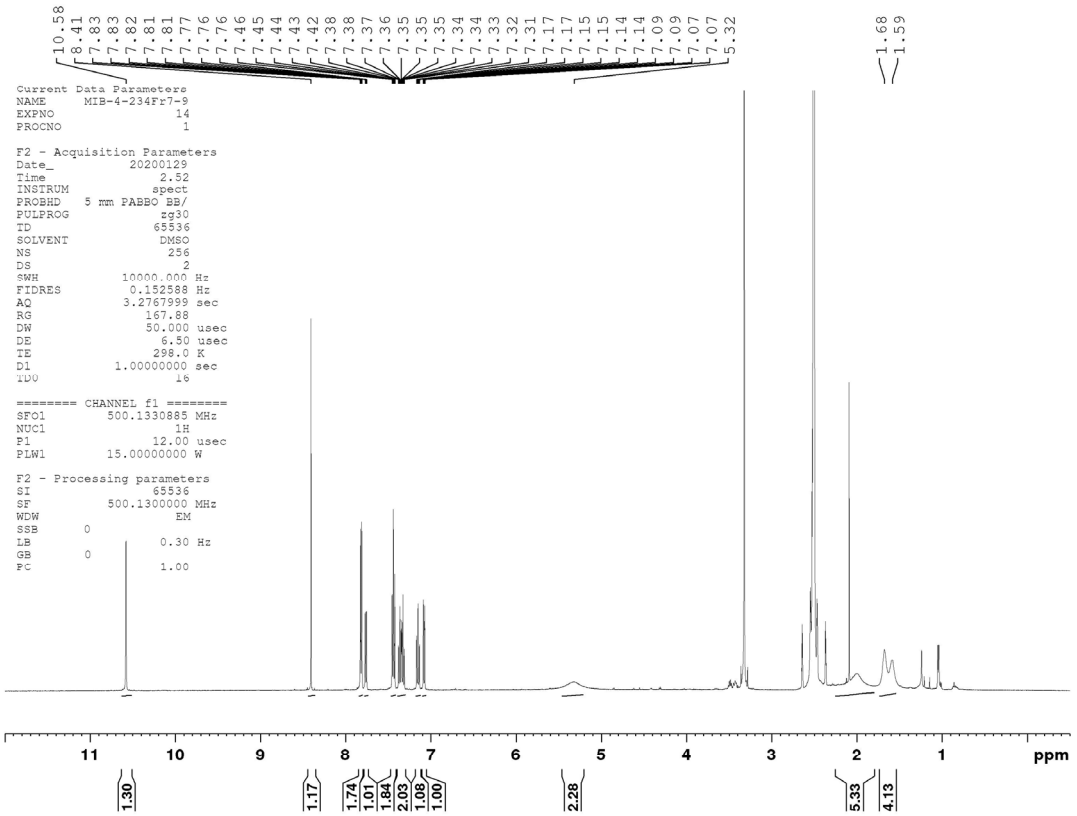


^{13}C-NMR

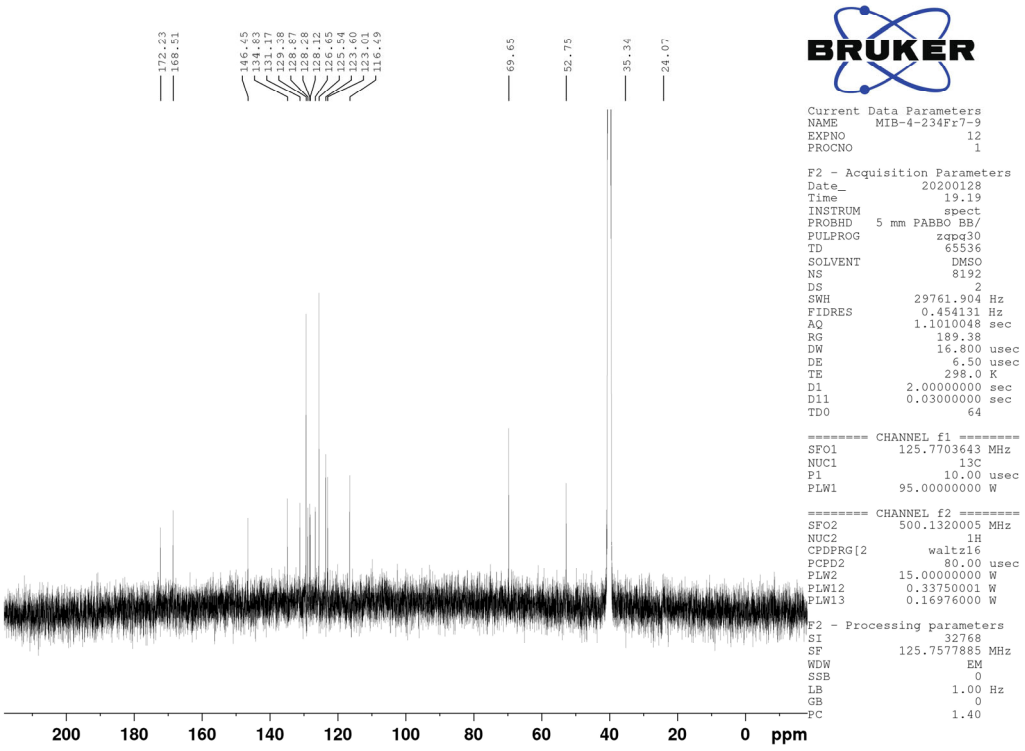


Compound 44

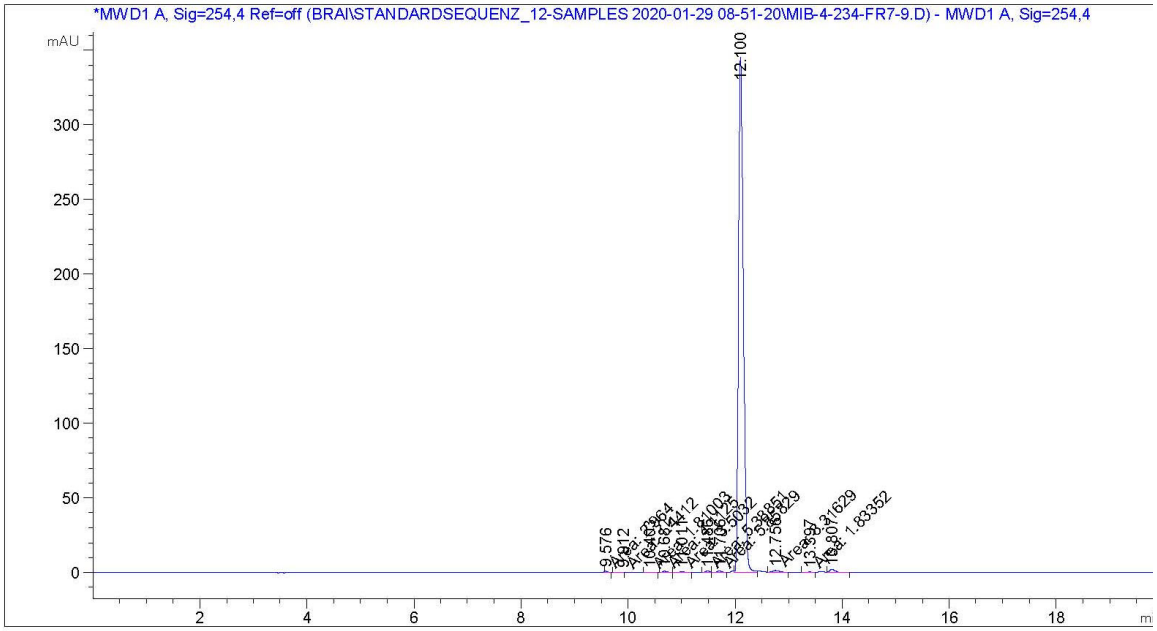
^{1}H-NMR



^{13}C-NMR



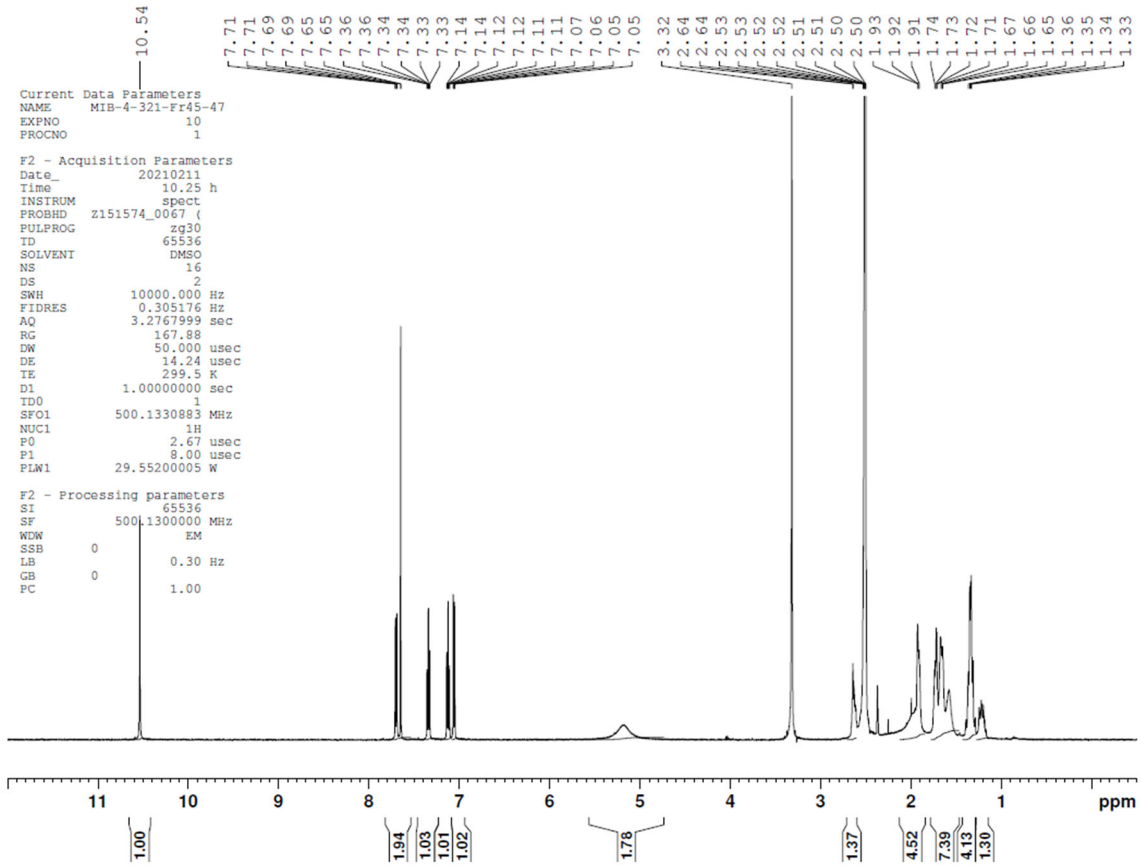
LC



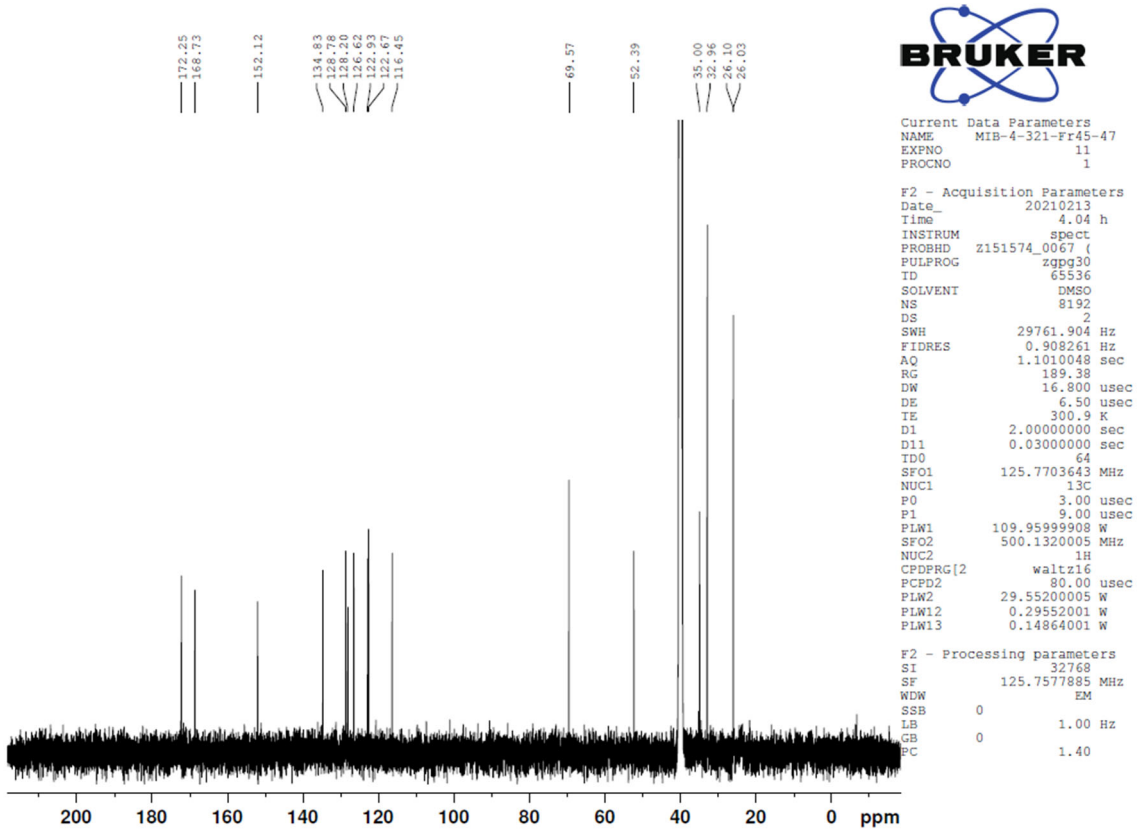

```
================================================================================
                          Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.576 MM    0.0652    2.96400 7.57965e-1   0.1343
   2   9.912 MM    0.0793    1.44120 3.03079e-1   0.0653
   3  10.403 MM    0.1256    1.81003 2.40131e-1   0.0820
   4  10.682 MM    0.1006    4.11250 6.81531e-1   0.1863
   5  11.011 MM    0.1182    3.50320 4.94089e-1   0.1587
   6  11.486 MM    0.0972    5.38851 9.23937e-1   0.2441
   7  11.706 MM    0.1071    5.85829 9.11943e-1   0.2654
   8  12.100 VV    0.0970 2157.63428  344.96829  97.7415
   9  12.756 MM    0.1277    8.31629    1.08515   0.3767
  10  13.397 MM    0.1309    1.83352 2.33445e-1   0.0831
  11  13.807 VV    0.1230   14.62966    1.83569   0.6627
```

Compound 45

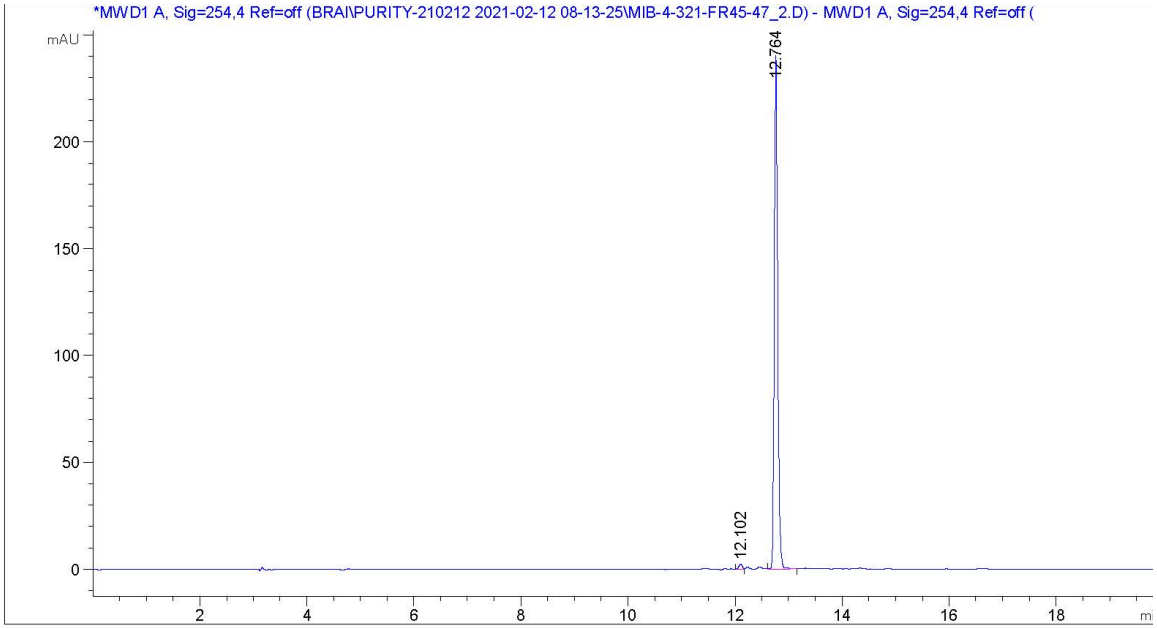
^{1}H-NMR



^{13}C-NMR



LC

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=====================================================================
                        Area Percent Report
=====================================================================

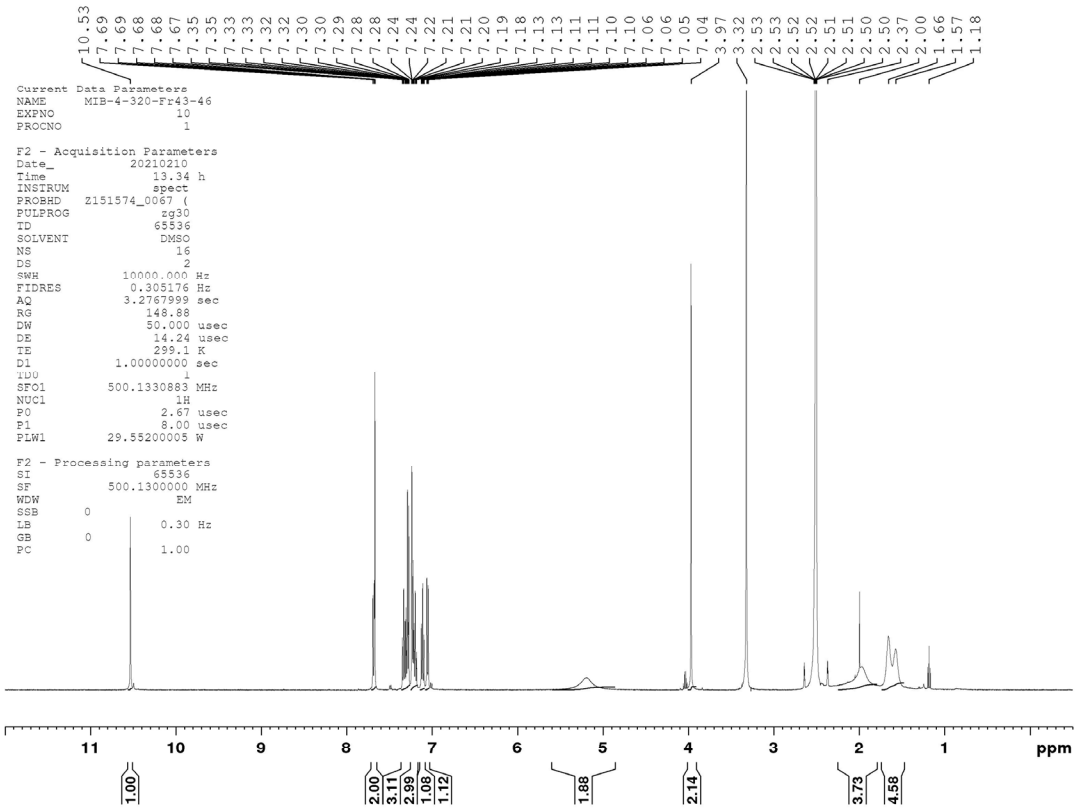
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

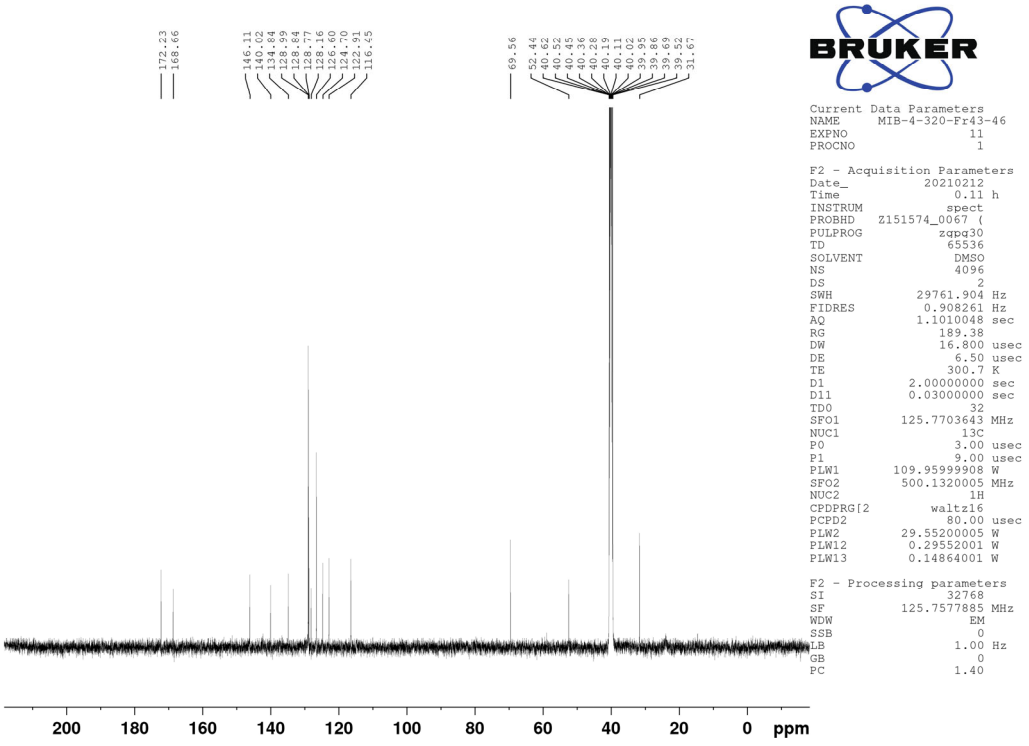
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.102 VV    0.0742   12.02480    2.49525   1.1109
   2  12.764 VB    0.0679 1070.39270  240.64124  98.8891
```

Compound 46

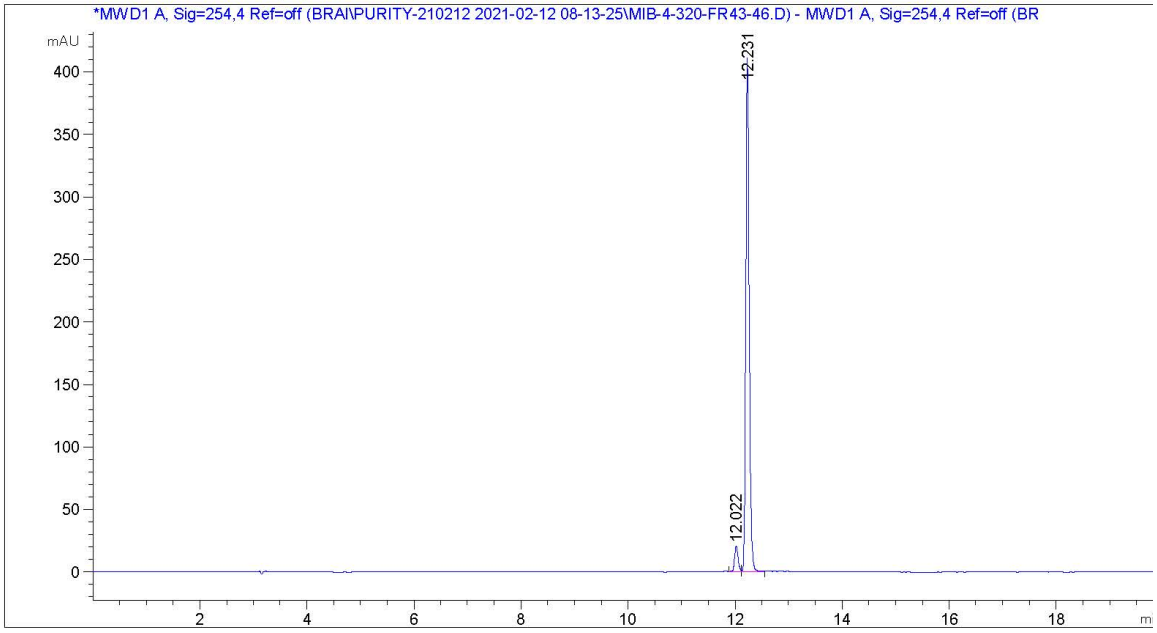
^{1}H-NMR



^{13}C-NMR



LC

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=====================================================================
                    Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.022 BV    0.0683   91.06959   20.31276   4.7026
   2  12.231 VV    0.0681 1845.51868  413.59122  95.2974
```
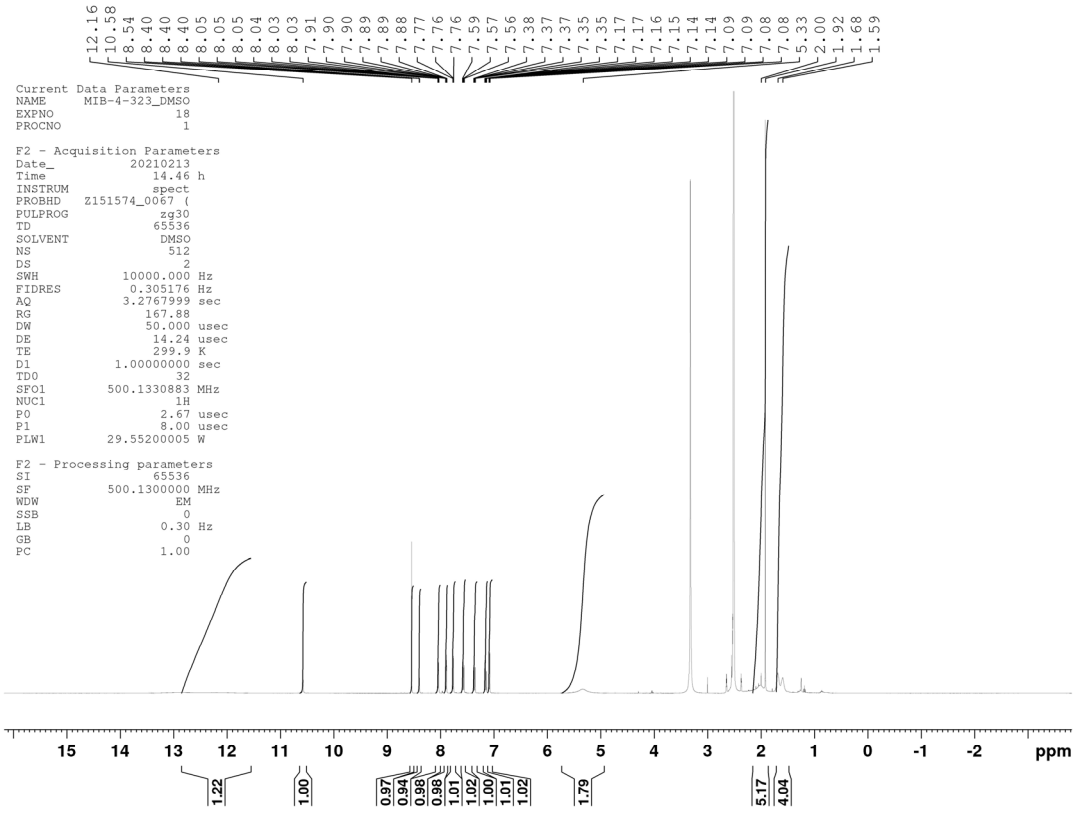
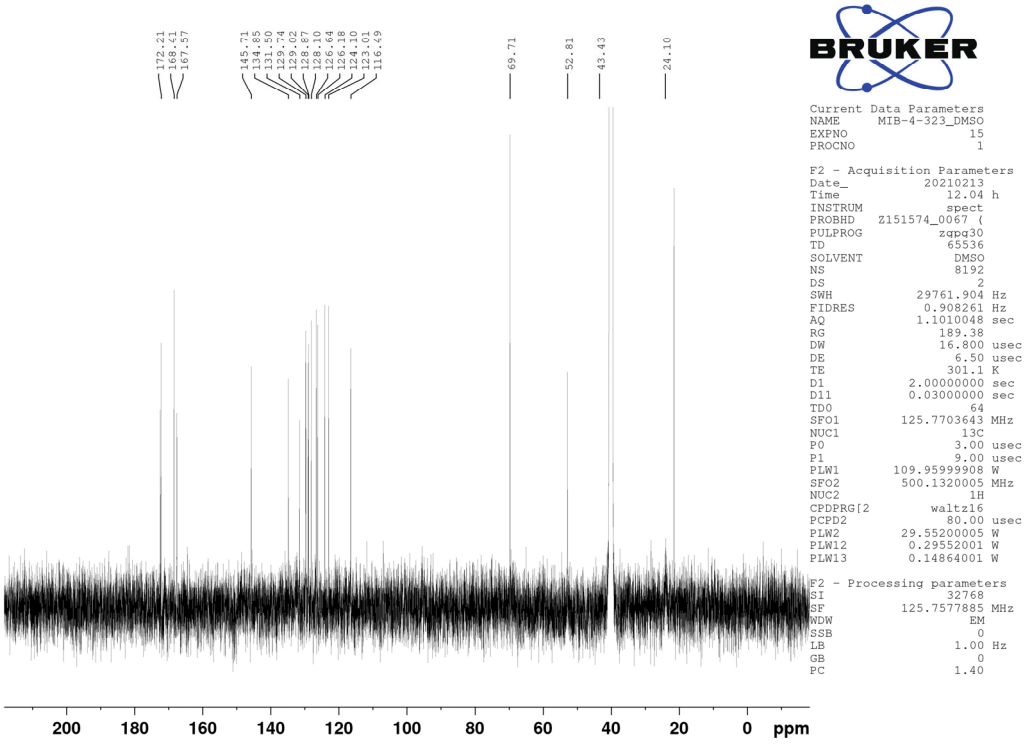

