

Exploration of hydrazine-based small molecules as metal chelators for KDM4 inhibition

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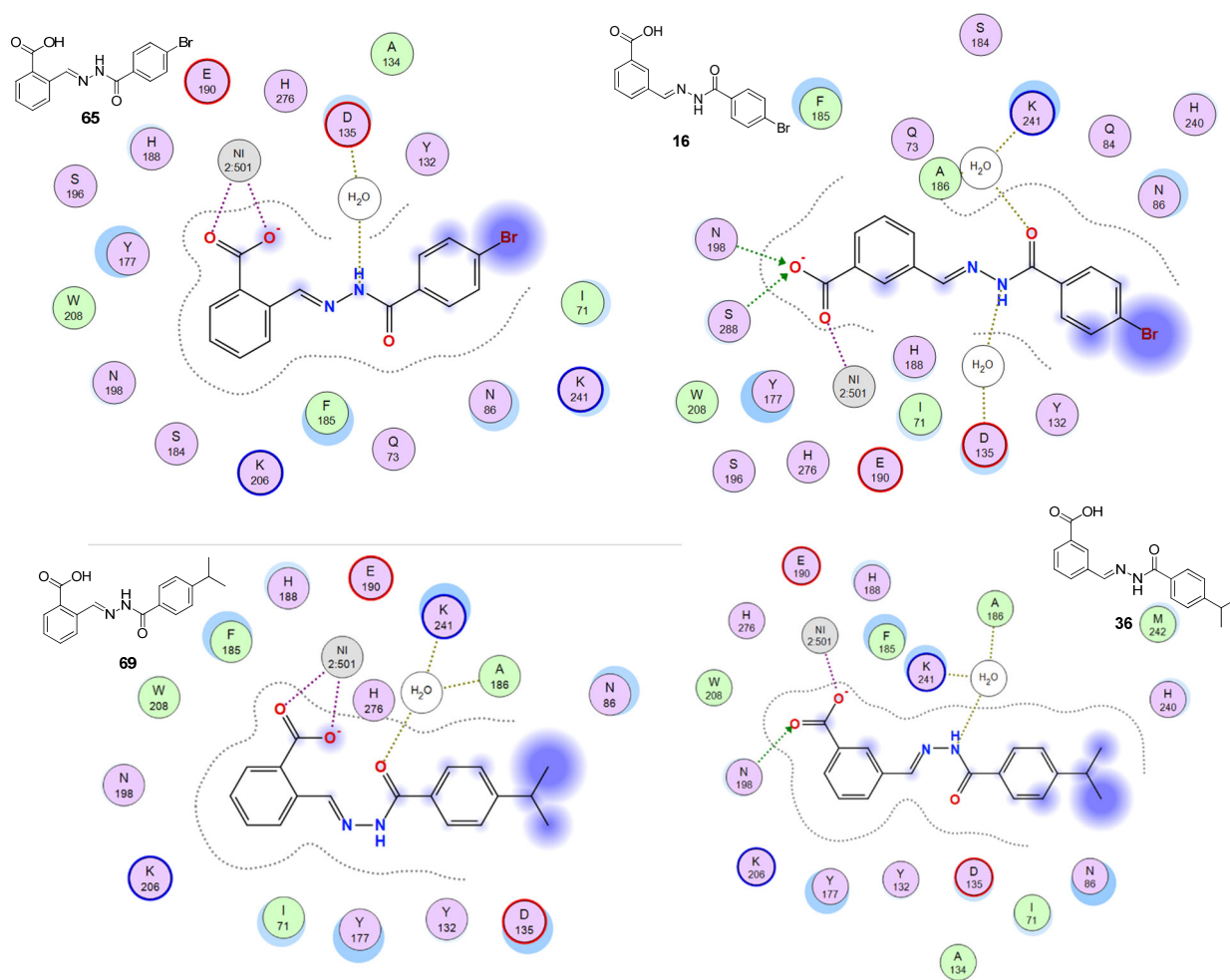
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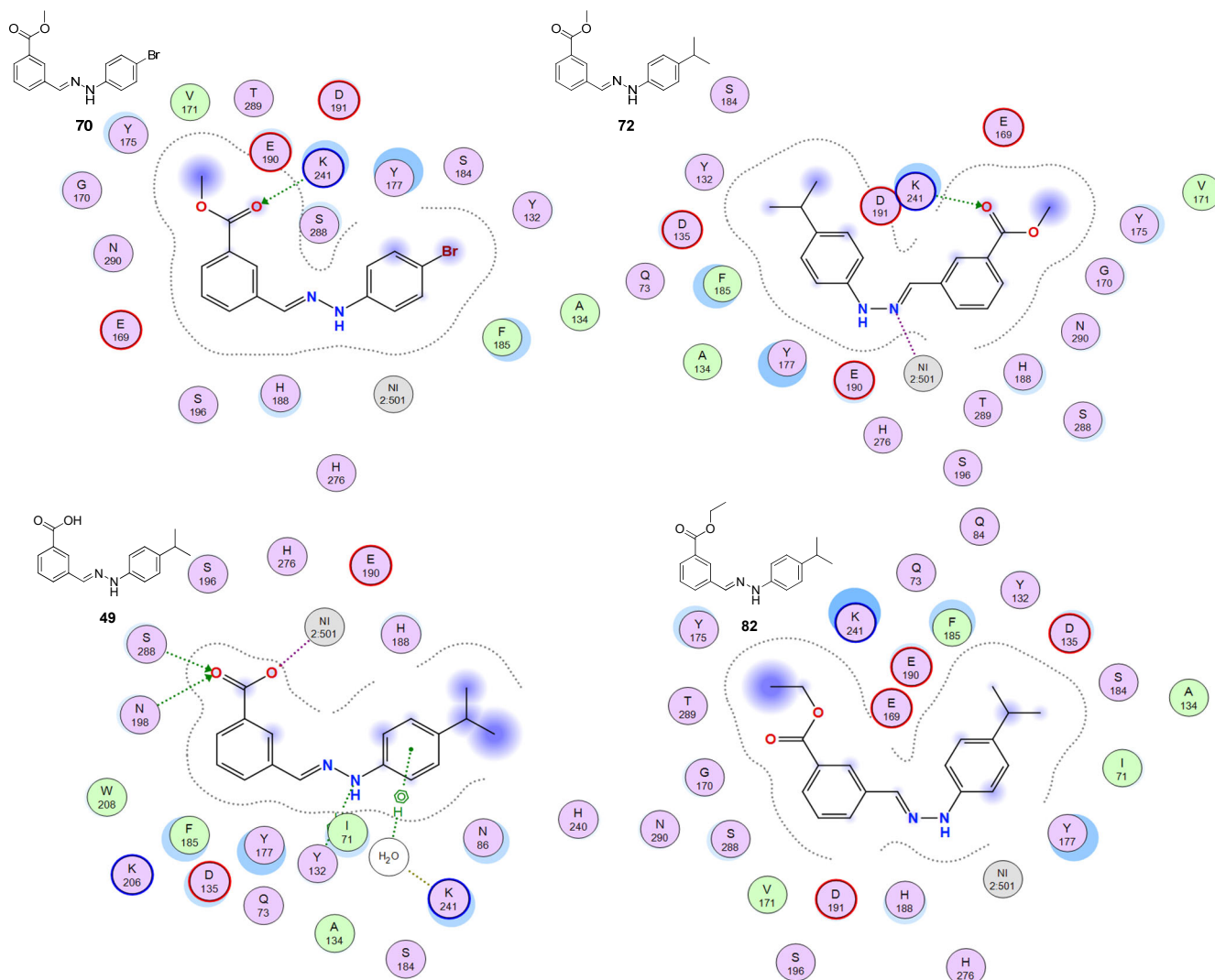
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Table S1. Selection of analogues from Library 1 that exhibited no KDM4A inhibitory activity.

Analogue	R ₁	R ₂	KDM4A activity at 20 μ M	KDM4A activity at 1 μ M
S1	H		97%	110%
S2	H		99%	105%
S3	H		104%	99%
S4	H		103%	95%
S5	H		98%	98%

Ligand interaction maps (Molecular Operating Environment)





Synthetic methods and characterisation

(*E*)-3-((2-carbamoylhydrazono)methyl)benzoic acid (9)

3-Formylbenzoic acid (300 mg, 2.0 mmol, 1.0 eq.) and semicarbazide dihydrochloride (444 mg, 4.0 mmol, 2.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and irradiated at 120 °C for 20 min. The reaction mixture was chilled at -20 °C for 19 h and filtered under vacuum. The crude solid was recrystallised from ethanol to afford the desired product as a white solid (170 mg, 35%). Mp 189-191 °C. ^1H NMR (600 MHz, DMSO- d_6) δ 13.04 (bs, 1H), 10.28 (s, 1H), 8.14 (s, 1H), 8.02 (d, J = 7.8 Hz, 1H), 7.91 (s, 1H), 7.90 (d, J = 7.8 Hz, 1H), 7.51 (t, J = 7.8 Hz, 1H), 6.48 (bs, 2H). ^{13}C NMR (151 MHz, DMSO- d_6) δ 167.1, 156.6, 138.5, 135.2, 131.4, 130.3, 129.6, 128.9, 127.4. IR (neat) ν_{max} : 3477 (N-H), 3151 (N-H), 3000 (O-H), 1703 (C=O), 1695 (C=O). UPLC-MS (80% Solvent B) t_{R} 1.167 min, (ESI-) m/z : 206 ($\text{C}_9\text{H}_9\text{N}_3\text{O}_3$) [M, 100%].

(*E*)-3-((2-(4-methoxybenzoyl)hydrazono)methyl)benzoic acid (10)

3-Formylbenzoic acid (108 mg, 0.7 mmol, 1.0 eq.) and 4-methoxybenzhydrazide (121 mg, 0.7 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and irradiated at 120 °C for 20 min. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (186

mg, 86%). Mp 317-319 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 13.15 (bs, 1H), 11.84 (s, 1H), 8.50 (s, 1H), 8.32 (s, 1H), 7.98 (d, *J* = 7.2 Hz, 1H), 7.92 (d, *J* = 7.8 Hz, 1H), 7.92 (d, *J* = 7.8 Hz, 2H), 7.59 (t, *J* = 7.8 Hz, 1H), 7.07 (d, *J* = 9.0 Hz, 2H), 3.84 (s, 3H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 167.0, 162.7, 162.1, 146.1, 135.0, 131.5, 131.4, 130.5, 129.6, 129.3, 127.3, 125.3, 113.8, 55.5. IR (neat) *v*_{max}: 3262 (N-H), 3000 (O-H), 2838 (O-CH₃), 1693 (C=O), 1690 (C=O). UPLC-MS (80% Solvent B) *t*_R 0.506 min, (ESI+) *m/z*: 299 (C₁₆H₁₅N₂O₄) [M+H, 100%]; (ESI-) *m/z*: 297 (C₁₆H₁₃N₂O₄) [M-H, 100%].

(*E*)-3-((2-(3-methoxybenzoyl)hydrazono)methyl)benzoic acid (11)

3-Formylbenzoic acid (102 mg, 0.7 mmol, 1.0 eq.) and 3-methoxybenzhydrazide (114 mg, 0.7 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and irradiated at 120 °C for 20 min. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a brown solid (176 mg, 87%). Mp 300-303 °C. ¹H NMR (600 MHz, methanol-*d*₄) δ 8.40 (s, 1H), 8.36 (s, 1H), 8.19 (d, *J* = 7.8 Hz, 1H), 8.09 (d, *J* = 7.8 Hz, 1H), 7.55 (t, *J* = 7.8 Hz, 1H), 7.52-7.50 (m, 2H), 7.42 (t, *J* = 7.8 Hz, 1H), 7.13 (dd, *J* = 7.8, 1.8 Hz, 1H), 3.89 (s, 3H). ¹³C NMR (151 MHz, methanol-*d*₄) δ 168.2, 165.5, 159.8, 148.3, 134.5, 134.0, 131.4, 131.2, 131.0, 129.6, 129.6, 128.8, 119.6, 118.1, 112.8, 55.0. IR (neat) *v*_{max}: 3247 (N-H), 2900 (O-H), 2834 (O-CH₃), 1675 (C=O), 1656 (C=O). UPLC-MS (80% Solvent B) *t*_R 0.511 min, (ESI+) *m/z*: 299 (C₁₆H₁₅N₂O₄) [M+H, 100%]; (ESI-) *m/z*: 297 (C₁₆H₁₃N₂O₄) [M-H, 100%].

(*E*)-3-((2-(2-methoxybenzoyl)hydrazono)methyl)benzoic acid (12)

3-Formylbenzoic acid (150 mg, 1.0 mmol, 1.0 eq.) and 2-methoxybenzhydrazide (166 mg, 1.0 mmol, 1.0 eq.) were combined with methanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold methanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) and recrystallised from methanol to afford the desired product as a white crystalline solid (236 mg, 79%). Mp 252-254 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 11.57 (s, 1H), 8.40 (s, 1H), 8.31 (s, 1H), 7.98 (d, *J* = 7.7 Hz, 1H), 7.92 (d, *J* = 7.7 Hz, 1H), 7.63 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.59 (t, *J* = 7.7 Hz, 1H), 7.54-7.49 (m, 1H), 7.18 (d, *J* = 8.3 Hz, 1H), 7.07 (t, *J* = 7.4 Hz, 1H), 3.89 (s, 3H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 167.0, 162.5, 156.7, 146.4, 134.8, 132.3, 131.5, 131.4, 130.5, 129.9, 129.3, 127.4, 123.3, 120.6, 112.0, 55.9. IR (neat) *v*_{max}: 3277 (N-H), 3000 (O-H, acid), 2850 (O-CH₃), 1714 (C=O), 1704 (C=O). UPLC-MS (80% Solvent B) *t*_R 0.553 min, (ESI+) *m/z*: 299 (C₁₆H₁₅N₂O₄) [M+H, 100%]; (ESI-) *m/z*: 297 (C₁₆H₁₃N₂O₄) [M-H, 100%].

(*E*)-3-((2-(4-chlorobenzoyl)hydrazono)methyl)benzoic acid (13)

3-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) and 4-chlorobenzhydrazide (112 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 1 mL) and cold diethyl ether (2 x 1 mL) to afford the desired product as a white solid (140 mg, 70%). Mp 292-294 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.03 (s, 1H), 8.50 (s, 1H), 8.33 (s, 1H), 7.99 (d, *J* = 7.7 Hz, 1H), 7.95 (d, *J* = 8.3 Hz, 3H), 7.62 (d, *J* = 8.3 Hz, 2H), 7.59 (d, *J* = 7.7 Hz, 1H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 167.0, 162.2, 147.1, 136.7, 134.7, 132.0, 131.6, 131.5, 130.7, 129.7 (2C), 129.3, 128.7 (2C), 127.4. IR (neat) *v*_{max}: 3207 (N-H), 2800 (O-H), 1683 (C=O), 1645

(C=O), 753 (C-Cl). UPLC-MS (80% Solvent B) t_R 0.545 min, (ESI-) m/z : 300 ($C_{15}H_9^{35}ClN_2O_3$) [M-2H, 100%], m/z : 302 ($C_{15}H_9^{37}ClN_2O_3$) [M-H, 35%].

(E)-3-((2-(3-chlorobenzoyl)hydrazono)methyl)benzoic acid (14)

3-Formylbenzoic acid (150 mg, 1.0 mmol, 1.0 eq.) and 3-chlorobenzhydrazide (171 mg, 1.0 mmol, 1.0 eq.) were combined with methanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold methanol (2 x 1 mL) and cold diethyl ether (2 x 1 mL) to afford the desired product as a white solid (303 mg, 75%). Mp 269-271 °C. 1H NMR (600 MHz, DMSO- d_6) δ 13.16 (bs, 1H), 12.05 (s, 1H), 8.50 (s, 1H), 8.33 (s, 1H), 8.00 (d, J = 7.7 Hz, 1H), 7.97 (s, 1H), 7.96 (d, J = 7.9 Hz, 1H), 7.89 (d, J = 7.7 Hz, 1H), 7.69 (d, J = 7.9 Hz, 1H), 7.61 (t, J = 6.5 Hz, 1H), 7.58 (t, J = 6.5 Hz, 1H). ^{13}C NMR (101 MHz, DMSO- d_6) δ 166.9, 161.8, 147.3, 135.3, 134.7, 133.3, 131.7, 131.6, 131.5, 130.7, 130.6, 129.3, 127.42, 127.37, 126.5. IR (neat) ν_{max} : 3217 (N-H), 3000 (O-H), 1684 (C=O), 1645 (C=O), 753 (C-Cl). UPLC-MS (80% Solvent B) t_R 0.545 min, (ESI+) m/z : 303 ($C_{15}H_{12}^{35}ClN_2O_3$) [M+H, 30%], m/z : 305 ($C_{15}H_{12}^{37}ClN_2O_3$) [M+H, 10%]; (ESI-) m/z : 301 ($C_{15}H_{10}^{35}ClN_2O_3$) [M-H, 100%], m/z : 303 ($C_{15}H_{10}^{37}ClN_2O_3$) [M-H, 35%].

(E)-3-((2-(2-chlorobenzoyl)hydrazono)methyl)benzoic acid (15)

3-Formylbenzoic acid (104 mg, 0.7 mmol, 1.0 eq.) and 2-chlorobenzhydrazide (121 mg, 0.7 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and irradiated at 120 °C for 20 min. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (151 mg, 73%). Mp 252-254 °C. 1H NMR (600 MHz, DMSO- d_6) δ 13.07 (bs, 1H), 12.05 (s, 1H), 8.33 (s, 1H), 8.32 (s, 1H), 8.00 (dt, J = 7.8, 1.2 Hz, 1H), 7.95 (d, J = 7.8 Hz, 1H), 7.61-7.57 (m, 3H), 7.53 (t, J = 7.2 Hz, 1H), 7.47 (t, J = 7.2 Hz, 1H). ^{13}C NMR (151 MHz, DMSO- d_6) δ 166.9, 162.6, 147.0, 135.2, 134.5, 131.5, 131.5, 131.4, 131.3, 130.8, 129.8, 129.3, 123.3, 127.5, 127.3. IR (neat) ν_{max} : 3190 cm^{-1} (N-H), 2850 cm^{-1} (O-H), 1695 cm^{-1} (C=O), 1661 cm^{-1} (C=O), 752 cm^{-1} (C-Cl). UPLC-ms (80% Solvent B) t_R 0.517 min, (ESI+) m/z : 303 ($C_{15}H_{12}^{35}ClN_2O_3$) [M+H, 100%], m/z : 305 ($C_{15}H_{12}^{37}ClN_2O_3$) [M+H, 35%]; (ESI-) m/z : 301 ($C_{15}H_{10}^{35}ClN_2O_3$) [M-H, 100%], m/z : 303 ($C_{15}H_{10}^{37}ClN_2O_3$) [M-H, 35%].

* 1H NMR (600 MHz, DMSO- d_6) δ 13.07 (bs, 1H), 12.07 (s, 1H), 8.13 (s, 1H), 7.94 (s, 1H), 7.89 (dt, J = 7.8, 1.2 Hz, 1H), 7.59 (d, J = 7.8 Hz, 1H), 7.53 (t, J = 7.2 Hz, 1H), 7.50-7.43 (m, 4H). ^{13}C NMR (151 MHz, DMSO- d_6) δ 168.7, 166.7, 143.4, 135.8, 134.4, 130.6, 130.5, 130.4, 130.4, 129.8, 129.1, 129.0, 128.8, 127.5, 126.9.

(E)-3-((2-(4-bromobenzoyl)hydrazono)methyl)benzoic acid (16)

3-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) and 4-bromobenzhydrazide (118 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 1 mL) and cold diethyl ether (2 x 1 mL) to afford the desired product as a white solid (181 mg, 75%). Mp 296-298 °C. 1H NMR (600 MHz, DMSO- d_6) δ 13.18 (bs, 1H), 12.03 (s, 1H), 8.51 (s, 1H), 8.33 (s, 1H), 7.99 (d, J = 7.6 Hz, 1H), 7.95 (d, J = 7.6 Hz, 1H), 7.88 (d, J = 8.4 Hz, 2H), 7.77 (d, J = 8.4 Hz, 2H), 7.60 (t, J = 7.6 Hz, 1H). ^{13}C NMR (151 MHz, DMSO- d_6) δ 166.9, 162.3, 147.1, 134.7, 132.4, 131.6 (2C), 131.5, 130.7, 129.8 (2C), 129.3 (2C), 127.4, 125.7. IR (neat) ν_{max} : 3000 (O-H), 2974 (NH), 1684 (C=O), 1645 (C=O). UPLC-MS (80% Solvent B) t_R 0.548 min, (ESI+) m/z : 347

(C₁₅H₁₂⁷⁹BrN₂O₃) [M+H, 10%], *m/z*: 349 (C₁₅H₁₂⁸¹BrN₂O₃) [M+H, 10%]; (ESI-) *m/z*: 345 (C₁₅H₁₀⁷⁹BrN₂O₃) [M-H, 85%], *m/z*: 347 (C₁₅H₁₀⁸¹BrN₂O₃) [M-H, 100%].

(E)-5-((2-(4-bromobenzoyl)hydrazono)methyl)-2-hydroxybenzoic acid (17)

5-Formyl-2-hydroxybenzoic acid (100 mg, 0.6 mmol, 1.0 eq.) and 4-bromobenzhydrazide (129 mg, 0.6 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 1 mL) and cold diethyl ether (2 x 1 mL) to afford the desired product as a white solid (78 mg, 36%). Mp 265-267 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 11.87 (s, 1H), 8.39 (s, 1H), 8.15 (d, *J* = 1.8 Hz, 1H), 7.88 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.86 (d, *J* = 8.4 Hz, 2H), 7.75 (d, *J* = 8.4 Hz, 2H), 7.06 (d, *J* = 8.6 Hz, 1H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 171.5, 162.5, 162.1, 147.2, 133.9, 132.5, 131.5 (2C), 129.7 (2C), 129.3, 125.6, 125.5, 117.9, 113.5. IR (neat) ν_{max} : 3229 (N-H), 3100 (O-H), 2900 (O-H), 1673 (C=O), 1655 (C=O). UPLC-MS (80% Solvent B) *t*_R 0.579 min, (ESI+) *m/z*: 363 (C₁₅H₁₂⁷⁹BrN₂O₄) [M+H, 25%], *m/z*: 365 (C₁₅H₁₂⁸¹BrN₂O₄) [M+H, 20%]; (ESI-) *m/z*: 361 (C₁₅H₁₀⁷⁹BrN₂O₄) [M-H, 100%], *m/z*: 363 (C₁₅H₁₀⁸¹BrN₂O₄) [M-H, 100%].

(E)-5-((2-(4-bromobenzoyl)hydrazono)methyl)-2-fluorobenzoic acid (18)

5-Formyl-2-fluorobenzoic acid (84 mg, 0.5 mmol, 1.0 eq.) and 4-bromobenzhydrazide (108 mg, 0.5 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold methanol (2 x 1 mL) and cold diethyl ether (2 x 1 mL) to afford the desired product as a white solid (120 mg, 66%). Mp 279-281 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 13.36 (bs, 1H), 12.03 (s, 1H), 8.46 (s, 1H), 8.25 (d, *J* = 5.3 Hz, 1H), 7.98-7.97 (m, 1H), 7.87 (d, *J* = 8.4 Hz, 2H), 7.76 (d, *J* = 8.4 Hz, 2H), 7.42 (t, *J* = 9.5 Hz, 1H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 164.6 (d, ³*J*_{CF} = 3.0 Hz), 161.8 (d, ¹*J*_{CF} = 261 Hz), 162.3, 146.1, 133.2 (d, ³*J*_{CF} = 9.1 Hz), 132.3, 131.6, 130.8 (d, ⁴*J*_{CF} = 3.0 Hz), 130.3, 129.8, 125.7, 119.9 (d, ³*J*_{CF} = 11.1 Hz), 117.8 (d, ²*J*_{CF} = 24.2 Hz). ¹⁹F NMR (376 MHz, DMSO-*d*₆, TFA) δ -106.28. IR (neat) ν_{max} : 3213 (N-H), 3000 (O-H), 1685 (C=O), 1654 (C=O). UPLC-MS (80% Solvent B) *t*_R 0.556 min, (ESI+) *m/z*: 365 (C₁₅H₁₂⁷⁹BrFN₂O₃) [M+H, 10%], *m/z*: 367 (C₁₅H₁₂⁸¹BrFN₂O₃) [M+H, 10%]; (ESI-) *m/z*: 363 (C₁₅H₁₀⁷⁹BrFN₂O₃) [M-H, 100%], *m/z*: 365 (C₁₅H₁₀⁸¹BrFN₂O₃) [M-H, 85%].

(E)-3-((2-(3-bromobenzoyl)hydrazono)methyl)benzoic acid (19)

3-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) and 3-bromobenzhydrazide (118 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 1 mL) and cold diethyl ether (2 x 1 mL) to afford the desired product as a white solid (191 mg, 92%). Mp 270-272 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 13.16 (bs, 1H), 12.05 (s, 1H), 8.50 (s, 1H), 8.33 (s, 1H), 8.10 (s, 1H), 8.00 (d, *J* = 7.7 Hz, 1H), 7.95 (d, *J* = 7.7 Hz, 1H), 7.93 (d, *J* = 7.9 Hz, 1H), 7.81 (dd, *J* = 7.9, 0.7 Hz, 1H), 7.60 (t, *J* = 7.7 Hz, 1H), 7.51 (t, *J* = 7.9 Hz, 1H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 166.9, 161.8, 147.4, 135.5, 134.7, 134.6, 131.6, 131.5, 130.8, 130.7, 130.2, 129.3, 127.5, 126.9, 121.8. IR (neat) ν_{max} : 3066 (N-H), 3000 (O-H), 1684 (C=O), 1645 (C=O). UPLC-MS (50% Solvent B) *t*_R 1.160 min, (ESI+) *m/z*: 346 (C₁₅H₁₂⁷⁹BrN₂O₃) [M+H, 100%], *m/z*: 348 (C₁₅H₁₂⁸¹BrN₂O₃) [M+H, 100%]; (ESI-) *m/z*: 344 (C₁₅H₁₀⁷⁹BrN₂O₃) [M-H, 100%], *m/z*: 346 (C₁₅H₁₀⁸¹BrN₂O₃) [M-H, 100%].

(E)-3-((2-(2-bromobenzoyl)hydrazono)methyl)benzoic acid (20)

3-Formylbenzoic acid (101 mg, 0.7 mmol, 1.0 eq.) and 2-bromobenzhydrazide (145 mg, 0.7 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and irradiated at 120 °C for 20 min. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (188 mg, 81%). Mp 264-267 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 12.83 (bs, 1H), 12.03 (s, 1H), 8.33 (s, 1H), 8.32 (s, 1H), 8.00 (dt, *J* = 7.8, 1.8 Hz, 1H), 7.95 (dt, *J* = 7.8, 1.8 Hz, 1H), 7.73 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.60 (t, *J* = 7.8 Hz, 1H), 7.56 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.51 (td, *J* = 7.2, 1.2 Hz, 1H), 7.49-7.38 (m, 1H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 167.4, 164.0, 147.4, 137.8, 135.0, 133.3, 132.1, 132.0, 131.9, 131.2, 129.8, 129.8, 128.2, 128.0, 120.0. IR (neat) ν_{max} : 3190 (N-H), 2800 (O-H), 1696 (C=O), 1659 (C=O), 688 (C-Br). UPLC-MS (80% Solvent B) *t*_R 0.519 min, (ESI+) *m/z*: 347 (C₁₅H₁₂⁷⁹BrN₂O₃) [M+H, 95%], *m/z*: 349 (C₁₅H₁₂⁸¹BrN₂O₃) [M+H, 100%]; (ESI-) *m/z*: 345 (C₁₅H₁₀⁷⁹BrN₂O₃) [M-H, 75%], *m/z*: 347 (C₁₅H₁₀⁸¹BrN₂O₃) [M-H, 75%].

* ¹H NMR (600 MHz, DMSO-*d*₆) δ 12.83 (bs, 1H), 12.06 (s, 1H), 8.14 (s, 1H), 7.94 (s, 1H), 7.89 (dt, *J* = 7.8, 1.8 Hz, 1H), 7.69 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.59 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.49-7.38 (m, 4H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 169.9, 167.2, 143.8, 138.5, 134.9, 132.5, 131.9, 131.1, 131.0, 130.9, 129.6, 129.3, 128.0, 127.8, 119.4.

(E)-3-((2-(4-nitrobenzoyl)hydrazono)methyl)benzoic acid (21)

3-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) and 4-nitrobenzhydrazide (120 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 1 mL) and cold diethyl ether (2 x 1 mL) to afford the desired product as a yellow solid (192 mg, 97%). Mp 290-292 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 12.61 (bs, 1H), 12.25 (s, 1H), 8.53 (s, 1H), 8.39 (d, *J* = 8.7 Hz, 2H), 8.34 (s, 1H), 8.17 (d, *J* = 8.7 Hz, 2H), 8.01 (d, *J* = 7.7 Hz, 1H), 7.97 (d, *J* = 7.7 Hz, 1H), 7.61 (t, *J* = 7.7 Hz, 1H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 166.9, 161.7, 149.4, 147.9, 139.0, 134.5, 131.7, 131.5, 130.9, 129.32, 129.25 (2C), 127.5, 123.7 (2C). IR (neat) ν_{max} : 3389 (N-H), 2820 (O-H), 1688 (C=O), 1662 (C=O), 1522 (NO₂), 1344 (NO₂). UPLC-MS (80% Solvent B) *t*_R 0.520 min, (ESI-) *m/z*: 311 (C₁₅H₉N₃O₅) [M-2H, 100%].

(E)-3-((2-(4-hydroxybenzoyl)hydrazono)methyl)benzoic acid (22)

3-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) and 4-hydroxybenzhydrazide (91 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. After this period, the solution was filtered, and the resultant solid was washed with cold ethanol (2 x 1 mL) and cold diethyl ether (2 x 1 mL) to afford the desired product as a white solid (113 mg, 66%). Mp 272-275 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 13.11 (bs, 1H), 11.75 (s, 1H), 10.15 (s, 1H), 8.48 (s, 1H), 8.30 (s, 1H), 7.97 (d, *J* = 7.6 Hz, 1H), 7.92 (d, *J* = 7.6 Hz, 1H), 7.81 (d, *J* = 8.6 Hz, 2H), 7.58 (t, *J* = 7.6 Hz, 1H), 6.87 (d, *J* = 8.6 Hz, 2H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 167.0, 162.9, 160.8, 145.8, 135.0, 131.44, 131.40, 130.4, 129.8, 129.3 (2C), 127.3 (2C), 123.8, 115.1. IR (neat) ν_{max} : 3285 (N-H), 3200 (O-H), 3000 (O-H), 1684 (C=O), 1622 (C=O). UPLC-MS (80% Solvent B) *t*_R 0.485 min, (ESI+) *m/z*: 284 (C₁₅H₁₂N₂O₄) [M, 45%].

(E)-3-((2-(3-hydroxybenzoyl)hydrazono)methyl)benzoic acid (23)

3-Formylbenzoic acid (150 mg, 1.0 mmol, 1.0 eq.) and 3-hydroxybenzhydrazide (152 mg, 1.0 mmol, 1.0 eq.) were combined with methanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold methanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford a 1:1 co-crystal of the desired product and methanol as a white solid (170 mg, 54%). Mp 153-156 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 13.17 (bs, 1H), 11.88 (s, 1H), 9.77 (bs, 1H), 8.50 (s, 1H), 8.31 (s, 1H), 7.98 (d, *J* = 7.7 Hz, 1H), 7.93 (d, *J* = 7.6 Hz, 1H), 7.59 (t, *J* = 7.7 Hz, 1H), 7.37-7.28 (m, 3H), 6.98 (d, *J* = 7.5 Hz, 1H), 4.09 (d, *J* = 5.1 Hz, 1H, methanol), 3.17 (d, *J* = 4.5 Hz, 3H, methanol). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 166.9, 163.3, 157.4, 146.6, 134.9, 134.7, 131.5, 131.4, 130.5, 129.6, 129.3, 127.3, 118.8, 118.1, 114.6, 48.6 (methanol). IR (neat) ν_{max} : 3390 (O-H), 3210 (N-H), 3000 (O-H), 1690 (C=O), 1631 (C=O). UPLC-MS (80% Solvent B) *t*_R 0.487 min, (ESI+) *m/z*: 285 (C₁₅H₁₃N₂O₄) [M+H, 50%]; (ESI-) *m/z*: 283 (C₁₅H₁₁N₂O₄) [M+H, 90%].

(*E*)-3-((2-(2-hydroxybenzoyl)hydrazono)methyl)benzoic acid (24)

3-Formylbenzoic acid (105 mg, 0.7 mmol, 1.0 eq.) and 2-hydroxybenzhydrazide (108 mg, 0.7 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL MW vial. A Teflon-coated stirrer bar was added, and the vial was capped and irradiated at 120 °C for 20 min. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (176 mg, 88%). Mp 291-295 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 13.11 (bs, 1H), 11.93 (s, 1H), 11.78 (bs, 1H), 8.53 (s, 1H), 8.34 (s, 1H), 8.00 (d, *J* = 7.8 Hz, 1H), 7.96 (d, *J* = 7.8 Hz, 1H), 7.90 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.61 (t, *J* = 7.8 Hz, 1H), 7.45 (t, *J* = 7.2 Hz, 1H), 6.99 (d, *J* = 8.4 Hz, 1H), 6.97 (t, *J* = 7.2 Hz, 1H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 166.9, 164.7, 158.8, 147.6, 134.6, 133.9, 131.6, 131.4, 130.8, 129.3, 128.7, 127.5, 119.0, 117.3, 116.1. IR (neat) ν_{max} : 3243 (N-H), 3053 (O-H), 2900 (O-H), 1677 (C=O), 1637 (C=O). UPLC-MS (80% Solvent B) *t*_R 0.527 min, (ESI+) *m/z*: 285 (C₁₅H₁₃N₂O₄) [M+H, 100%], *m/z*: 307 (C₁₅H₁₂N₂O₄Na) [M+Na, 55%]; (ESI-) *m/z*: 283 (C₁₅H₁₁N₂O₄) [M-H, 100%].

(*E*)-3-((2-isonicotinoylhydrazono)methyl)benzoic acid (25)

3-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) and nicotinohydrazide (90 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (143 mg, 89%). Mp 384-387 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.48 (bs, 1H), 12.19 (s, 1H), 8.80 (dd, *J* = 4.5, 1.5 Hz, 2H), 8.53 (s, 1H), 8.34 (s, 1H), 7.99 (dd, *J* = 15.5, 7.8 Hz, 2H), 7.84 (dd, *J* = 4.5, 1.5 Hz, 2H), 7.61 (t, *J* = 7.8 Hz, 1H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 166.9, 161.8, 150.4 (2C), 148.0, 140.4, 134.5, 131.7, 131.5, 130.9, 129.3, 127.5, 121.6 (2C). IR (neat) ν_{max} : 3200 (N-H), 3000 (O-H), 1713 (C=O), 1651 (C=O). UPLC-MS (80% solvent B) *t*_R 0.491 min, (ESI+) *m/z*: 269 (C₁₄H₁₁N₃O₃) [M, 100%].

(*E*)-2-hydroxy-5-((2-isonicotinoylhydrazono)methyl)benzoic acid (26)

5-Formyl-2-hydroxybenzoic acid (100 mg, 0.6 mmol, 1.0 eq.) and isonicotinohydrazide (82 mg, 0.6 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated (in a sand bath) at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired

product as a yellow solid (70 mg, 41%). Mp 273-275 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 12.03 (s, 1H), 8.79 (d, *J* = 4.6 Hz, 2H), 8.41 (s, 1H), 8.17 (s, 1H), 7.90 (d, *J* = 8.6 Hz, 1H), 7.82 (d, *J* = 4.6 Hz, 2H), 7.06 (d, *J* = 8.6 Hz, 1H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 171.4, 162.7, 161.5, 150.3 (2C), 148.1, 140.6, 134.0, 129.5, 125.4, 121.6 (2C), 118.0, 113.6. IR (neat) ν_{max} : 3305 (N-H), 3000 (O-H), 1660 (C=O), 1657 (C=O). UPLC-MS (80% Solvent B) *t*_R 0.507 min, (ESI+) *m/z*: 286 (C₁₄H₁₂N₃O₄) [M+H, 100%]; (ESI-) *m/z*: 284 (C₁₄H₁₀N₃O₄) [M-H, 100%].

(*E*)-2-fluoro-5-((2-isonicotinoylhydrazono)methyl)benzoic acid (27)

5-Formyl-2-fluorobenzoic acid (84 mg, 0.5 mmol, 1.0 eq.) and isonicotinohydrazide (69 mg, 0.5 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold methanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (120 mg, 66%). Mp 265-267 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 13.45 (bs, 1H), 12.19 (s, 1H), 8.79 (dd, *J* = 4.5, 1.4 Hz, 2H), 8.48 (s, 1H), 8.26 (dd, *J* = 7.1, 2.1 Hz, 1H), 8.01-7.99 (m, 1H), 7.82 (dd, *J* = 4.5, 1.4 Hz, 2H), 7.45-7.42 (m, 1H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 164.6 (d, ³*J*_{CF} = 2.9 Hz), 162.0 (d, ¹*J*_{CF} = 261 Hz), 161.8, 150.4, 147.0, 140.4, 133.3 (d, ³*J*_{CF} = 8.3 Hz), 130.6 (d, ⁴*J*_{CF} = 3.3 Hz), 130.4, 131.6, 119.9 (d, ³*J*_{CF} = 11.1 Hz), 117.8 (d, ²*J*_{CF} = 23.5 Hz). ¹⁹F NMR (376 MHz, DMSO-*d*₆, TFA) δ -106.13. IR (neat) ν_{max} : 3175 (N-H), 3000 (O-H), 1668 (C=O), 1611 (C=O). UPLC-MS (80% Solvent B) *t*_R 0.492 min, (ESI+) *m/z*: 288 (C₁₄H₁₁FN₃O₃) [M+H, 55%]; (ESI-) *m/z*: 286 (C₁₄H₉FN₃O₃) [M-H, 90%].

(*E*)-3-((2-nicotinoylhydrazono)methyl)benzoic acid (28)

3-Formylbenzoic acid (150 mg, 1.0 mmol, 1.0 eq.) and nicotinohydrazide (151 mg, 1.1 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and irradiated at 120 °C for 20 min. Upon completion, the reaction mixture was chilled at -20 °C for 3 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (145 mg, 77%). Mp 288-290 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 12.94 (bs, 1H), 12.14 (s, 1H), 9.08 (s, 1H), 8.78 (d, *J* = 3.7 Hz, 1H), 8.50 (s, 1H), 8.34 (s, 1H), 8.27 (d, *J* = 7.8 Hz, 1H), 8.00 (d, *J* = 7.6 Hz, 1H), 7.97 (d, *J* = 7.6 Hz, 1H), 7.63-7.57 (m, 2H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 166.9, 161.9, 152.4, 148.6, 147.4, 135.5, 134.6, 131.6, 131.5, 130.8, 129.3, 129.1, 127.5, 123.7. IR (neat) ν_{max} : 3185 (N-H), 3000 (O-H), 1648 (C=O), 1646 (C=O). UPLC-MS (80% Solvent B) *t*_R 0.478 min, (ESI+) *m/z*: 270 (C₁₄H₁₂N₃O₃) [M+H, 100%]; (ESI-) *m/z*: 268 (C₁₄H₁₀N₃O₃) [M-H, 100%].

(*E*)-2-hydroxy-5-((2-nicotinoylhydrazono)methyl)benzoic acid (29)

5-Formyl-2-hydroxybenzoic acid (100 mg, 0.6 mmol, 1.0 eq.) and nicotinohydrazide (85 mg, 0.6 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 70 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 3 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (81 mg, 47%). Mp 284-287 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 11.98 (s, 1H), 9.06 (s, 1H), 8.76 (s, 1H), 8.39 (s, 1H), 8.25 (d, *J* = 6.2 Hz, 1H), 8.16 (s, 1H), 7.90 (d, *J* = 7.6 Hz, 1H), 7.57 (s, 1H), 7.06 (d, *J* = 8.0 Hz, 1H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 171.5, 162.6, 161.6, 152.2, 148.5, 147.5, 135.6, 134.0, 129.4, 129.3, 125.5, 123.7, 118.0, 113.6. IR (neat) ν_{max} : 3301 (N-H), 3000 (O-H), 1685 (C=O), 1675 (C=O). UPLC-MS (80% Solvent B) *t*_R 0.509 min, (ESI+) *m/z*: 286 (C₁₄H₁₂N₃O₄) [M+H, 80%]; (ESI-) *m/z*: 284 (C₁₄H₁₀N₃O₄) [M-H, 100%].

(E)-2-fluoro-5-((2-nicotinoylhydrazono)methyl)benzoic acid (30)

5-Formyl-2-fluorobenzoic acid (84 mg, 0.5 mmol, 1.0 eq.) and nicotinohydrazide (69 mg, 0.5 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 3 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (113 mg, 78%). Mp 267-268 °C. ^1H NMR (600 MHz, DMSO- d_6) δ 13.23 (bs, 1H), 12.14 (s, 1H), 9.07 (d, J = 1.2 Hz, 1H), 8.77 (d, J = 3.7 Hz, 1H), 8.46 (s, 1H), 8.26 (d, J = 7.5 Hz, 2H), 8.00-7.99 (m, 1H), 7.58 (dd, J = 7.7, 4.9 Hz, 1H), 7.46-7.40 (m, 1H). ^{13}C NMR (151 MHz, DMSO- d_6) δ 164.6 (d, $^3J_{\text{CF}}$ = 2.6 Hz), 161.94 (d, $^1J_{\text{CF}}$ = 261 Hz), 161.86, 152.4, 148.6, 146.4, 140.4, 135.5, 133.2 (d, $^3J_{\text{CF}}$ = 9.1 Hz), 130.7 (d, $^4J_{\text{CF}}$ = 3.0 Hz), 130.4, 129.1, 123.7, 119.9 (d, $^3J_{\text{CF}}$ = 11.2 Hz), 117.8 (d, $^2J_{\text{CF}}$ = 23.3 Hz). ^{19}F NMR (376 MHz, DMSO- d_6 , TFA) δ -106.55. IR (neat) ν_{max} : 3195 (N-H), 3000 (O-H), 1692 (C=O), 1648 (C=O). UPLC-MS (80% Solvent B) t_{R} 0.494 min, (ESI+) m/z : 288 (C₁₄H₁₁FN₃O₃) [M+H, 95%]; (ESI-) m/z : 286 (C₁₄H₉FN₃O₃) [M-H, 100%].

(E)-3-((2-picolinoylhydrazono)methyl)benzoic acid (31)

3-Formylbenzoic acid (150 mg, 1.0 mmol, 1.0 eq.) and picolinohydrazide (137 mg, 1.0 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 3 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 5 mL) and cold diethyl ether (2 x 5 mL) to afford the desired product as a white solid (202 mg, 75%). Mp 242-245 °C. ^1H NMR (600 MHz, DMSO- d_6) δ 13.17 (bs, 1H), 12.25 (s, 1H), 8.73 (2 overlapping singlets, 2H), 8.30 (s, 1H), 8.15 (d, J = 7.8 Hz, 1H), 8.07 (td, J = 7.7, 1.6 Hz, 1H), 8.00 (d, J = 7.7 Hz, 1H), 7.93 (d, J = 7.7 Hz, 1H), 7.69-7.67 (m, 1H), 7.60 (t, J = 7.7 Hz, 1H). ^{13}C NMR (151 MHz, DMSO- d_6) δ 166.9, 160.5, 149.5, 148.5, 148.2, 138.1, 134.8, 131.43, 131.42, 130.7, 129.3, 127.6, 127.1, 122.8. IR (neat) ν_{max} : 3277 (N-H), 3000 (O-H), 1711 (C=O), 1656 (C=O). UPLC-MS (80% Solvent B) t_{R} 0.518 min, (ESI+) m/z : 270 (C₁₄H₁₂N₃O₃) [M+H, 100%]; (ESI-) m/z : 268 (C₁₄H₁₀N₃O₃) [M-H, 100%].

(E)-3-((2-(1H-pyrrole-2-carbonyl)hydrazono)methyl)benzoic acid (32)

3-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) and 1H-pyrrole-2-carbohydrazide (83 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 100 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 3 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 5 mL) and cold diethyl ether (2 x 5 mL) to afford the desired product as an off-white solid (110 mg, 71%). Mp 243-245 °C. ^1H NMR (600 MHz, DMSO- d_6) δ 13.34 (bs, 1H), 12.07 (s, 1H), 9.17 (s, 1H), 8.04 (d, J = 7.3 Hz, 1H), 7.95 (s, 1H), 7.90 (dd, J = 7.8, 1.1 Hz, 1H), 7.64 (t, J = 7.5 Hz, 1H), 7.53 (td, J = 7.7, 1.2 Hz, 1H), 7.34 (s, 1H), 6.70 (dd, J = 3.4, 1.7 Hz, 1H). ^{13}C NMR (151 MHz, DMSO- d_6) δ 168.1 (2C), 154.4, 146.6, 146.0, 134.6, 132.0, 130.7, 130.3, 129.6, 126.7, 115.0, 112.0. IR (neat) ν_{max} : 3360 (N-H), 3000 (O-H), 2942 (N-H), 1678 (C=O), 1616 (C=O). UPLC-MS (50% Solvent B) t_{R} 0.678 min, (ESI+) m/z : 257 (C₁₃H₁₁N₃O₃) [M, 100%].