Compound 47

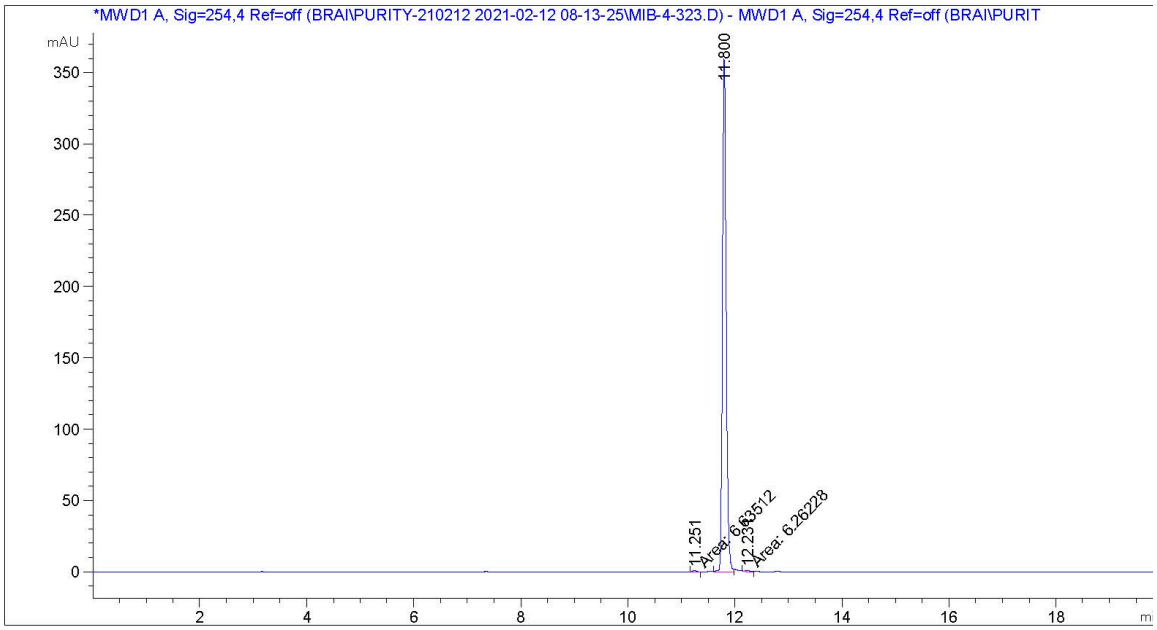
^{1}H-NMR



^{13}C-NMR



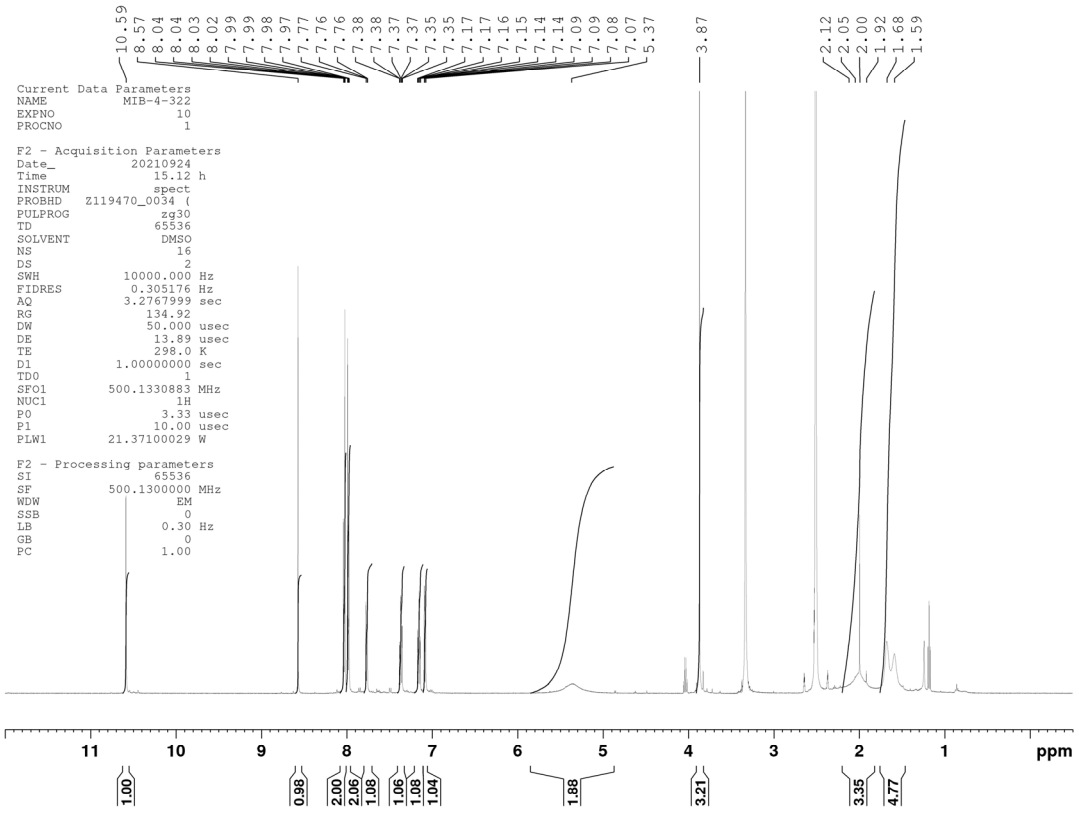
LC



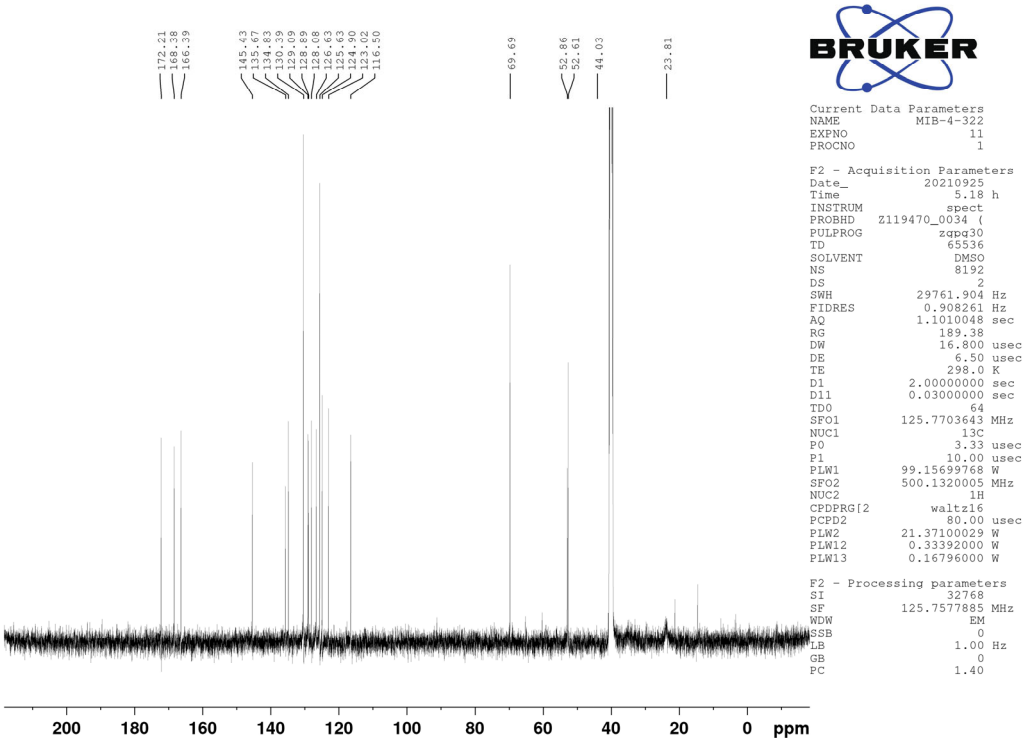

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.251 MM    0.1223    6.63512 9.04162e-1   0.3895
   2  11.800 VV    0.0727 1690.51233  360.55911  99.2428
   3  12.231 MM    0.1285    6.26228 8.11981e-1   0.3676
```

Compound 48

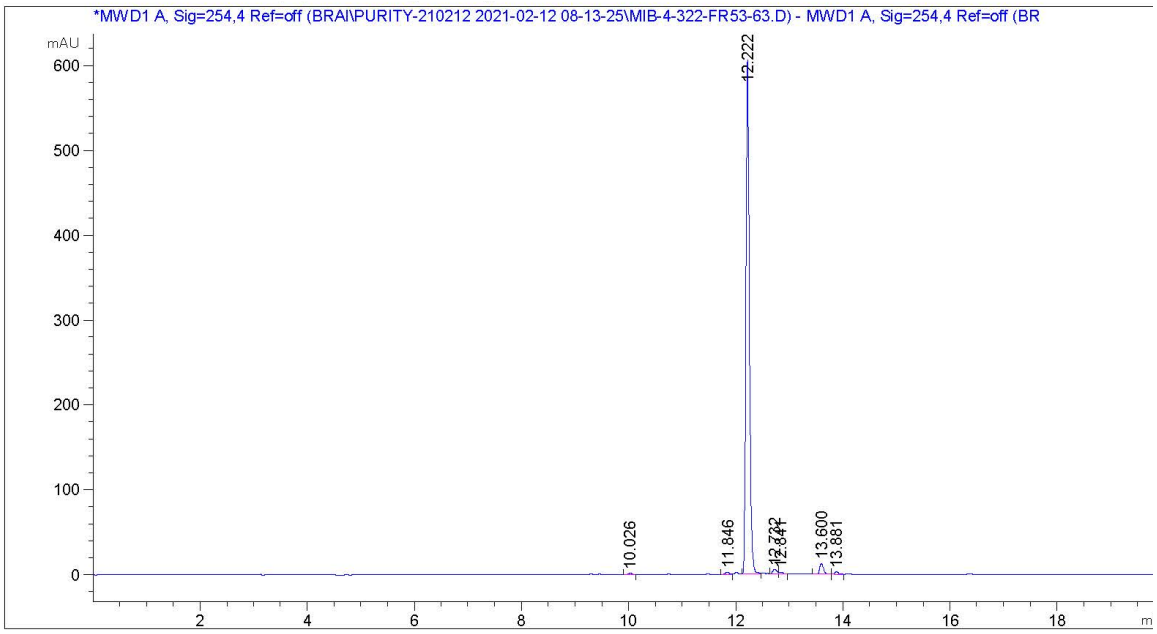
^{1}H-NMR



^{13}C-NMR



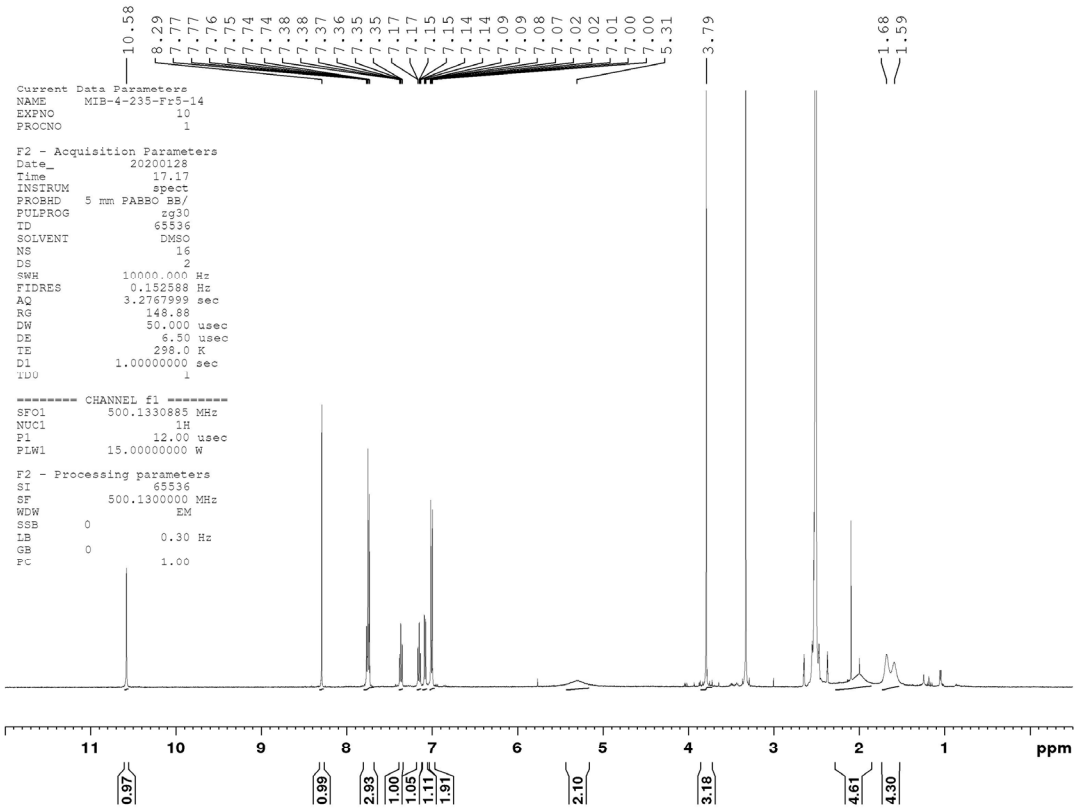
LC



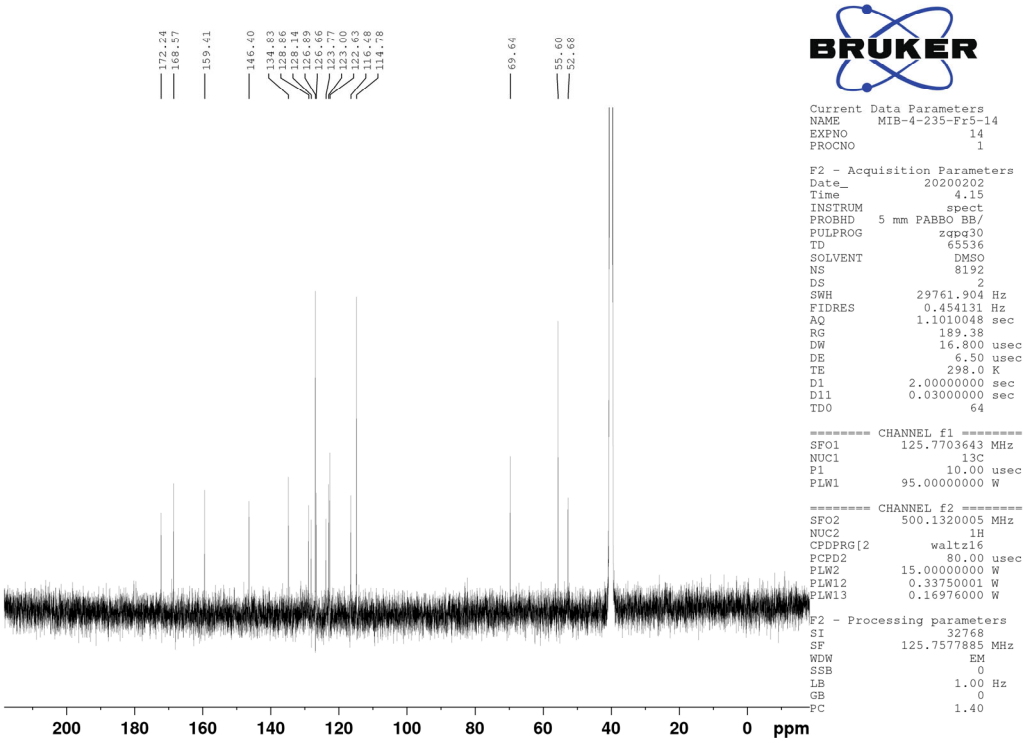

```
=====================================================================
                    Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.026 BV    0.0675    8.21501    1.86211   0.2862
   2  11.846 BV    0.0720   14.66877    3.05846   0.5110
   3  12.222 BV    0.0706 2731.29468  606.05725  95.1508
   4  12.732 BV    0.0938   27.99298    4.81930   0.9752
   5  12.841 VB    0.0663   10.42537    2.32458   0.3632
   6  13.600 BV    0.0736   62.51662   13.10691   2.1779
   7  13.881 VB    0.0762   15.37740    3.08325   0.5357
```

Compound 49

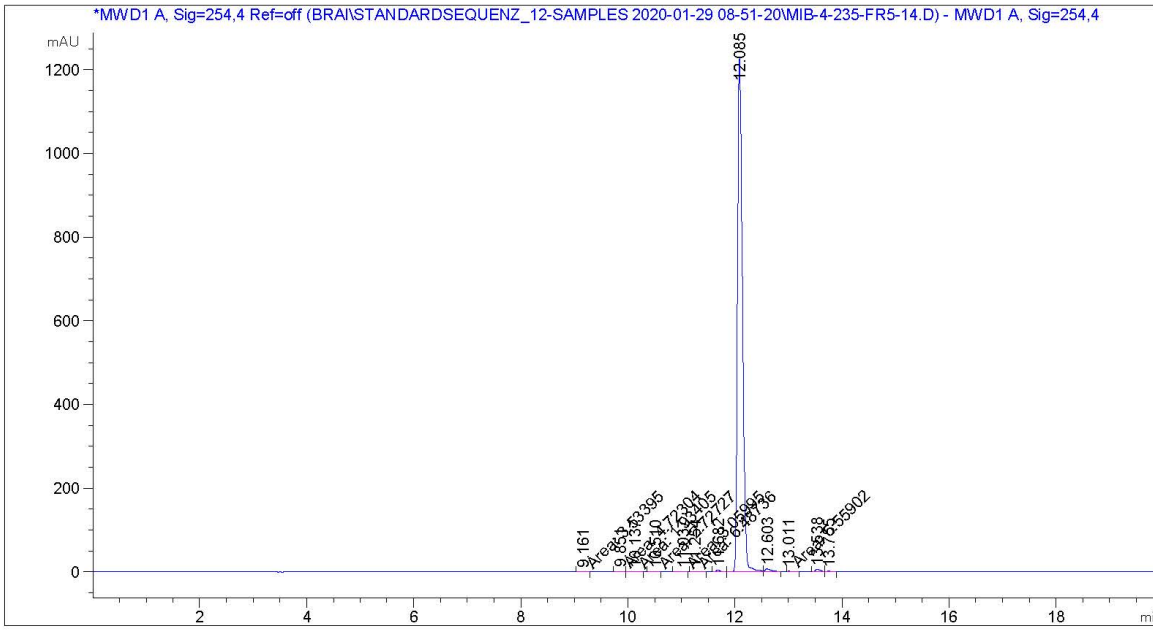
^{1}H-NMR



^{13}C-NMR



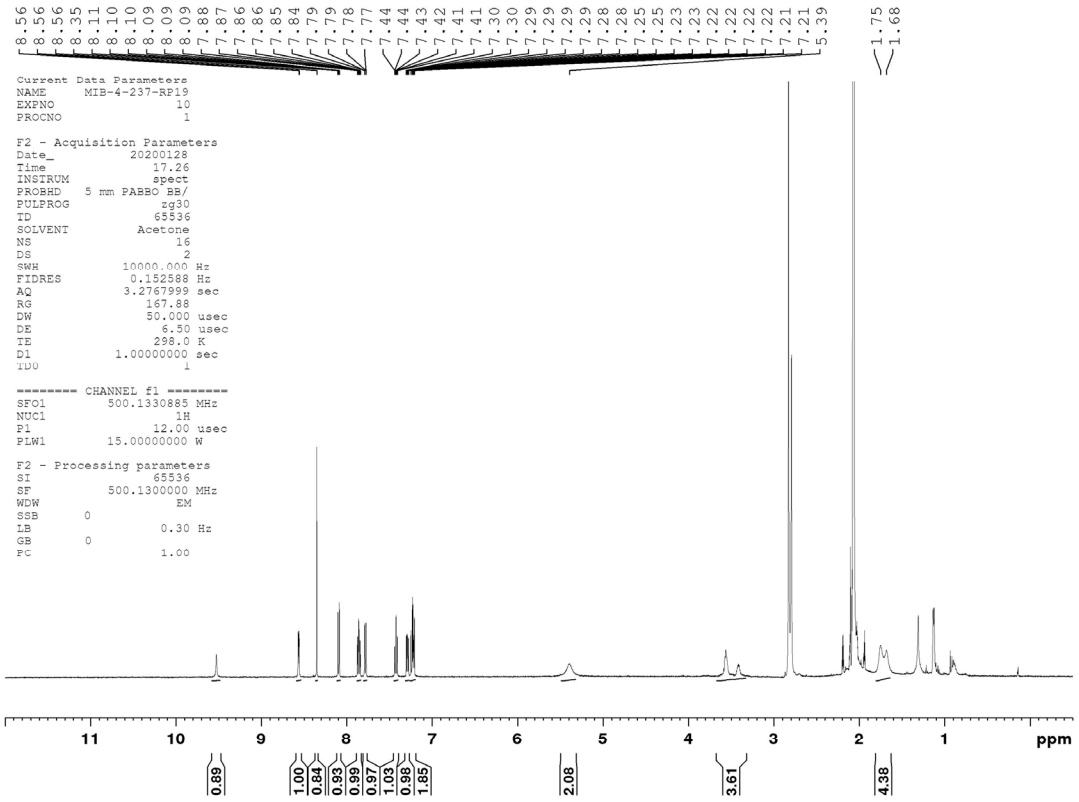
LC



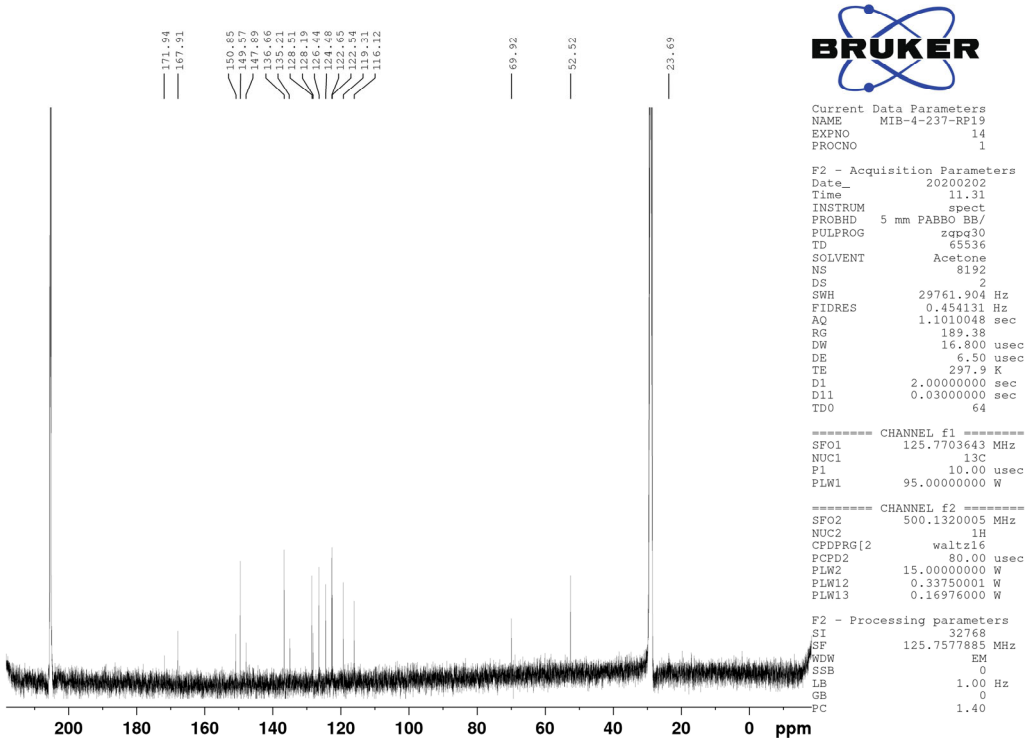

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.161 MM    0.1302    3.53395 4.52261e-1   0.0447
   2   9.851 MM    0.0864    4.72304 9.10863e-1   0.0597
   3  10.137 MM    0.1061    1.93405 3.03688e-1   0.0244
   4  10.510 MM    0.0853    2.72727 5.32622e-1   0.0345
   5  11.037 MM    0.1377    3.05995 3.70439e-1   0.0387
   6  11.254 MM    0.1800    6.48736 6.00588e-1   0.0820
   7  11.682 BB    0.1015   24.65386    3.91296   0.3116
   8  12.085 BV    0.0977 7755.65039 1226.99341  98.0098
   9  12.603 VB    0.1208   49.41617    6.07977   0.6245
  10  13.011 MM    0.0971    5.55902 9.54264e-1   0.0703
  11  13.538 BV    0.1221   41.98141    5.56161   0.5305
  12  13.755 VV    0.1135   13.41397    1.82965   0.1695
```

Compound 50

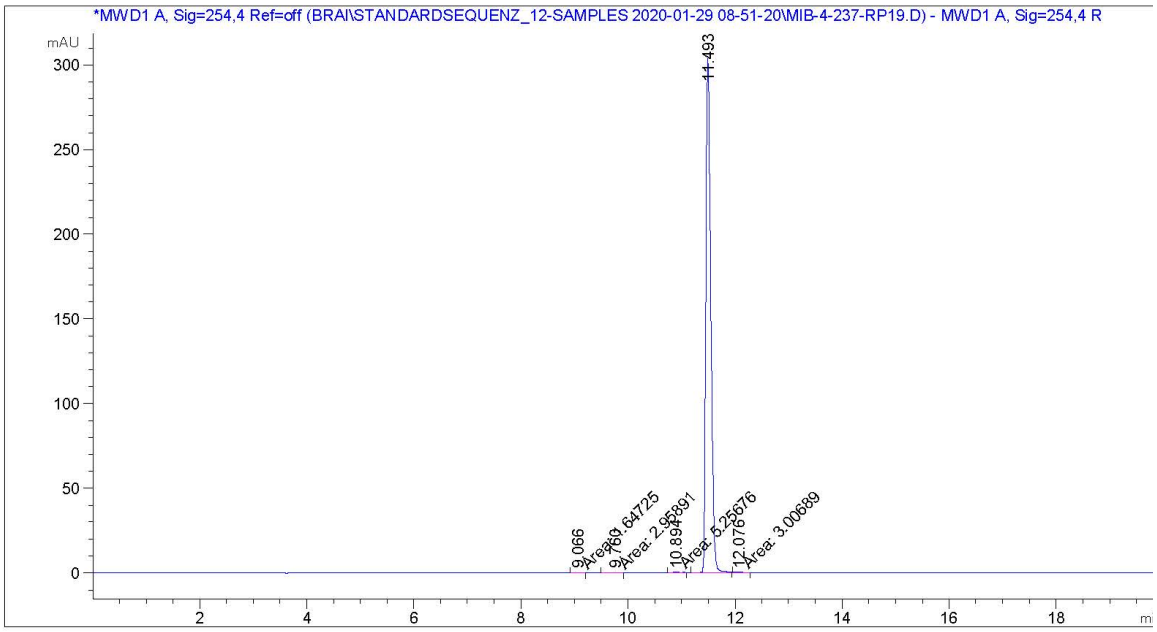
^{1}H-NMR



^{13}C-NMR



LC

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=====================================================================
                        Area Percent Report
=====================================================================

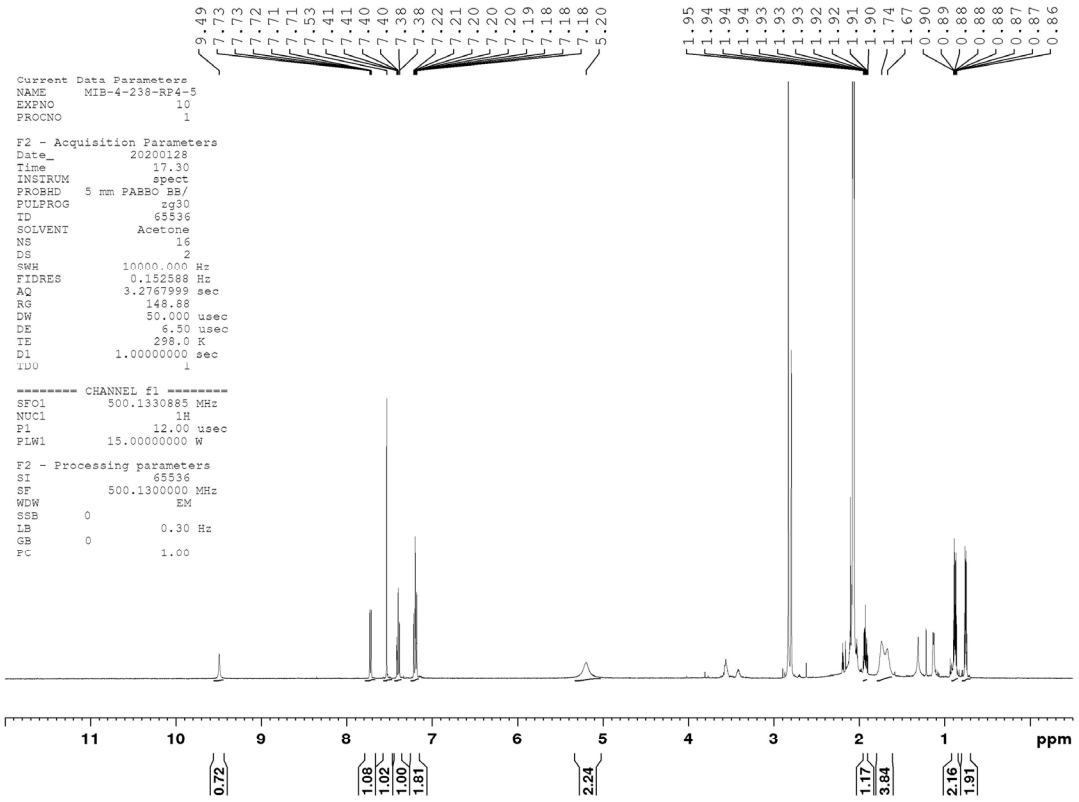
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

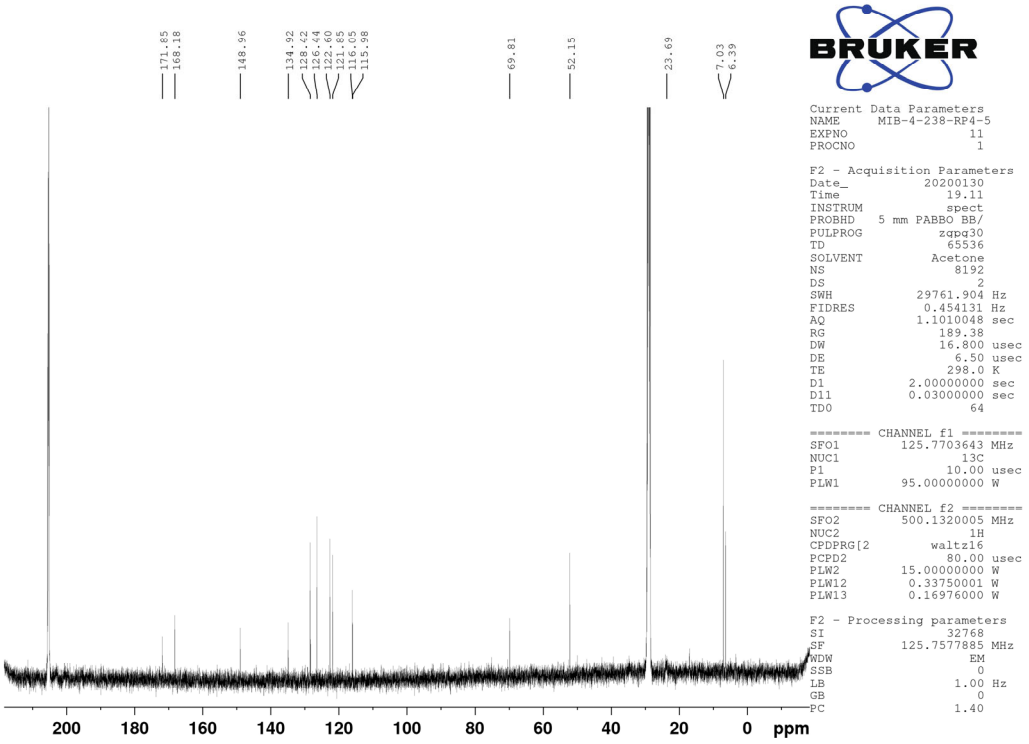
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.066 MM    0.1325    1.64725 2.07139e-1   0.0858
   2   9.760 MM    0.2369    2.95891 2.08200e-1   0.1541
   3  10.894 MM    0.1739    5.25676 5.03742e-1   0.2738
   4  11.493 BV    0.0952 1907.04333  304.07443  99.3297
   5  12.076 MM    0.2205    3.00689 2.27270e-1   0.1566
```

Compound 51

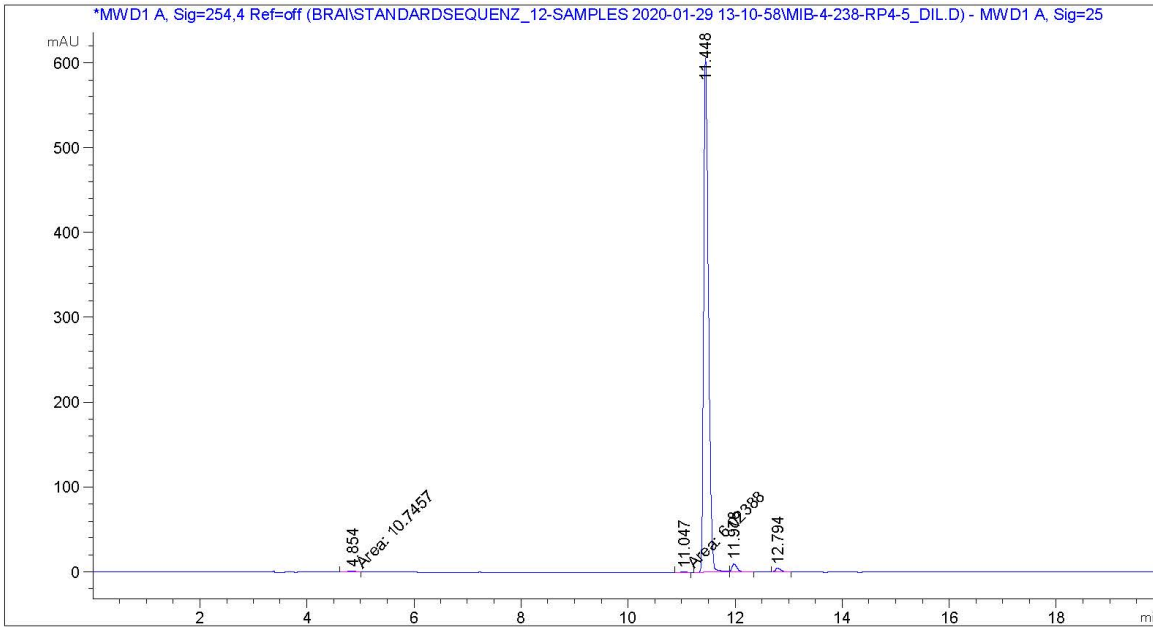
^{1}H-NMR



^{13}C-NMR



LC

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=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.854 MM    0.1895   10.74570 9.44862e-1   0.2774
   2  11.047 MM    0.1669    6.02388 6.01699e-1   0.1555
   3  11.448 BV    0.0964 3761.81274  606.09668  97.1119
   4  11.978 VB    0.1020   64.92233    9.71219   1.6760
   5  12.794 BB    0.1133   30.18341    4.33205   0.7792
```
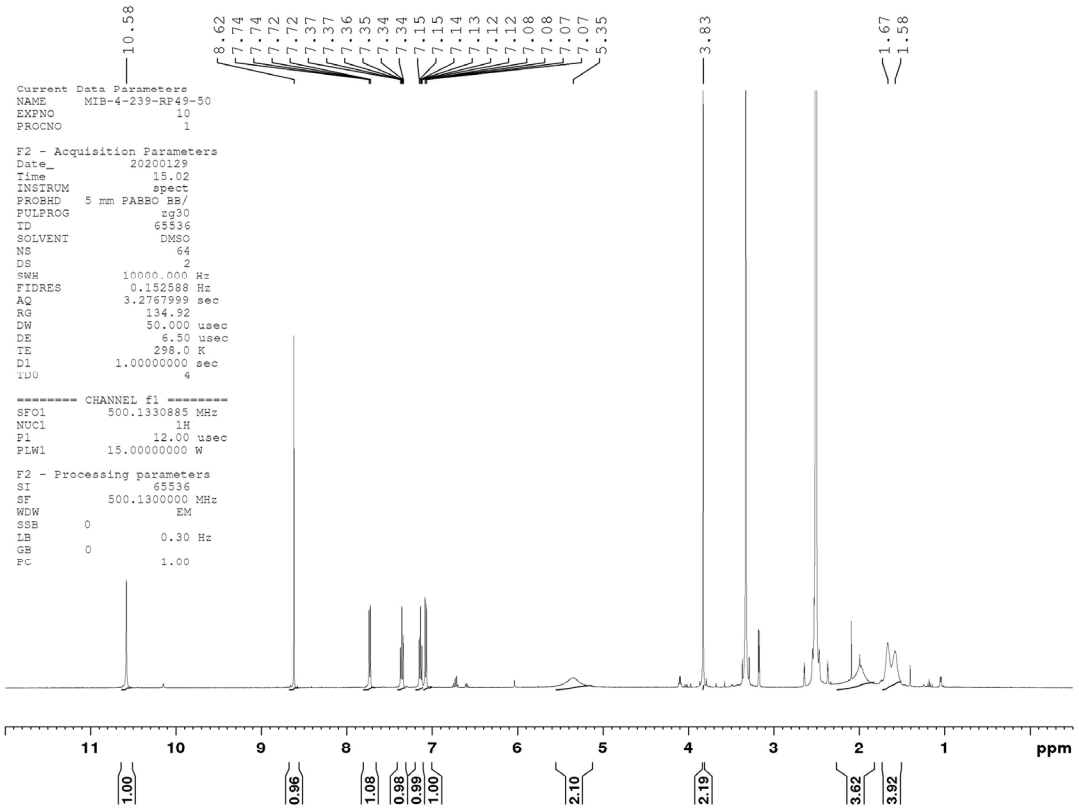
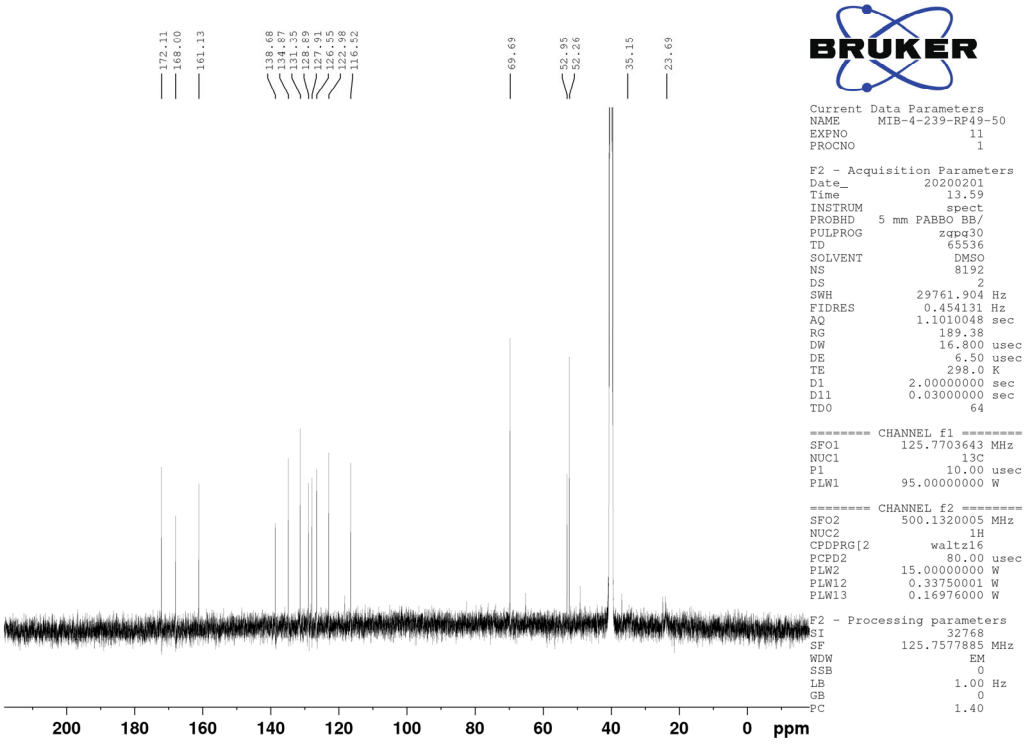

Compound 52

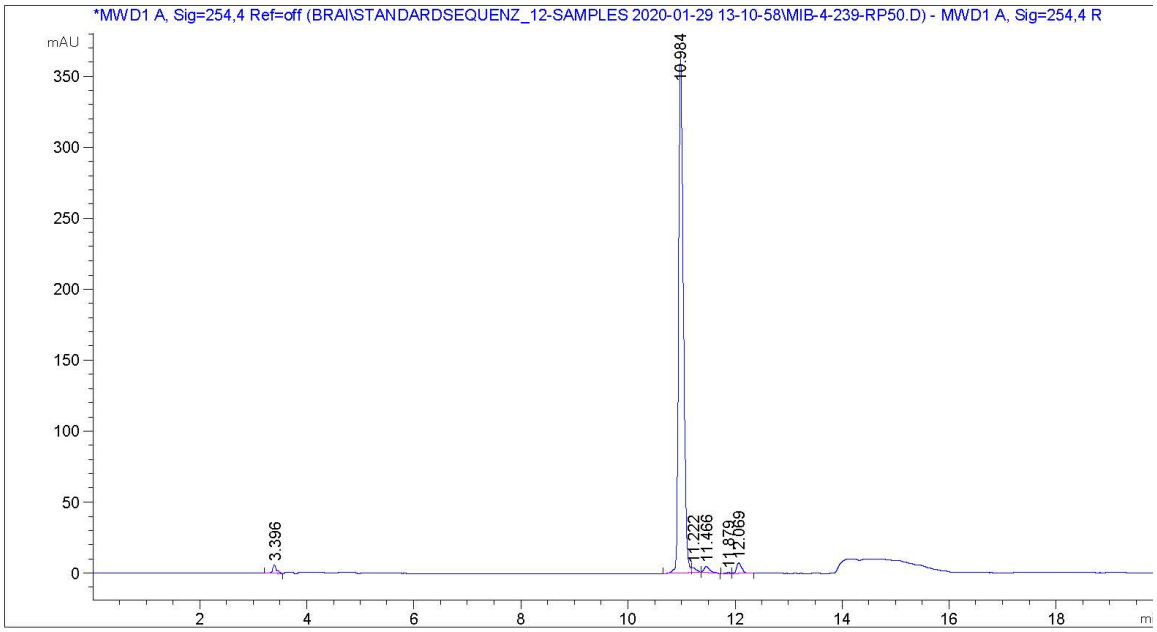
^{1}H-NMR



^{13}C-NMR



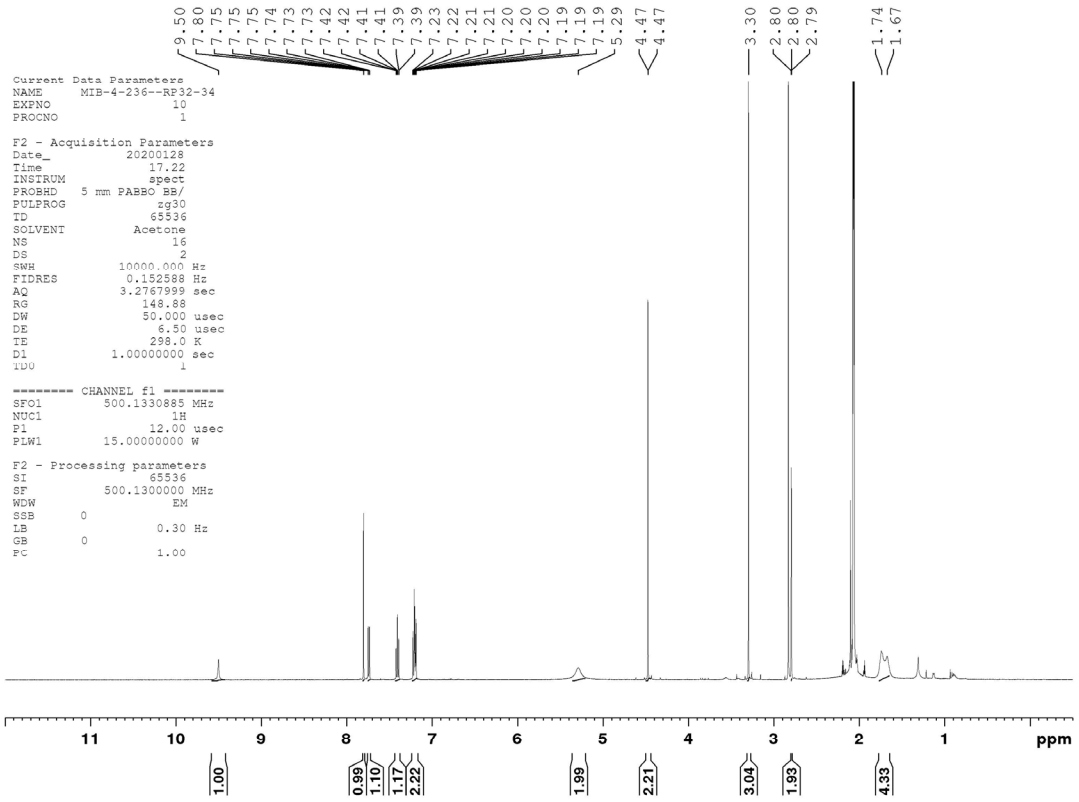
LC



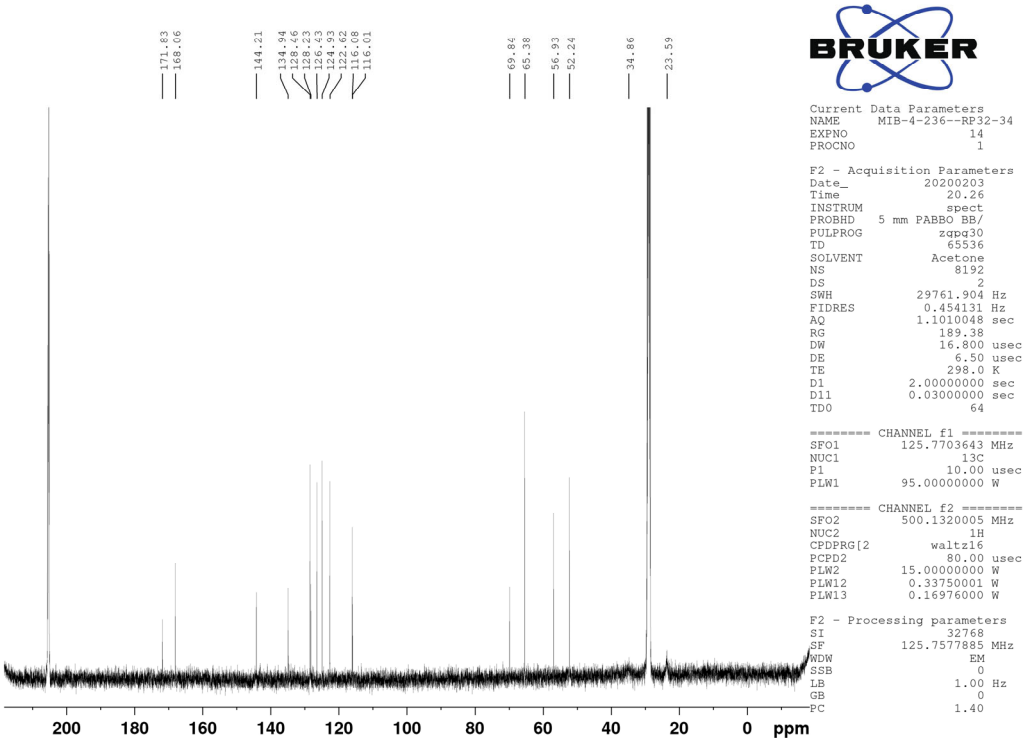

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   3.396 BB    0.0783   31.21430    5.84831   1.3368
   2  10.984 BV    0.0928 2197.71777  362.15585  94.1194
   3  11.222 VB    0.0881   19.79609    3.39032   0.8478
   4  11.466 BB    0.1102   31.28835    4.23284   1.3400
   5  11.879 BV    0.1114    4.71324 5.88426e-1   0.2018
   6  12.069 VB    0.1019   50.30114    7.53028   2.1542
```

Compound 53

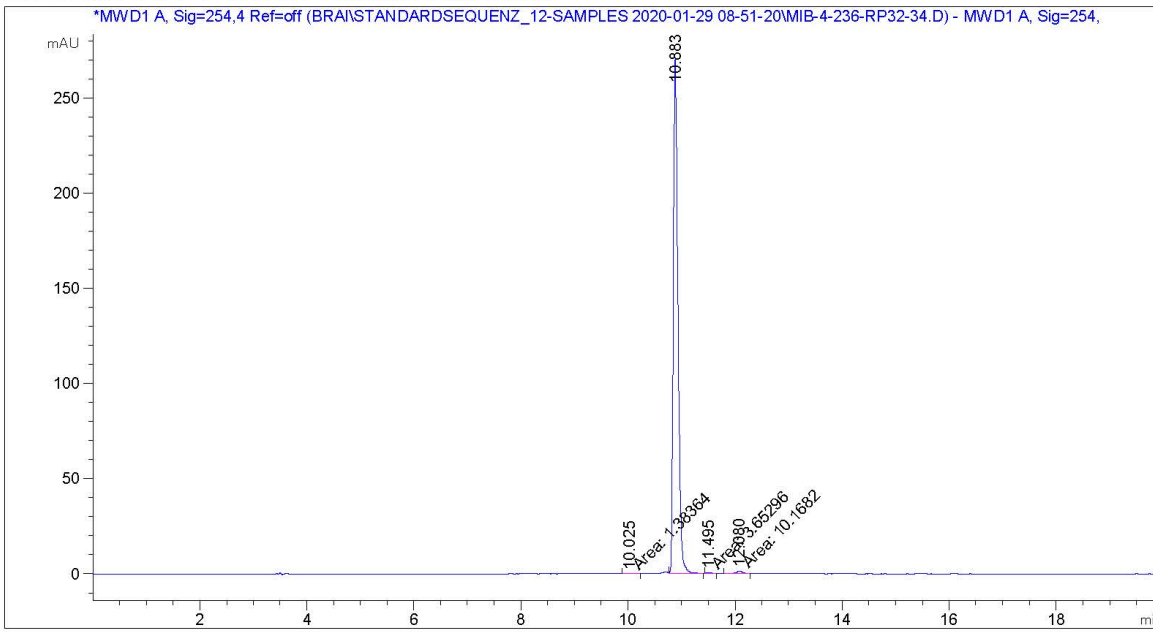
^{1}H-NMR



^{13}C-NMR



LC

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=====================================================================
                        Area Percent Report
=====================================================================

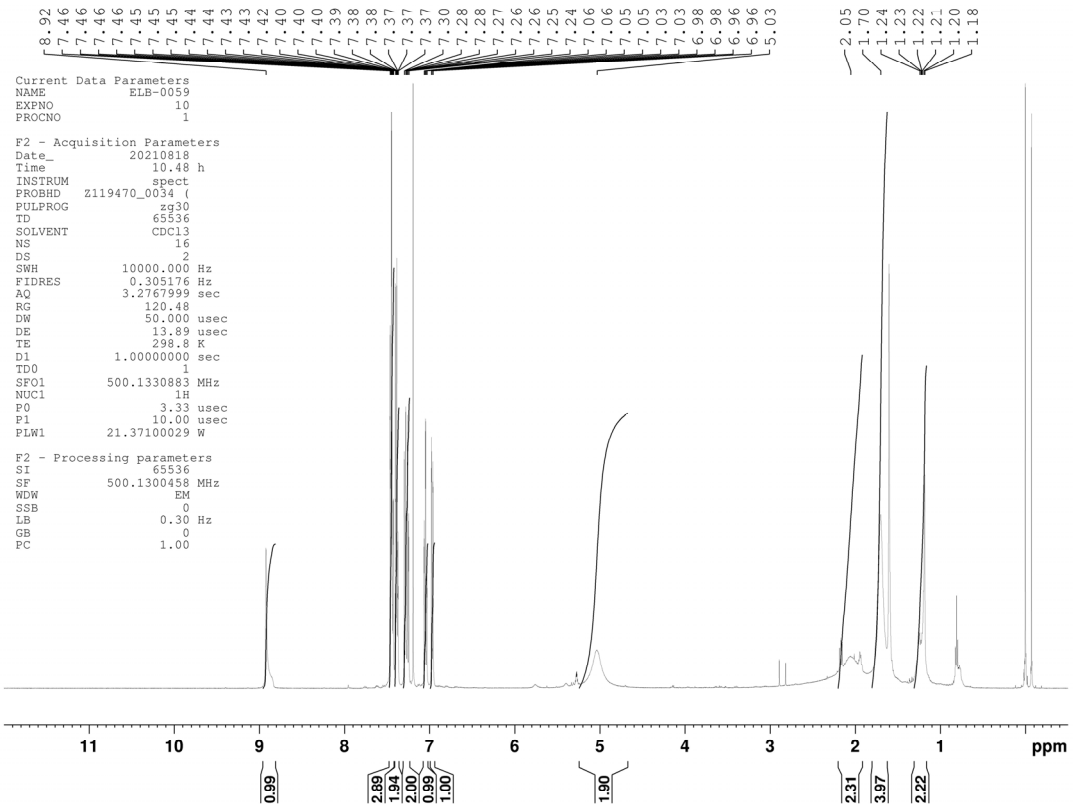
Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

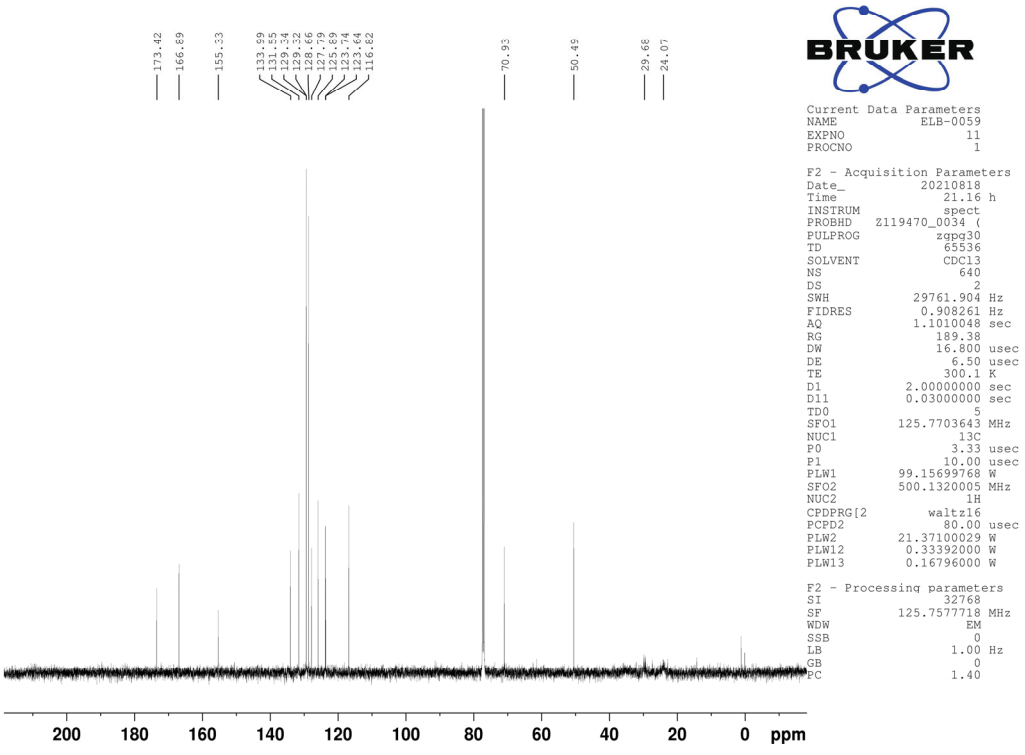
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.025 MM    0.1318    1.38364 1.74931e-1   0.0835
   2  10.883 VV    0.0929 1642.53210  270.19199  99.0828
   3  11.495 MM    0.1076    3.65296 5.65791e-1   0.2204
   4  12.080 MM    0.1180   10.16818    1.43630   0.6134
```

Compound 54

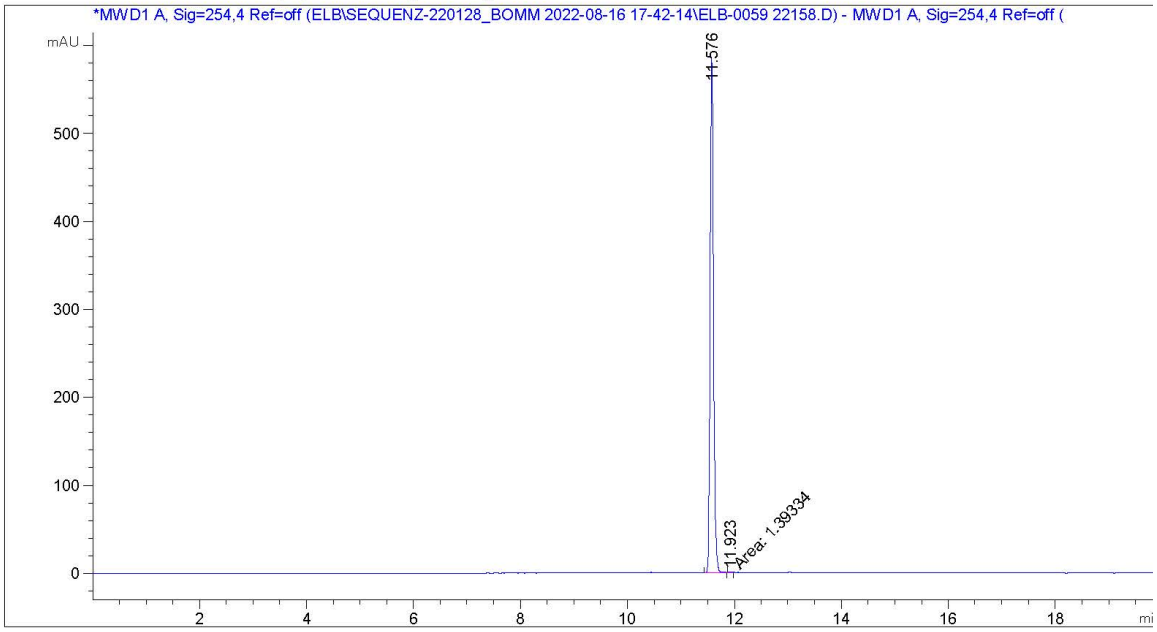
^{1}H-NMR



^{13}C-NMR



LC




```
=====================================================================
                    Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs

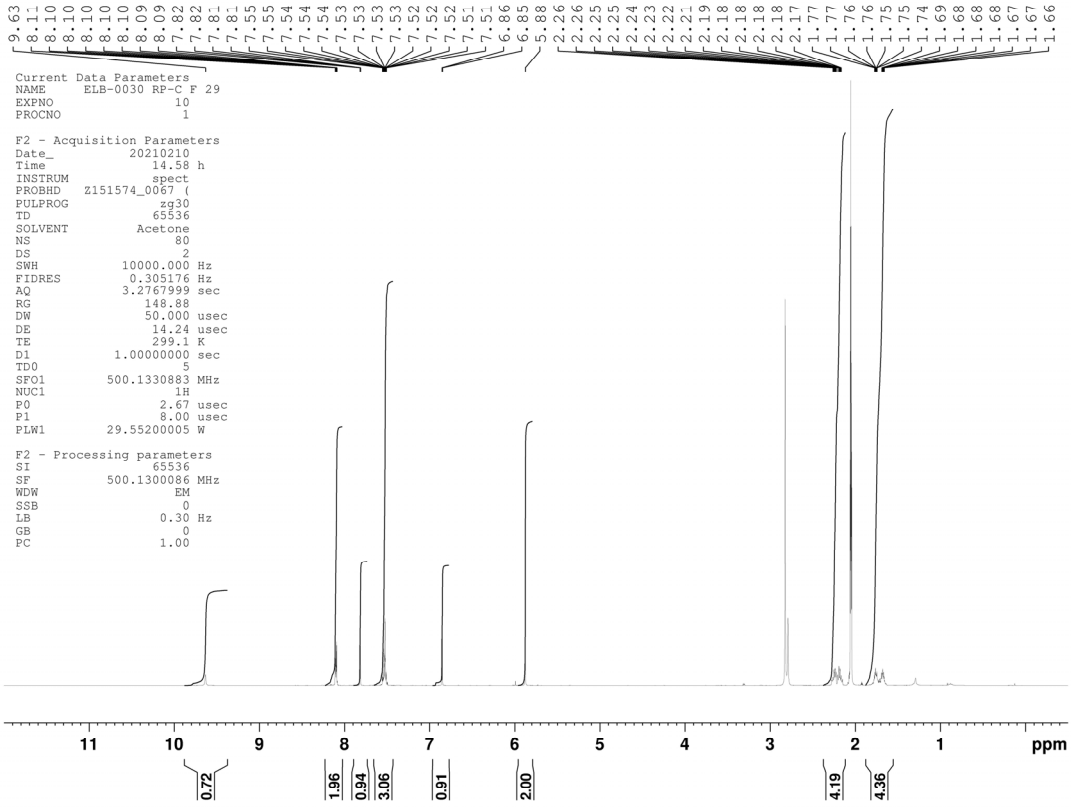

Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.576 BV    0.0693 2570.32397  584.90930  99.9458
   2  11.923 MM    0.0672    1.39334 3.45459e-1   0.0542

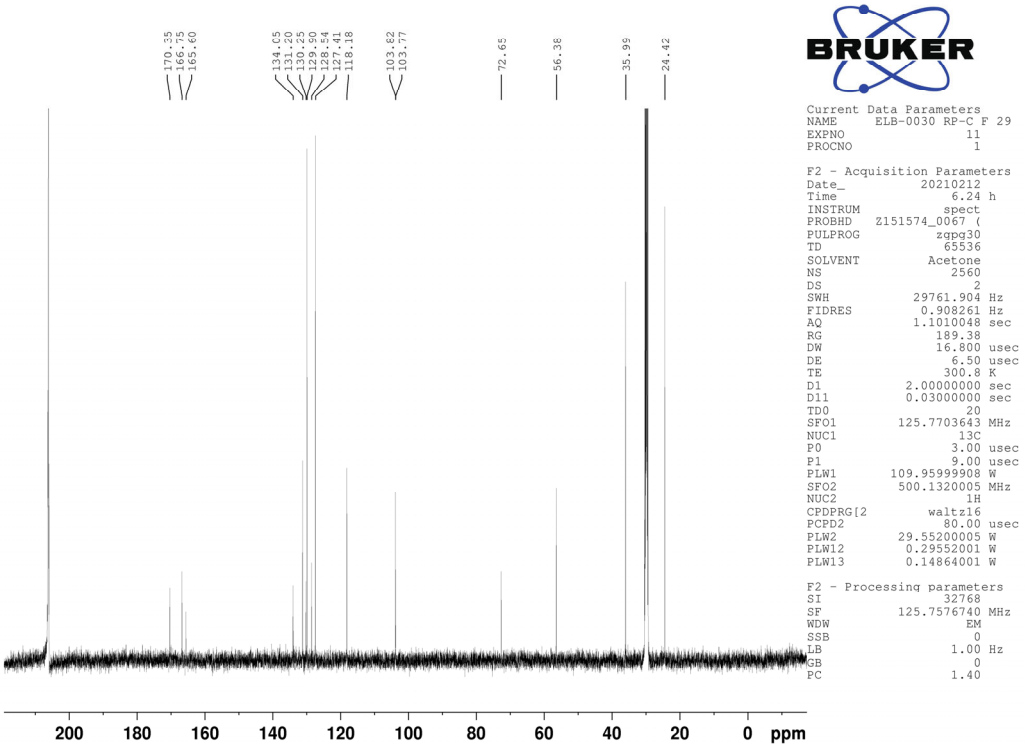
Totals :                  2571.71732  585.25476
```

Compound 55

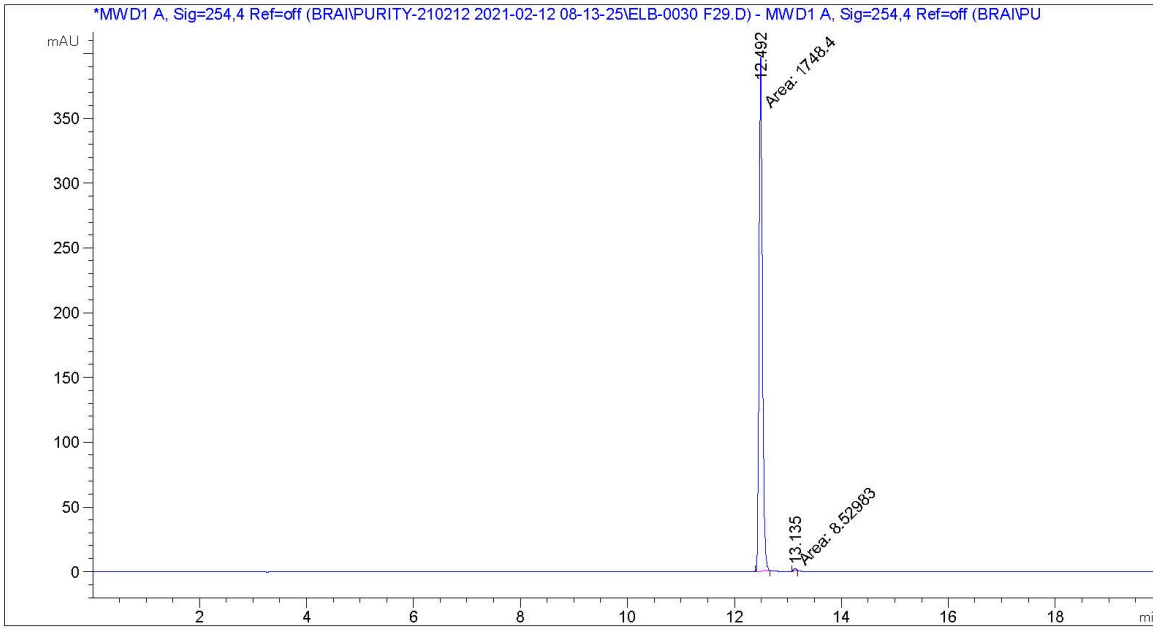
^{1}H-NMR



^{13}C-NMR



LC

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=====================================================================
                    Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.492 MM    0.0729 1748.40356  399.80600  99.5145
   2  13.135 MM    0.0650    8.52983    2.18628   0.4855