(E)-3-((2-(1-methyl-1H-imidazole-5-carbonyl)hydrazono)methyl)benzoic acid (33)

3-Formylbenzoic acid (101 mg, 0.7 mmol, 1.0 eq.) and 1-methyl-1H-imidazole-5-carbohydrazide (96 mg, 0.7 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and irradiated at 120 °C for 20 min. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and filtered under vacuum. The

crude solid was washed with cold ethanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (163 mg, 89%). Mp 299-301 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 12.96 (bs, 1H), 11.79 (s, 1H), 8.41 (s, 1H), 8.29 (s, 1H), 7.97 (d, *J* = 7.8 Hz, 1H), 7.92 (d, *J* = 7.8 Hz, 1H), 7.87 (s, 1H), 7.73 (s, 1H), 7.59 (t, *J* = 7.8 Hz, 1H), 3.87 (s, 3H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 166.9, 157.7, 145.8, 142.7, 134.8, 132.9, 131.5, 131.4, 130.5, 129.3, 127.3, 124.5, 33.6. IR (neat) ν_{max} : 3232 (N-H), 3054 (N-CH₃), 3000 (O-H), 1878 (C=N), 1698 (C=O), 1659 (C=O). UPLC-MS (80% Solvent B) *t*_R 0.493 min, (ESI+) *m/z*: 273 (C₁₃H₁₃N₄O₃) [M+H, 100%]; (ESI-) *m/z*: 271 (C₁₃H₁₁N₄O₃) [M-H, 100%].

(*E*)-3-((2-(adamantane-1-carbonyl)hydrazono)methyl)benzoic acid (34)

3-Formylbenzoic acid (150 mg, 1.0 mmol, 1.0 eq.) and adamantane carbohydrazide (213 mg, 1.1 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and irradiated at 120 °C for 20 min. Upon completion, the reaction mixture was chilled at -20 °C for 3 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 5 mL) and cold diethyl ether (2 x 5 mL) to afford a 1:1 co-crystal of the desired product and ethanol as a white crystalline solid (205 mg, 58%). Mp 261-263 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 13.09 (bs, 1H), 10.91 (s, 1H), 8.44 (s, 1H), 8.25 (s, 1H), 7.95 (d, *J* = 7.7 Hz, 1H), 7.86 (d, *J* = 7.7 Hz, 1H), 7.56 (t, *J* = 7.7 Hz, 1H), 4.34 (s, 1H), 3.44 (q, *J* = 6.8 Hz, 2H, ethanol), 2.01 (s, 3H), 1.88 (s, 6H), 1.70 (s, 5H), 1.05 (t, *J* = 6.8 Hz, 3H, ethanol). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 173.4, 167.0, 145.5, 135.0, 131.4, 131.3, 130.3, 129.2, 127.1, 56.0 (ethanol), 38.3 (4C), 36.0 (3C), 27.6 (3C), 18.6 (ethanol). IR (neat) ν_{max} : 3230 (N-H), 3000 (O-H), 2974 (C-H), 2909 (C-H), 2852 (C-H), 1688 (C=O), 1660 (C=O). UPLC-MS (80% Solvent B) *t*_R 0.626 min, (ESI+) *m/z*: 327 (C₁₉H₂₃N₂O₃) [M+H, 100%]; (ESI-) *m/z*: 325 (C₁₉H₂₁N₂O₃) [M-H, 100%].

(*E*)-3-((2-(4-(dimethylamino)benzoyl)hydrazono)methyl)benzoic acid (35)

3-Formylbenzoic acid (105 mg, 0.7 mmol, 1.0 eq.) and 4-dimethylaminobenzhydrazide (138 mg, 0.77 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and irradiated at 120 °C for 20 min. Upon completion, the reaction mixture was chilled at -20 °C for 3 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a creamy-coloured solid (122 mg, 56%). Mp 260-262 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 13.13 (bs, 1H), 11.65 (s, 1H), 8.48 (s, 1H), 8.30 (s, 1H), 7.96 (d, *J* = 7.7 Hz, 1H), 7.91 (d, *J* = 7.7 Hz, 1H), 7.83 (d, *J* = 8.9 Hz, 2H), 7.58 (t, *J* = 7.7 Hz, 1H), 6.76 (d, *J* = 8.9 Hz, 2H), 3.33 (s, 6H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 167.0 (2C), 152.5, 145.1, 135.2, 131.4, 131.3, 130.2 (2C), 129.2 (2C), 127.1, 119.3, 110.8 (2C), 39.7 (2C). IR (neat) ν_{max} : 3000 (O-H), 2980 (NH), 2922 (C-H), 1679 (C=O), 1595 (C=O). UPLC-MS (80% Solvent B) *t*_R 0.512 min, (ESI+) *m/z*: 312 (C₁₇H₁₈N₃O₃) [M+H, 100%]; (ESI-) *m/z*: 310 (C₁₇H₁₆N₃O₃) [M-H, 100%].

(*E*)-3-((2-(4-isopropylbenzoyl)hydrazono)methyl)benzoic acid (36)

3-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) and (4-isopropyl)benzhydrazide (107 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 3 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (68 mg, 37%). Mp 219-222 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 13.04 (bs, 1H), 11.89 (s, 1H), 8.50 (s, 1H), 8.32 (s, 1H), 7.98 (d, *J* = 7.6 Hz, 1H), 7.94 (d, *J* = 7.6 Hz, 1H), 7.86 (d, *J* = 7.8 Hz, 2H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.41 (d, *J* = 7.8 Hz, 2H), 2.97 (sept, *J* = 6.9 Hz, 1H), 1.24 (d, *J* = 6.9 Hz, 6H).

^{13}C NMR (101 MHz, DMSO- d_6) δ 167.0, 163.2, 152.6, 146.5, 134.9, 131.50, 131.45, 130.9, 130.5, 129.3 (2C), 127.8, 127.3, 126.5 (2C), 33.4, 23.6 (2C). IR (neat) ν_{max} : 3233 (NH), 3000 (O-H), 2958 (C-H), 1703 (C=O), 1687 (C=O). UPLC-MS (80% Solvent B) t_{R} 0.593 min, (ESI-) m/z : 308 ($\text{C}_{18}\text{H}_{16}\text{N}_2\text{O}_3$) [M-2H, 100%].

(E)-3-((2-(4-(*tert*-butyl)benzoyl)hydrazono)methyl)benzoic acid (37)

3-Formylbenzoic acid (150 mg, 1.0 mmol, 1.0 eq.) and 4-(*tert*-butyl)benzhydrazide (192 mg, 1.0 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 3 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 5 mL) and cold diethyl ether (2 x 5 mL) to afford the desired product as a white solid (213 mg, 78%). Mp decomp. >265 °C. ^1H NMR (600 MHz, DMSO- d_6) δ 13.17 (bs, 1H), 11.89 (s, 1H), 8.50 (s, 1H), 8.32 (s, 1H), 7.98 (d, J = 7.6 Hz, 1H), 7.94 (d, J = 7.6 Hz, 1H), 7.86 (d, J = 8.1 Hz, 2H), 7.59 (t, J = 7.6 Hz, 1H), 7.55 (d, J = 8.1 Hz, 2H), 1.32 (s, 9H). ^{13}C NMR (151 MHz, DMSO- d_6) δ 166.9, 163.2, 154.8, 146.5, 134.9, 131.48, 131.45, 130.6, 130.5, 129.2 (2C), 127.5, 127.3, 125.3 (2C), 34.7, 30.9 (3C). IR (neat) ν_{max} : 3217 (NH), 3000 (O-H), 2964 (C-H), 1725 (C=O), 1687 (C=O). UPLC-MS (80% Solvent B) t_{R} 0.636 min, (ESI-) m/z : 323 ($\text{C}_{19}\text{H}_{19}\text{N}_2\text{O}_3$) [M-H, 100%].

(E)-3-((2-(4-(trifluoromethyl)benzoyl)hydrazono)methyl)benzoic acid (38)

3-Formylbenzoic acid (104 mg, 0.7 mmol, 1.0 eq.) and 4-(trifluoromethyl)benzhydrazide (142 mg, 0.7 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and irradiated at 120 °C for 20 min. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (193 mg, 83%). Mp 288-291 °C. ^1H NMR (600 MHz, DMSO- d_6) δ 13.20 (bs, 1H), 12.17 (s, 1H), 8.53 (s, 1H), 8.34 (s, 1H), 8.13 (d, J = 7.8 Hz, 2H), 8.00 (dt, J = 7.8, 1.8 Hz, 1H), 7.97 (dt, J = 7.8, 1.8 Hz, 1H), 7.93 (d, J = 8.4 Hz, 2H), 7.61 (t, J = 7.8 Hz, 1H). ^{13}C NMR (151 MHz, DMSO- d_6) δ 166.9, 162.1, 147.6, 137.1, 134.6, 131.6, 131.6 (q, $^2J_{\text{CF}}$ = 31.7 Hz), 131.5, 130.8, 129.3, 128.6, 127.5, 125.5 (q, $^3J_{\text{CF}}$ = 3.0 Hz), 123.9 (q, $^1J_{\text{CF}}$ = 271.8 Hz). ^{19}F NMR (376 MHz, DMSO- d_6 , TFA) δ -59.66. IR (neat) ν_{max} : 3477 (N-H), 3224 (N-H), 2900 (O-H), 1685 (C=O), 1652 (C=O), 1132 (C-F). UPLC-MS (80% Solvent B) t_{R} 0.557 min, (ESI+) m/z : 337 ($\text{C}_{16}\text{H}_{12}\text{F}_3\text{N}_2\text{O}_3$) [M+H, 40%], 359 ($\text{C}_{16}\text{H}_{11}\text{F}_3\text{N}_2\text{O}_3\text{Na}$) [M+Na, 100%], 375 ($\text{C}_{16}\text{H}_{11}\text{F}_3\text{N}_2\text{O}_3\text{K}$) [M+K, 15%]; (ESI-) m/z : 335 ($\text{C}_{16}\text{H}_{10}\text{F}_3\text{N}_2\text{O}_3$) [M-H, 100%].

(E)-3-((2-(3-(trifluoromethyl)benzoyl)hydrazono)methyl)benzoic acid (39)

3-Formylbenzoic acid (100 mg, 0.7 mmol, 1.0 eq.) and 3-(trifluoromethyl)benzhydrazide (139 mg, 0.7 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and irradiated at 120 °C for 20 min. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (187 mg, 76%). Mp 308-311 °C. ^1H NMR (600 MHz, DMSO- d_6) δ 13.17 (bs, 1H), 12.17 (s, 1H), 8.53 (s, 1H), 8.35 (s, 1H), 8.26 (s, 1H), 8.24 (d, J = 7.8 Hz, 1H), 8.00 (d, J = 7.8 Hz, 1H), 7.99-7.95 (m, 2H), 7.79 (t, J = 7.8 Hz, 1H), 7.60 (t, J = 7.8 Hz, 1H). ^{13}C NMR (151 MHz, DMSO- d_6) δ 167.4, 162.3, 148.0, 135.1, 134.7, 132.3, 132.1, 131.9, 131.2, 130.3, 129.7, 129.7 (q, $^2J_{\text{CF}}$ = 32.2 Hz), 127.9, 124.7 (q, $^3J_{\text{CF}}$ = 3.9 Hz), 124.4 (q, $^1J_{\text{CF}}$ = 272.7 Hz). ^{19}F NMR (376 MHz, DMSO- d_6 , TFA) δ -59.36. IR (neat) ν_{max} : 3470 cm^{-1} (N-H), 2900 cm^{-1} (O-H), 1675 cm^{-1} (C=O), 1643 cm^{-1} (C=O), 1132 cm^{-1} (C-F). UPLC-MS (80% Solvent B) t_{R} 0.557 min, (ESI+) m/z : 337 ($\text{C}_{16}\text{H}_{12}\text{F}_3\text{N}_2\text{O}_3$) [M+H, 100%], 359

(C₁₆H₁₁F₃N₂O₃Na) [M+Na, 25%], 375 (C₁₆H₁₁F₃N₂O₃K) [M+K, 5%]; (ESI-) *m/z*: 335 (C₁₆H₁₀F₃N₂O₃) [M-H, 100%].

(E)-3-((2-(3,5-bis(trifluoromethyl)benzoyl)hydrazono)methyl)benzoic acid (40)

3-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) and 3,5-(bis-trifluoromethyl)benzhydrazide (180 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 3 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 5 mL) and cold diethyl ether (2 x 5 mL) to afford the desired product as a white solid (176 mg, 73%). Mp 292-293 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.33 (s, 1H), 8.57 (s, 2H), 8.53 (s, 1H), 8.40 (s, 1H), 8.36 (s, 1H), 8.00 (dd, *J* = 12.0, 7.8 Hz, 2H), 7.62 (t, *J* = 7.7 Hz, 1H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 166.9, 160.4, 148.2, 144.2, 135.6, 134.5, 131.7, 131.5, 131.0, 130.6 (q, ²*J*_{CF} = 33.4 Hz, 2C), 129.4, 128.6 (q, ⁴*J*_{CF} = 2.9 Hz, 2C), 127.6, 125.5 (unresolved multiplet), 123.1 (q, ¹*J*_{CF} = 274 Hz, 2C). ¹⁹F NMR (376 MHz, DMSO-*d*₆, TFA) δ -58.88. IR (neat) ν_{max} : 3196 (N-H), 3000 (O-H), 1687 (C=O), 1684 (C=O). UPLC-MS (80% Solvent B) *t*_R 0.667 min, (ESI+) *m/z*: 404 (C₁₇H₁₀F₆N₂O₃) [M, 80%], *m/z*: 426 (C₁₇H₁₀F₆N₂O₃Na) [M+Na, 30%]; (ESI-) *m/z*: 402 (C₁₇H₈F₆N₂O₃) [M-2H, 100%].

(E)-3-((2-(4-(trifluoromethoxy)benzoyl)hydrazono)methyl)benzoic acid (41)

3-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) and 4-(trifluoromethoxy)benzhydrazide (145 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 3 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 1 mL) and cold diethyl ether (2 x 1 mL) to afford the desired product as a white solid (135 mg, 64%). Mp 281-283 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 13.18 (bs, 1H), 12.07 (s, 1H), 8.51 (s, 1H), 8.34 (s, 1H), 8.06 (d, *J* = 8.4 Hz, 2H), 7.98 (dd, *J* = 15.8, 7.7 Hz, 3H), 7.60 (t, *J* = 7.7 Hz, 1H), 7.55 (d, *J* = 8.4 Hz, 2H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 166.9, 162.1, 150.6, 147.2, 134.7, 132.4, 131.6, 131.5, 130.7, 130.1 (2C), 129.3, 127.4, 120.9 (2C), 120.1 (q, ¹*J*_{CF} = 258 Hz). ¹⁹F NMR (376 MHz, DMSO-*d*₆, TFA) δ -54.94. IR (neat) ν_{max} : 3215 (N-H), 3000 (O-H), 1687 (C=O), 1644 (C=O), 1147 (O-C). UPLC-MS (80% Solvent B) *t*_R 0.575 min, (ESI-) *m/z*: 352 (C₁₆H₁₁F₃N₂O₄) [M, 100%]; (ESI-) *m/z*: 350 (C₁₆H₉F₃N₂O₄) [M-2H, 100%].

(E)-3-((2-(pyridin-4-yl)hydrazono)methyl)benzoic acid (42)

3-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) and 4-hydrazinylpyridine hydrochloride (96 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 1 mL) and cold diethyl ether (2 x 1 mL) to afford the desired product as a white solid (117 mg, 81%). Mp 305-308 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 12.81 (s, 1H), 8.40 (s, 1H), 8.37-8.36 (m, 2H), 8.34 (s, 1H), 8.06 (d, *J* = 7.6 Hz, 1H), 8.01 (d, *J* = 7.7 Hz, 1H), 7.61 (t, *J* = 7.7 Hz, 1H), 7.23 (s, 1H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 166.9, 155.0, 146.6, 134.1, 131.5, 131.4, 131.0, 129.4 (2C), 127.8 (2C). IR (neat) ν_{max} : 3486 (N-H), 3000 (O-H), 1700 (C=O), 1645 (C=O). UPLC-MS (80% Solvent B) *t*_R 0.505 min, (ESI+) *m/z*: 242 (C₁₃H₁₂N₃O₂) [M+H, 100%].

(E)-3-((2-(3-chloro-4-methylphenyl)hydrazono)methyl)benzoic acid (43)

3-Chloro-4-methylphenylhydrazine hydrochloride (127 mg, 0.66 mmol, 1.1 eq.) and sodium hydroxide (26 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A

Teflon-coated stirrer bar was added, and the solution was stirred at ambient temperature for 20 min. 3-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) was added and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the solvent was removed *in vacuo*, the resultant residue taken up in ethyl acetate (10 mL) and washed with water (3 x 10 mL). The organic residue was dried over MgSO₄ and dried *in vacuo* to afford the desired product as a pale brown solid (131 mg, 76%). Mp 187-190 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 10.52 (s, 1H), 8.17 (s, 1H), 7.91 (s, 1H), 7.89 (d, *J* = 7.8 Hz, 1H), 7.85 (d, *J* = 7.7 Hz, 1H), 7.51 (t, *J* = 7.7 Hz, 1H), 7.18 (d, *J* = 8.3 Hz, 1H), 7.11 (d, *J* = 2.0 Hz, 1H), 6.92 (dd, *J* = 8.3, 2.0 Hz, 1H), 2.23 (s, 3H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 167.3, 144.5, 136.3, 136.0, 133.8, 131.7, 131.6, 129.7, 129.0, 128.8, 126.4, 124.9, 111.9, 111.1, 18.7. IR (neat) ν_{max} : 3375 (N-H), 3278 (C-H), 3200 (O-H), 1691 (C=O), 683 (C-Cl). UPLC-MS (80% Solvent B) *t*_R 0.889 min, (ESI+) *m/z*: 289 (C₁₅H₁₄³⁵ClN₂O₂) [M+H, 35%], *m/z*: 305 (C₁₅H₁₄³⁷ClN₂O₂) [M+H, 10%]; (ESI-) *m/z*: 287 (C₁₅H₁₂³⁵ClN₂O₂) [M-H, 100%], *m/z*: 289 (C₁₅H₁₂³⁷ClN₂O₂) [M-H, 35%].

(E)-3-((2-(3,4-dichlorophenyl)hydrazono)methyl)benzoic acid (44)

3,4-Dichlorophenylhydrazine hydrochloride (141 mg, 0.66 mmol, 1.1 eq.) and sodium hydroxide (26 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the solution was stirred at ambient temperature for 20 min. 3-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) was added and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the solvent was removed *in vacuo*, the resultant residue taken up in ethyl acetate (10 mL) and washed with water (3 x 10 mL). The organic residue was dried over MgSO₄ and dried *in vacuo* to afford the desired product as a brown solid (148 mg, 80%). Mp 184-187 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 13.14 (bs, 1H), 10.76 (s, 1H), 8.20 (s, 1H), 7.96 (s, 1H), 7.90 (dd, *J* = 17.5, 7.7 Hz, 2H), 7.52 (t, *J* = 7.7 Hz, 1H), 7.44 (d, *J* = 8.8 Hz, 1H), 7.25 (d, *J* = 2.4 Hz, 1H), 7.02 (dd, *J* = 8.8, 2.4 Hz, 1H). (Residual EtOAc peaks at 4.02, 1.98 and 1.17 ppm. Product contains 4.9% EtOAc by mass, calculated from the peak at 4.01 ppm that integrates to 0.36 and is representative of 2 protons). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 167.3, 145.2 (2C), 137.8, 135.7, 131.6, 131.0, 129.9, 129.1, 129.0, 126.7, 119.7, 113.0, 112.4. (Residual EtOAc peaks at 59.8, 20.8, 14.1 ppm). IR (neat) ν_{max} : 3297 (N-H), 3000 (O-H), 1710 (C=O), 685 (C-Cl), 676 (C-Cl). UPLC-MS (80% Solvent B) *t*_R 0.902 min, (ESI+) *m/z*: 309 (C₁₄H₁₁³⁵Cl₂N₂O₂) [M+H, 40%], *m/z*: 311 (C₁₄H₁₁³⁵Cl³⁷ClN₂O₂) [M+H, 25%], *m/z*: 313 (C₁₄H₁₁³⁷Cl₂N₂O₂) [M+H, 5%]; (ESI-) *m/z*: 307 (C₁₄H₉³⁵Cl₂N₂O₂) [M-H, 100%], *m/z*: 309 (C₁₄H₉³⁵Cl³⁷ClN₂O₂) [M-H, 65%], *m/z*: 311 (C₁₄H₉³⁷Cl₂N₂O₂) [M-H, 10%].

(E)-3-((2-(4-bromophenyl)hydrazono)methyl)benzoic acid (45)

4-Bromophenylhydrazine hydrochloride (147 mg, 0.66 mmol, 1.1 eq.) and sodium hydroxide (26 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the solution was stirred at ambient temperature for 20 min. 3-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) was added and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the solvent was removed *in vacuo*, the resultant residue taken up in ethyl acetate (10 mL) and washed with water (3 x 10 mL). The organic residue was dried over MgSO₄ and concentrated *in vacuo* to afford the desired product as an off-white solid (46 mg, 24%). Mp decomp. >225 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 13.05 (bs, 1H), 10.88 (s, 1H), 8.18 (s, 1H), 7.98 (s, 1H), 7.86 (t, *J* = 8.3 Hz, 2H), 7.50 (t, *J* = 7.7 Hz, 1H), 7.37 (d, *J* = 8.8 Hz, 2H), 7.05 (d, *J* = 8.8 Hz, 2H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 167.2, 144.5, 136.4, 136.1, 131.8 (2C), 131.4, 129.8, 129.0, 128.7, 126.2, 114.0 (2C), 109.7. IR (neat) ν_{max} : 3315 (N-H), 3069 (O-H), 1684 (C=O), 504 (C-Br). UPLC-MS (80% Solvent B) *t*_R 0.790 min, (ESI-) *m/z*: 317 (C₁₄H₁₀⁷⁹BrN₂O₂) [M-H, 100%], *m/z*: 319 (C₁₄H₁₀⁸¹BrN₂O₂) [M-H, 100%].

(E)-3-((2-(4-chlorophenyl)hydrazono)methyl)benzoic acid (46)

4-Chlorophenylhydrazine hydrochloride (118 mg, 0.66 mmol, 1.1 eq.) and sodium hydroxide (26 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the solution was stirred at ambient temperature for 20 min. 3-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) was added and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the solvent was removed *in vacuo*, the resultant residue taken up in ethyl acetate (10 mL) and washed with water (3 x 10 mL). The organic residue was dried over MgSO_4 and concentrated *in vacuo* to afford the desired product as an off-white solid (117 mg, 71%). Mp 216-217 °C. ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 13.03 (bs, 1H), 10.60 (s, 1H), 8.19 (s, 1H), 7.93 (s, 1H), 7.90-7.83 (m, 2H), 7.51 (t, $J = 7.7$ Hz, 1H), 7.30-7.24 (m, 2H), 7.12-7.04 (m, 2H). ^{13}C NMR (101 MHz, $\text{DMSO}-d_6$) δ 167.2, 144.1, 136.4, 136.1, 131.3, 129.9, 129.09, 129.05 (2C), 128.8, 126.3, 122.3, 113.6 (2C). IR (neat): ν_{max} : 3371 (N-H), 3319 (O-H), 1682 (C=O), 685 (C-Cl). UPLC-MS (80% Solvent B) t_R 0.753 min, (ESI+) m/z : 275 ($\text{C}_{14}\text{H}_{12}^{35}\text{ClN}_2\text{O}_2$) [M+H, 50%], m/z : 277 ($\text{C}_{14}\text{H}_{12}^{37}\text{ClN}_2\text{O}_2$) [M+H, 15%]; (ESI-) m/z : 273 ($\text{C}_{14}\text{H}_{10}^{35}\text{ClN}_2\text{O}_2$) [M-H, 100%], m/z : 275 ($\text{C}_{14}\text{H}_{10}^{37}\text{ClN}_2\text{O}_2$) [M-H, 35%].

(E)-3-((2-(2,4-dichlorophenyl)hydrazono)methyl)benzoic acid (47)

2,4-Dichlorophenylhydrazine hydrochloride (143 mg, 0.66 mmol, 1.1 eq.) and sodium hydroxide (26 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the solution was stirred at ambient temperature for 20 min. 3-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) was added and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 1 mL) and cold diethyl ether (2 x 1 mL) to afford the desired product as an off-white solid (59 mg, 32%). Mp decomp. 250 °C. ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 13.06 (bs, 1H), 10.20 (s, 1H), 8.38 (s, 1H), 8.18 (s, 1H), 7.90 (d, $J = 7.7$ Hz, 2H), 7.55 (dd, $J = 12.3, 6.0$ Hz, 2H), 7.48 (d, $J = 2.3$ Hz, 1H), 7.34 (dd, $J = 8.9, 2.3$ Hz, 1H). ^{13}C NMR (101 MHz, $\text{DMSO}-d_6$) δ 167.1, 140.5, 140.2, 135.7, 131.4, 130.3, 129.4, 129.2, 128.7, 128.2, 126.6, 122.5, 116.8, 115.1. IR (neat) ν_{max} : 3321 (N-H), 3100 (O-H), 1699 (C=O), 680 (C-Cl). UPLC-MS (80% Solvent B) t_R 1.059 min, (ESI+) m/z : 309 ($\text{C}_{14}\text{H}_{11}^{35}\text{Cl}_2\text{N}_2\text{O}_2$) [M+H, 25%], m/z : 311 ($\text{C}_{14}\text{H}_{11}^{35}\text{Cl}^{37}\text{Cl}_2\text{N}_2\text{O}_2$) [M+H, 15%]; (ESI-) m/z : 307 ($\text{C}_{14}\text{H}_9^{35}\text{Cl}_2\text{N}_2\text{O}_2$) [M-H, 100%], m/z : 309 ($\text{C}_{14}\text{H}_9^{35}\text{Cl}^{37}\text{Cl}_2\text{N}_2\text{O}_2$) [M-H, 70%], m/z : 311 ($\text{C}_{14}\text{H}_9^{37}\text{Cl}_2\text{N}_2\text{O}_2$) [M-H, 10%].

(E)-3-((2-(2,4-difluorophenyl)hydrazono)methyl)benzoic acid (48)

2,4-Difluorophenylhydrazine hydrochloride (119 mg, 0.66 mmol, 1.1 eq.) and sodium hydroxide (26 mg, 0.66 mmol, 1.1 eq.) were combined with methanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the solution was stirred at ambient temperature for 20 min. 3-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) was added and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the solvent was removed *in vacuo*, the residue was taken up in ethyl acetate (20 mL) and washed with water (2 x 20 mL). The organic solution was reduced *in vacuo*, and the residue loaded onto silica and purified by column chromatography (0-10% MeOH in DCM) to afford the desired product as a tan solid (146 mg, 88%). Mp 150-152 °C. ^1H NMR (600 MHz, methanol- d_4) δ 8.29 (t, $J = 1.7$ Hz, 1H), 8.00 (s, 1H), 7.94 (dt, $J = 7.8, 1.7$ Hz, 1H), 7.88 (dt, $J = 7.8, 1.7$ Hz, 1H), 7.60-7.54 (m, 1H), 7.48 (t, $J = 7.8$ Hz, 1H), 6.93-6.88 (m, 2H). ^{13}C NMR (151 MHz, methanol- d_4) δ 170.0, 157.0 (dd, $^1J_{\text{CF}} = 238.4$, $^3J_{\text{CF}} = 10.8$ Hz), 150.4 (dd, $^1J_{\text{CF}} = 242.6$, $^3J_{\text{CF}} = 11.7$ Hz), 139.2, 137.8, 132.5, 131.8*, 131.2, 130.3, 129.8, 128.2, 115.7 (dd, $^3J_{\text{CF}} = 8.7$, $^3J_{\text{CF}} = 4.3$ Hz), 112.1 (d, $^2J_{\text{CF}} = 22.0$, $^4J_{\text{CF}} = 3.5$ Hz), 104.3 (d, $^2J_{\text{CF}} = 27.0$, $^2J_{\text{CF}} = 22.5$ Hz). ^{19}F NMR (376 MHz, $\text{DMSO}-d_6$, TFA) δ -121.96, -127.91. IR (neat): ν_{max} : 3352 (N-H), 3000 (O-H), 1689 (C=O), 752 (C-F), 724 (C-F). UPLC-MS (50% Solvent B) t_R 2.583 min; (ESI-) m/z : 275 ($\text{C}_{14}\text{H}_8\text{F}_2\text{N}_2\text{O}_2$) [M-H, 100%]. * Not observed but confirmed by HSQC and HMBC correlations

(E)-3-((2-(4-isopropylphenyl)hydrazono)methyl)benzoic acid (49)

3-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) and (4-isopropylphenyl)hydrazine hydrochloride (123 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 100 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h. The reaction mixture was loaded onto silica and purified by column chromatography (0-10% MeOH in DCM) to afford the desired product as an orange solid (98 mg, 51%). Mp decomp. >170 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 10.36 (s, 1H), 8.16 (s, 1H), 7.88 (s, 1H), 7.85 (d, *J* = 7.7 Hz, 1H), 7.82 (d, *J* = 7.7 Hz, 1H), 7.50 (t, *J* = 7.7 Hz, 1H), 7.11 (d, *J* = 8.4 Hz, 2H), 7.01 (d, *J* = 8.4 Hz, 2H), 2.79 (sept, *J* = 6.9 Hz, 1H), 1.17 (d, *J* = 6.9 Hz, 6H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 167.3, 143.2, 139.1, 136.5, 134.8, 131.3, 129.6, 129.0, 128.3, 126.9 (2C), 126.1, 112.1 (2C), 32.7, 24.2 (2C). IR (neat) ν_{max} : 3294 (N-H), 2900 (O-H), 2948 (N-H), 1680 (C=O). UPLC-MS (80% Solvent B) *t*_R 0.947 min, (ESI+) *m/z*: 282 (C₁₇H₁₈N₂O₂) [M, 100%]; (ESI-) *m/z*: 280 (C₁₇H₁₆N₂O₂) [M-2H, 100%].

(E)-2-((2-(4-bromobenzoyl)hydrazono)methyl)benzoic acid (50)

2-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) and 4-bromobenzhydrazide (118 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 100 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 1 mL) and cold diethyl ether (2 x 1 mL) to afford the desired product as a fluffy white solid (113 mg, 54%). Mp 205-207 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 12.13 (s, 1H), 9.20 (s, 1H), 8.07 (d, *J* = 7.8 Hz, 1H), 7.90 (t, *J* = 7.4 Hz, 3H), 7.75 (dd, *J* = 8.3, 4.0 Hz, 2H), 7.65 (t, *J* = 8.3 Hz, 1H), 7.54 (t, *J* = 7.4 Hz, 1H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 168.1, 162.3, 146.9, 134.5, 132.4, 132.0, 131.5, 131.4, 130.7, 130.3, 129.9, 129.7, 129.1, 126.7, 125.6. IR (neat) ν_{max} : 3000 (O-H), 2974 (NH), 1692 (C=O), 1684 (C=O). UPLC-MS (80% Solvent B) *t*_R 0.556 min, (ESI+) *m/z*: 347 (C₁₅H₁₂⁷⁹BrN₂O₃) [M+H, 35%], *m/z*: 349 (C₁₅H₁₂⁸¹BrN₂O₃) [M+H, 30%]; (ESI-) *m/z*: 345 (C₁₅H₁₀⁷⁹BrN₂O₃) [M-H, 100%], *m/z*: 347 (C₁₅H₁₀⁸¹BrN₂O₃) [M-H, 100%].

(E)-2-((2-(3-bromobenzoyl)hydrazono)methyl)benzoic acid (51)

2-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) and 3-bromobenzhydrazide (142 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 100 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 3 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 5 mL) and cold diethyl ether (2 x 5 mL) to afford the desired product as a fluffy white solid (160 mg, 77%). Mp 205-207 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 13.36 (bs, 1H), 12.15 (bs, 1H), 9.20 (s, 1H), 8.13 (s, 1H), 8.08 (d, *J* = 7.8 Hz, 1H), 7.94 (d, *J* = 7.8 Hz, 1H), 7.91 (d, *J* = 7.4 Hz, 1H), 7.81 (d, *J* = 7.8 Hz, 1H), 7.66 (t, *J* = 7.4 Hz, 1H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.50 (t, *J* = 7.8 Hz, 1H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 168.1, 161.7, 147.1, 135.5, 134.54, 134.49, 132.0, 130.7, 130.8, 130.4, 130.2, 129.8, 127.0, 126.7, 121.7. IR (neat) ν_{max} : 3200 (O-H), 2974 (N-H), 1688 (C=O), 1634 (C=O), 753 (C-Br). UPLC-MS (80% Solvent B) *t*_R 0.557 min, (ESI-) *m/z*: 345 (C₁₅H₁₀⁷⁹BrN₂O₃) [M-H, 100%], *m/z*: 347 (C₁₅H₁₀⁸¹BrN₂O₃) [M-H, 100%].

(E)-2-((2-isonicotinoylhydrazono)methyl)benzoic acid (52)

2-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) and isonicotinohydrazide (90 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 100 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 3 h and filtered under vacuum. The crude solid was washed

with cold ethanol (2 x 5 mL) and cold diethyl ether (2 x 5 mL) to afford the desired product as a white solid (94 mg, 58%). Mp 189-191 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 13.37 (bs, 1H), 12.29 (s, 1H), 9.22 (s, 1H), 8.78 (d, *J* = 5.6 Hz, 2H), 8.08 (d, *J* = 7.8 Hz, 1H), 7.92 (d, *J* = 7.6 Hz, 1H), 7.85 (d, *J* = 5.8 Hz, 2H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.55 (t, *J* = 7.4 Hz, 1H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 168.1, 161.8, 150.3 (2C), 147.8, 140.4, 134.4, 132.1, 130.8, 130.4, 129.9, 126.8, 121.6 (2C). IR (neat) ν_{max} : 3150 (O-H), 2986 (N-H), 1656 (C=O), 1645 (C=O). UPLC-MS (80% Solvent B) *t*_R 0.488 min, (ESI+) *m/z*: 270 (C₁₄H₁₂N₃O₃) [M+H, 100%]; (ESI-) *m/z*: 268 (C₁₄H₁₀N₃O₃) [M-H, 100%].

(*E*)-2-((2-nicotinoylhydrazono)methyl)benzoic acid (53)

2-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) and nicotinohydrazide (90 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 100 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 3 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 5 mL) and cold diethyl ether (2 x 5 mL) to afford the desired product as a white solid (108 mg, 67%). Mp 191-193 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 13.36 (bs, 1H), 12.24 (s, 1H), 9.20 (s, 1H), 9.08 (s, 1H), 8.77 (d, *J* = 3.8 Hz, 1H), 8.28 (d, *J* = 7.8 Hz, 1H), 8.09 (d, *J* = 7.8 Hz, 1H), 7.92 (d, *J* = 7.7 Hz, 1H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.58-7.53 (m, 2H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 168.1, 162.0, 152.3, 148.7, 147.2, 135.6, 134.5, 132.1, 130.7, 130.4, 129.8, 129.1, 126.7, 123.6. IR (neat) ν_{max} : 3220 (O-H), 2974 (N-H), 1695 (C=O), 1657 (C=O). UPLC-MS (80% Solvent B) *t*_R 0.489 min, (ESI+) *m/z*: 270 (C₁₄H₁₂N₃O₃) [M+H, 100%]; (ESI-) *m/z*: 268 (C₁₄H₁₀N₃O₃) [M-H, 100%].

(*E*)-2-((2-(4-(dimethylamino)benzoyl)hydrazono)methyl)benzoic acid (54)

2-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) and 4-(dimethylamino)benzhydrazide (118 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 100 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 3 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 2 mL) and cold diethyl ether (1 x 2 mL) to afford the desired product as a yellow solid (94 mg, 50%). Mp 210-212 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 13.26 (bs, 1H), 11.76 (s, 1H), 9.14 (s, 1H), 8.06 (d, *J* = 6.5 Hz, 1H), 7.88 (d, *J* = 7.7 Hz, 1H), 7.85 (d, *J* = 8.9 Hz, 2H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.50 (t, *J* = 7.5 Hz, 1H), 6.75 (d, *J* = 8.9 Hz, 2H), 3.00 (s, 6H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 168.2 (2C), 152.5, 135.0, 131.9 (2C), 130.5, 130.2 (2C), 129.2 (2C), 126.5, 119.4, 110.8 (2C), 39.7 (2C). IR (neat) ν_{max} : 3200 (O-H), 2974 (N-H), 1674 (C=O), 1600 (C=O). UPLC-MS (80% Solvent B) *t*_R 0.518 min, (ESI+) *m/z*: 312 (C₁₇H₁₈N₃O₃) [M+H, 70%]; (ESI-) *m/z*: 310 (C₁₇H₁₆N₃O₃) [M-H, 100%].

(*E*)-2-((2-(4-isopropylbenzoyl)hydrazono)methyl)benzoic acid (55)

2-Formylbenzoic acid (75 mg, 0.5 mmol, 1.0 eq.) and (4-isopropyl)benzhydrazide (89 mg, 0.5 mmol, 1.0 eq.) were combined with ethanol (4 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (94 mg, 59%). Mp 191-193 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 13.34 (bs, 1H), 12.00 (s, 1H), 9.18 (s, 1H), 8.07 (d, *J* = 7.6 Hz, 1H), 7.90 (d, *J* = 7.966 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 2H), 7.65 (t, *J* = 7.6 Hz, 1H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 2H), 2.97 (sept, *J* = 6.9 Hz, 1H), 1.24 (d, *J* = 6.9 Hz, 6H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 168.1, 163.2, 152.5, 146.2, 134.7, 132.0, 130.9, 130.7, 130.3, 129.6, 127.9 (2C), 126.6, 126.4 (2C), 33.4, 23.7 (2C). IR (neat) ν_{max} : 2900 (O-H), 2871 (N-H),

1675 (C=O), 1626 (C=O). UPLC-MS (80% Solvent B) t_R 0.618 min, (ESI+) m/z : 311 (C₁₈H₁₉N₂O₃) [M+H, 35%]; (ESI-) m/z : 309 (C₁₈H₁₇N₂O₃) [M-H, 100%].

(E)-2-((2-(4-(trifluoromethyl)benzoyl)hydrazono)methyl)benzoic acid (56)

2-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) and 4-(trifluoromethyl)benzhydrazide (135 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (4 mL) in a 2-5 μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 5 mL) and cold diethyl ether (2 x 5 mL) to afford the desired product as a white solid (125 mg, 62%). Mp 209-211 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 13.36 (bs, 1H), 12.27 (s, 1H), 9.23 (s, 1H), 8.14 (d, J = 7.8 Hz, 2H), 8.09 (d, J = 7.8 Hz, 1H), 7.92-7.91 (m, 3H), 7.66 (t, J = 7.3 Hz, 1H), 7.55 (t, J = 7.3 Hz, 1H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 168.1, 162.2, 147.4, 137.1, 134.5, 132.1, 131.6 (q, ² J_{CF} = 32.0 Hz), 130.8, 130.4, 129.8, 128.7 (2C), 126.7, 125.4 (q, ³ J_{CF} = 3.0 Hz, 2C), 124.4 (q, ¹ J_{CF} = 271.8 Hz). ¹⁹F NMR (376 MHz, DMSO-*d*₆, TFA) δ -59.27. IR (neat) ν_{max} : 2900 (O-H), 2871 (N-H), 1675 (C=O), 1626 (C=O). UPLC-MS (80% Solvent B) t_R 0.563 min, (ESI-) m/z : 335 (C₁₆H₁₀F₃N₂O₃) [M-H, 100%].

(E)-2-((2-(4-(*tert*-butyl)benzoyl)hydrazono)methyl)benzoic acid (57)

2-Formylbenzoic acid (96 mg, 0.64 mmol, 1.0 eq.) and 4-(*tert*-butyl)benzhydrazide (137 mg, 0.70 mmol, 1.1 eq.) were combined with ethanol (4 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 5 mL) and cold diethyl ether (2 x 5 mL) to afford the desired product as a white solid (138 mg, 67%). Mp 198-200 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 13.33 (bs, 1H), 12.01 (s, 1H), 9.18 (s, 1H), 8.08 (d, J = 7.7 Hz, 1H), 7.89 (m, 3H), 7.65 (t, J = 7.7 Hz, 1H), 7.53 (t, J = 9.6 Hz, 3H), 1.32 (s, 9H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 168.1, 163.2, 154.7, 146.3, 134.7, 132.0, 130.7, 130.5, 130.3, 129.6, 127.6 (2C), 126.6, 125.2 (2C), 34.7, 30.9 (3C). IR (neat) ν_{max} : 2961 (N-H), 2900 (O-H), 1677 (C=O), 1627 (C=O). UPLC-MS (80% Solvent B) t_R 0.629 min, (ESI+) m/z : 325 (C₁₉H₂₁N₂O₃) [M+H, 100%]; (ESI-) m/z : 323 (C₁₉H₁₉N₂O₃) [M-H, 100%].

(E)-2-((2-(1H-pyrrole-2-carbonyl)hydrazono)methyl)benzoic acid (58)

2-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) and 1H-pyrrole-2-carbohydrazide (83 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (4 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 5 mL) and cold diethyl ether (2 x 5 mL) to afford the desired product as a white solid (118 mg, 77%). Mp 200-202 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 13.29 (s, 1H), 11.69 (2 overlapping signals, 2H), 9.08 (s, 1H), 8.05 (d, J = 7.7 Hz, 1H), 7.89 (dd, J = 7.7, 1.2 Hz, 1H), 7.64 (t, J = 7.7 Hz, 1H), 7.51 (td, J = 7.7, 1.2 Hz, 1H), 7.01 (2 overlapping signals, 2H), 6.17 (s, 1H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 168.2 (2 overlapping signals), 134.9 (2 overlapping signals), 132.0, 130.4, 130.3, 129.2 (2 overlapping signals), 126.5, 122.8 (2 overlapping signals), 109.0. IR (neat) ν_{max} : 3346 (N-H), 3000 (O-H), 1680 (C=O), 1678 (C=O). UPLC-MS (80% Solvent B) t_R 0.499 min, (ESI+) m/z : 258 (C₁₃H₁₂N₃O₃) [M+H, 65%]; (ESI-) m/z : 256 (C₁₃H₁₀N₃O₃) [M-H, 100%].

(E)-2-((2-(1-methyl-1H-imidazole-5-carbonyl)hydrazono)methyl)benzoic acid (59)

2-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) and 1-methyl-1H-imidazole-5-carbohydrazide (92 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (4 mL) in a 2-5 mL μ wave

vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 5 mL) and cold diethyl ether (2 x 5 mL) to afford the desired product as a white solid (103 mg, 63%). Mp 204-205 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 13.32 (bs, 1H), 11.90 (s, 1H), 9.10 (s, 1H), 8.03 (s, 1H), 7.90 (dd, *J* = 7.7, 1.0 Hz, 1H), 7.86 (s, 1H), 7.76 (s, 1H), 7.64 (t, *J* = 7.7 Hz, 1H), 7.52 (td, *J* = 7.7, 1.0 Hz, 1H), 3.86 (s, 3H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 168.1, 156.5, 145.6, 142.7, 134.7, 133.0, 132.0, 130.6, 130.4, 129.5, 126.5, 124.5, 33.6. IR (neat) ν_{max} : 3050 (O-H), 2961 (N-H), 1647 (C=O), 1644 (C=O). UPLC-MS (80% Solvent B) *t*_R 0.513 min, (ESI+) *m/z*: 273 (C₁₃H₁₃N₄O₃) [M+H, 100%]; (ESI-) *m/z*: 271 (C₁₃H₁₁N₄O₃) [M-H, 100%].

(*E*)-2-((2-(3-(4-hydroxyphenyl)propanoyl)hydrazono)methyl)benzoic acid (60)

2-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) and 3-(4-hydroxyphenyl)propanehydrazide (119 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (4 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 5 mL) and cold diethyl ether (2 x 5 mL) to afford the desired product as a fluffy white solid (0.4:0.6 isomers) (117 mg, 63%). Mp 191-193 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 13.28 (bs, 1H), 11.52 (s, 0.4H), 11.37 (s, 0.6H), 9.14 (d, *J* = 13.7 Hz, 1H), 8.89 (s, 0.4H), 8.69 (s, 0.6H), 7.96 (dd, *J* = 37.0, 7.8 Hz, 1H), 7.90-7.83 (m, 1H), 7.60 (dt, *J* = 12.3, 7.6 Hz, 1H), 7.49 (ddd, *J* = 15.0, 8.1, 1.0 Hz, 1H), 7.03 (dd, *J* = 13.4, 8.4 Hz, 2H), 6.70-6.62 (m, 2H), 2.87 (t, *J* = 7.5 Hz, 1H), 2.78 (dd, *J* = 12.3, 5.3 Hz, 2H), 2.45 (t, *J* = 7.7 Hz, 1H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 173.8 (2 overlapping signals), 168.13, 168.09, 155.53, 155.46, 144.6, 141.7, 134.7, 134.5, 131.99, 131.95, 131.4, 131.1, 130.5, 130.4 (2 overlapping signals), 130.2, 129.4, 129.21, 129.18 (2C), 129.1 (2C), 126.5, 126.4, 115.10 (2C), 115.06 (2C), 36.3, 34.3, 29.9, 29.3. IR (neat) ν_{max} : 3416 (O-H), 3000 (O-H), 2974 (N-H), 1686 (C=O), 1644 (C=O). UPLC-MS (70% Solvent B) *t*_R 0.524 min, (ESI+) *m/z*: 313 (C₁₇H₁₇N₂O₄) [M+H, 35%], *m/z*: 335 (C₁₇H₁₇N₂O₄Na) [M+H, 50%]; (ESI-) *m/z*: 311 (C₁₇H₁₅N₂O₄) [M-H, 100%].