Totals :                  1756.93340  401.99228
```
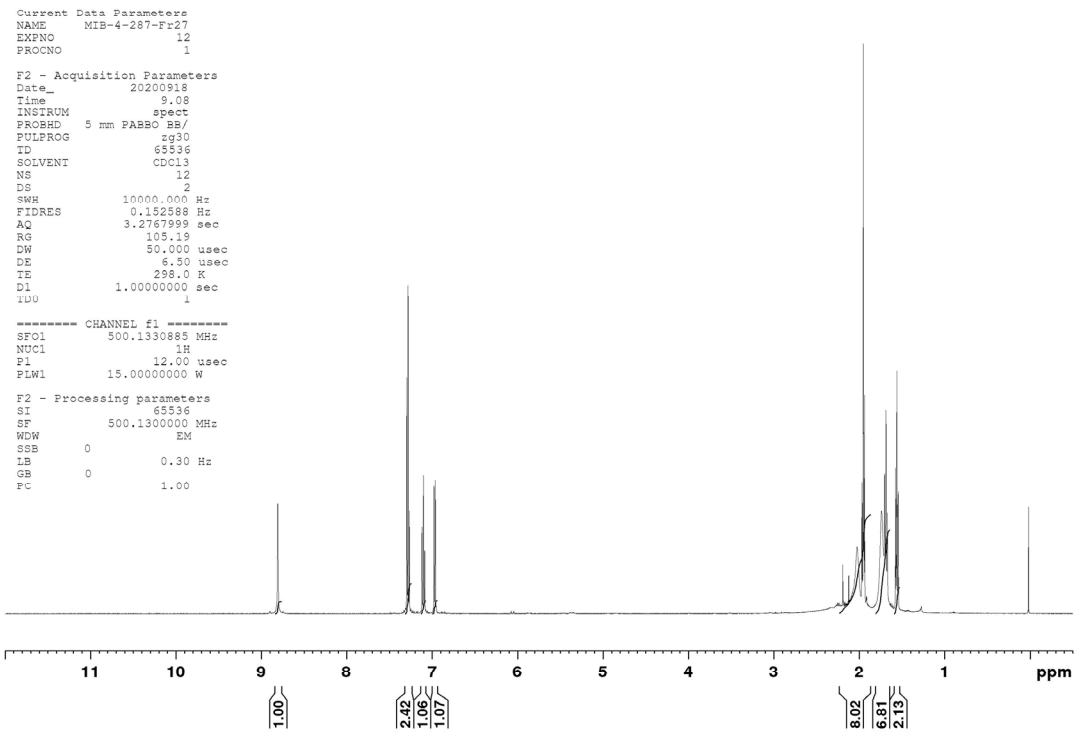
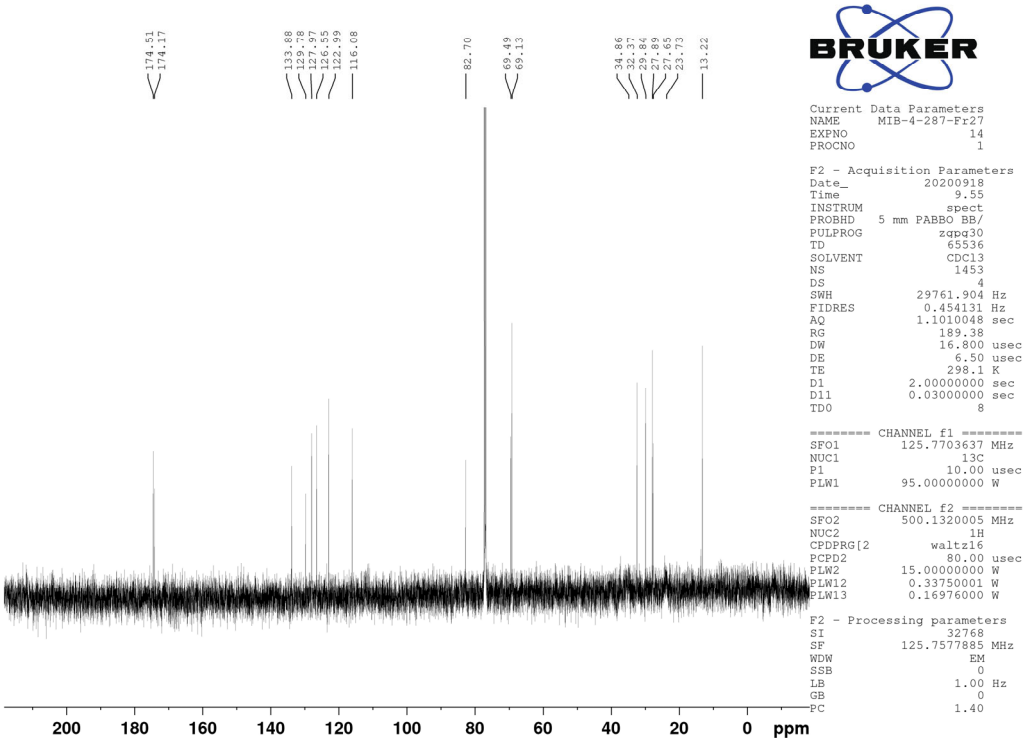

Compound 56

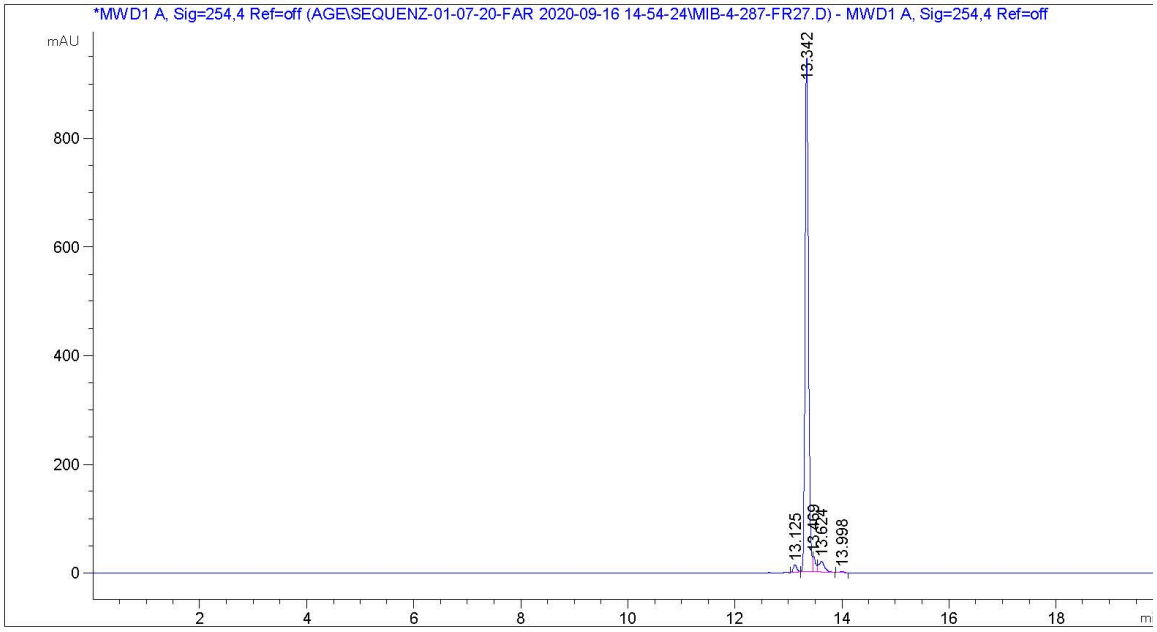
^{1}H-NMR



^{13}C-NMR



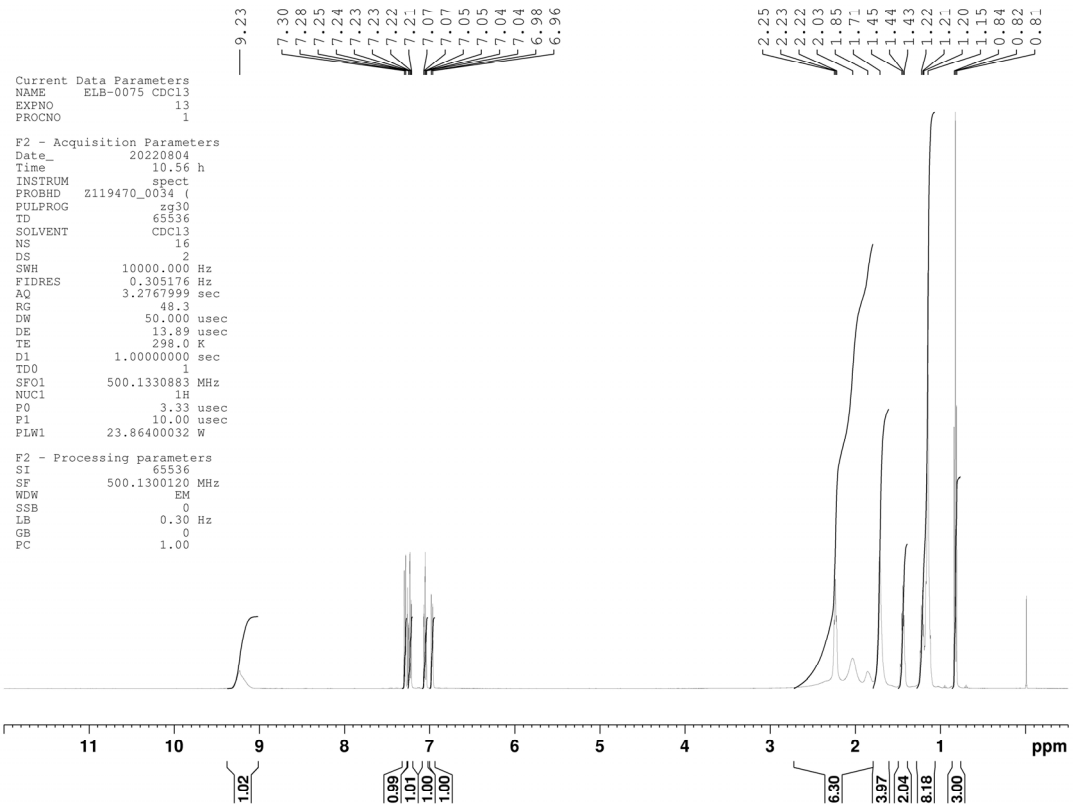
LC



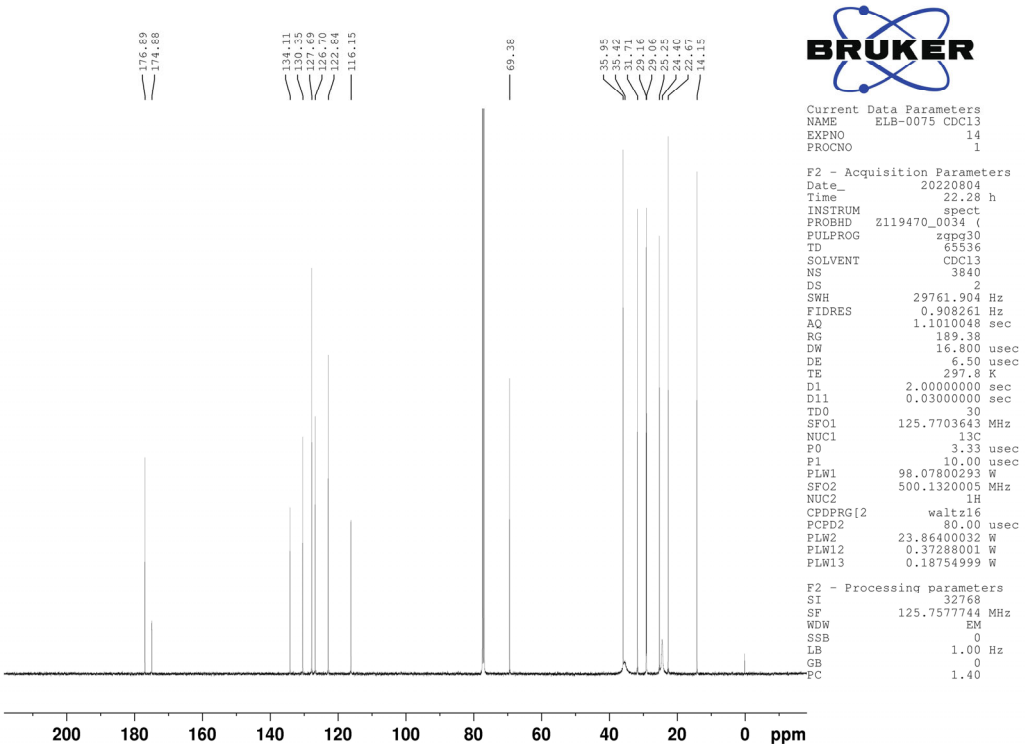

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  13.125 BB    0.0705   59.63300   13.24950   1.3170
   2  13.342 BV    0.0675 4192.39502  949.02539  92.5895
   3  13.469 VV    0.0543  108.75386   28.63091   2.4018
   4  13.624 VB    0.1054  156.64952   20.43171   3.4596
   5  13.998 BB    0.0777   10.50593    2.05454   0.2320
```

Compound 57

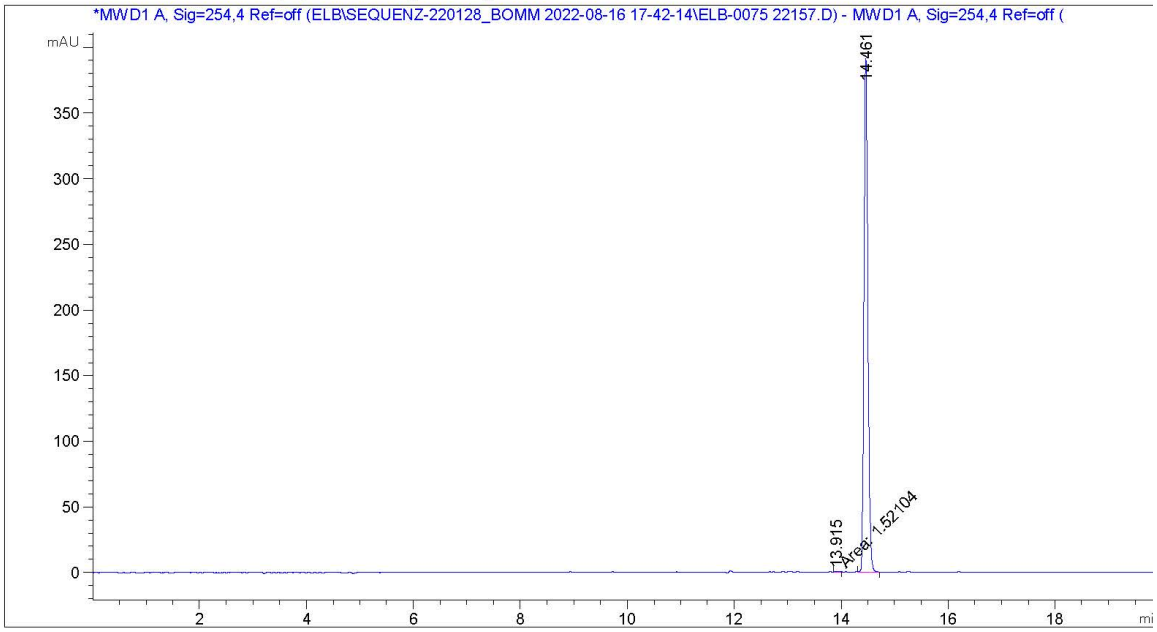
^{1}H-NMR



^{13}C-NMR



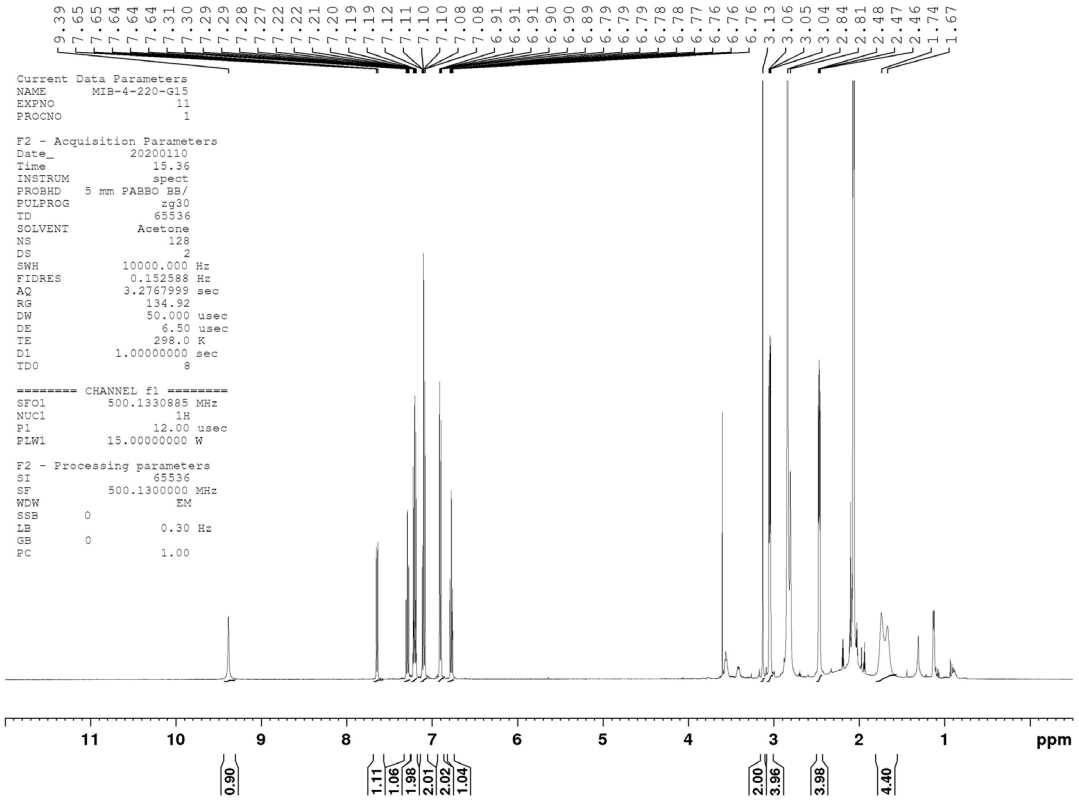
LC



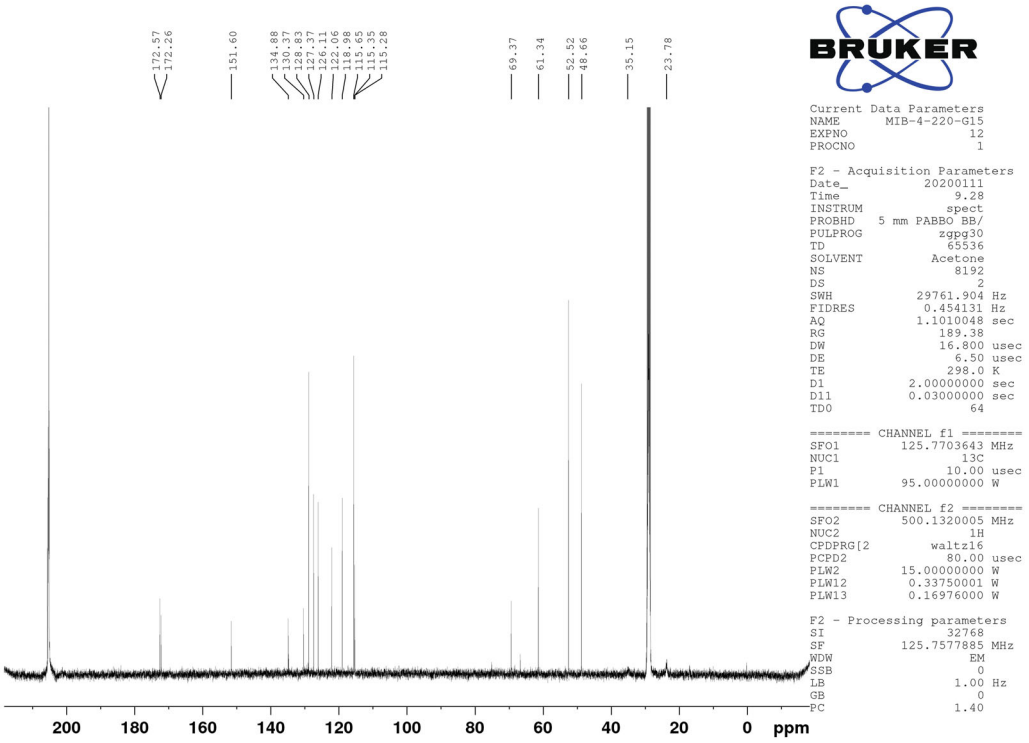

```
=====================================================================
                    Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  13.915 MM    0.0727    1.52104 3.48565e-1   0.0787
   2  14.461 VV    0.0754 1930.66223  392.51517  99.9213

Totals :                  1932.18327  392.86373
```

Compound S1

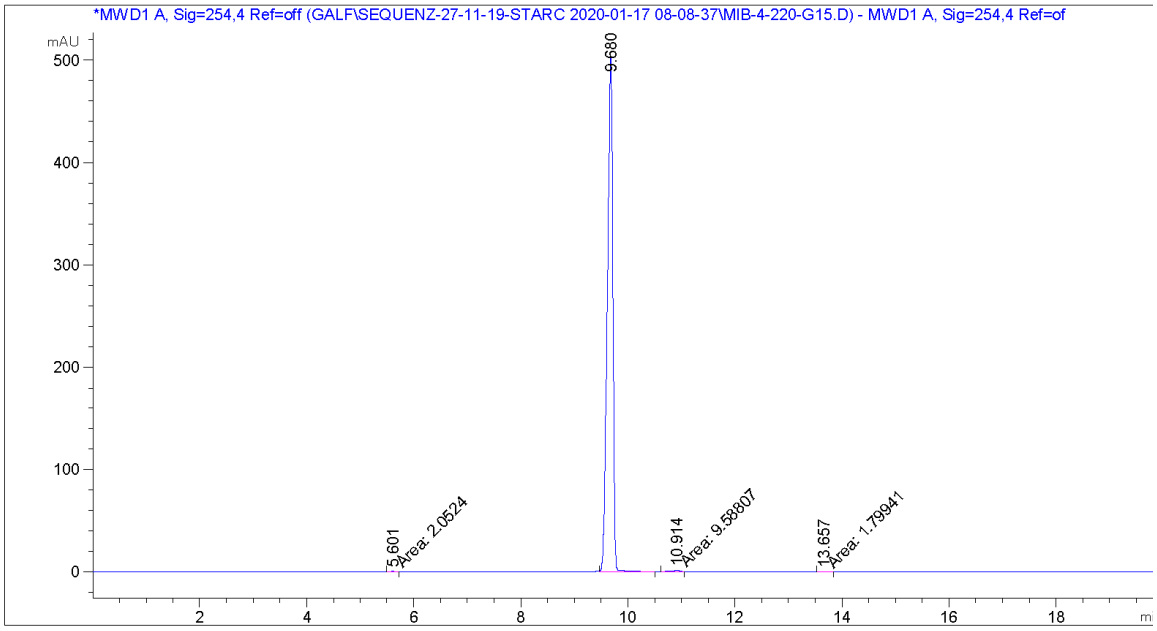
^{1}H-NMR



^{13}C-NMR



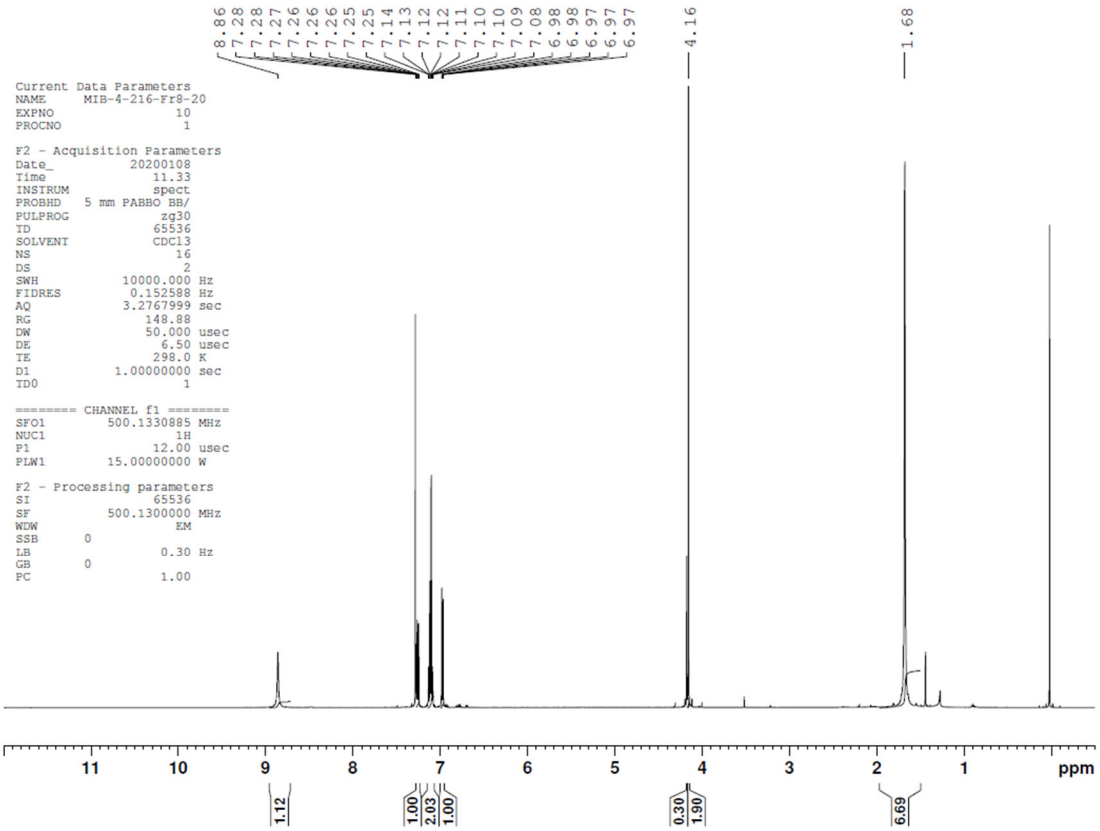
LC



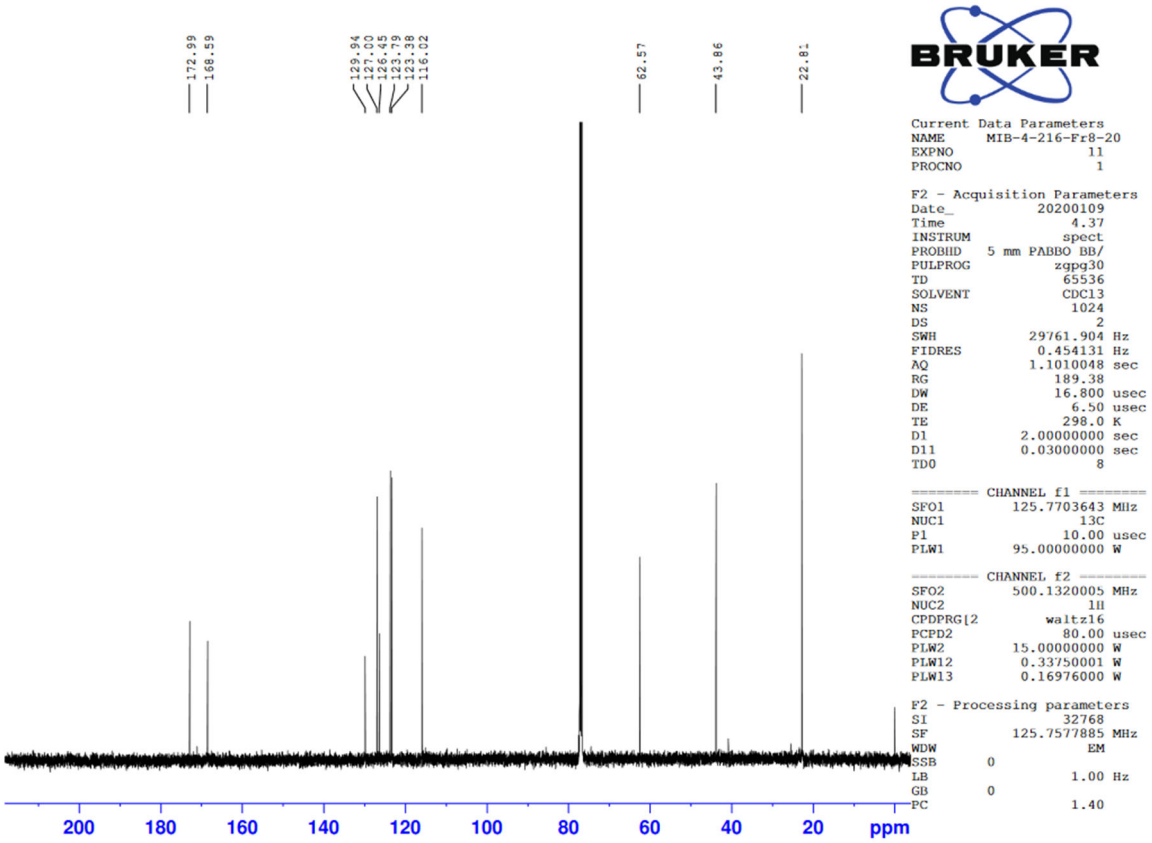

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.601 MM    0.0631    2.05240 5.42125e-1   0.0582
   2   9.680 VB    0.1015 3515.44995  503.16556  99.6191
   3  10.914 MM    0.1296    9.58807    1.23314   0.2717
   4  13.657 MM    0.1266    1.79941 2.36958e-1   0.0510
```

Compound S16

^{1}H-NMR

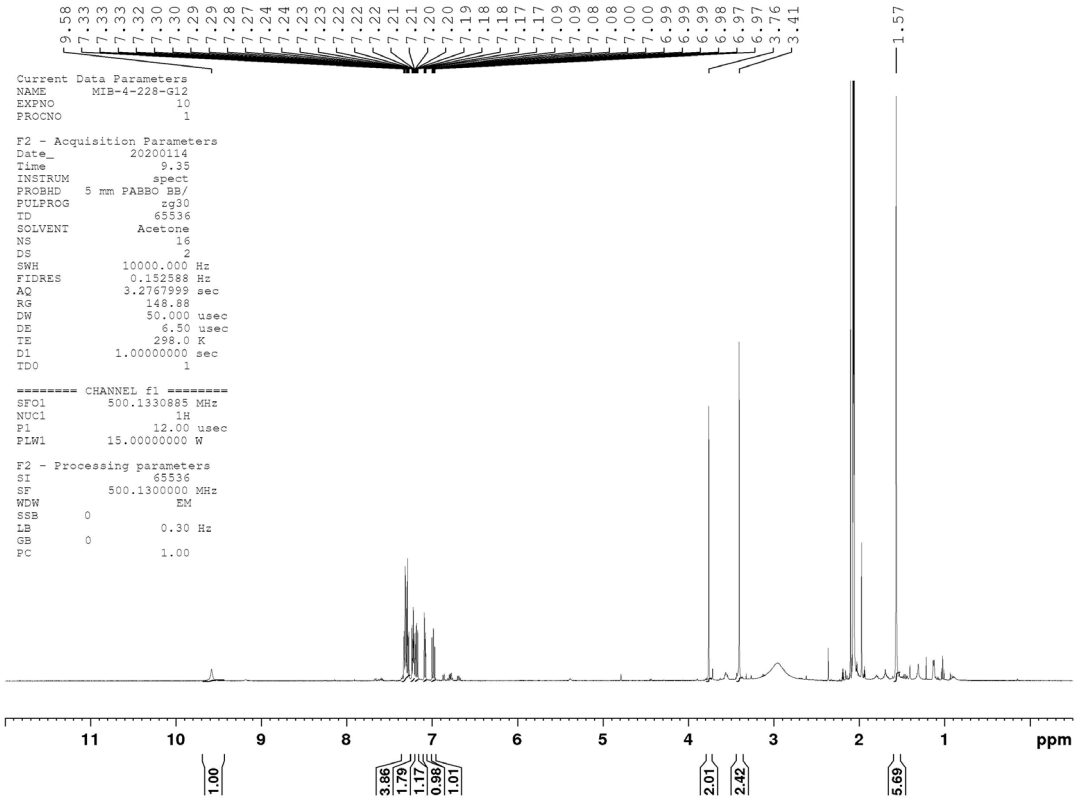


^{13}C-NMR

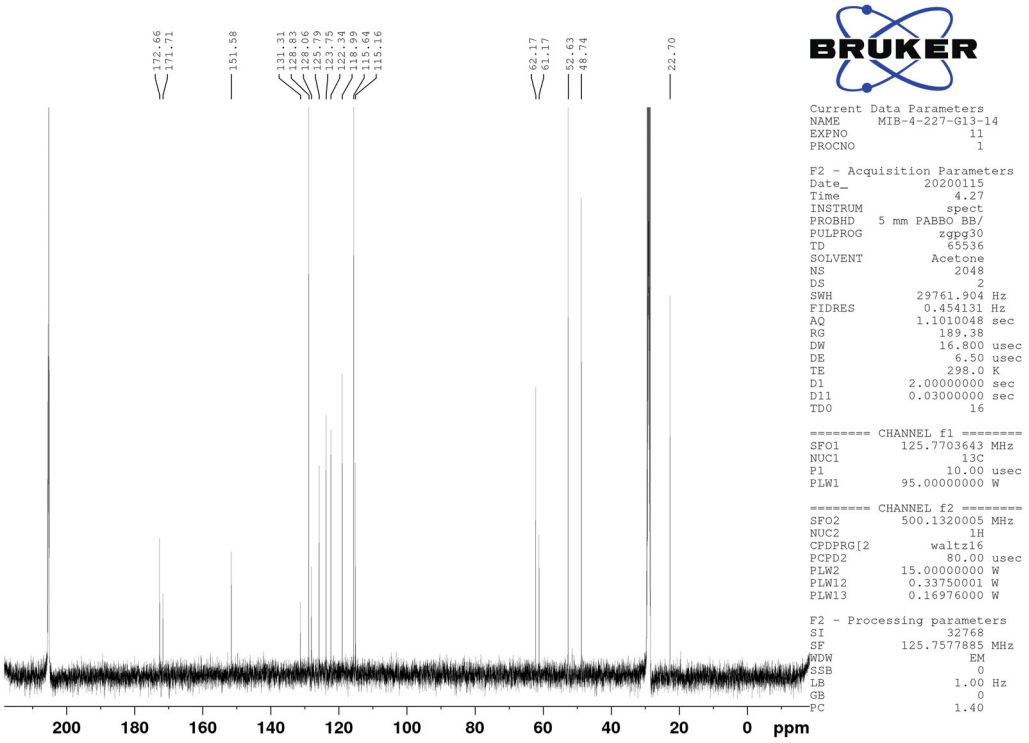


Compound S2

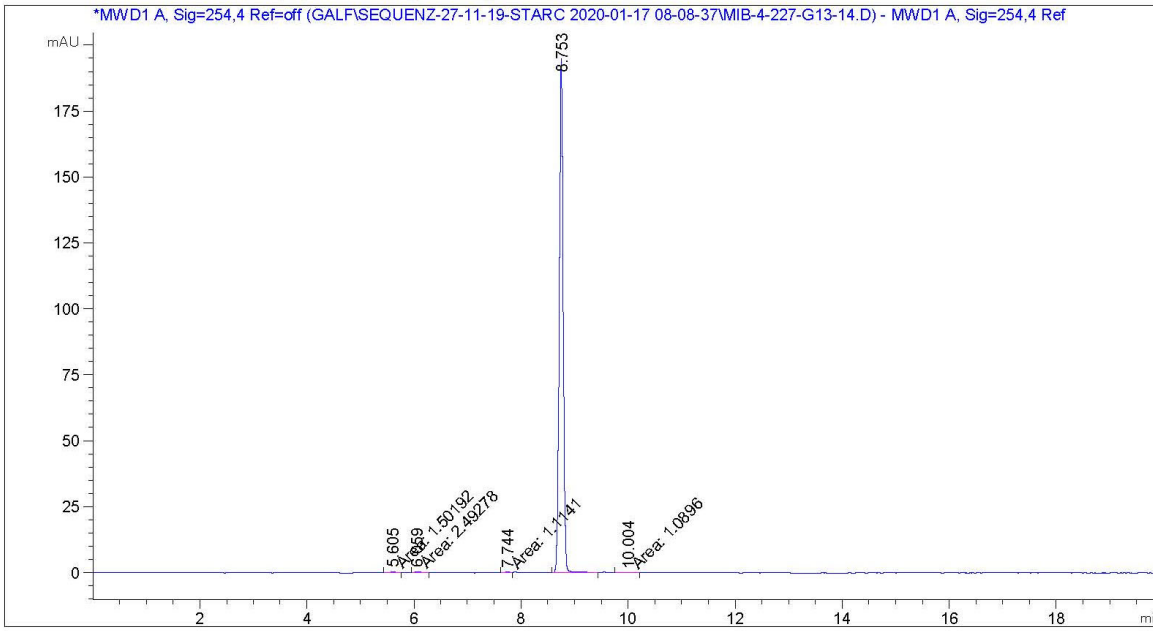
^{1}H-NMR



^{13}C-NMR



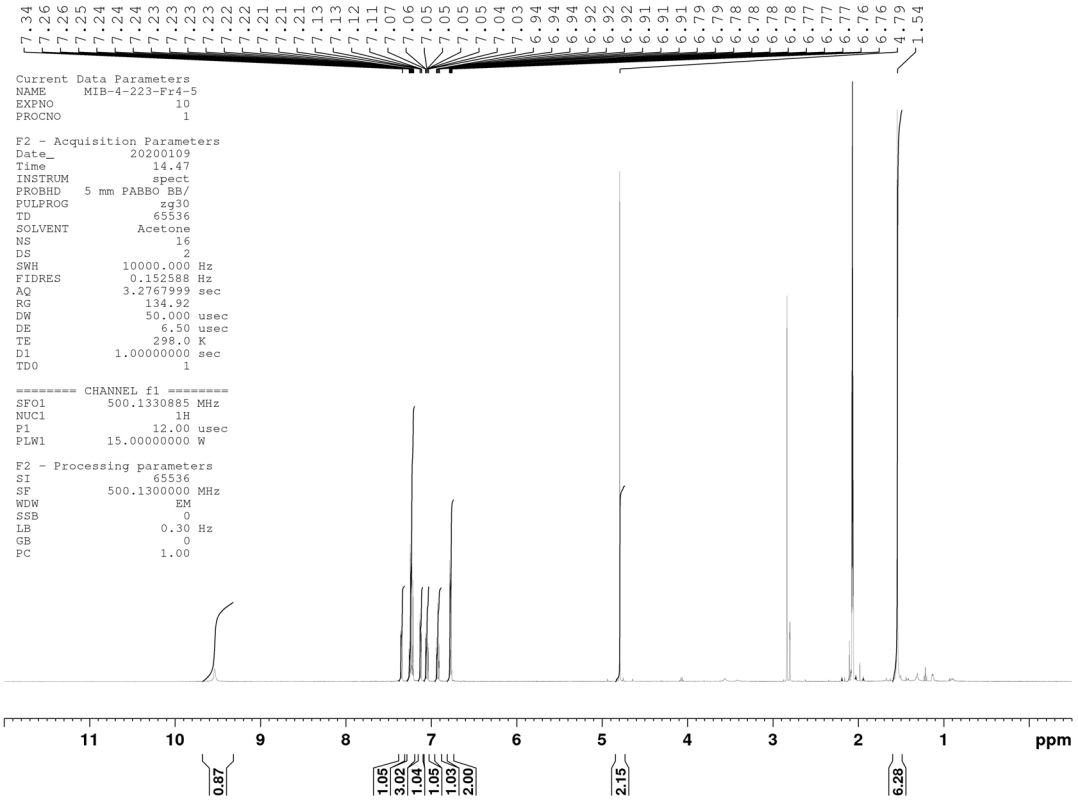
LC



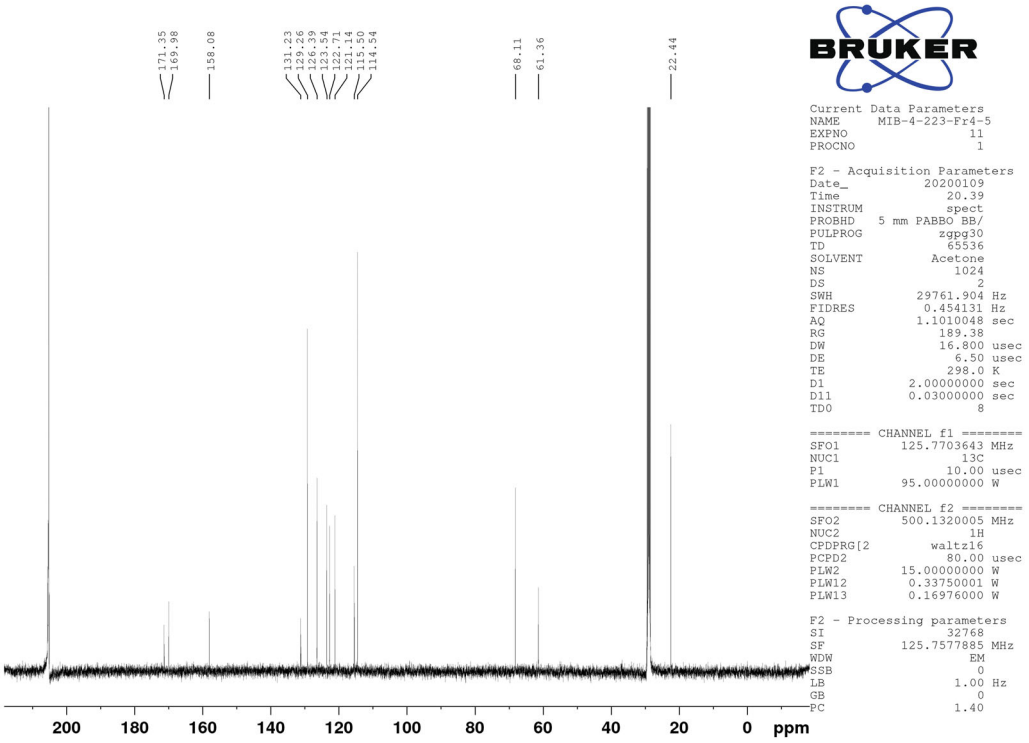