(*E*)-2-((2-(furan-2-carbonyl)hydrazono)methyl)benzoic acid (61)

2-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) and furan-2-carbohydrazide (83 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (4 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 5 mL) and cold diethyl ether (2 x 5 mL) to afford the desired product as a white solid (73 mg, 47%). Mp 187-189 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 13.34 (bs, 1H), 12.07 (s, 1H), 9.17 (s, 1H), 8.04 (d, *J* = 7.3 Hz, 1H), 7.95 (s, 1H), 7.90 (dd, *J* = 7.8, 1.1 Hz, 1H), 7.64 (t, *J* = 7.5 Hz, 1H), 7.53 (td, *J* = 7.7, 1.2 Hz, 1H), 7.34 (s, 1H), 6.70 (dd, *J* = 3.4, 1.7 Hz, 1H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 168.1 (2 overlapping signals), 154.4, 146.6, 146.0, 134.6, 132.0, 130.7, 130.3, 129.6, 126.7, 115.0, 112.0. IR (neat) ν_{max} : 3000 (O-H), 2781 (N-H), 1678 (C=O). UPLC-MS (50% Solvent B) *t*_R 0.655 min, (ESI+) *m/z*: 259 (C₁₃H₁₁N₂O₄) [M+H, 100%]; (ESI-) *m/z*: 257 (C₁₃H₉N₂O₄) [M-H, 100%].

(*E*)-2-((2-(3-chloro-4-methylphenyl)hydrazono)methyl)benzoic acid (62)

3-Chloro-4-methylphenylhydrazine hydrochloride (167 mg, 0.9 mmol, 1.0 eq.) and sodium hydroxide (35 mg, 0.9 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the solution was stirred at ambient temperature for 20 min. 2-Formylbenzoic acid (129 mg, 0.9 mmol, 1.0 eq.) was added and the vial was capped and heated (in a sand bath) at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and

filtered under vacuum. The crude solid was washed with cold water (2 x 5 mL), cold ethanol (2 x 2 mL), and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (215 mg, 87%). Mp 160-162 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 8.58 (s, 1H), 8.32 (d, *J* = 7.8 Hz, 1H), 8.03-8.00 (m, 2H), 7.92 (td, *J* = 7.8, 1.8 Hz, 1H), 7.72 (d, *J* = 1.8 Hz, 1H), 7.54-7.48 (m, 2H), 2.40 (s, 3H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 158.3, 140.7, 139.0, 134.9, 134.1, 132.7, 132.5, 131.0, 129.2, 127.6, 127.1, 126.3, 126.2, 124.6, 19.3. IR (neat) ν_{max} : 3058 (N-H), 1655 (C=O), 761 (C-Cl). UPLC-MS (80% Solvent B) *t*_R 1.084 min, (ESI+) *m/z*: 271 (C₁₅H₁₂³⁵ClN₂O) [M+H-H₂O, 100%], *m/z*: 273 (C₁₅H₁₂³⁷ClN₂O) [M+H-H₂O, 35%]; (ESI-) *m/z*: 287 (C₁₅H₁₂³⁵ClN₂O₂) [M-H, 70%], *m/z*: 289 (C₁₅H₁₂³⁷ClN₂O₂) [M-H, 30%].

(E)-2-((2-(3,4-dichlorophenyl)hydrazono)methyl)benzoic acid (63)

3,4-Dichlorophenylhydrazine hydrochloride (187 mg, 0.9 mmol, 1.0 eq.) and sodium hydroxide (35 mg, 0.9 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the solution was stirred at ambient temperature for 20 min. 2-Formylbenzoic acid (132 mg, 0.9 mmol, 1.0 eq.) was added and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and filtered under vacuum. The crude solid was washed with cold water (2 x 5 mL), cold ethanol (2 x 2 mL), and cold diethyl ether (2 x 2 mL) to afford the desired product as a yellow solid (111 mg, 41%). Mp 203-206 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 13.21 (bs, 1H), 10.90 (s, 1H), 8.70 (s, 1H), 8.10 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.85 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.58 (td, *J* = 7.8, 1.2 Hz, 1H), 7.43-7.40 (m, 2H), 7.26 (d, *J* = 2.4 Hz, 1H), 7.01 (dd, *J* = 9.0, 2.4 Hz, 1H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 168.5, 145.3, 137.4, 135.4, 131.9, 131.7, 131.0, 130.4, 129.1, 128.1, 125.9, 119.7, 113.0, 112.5. IR (neat) ν_{max} : 3326 (N-H), 2900 (O-H), 1697 (C=O), 807 (C-Cl), 750 (C-Cl). UPLC-MS (80% Solvent B) *t*_R 1.158 min, (ESI+) *m/z*: 309 (C₁₄H₁₁³⁵Cl₂N₂O₂) [M+H, 100%], *m/z*: 311 (C₁₄H₁₁³⁵Cl³⁷ClN₂O₂) [M+H, 65%], *m/z*: 313 (C₁₄H₁₁³⁷Cl₂N₂O₂) [M+H, 10%]; (ESI-) *m/z*: 307 (C₁₄H₁₀³⁵Cl₂N₂O₂) [M-H, 100%], *m/z*: 309 (C₁₄H₁₀³⁵Cl³⁷ClN₂O₂) [M-H, 70%], *m/z*: 311 (C₁₄H₁₀³⁷Cl₂N₂O₂) [M-H, 10%].

(E)-2-((2-(3-bromophenyl)hydrazono)methyl)benzoic acid (64)

3-Bromophenylhydrazine hydrochloride (179 mg, 0.8 mmol, 1.0 eq.) and sodium hydroxide (32 mg, 0.8 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the solution was stirred at ambient temperature for 20 min. 2-Formylbenzoic acid (120 mg, 0.8 mmol, 1.0 eq.) was added and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and filtered under vacuum. The crude solid was washed with cold water (2 x 5 mL), cold ethanol (2 x 2 mL), and cold diethyl ether (2 x 2 mL) to afford the desired product as a brown solid (196 mg, 77%). Mp 139-141 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 8.58 (s, 1H), 8.31 (d, *J* = 7.8 Hz, 1H), 8.01-7.97 (m, 2H), 7.91 (ddd, *J* = 8.4, 6.8, 1.8 Hz, 1H), 7.87 (t, *J* = 1.8 Hz, 1H), 7.67 (ddd, *J* = 8.1, 2.0, 1.0 Hz, 1H), 7.61 (ddd, *J* = 8.1, 2.0, 1.0 Hz, 1H), 7.48 (t, *J* = 7.8 Hz, 1H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 158.3, 143.1, 139.2, 134.1, 132.5, 130.5, 130.4, 129.2, 128.7, 127.6, 127.2, 126.3, 125.1, 120.9. IR (neat) ν_{max} : 3050 (C-H), 1654 (C=O), 677 (C-Br). UPLC-MS (80% Solvent B) *t*_R 0.927 min, (ESI+) *m/z*: 301 (C₁₄H₁₀⁷⁹BrN₂O) [M+H-H₂O, 100%], *m/z*: 303 (C₁₄H₁₀⁸¹BrN₂O) [M+H-H₂O, 100%].

(E)-2-((2-(4-bromophenyl)hydrazono)methyl)benzoic acid (65)

4-Bromophenylhydrazine hydrochloride (179 mg, 0.8 mmol, 1.0 eq.) and sodium hydroxide (32 mg, 0.9 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the solution was stirred at ambient temperature for 20 min. 2-Formylbenzoic acid (120 mg, 0.8 mmol, 1.0 eq.) was added and the vial was capped and heated in a sand bath at 50 °C

for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and filtered under vacuum. The crude solid was washed with cold water (2 x 5 mL), cold ethanol (2 x 2 mL), and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (223 mg, 87%). Mp 169-172 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 8.60 (s, 1H), 8.33 (d, *J* = 7.8 Hz, 1H), 8.03-7.99 (m, 2H), 7.93 (ddd, *J* = 7.8, 6.6, 1.8 Hz, 1H), 7.71 (d, *J* = 9.0 Hz, 2H), 7.61 (d, *J* = 9.0 Hz, 2H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 158.3, 141.1, 139.2, 134.1, 132.6, 131.5, 129.3, 128.1, 127.6, 127.2, 126.3, 120.3. IR (neat) ν_{max} : 3061 (C-H), 1656 (C=O), 683 (C-Br). UPLC-MS (80% Solvent B) *t*_R 0.907 min, (ESI+) *m/z*: 301 (C₁₄H₁₀⁷⁹BrN₂O) [M+H-H₂O, 100%], *m/z*: 303 (C₁₄H₁₀⁸¹BrN₂O) [M+H-H₂O, 100%].

(E)-2-((2-(4-chlorophenyl)hydrazono)methyl)benzoic acid (66)

4-Chlorophenylhydrazine hydrochloride (152 mg, 0.9 mmol, 1.0 eq.) and sodium hydroxide (34 mg, 0.9 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the solution was stirred at ambient temperature for 20 min. 2-Formylbenzoic acid (128 mg, 0.9 mmol, 1.0 eq.) was added and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and filtered under vacuum. The crude solid was washed with cold water (2 x 5 mL), cold ethanol (2 x 2 mL), and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (188 mg, 81%). Mp 165-167 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 8.59 (s, 1H), 8.32 (d, *J* = 7.8 Hz, 1H), 8.03-7.98 (m, 2H), 7.92 (ddd, *J* = 7.8, 6.6, 1.8 Hz, 1H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.57 (d, *J* = 8.4 Hz, 2H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 158.3, 140.7, 139.1, 134.1, 132.5, 131.9, 129.3, 128.6, 127.8, 127.6, 127.2, 126.3. IR (neat) ν_{max} : 3058 (C-H), 1655 (C=O), 599 (C-Cl). UPLC-MS (80% Solvent B) *t*_R 0.855 min, (ESI+) *m/z*: 257 (C₁₄H₁₀³⁵ClN₂O) [M+H-H₂O, 100%], *m/z*: 259 (C₁₄H₁₀³⁷ClN₂O) [M+H-H₂O, 35%]; (ESI-) *m/z*: 275 (C₁₄H₁₀³⁷ClN₂O₂) [M-H, 100%].

(E)-2-((2-(2,4-dichlorophenyl)hydrazono)methyl)benzoic acid (67)

2,4-Dichlorophenylhydrazine hydrochloride (183 mg, 0.9 mmol, 1.0 eq.) and sodium hydroxide (34 mg, 0.9 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the solution was stirred at ambient temperature for 20 min. 2-Formylbenzoic acid (128 mg, 0.9 mmol, 1.0 eq.) was added and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and filtered under vacuum. The crude solid was washed with cold water (2 x 5 mL), cold ethanol (2 x 2 mL), and cold diethyl ether (2 x 2 mL) to afford the desired product as a yellow solid (209 mg, 79%). Mp 225-228 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 13.12 (bs, 1H), 10.35 (s, 1H), 8.97 (s, 1H), 8.07 (d, *J* = 7.8 Hz, 1H), 7.82 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.57 (t, *J* = 7.8 Hz, 1H), 7.57 (d, *J* = 8.4 Hz, 1H), 7.46 (d, *J* = 2.4 Hz, 1H), 7.42 (td, *J* = 7.8, 1.2 Hz, 1H), 7.30 (dd, *J* = 9.0, 2.4 Hz, 1H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 168.5, 140.7, 139.7, 135.3, 131.7, 130.1, 129.9, 128.7, 128.3, 128.1, 126.1, 122.5, 116.9, 115.3. IR (neat) ν_{max} : 3326 (N-H), 3073 (C-H), 3000 (O-H), 1700 (C=O), 749.6 (C-Cl). UPLC-MS (80% Solvent B) *t*_R 1.215 min, (ESI+) *m/z*: 309 (C₁₄H₁₁³⁵Cl₂N₂O₂) [M+H, 100%], *m/z*: 311 (C₁₄H₁₁³⁵Cl³⁷ClN₂O₂) [M+H, 75%], *m/z*: 313 (C₁₄H₁₁³⁷Cl₂N₂O₂) [M+H, 10%]; (ESI-) *m/z*: 307 (C₁₄H₉³⁵Cl₂N₂O₂) [M-H, 100%], *m/z*: 309 (C₁₄H₉³⁵Cl³⁷ClN₂O₂) [M-H, 75%], *m/z*: 311 (C₁₄H₉³⁷Cl₂N₂O₂) [M-H, 10%].

(E)-2-((2-(2,4-difluorophenyl)hydrazono)methyl)benzoic acid (68)

2,4-Difluorophenylhydrazine hydrochloride (151 mg, 0.8 mmol, 1.0 eq.) and sodium hydroxide (33 mg, 0.8 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the solution was stirred at ambient temperature for 20 min. 2-Formylbenzoic acid (126 mg, 0.8 mmol, 1.0 eq.) was added and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and filtered under

vacuum. The crude solid was washed with cold water (2 x 5 mL), cold ethanol (2 x 2 mL), and cold diethyl ether (2 x 2 mL) to afford the desired product as a yellow solid (150 mg, 65%). Mp 176-178 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 13.16 (bs, 1H), 10.49 (s, 1H), 8.82 (s, 1H), 8.07 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.81 (d, *J* = 7.8, 1.2 Hz, 1H), 7.57-7.54 (m, 1H), 7.50 (td, *J* = 9.0, 6.0 Hz, 1H), 7.39 (td, *J* = 7.8, 1.2 Hz, 1H), 7.20 (ddd, *J* = 12.0, 9.0, 3.0 Hz), 7.01-6.98 (m, 1H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 168.6, 154.9 (dd, ¹*J*_{CF} = 237.5 Hz, ³*J*_{CF} = 11.0 Hz), 148.5 (dd, ¹*J*_{CF} = 243.1 Hz, ³*J*_{CF} = 12.1 Hz), 138.0, 135.6, 131.6, 130.4 (dd, ²*J*_{CF} = 9.7 Hz, ⁴*J*_{CF} = 3.0 Hz), 130.1, 129.5, 127.9, 125.9, 114.4 (dd, ³*J*_{CF} = 4.5 Hz, ³*J*_{CF} = 4.5 Hz), 111.5 (dd, ²*J*_{CF} = 21.7 Hz, ⁴*J*_{CF} = 3.4 Hz), 103.9 (dd, ²*J*_{CF} = 27.1 Hz, ²*J*_{CF} = 22.3 Hz). IR (neat) ν_{max}: 3368 (N-H), 3065 (C-H), 2900 (O-H), 1695 (C=O), 1269 (C-F), 1253 (C-F). UPLC-MS t_R 0.766 min, (ESI+) *m/z*: 277 (C₁₄H₁₂F₂N₂O₂) [M+H, 100%]; (ESI-) *m/z*: 275 (C₁₄H₁₀F₂N₂O₂) [M-H, 100%].

(*E*)-2-((2-(4-isopropylphenyl)hydrazono)methyl)benzoic acid (69)

2-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) and (4-isopropylphenyl)hydrazine hydrochloride (123 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (4 mL) in a 2-5 mL μwave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated (in a sand bath) at 100 °C for 18 h. Upon completion, the reaction mixture was reduced by half and chilled at -20 °C for 19 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a golden crystalline solid (26 mg, 14%). Mp 86-88 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 8.57 (s, 1H), 8.32 (d, *J* = 7.9 Hz, 1H), 8.02-7.98 (m, 2H), 7.93-7.90 (m, 1H), 7.51 (d, *J* = 8.4 Hz, 2H), 7.37 (d, *J* = 8.4 Hz, 2H), 2.97 (sept, *J* = 6.9 Hz, 1H), 1.25 (d, *J* = 6.9 Hz, 6H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 158.3, 147.8, 139.7, 138.6, 133.9, 132.3, 129.3, 127.7, 127.0, 126.4 (2C), 126.2, 125.9 (2C), 33.2, 23.9 (2C). IR (neat) ν_{max}: 2955 (N-H), 2896 (C-H), 1757 (C=O). UPLC-MS (80% Solvent B) t_R 1.045 min, (ESI+) *m/z*: 265 (C₁₇H₁₇N₂O) [M+H-H₂O, 100%].

(*E*)-methyl 3-((2-(4-bromophenyl)hydrazono)methyl)benzoate (70)

4-Bromophenylhydrazine hydrochloride (182 mg, 0.8 mmol, 1.0 eq.) and sodium hydroxide (33 mg, 0.8 mmol, 1.0 eq.) were combined with methanol (3 mL) in a 2-5 mL μwave vial. A Teflon-coated stirrer bar was added, and the solution was stirred at ambient temperature for 20 min. Methyl-3-formylbenzoate (133 mg, 0.8 mmol, 1.0 eq.) was added and the vial was capped and irradiated at 120 °C for 20 min. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and filtered under vacuum. The crude solid was washed with cold water (2 x 5 mL), cold ethanol (2 x 2 mL), and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (156 mg, 59%). Mp 200-203 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 10.65 (s, 1H), 8.19 (s, 1H), 7.94 (s, 1H), 7.93 (dt, *J* = 7.8, 1.2 Hz, 1H), 7.87 (dt, *J* = 7.8, 1.2 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 1H), 7.39 (d, *J* = 8.4 Hz, 2H), 7.04 (d, *J* = 8.4 Hz, 2H), 3.88 (s, 3H). 166.1, 144.4, 136.2, 136.2, 131.8 (2C), 130.2, 130.2, 129.2, 128.6, 126.1, 114.1 (2C), 109.9, 52.3. IR (neat) ν_{max}: 3304 (N-H), 2948 (C-H), 1712 (C=O), 1645 (C=O), 752 (C-Br). UPLC-MS (80% Solvent B) t_R 1.484 min, (ESI+) *m/z*: 333 (C₁₅H₁₃⁷⁹BrN₂O₂) [M+H, 100%], *m/z*: 335 (C₁₅H₁₃⁸¹BrN₂O₂) [M+H, 100%]; (ESI-) *m/z*: 331 (C₁₅H₁₃⁷⁹BrN₂O₂) [M-H, 100%], *m/z*: 333 (C₁₅H₁₃⁸¹BrN₂O₂) [M-H, 100%].

(*E*)-methyl 3-((2-(3-bromophenyl)hydrazono)methyl)benzoate (71)

Methyl-3-formylbenzoate (100 mg, 0.61 mmol, 1.0 eq.) and 3-bromophenylhydrazine hydrochloride (144 mg, 0.67 mmol, 1.1 eq.) were combined with methanol (4 mL) in a 2-5 mL μwave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 100 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold methanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford

the desired product as a creamy yellow solid (125 mg, 53%). Mp 150-152 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 10.67 (s, 1H), 8.19 (s, 1H), 7.96-7.95 (m, 2H), 7.88 (d, *J* = 7.7 Hz, 1H), 7.55 (t, *J* = 7.7 Hz, 1H), 7.25 (s, 1H), 7.18 (t, *J* = 8.0 Hz, 1H), 7.04 (d, *J* = 8.0 Hz, 1H), 6.92 (d, *J* = 8.0 Hz, 1H), 3.88 (s, 3H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 166.1, 146.7, 136.9, 136.1, 131.2, 130.3, 130.2, 129.3, 128.7, 126.3, 122.5, 121.4, 114.2, 111.2, 52.3. IR (neat) ν_{max} : 3305 (N-H), 2952 (C-H), 1708 (C=O), 678 (C-Br). UPLC-MS (80% Solvent B) *t*_R 1.330 min, (ESI+) *m/z*: 331 (C₁₅H₁₄⁷⁹BrN₂O₂) [M+H, 75%], *m/z*: 333 (C₁₅H₁₄⁸¹BrN₂O₂) [M+H, 90%]; (ESI-) *m/z*: 331 (C₁₅H₁₂⁷⁹BrN₂O₂) [M-H, 70%], *m/z*: 333 (C₁₅H₁₂⁸¹BrN₂O₂) [M-H, 75%].

(*E*)-methyl 3-((2-(4-isopropylphenyl)hydrazono)methyl)benzoate (72)

Methyl-3-formylbenzoate (100 mg, 0.61 mmol, 1.0 eq.) and (4-isopropylphenyl)hydrazine hydrochloride (125 mg, 0.67 mmol, 1.1 eq.) were combined with methanol (4 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 100 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a golden crystalline solid (51 mg, 26%). Mp 127-129 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 10.39 (s, 1H), 8.17 (s, 1H), 7.89-7.89 (m, 2H), 7.84 (d, *J* = 7.7 Hz, 1H), 7.52 (t, *J* = 7.7 Hz, 1H), 7.11 (d, *J* = 8.5 Hz, 2H), 7.01 (d, *J* = 8.5 Hz, 2H), 3.88 (s, 3H), 2.80 (hept, *J* = 6.9 Hz, 1H), 1.17 (d, *J* = 6.9 Hz, 6H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 166.2, 143.1, 139.1, 136.7, 134.5, 130.1, 129.9, 129.2, 128.1, 126.9 (2C), 125.8, 112.1 (2C), 52.3, 32.7, 24.2 (2C). IR (neat) ν_{max} : 3300 (N-H), 2954 (C-H), 1695 (C=O), 1648. UPLC-MS (80% Solvent B) *t*_R 1.715 min, (ESI+) *m/z*: 297 (C₁₈H₂₀N₂O₂) [M-H, 100%]; (ESI-) *m/z*: 295 (C₁₈H₁₈N₂O₂) [M-H, 100%].

(*E*)-methyl 3-((2-(4-chlorophenyl)hydrazono)methyl)benzoate (73)

4-Chlorophenylhydrazine hydrochloride (147 mg, 0.8 mmol, 1.0 eq.) and sodium hydroxide (33 mg, 0.8 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the solution was stirred at ambient temperature for 20 min. Methyl-3-formylbenzoate (133 mg, 0.8 mmol, 1.0 eq.) was added and the vial was capped and irradiated at 120 °C for 20 min. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and filtered under vacuum. The crude solid was washed with cold water (2 x 5 mL), cold ethanol (2 x 2 mL), and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (185 mg, 79%). Mp 199-201 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 10.64 (s, 1H), 8.20 (t, *J* = 1.8 Hz, 1H), 7.94 (s, 1H), 7.93 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.87 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 1H), 7.27 (d, *J* = 7.2 Hz, 2H), 7.09 (d, *J* = 7.2 Hz, 2H), 3.88 (s, 3H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 166.1, 144.0, 136.3, 136.1, 130.2, 130.2, 129.2, 129.0, 128.5, 126.1, 122.3, 113.6, 52.3. IR (neat) ν_{max} : 3307 (N-H), 2948 (C-H), 1712 (C=O). UPLC-MS (80% Solvent B) *t*_R 1.366 min, (ESI+) *m/z*: 289 (C₁₅H₁₄³⁵ClN₂O₂) [M+H, 100%], *m/z*: 291 (C₁₅H₁₄³⁷ClN₂O₂) [M+H, 35%]; (ESI-) *m/z*: 287 (C₁₅H₁₂³⁵ClN₂O₂) [M-H, 100%], *m/z*: 289 (C₁₅H₁₂³⁷ClN₂O₂) [M-H, 35%].

(*E*)-methyl 3-((2-(2,4-dichlorophenyl)hydrazono)methyl)benzoate (74)

2,4-Dichlorophenylhydrazine hydrochloride (172 mg, 0.8 mmol, 1.0 eq.) and sodium hydroxide (35 mg, 0.9 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the solution was stirred at ambient temperature for 20 min. Methyl-3-formylbenzoate (131 mg, 0.8 mmol, 1.0 eq.) was added and the vial was capped and irradiated at 120 °C for 20 min. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and filtered under vacuum. The crude solid was washed with cold water (2 x 5 mL), cold ethanol (2 x 2 mL), and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (110 mg, 43%). Mp 179-181 °C.

¹H NMR (600 MHz, DMSO-*d*₆) δ 10.20 (s, 1H), 8.36 (s, 1H), 8.19 (t, *J* = 1.8 Hz, 1H), 7.95 (dt, *J* = 7.8, 1.2 Hz, 1H), 7.92 (dt, *J* = 7.8, 1.2 Hz, 1H), 7.58-7.55 (m, 2H), 7.48 (d, *J* = 2.4 Hz, 1H), 7.34 (dd, *J* = 9.0, 2.4 Hz, 1H), 3.89 (s, 3H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 166.0, 140.4, 140.0, 135.9, 130.6, 130.2, 129.4, 129.1, 128.7, 128.2, 122.6, 116.9, 115.2, 52.3. IR (neat) ν_{max} : 3326 (N-H), 2959 (C-H), 1721 (C=O). UPLC-MS (80% Solvent B) *t*_R 2.371 min, (ESI+) *m/z*: 323 (C₁₅H₁₃³⁵Cl₂N₂O₂) [M+H, 100%], *m/z*: 325 (C₁₅H₁₃³⁵Cl³⁷ClN₂O₂) [M+H, 75%], *m/z*: 327 (C₁₅H₁₃³⁷Cl₂N₂O₂) [M+H, 10%]; (ESI-) *m/z*: 321 (C₁₅H₁₁³⁵Cl₂N₂O₂) [M-H, 100%], *m/z*: 323 (C₁₅H₁₁³⁵Cl³⁷ClN₂O₂) [M-H, 75%], *m/z*: 325 (C₁₅H₁₁³⁷Cl₂N₂O₂) [M-H, 10%].

(*E*)-methyl 3-((2-(2,4-difluorophenyl)hydrazono)methyl)benzoate (75)

2,4-Difluorophenylhydrazine hydrochloride (145 mg, 0.8 mmol, 1.0 eq.) and sodium hydroxide (33 mg, 0.8 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the solution was stirred at ambient temperature for 20 min. Methyl-3-formylbenzoate (130 mg, 0.8 mmol, 1.0 eq.) was added and the vial was capped and irradiated at 120 °C for 20 min. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and filtered under vacuum. The crude solid was washed with cold water (2 x 5 mL), cold ethanol (2 x 2 mL), and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (159 mg, 70%). Mp 186-188 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 10.38 (s, 1H), 8.17 (t, *J* = 1.8 Hz, 1H), 8.17 (s, 1H), 7.92 (dt, *J* = 7.8, 1.2 Hz, 1H), 7.89 (dt, *J* = 7.8, 1.2 Hz, 1H), 7.55 (t, *J* = 7.8 Hz, 1H), 7.50 (td, *J* = 9.6, 5.4 Hz, 1H), 7.25-7.21 (m, 1H), 7.05-7.01 (m, 1H), 3.88 (s, 1H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 166.1, 154.9 (dd, ¹*J*_{CF} = 237.1, ³*J*_{CF} = 10.6 Hz), 148.5 (dd, ¹*J*_{CF} = 243.1, ³*J*_{CF} = 12.1 Hz), 138.2, 136.1, 130.3, 130.2 (dd, ³*J*_{CF} = 10.6, ³*J*_{CF} = 3.0 Hz), 130.2, 129.3, 128.7, 126.1, 114.3 (dd, ³*J*_{CF} = 9.6, ³*J*_{CF} = 4.5 Hz), 111.5 (dd, ²*J*_{CF} = 22.7, ³*J*_{CF} = 3.0 Hz), 103.9 (dd, ²*J*_{CF} = 27.2, ²*J*_{CF} = 22.7 Hz), 52.3. ¹⁹F NMR (376 MHz, DMSO-*d*₆, TFA) δ -121.53, -127.48. IR (neat) ν_{max} : 3323 (N-H), 2971 (C-H), 1714 (C=O), 751 (C-F). UPLC-MS (80% Solvent B) *t*_R 1.227 min, (ESI+) *m/z*: 291 (C₁₅H₁₃F₂N₂O₂) [M+H, 100%]; (ESI-) *m/z*: 289 (C₁₅H₁₁F₂N₂O₂) [M-H, 100%].

(*E*)-methyl 3-((2-(3-chloro-4-methylphenyl)hydrazono)methyl)benzoate (76)

3-Chloro-4-methylphenylhydrazine hydrochloride (153 mg, 0.8 mmol, 1.0 eq.) and sodium hydroxide (34 mg, 0.9 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the solution was stirred at ambient temperature for 20 min. Methyl-3-formylbenzoate (129 mg, 0.8 mmol, 1.0 eq.) was added and the vial was capped and irradiated at 120 °C for 20 min. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and filtered under vacuum. The crude solid was washed with cold water (2 x 5 mL), cold ethanol (2 x 2 mL), and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (182 mg, 76%). Mp 176-178 °C. ¹H NMR (600 MHz, CDCl₃) δ 8.21 (s, 1H), 7.96 (d, *J* = 7.8 Hz, 1H), 7.91 (d, *J* = 7.8 Hz, 1H), 7.87 (s, 1H), 7.45 (t, *J* = 7.2 Hz, 1H), 7.19 (s, 1H), 7.10 (d, *J* = 8.4 Hz, 1H), 6.88 (d, *J* = 7.8 Hz, 1H), 3.95 (s, 3H), 2.30 (s, 3H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 167.0, 143.5, 136.6, 135.7, 135.2, 131.5, 130.8, 130.2, 129.6, 128.9, 127.7, 127.5, 113.5, 111.4, 52.4, 19.3. IR (neat) ν_{max} : 3296 (N-H), 2952 (C-H), 2921 (C-H), 1704 (C=O). UPLC-MS (80% Solvent B) *t*_R 1.790 min, (ESI+) *m/z*: 303 (C₁₆H₁₄³⁵ClN₂O₂) [M+H, 100%], *m/z*: 305 (C₁₆H₁₄³⁷ClN₂O₂) [M+H, 35%]; (ESI-) *m/z*: 301 (C₁₆H₁₂³⁵ClN₂O₂) [M-H, 100%], *m/z*: 303 (C₁₆H₁₂³⁷ClN₂O₂) [M-H, 35%].

(*E*)-methyl 3-((2-(4-bromobenzoyl)hydrazono)methyl)benzoate (77)

Methyl-3-formyl benzoate (164 mg, 1.0 mmol, 1.1 eq.) and 4-bromobenzhydrazide (196 mg, 0.91 mmol, 1.0 eq.) were combined with ethanol (40 mL) in a 100 mL round-bottomed flask. A Teflon-coated stirrer bar was added, and the reaction was heated at 100 °C for 19 h. Upon completion, the

reaction mixture was chilled at -20 °C for 3 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 5 mL) and cold diethyl ether (2 x 5 mL) to afford the desired product as a fluffy white solid (230 mg, 70%). Mp 179-180 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.05 (s, 1H), 8.51 (s, 1H), 8.36 (s, 1H), 8.01 (d, *J* = 7.7 Hz, 1H), 7.97 (d, *J* = 7.7 Hz, 1H), 7.88 (d, *J* = 8.4 Hz, 2H), 7.77 (d, *J* = 8.4 Hz, 2H), 7.63 (t, *J* = 7.7 Hz, 1H), 3.90 (s, 3H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 165.9, 162.4, 146.9, 134.9, 132.3, 132.2, 131.6 (2C), 130.5, 130.3, 129.8 (2C), 129.5, 127.0, 125.7, 52.4. IR (neat) ν_{max} : 3205 (N-H, amine), 3063 (C-H), 1722 (C=O), 1645 (C=O), 750 (C-Br). UPLC-MS (50% Solvent B) *t*_R 2.133 min, (ESI+) *m/z*: 361 (C₁₆H₁₄⁷⁹BrN₂O₃) [M+H, 100%], *m/z*: 363 (C₁₆H₁₄⁸¹BrN₂O₃) [M+H, 100%]; (ESI-) *m/z*: 359 (C₁₆H₁₂⁷⁹BrN₂O₃) [M-H, 100%], *m/z*: 361 (C₁₆H₁₂⁸¹BrN₂O₃) [M-H, 100%].

(*E*)-methyl 3-((2-(3-bromobenzoyl)hydrazono)methyl)benzoate (78)

Methyl-3-formyl benzoate (100 mg, 0.61 mmol, 1.0 eq.) and 3-bromobenzhydrazide (144 mg, 0.67 mmol, 1.1 eq.) were combined with methanol (4 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated (in a sand bath) at 100 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold methanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (154 mg, 70%). Mp 146-147 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 12.07 (s, 1H), 8.50 (s, 1H), 8.36 (s, 1H), 8.10 (s, 1H), 8.02 (d, *J* = 7.7 Hz, 1H), 7.98 (d, *J* = 7.7 Hz, 1H), 7.93 (d, *J* = 7.9 Hz, 1H), 7.82 (d, *J* = 7.9 Hz, 1H), 7.63 (t, *J* = 7.7 Hz, 1H), 7.52 (t, *J* = 7.9 Hz, 1H), 3.90 (s, 3H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 165.9, 161.8, 147.2, 135.5, 134.8, 134.6, 132.2, 130.8, 130.5, 130.3, 130.2, 129.5, 127.1, 126.9, 121.8, 52.4. IR (neat) ν_{max} : 3300 (N-H, amine), 2961 (C-H), 1724 (C=O), 1640 (C=O), 751 (C-Br). UPLC-MS (80% Solvent B) *t*_R 0.708 min, (ESI-) *m/z*: 359 (C₁₆H₁₂⁷⁹BrN₂O₃) [M-H, 100%]; *m/z*: 361 (C₁₆H₁₂⁸¹BrN₂O₃) [M-H, 100%].

(*E*)-methyl 3-((2-(nicotinoyl)hydrazono)methyl)benzoate (79)

Methyl-3-formyl benzoate (180 mg, 1.1 mmol, 1.1 eq.) and pyridine-3-carbohydrazide (137 mg, 1.0 mmol, 1.0 eq.) were combined with methanol (40 mL) in a 100 mL round-bottomed flask. A Teflon-coated stirrer bar was added, and the reaction was heated at 100 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 3 h and filtered under vacuum. The crude solid was washed with cold methanol (2 x 5 mL) and cold diethyl ether (2 x 5 mL) to afford the desired product as a crystalline white solid (258 mg, 91%). Mp 165-166 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 12.16 (s, 1H), 9.08 (s, 1H), 8.78 (d, *J* = 4.0 Hz, 1H), 8.51 (s, 1H), 8.37 (s, 1H), 8.27 (d, *J* = 7.6 Hz, 1H), 8.02 (d, *J* = 7.7 Hz, 1H), 7.99 (d, *J* = 7.7 Hz, 1H), 7.63 (t, *J* = 7.7 Hz, 1H), 7.58 (d, *J* = 7.6, 4.0 Hz, 1H), 3.90 (s, 3H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 165.9, 161.9, 152.4, 148.6, 147.2, 135.6, 134.8, 132.2, 130.6, 130.3, 129.5, 129.1, 127.1, 123.7, 52.4. IR (neat) ν_{max} : 3179 (N-H, amine), 3025 (C-H), 1725 (C=O), 1652 (C=O). UPLC-MS (80% Solvent B) *t*_R 0.519 min, (ESI+) *m/z*: 284 (C₁₅H₁₄N₃O₃) [M+H, 100%]; (ESI-) *m/z*: 282 (C₁₅H₁₂N₃O₃) [M-H, 100%].

(*E*)-methyl 3-((2-(4-isopropylbenzoyl)hydrazono)methyl)benzoate (80)

Methyl-3-formylbenzoate (82 mg, 0.5 mmol, 1.0 eq.) and (4-isopropyl)benzhydrazide (89 mg, 0.5 mmol, 1.0 eq.) were combined with ethanol (4 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 100 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (115 mg, 74%). Mp 189-191 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 11.92 (s, 1H), 8.51 (s, 1H), 8.36 (s, 1H), 8.00 (d, *J* = 7.7 Hz, 1H), 7.96 (d, *J* = 7.7 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 2H), 7.62 (t, *J* = 7.7 Hz, 1H), 7.41 (d, *J* = 8.0 Hz, 2H), 3.90 (s, 3H), 2.97 (sept, *J* = 6.9 Hz, 1H), 1.24 (d, *J* = 6.9 Hz, 6H). ¹³C

NMR (151 MHz, DMSO-*d*₆) δ 165.9, 163.2, 152.6, 146.3, 135.1, 132.1, 130.9, 130.32, 130.25, 129.5 (2C), 127.8, 126.9, 126.5 (2C), 52.4, 33.5, 23.6 (2C). IR (neat) ν_{max} : 2964 (N-H), 2880 (C-H), 1723 (C=O), 1648 (C=O). UPLC-MS (80% Solvent B) t_R 0.789 min, (ESI-) m/z : 323 (C₁₉H₁₉N₂O₃) [M-H, 100%].

(E)-methyl 3-((2-(1H-pyrrole-2-carbonyl)hydrazono)methyl)benzoate (81)

Methyl-3-formylbenzoate (82 mg, 0.5 mmol, 1.0 eq.) and 1H-pyrrole-2-carbohydrazide (63 mg, 0.5 mmol, 1.0 eq.) were combined with methanol (4 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 100 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold methanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (62 mg, 46%). Mp 198-200 °C. ¹H NMR (600 MHz, DMSO-*d*₆) δ 11.75 (s, 1H), 11.57 (s, 1H), 8.41 (s, 1H), 8.32 (s, 1H), 8.00-7.97 (m, 1H), 7.94 (d, J = 7.4 Hz, 1H), 7.62 (t, J = 7.7 Hz, 1H), 6.99 (s, 1H), 6.19 (s, 1H), 3.90 (s, 3H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 165.9 (2C), 135.2, 130.2 (2C), 130.0 (2C), 129.4 (2C), 123.0 (2C), 109.1 (2C), 52.4. IR (neat) ν_{max} : 3295 (C-H), 3259 (C-H), 2952 (N-H), 1710 (C=O), 1626 (C=O). UPLC-MS (80% Solvent B) t_R 0.562 min, (ESI+) m/z : 272 (C₁₄H₁₄N₃O₃) [M+H, 85%], (ESI-) m/z : 270 (C₁₄H₁₂N₃O₃) [M-H, 100%], m/z : 306 (C₁₄H₁₂N₃O₃Cl) [M-H+Cl, 100%].

(E)-ethyl 3-((2-(4-isopropylphenyl)hydrazono)methyl)benzoate (82)

3-Formylbenzoic acid (985 mg, 6.57 mmol, 1.0 eq.), (4-isopropylphenyl)hydrazine hydrochloride (1351 mg, 7.23 mmol, 1.1 eq.) and ethanol (15 mL) were combined in a 10-20 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 80 °C for 4 h. Upon completion, the crude mixture was dried *in vacuo*, loaded onto silica and purified by column chromatography (0-10% MeOH in DCM + 1% acetic acid) to afford the desired product as an orange solid (688 mg, 35%). Mp 128-130 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 10.39 (s, 1H), 8.17 (s, 1H), 7.87 (dd, J = 22.3, 6.9 Hz, 3H), 7.52 (t, J = 7.7 Hz, 1H), 7.06 (dd, J = 39.1, 8.5 Hz, 4H), 4.34 (q, J = 6.9 Hz, 2H), 2.79 (dt, J = 13.7, 6.9 Hz, 1H), 1.34 (t, J = 6.9 Hz, 3H), 1.17 (d, J = 6.9 Hz, 6H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 165.7, 143.1, 139.1, 136.6, 134.6, 130.4, 129.8, 129.1, 128.1, 126.9 (2C), 125.8, 112.1 (2C), 60.9, 32.7, 24.2 (2C), 14.2. IR (neat) ν_{max} : 3297 (C-H), 2958 (N-H), 1699 (C=O), 1568 (C-C). UPLC-MS (80% Solvent B) t_R 2.436 min, (ESI+) m/z : 310 (C₁₉H₂₂N₂O₂) [M, 100%]; (ESI-) m/z : 308 (C₁₉H₂₀N₂O₂) [M-2H, 100%], m/z : 344 (C₁₉H₂₀N₂O₂Cl) [M-2H+Cl, 100%].

(E)-ethyl 3-((2-(4-chlorophenyl)hydrazono)methyl)benzoate (83)

3-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.), 4-chlorophenylhydrazine hydrochloride (118 mg, 0.66 mmol, 1.1 eq.) and ethanol (3 mL) were combined in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 1 mL) and cold diethyl ether (2 x 1 mL) to afford the desired product as a white solid (47 mg, 26%). Mp 167-169 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 10.62 (s, 1H), 8.19 (s, 1H), 7.93 (d, J = 5.6 Hz, 2H), 7.89-7.85 (m, 1H), 7.54 (t, J = 7.7 Hz, 1H), 7.30-7.24 (m, 2H), 7.12-7.06 (m, 2H), 4.35 (q, J = 7.1 Hz, 2H), 1.35 (t, J = 7.1 Hz, 3H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 165.6, 144.0, 136.2, 136.2, 130.5, 130.1, 129.2 (2C), 129.0, 128.5, 126.1, 122.3, 113.56 (2C), 60.9, 14.2. IR (neat) ν_{max} : 3293 (C-H), 2995 (N-H), 1694 (C=O), 1530 (C-C), 753 (C-Cl). UPLC-MS (80% Solvent B) t_R 1.727 min, (ESI-) m/z : 300 (C₁₆H₁₃³⁵ClN₂O₂) [M-2H, 100%], m/z : 302 (C₁₆H₁₃³⁷ClN₂O₂) [M-2H, 35%].

(E)-ethyl 3-((2-(4-bromophenyl)hydrazono)methyl)benzoate (84)

3-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.), 4-bromophenylhydrazine hydrochloride (134 mg, 0.66 mmol, 1.1 eq.) and ethanol (3 mL) were combined in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 1 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 1 mL) and cold diethyl ether (2 x 1 mL) to afford the desired product as a white solid (73 mg, 26%). Mp 170-172 °C. ^1H NMR (400 MHz, DMSO- d_6) δ 10.63 (s, 1H), 8.19 (s, 1H), 7.93 (d, J = 6.3 Hz, 2H), 7.88 (dt, J = 7.8, 1.3 Hz, 1H), 7.54 (t, J = 7.7 Hz, 1H), 7.45-7.33 (m, 2H), 7.09-7.01 (m, 2H), 4.35 (q, J = 7.1 Hz, 2H), 1.35 (t, J = 7.1 Hz, 3H). ^{13}C NMR (151 MHz, DMSO- d_6) δ 165.6, 144.4, 136.3, 136.2, 131.8 (2C), 130.4, 130.1, 129.2, 128.5, 126.1, 114.1 (2C), 109.9, 60.9, 14.2. IR (neat) ν_{max} : 3288 (N-H), 1695 (C=O), 1529 (C-C), 753 (C-Br). UPLC-MS (80% Solvent B) t_{R} 1.885 min, (ESI-) m/z : 346 ($\text{C}_{16}\text{H}_{14}^{79}\text{BrN}_2\text{O}_2$) [M-H, 100%], m/z : 348 ($\text{C}_{16}\text{H}_{14}^{81}\text{BrN}_2\text{O}_2$) [M-H, 100%].

(E)-3-((2-(1-phenyl-5-(trifluoromethyl)-1H-pyrazole-4-carbonyl)hydrazono)methyl)benzoic acid (S1)

3-Formylbenzoic acid (100 mg, 0.7 mmol, 1.0 eq.) and 1-phenyl-5-(trifluoromethyl)-1H-pyrazole-4-carbohydrazide (183 mg, 0.7 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and irradiated at 120 °C for 20 min. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (230 mg, 85%). Mp 270-272 °C. ^1H NMR (600 MHz, DMSO- d_6) δ 13.14 (bs, 1H), 12.13 (s, 1H), 8.40 (s, 1H), 8.34 (s, 1H), 8.29 (s, 1H), 8.01 (d, J = 7.8 Hz, 1H), 7.96 (d, J = 7.8 Hz, 1H), 7.64-7.54 (m, 6H). ^{13}C NMR (151 MHz, DMSO- d_6) δ 166.9, 163.0, 147.0, 139.8, 138.7, 134.5, 131.6, 131.5, 130.8, 130.2, 129.8 (q, $^2J_{\text{CF}}$ = 39.3 Hz), 129.5, 129.3, 127.5, 126.0, 119.6, 119.3 (q, $^1J_{\text{CF}}$ = 271.8 Hz). ^{19}F NMR (376 MHz, DMSO- d_6 , TFA) δ -52.67. IR (neat) ν_{max} : 3035 (N-H), 3000 (O-H), 1684 (C=O), 1645 (C=O), 1136 (C-F). UPLC-MS (80% Solvent B) t_{R} 0.556 min, (ESI+) m/z : 403 ($\text{C}_{19}\text{H}_{14}\text{F}_3\text{N}_4\text{O}_3$) [M+H, 100%]; (ESI-) m/z : 401 ($\text{C}_{19}\text{H}_{12}\text{F}_3\text{N}_4\text{O}_3$) [M-H, 100%].

* ^1H NMR (600 MHz, DMSO- d_6) δ 13.14 (bs, 1H), 12.15 (s, 1H), 8.22 (s, 1H), 8.19 (s, 1H), 8.18 (s, 1H), 7.96 (d, J = 7.8 Hz, 1H), 7.81 (d, J = 7.8 Hz, 1H), 7.64-7.54 (m, 6H). ^{13}C NMR (151 MHz, DMSO- d_6) δ 167.0, 156.8, 143.4, 140.4, 138.6, 134.3, 131.7, 131.3, 130.5, 130.1, 129.8 (q, J = 39.3 Hz), 129.5, 129.2, 127.0, 126.1, 119.4 (q, J = 271.8 Hz), 118.9. ^{19}F NMR (376 MHz, DMSO- d_6 , TFA) δ -53.43.