```
=====================================================================
                      Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.605 MM    0.0717    1.50192 3.49111e-1   0.1508
   2   6.059 MM    0.0970    2.49278 4.28321e-1   0.2503
   3   7.744 MM    0.0747    1.11410 2.48439e-1   0.1119
   4   8.753 BB    0.0773  989.83307  194.83113  99.3777
   5  10.004 MM    0.1779    1.08960 1.02083e-1   0.1094
```

Compound S3

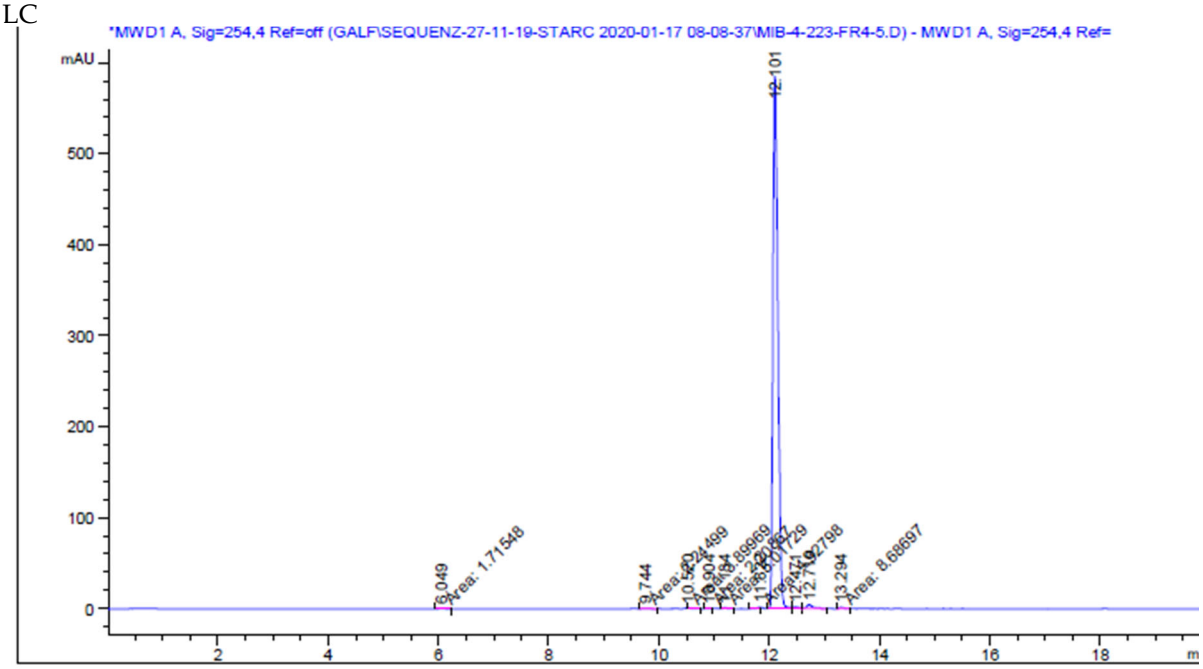
^{1}H-NMR



^{13}C-NMR



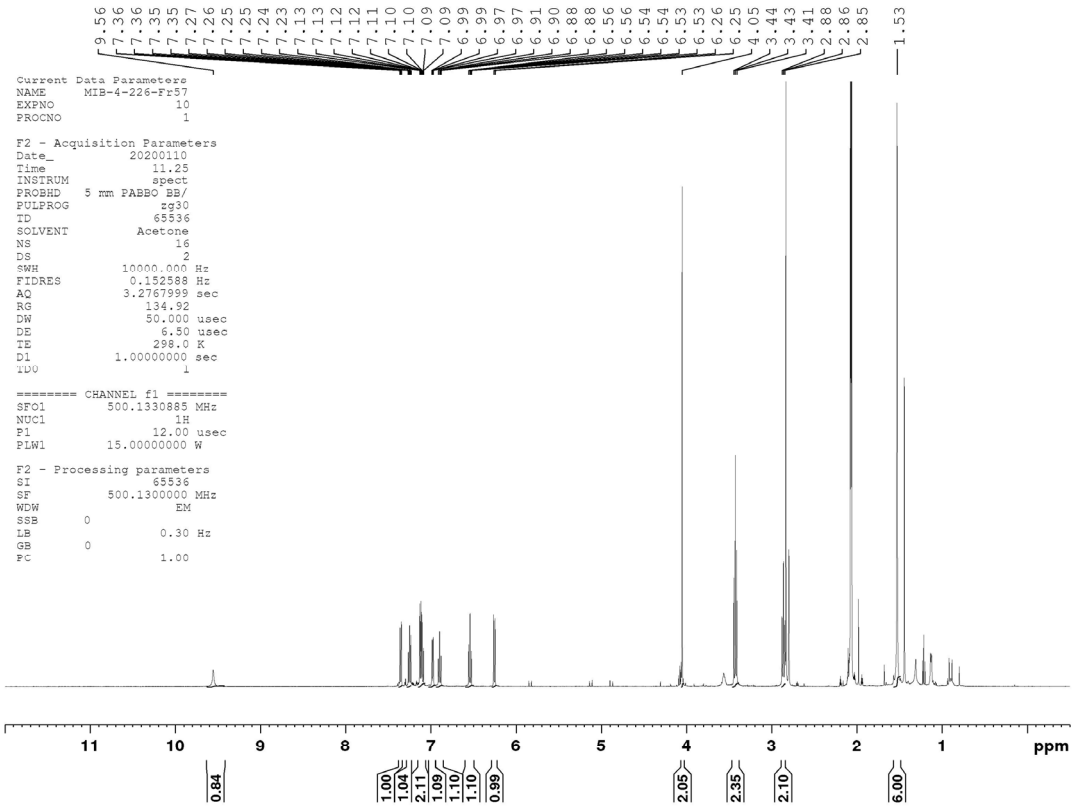
LC



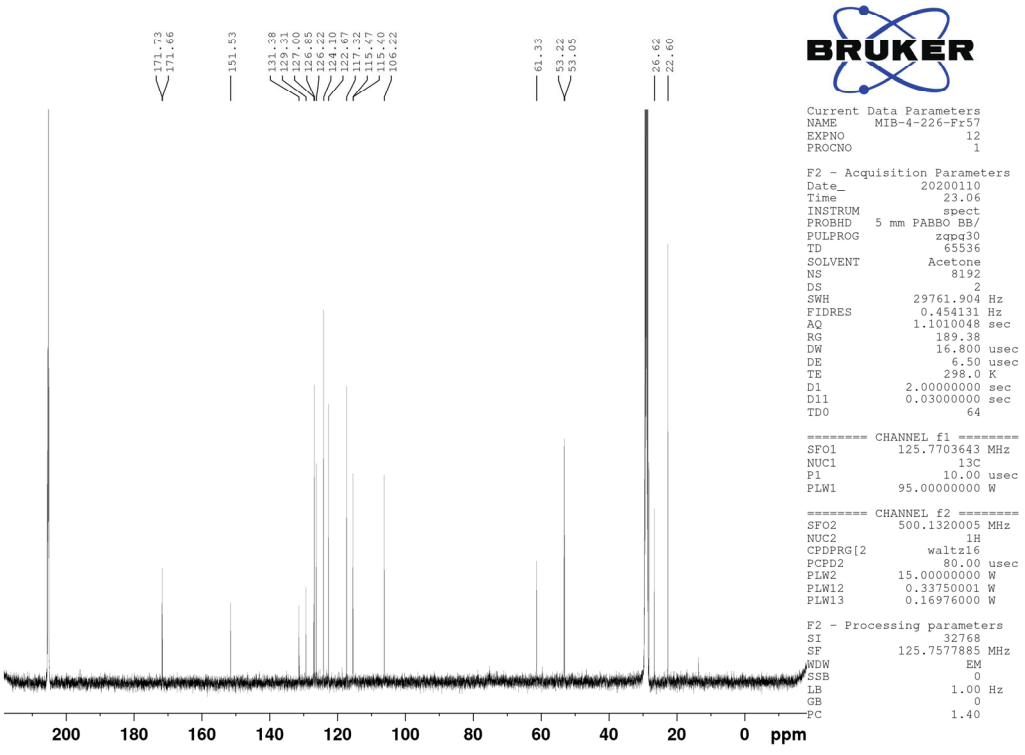

```
=====================================================================
                      Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.049 MM    0.1192    1.71548 2.39828e-1   0.0465
   2   9.744 MM    0.1080    2.24499 3.46585e-1   0.0609
   3  10.520 MM    0.0773    3.89969 8.40470e-1   0.1057
   4  10.904 MM    0.0900    2.20867 4.09218e-1   0.0599
   5  11.184 MM    0.0968    5.01729 8.64126e-1   0.1361
   6  11.822 MM    0.0696    4.92798    1.18017   0.1336
   7  12.101 BV    0.0958 3606.28735  585.83331  97.7934
```

Compound S4

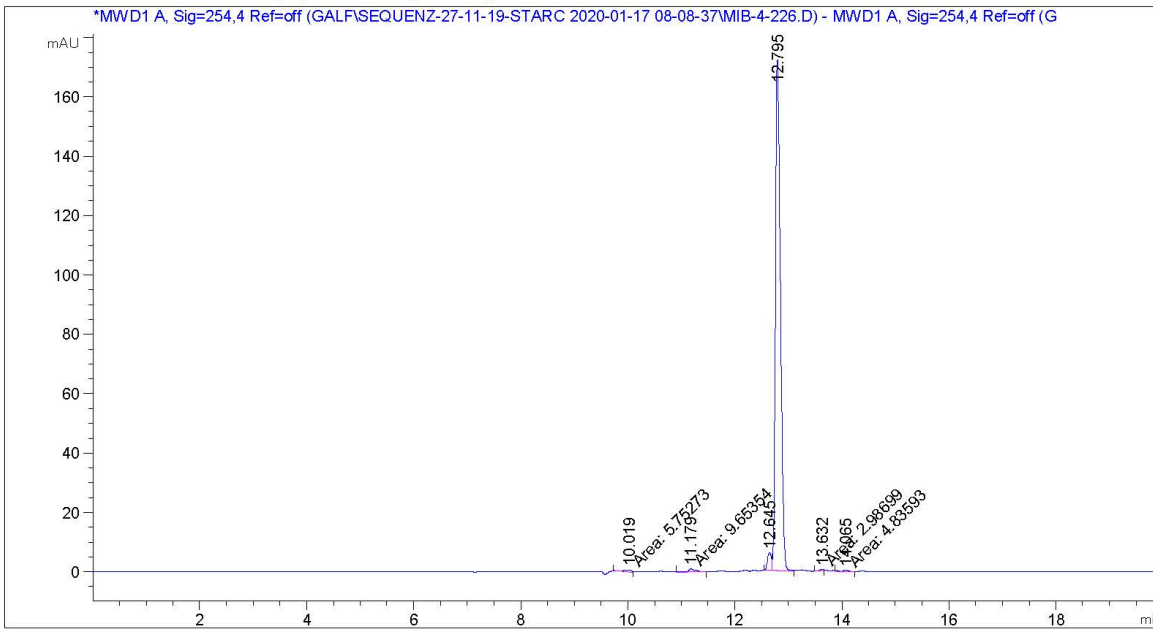
^{1}H-NMR



^{13}C-NMR



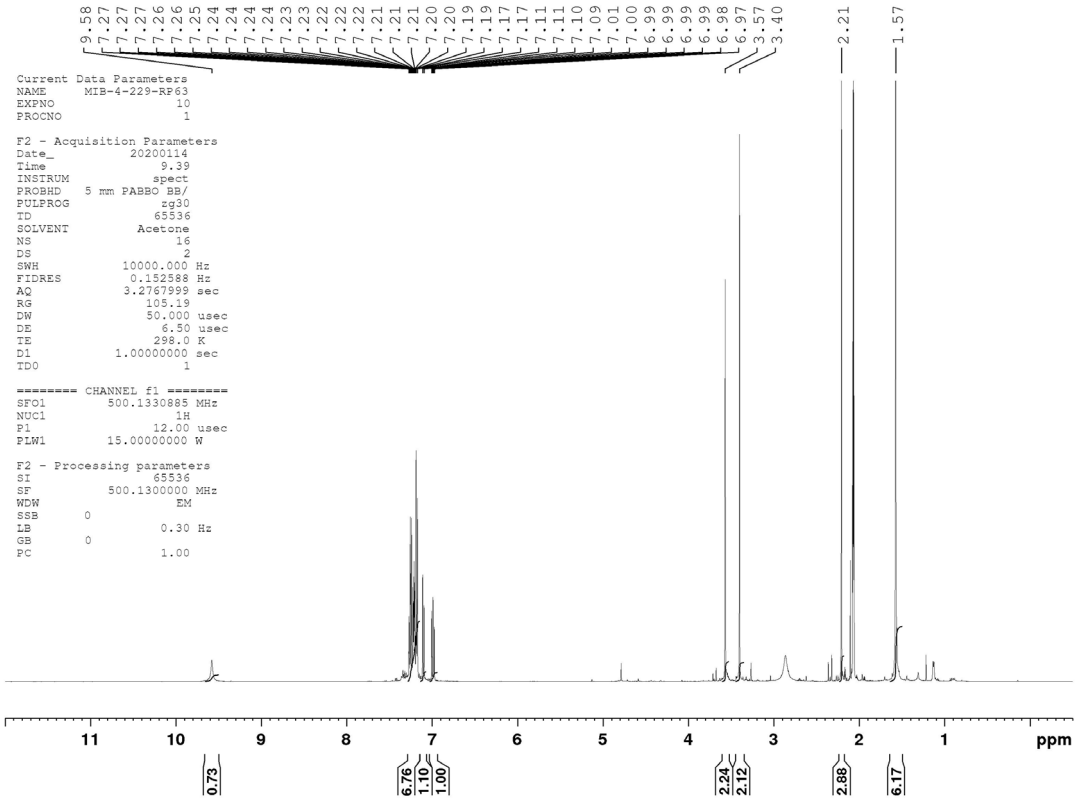
LC



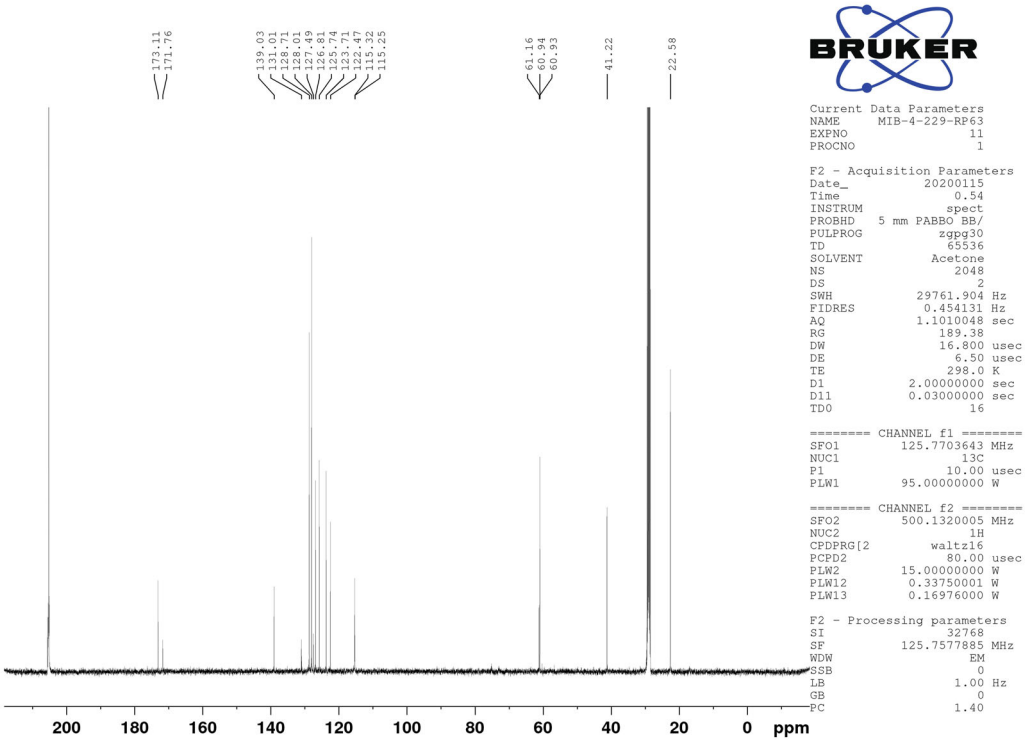

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.019 MM    0.1493    5.75273 6.42100e-1   0.4942
   2  11.179 MM    0.1706    9.65354 9.43049e-1   0.8292
   3  12.645 BV    0.0792   30.15967    5.94530   2.5907
   4  12.795 VV    0.1031 1110.74243  172.51054  95.4138
   5  13.632 MM    0.0877    2.98699 5.67707e-1   0.2566
   6  14.065 MM    0.1874    4.83593 4.29990e-1   0.4154
```

Compound S5

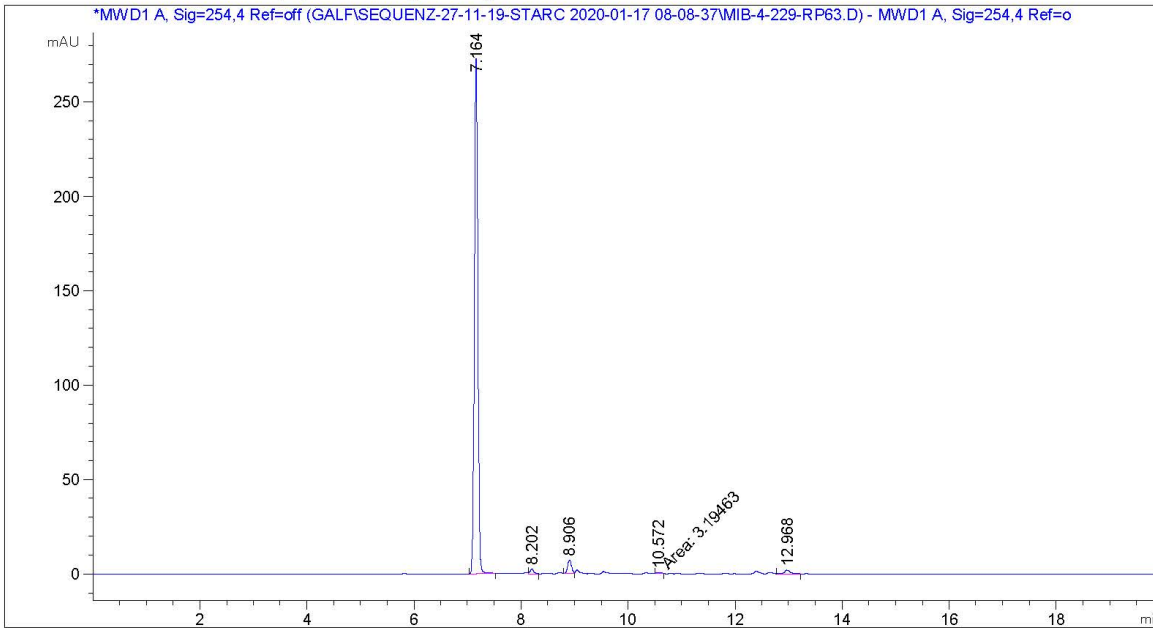
^{1}H-NMR



^{13}C-NMR



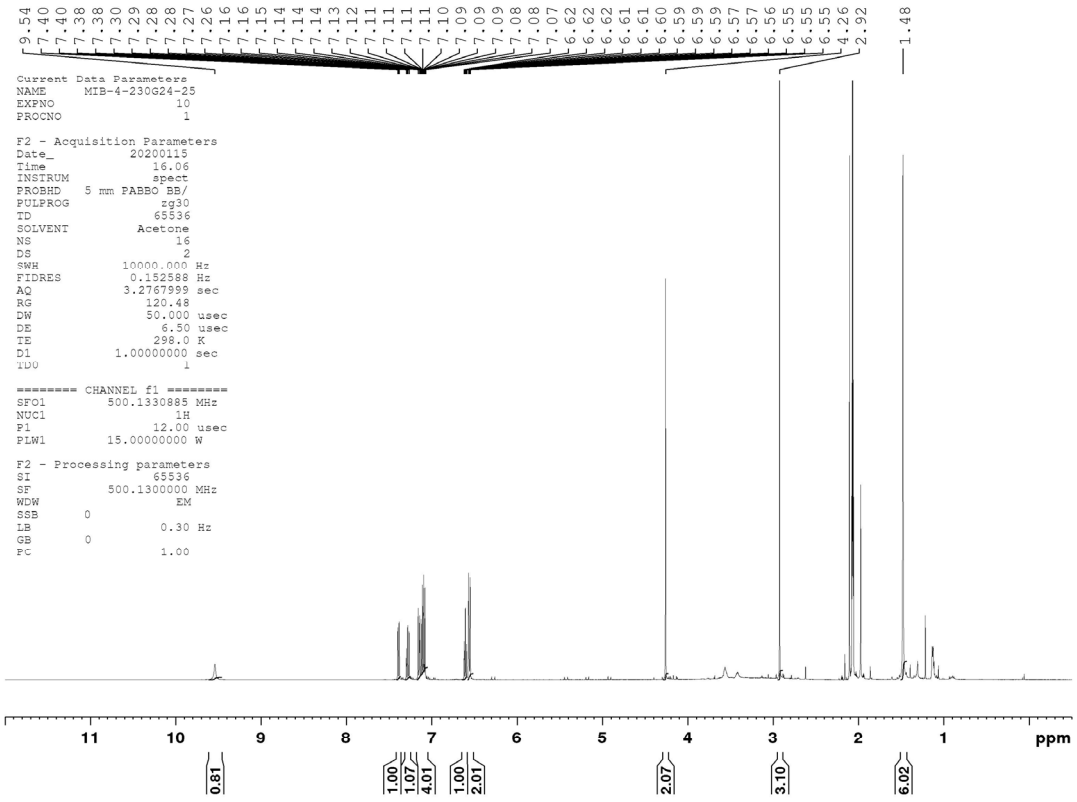
LC



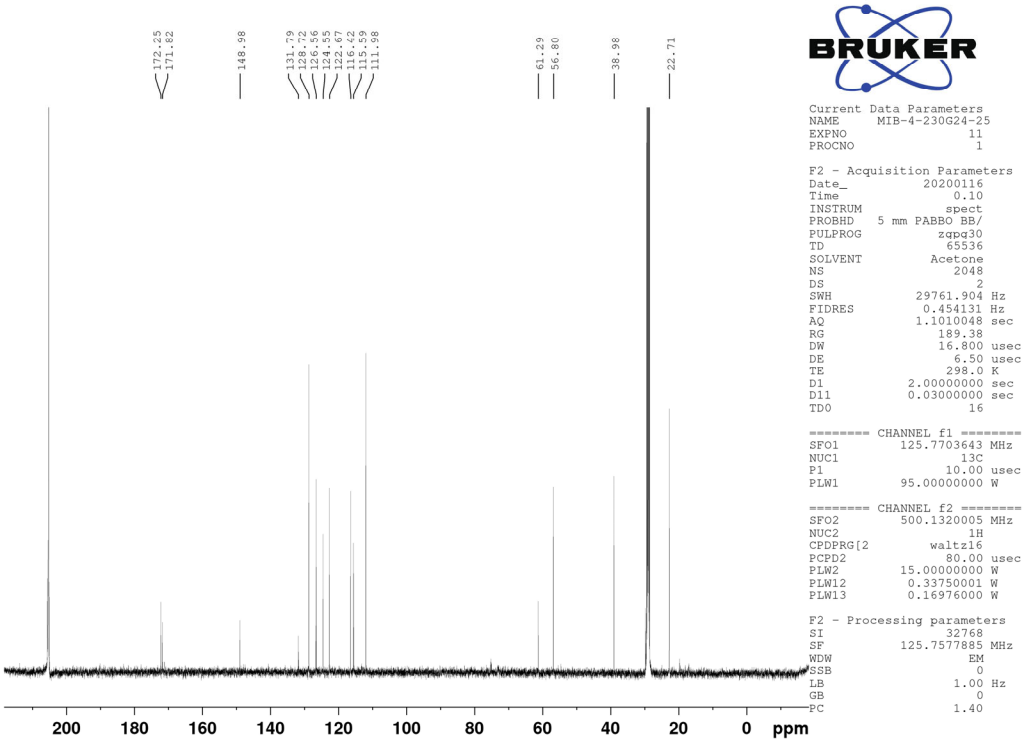

```
=====================================================================
                    Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.164 BB    0.0682 1226.65686  273.96463  95.0209
   2   8.202 VB    0.0727   11.47877    2.45046   0.8892
   3   8.906 BV    0.0747   34.56721    7.10991   2.6777
   4  10.572 MM    0.0875    3.19463 6.08688e-1   0.2475
   5  12.968 VB    0.1181   15.03613    1.90542   1.1647
```

Compound S6

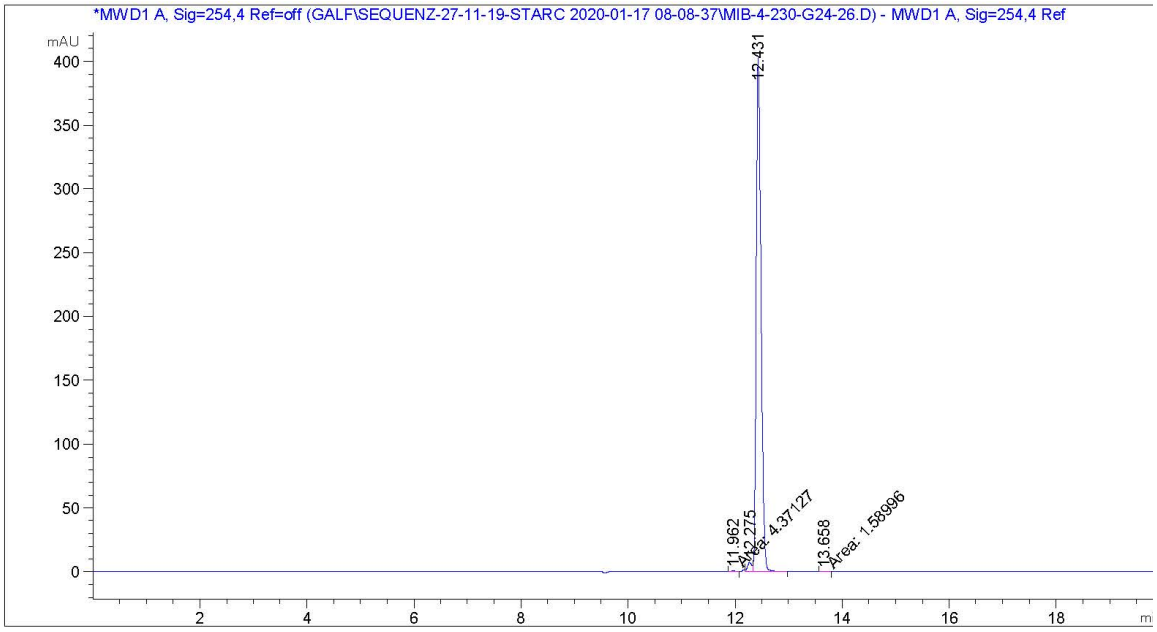
^{1}H-NMR



^{13}C-NMR



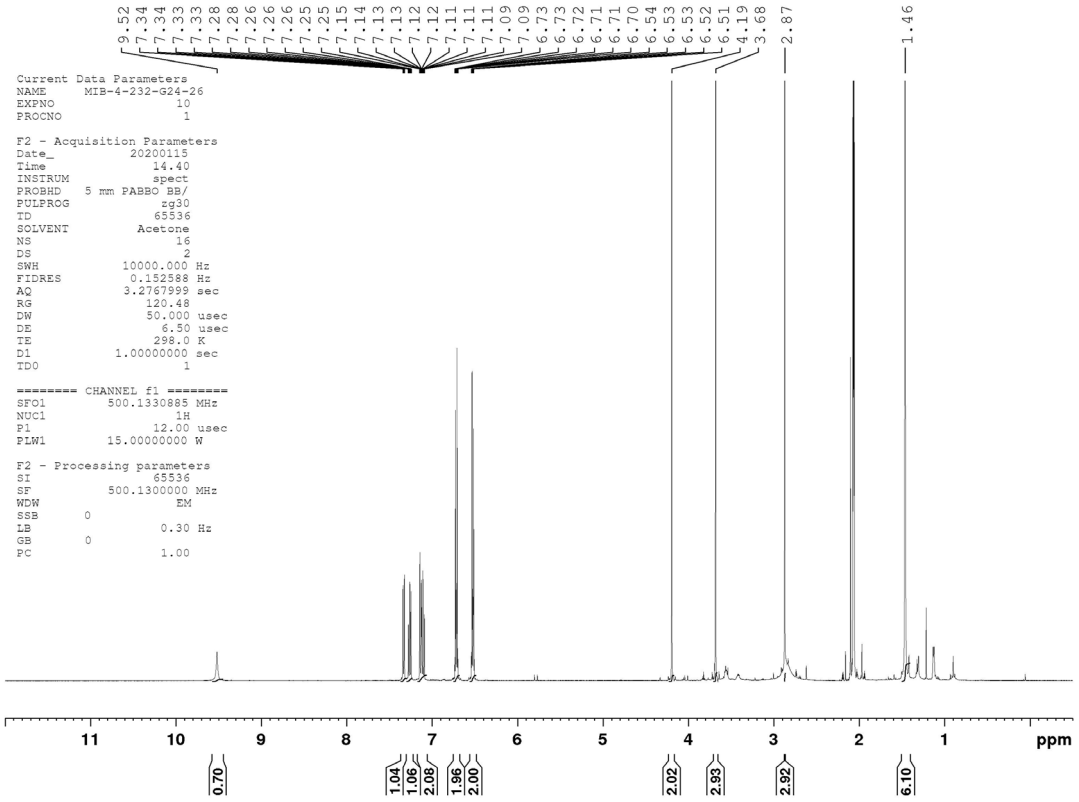
LC



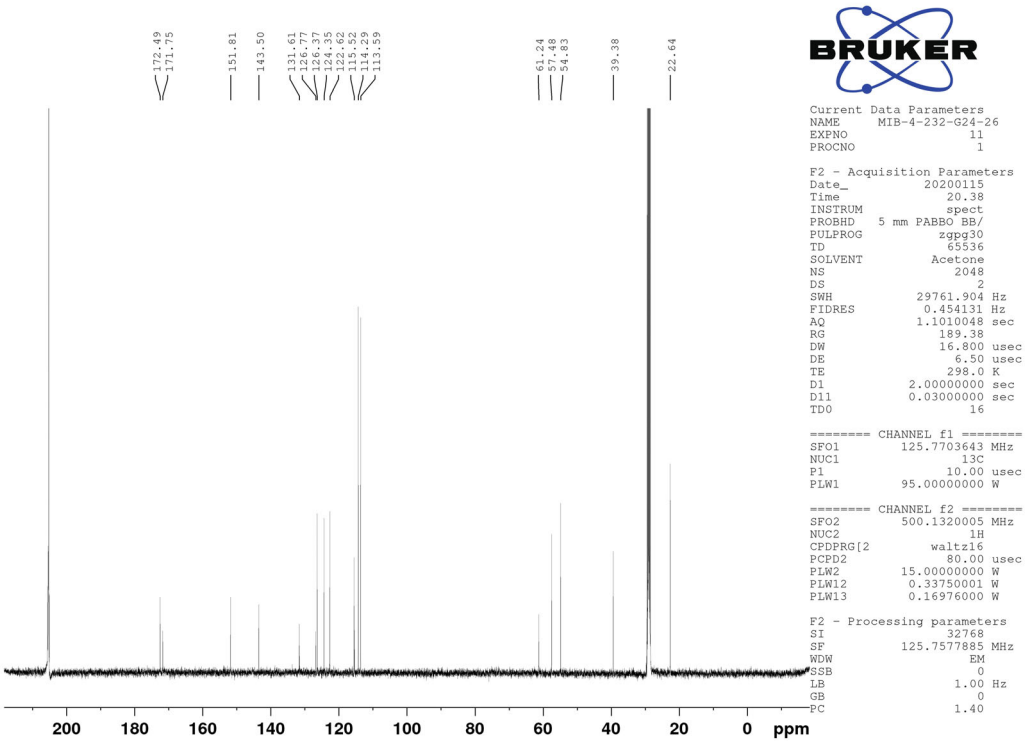

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.962 MM    0.1017    4.37127 7.16553e-1   0.1694
   2  12.275 VV    0.0831   37.99773    7.02580   1.4728
   3  12.431 VB    0.0994 2536.02856  403.13416  98.2962
   4  13.658 MM    0.1413    1.58996 1.87573e-1   0.0616
```

Compound S7

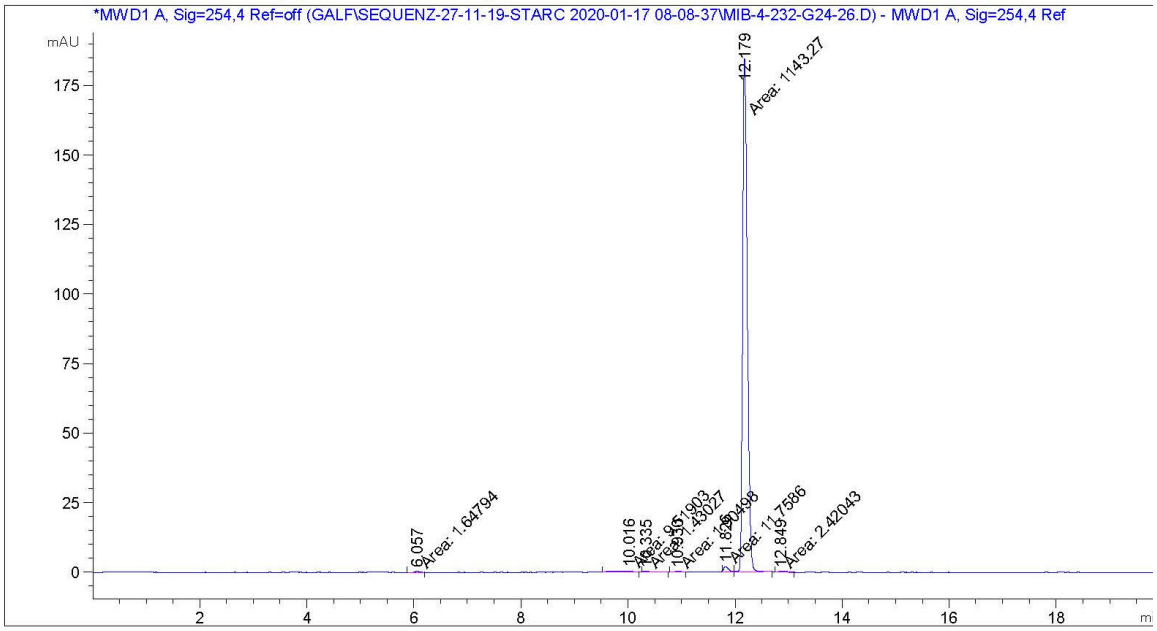
^{1}H-NMR



^{13}C-NMR



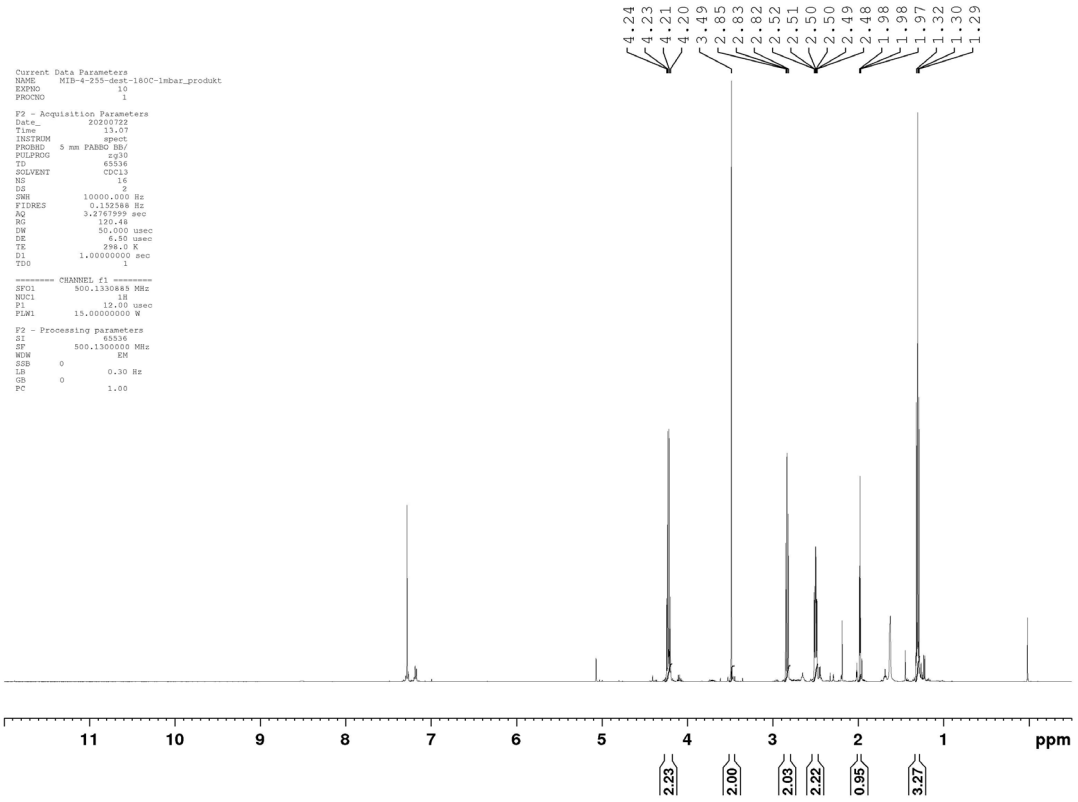
LC



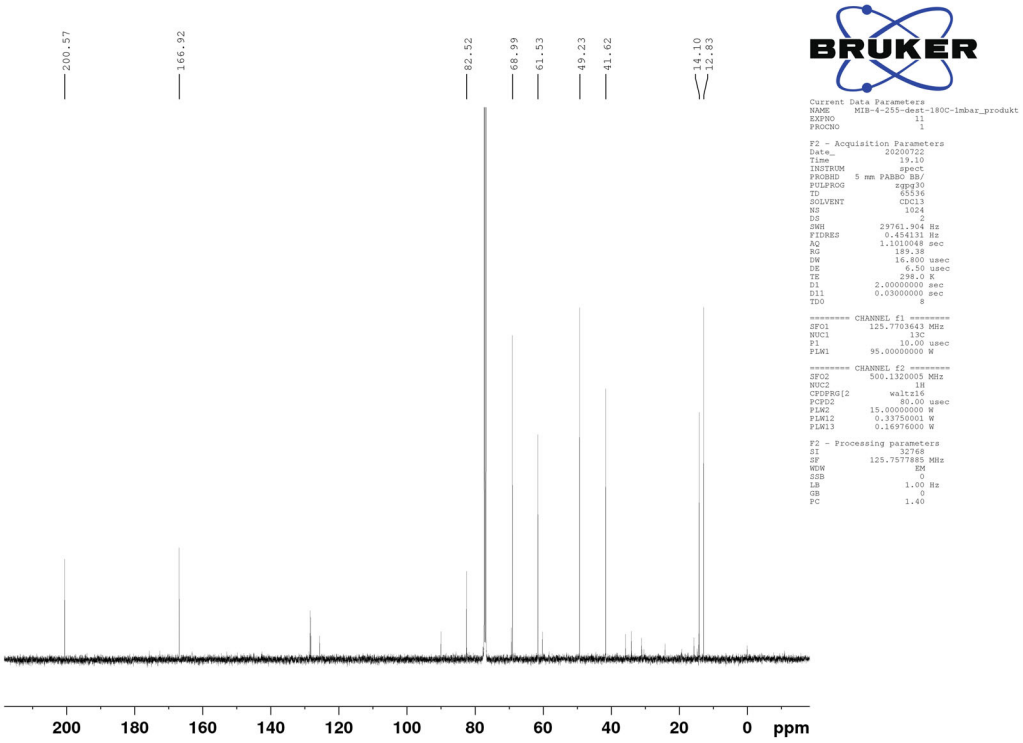