(E)-3-((2-(3-(2,5-dimethyl-1H-pyrrol-1-yl)thiophene-2-carbonyl)hydrazono)methyl)benzoic acid (S2)

3-Formylbenzoic acid (100 mg, 0.7 mmol, 1.0 eq.) and 3-(2,5-dimethyl-1H-pyrrol-1-yl)-2-thiophenecarbohydrazide (161 mg, 0.7 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and irradiated at 120 °C for 20 min. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a yellow solid (172 mg, 76%). Mp 220-223 °C. ^1H NMR (600 MHz, methanol- d_4) δ 8.25 (s, 1H), 8.08 (d, J = 7.8 Hz, 1H), 8.06 (d, J = 7.8 Hz, 1H), 7.86 (d, J = 5.4 Hz, 1H), 7.51 (t, J = 7.8 Hz, 1H), 7.41 (s, 1H), 7.15 (d, J = 4.8 Hz, 1H), 6.17 (s, 2H), 2.05 (s, 6H). ^{13}C NMR (151 MHz, methanol- d_4) δ 168.6, 157.8, 148.9, 137.4, 134.0, 134.0, 132.4, 133.0, 131.9, 131.7, 130.3, 129.6, 129.4, 129.0, 108.8, 12.5. IR (neat) ν_{max} : 3039 (N-H), 2937 (C-H), 2900 (O-H), 1682 (C=O), 1632 (C=O).

UPLC-MS (80% Solvent B) t_R 0.661 min, (ESI+) m/z : 368 ($C_{19}H_{17}N_3O_3S$) [M+H, 100%], (ESI-) m/z : 366 ($C_{19}H_{17}N_3O_3S$) [M-H, 100%].

(E)-3-((2-(furan-2-carbonyl)hydrazono)methyl)benzoic acid (S3)

3-Formylbenzoic acid (90 mg, 0.6 mmol, 1.0 eq.) and furan-2-carbohydrazide (83 mg, 0.66 mmol, 1.1 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and heated in a sand bath at 50 °C for 19 h. Upon completion, the reaction mixture was chilled at -20 °C for 3 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 5 mL) and cold diethyl ether (2 x 5 mL) to afford the desired product as a creamy-coloured solid (133 mg, 85%). Mp 265-267 °C. 1H NMR (600 MHz, DMSO- d_6) δ 13.16 (bs, 1H), 11.96 (s, 1H), 8.50 (s, 1H), 8.30 (s, 1H), 7.99 (dt, J = 7.8, 1.2 Hz, 1H), 7.96 (s, 1H), 7.93 (d, J = 7.4 Hz, 1H), 7.59 (t, J = 7.8 Hz, 1H), 7.32 (s, 1H), 6.72 (s, 1H). ^{13}C NMR (151 MHz, DMSO- d_6) δ 166.9, 154.3, 146.9, 146.5, 146.0, 134.7, 131.5, 131.4, 130.6, 129.3, 127.4, 115.2, 112.2. IR (neat) ν_{max} : 3085 (N-H), 3000 (O-H), 1695 (C=O), 1670 (C=O). UPLC-MS (50% Solvent B) t_R 0.651 min, (ESI+) m/z : 259 ($C_{13}H_{11}N_2O_4$) [M+H, 100%], (ESI-) m/z : 257 ($C_{13}H_9N_2O_4$) [M-H, 100%].

(E)-3-((2-(benzo[b]thiophene-2-carbonyl)hydrazono)methyl)benzoic acid (S4)

3-Formylbenzoic acid (101 mg, 0.7 mmol, 1.0 eq.) and benzo[b]thiophene-2-carbohydrazide (132 mg, 0.7 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and irradiated at 120 °C for 20 min. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (191 mg, 88%). Mp 277-280 °C. 1H NMR (600 MHz, DMSO- d_6) δ 13.16 (bs, 1H), 12.15 (s, 1H), 8.45 (s, 1H), 8.41 (s, 1H), 8.24 (s, 1H), 8.14 (d, J = 7.8 Hz, 1H), 8.08-7.97 (m, 3H), 7.66 (t, J = 8.4 Hz, 1H), 7.52-7.48 (m, 2H). ^{13}C NMR (151 MHz, DMSO- d_6) δ 167.0, 158.4, 147.2, 140.4, 139.1, 138.2, 134.6, 131.8, 131.5, 130.8, 129.3, 127.6, 126.7, 126.0, 125.5, 125.2, 122.9. IR (neat) ν_{max} : 3273 (N-H), 2900 (O-H), 1684 (C=O), 1626 (C=O), 748 (C-S). UPLC-MS (80% Solvent B) t_R 0.580 min, (ESI+) m/z : 325 ($C_{17}H_{13}N_2O_3S$) [M+H, 100%], m/z : 347 ($C_{17}H_{12}N_2O_3SNa$) [M+Na, 100%], m/z : 363 ($C_{17}H_{12}N_2O_3SK$) [M+K, 50%], (ESI-) m/z : 323 ($C_{17}H_{11}N_2O_3S$) [M-H, 100%].

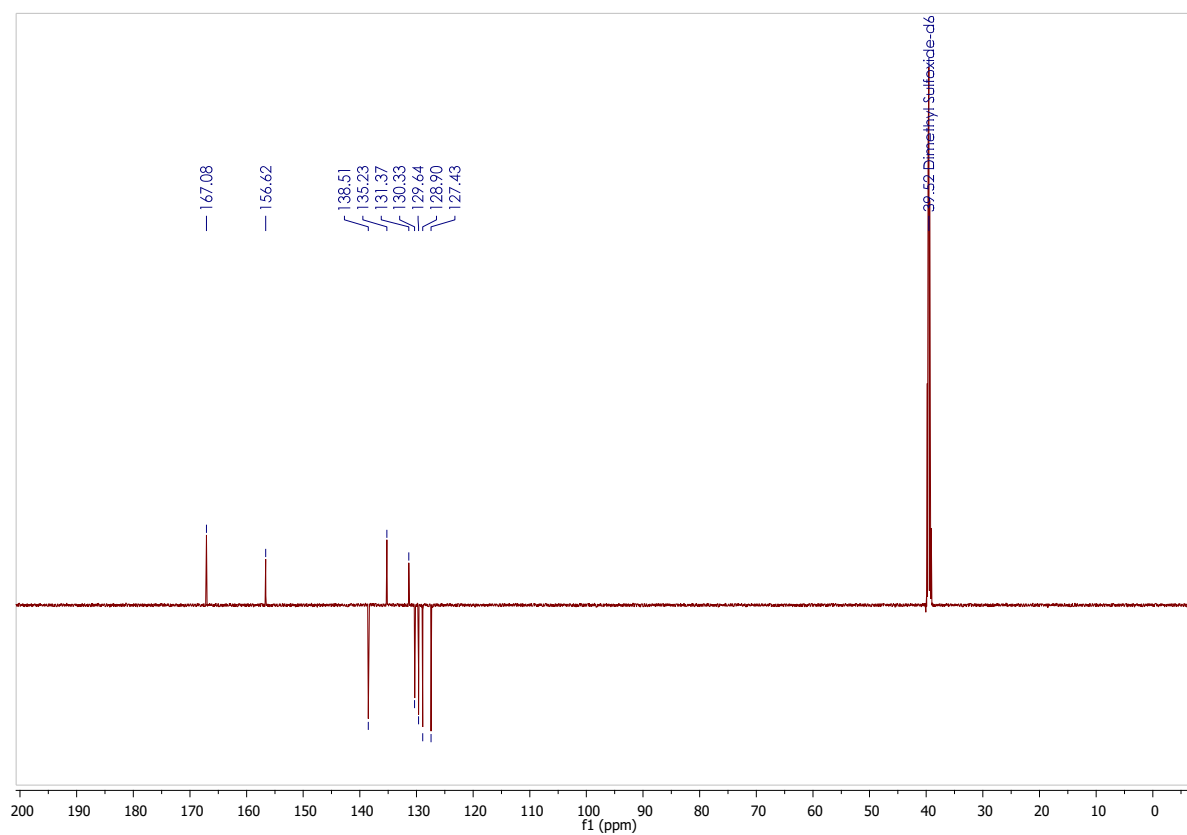
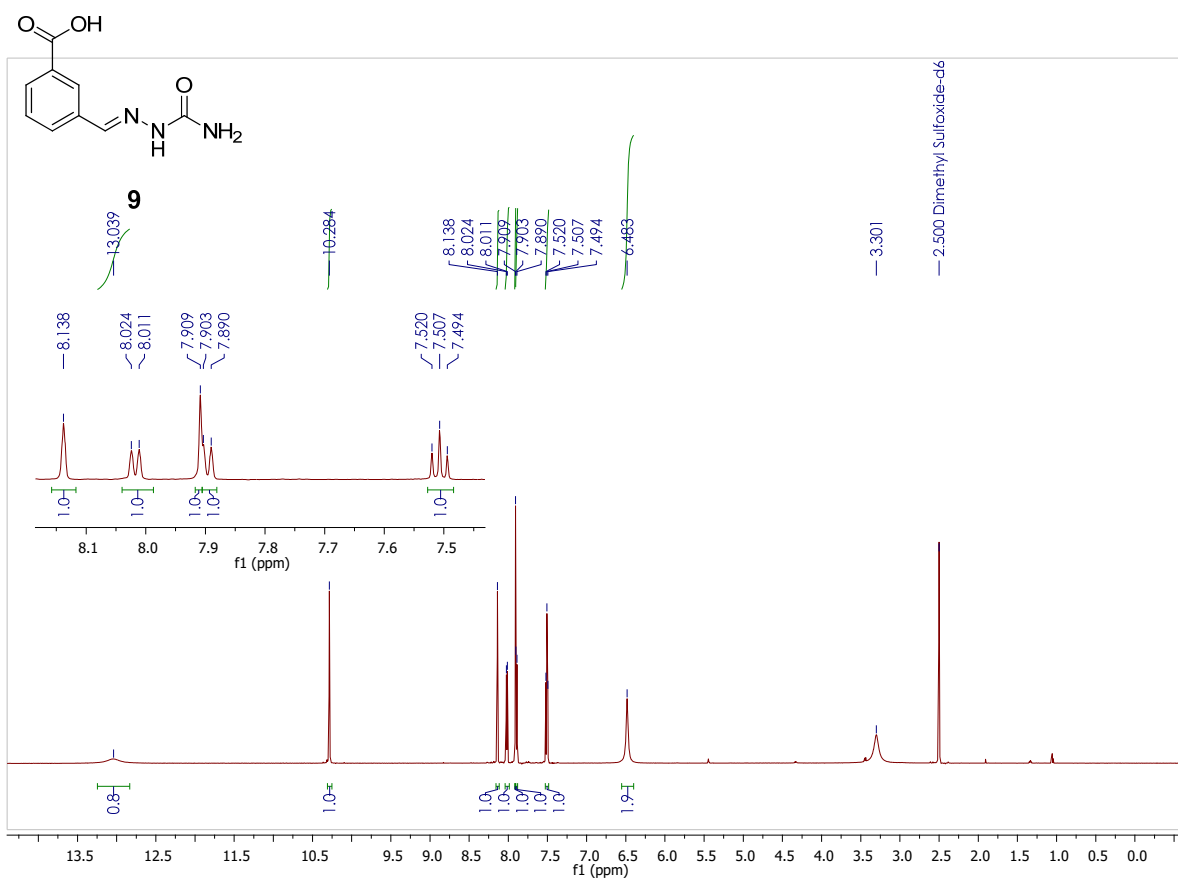
* 1H NMR (600 MHz, DMSO- d_6) δ 13.16 (bs, 1H), 12.27 (s, 1H), 8.53 (s, 1H), 8.35 (s, 1H), 8.28 (s, 1H), 8.08-7.97 (m, 4H), 7.62 (t, J = 7.8 Hz, 1H), 7.52-7.48 (m, 2H). ^{13}C NMR (151 MHz, DMSO- d_6) δ 161.8, 143.9, 143.0, 140.5, 137.4, 134.5, 133.3, 132.0, 131.9, 131.0, 130.7, 129.5, 128.6, 126.9, 125.7, 125.0, 122.5.

(E)-3-((2-(2-(3-(pyrazin-2-yl)-1,2,4-oxadiazol-5-yl)acetyl)hydrazono)methyl)benzoic acid (S5)

3-Formylbenzoic acid (102 mg, 0.7 mmol, 1.0 eq.) and 2-(3-pyrazin-2-yl-1,2,4-oxadiazol-5-yl)ethanohydrazide (150 mg, 0.7 mmol, 1.0 eq.) were combined with ethanol (3 mL) in a 2-5 mL μ wave vial. A Teflon-coated stirrer bar was added, and the vial was capped and irradiated at 120 °C for 20 min. Upon completion, the reaction mixture was chilled at -20 °C for 19 h and filtered under vacuum. The crude solid was washed with cold ethanol (2 x 2 mL) and cold diethyl ether (2 x 2 mL) to afford the desired product as a white solid (219 mg, 91%). Mp 245-248 °C. 1H NMR (600 MHz, DMSO- d_6) δ 13.04 (bs, 1H), 11.93 (s, 1H), 9.26 (d, J = 1.2 Hz, 1H), 8.89-8.85 (m, 2H), 8.19 (s, 1H), 8.10 (s, 1H), 7.95 (d, J = 7.8 Hz, 1H), 7.90 (d, J = 7.8 Hz, 1H), 7.53 (t, J = 7.8 Hz, 1H), 4.64 (s, 2H). ^{13}C NMR (151 MHz, DMSO- d_6) δ 176.2, 167.2, 166.9, 166.2, 147.2, 145.3, 143.8, 143.6, 141.5, 134.2, 131.7, 130.8, 130.6, 129.1, 127.6, 32.4. IR (neat) ν_{max} : 3274 (N-H), 3080 (C-H), 3000 (O-H), 1687 (C=O), 1677 (C=O). UPLC-MS (80% Solvent B) t_R 0.480 min, (ESI+) m/z : 353 ($C_{16}H_{12}N_6O_4$) [M+H, 35%], m/z : 375

(C₁₆H₁₂N₆O₄Na) [M+Na, 100%], *m/z*: 391 (C₁₆H₁₂N₆O₄K) [M+K, 35%]; (ESI-) *m/z*: 351 (C₁₆H₁₁N₆O₄) [M-H, 100%].

* ¹H NMR (600 MHz, DMSO-*d*₆) δ 13.04 (bs, 1H), 12.04 (s, 1H), 9.27 (d, *J* = 1.2 Hz, 1H), 8.89-8.85 (m, 2H), 8.31 (s, 1H), 8.30 (s, 1H), 7.99 (d, *J* = 7.8 Hz, 1H), 7.95 (d, *J* = 7.8 Hz, 1H), 7.58 (t, *J* = 7.8 Hz, 1H), 4.28 (s, 2H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 175.7, 166.9, 166.3, 161.3, 147.2, 146.8, 145.3, 143.8, 141.5, 134.4, 131.6, 131.4, 130.8, 129.2, 127.7, 33.3.

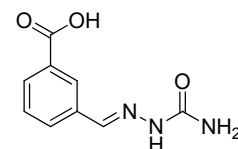


LCMS Report



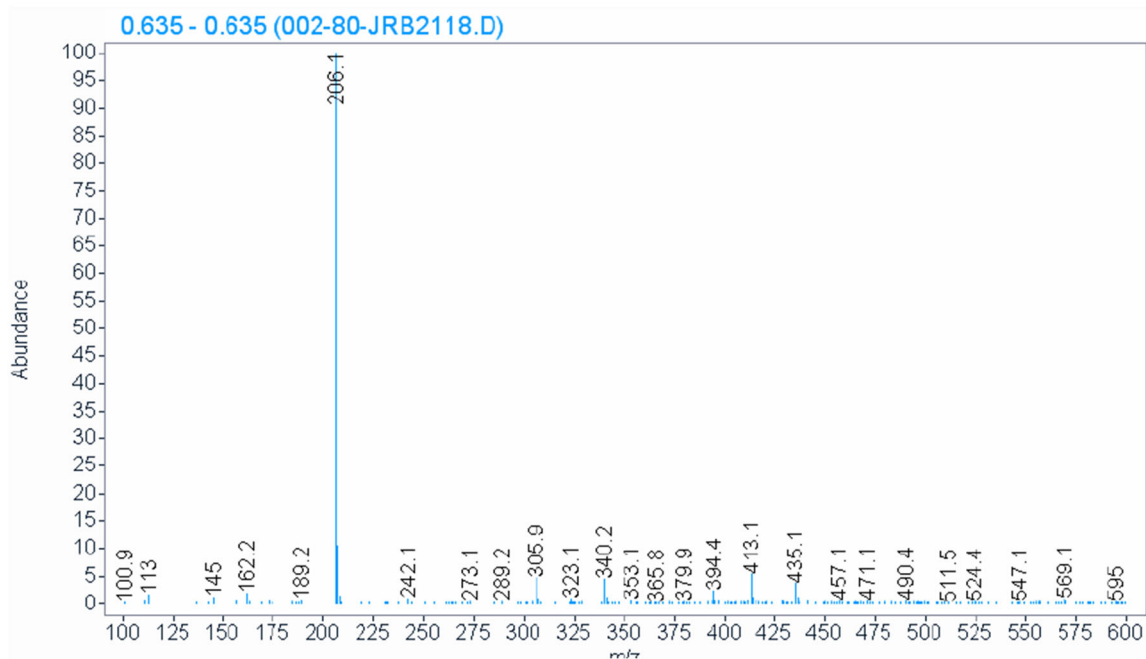
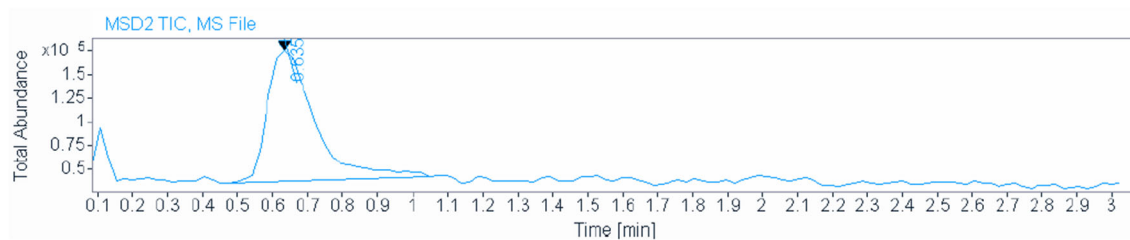
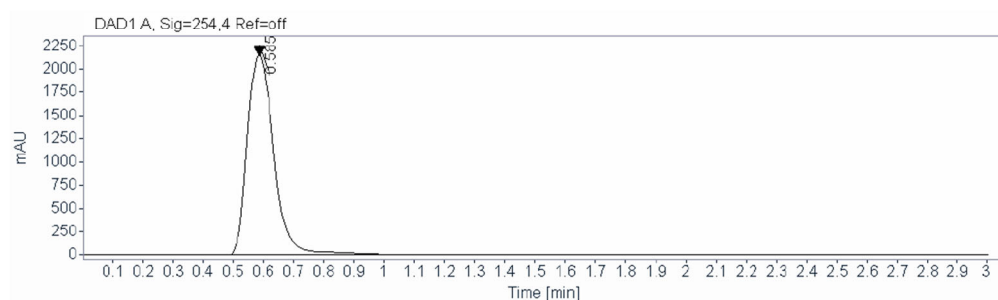
Agilent Technologies

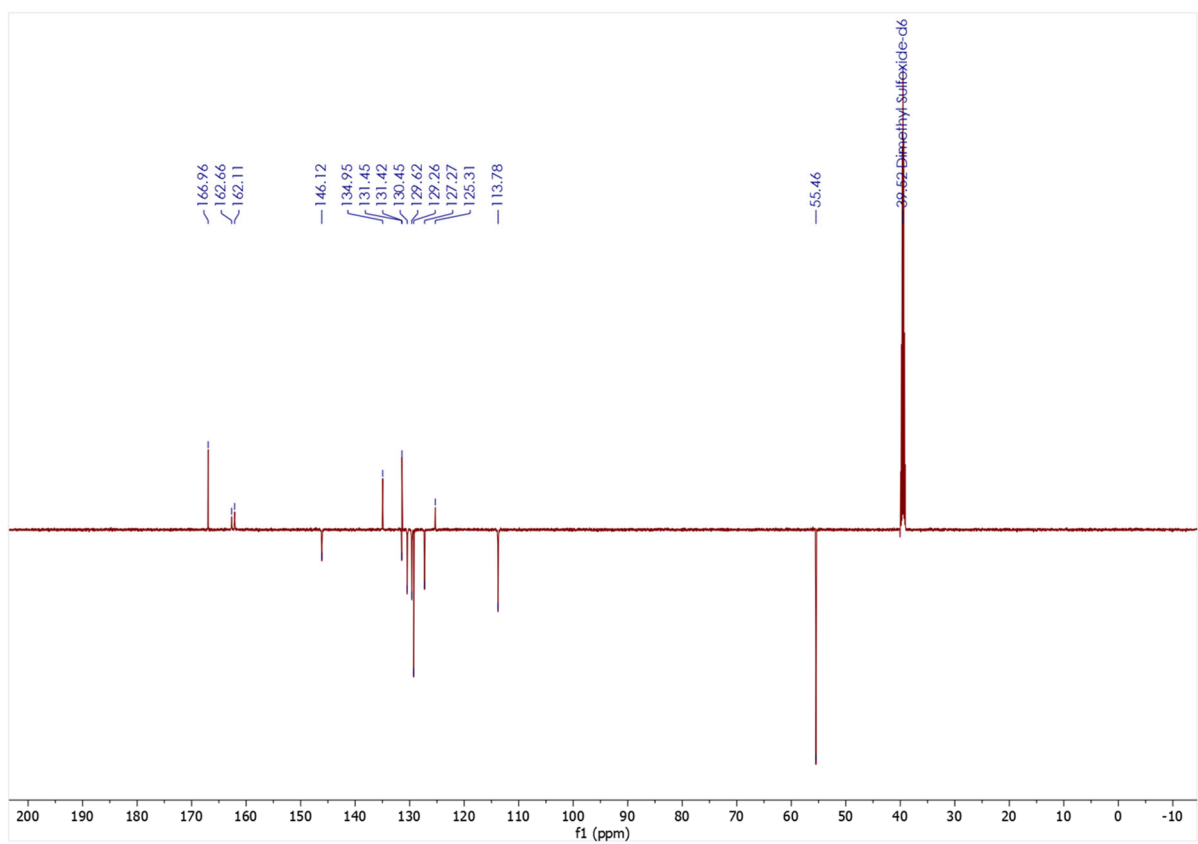
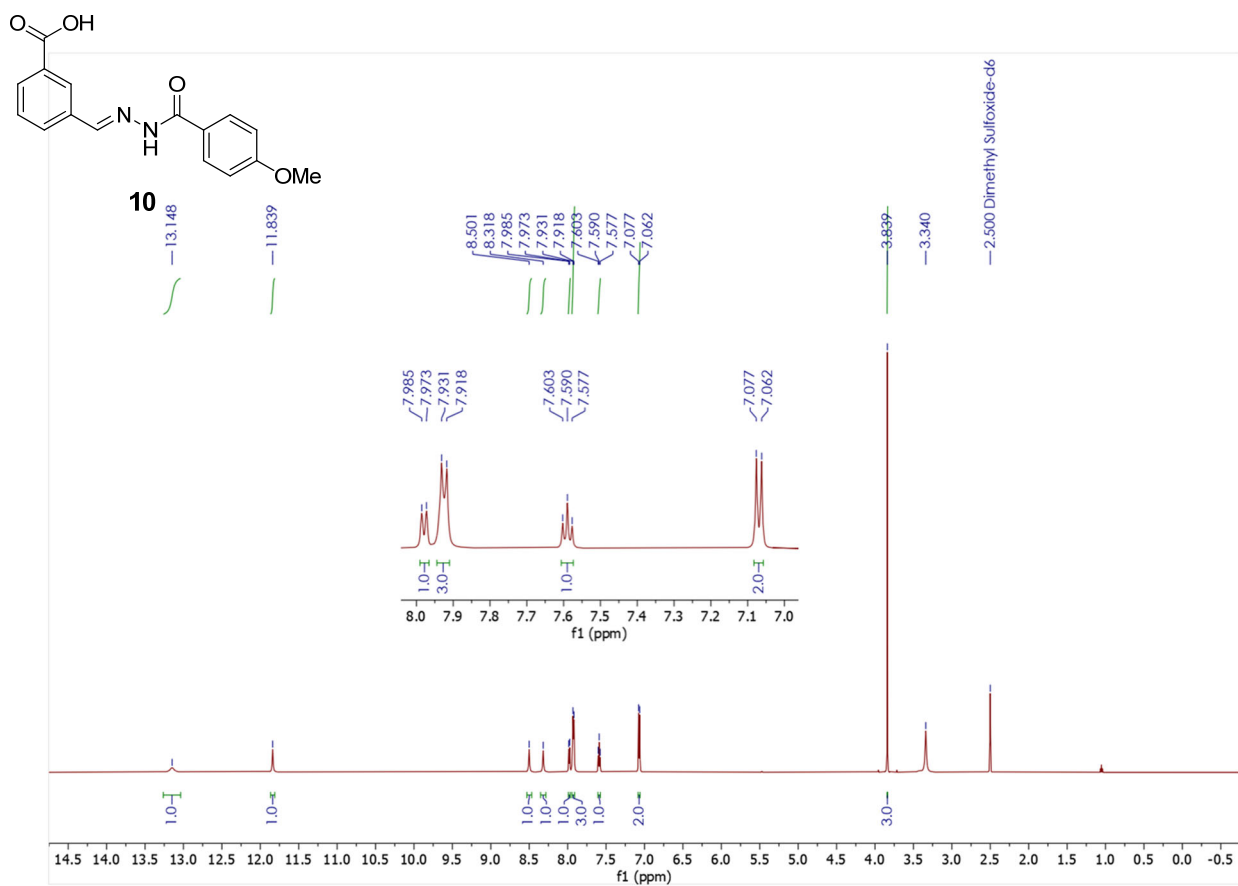
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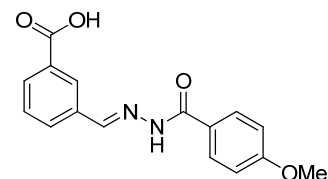
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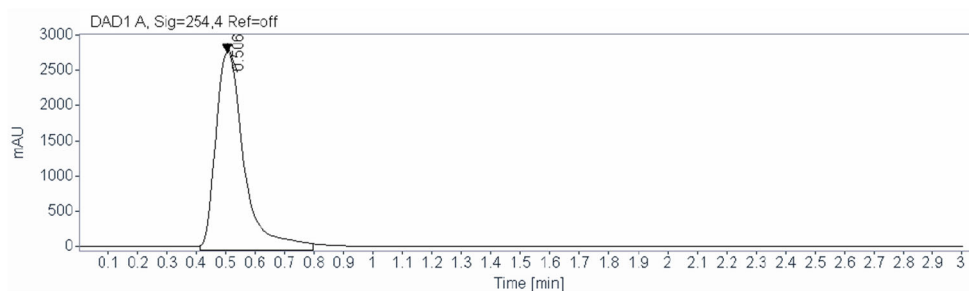


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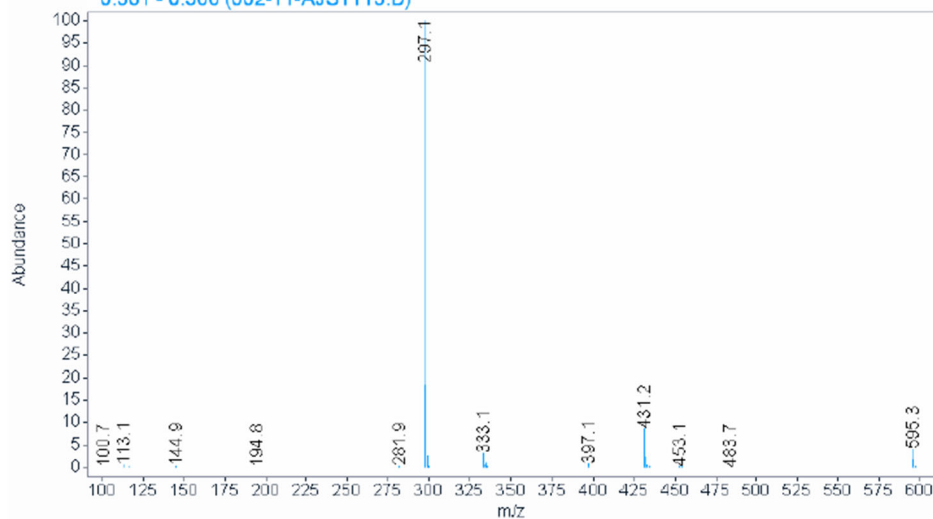


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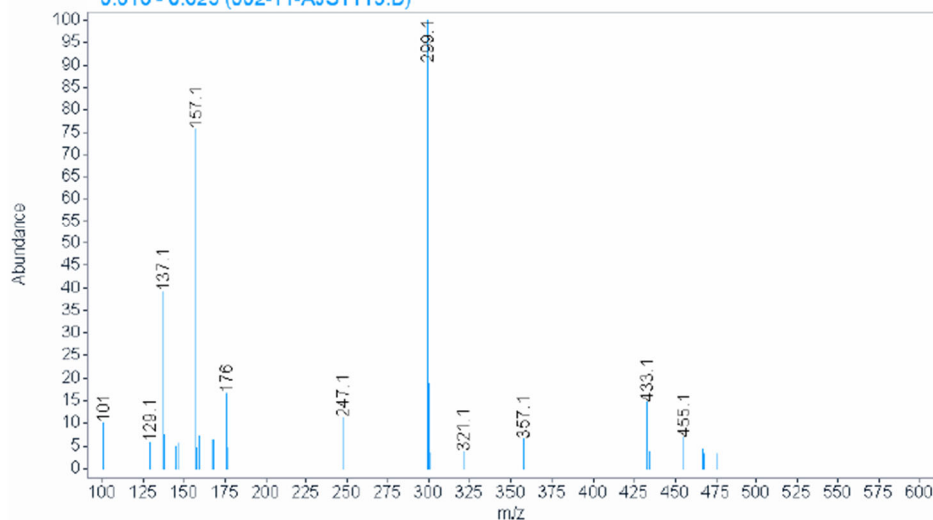
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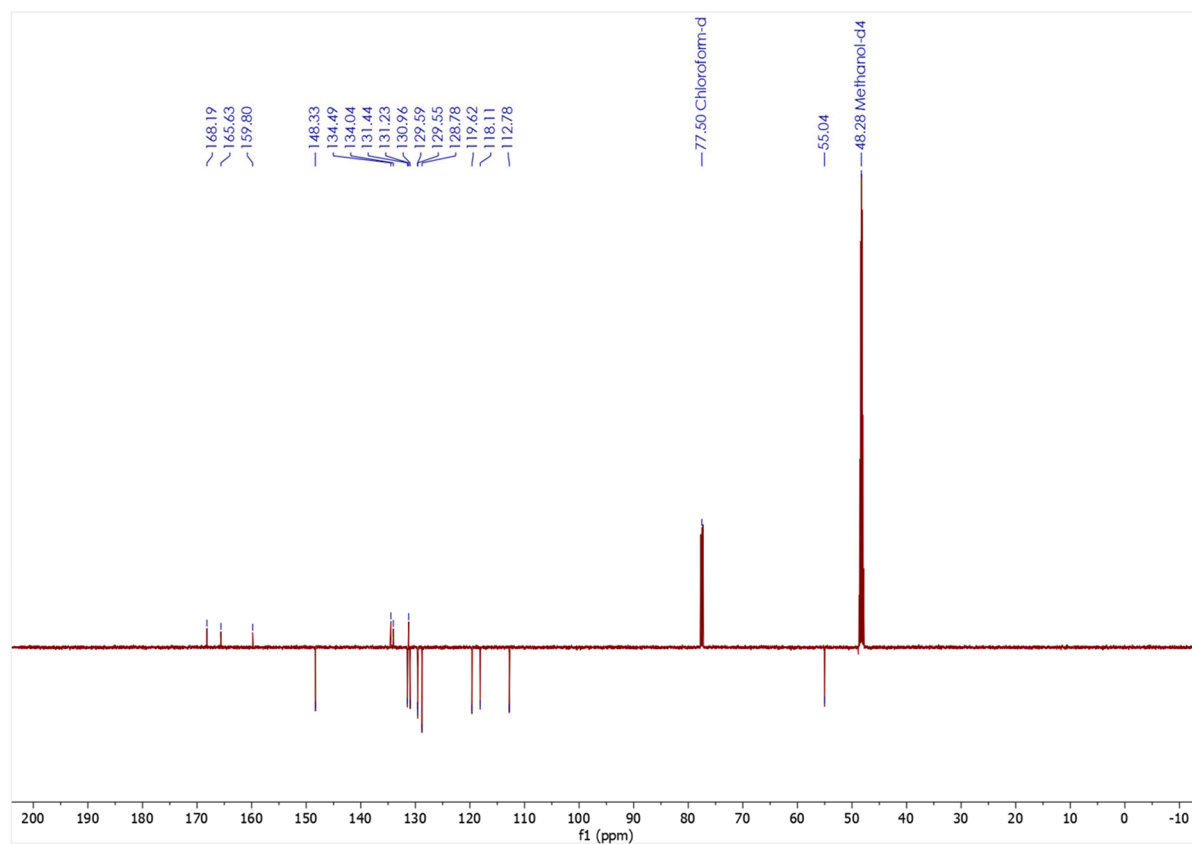
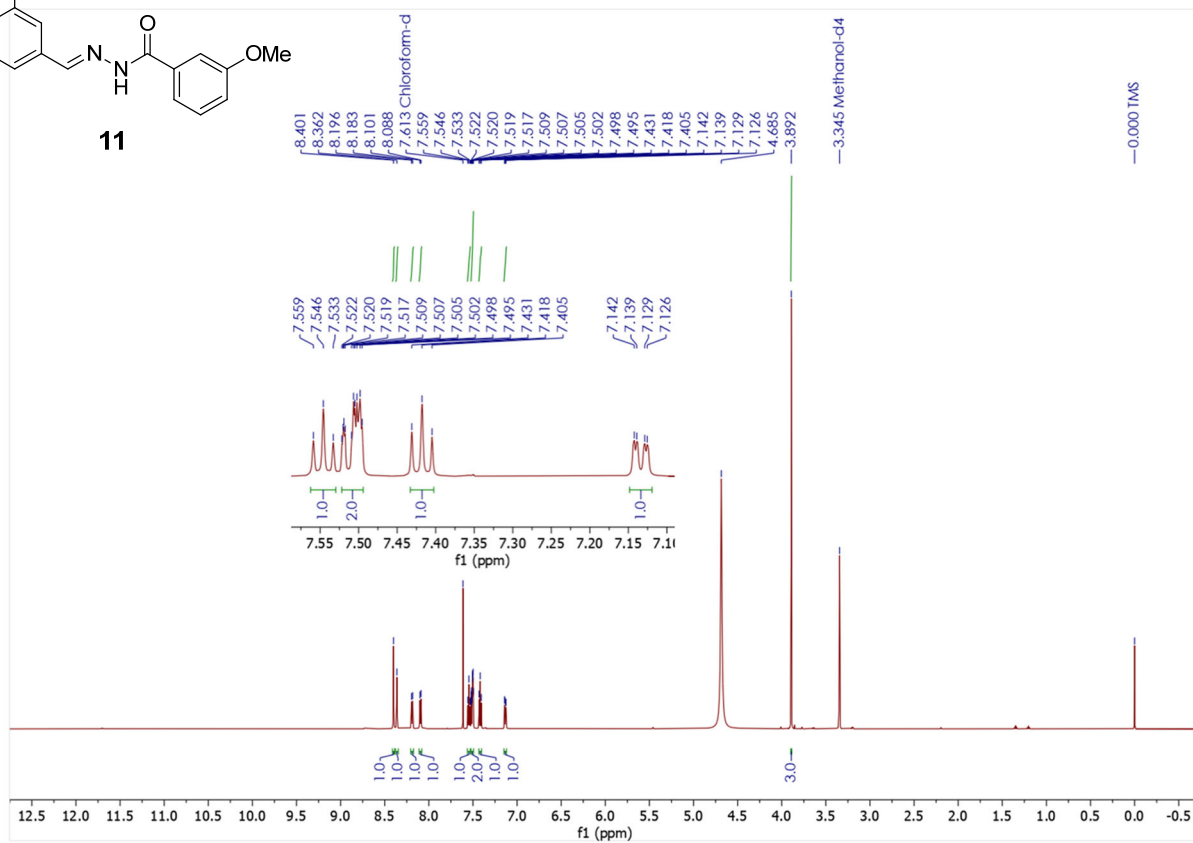
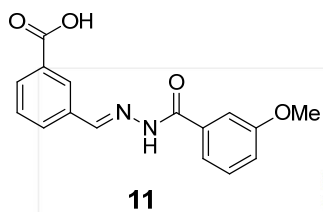


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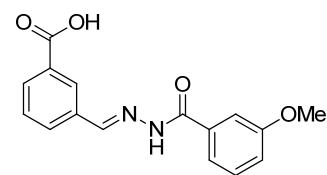
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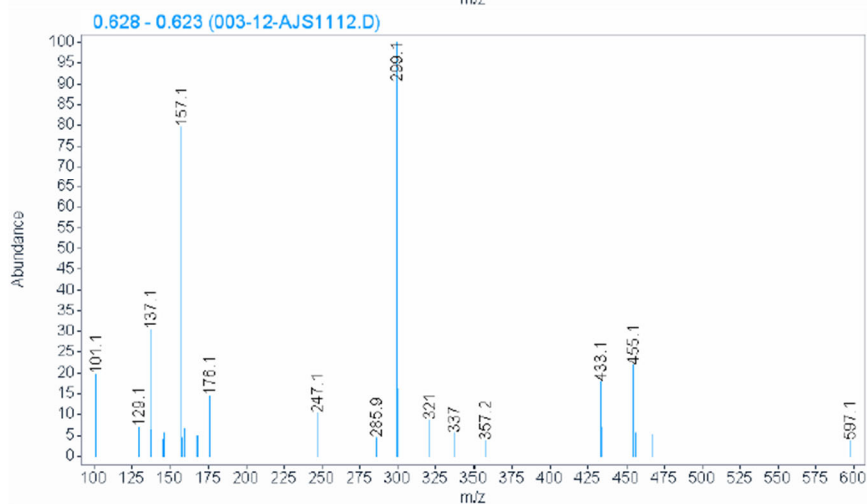
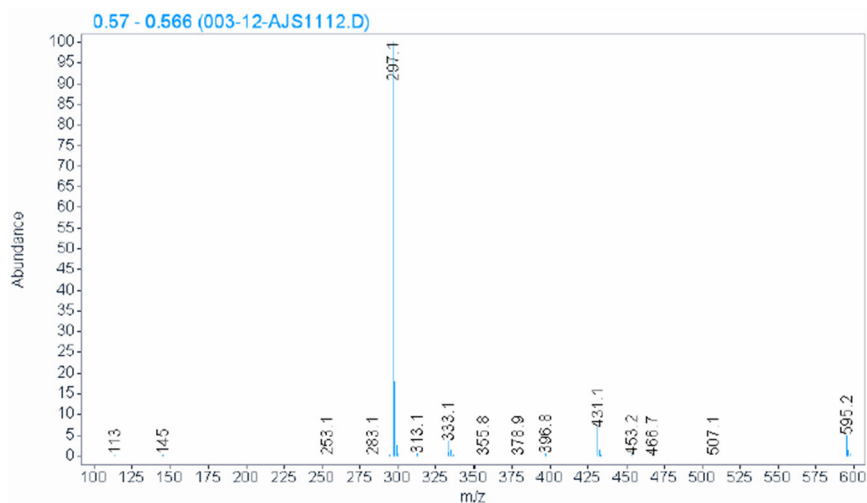
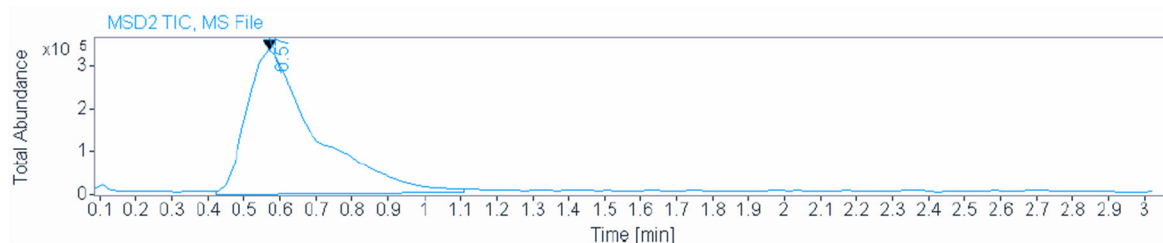
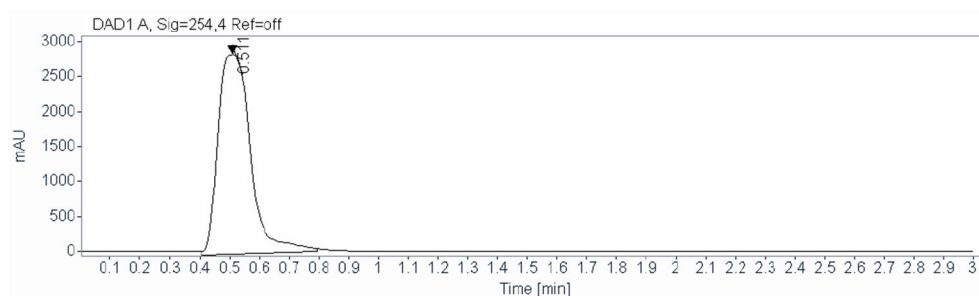


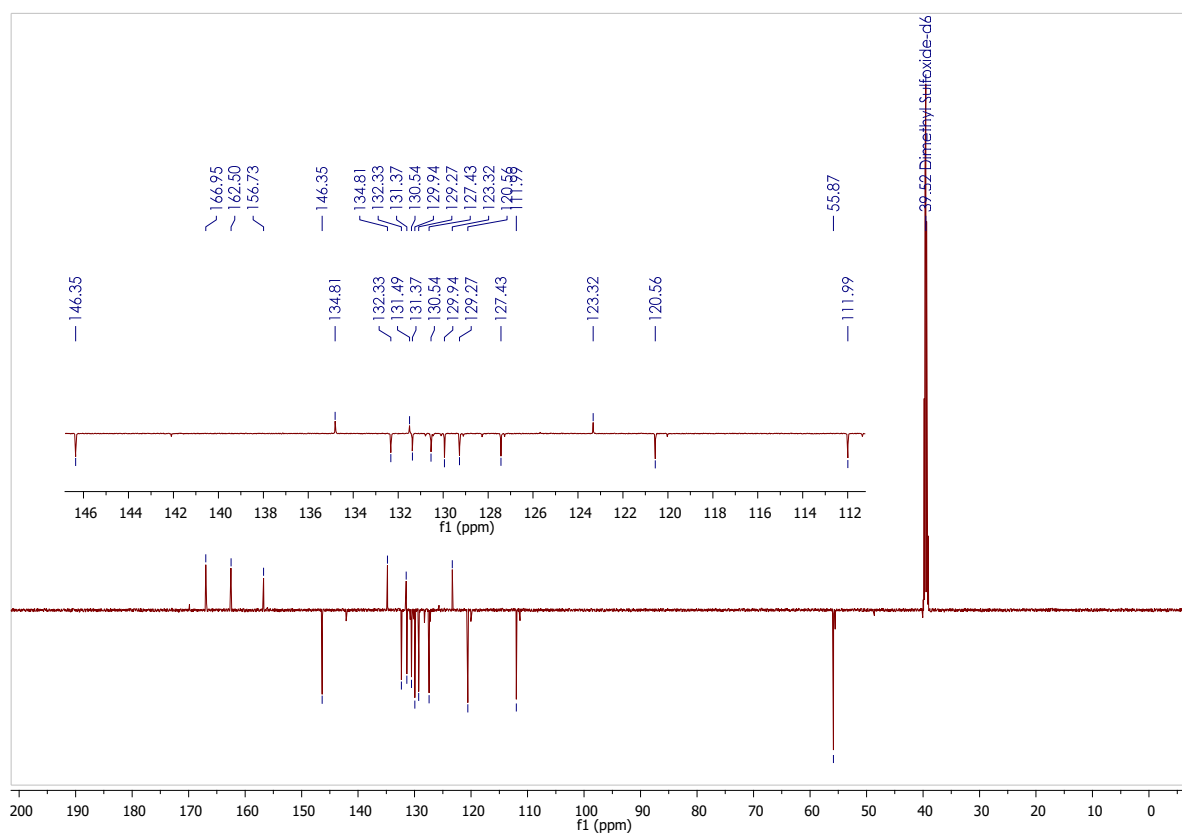
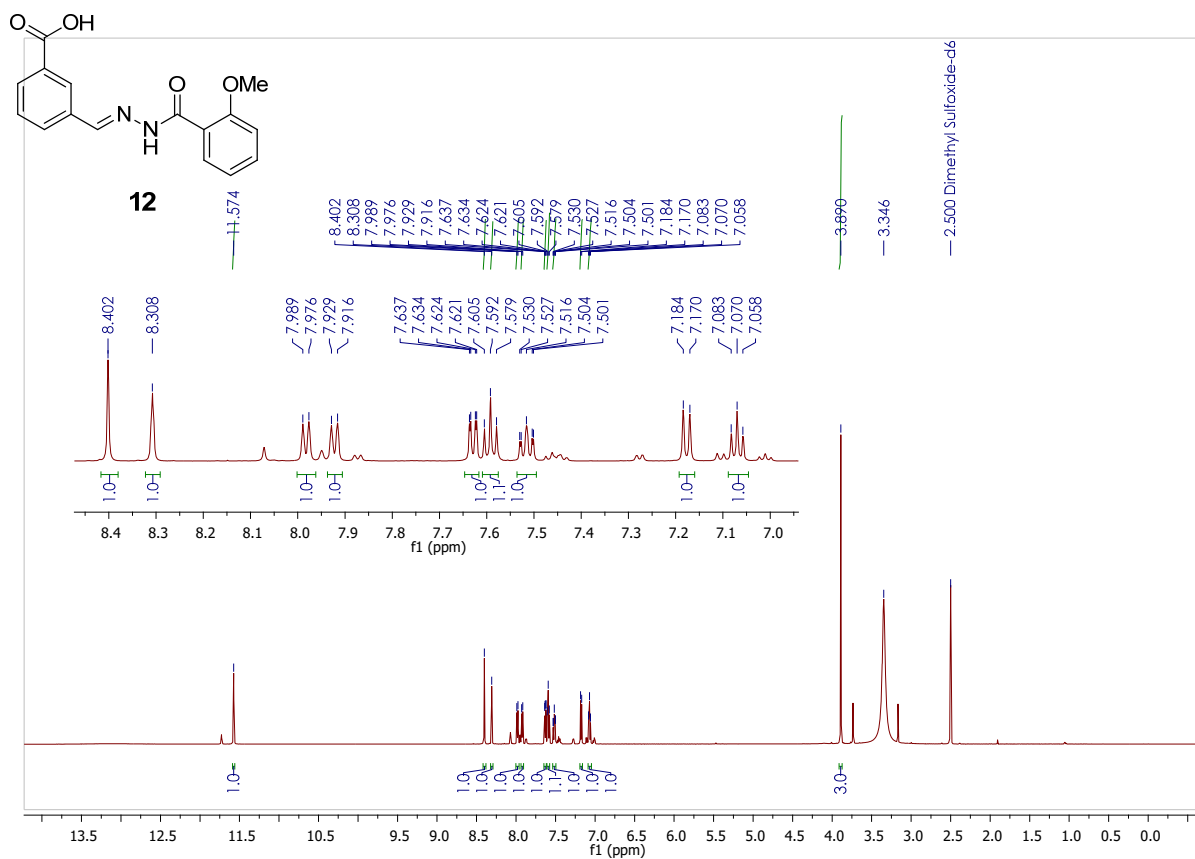
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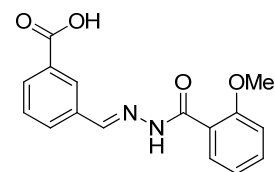


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Sample type: Sample

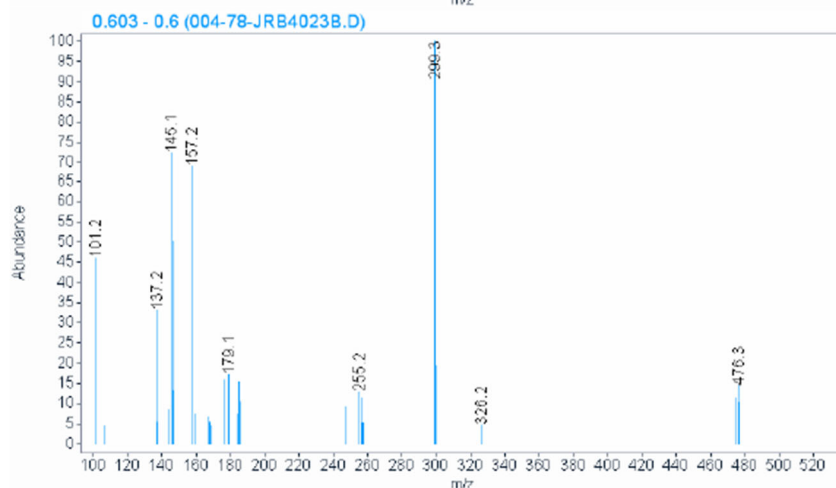
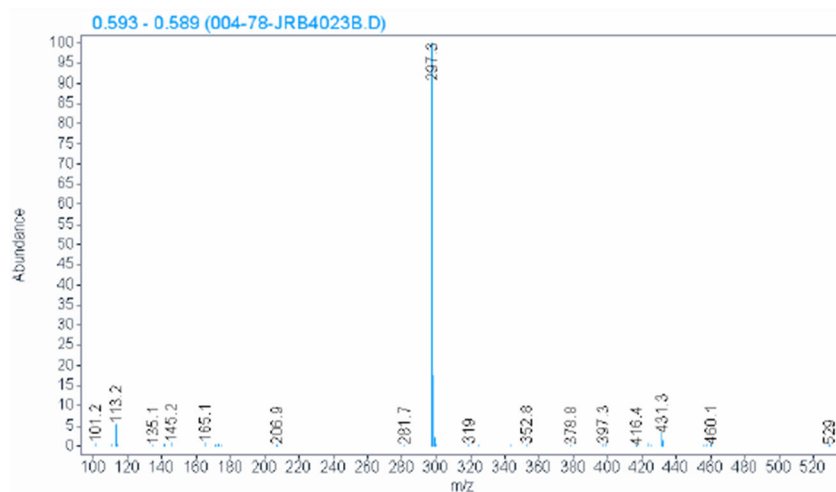
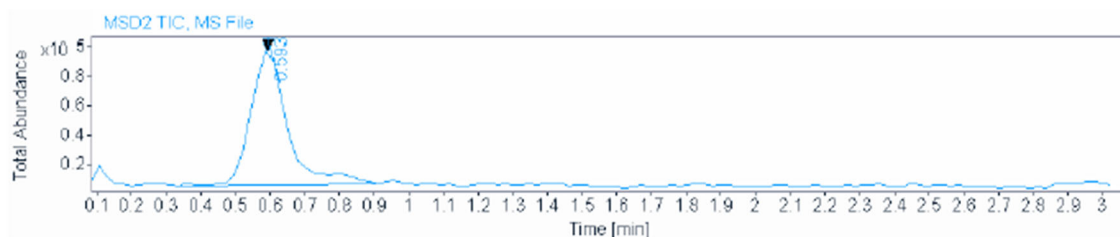
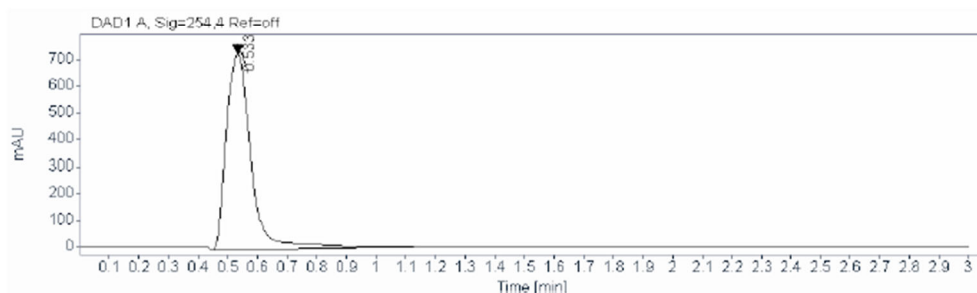
Location: 78
Injection: 1 of 1
Injection volume: 2.000

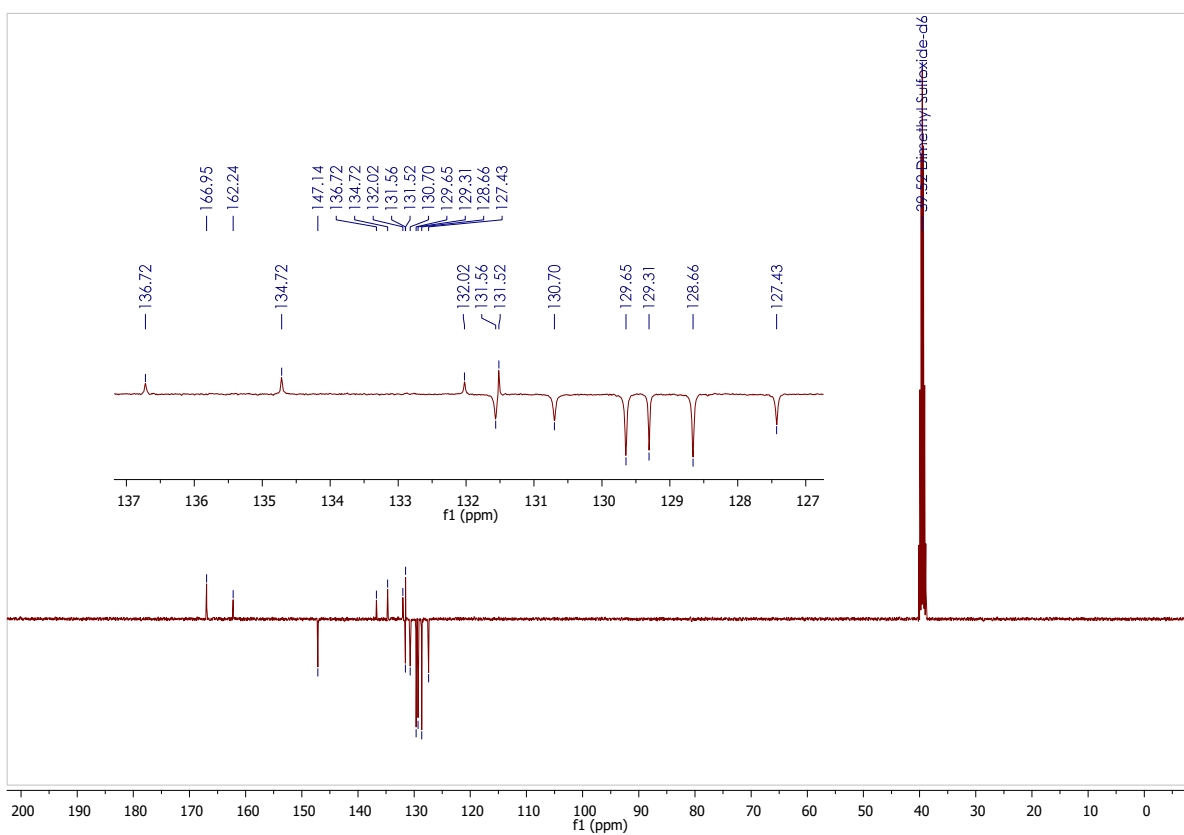
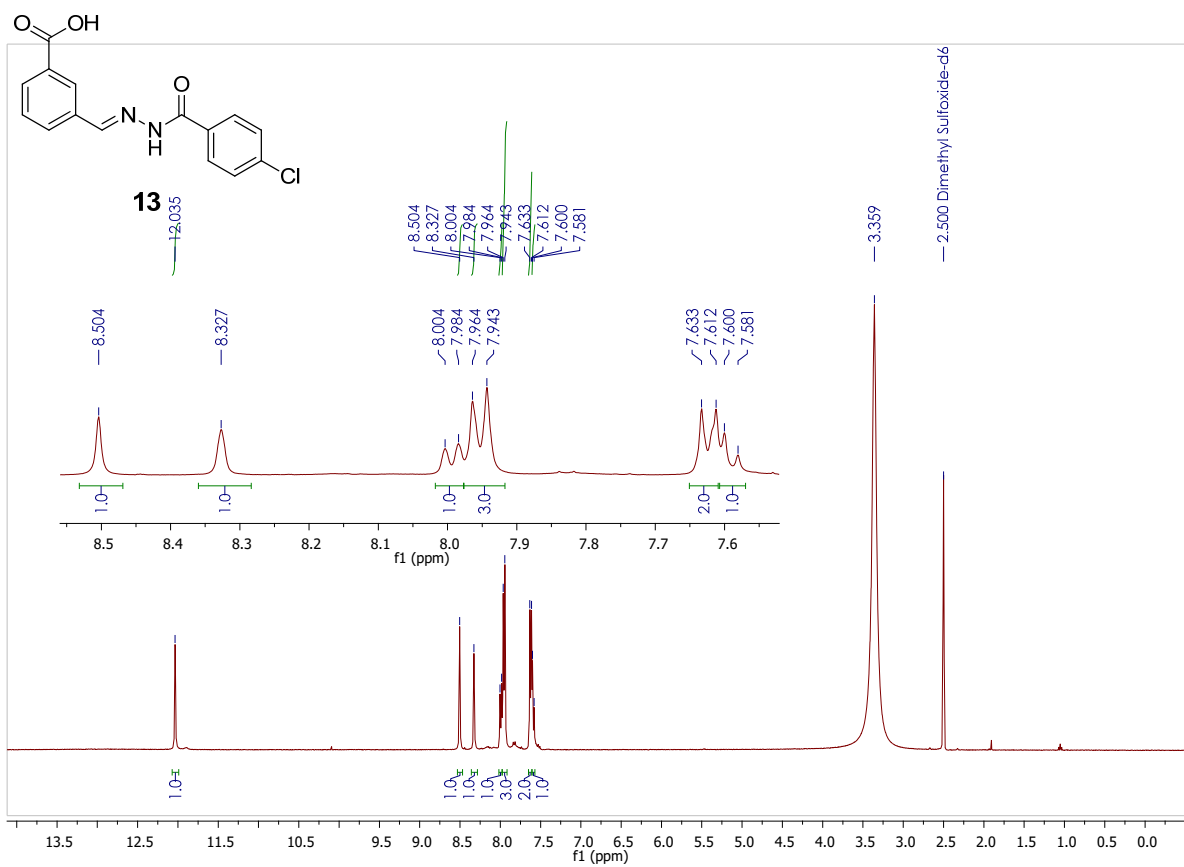
Acq. operator: SYSTEM



Molecular Weight: 298.293

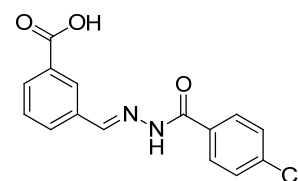
12





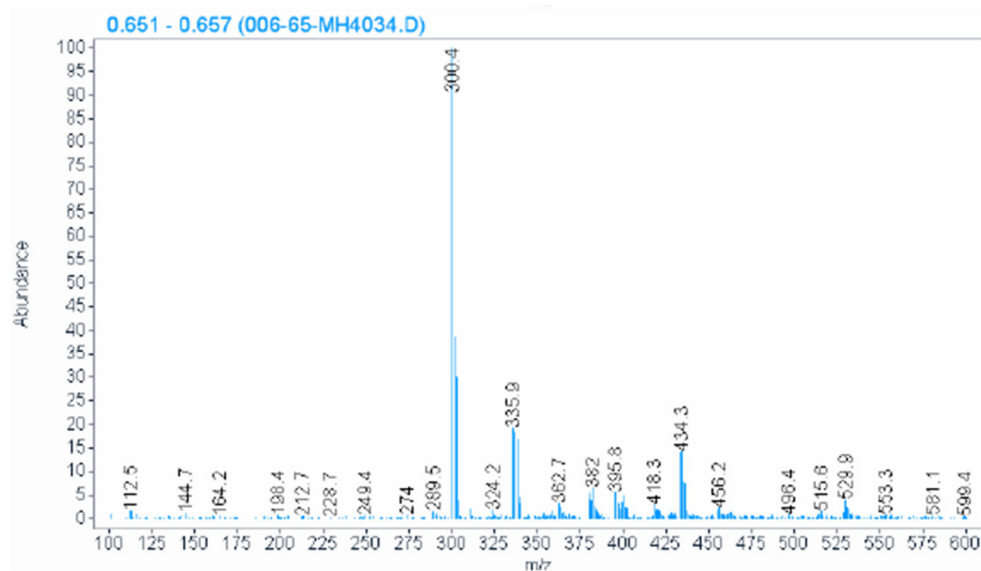
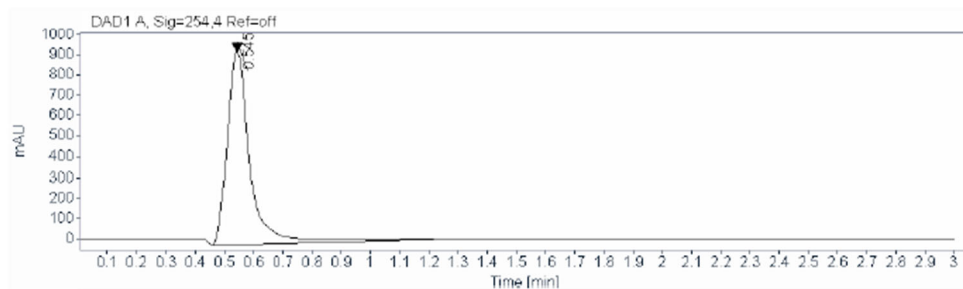


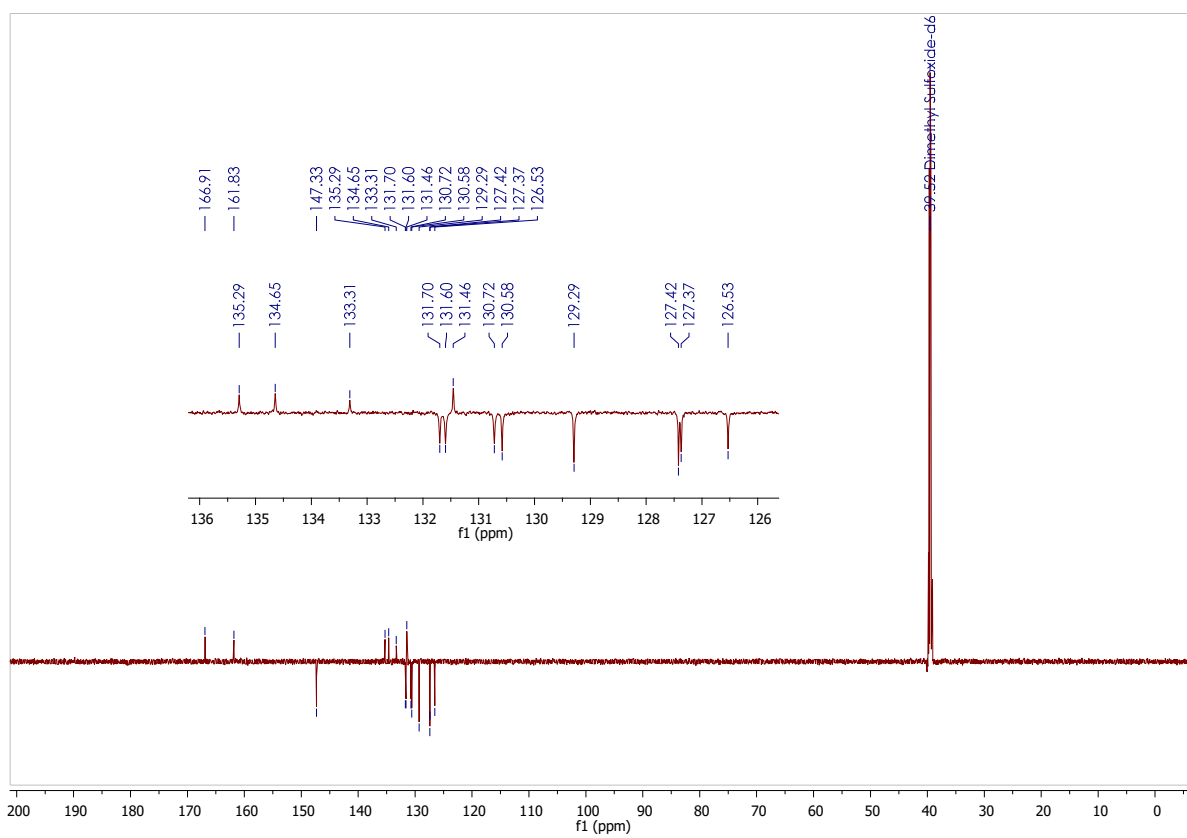
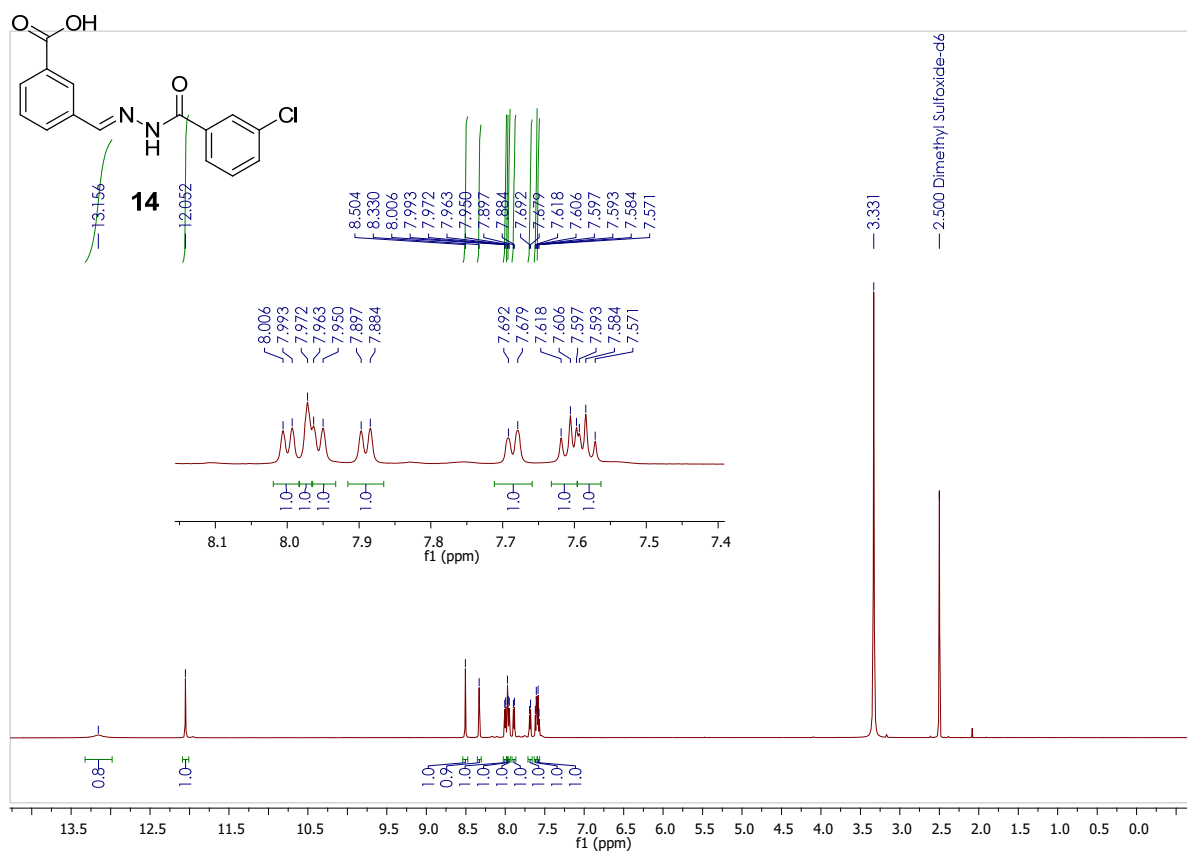
Data file: D:\Chem32\1\Data\MH\MH4030-4036 2022-03-07 10-54-23\006-65-MH4034.D
Sample name: MH4034
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Location: 65
Injection date: 3/7/2022 11:19:16 AM
Injection: 1 of 1
Acq. method: LCMS ISOCRATIC 80%
B_3 MINS.M
Injection volume: 2.000
Analysis method: LCMS ISOCRATIC
80%B_3 MINS.M
Acq. operator: SYSTEM
Last changed: 11/26/2021 9:20:48 AM



Molecular Weight: 302.712

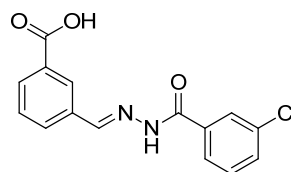
13





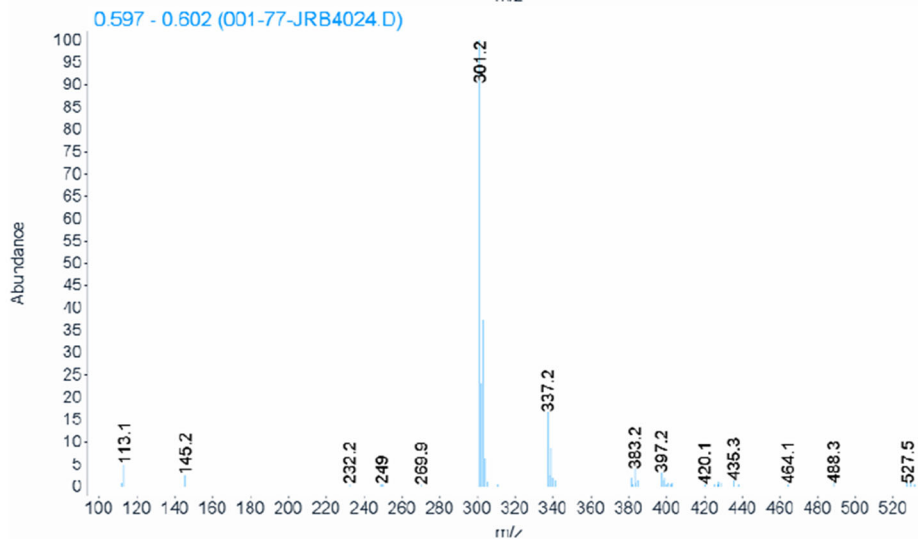
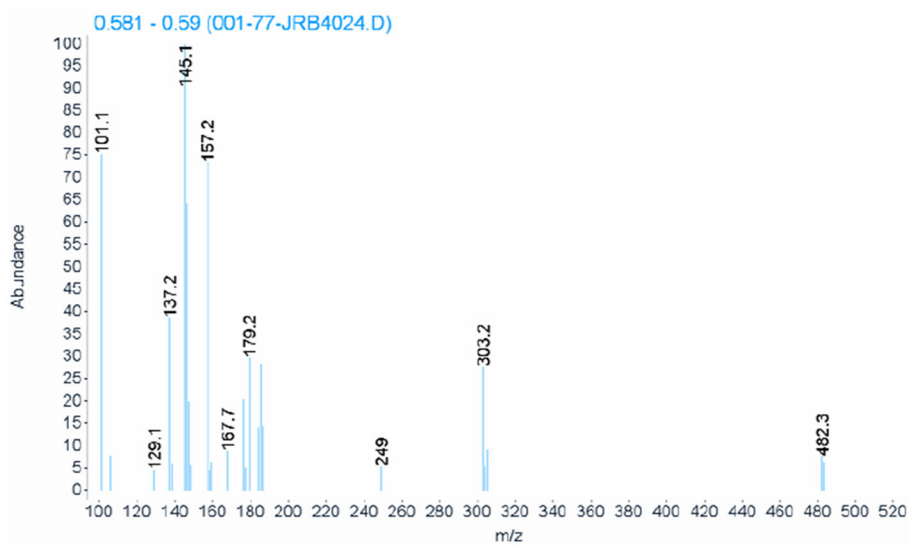
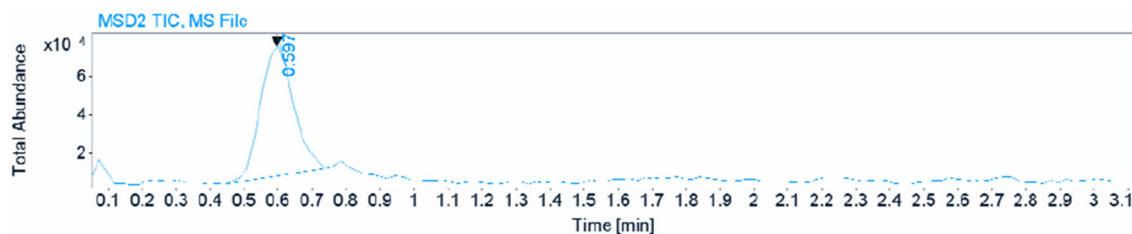


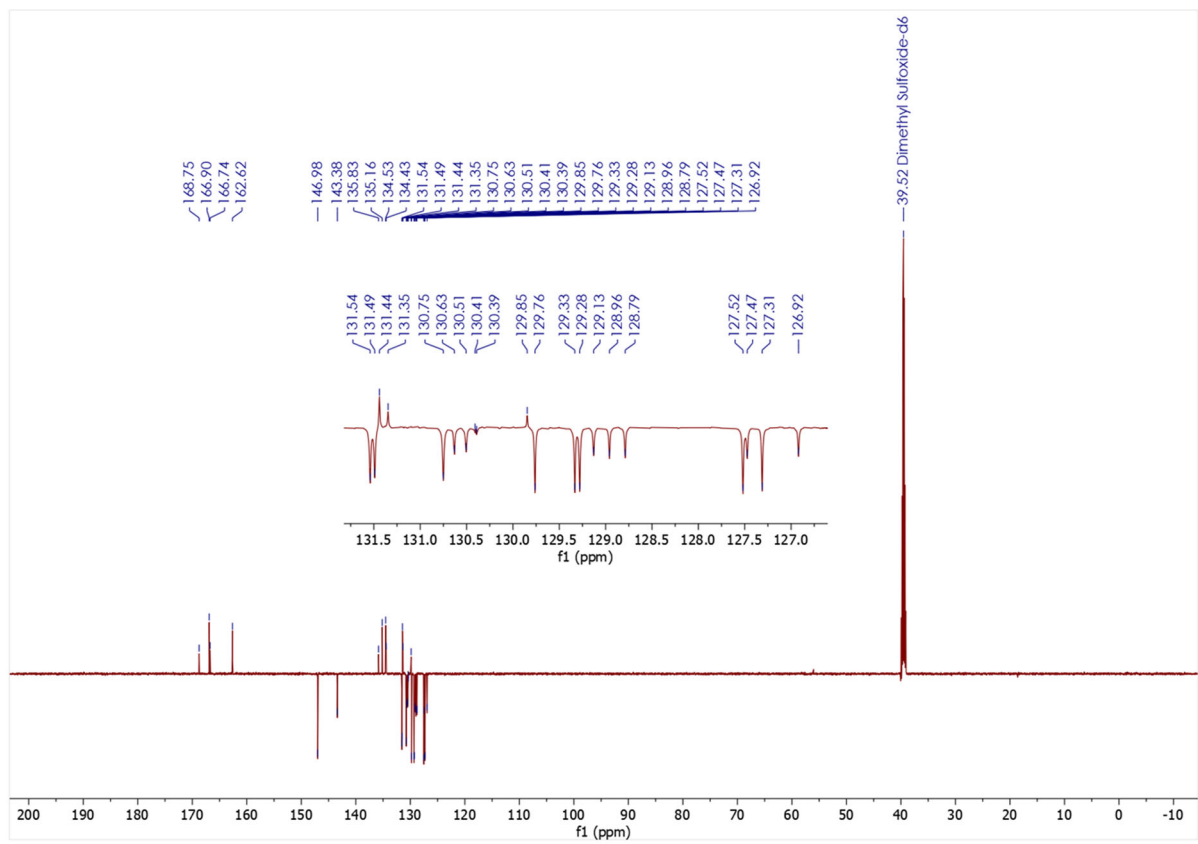
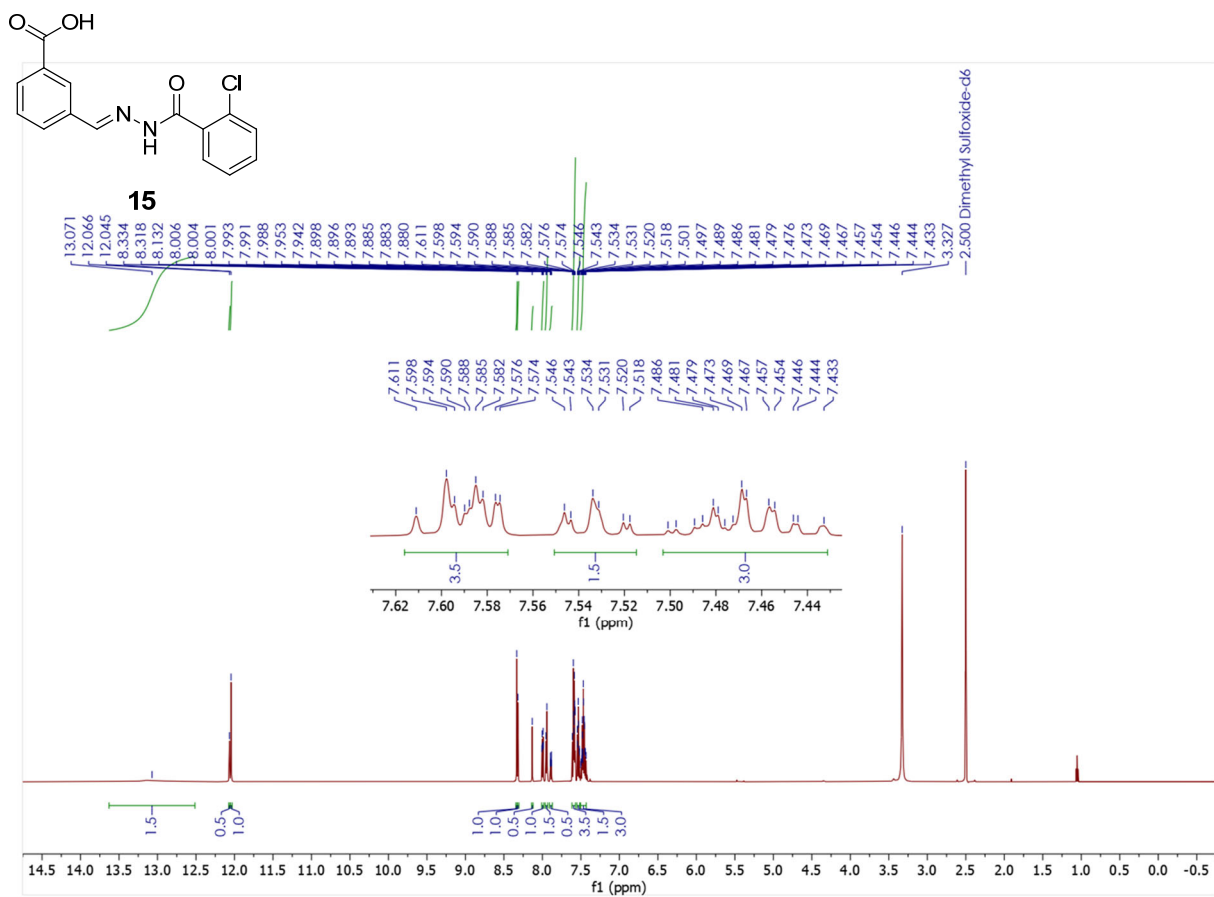
Data file: D:\Chem32\1\Data\JRB\JRB4024 2023-07-24 16-11-49\001-77-JRB4024.D
Sample name: JRB4024
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Injection date: 7/24/2023 4:13:42 PM
Acq. method: LCMS ISOCRATIC 80%
B_3 MINS.M
Analysis method: LCMS ISOCRATIC
80%B_3 MINS.M
Last changed: 11/26/2021 9:20:48 AM
Location: 77
Injection: 1 of 1
Injection volume: 2.000
Acq. operator: SYSTEM



Molecular Weight: 302.712

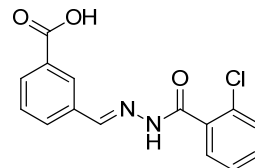
14





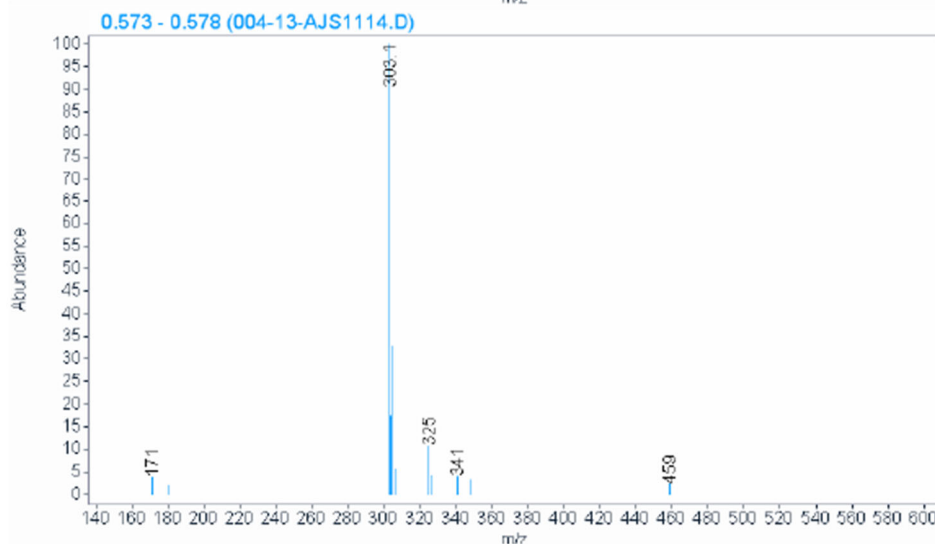
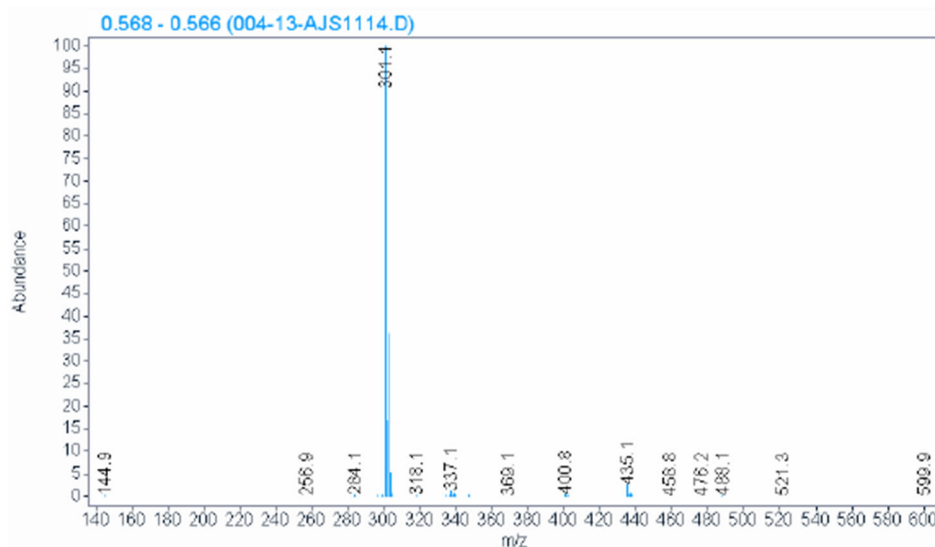
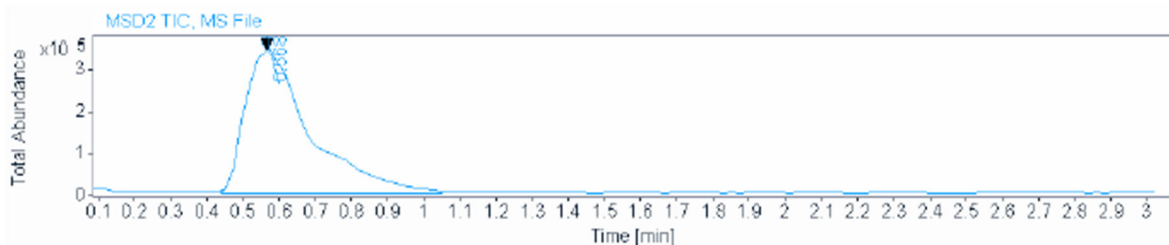


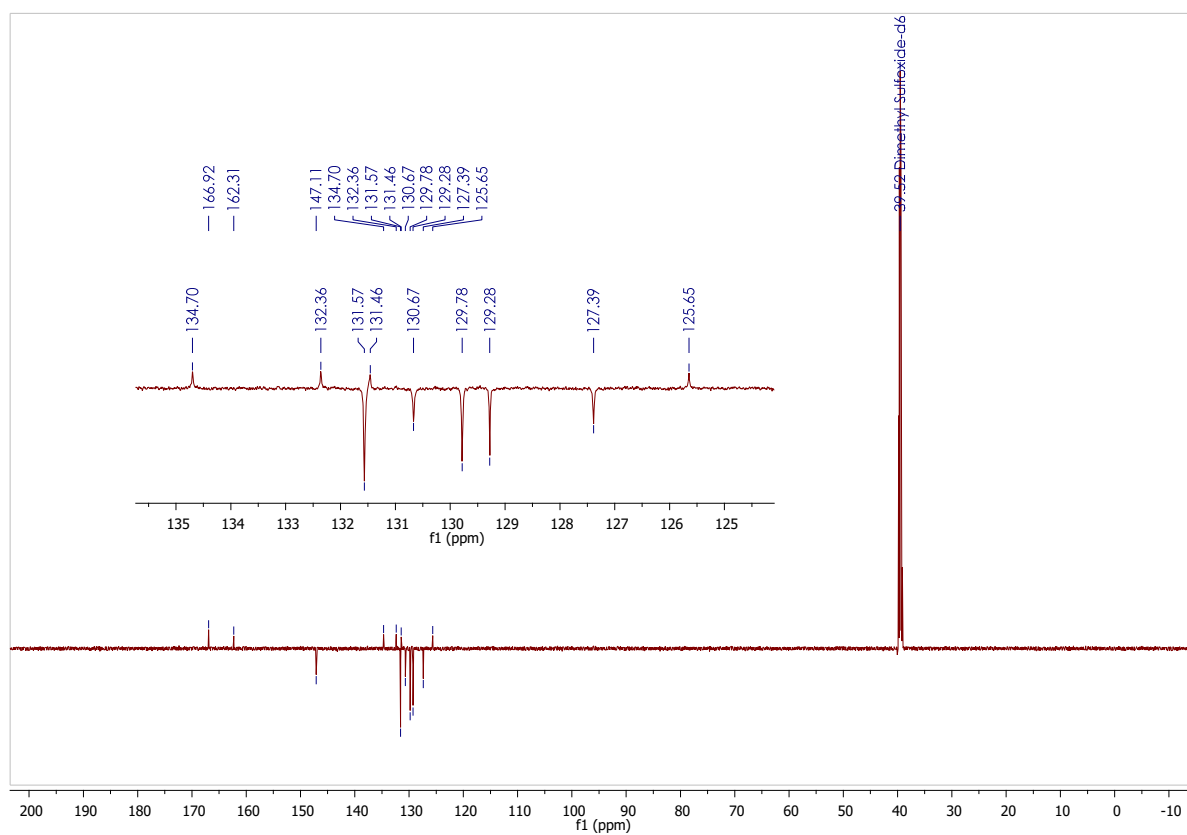
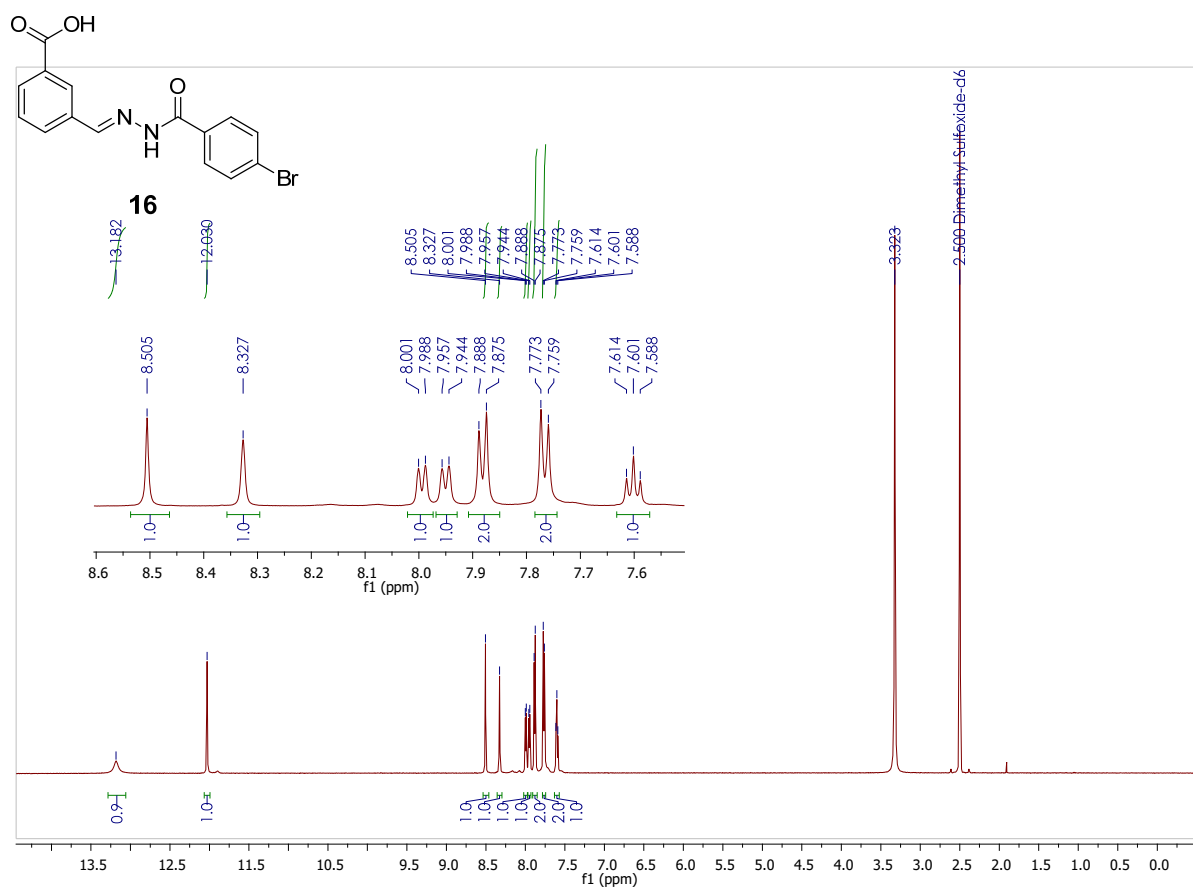
Data file: D:\Chem32\1\Data\AJS\AJS Table1 2023-07-25 14-45-29\004-13-AJS1114.D
 Sample name: AJS1114
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 13
 Injection date: 7/25/2023 3:00:05 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 Injection volume: 2.000
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 80%B_3 MINS.M
 Last changed: 11/26/2021 9:20:48 AM