```
=====================================================================
                    Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: MWD1 A, Sig=254,4 Ref=off
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.057 MM    0.0964    1.64794 2.84888e-1   0.1406
   2  10.016 MM    0.3419    9.51903 4.64042e-1   0.8122
   3  10.335 MM    0.1199    1.43027 1.98747e-1   0.1220
   4  10.930 MM    0.1140    1.90498 2.78574e-1   0.1625
   5  11.826 MF    0.1023   11.75859    1.91577   1.0033
   6  12.179 FM    0.1028 1143.27441  185.28415  97.5527
   7  12.849 MM    0.1930    2.42043 2.09038e-1   0.2065
```

Compound S9

^{1}H-NMR

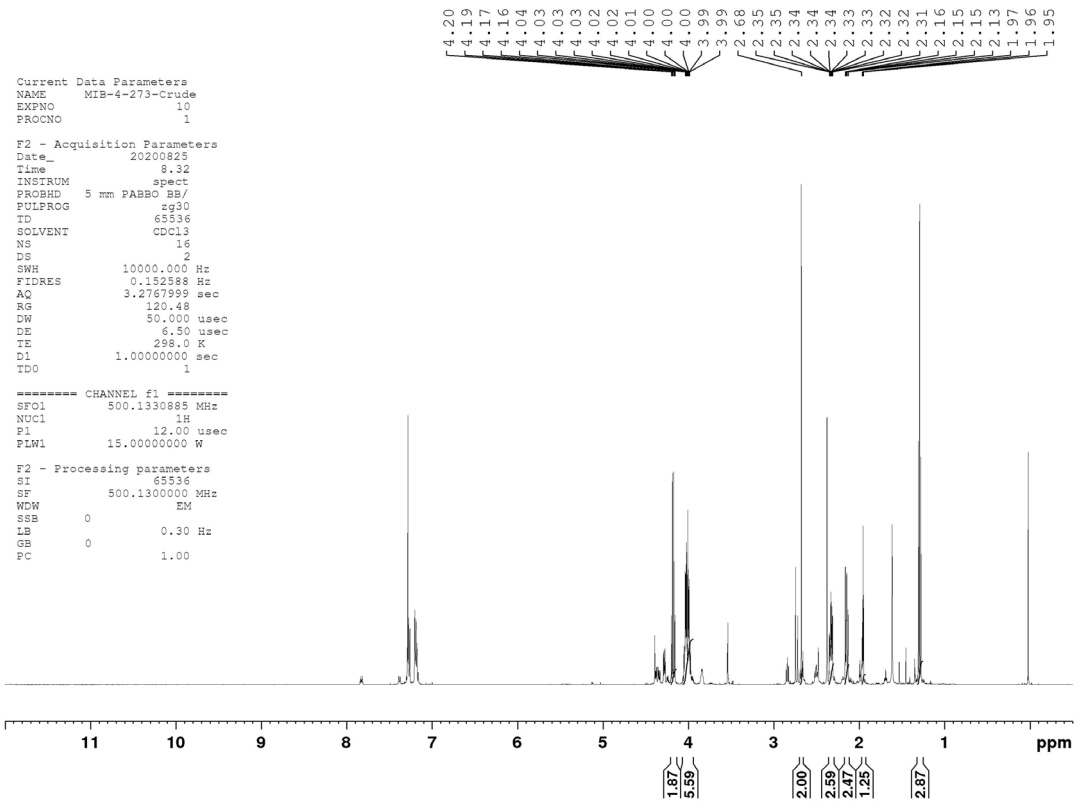


^{13}C-NMR



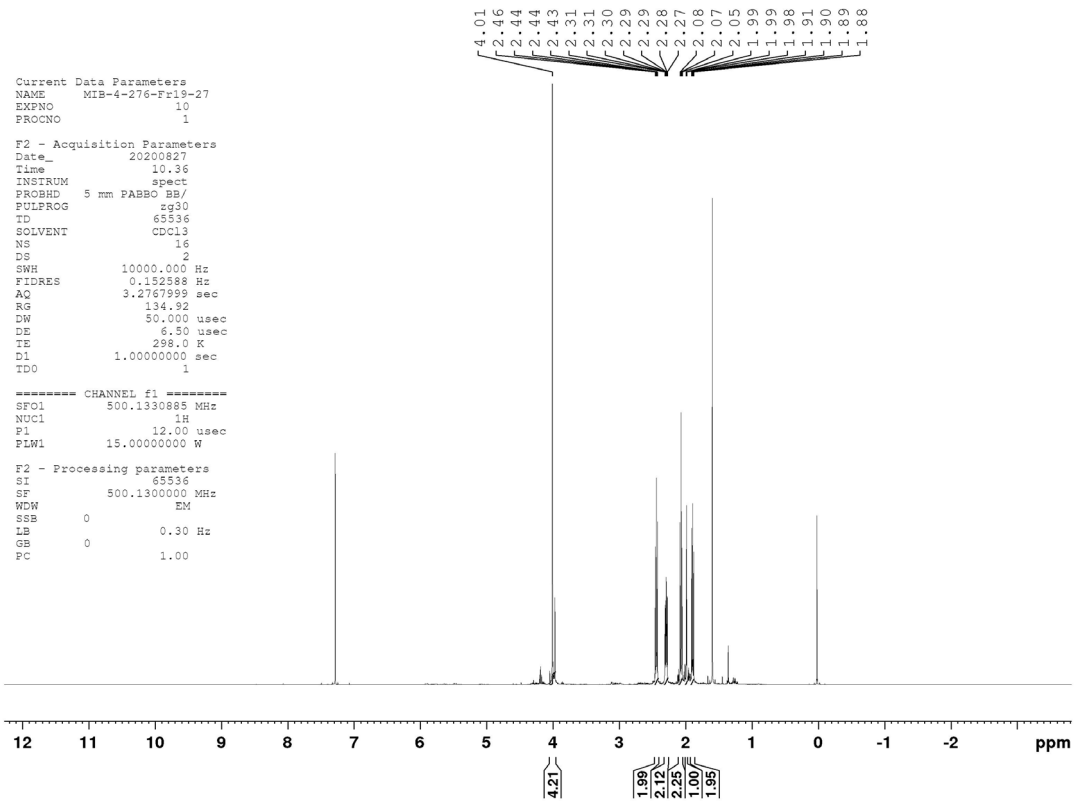
Compound S10

^{1}H-NMR

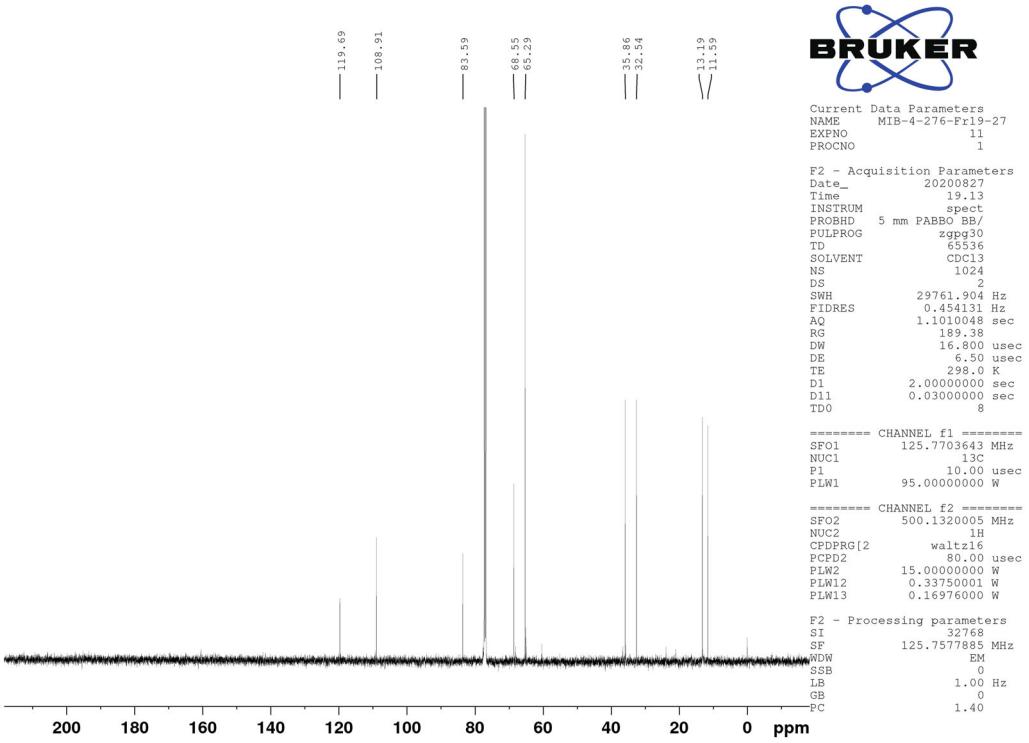


Compound S13

^{1}H-NMR

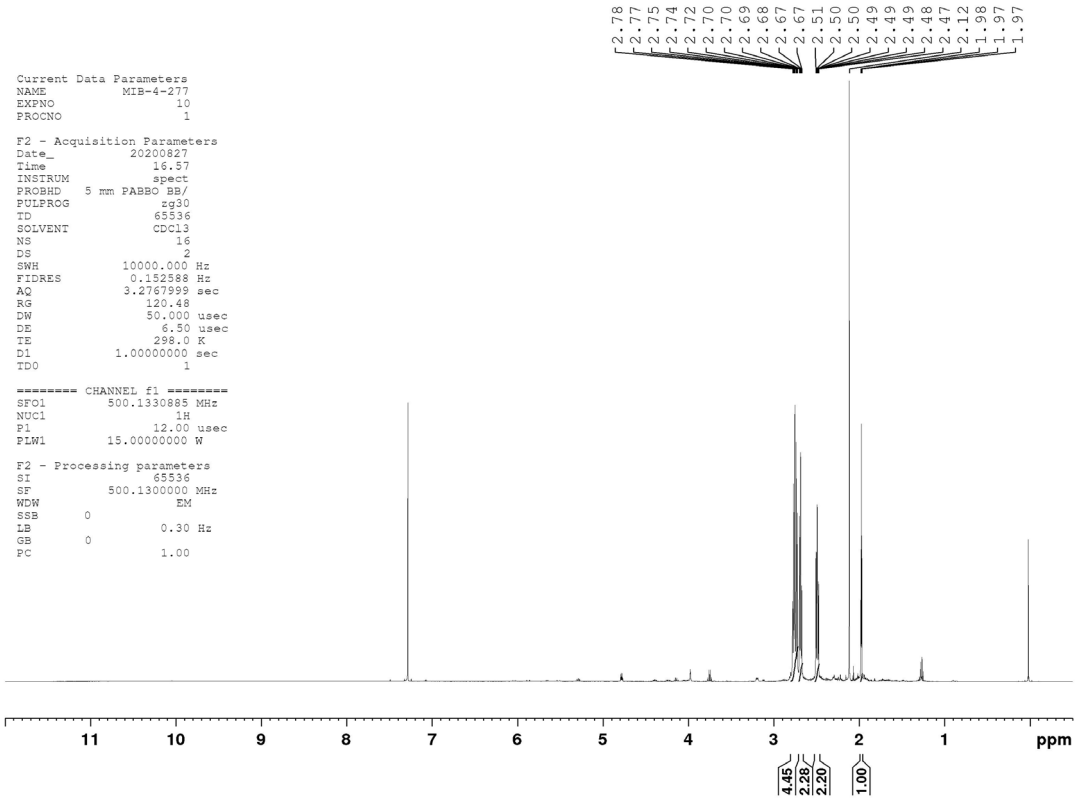


^{13}C-NMR

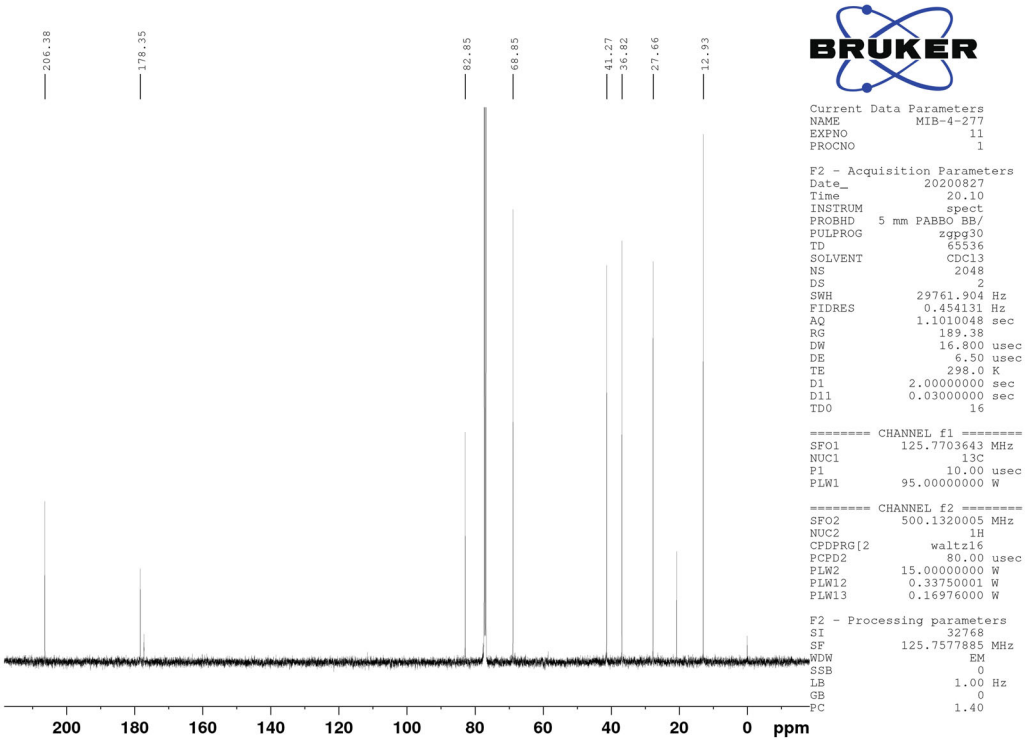


Compound S14

^{1}H-NMR

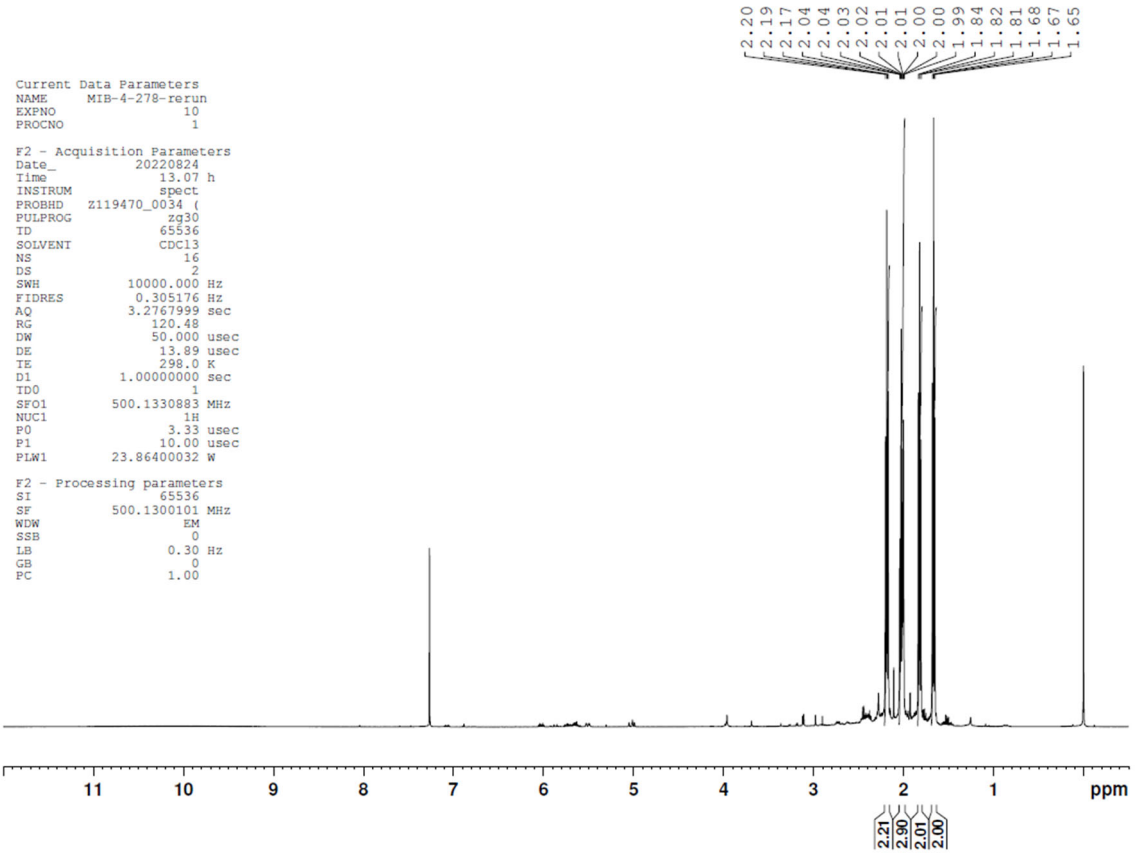


^{13}C-NMR

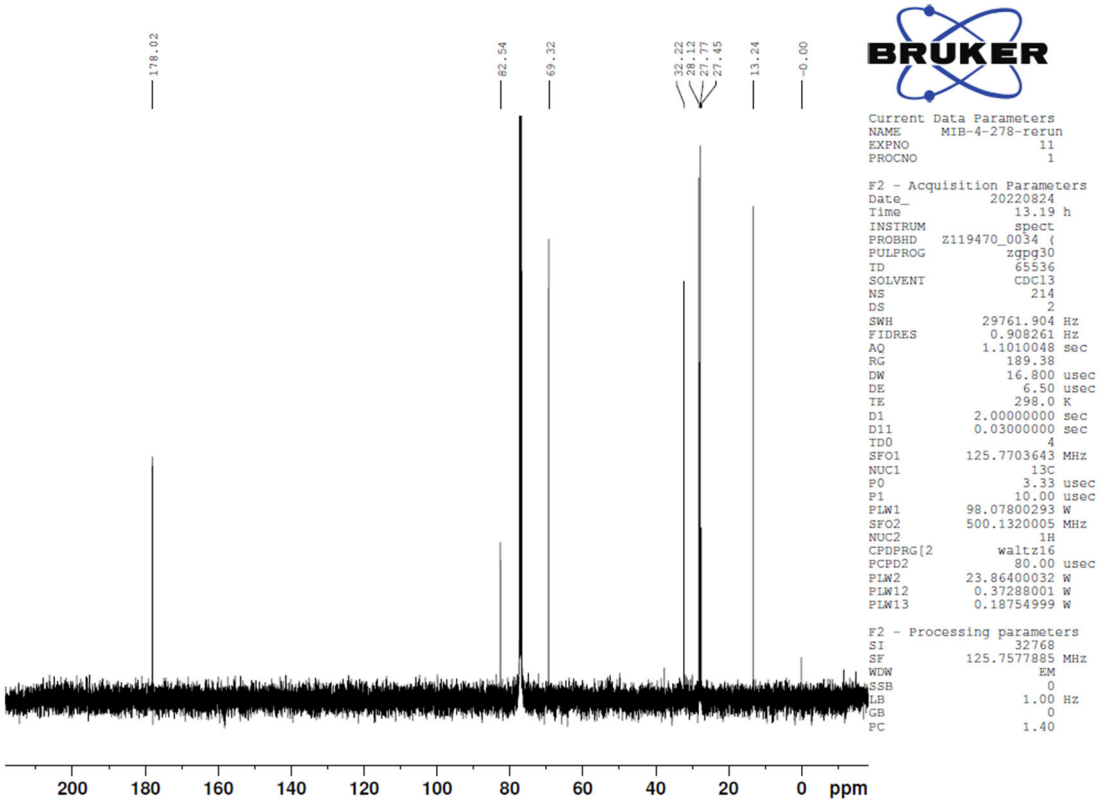


Compound S15

^{1}H-NMR



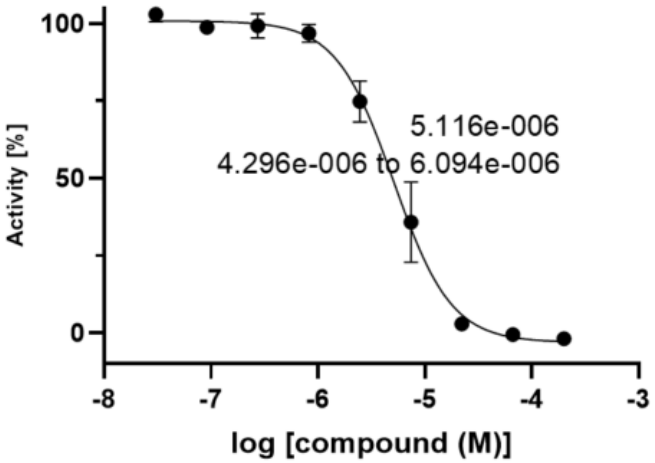
^{13}C-NMR



3.2. Biological assay results

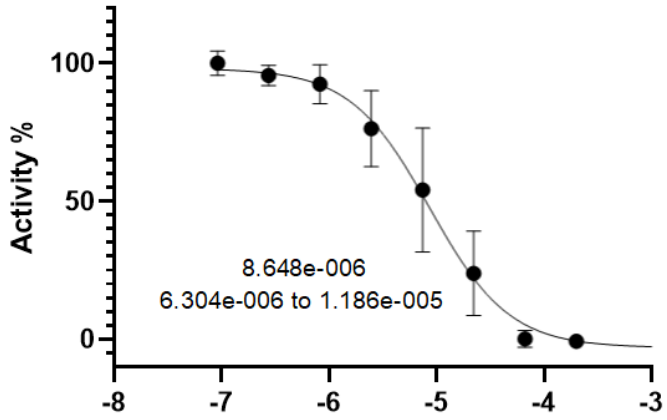
3.2.1.SENP1-SUMO1-AMC

Compound 11 screening library

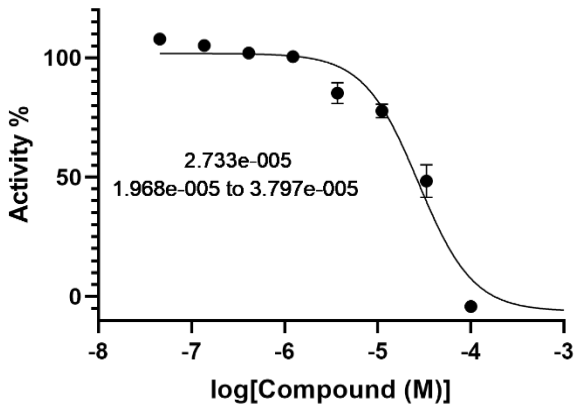


Conc log[M]	%	%
-3.70	-1.5	-2.4
-4.18	-0.9	-0.3
-4.65	2.0	3.8
-5.13	44.9	26.6
-5.61	79.5	70.0
-6.08	98.8	94.7
-6.56	102.0	96.4
-7.04	99.4	98.0
DMSO	104.6	101.3

Compound 11 synthesised

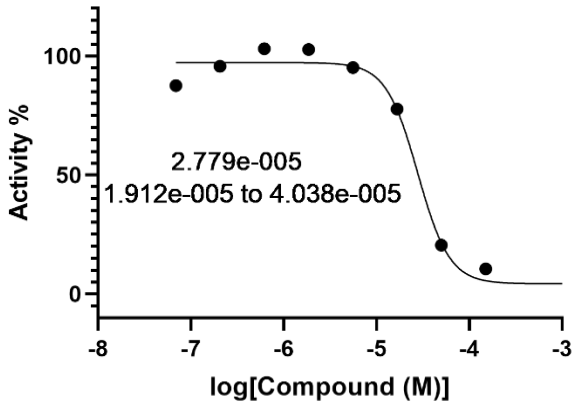


Compound 12



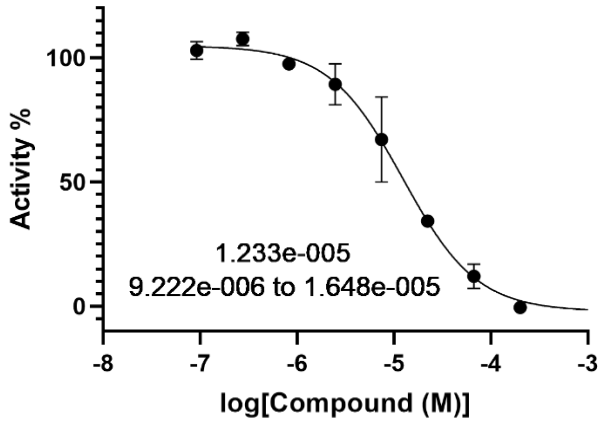
Conc log[M]	%	%
-3.82	-3.7	-4.7
-4.30	53.3	43.5
-4.78	79.7	75.7
-5.26	88.3	82.0
-5.73	100.2	100.7
-6.21	103.6	100.4
-6.69	104.4	105.8
-7.16	107.7	108.0
DMSO	97.3	97.3

Compound 13



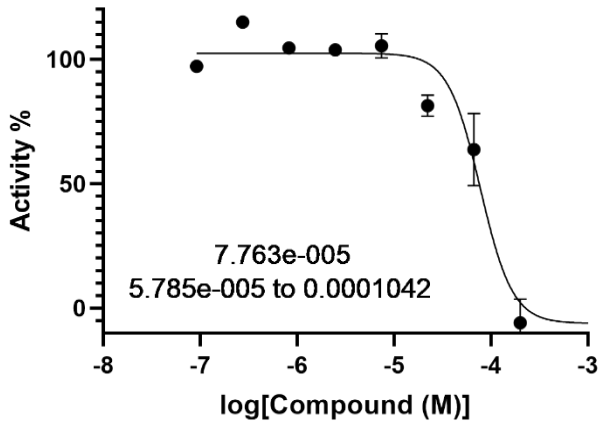
Conc log[M]	%
-3.82	10.6
-4.30	20.5
-4.78	77.7
-5.26	95.1
-5.73	102.7
-6.21	103.1
-6.69	95.7
-7.16	87.6
DMSO	97.3

Compound 23



Conc log[M]	%	%
-3.70	-0.8	-0.3
-4.18	15.5	8.5
-4.65	34.5	34.1
-5.13	79.2	55.0
-5.61	95.2	83.5
-6.08	98.8	96.2
-6.56	109.5	105.7
-7.04	105.5	100.4
DMSO	99.3	100.6

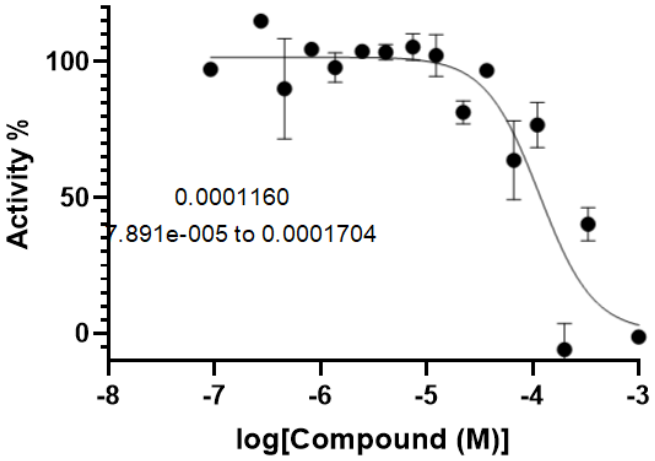
Compound 24



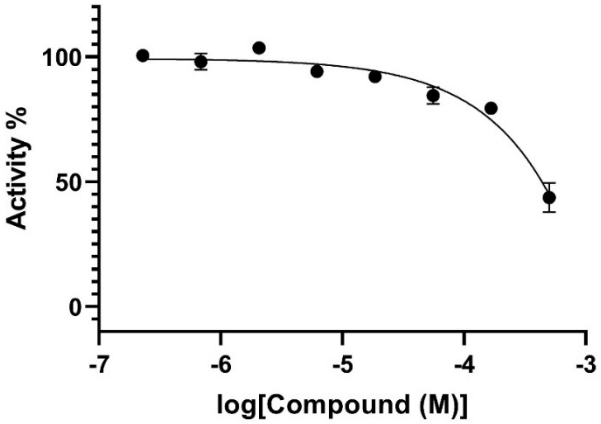
Conc log[M]	%	%
-3.70	-12.7	0.8
-4.18	74.0	53.4
-4.65	84.4	78.4
-5.13	108.9	102.0
-5.61	102.8	104.8
-6.08	103.0	106.1
-6.56	115.5	114.3
-7.04	98.0	96.4
DMSO	111.3	105.3

Fragments

Compound 15

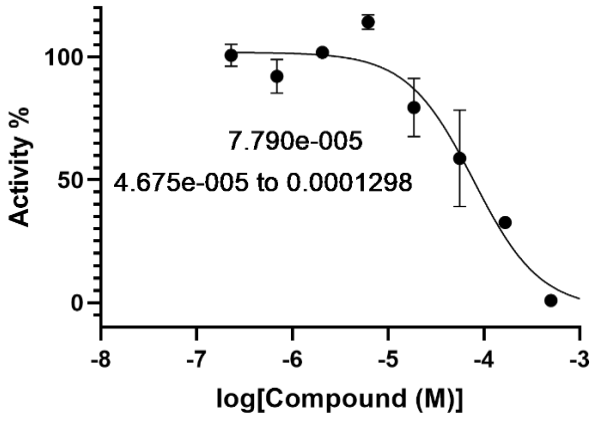


Compound 16



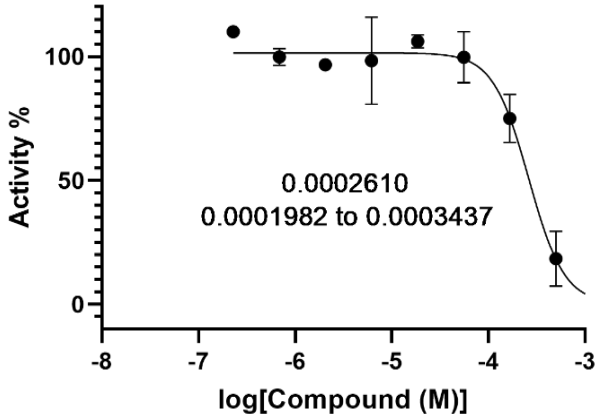
Conc log[M]	%	%
-3.30	39.6	47.8
-3.78	78.3	80.6
-4.26	82.2	86.9
-4.73	92.1	92.1
-5.21	95.1	93.3
-5.69	104.9	102.3
-6.16	100.4	95.7
-6.64	144.5	100.6
DMSO	103.2	102.1

Compound 26



Conc log[M]	%	%
-3.30	0.4	1.3
-3.78	31.0	34.3
-4.26	44.8	72.6
-4.73	71.0	87.8
-5.21	116.2	112.1
-5.69	101.7	102.1
-6.16	97.0	87.3
-6.64	103.8	97.5
DMSO	107.2	104.3

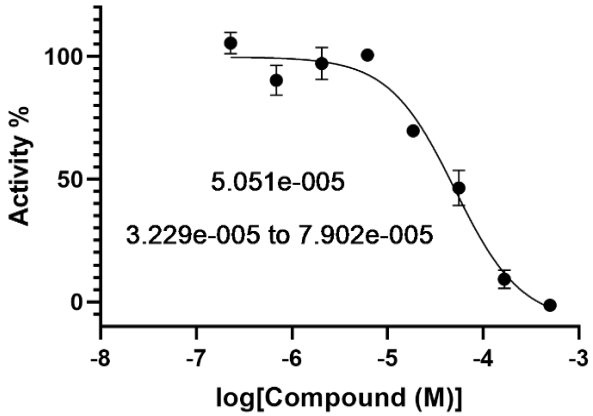
Compound 27



Conc log[M]	%	%
-3.30	26.3	10.6
-3.78	81.8	68.1
-4.26	107.0	92.4
-4.73	107.9	104.3
-5.21	85.9	110.7
-5.69	95.8	97.5
-6.16	97.5	102.2
-6.64	110.0	76.9
DMSO	102.3	106.9

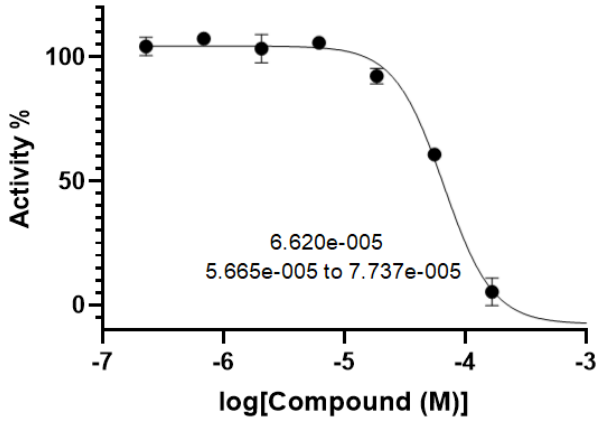
data point omitted

Compound 28



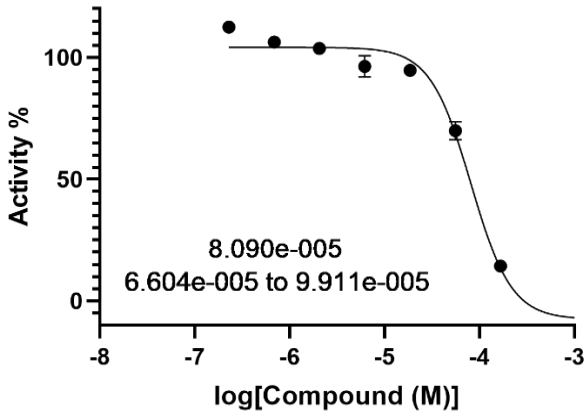
Conc log[M]	%	%
-3.30	-0.2	-2.7
-3.78	11.9	6.7
-4.26	51.5	41.3
-4.73	69.2	70.1
-5.21	98.8	102.4
-5.69	101.7	92.5
-6.16	94.6	86.0
-6.64	102.3	108.5
DMSO	93.2	104.7

Compound 29



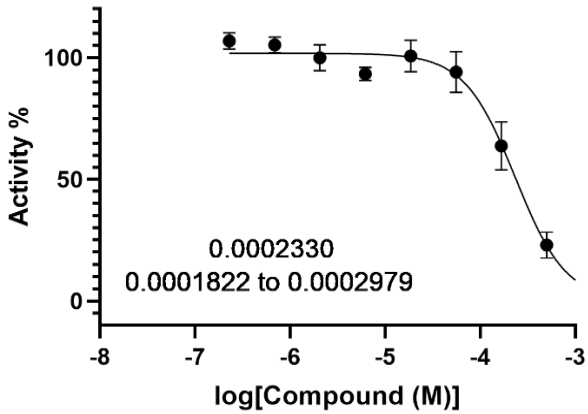
Conc log[M]	%	%
-3.30	-12.7	-14.7
-3.78	1.4	9.2
-4.26	60.7	60.7
-4.73	90.1	94.6
-5.21	104.6	106.8
-5.69	99.3	107.4
-6.16	106.1	108.6
-6.64	101.6	106.9
DMSO	105.3	102.8

Compound 30



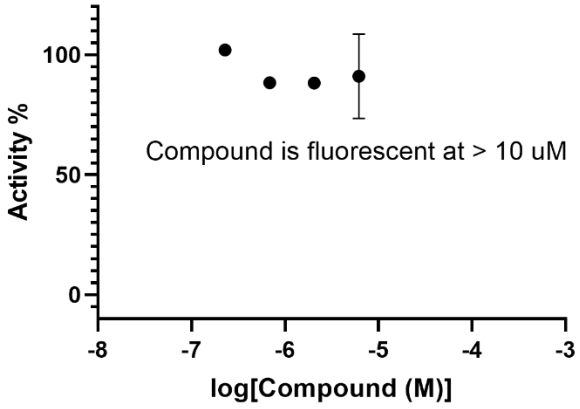
Conc log[M]	%	%
-3.30	-12.6	-14.7
-3.78	15.1	13.6
-4.26	72.5	67.2
-4.73	94.1	95.4
-5.21	99.4	93.2
-5.69	103.5	103.8
-6.16	106.3	106.4
-6.64	112.7	112.2
DMSO	107.4	99.6

Compound 31



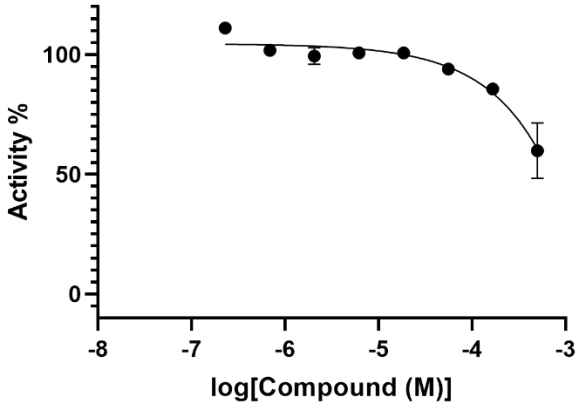
Conc log[M]	%	%
-3.30	19.3	26.8
-3.78	56.7	70.7
-4.26	88.1	100.0
-4.73	96.0	105.2
-5.21	91.3	95.2
-5.69	96.2	103.6
-6.16	102.9	107.6
-6.64	104.5	109.2
DMSO	100.0	112.3

Compound 32



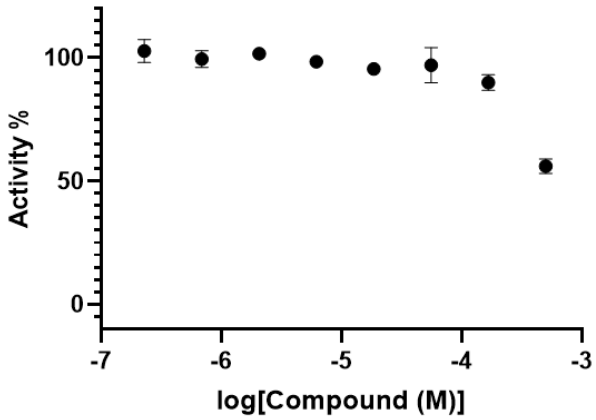
Conc log[M]	%	%
-3.30	fluorescent	
-3.78	fluorescent	
-4.26	fluorescent	
-4.73	fluorescent	
-5.21	103.5	78.5
-5.69	89.3	87.0
-6.16	90.0	86.7
-6.64	103.3	100.5
DMSO	107.4	99.6

Compound 33



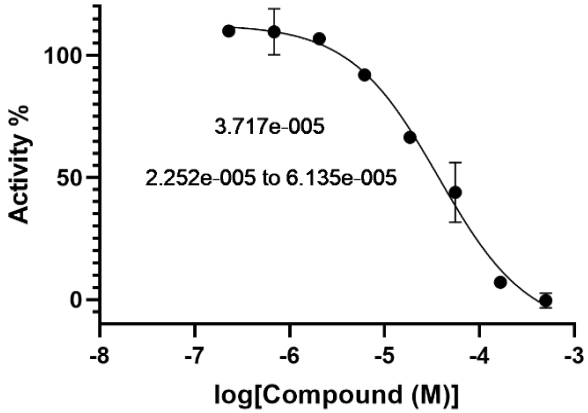
Conc log[M]	%	%
-3.30	51.6	68.1
-3.78	83.9	87.3
-4.26	92.1	95.7
-4.73	99.4	101.9
-5.21	101.2	100.1
-5.69	101.8	96.9
-6.16	101.7	101.9
-6.64	110.1	112.1
DMSO	103.4	99.2

Compound 34



Conc log[M]	%	%
-3.30	58.1	54.0
-3.78	87.6	92.2
-4.26	91.9	102.1
-4.73	95.9	95.0
-5.21	98.1	98.7
-5.69	103.1	100.1
-6.16	97.1	101.9
-6.64	106.1	99.4
DMSO	97.3	103.7

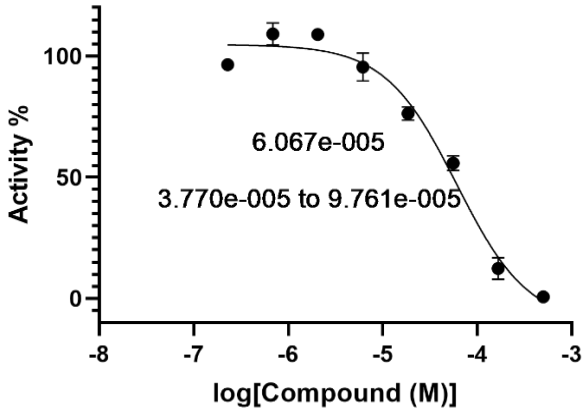
Compound 35



Conc log[M]	%	%
-3.30	1.8	-2.6
-3.78	8.0	6.2
-4.26	52.6	35.2
-4.73	66.5	66.3
-5.21	32.1	92.0
-5.69	108.6	105.0
-6.16	116.3	102.9
-6.64	110.0	68.9
DMSO	112.3	103.4

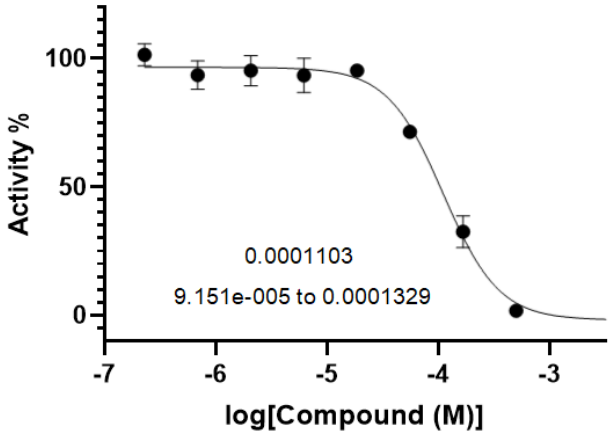
data point omitted

Compound 36



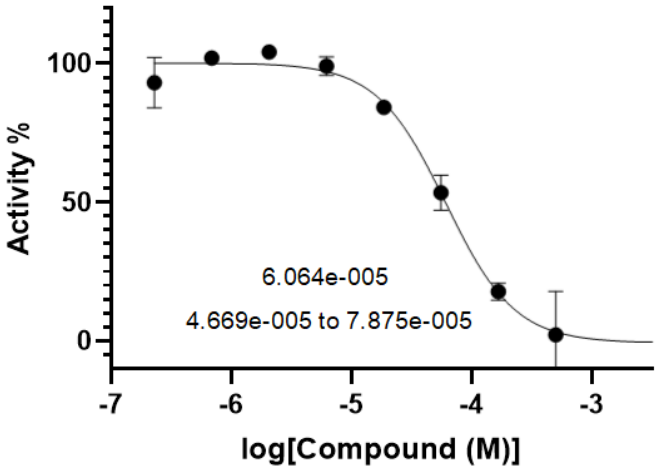
Conc log[M]	%	%
-3.30	-0.5	1.9
-3.78	9.3	15.5
-4.26	58.0	53.7
-4.73	74.4	78.2
-5.21	99.5	91.4
-5.69	108.4	109.3
-6.16	112.4	105.9
-6.64	95.3	97.5
DMSO	98.3	105.0

Compound 37



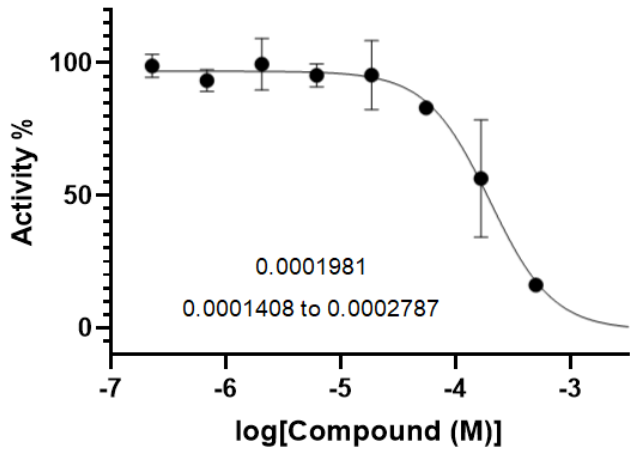
Conc log[M]	%	%
-3.30	2.4	1.1
-3.78	28.2	37.0
-4.26	69.6	73.3
-4.73	94.5	95.9
-5.21	98.1	88.8
-5.69	99.5	91.1
-6.16	97.4	89.6
-6.64	98.4	104.5
DMSO	100.2	97.8

Compound 38



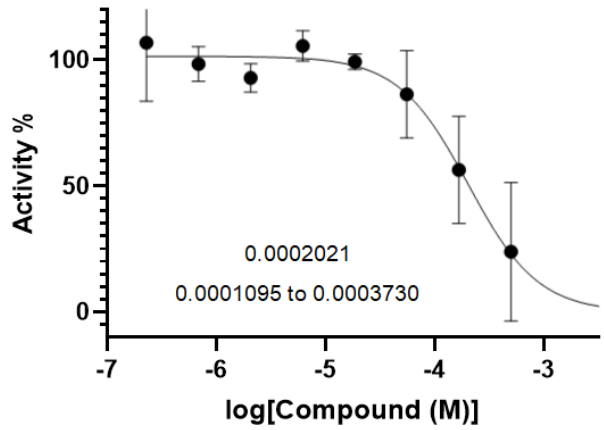
Conc log[M]	%	%
-3.30	13.3	-8.9
-3.78	19.9	15.6
-4.26	57.9	49.0
-4.73	83.1	85.3
-5.21	101.4	96.6
-5.69	104.4	103.8
-6.16	100.8	103.1
-6.64	99.5	86.7
DMSO	102.2	95.4

Compound 39



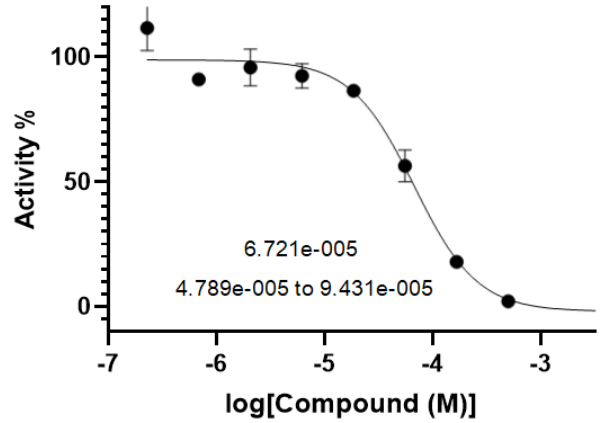
Conc log[M]	%	%
-3.30	14.4	17.9
-3.78	40.7	71.9
-4.26	84.1	81.8
-4.73	86.1	104.6
-5.21	92.2	98.4
-5.69	92.6	106.4
-6.16	90.4	96.3
-6.64	101.9	95.8
DMSO	97.5	95.4

Compound 40



Conc log[M]	%	%
-3.30	43.3	4.4
-3.78	71.3	41.3
-4.26	98.6	74.0
-4.73	97.1	101.4
-5.21	109.8	101.3
-5.69	88.9	96.8
-6.16	103.3	93.5
-6.64	123.2	90.5
DMSO	97.5	95.4

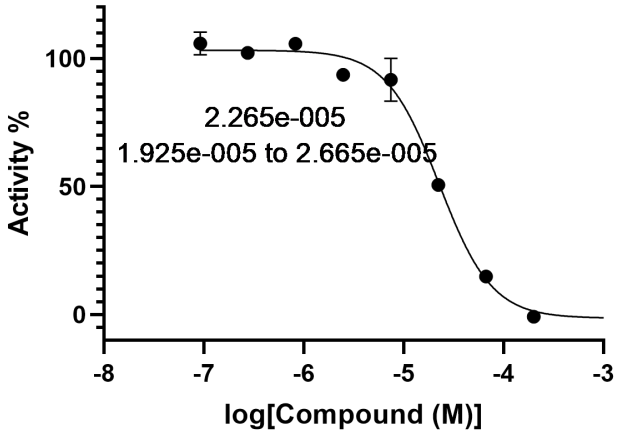
Compound 41



Conc log[M]	%	%
-3.30	0.9	3.3
-3.78	17.2	18.6
-4.26	51.8	60.9
-4.73	85.5	87.5
-5.21	89.0	95.9
-5.69	90.5	101.0
-6.16	92.2	89.7
-6.64	105.2	118.0
DMSO	103.2	107.5

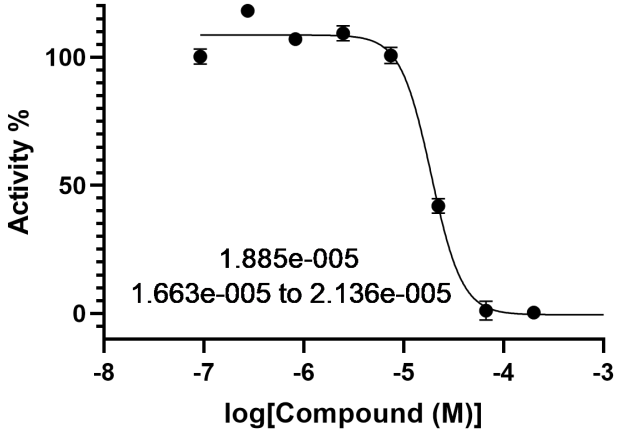
Tetrazol modifications

Compound 44



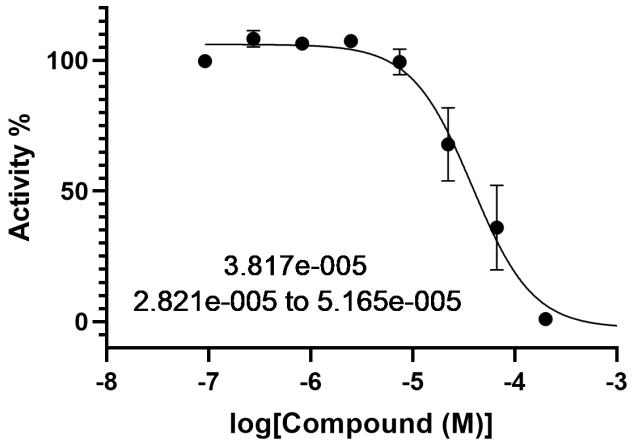
Conc log[M]	%	%
-3.70	-0.8	-0.9
-4.18	14.3	15.5
-4.65	51.7	49.5
-5.13	85.8	97.6
-5.61	95.5	91.8
-6.08	106.9	104.6
-6.56	100.7	103.7
-7.04	102.7	109.0
DMSO	104.0	106.3

Compound 45



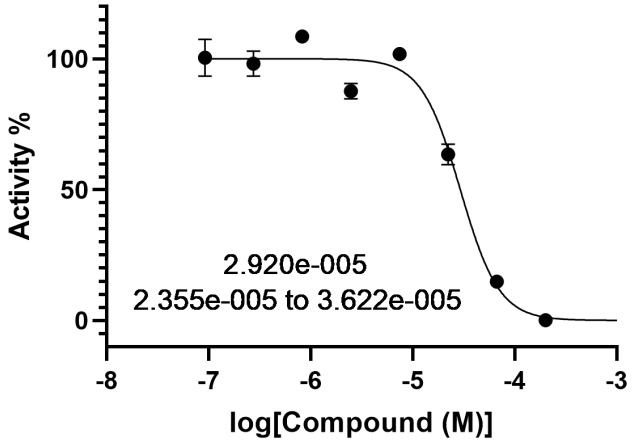
Conc log[M]	%	%
-3.70	-0.2	0.9
-4.18	3.7	-1.6
-4.65	44.0	40.0
-5.13	98.4	102.8
-5.61	107.3	111.4
-6.08	106.9	107.3
-6.56	118.6	117.7
-7.04	102.4	98.2
DMSO	100.2	107.3

Compound 46



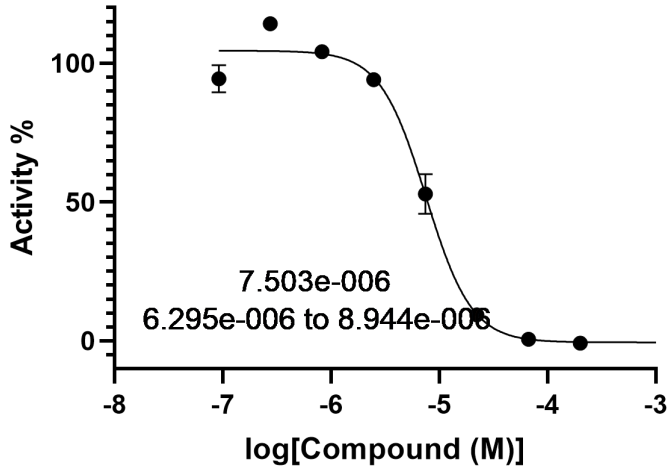
Conc log[M]	%	%
-3.70	0.4	1.5
-4.18	47.5	24.6
-4.65	77.7	57.9
-5.13	102.8	95.9
-5.61	107.4	107.3
-6.08	107.6	105.1
-6.56	110.5	106.0
-7.04	100.9	98.4
DMSO	98.1	103.4

Compound 47