Molecular Weight: 302.712

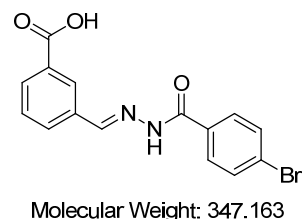
15



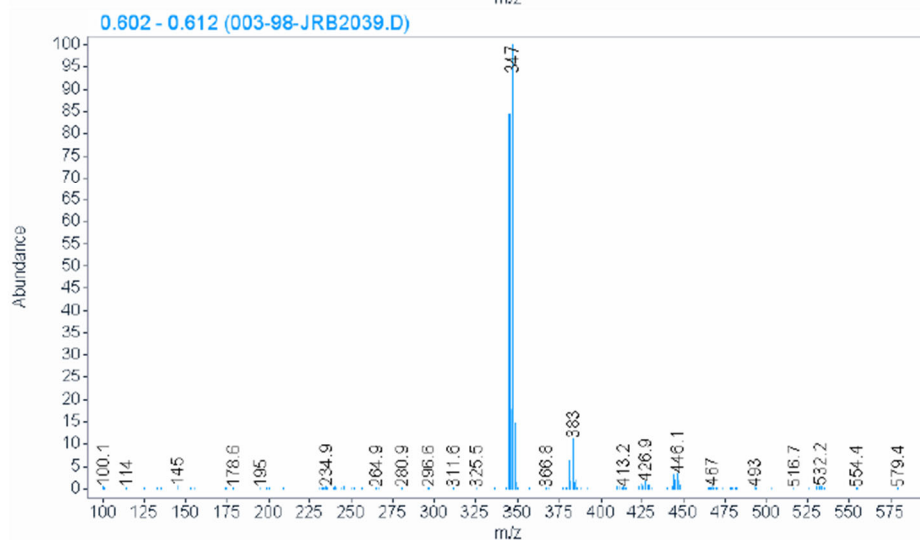
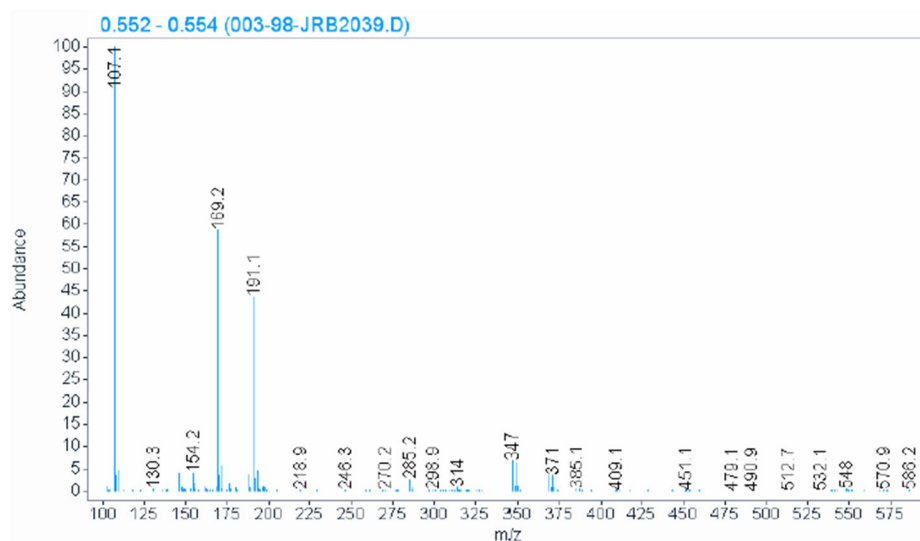
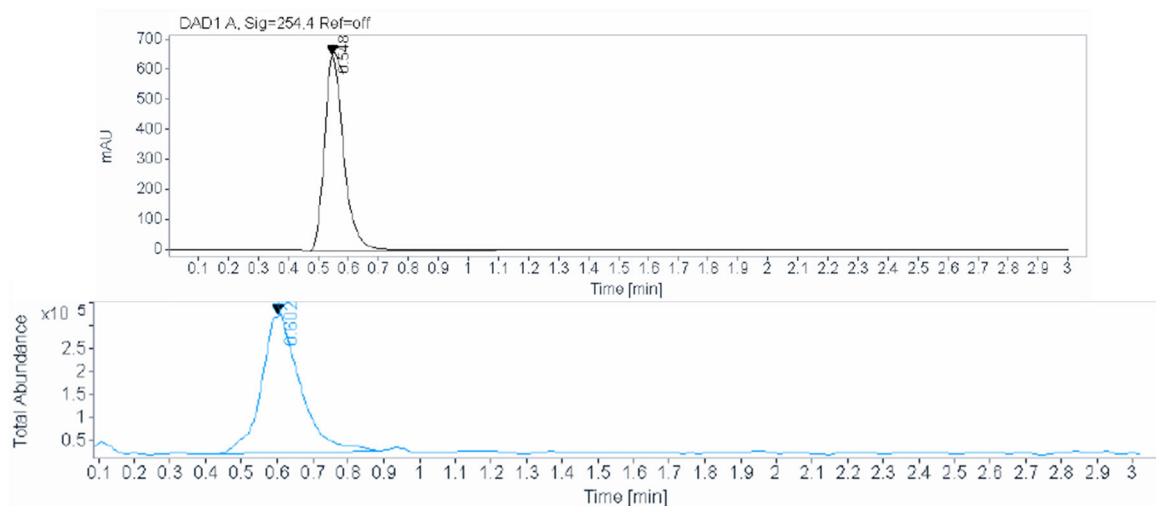


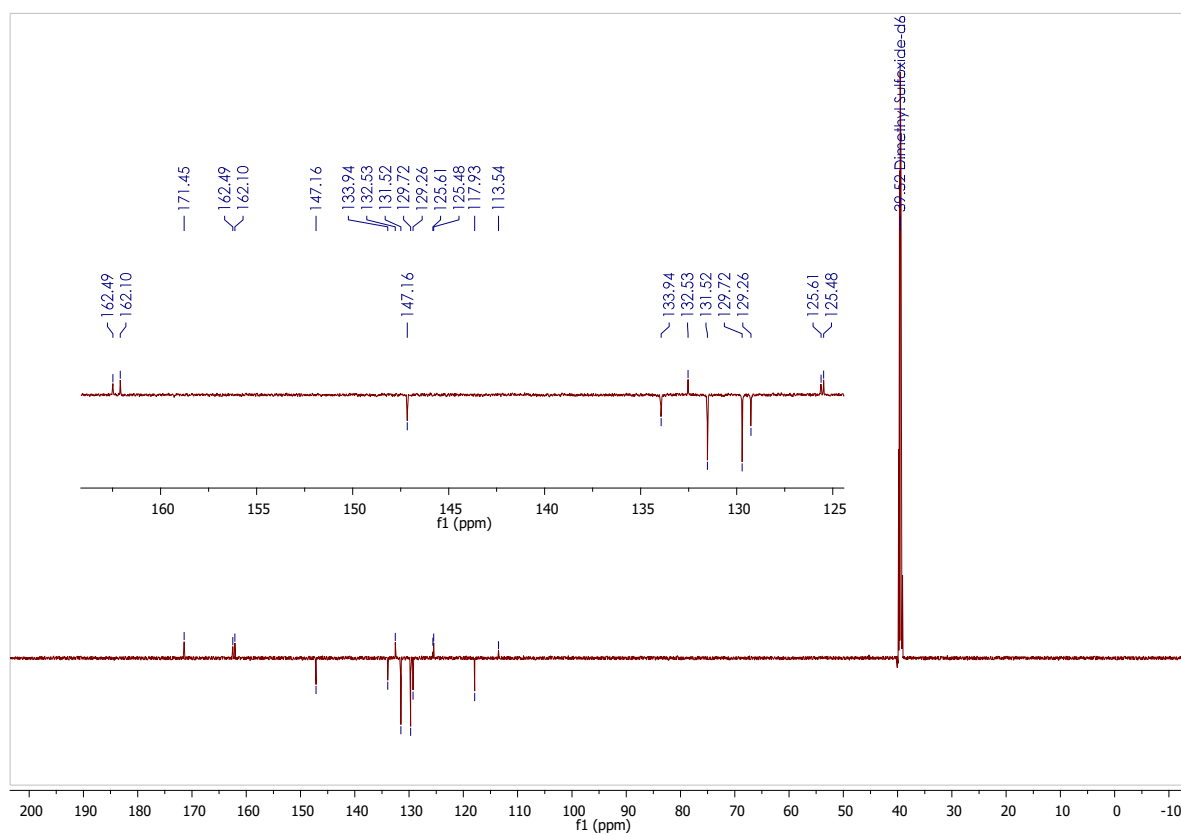
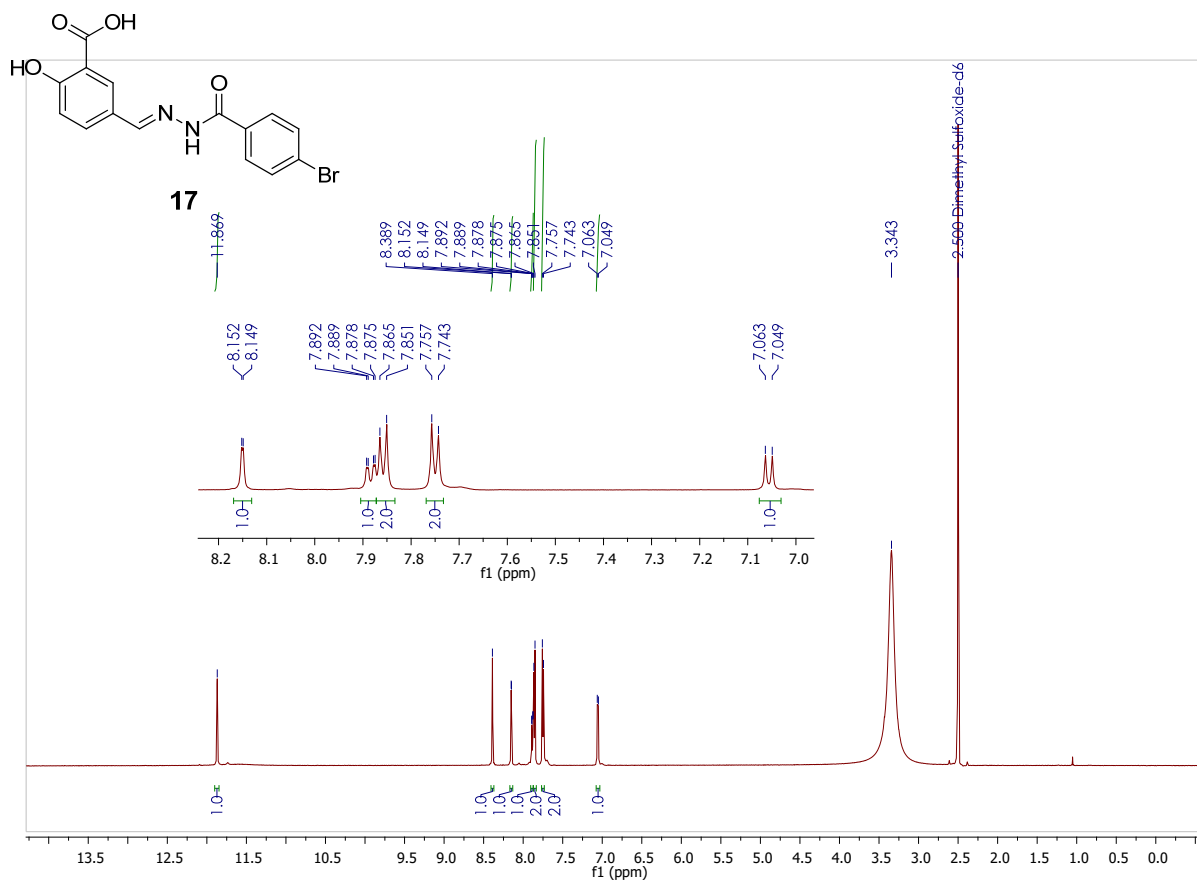


Data file: D:\Chem32\1\Data\JRB\JRB2031 2038 2039 2021-11-26 16-23-36\003-98-JRB2039.D
 Sample name: JRB2039
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 98
 Injection date: 11/26/2021 4:34:37 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80% B_3 MINS.M
 Injection volume: 2.000
 Analysis method: LCMS ISOCRATIC 80%B_3 MINS.M
 Acq. operator: SYSTEM
 Last changed: 11/26/2021 9:20:48 AM



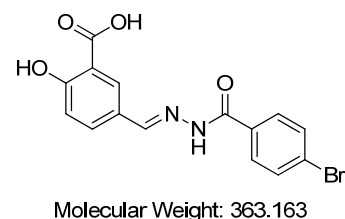
16



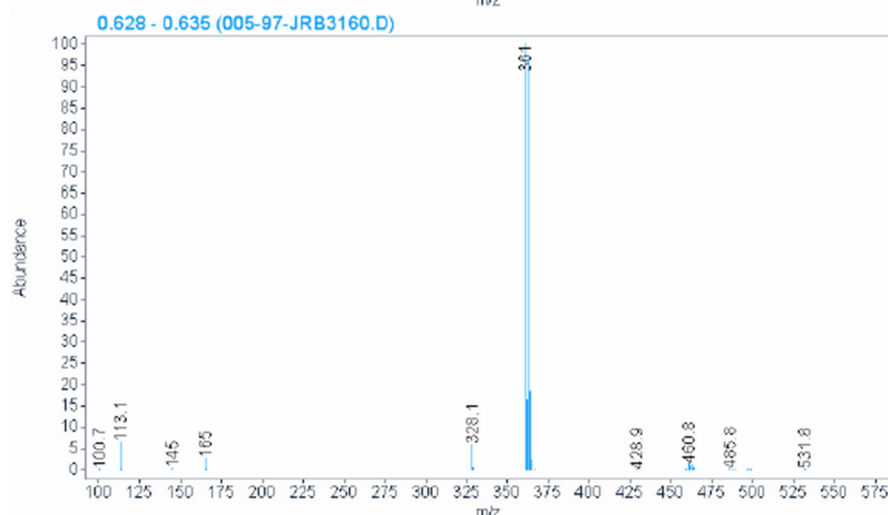
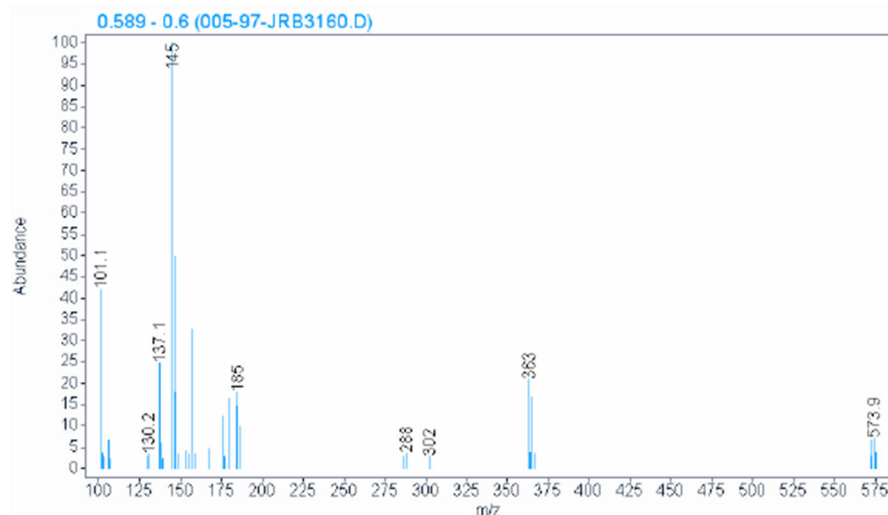
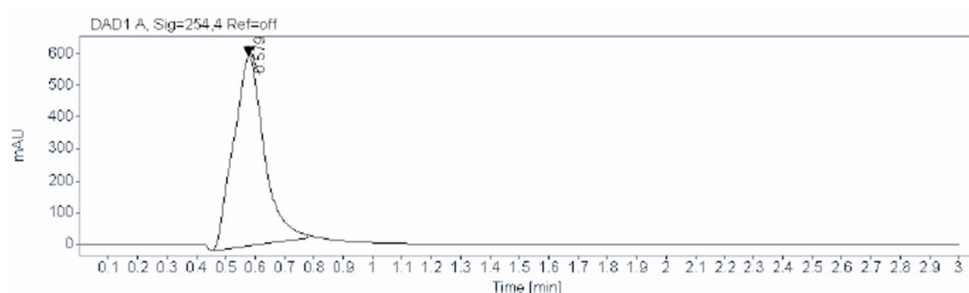


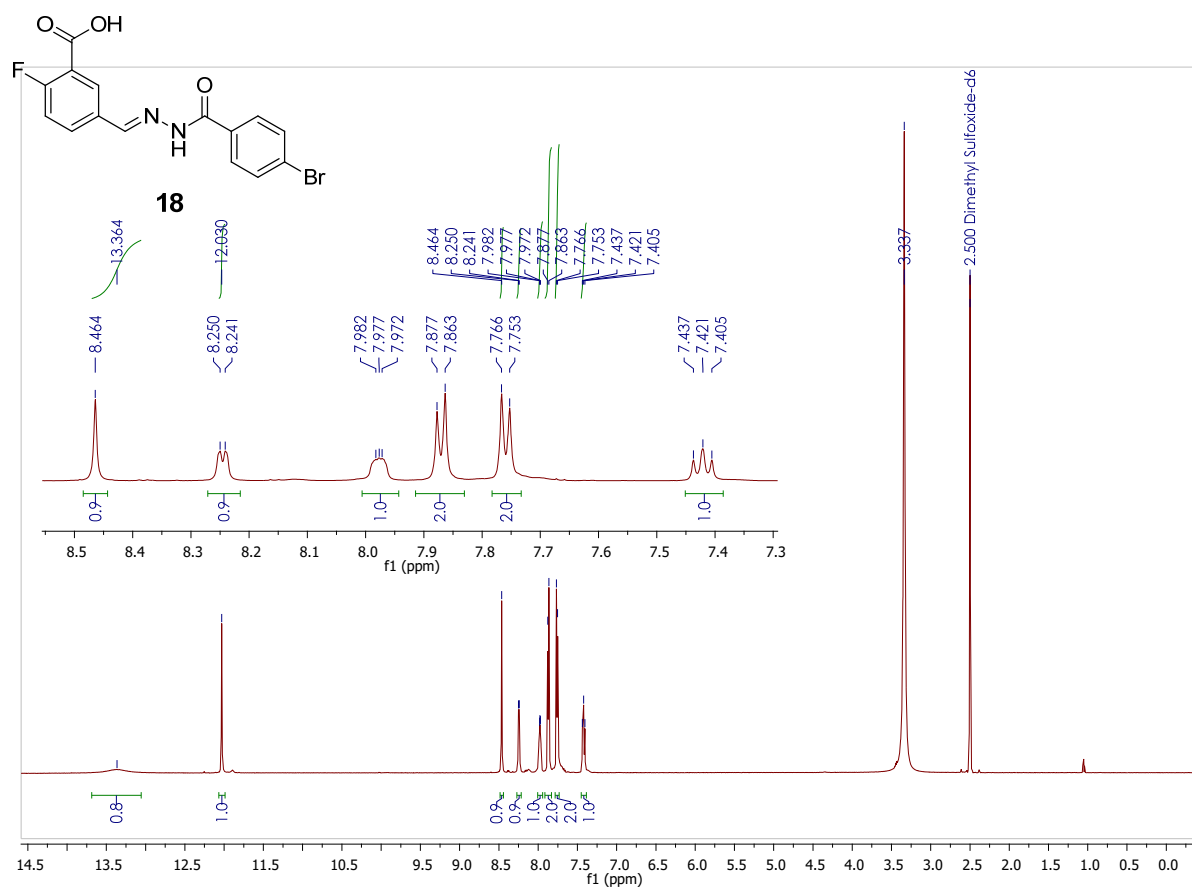


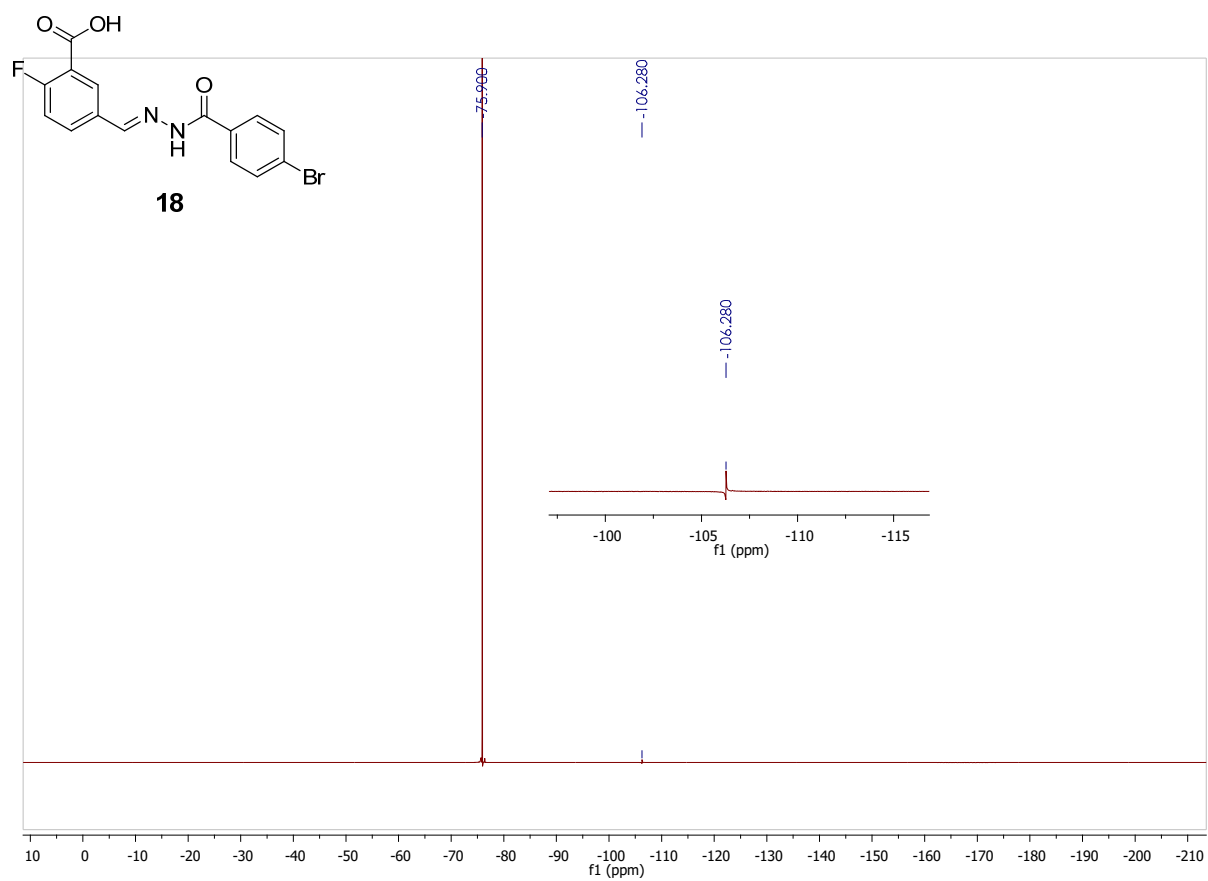
Data file: D:\Chem32\1\Data\JRB\JRB3066 3157 3158 3160 2023-07-24 12-35-44\005-97-JRB3160.D
 Sample name: JRB3160
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 97
 Injection date: 7/24/2023 12:56:33 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 Injection volume: 2.000
 B_3 MINS.M
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 80%B_3 MINS.M
 Last changed: 11/26/2021 9:20:48 AM



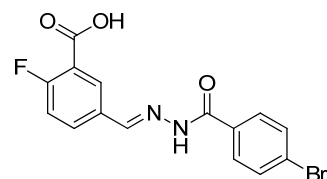
17





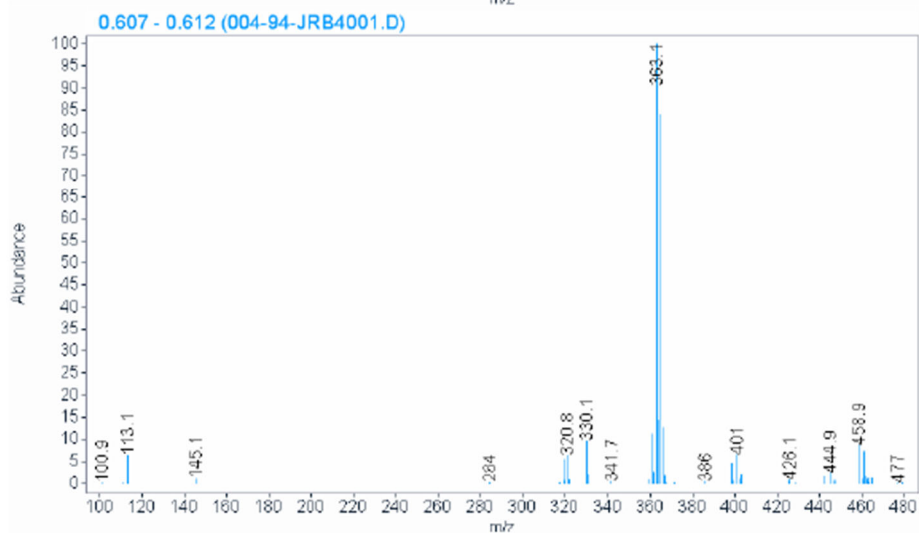
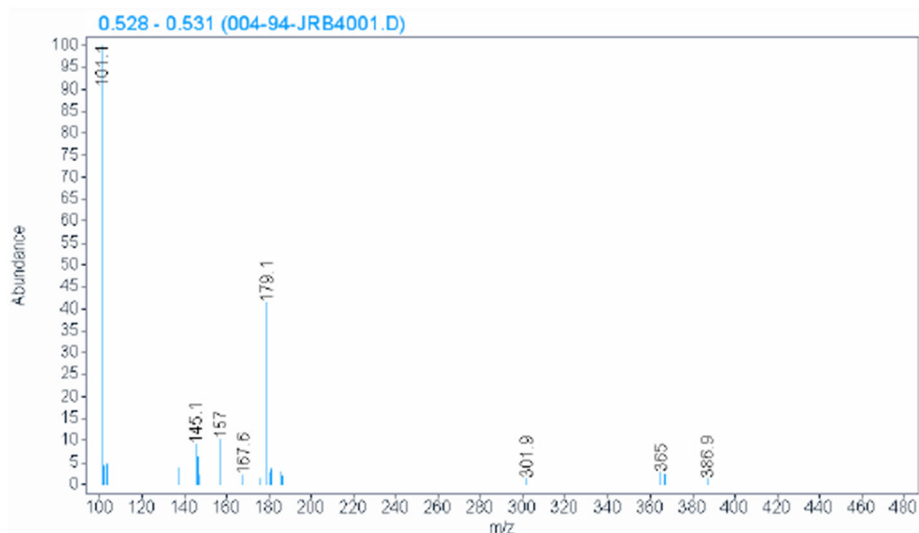
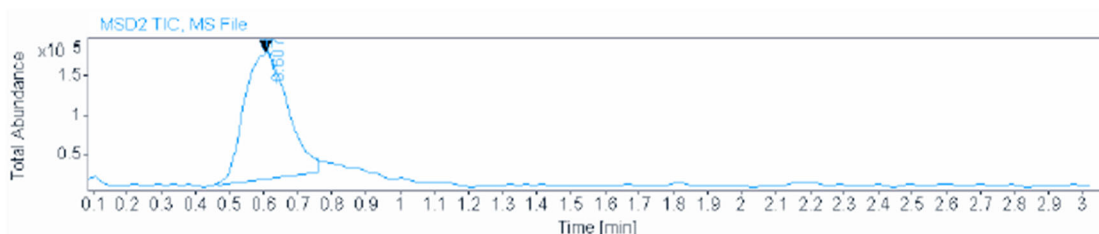
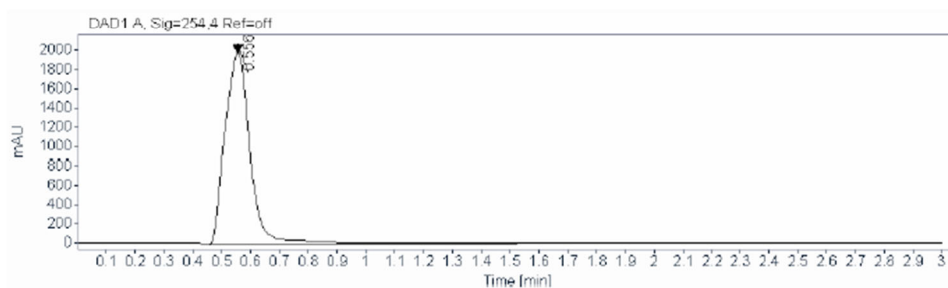


Data file: D:\Chem32\1\Data\JRB\JRB3189 3196 4001 4002 2023-07-24 12-59-52\004-94-JRB4001.D
 Sample name: JRB4001
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 94
 Injection date: 7/24/2023 1:15:35 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 Injection volume: 2.000
 B_3 MINS.M
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 80%B_3 MINS.M
 Last changed: 11/26/2021 9:20:48 AM

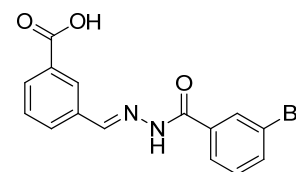


Molecular Weight: 365.154

18

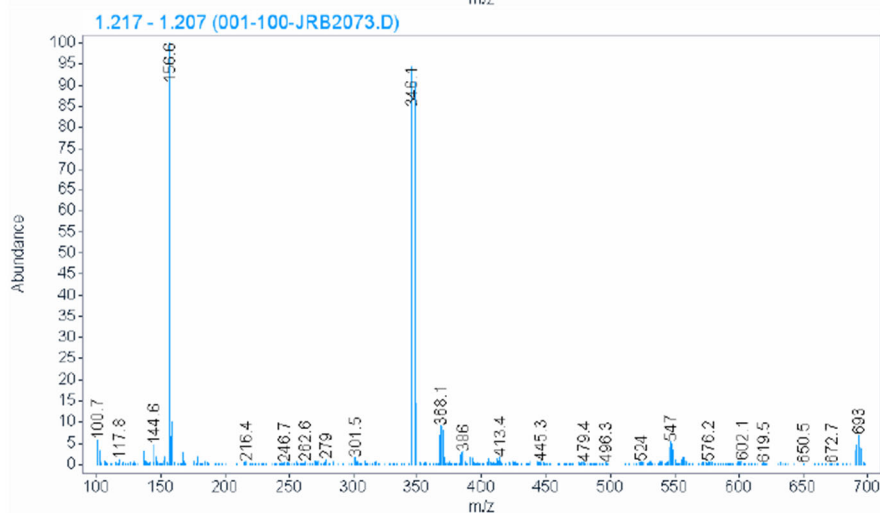
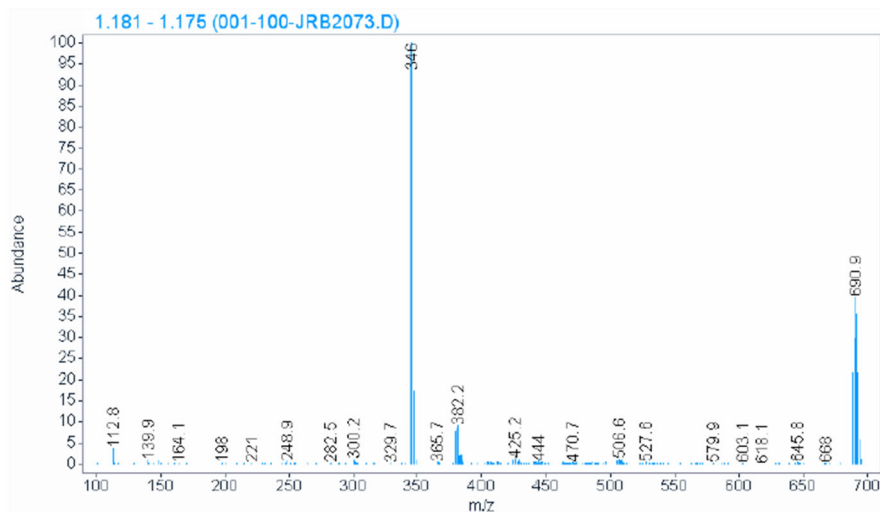
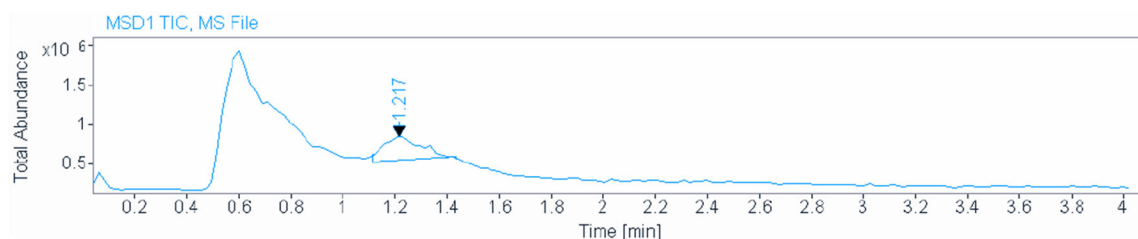
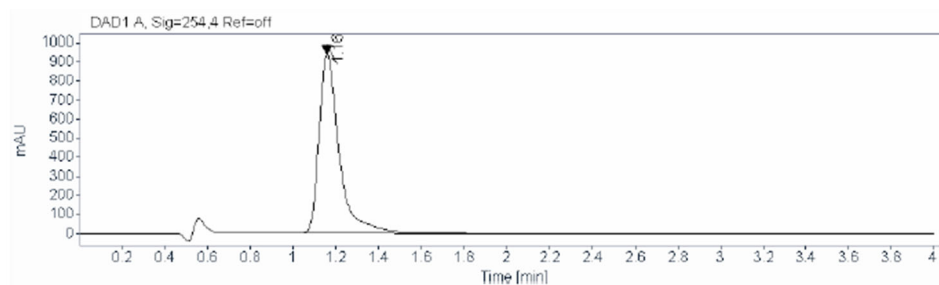


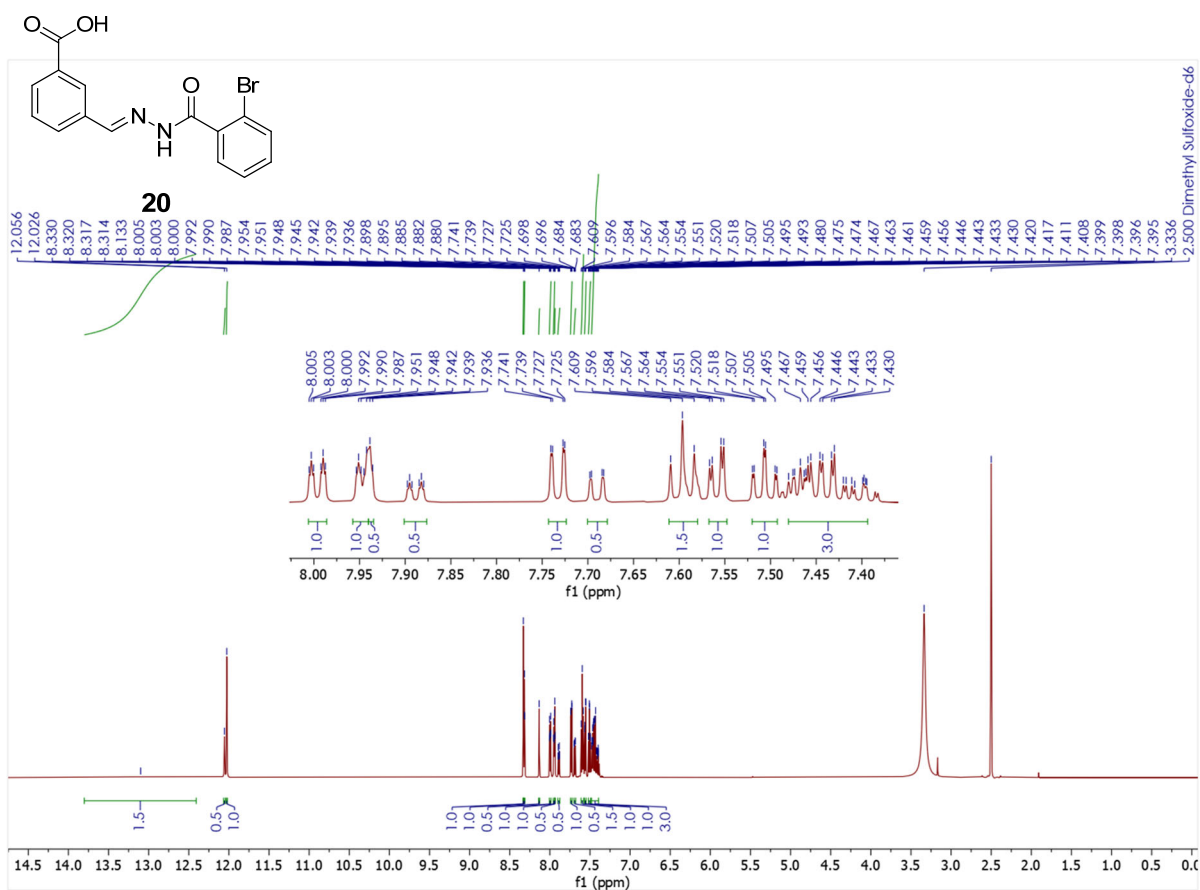
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 Sample name: JRB2073
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 100
 Injection date: 1/31/2022 3:45:53 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC_50%
 Injection volume: 2.000
 B_0.4MLMIN-1_4MINS.M
 Analysis method: LCMS
 Acq. operator: SYSTEM
 ISOCRATIC_50%
 B_0.4MLMIN-1_4MINS.M
 Last changed: 7/14/2016 12:06:24 PM



Molecular Weight: 347.163

19



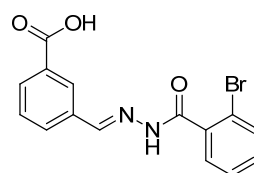


LCMS Report



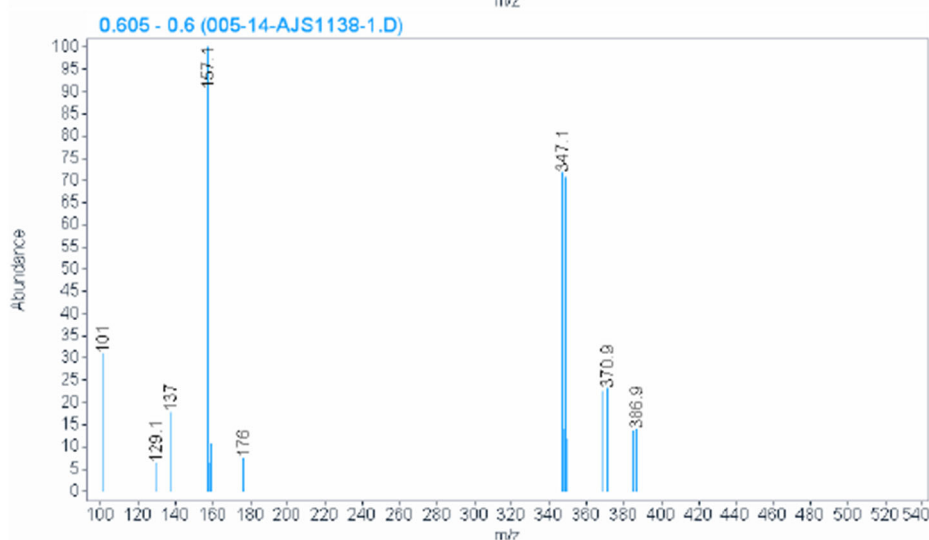
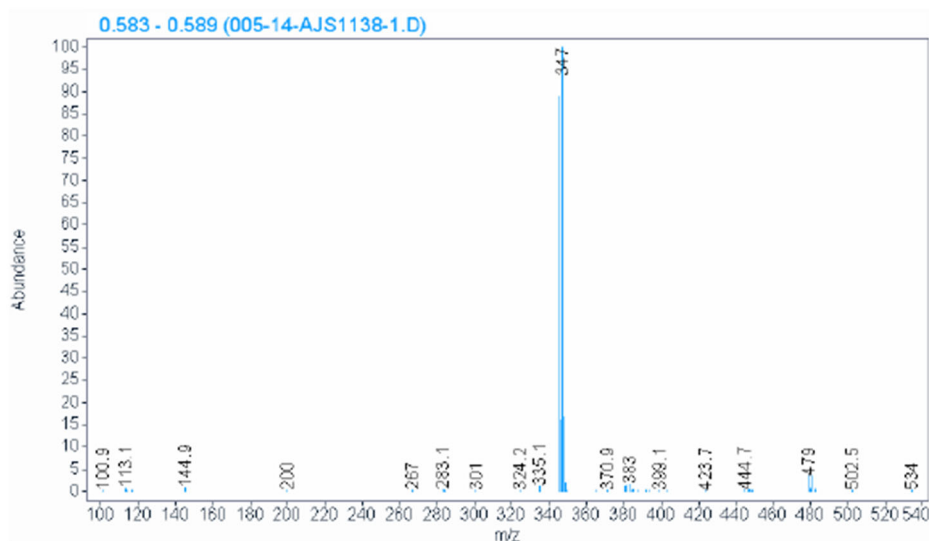
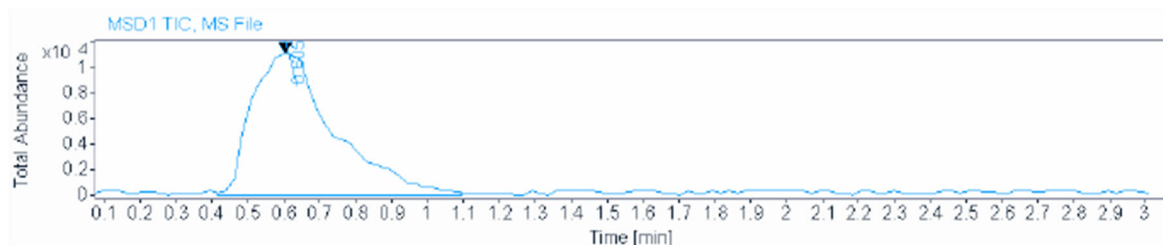
Agilent Technologies

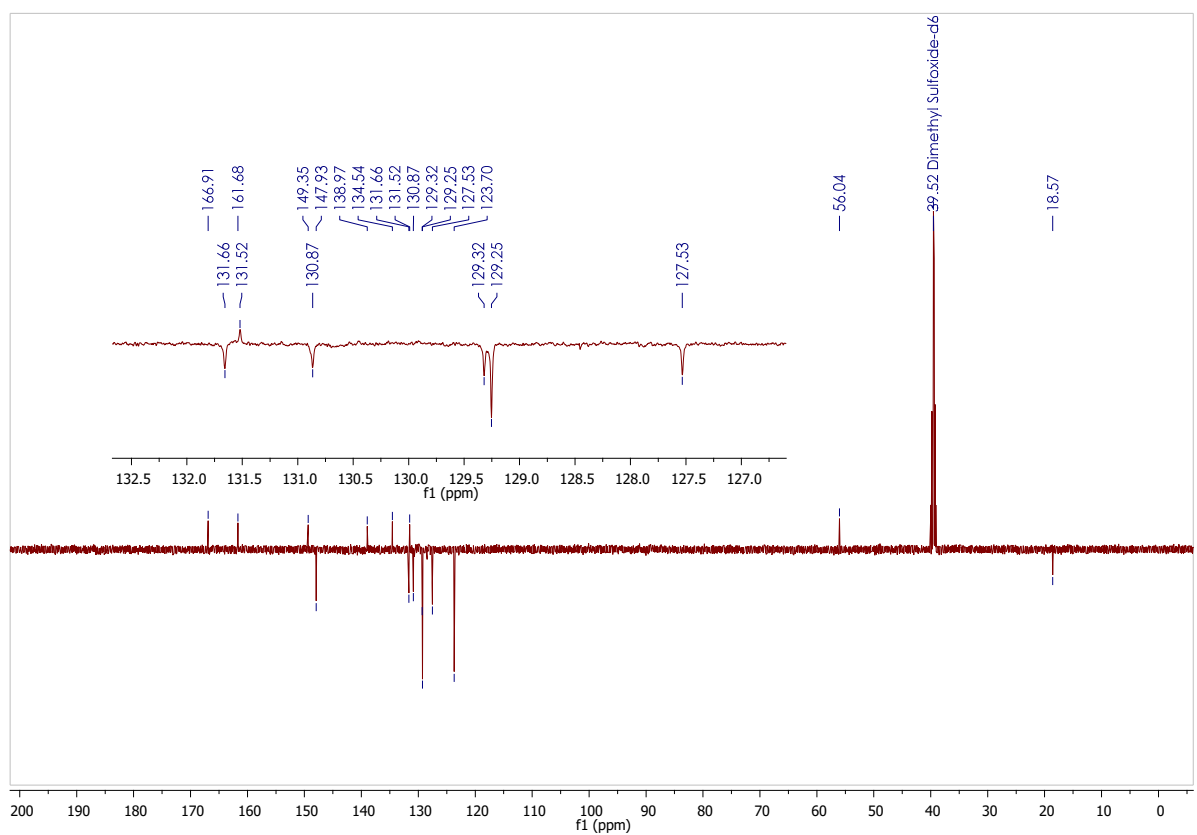
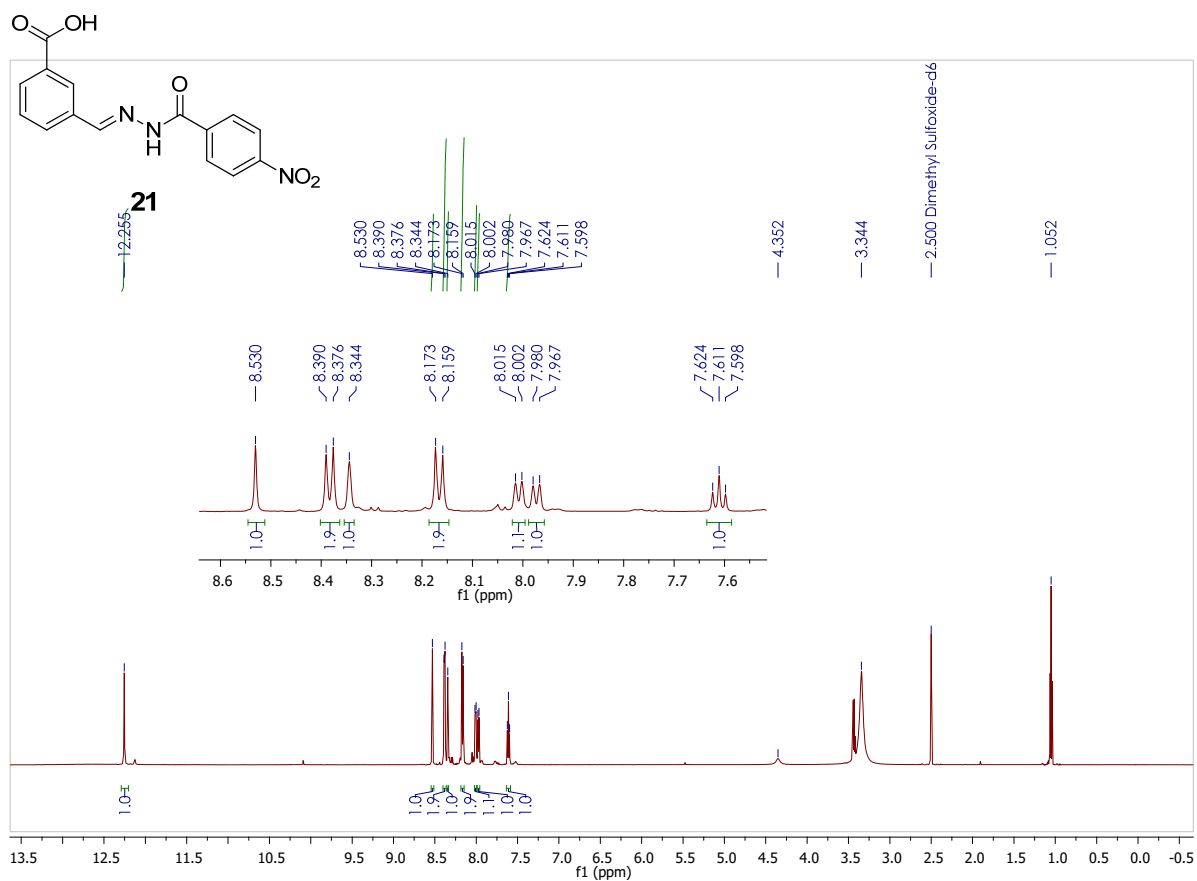
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 Sample name: AJS1138-1
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 14
 Injection date: 7/25/2023 3:04:49 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 Injection volume: 2.000
 B_3 MINS.M
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 80%B_3 MINS.M
 Last changed: 11/26/2021 9:20:48 AM



Molecular Weight: 347.163

20



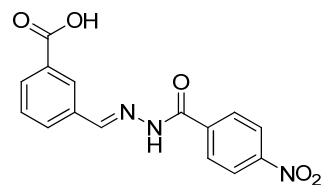


LCMS Report



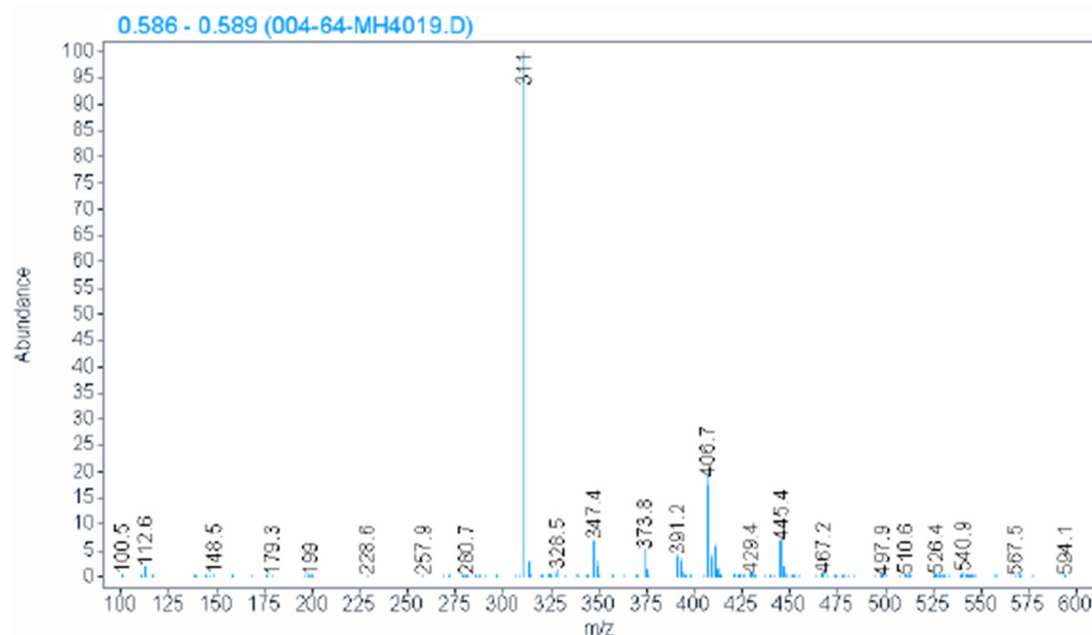
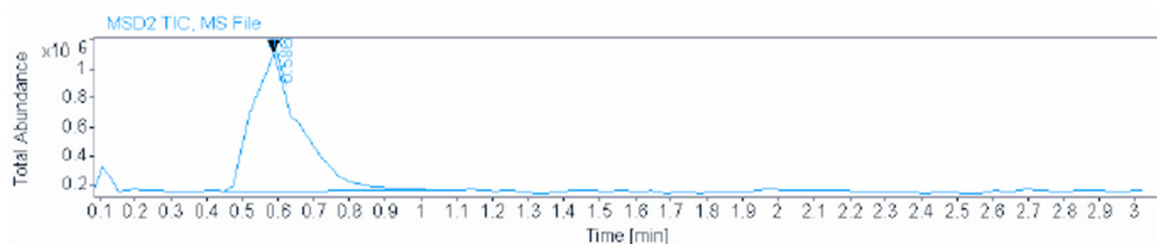
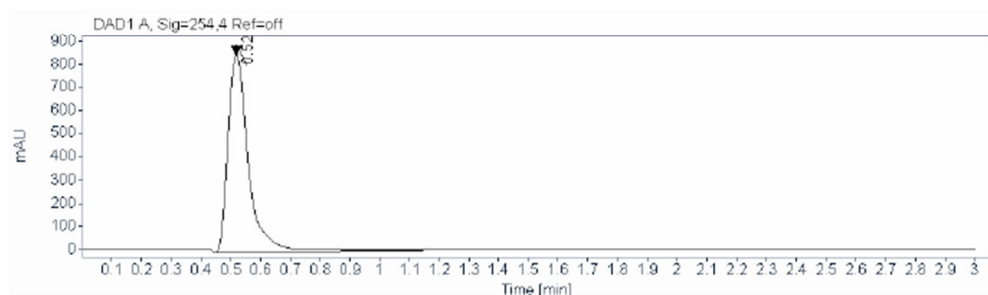
Agilent Technologies

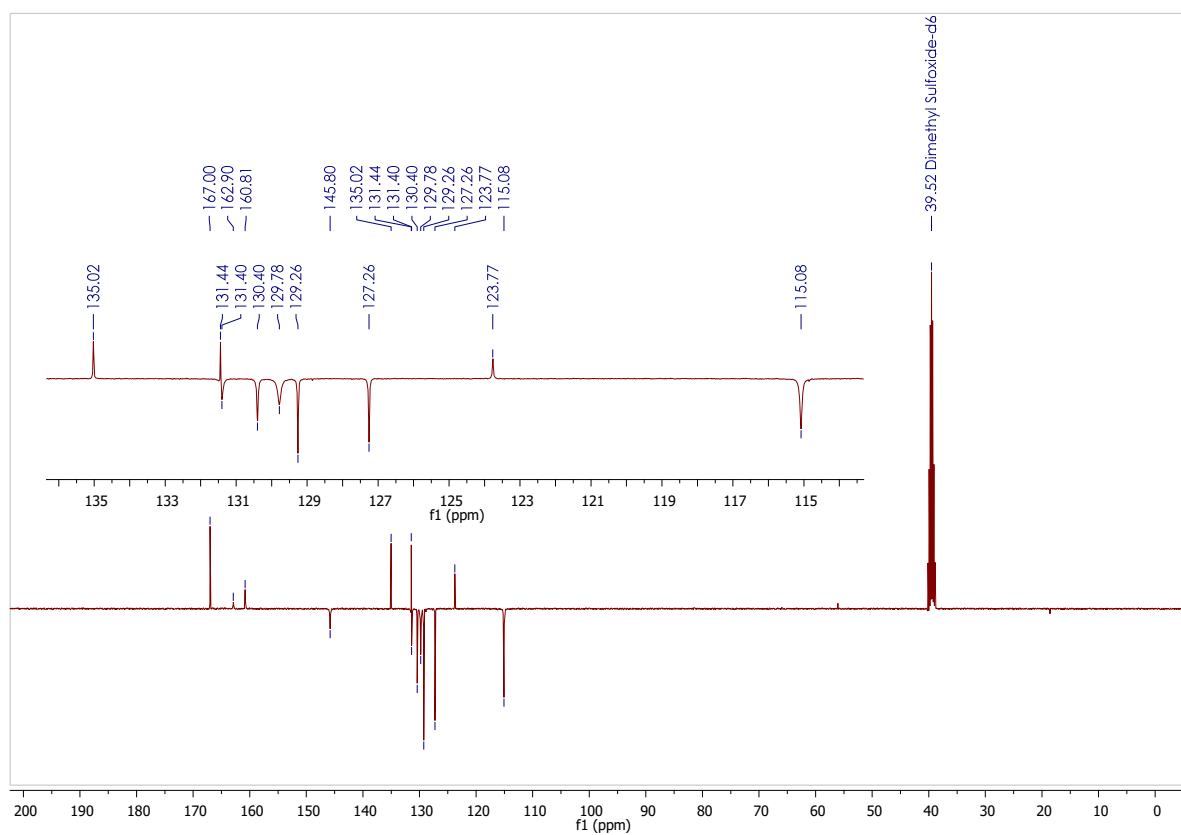
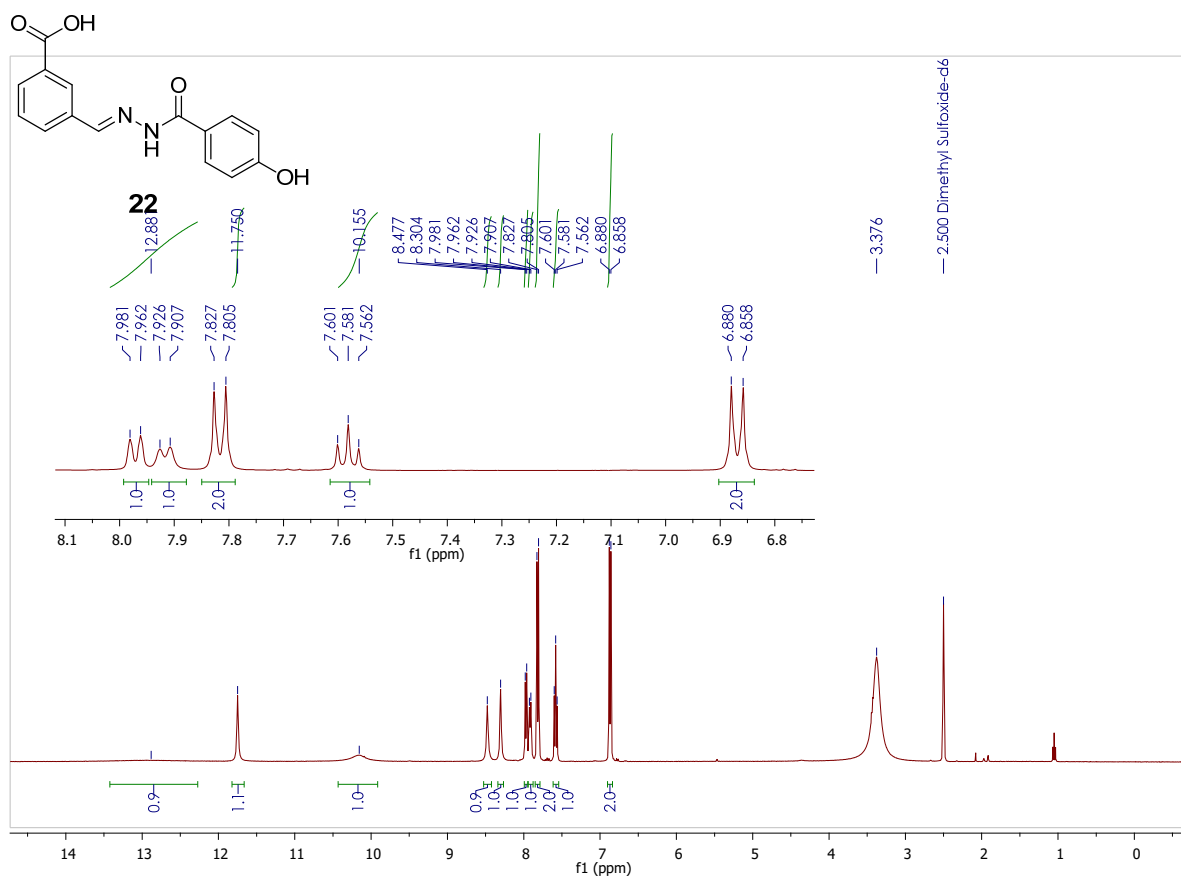
Data file: D:\Chem32\1\Data\MH\mh4017-4021 2022-03-04 11-47-59\004-64-MH4019.D
 Sample name: MH4019
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 64
 Injection date: 3/4/2022 12:03:36 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 Injection volume: 2.000
 B_3 MINS.M
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 80%B_3 MINS.M
 Last changed: 11/26/2021 9:20:48 AM



Molecular Weight: 313.265

21



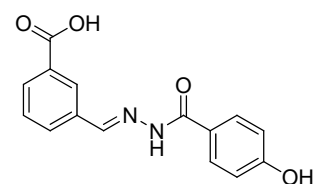


LCMS Report



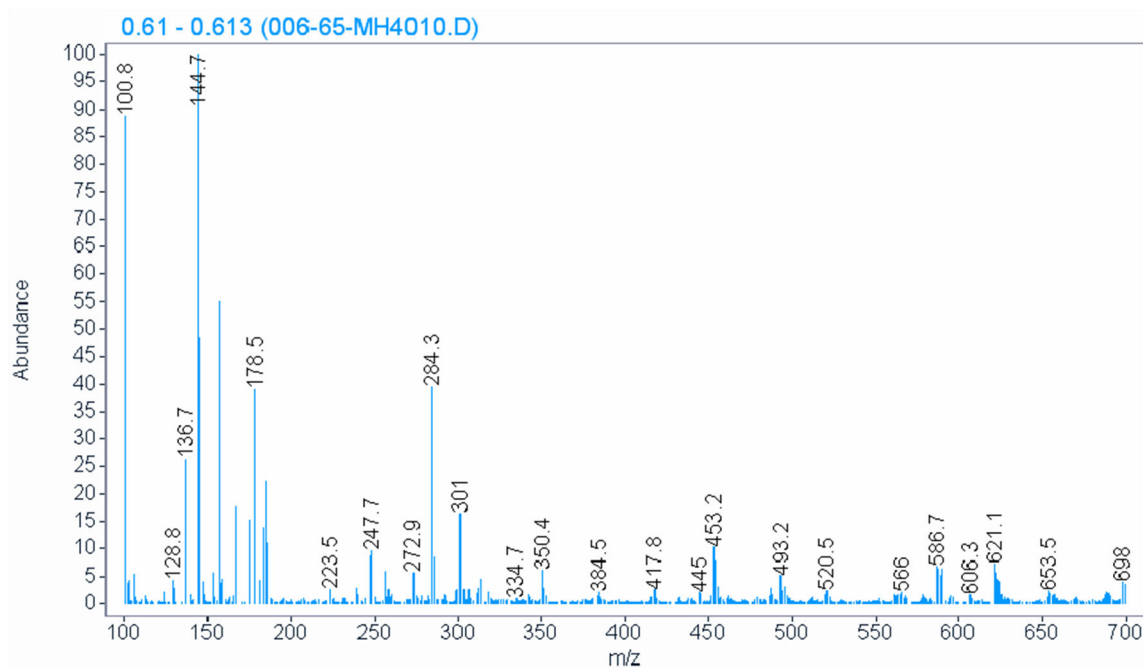
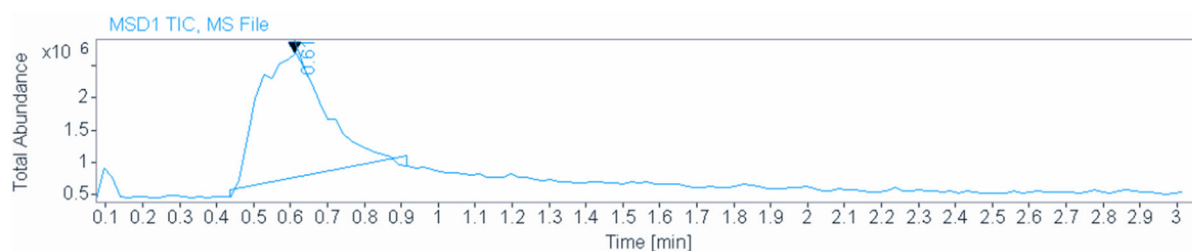
Agilent Technologies

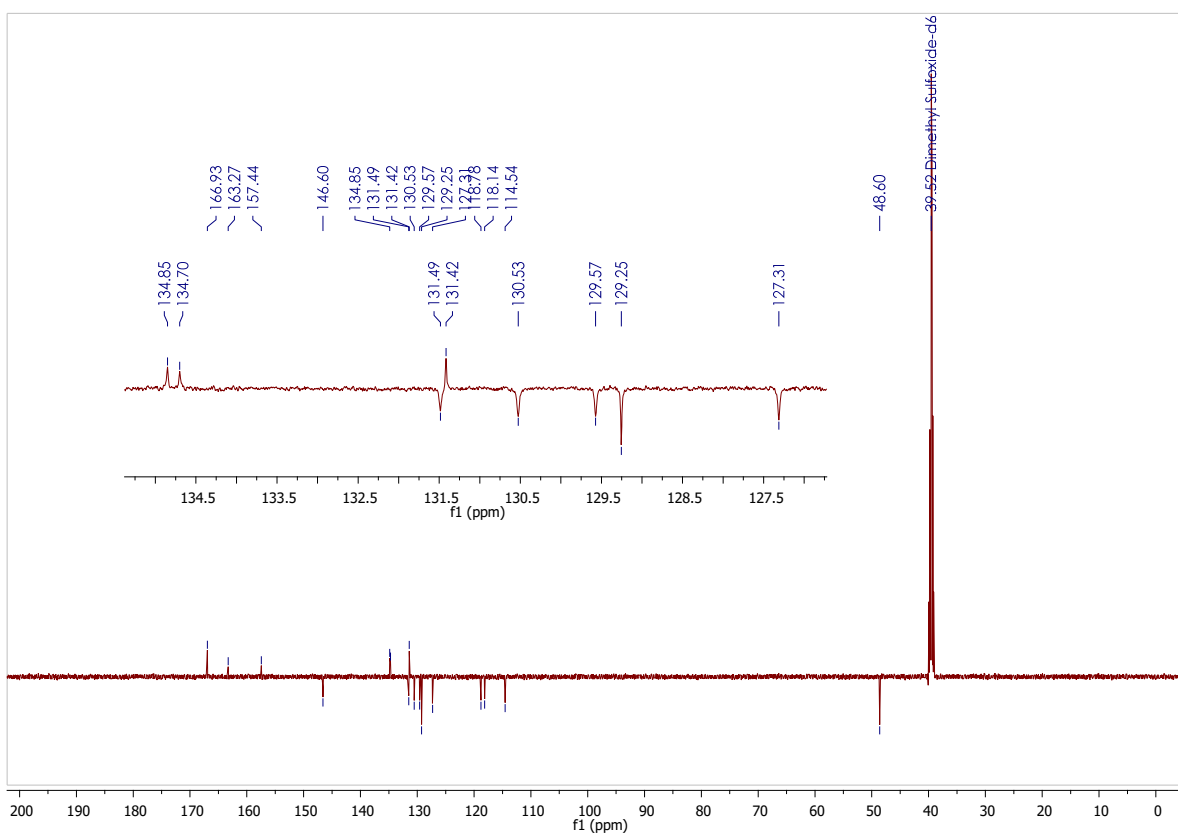
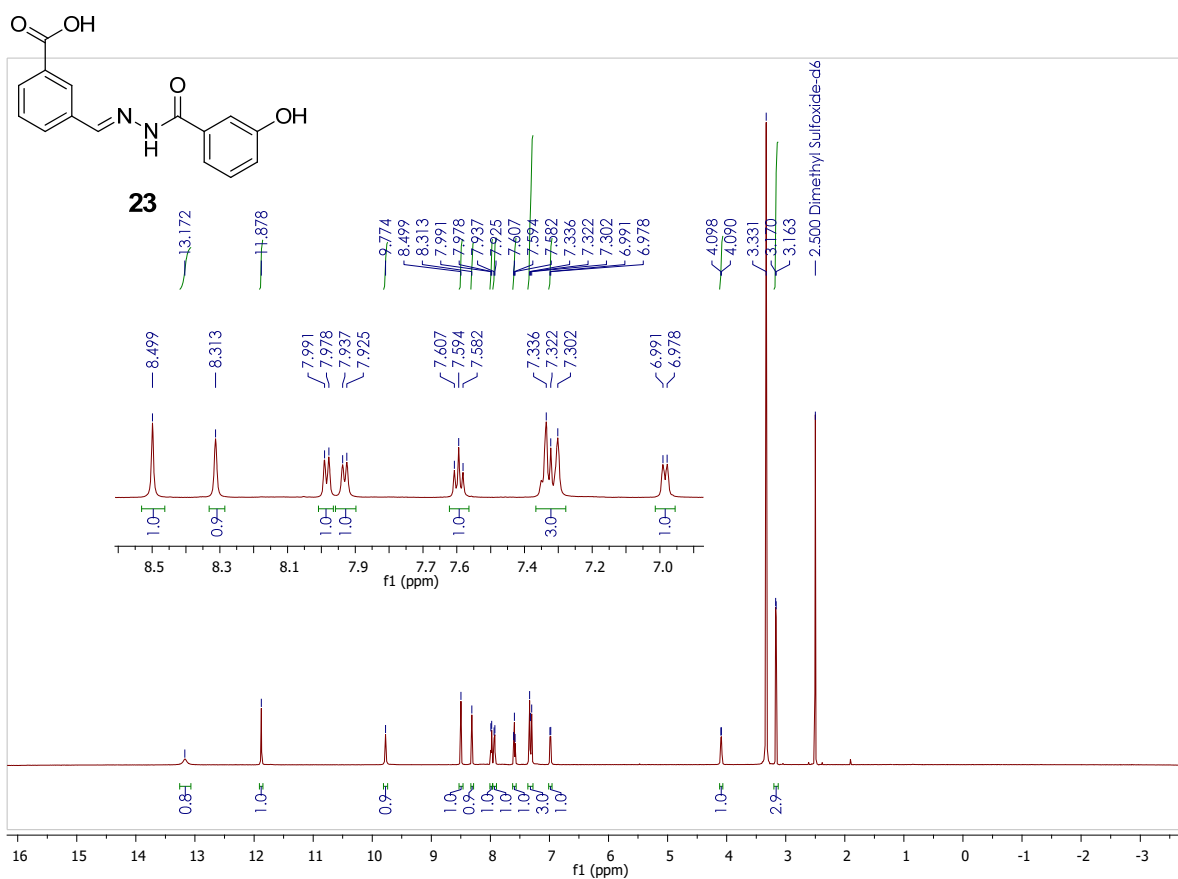
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Sample name: MH4010
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Location: 65
Injection date: 3/1/2022 12:37:39 PM
Injection: 1 of 1
Acq. method: LCMS ISOCRATIC_80% B_0.4MLMIN-1_4MINS.M
Injection volume: 2.000
Analysis method: LCMS ISOCRATIC_80% B_0.4MLMIN-1_4MINS.M
Acq. operator: SYSTEM
Last changed: 7/13/2021 10:05:44 AM



Molecular Weight: 284.267

22



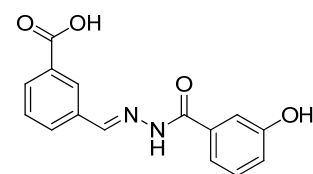


LCMS Report



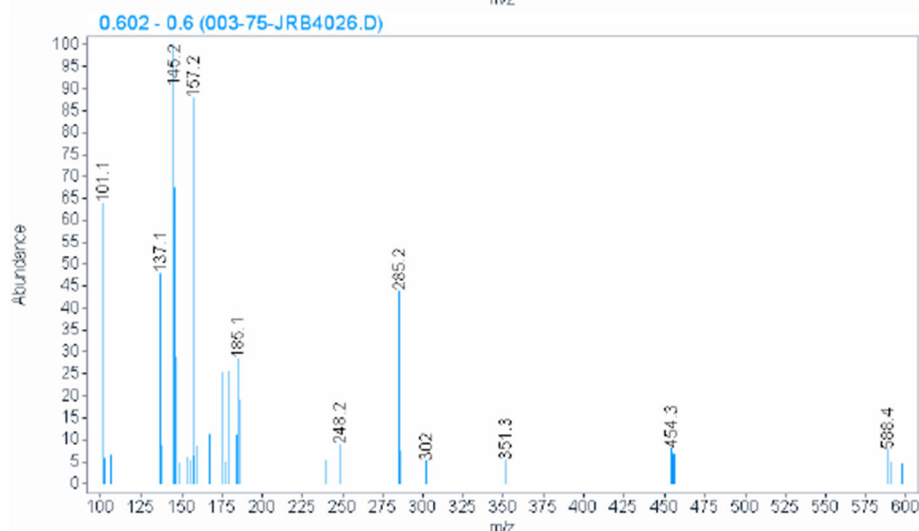
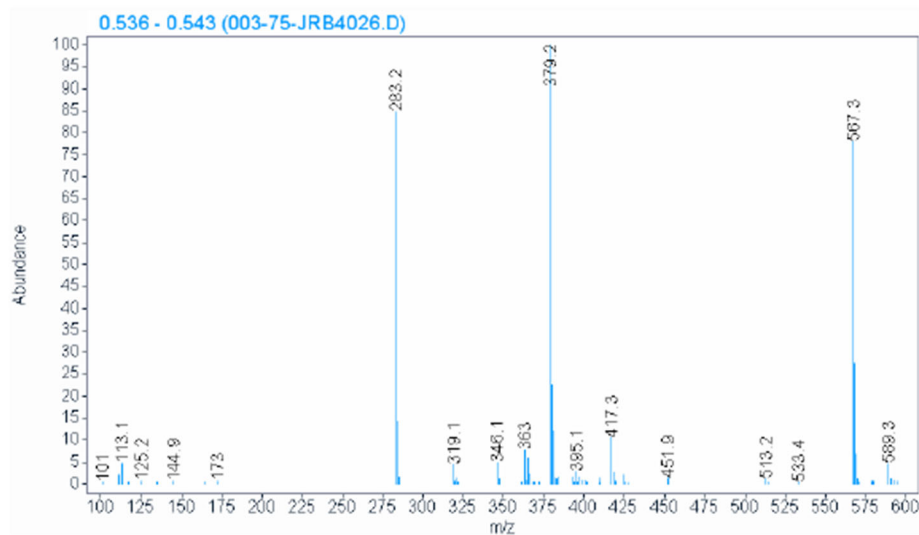
Agilent Technologies

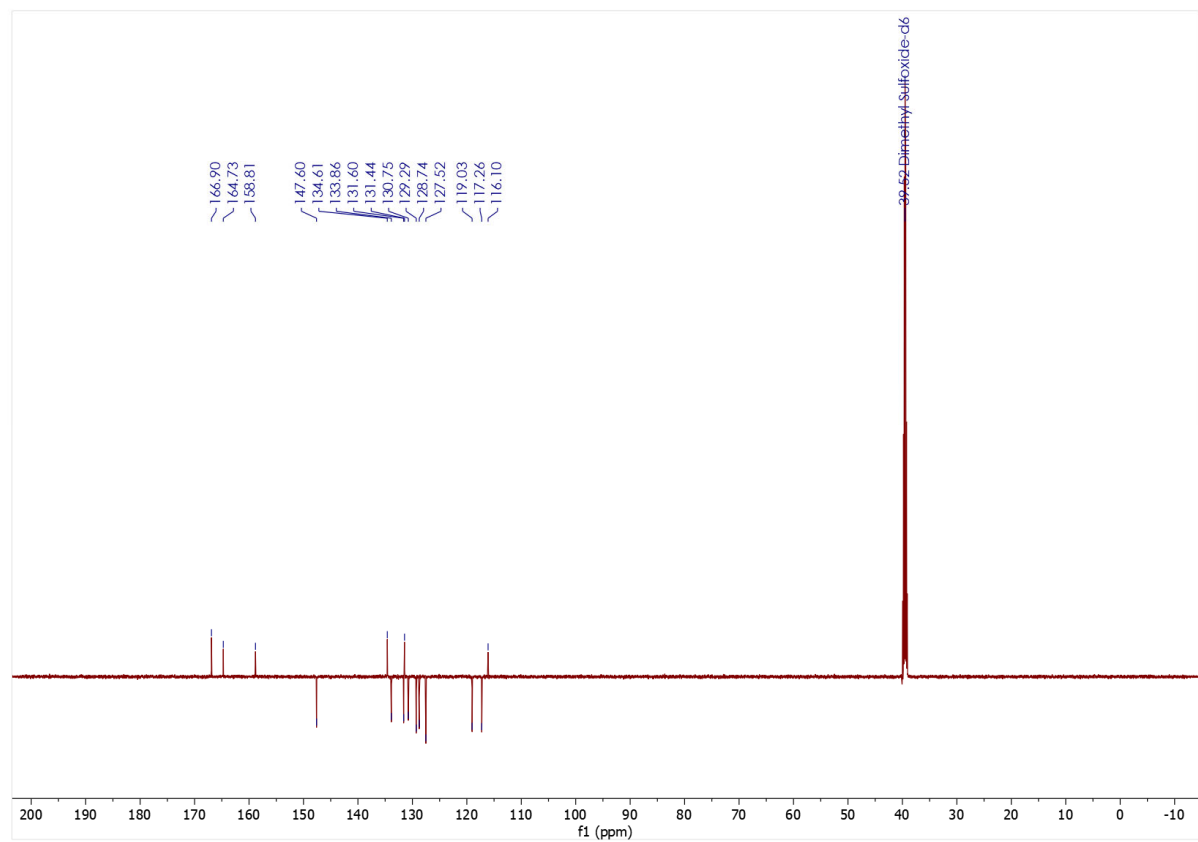
Data file: D:\Chem32\1\Data\JRB\JRB4025-4027-2 2023-07-24 15-27-22\003-75-JRB4026.D
 Sample name: JRB4026
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Injection date: 7/24/2023 3:40:18 PM
 Location: 75
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 Injection volume: 2.000
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 80%B_3 MINS.M
 Last changed: 11/26/2021 9:20:48 AM



Molecular Weight: 284.267

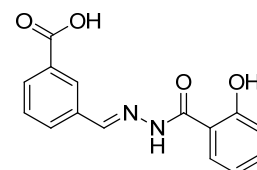
23





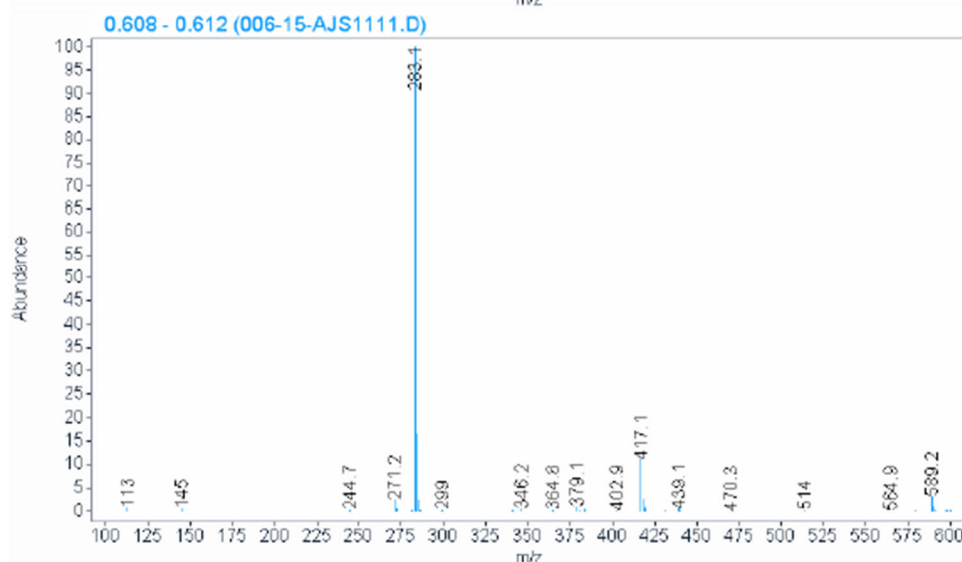
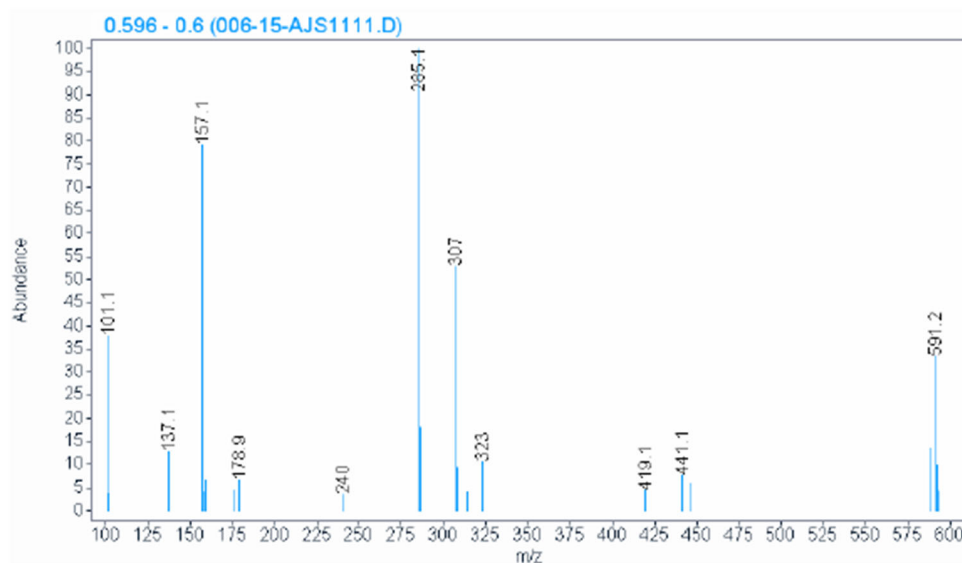
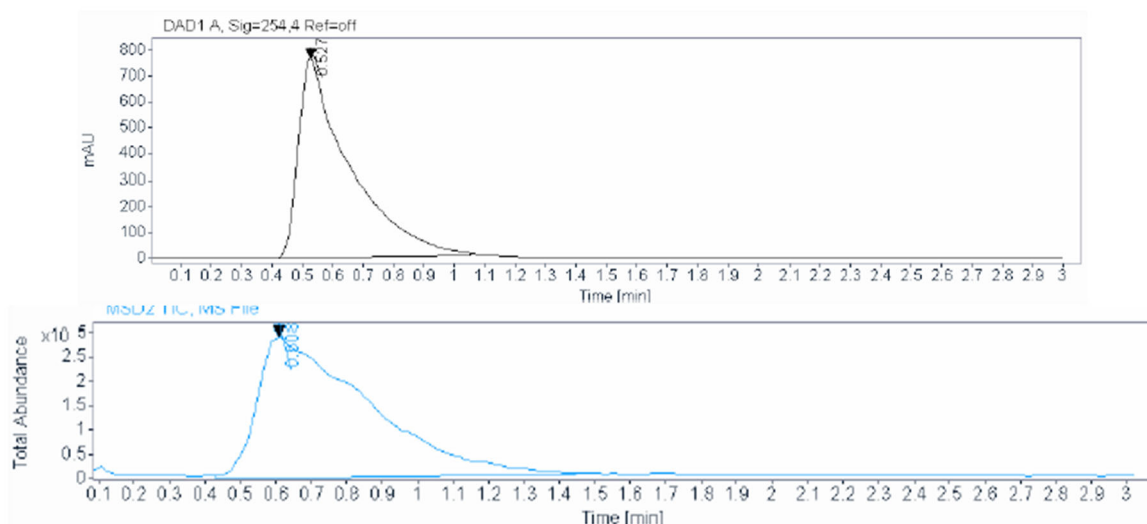


Data file: D:\Chem321\1\Data\AJS\AJS Table1 2023-07-25 14-45-29\006-15-AJS1111.D
Sample name: AJS1111
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Location: 15
Injection date: 7/25/2023 3:09:29 PM
Injection: 1 of 1
Acq. method: LCMS ISOCRATIC 80%
Injection volume: 2.000
B_3 MINS.M
Analysis method: LCMS ISOCRATIC
Acq. operator: SYSTEM
80%B_3 MINS.M
Last changed: 11/26/2021 9:20:48 AM



Molecular Weight: 284.267

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LCMS Report



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Data file: D:\Chem32\1\Data\MH\MH4027-29, MH4013-14 2022-03-04 13-12-27\004-74-MH4029.D
Sample name: MH4029
Description:
Sample amount: 0.000
Instrument: LCMS
Injection date: 3/4/2022 1:28:06 PM
Acq. method: LCMS ISOCRATIC 80% B_3 MINS.M
Analysis method: LCMS ISOCRATIC 80%B_3 MINS.M
Last changed: 11/26/2021 9:20:48 AM

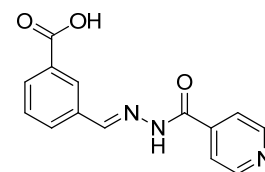
Sample type: Sample

Location: 74

Injection: 1 of 1

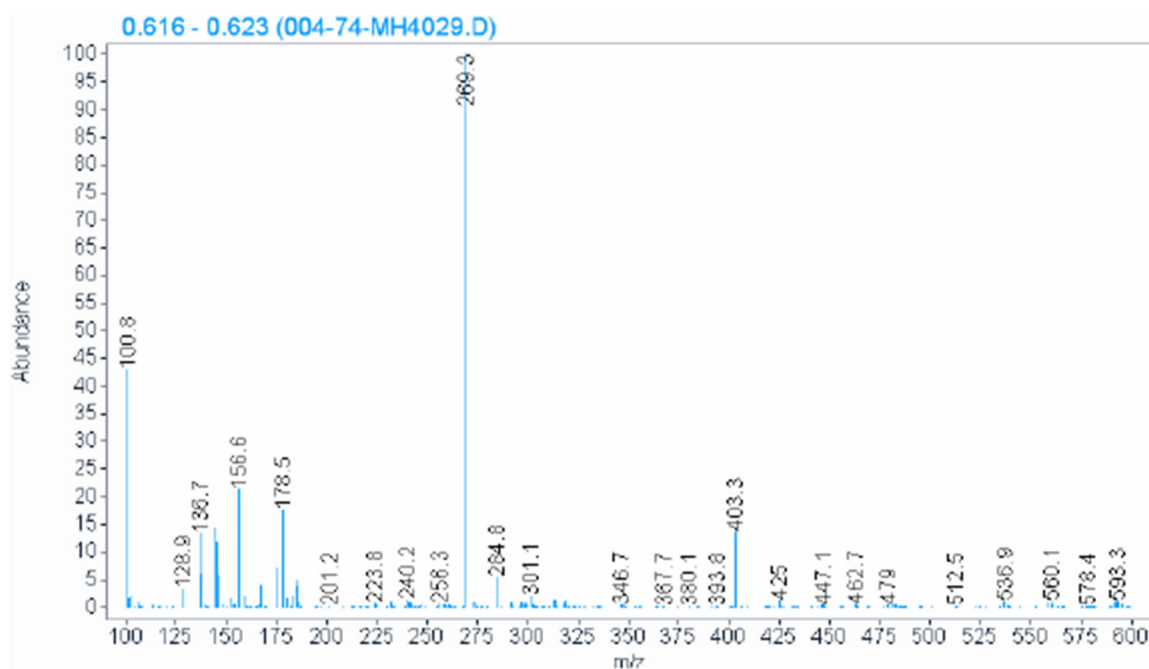
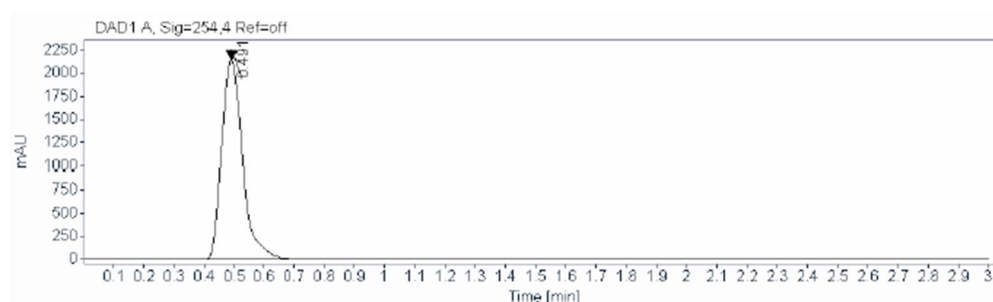
Injection volume: 2.000