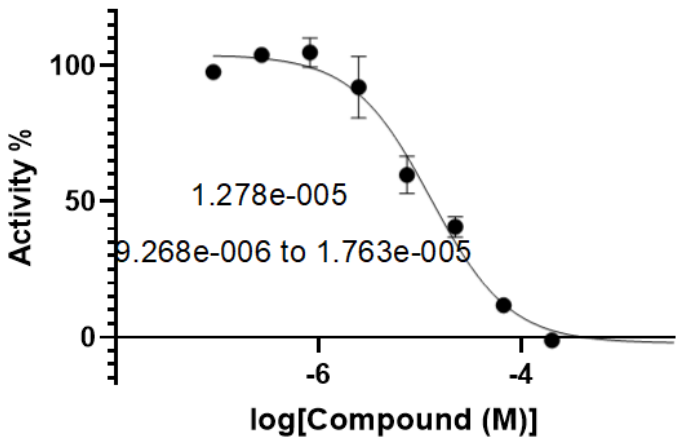
Conc log[M]	%	%
-3.70	0.1	0.3
-4.18	13.0	16.6
-4.65	60.7	66.3
-5.13	101.7	102.1
-5.61	85.6	89.7
-6.08	109.9	107.2
-6.56	94.8	101.6
-7.04	105.4	95.5
DMSO	103.0	97.8

Compound 48



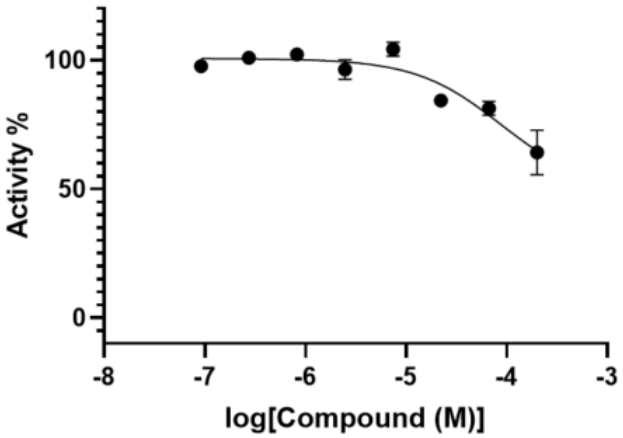
Conc log[M]	%	%
-3.70	-1.3	-0.5
-4.18	0.1	0.9
-4.65	10.6	8.1
-5.13	47.8	58.0
-5.61	95.4	92.6
-6.08	103.9	104.4
-6.56	114.9	113.6
-7.04	90.9	97.9
DMSO	94.3	97.8

Compound 49



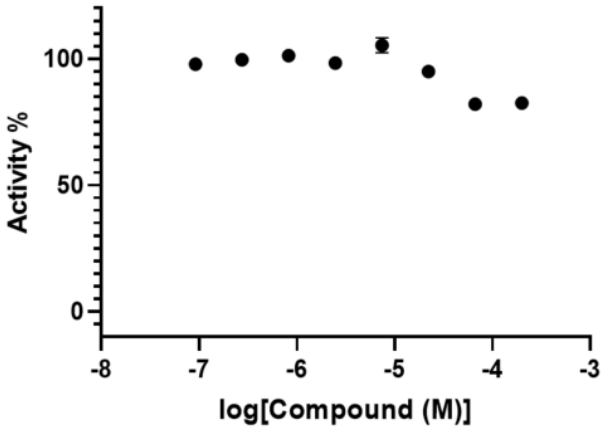
Conc log[M]	%	%
-3.70	-1.1	-1.3
-4.18	10.5	12.8
-4.65	37.9	43.2
-5.13	64.5	54.7
-5.61	100.1	84.0
-6.08	108.5	101.0
-6.56	104.5	103.1
-7.04	99.4	95.8
DMSO	106.7	102.5

Compound 50



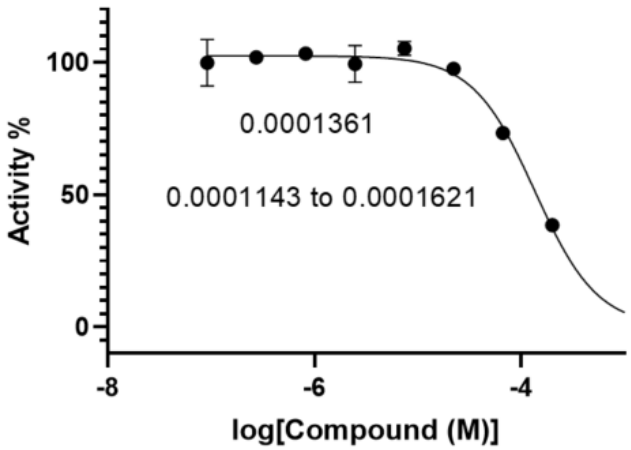
Conc log[M]	%	%
-3.70	58.1	70.3
-4.18	79.3	83.2
-4.65	84.9	83.7
-5.13	102.3	106.1
-5.61	93.6	99.1
-6.08	101.2	103.3
-6.56	101.4	100.3
-7.04	96.3	99.0
DMSO	104.0	106.3

Compound 51



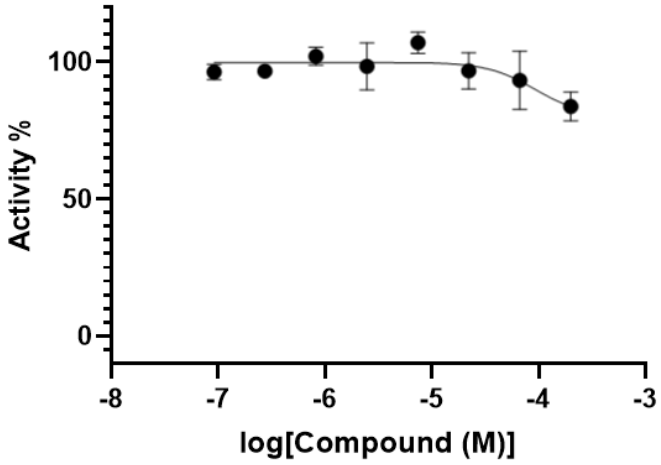
Conc log[M]	%	%
-3.70	82.1	82.8
-4.18	82.9	81.2
-4.65	96.6	93.2
-5.13	107.4	103.1
-5.61	99.6	97.0
-6.08	102.5	99.8
-6.56	99.3	99.8
-7.04	97.8	97.9
DMSO	104.0	106.3

Compound 52



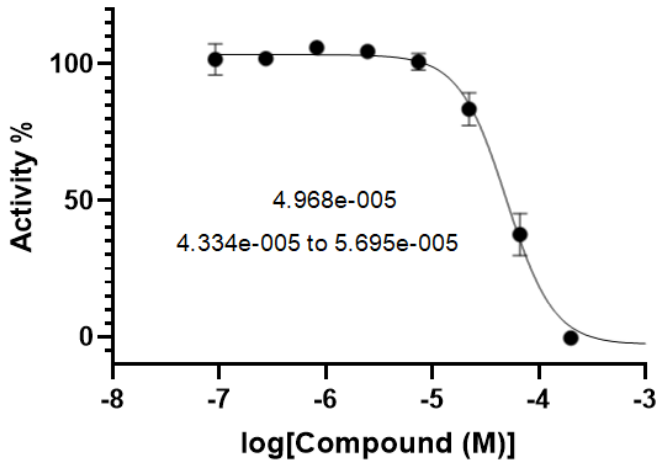
Conc log[M]	%	%
-3.70	37.4	39.4
-4.18	72.0	74.4
-4.65	97.6	97.5
-5.13	107.0	103.3
-5.61	104.3	94.5
-6.08	103.3	103.3
-6.56	101.1	102.6
-7.04	106.0	93.5
DMSO	104.0	106.3

Compound 53



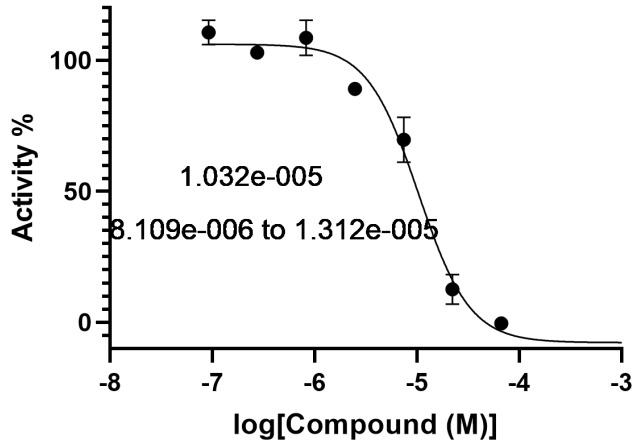
Conc log[M]	%	%
-3.70	80.1	87.5
-4.18	85.8	100.8
-4.65	92.0	101.4
-5.13	104.2	109.8
-5.61	92.3	104.5
-6.08	99.7	104.4
-6.56	95.9	97.5
-7.04	94.4	98.3
DMSO	104.0	106.3

Compound 54



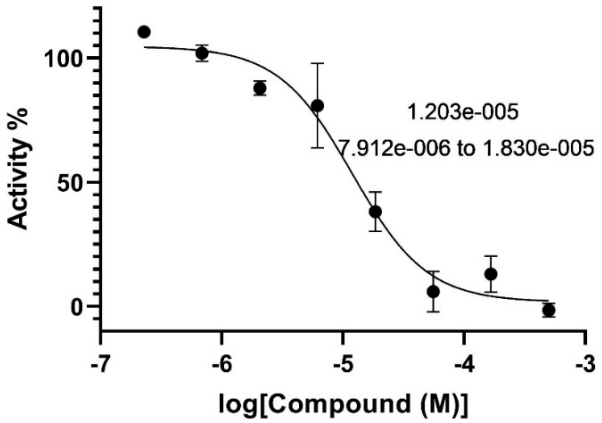
Conc log[M]	%	%
-3.70	-1.7	1.0
-4.18	42.9	32.0
-4.65	87.6	79.2
-5.13	102.9	98.6
-5.61	103.4	105.8
-6.08	105.0	106.8
-6.56	101.2	102.8
-7.04	97.5	105.7
DMSO	102.3	106.7

Compound 55



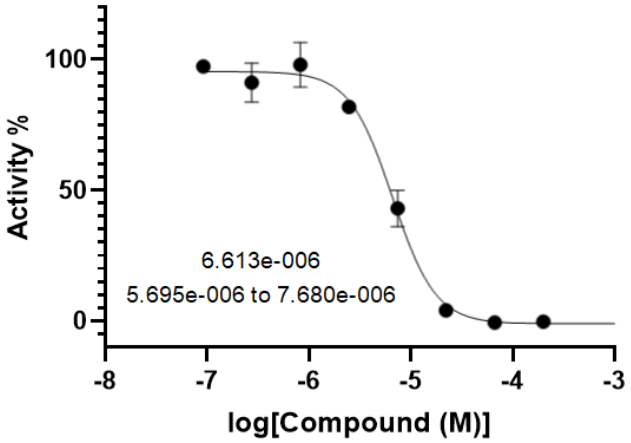
Conc log[M]	%	%
-3.70	-16.1	-16.3
-4.18	-0.2	-0.6
-4.65	8.6	16.6
-5.13	75.7	63.6
-5.61	88.7	89.5
-6.08	103.9	113.3
-6.56	104.5	101.3
-7.04	113.9	107.2
DMSO	106.3	100.8

Compound 56



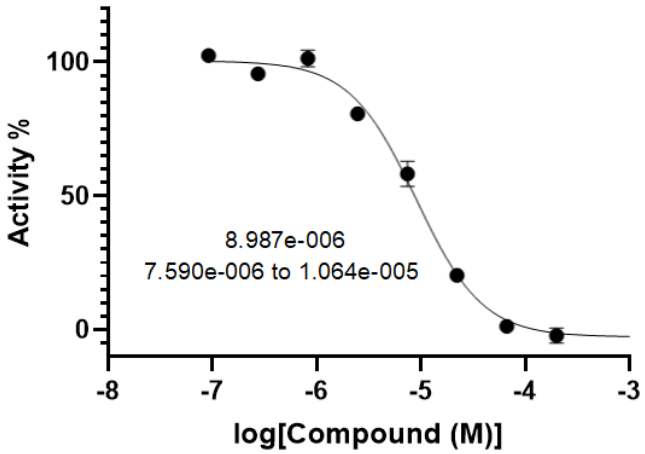
Conc log[M]	%	%
-3.30	-3.4	0.4
-3.78	7.8	18.2
-4.26	0.2	11.8
-4.73	43.7	32.5
-5.21	68.8	92.8
-5.69	85.9	89.9
-6.16	104.3	99.7
-6.64	111.4	109.6
DMSO	97.9	100.4

Compound 57



Conc log[M]	%	%
-3.70	1.1	-1.7
-4.18	-0.4	-0.8
-4.65	4.1	3.9
-5.13	47.9	38.1
-5.61	80.4	83.2
-6.08	104.1	91.9
-6.56	96.4	85.8
-7.04	98.6	95.9
DMSO	102.3	106.7

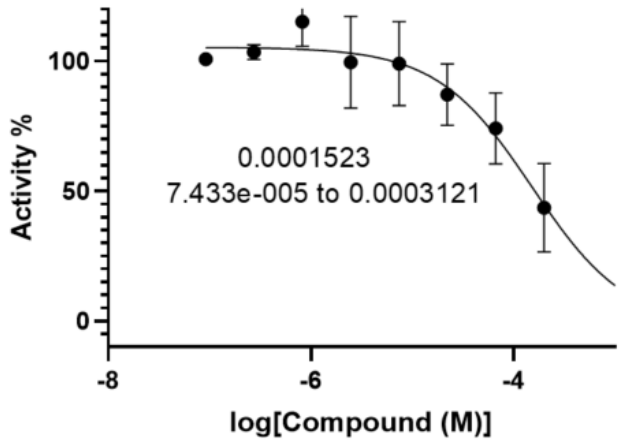
Compound 7



Conc log[M]	%	%
-3.70	-4.3	-0.3
-4.18	1.0	1.4
-4.65	21.4	19.2
-5.13	61.5	54.8
-5.61	81.8	79.5
-6.08	99.1	103.5
-6.56	95.8	95.4
-7.04	102.6	102.1
DMSO	97.3	102.0

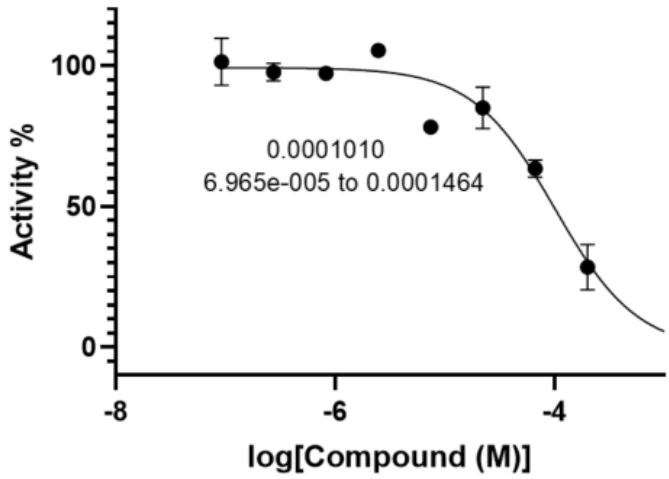
SI compounds

Compound S1



Conc log[M]	%	%
-3.70	55.6	31.4
-4.18	83.8	64.5
-4.65	95.6	78.8
-5.13	110.5	87.6
-5.61	112.1	87.0
-6.08	108.5	121.8
-6.56	101.5	105.5
-7.04	102.0	99.5
DMSO	103.2	99.7

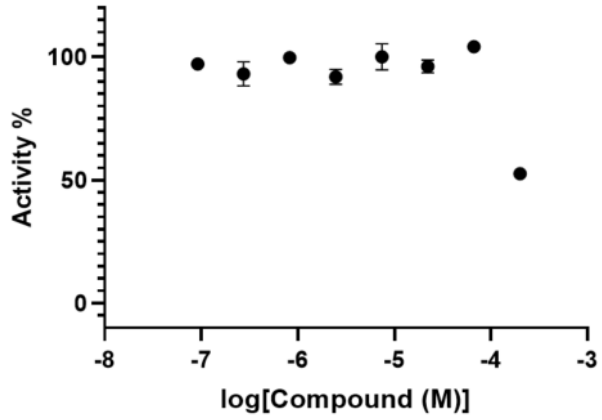
Compound S2



Conc log[M]	%	%
-3.70	34.1	22.8
-4.18	61.2	65.6
-4.65	79.7	90.2
-5.13	30.2	78.1
-5.61	105.7	104.8
-6.08	95.5	99.0
-6.56	95.4	99.8
-7.04	95.4	107.3
DMSO	103.2	99.7

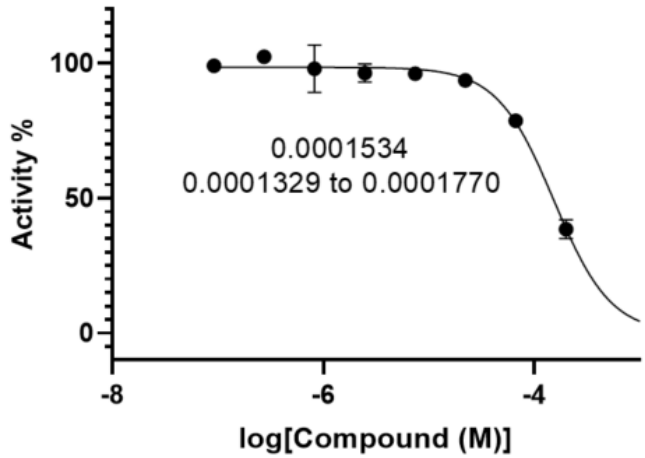
data point omitted

Compound S3



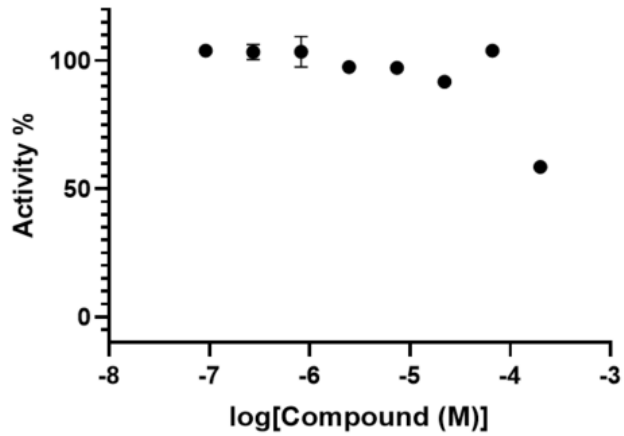
Conc log[M]	%	%
-3.70	51.4	53.7
-4.18	102.7	105.5
-4.65	97.9	94.2
-5.13	96.3	103.8
-5.61	94.1	89.7
-6.08	99.1	100.3
-6.56	89.6	96.6
-7.04	96.9	97.2
DMSO	98.4	101.2

Compound S4



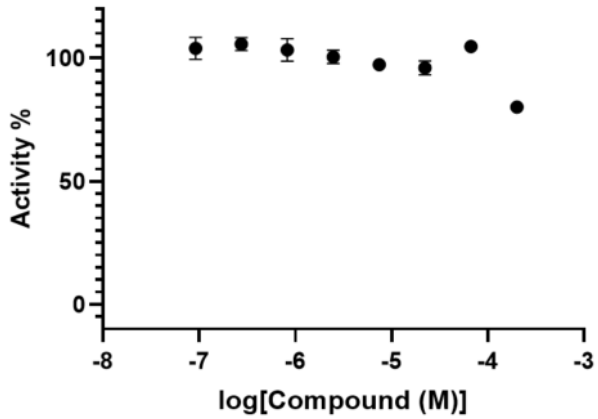
Conc log[M]	%	%
-3.70	41.0	36.0
-4.18	77.5	79.9
-4.65	95.2	92.1
-5.13	97.4	94.7
-5.61	98.7	94.0
-6.08	91.7	104.1
-6.56	104.0	100.7
-7.04	100.7	97.4
DMSO	98.4	101.2

Compound S5



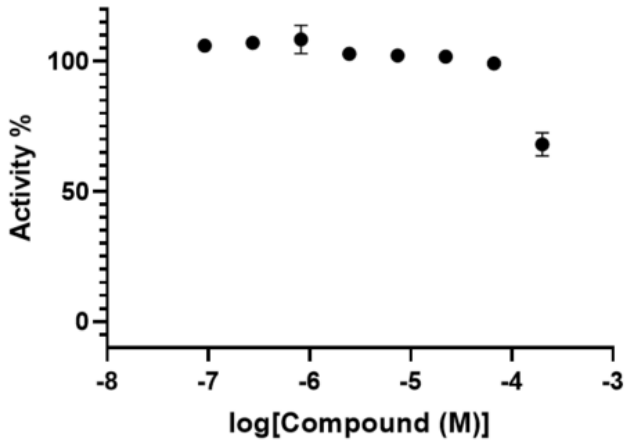
Conc log[M]	%	%
-3.70	57.6	59.4
-4.18	102.7	105.1
-4.65	93.5	90.1
-5.13	96.5	97.8
-5.61	98.2	96.8
-6.08	107.7	99.2
-6.56	105.5	101.3
-7.04	104.7	103.0
DMSO	98.4	101.2

Compound S6



Conc log[M]	%	%
-3.70	78.6	81.5
-4.18	105.9	103.5
-4.65	98.0	94.0
-5.13	99.1	95.6
-5.61	102.4	98.6
-6.08	106.5	100.1
-6.56	107.4	103.8
-7.04	107.1	100.8
DMSO	98.4	101.2

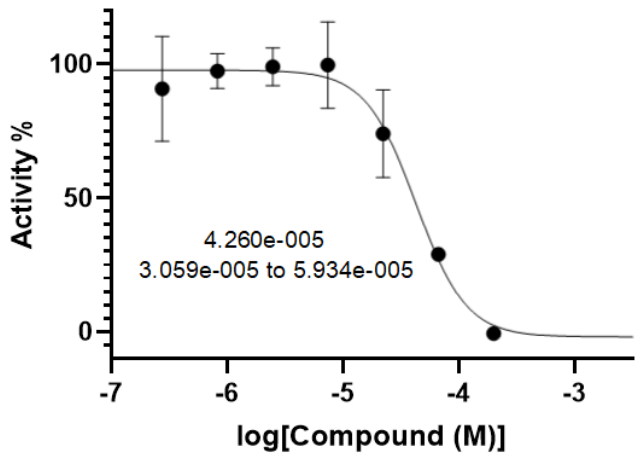
Compound S7



Conc log[M]	%	%
-3.70	64.8	71.2
-4.18	100.2	98.0
-4.65	99.9	103.5
-5.13	101.8	102.5
-5.61	104.2	101.5
-6.08	112.2	104.4
-6.56	107.2	107.0
-7.04	105.7	106.3
DMSO	98.4	101.2

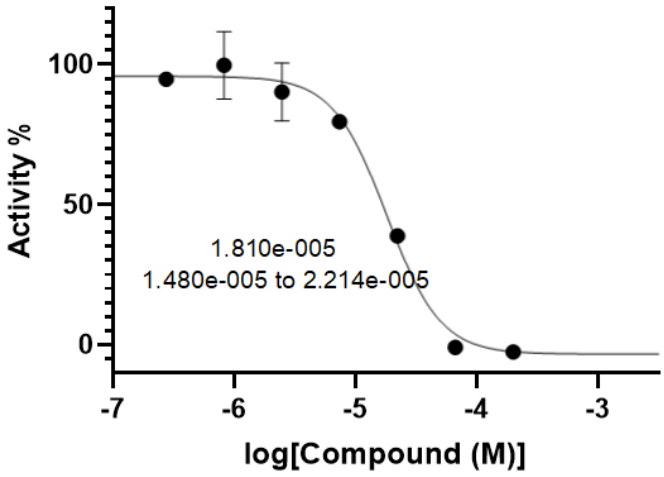
3.2.2.SENP1-SUMO2-AMC

Compound 11



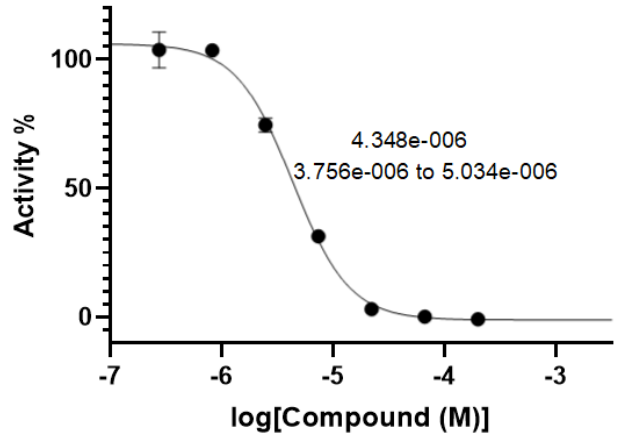
Conc log[M]	%	%
-3.70	-1.7	0.5
-4.18	30.6	27.2
-4.65	62.4	85.6
-5.13	88.3	111.1
-5.61	94.1	104.0
-6.08	102.1	92.8
-6.56	104.7	76.9
-7.04	102.9	97.5
DMSO	97.3	103.7

Compound 55



Conc log[M]	%	%
-3.70	-3.7	-1.5
-4.18	-0.8	-1.2
-4.65	38.6	39.0
-5.13	78.2	80.7
-5.61	82.9	97.4
-6.08	91.1	108.2
-6.56	93.1	96.3
-7.04	103.6	90.6
DMSO	95.3	98.7

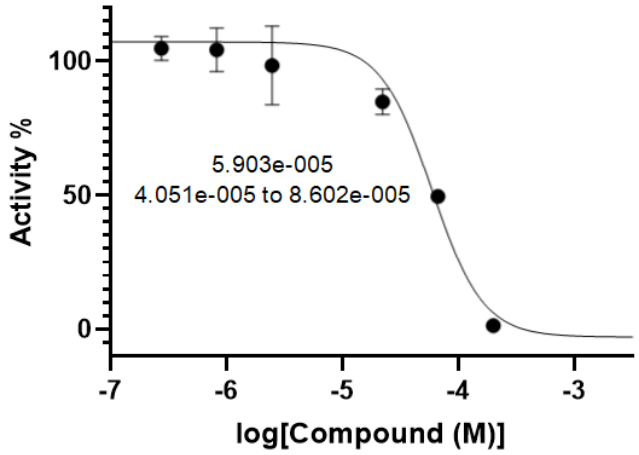
Compound 7



Conc log[M]	%	%
-3.82	-3.7	-4.7
-4.30	53.3	43.5
-4.78	79.7	75.7
-5.26	88.3	82.0
-5.73	100.2	100.7
-6.21	103.6	100.4
-6.69	104.4	105.8
-7.16	107.7	108.0
DMSO	97.3	97.3

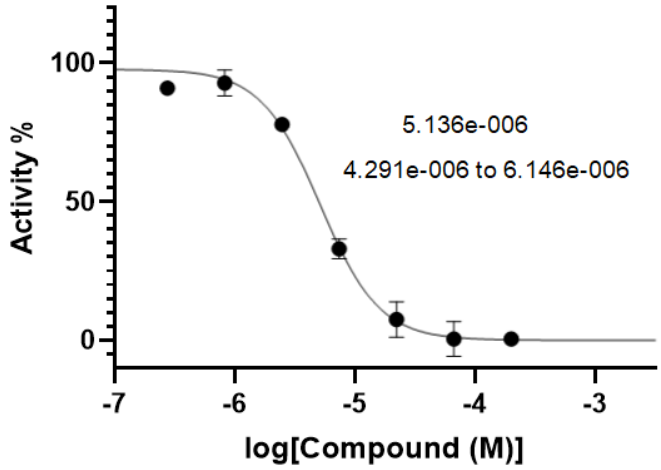
3.2.3.SENP1-SUMO3-AMC

4. Compound 11



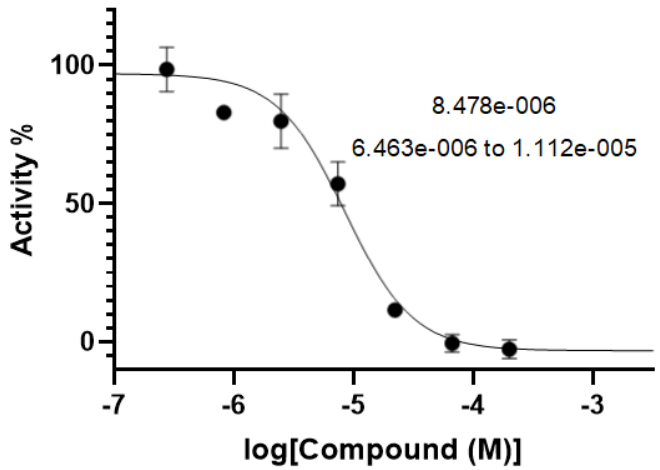
Conc log[M]	%	%
-3.70	0.4	2.2
-4.18	48.4	50.8
-4.65	81.5	88.2
-5.13	139.1	109.5
-5.61	88.0	108.8
-6.08	98.5	110.0
-6.56	107.9	101.6
-7.04	116.6	99.6
DMSO	105.4	109.3

Compound 55



Conc log[M]	%	%
-3.70	0.0	1.0
-4.18	5.0	-4.0
-4.65	12.0	3.0
-5.13	30.4	35.5
-5.61	79.5	76.1
-6.08	89.4	96.1
-6.56	89.6	92.2
-7.04	101.2	107.4
DMSO	102.4	96.9

Compound 7

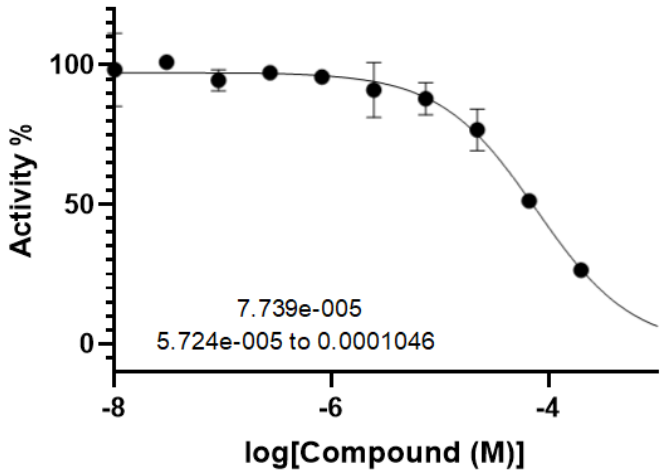


Conc log[M]	%	%
-3.70	-0.3	-5.0
-4.18	1.7	-2.8
-4.65	11.6	11.4
-5.13	62.7	51.4
-5.61	86.7	72.8
-6.08	137.2	82.9
-6.56	104.3	92.8
-7.04	100.4	103.2
DMSO	97.7	100.4

data point omitted

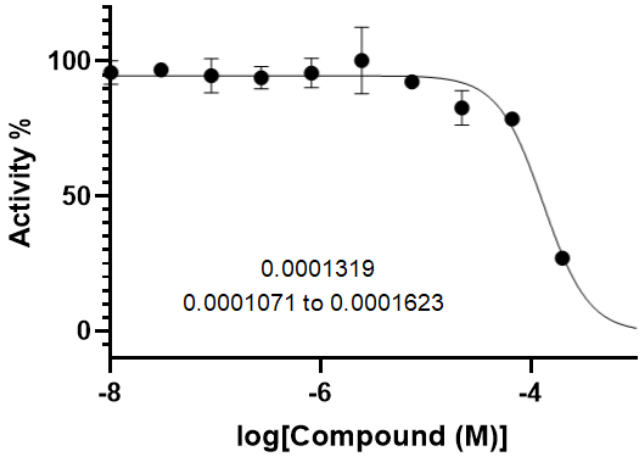
4.1.1.UCHL1

Compound 11



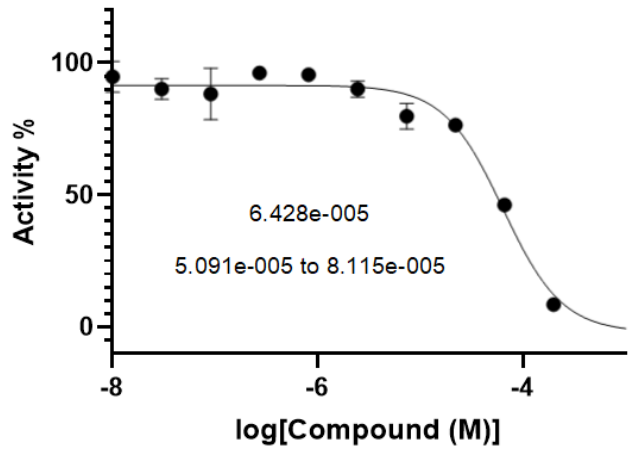
Conc log[M]	%	%
-3.70	26.2	26.7
-4.18	52.4	50.2
-4.65	82.0	71.4
-5.13	83.7	91.9
-5.61	98.0	84.1
-6.08	96.6	94.7
-6.56	98.9	95.5
-7.04	97.2	91.8
-7.52	102.23	99.83
-7.99	107.66	89.00

Compound 55



Conc log[M]	%	%
-3.70	26.4	27.6
-4.18	79.9	77.2
-4.65	87.2	78.2
-5.13	92.3	92.2
-5.61	91.5	109.0
-6.08	91.7	99.4
-6.56	90.9	96.7
-7.04	90.1	99.0
-7.52	97.70	95.80
-7.99	98.83	90.57

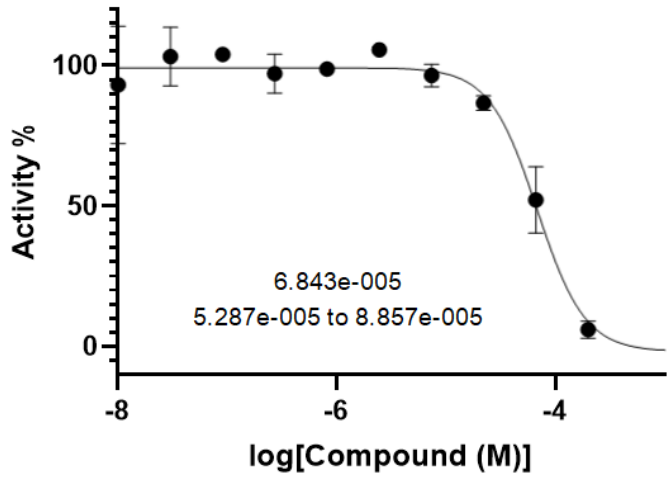
Compound 7



Conc log[M]	%	%
-3.70	7.1	9.8
-4.18	46.1	46.3
-4.65	75.3	77.6
-5.13	83.2	76.3
-5.61	92.3	87.9
-6.08	96.4	94.5
-6.56	95.3	96.8
-7.04	81.3	95.1
-7.52	87.29	92.89
-7.99	98.83	90.57

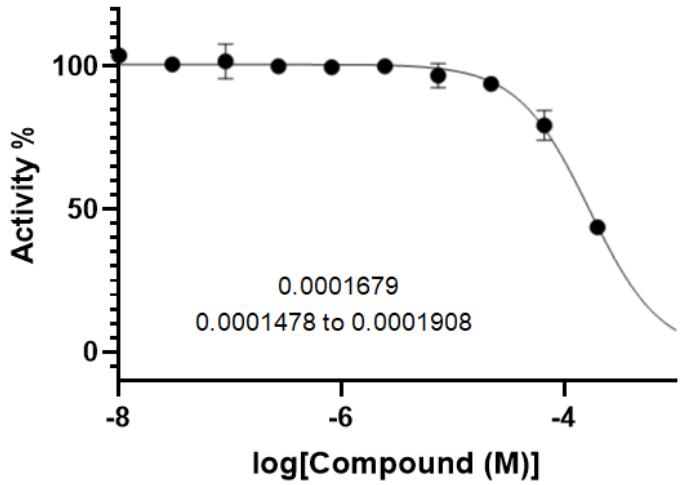
4.1.2. Ataxin-3

Compound 11



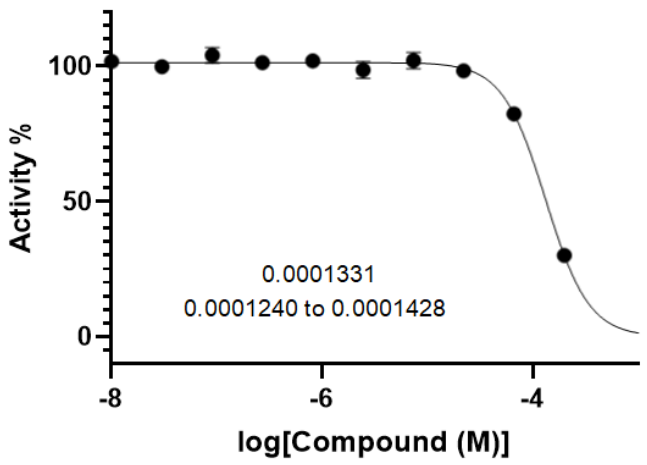
Conc log[M]	%	%
-3.70	8.1	3.9
-4.18	60.5	43.7
-4.65	88.5	84.7
-5.13	99.2	93.6
-5.61	105.5	
-6.08	98.1	99.3
-6.56	102.1	92.2
-7.04	104.8	102.9
-7.52	110.5	95.8
-7.99	78.3	107.8

Compound 55



Conc log[M]	%	%
-3.70	44.5	42.8
-4.18	75.7	83.0
-4.65	92.8	94.8
-5.13	93.8	99.8
-5.61	98.5	101.6
-6.08	98.8	100.6
-6.56	100.1	99.9
-7.04	97.4	106.1
-7.52	102.2	99.1
-7.99	103.0	104.5

Compound 7



Conc log[M]	%	%
-3.70	31.1	28.9
-4.18	82.8	82.0
-4.65	98.3	
-5.13	104.2	99.8
-5.61	100.8	96.3
-6.08	103.1	100.9
-6.56	102.3	100.4
-7.04	106.1	102.0
-7.52	99.2	100.4
-7.99	103.0	100.5