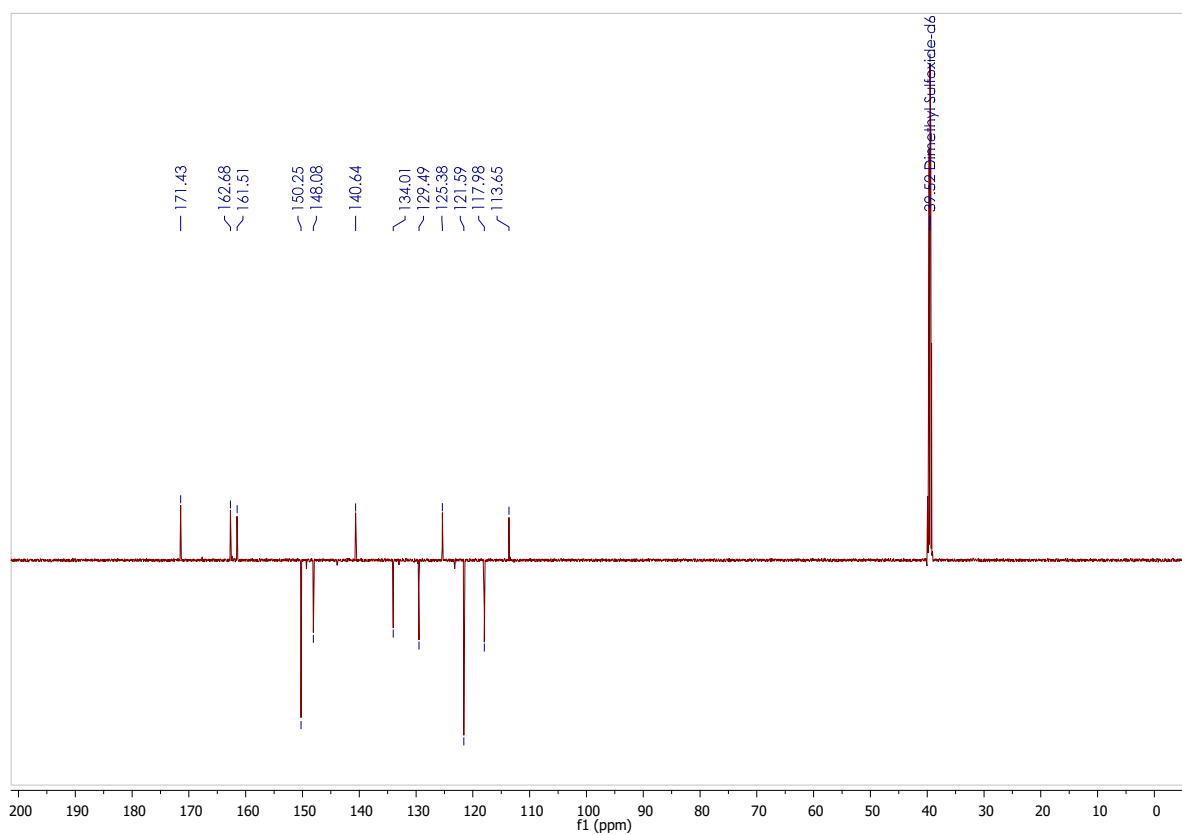
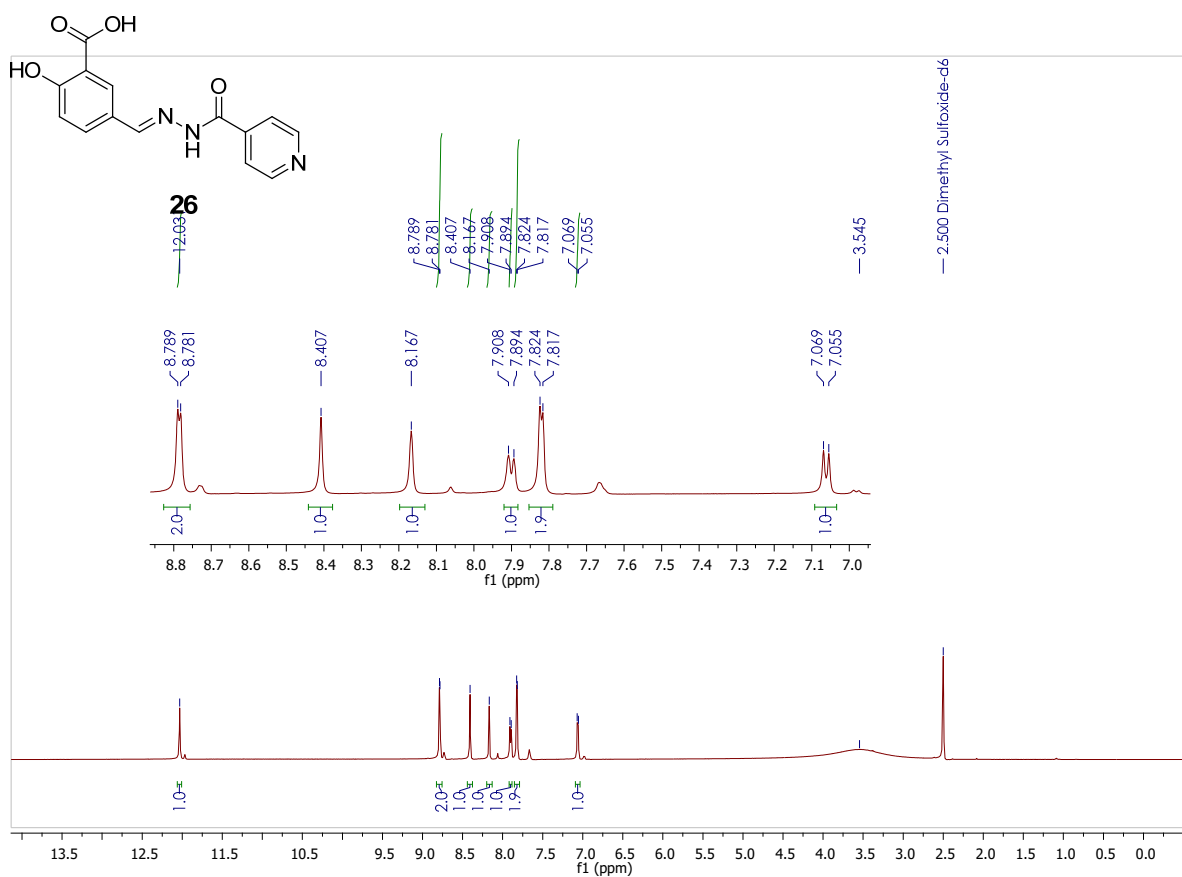
Acq. operator: SYSTEM



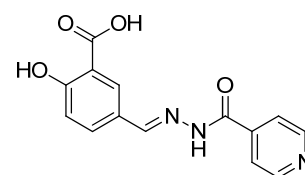
Molecular Weight: 269.255

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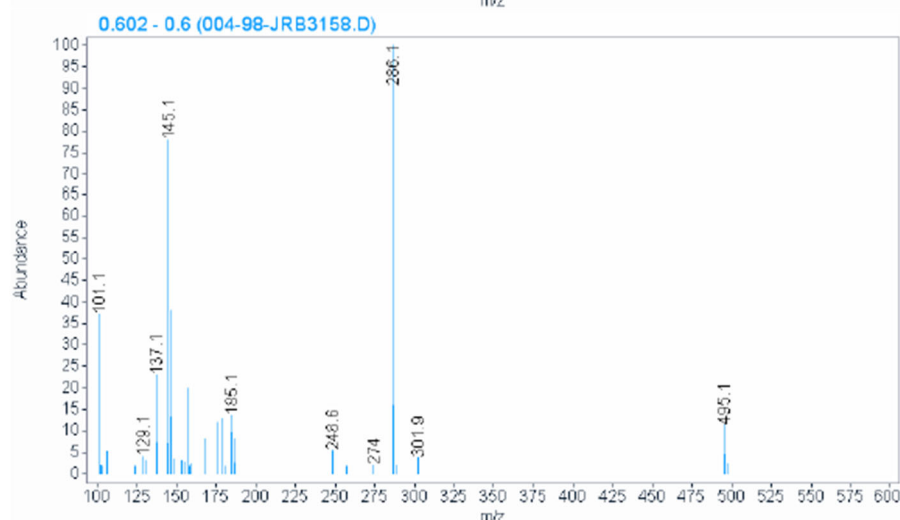
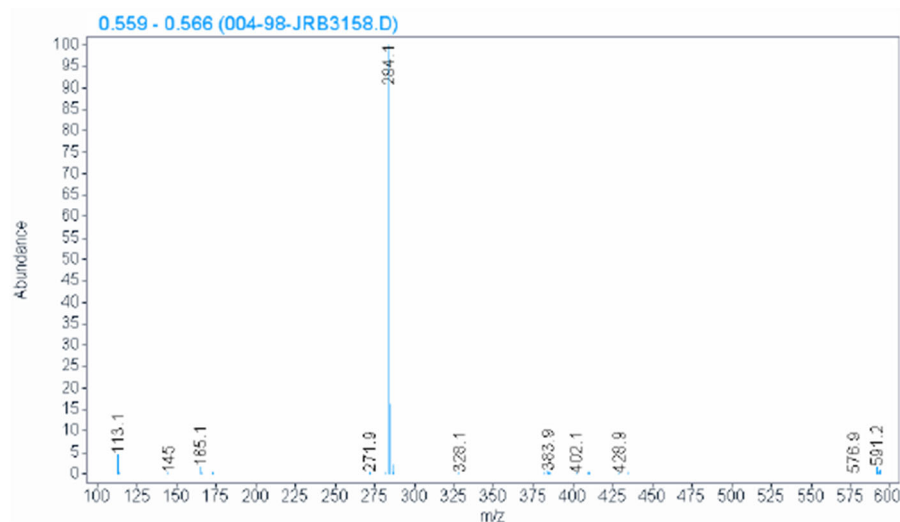
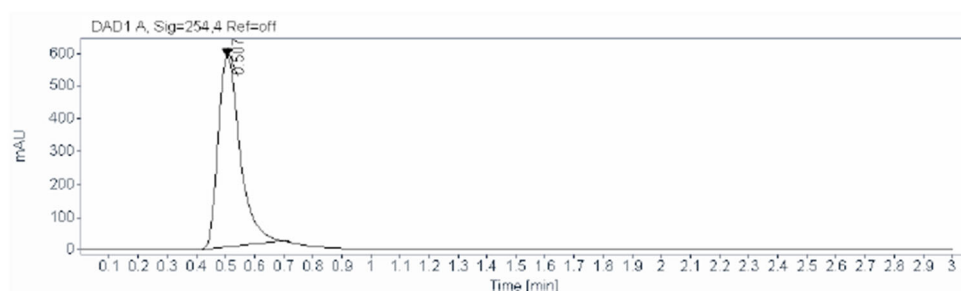


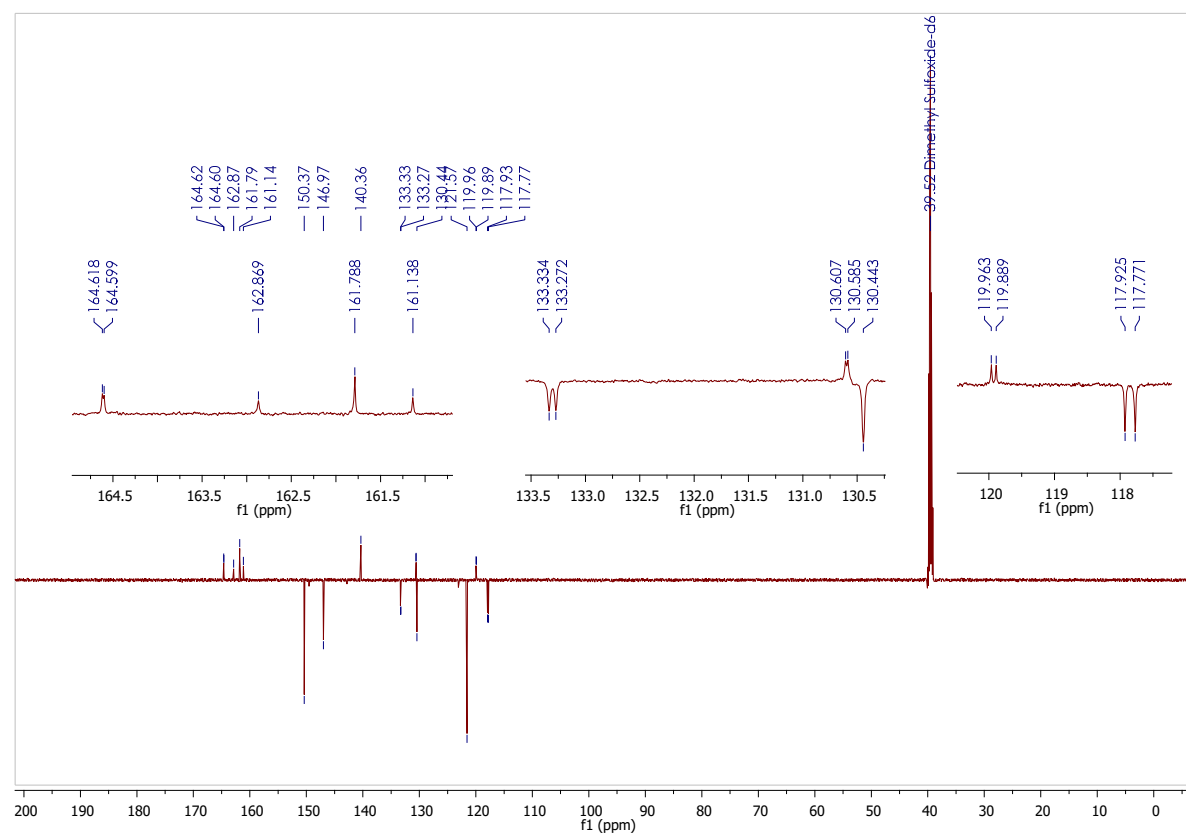
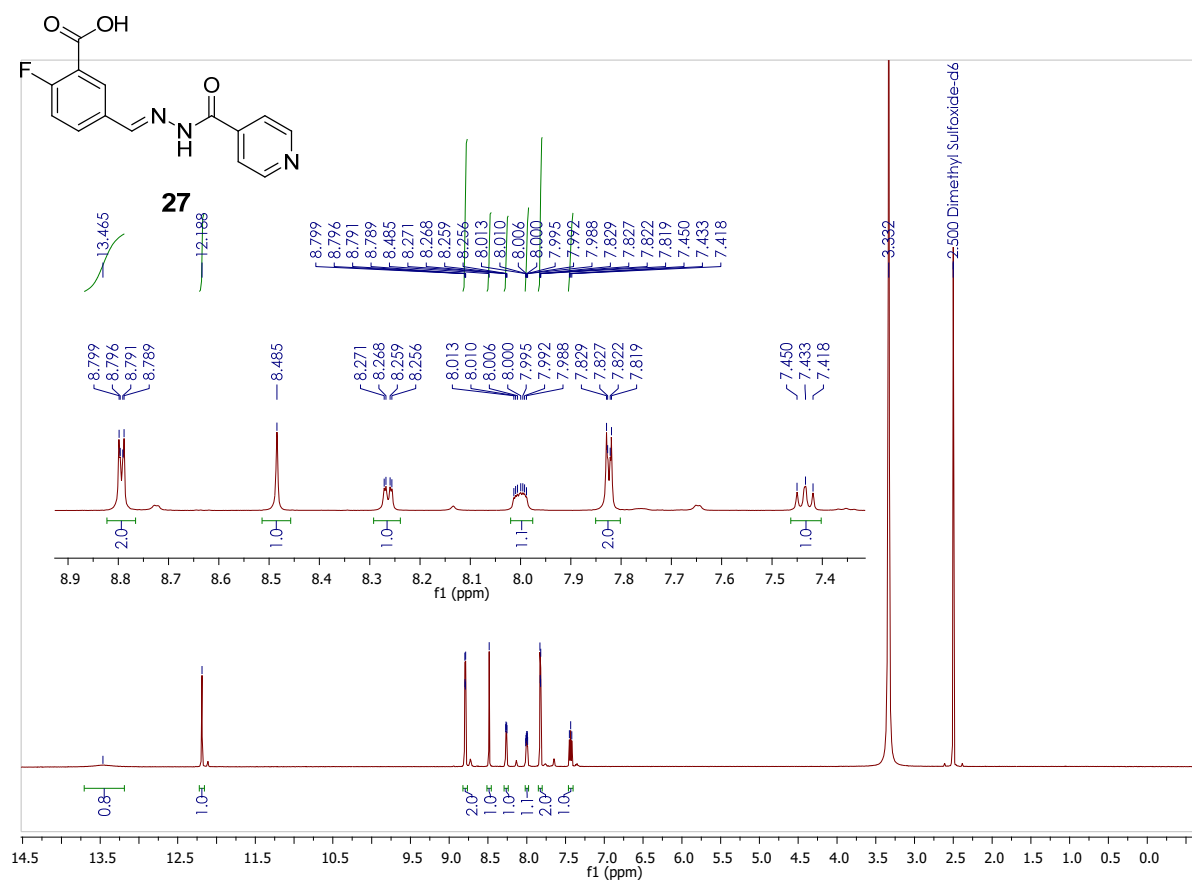
Data file: D:\Chem32\1\Data\JRB\JRB3066 3157 3158 3160 2023-07-24 12-35-44\004-98-JRB3158.D
 Sample name: JRB3158
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 98
 Injection date: 7/24/2023 12:51:52 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 Injection volume: 2.000
 B_3 MINS.M
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 80%B_3 MINS.M
 Last changed: 11/26/2021 9:20:48 AM

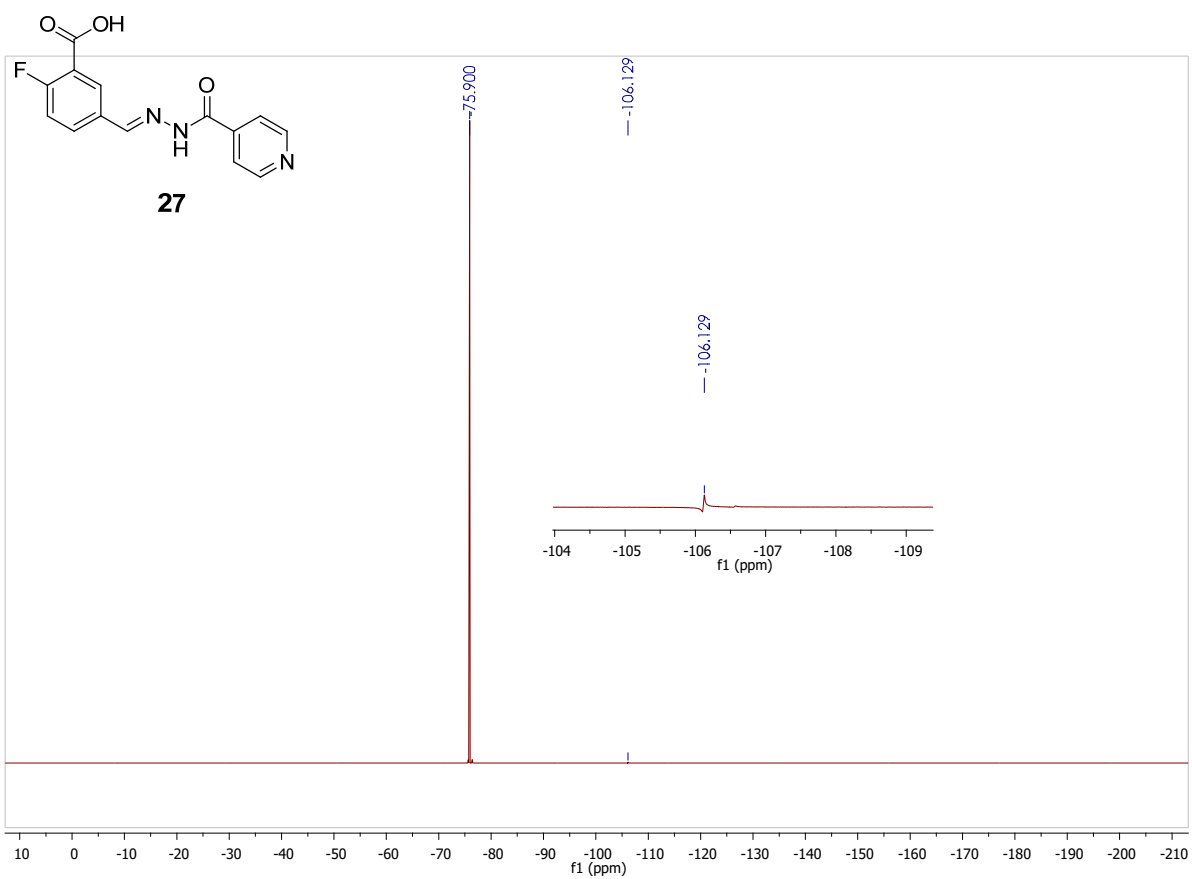


Molecular Weight: 285.255

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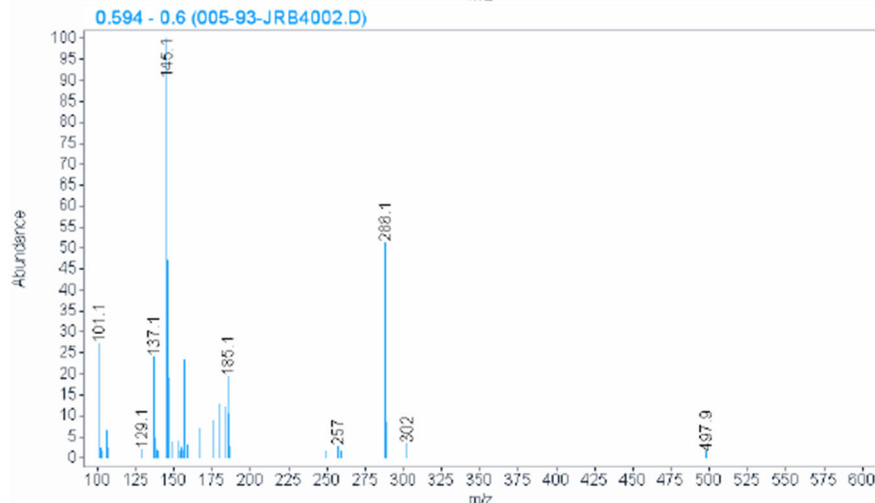
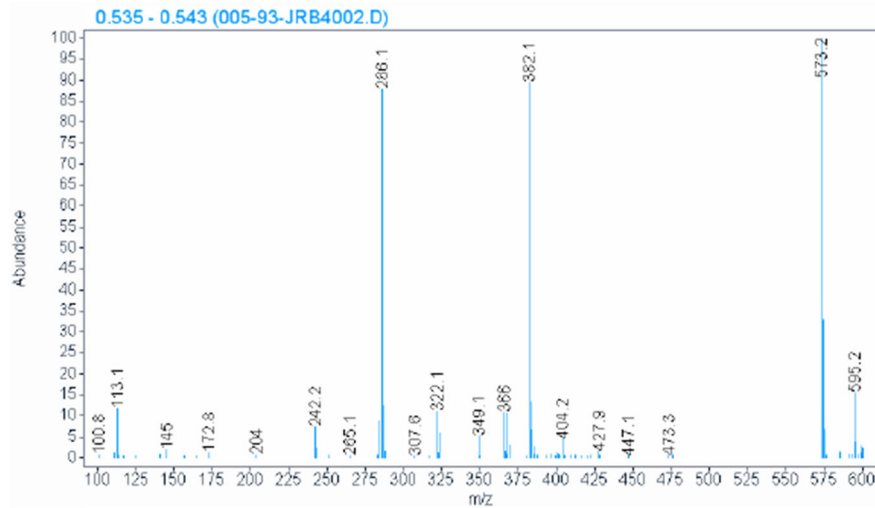
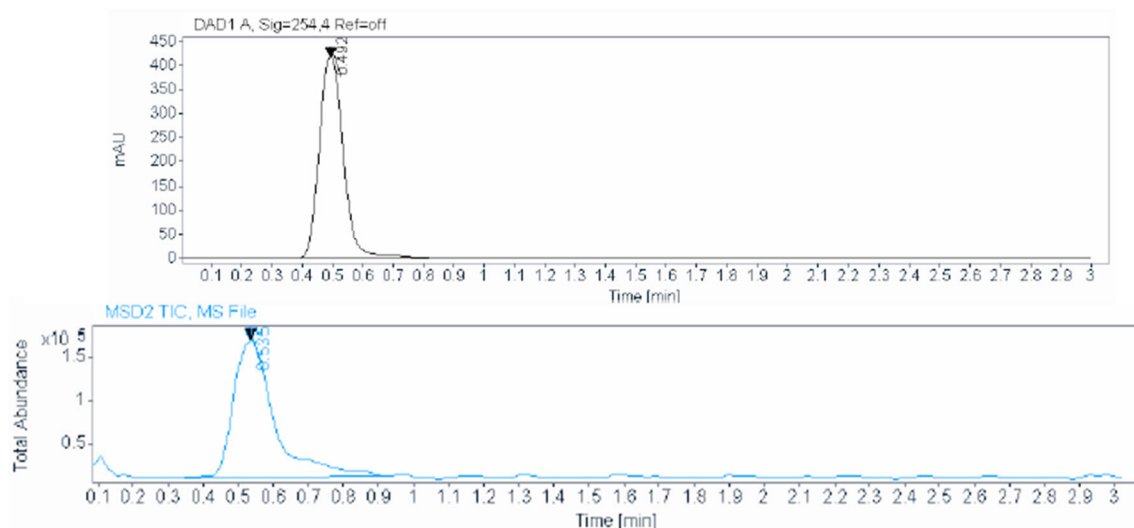
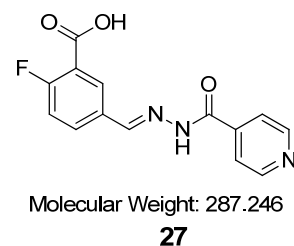


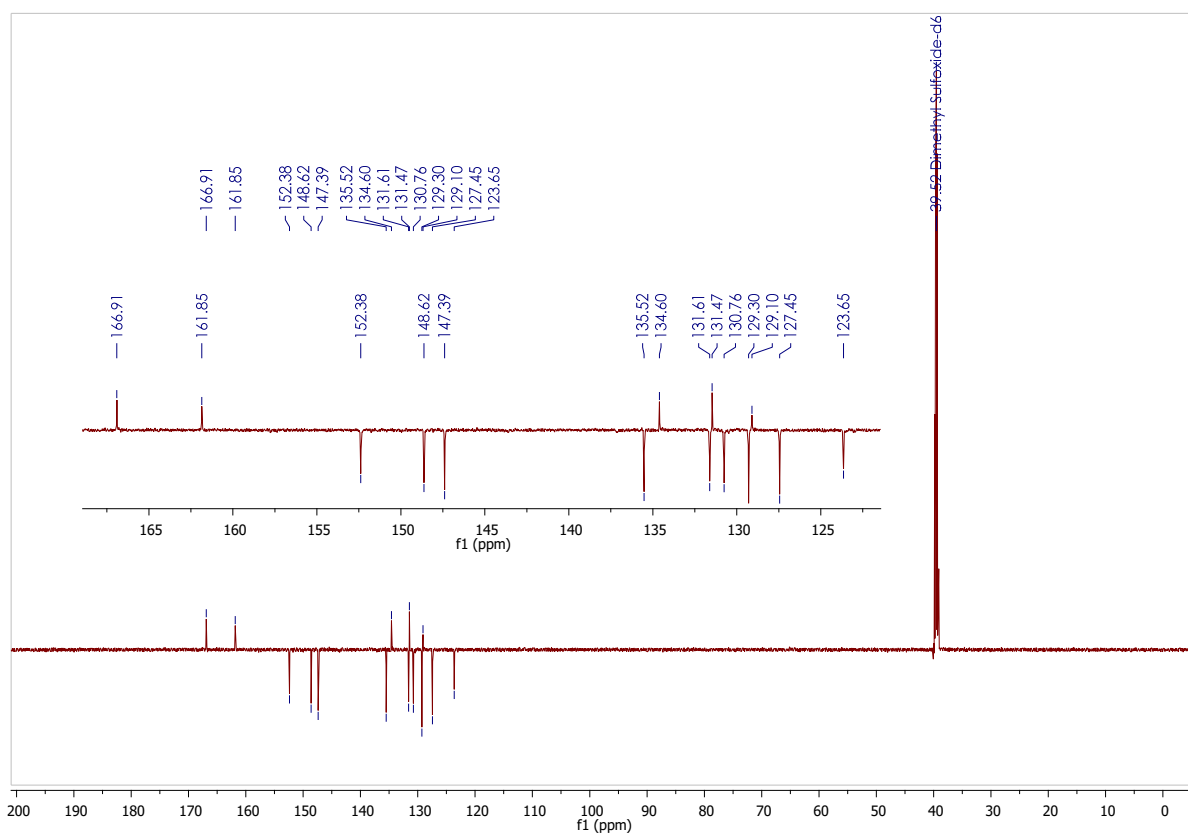
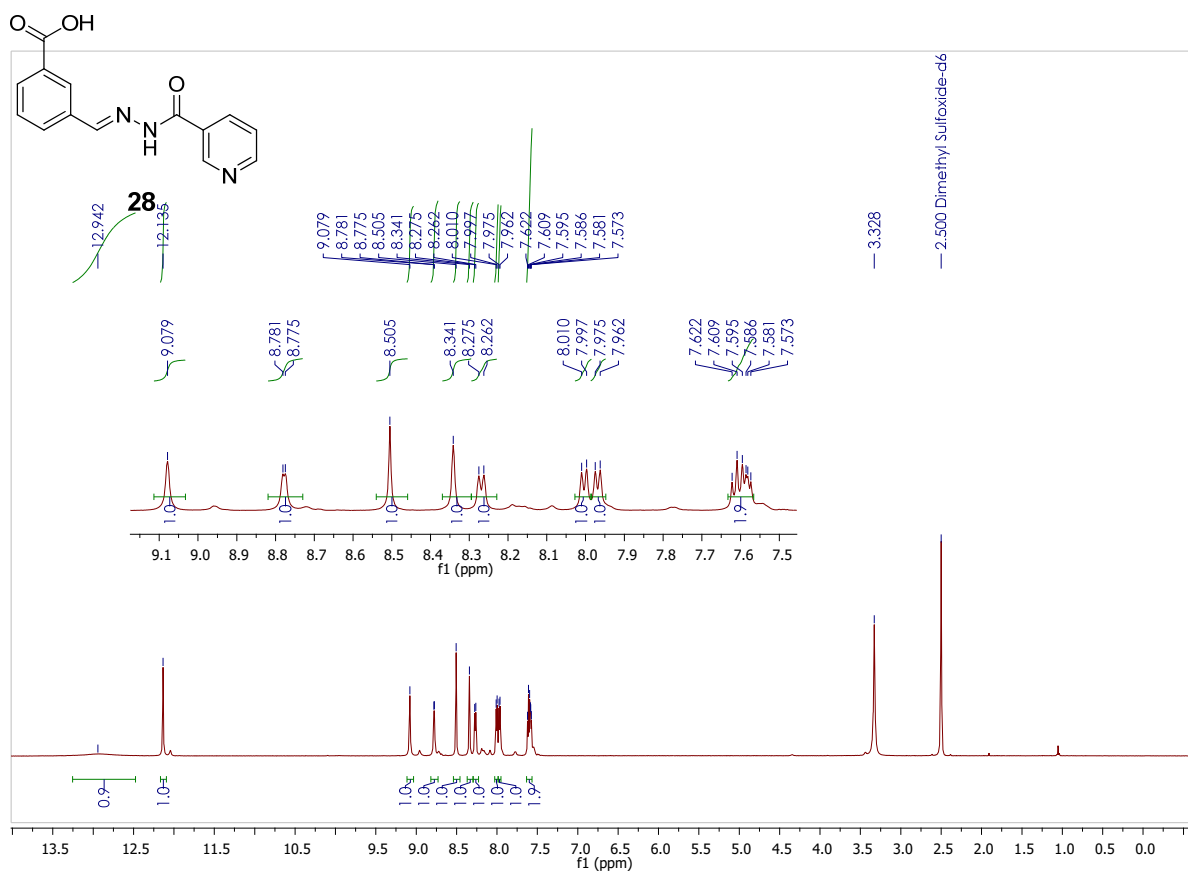




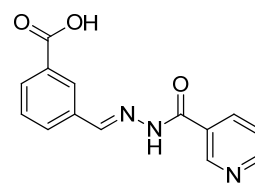


Data file:	D:\Chem32\1\Data\JRB\JRB3189 3196 4001 4002 2023-07-24 12-59-52\005-93-JRB4002.D		
Sample name:	JRB4002		
Description:			
Sample amount:	0.000	Sample type:	Sample
Instrument:	LCMS	Location:	93
Injection date:	7/24/2023 1:20:11 PM	Injection:	1 of 1
Acq. method:	LCMS ISOCRATIC 80% B_3 MINS.M	Injection volume:	2.000
Analysis method:	LCMS ISOCRATIC 80%B_3 MINS.M	Acq. operator:	SYSTEM
Last changed:	11/26/2021 9:20:48 AM		



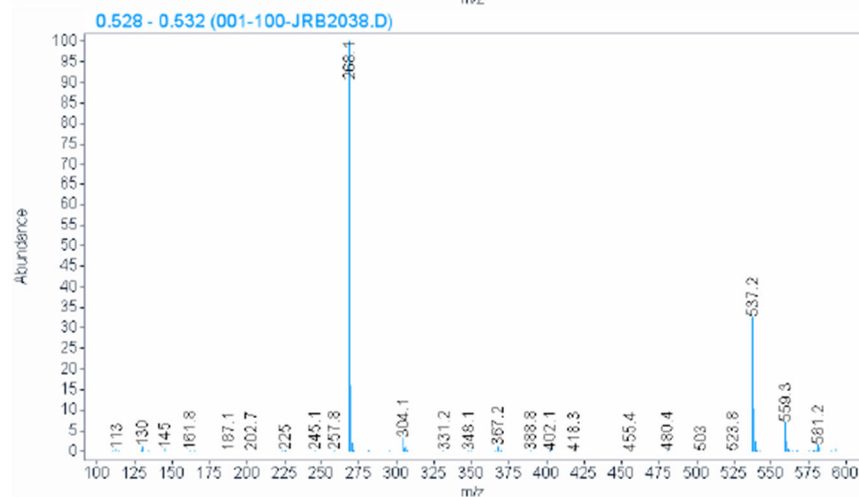
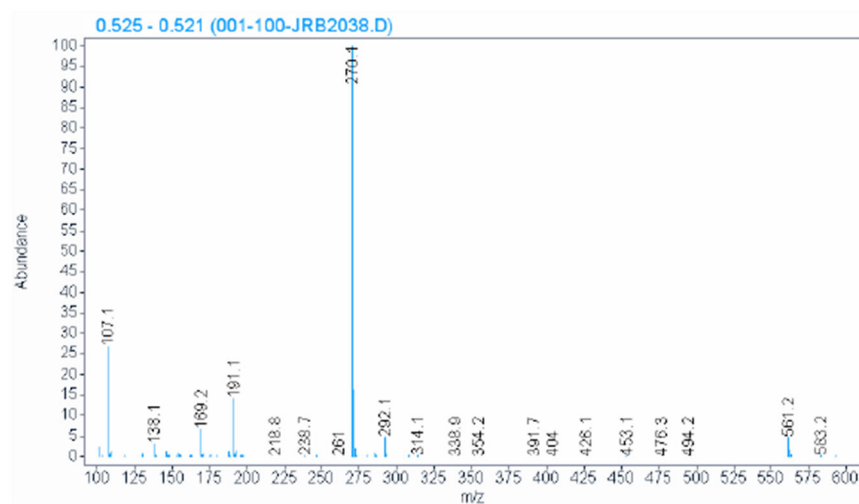
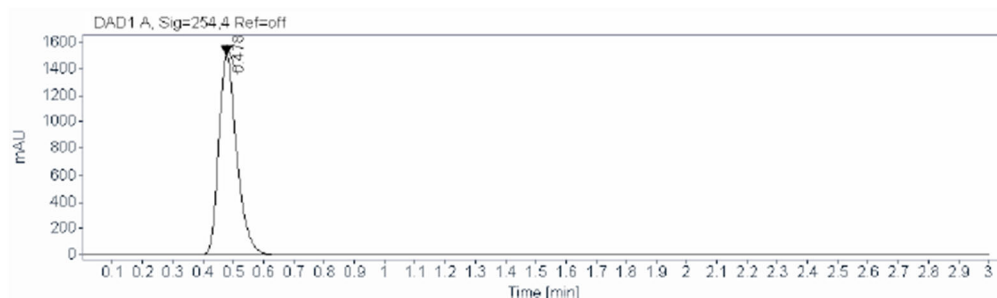


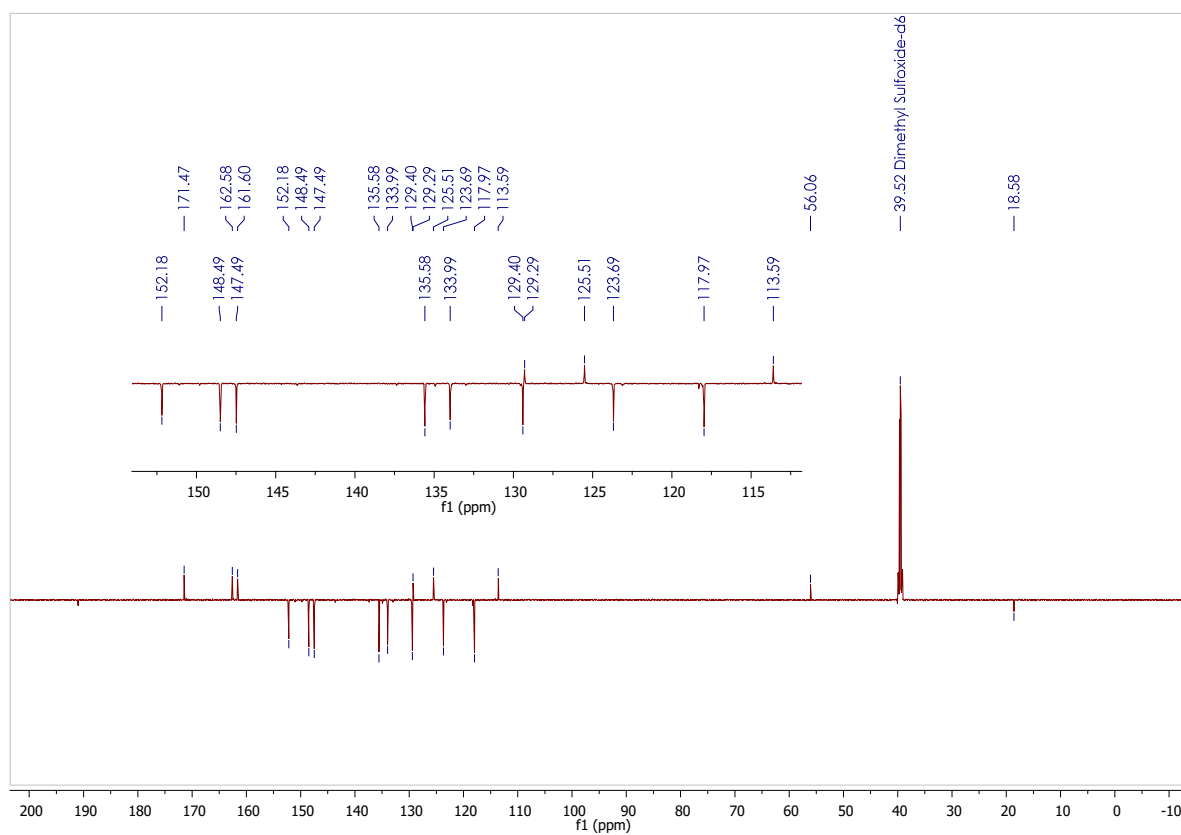
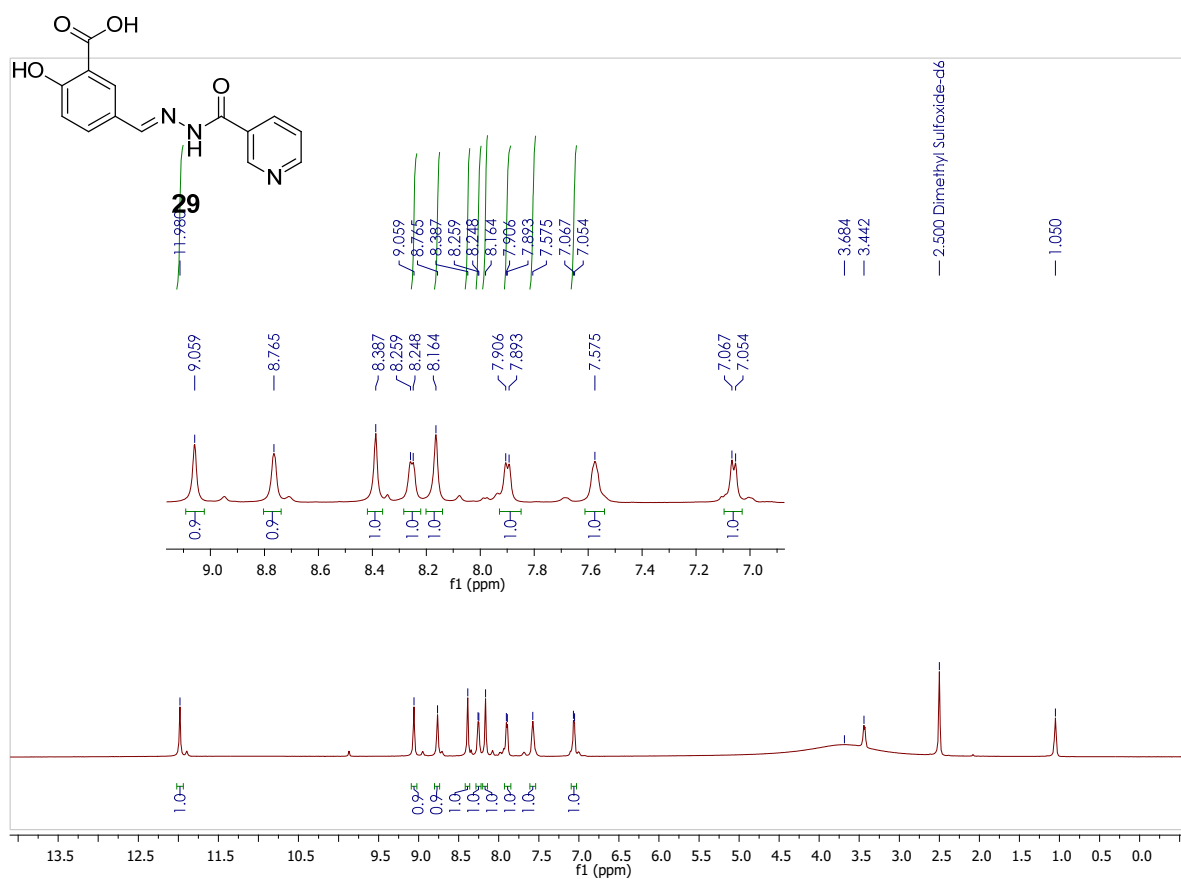
Data file: D:\Chem32\1\Data\JRB\JRB2031 2038 2039 2021-11-26 16-23-36\001-100-JRB2038.D
Sample name: JRB2038
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Location: 100
Injection date: 11/26/2021 4:25:21 PM
Injection: 1 of 1
Acq. method: LCMS ISOCRATIC 80%
Injection volume: 2.000
Analysis method: B_3 MINS.M
Acq. operator: SYSTEM
Last changed: 11/26/2021 9:20:48 AM
LCMS ISOCRATIC
80%B_3 MINS.M



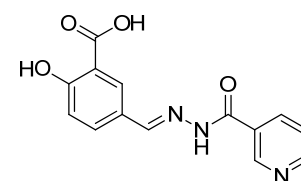
Molecular Weight: 269.255

28



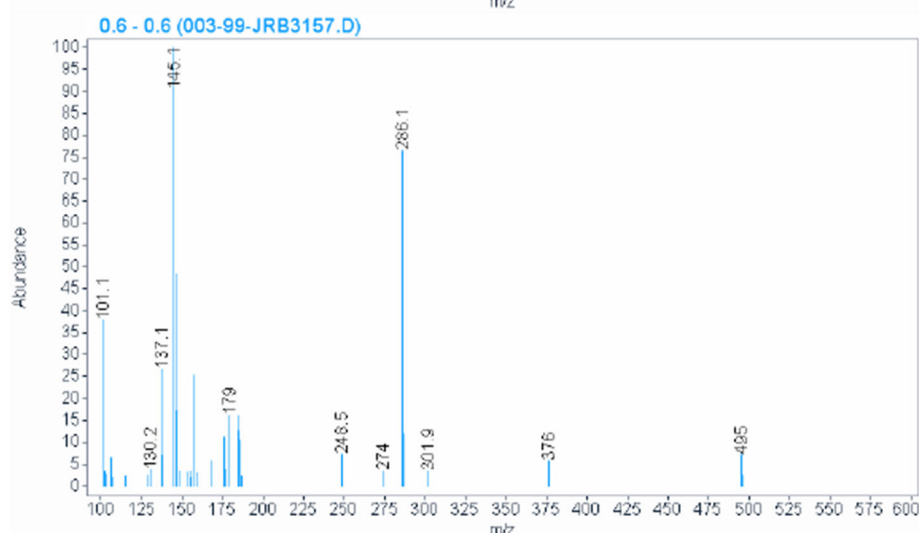
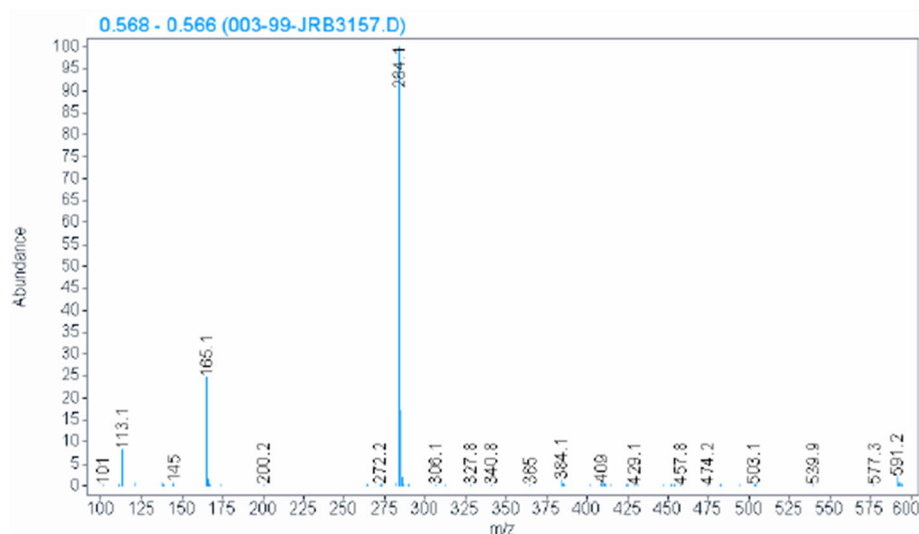
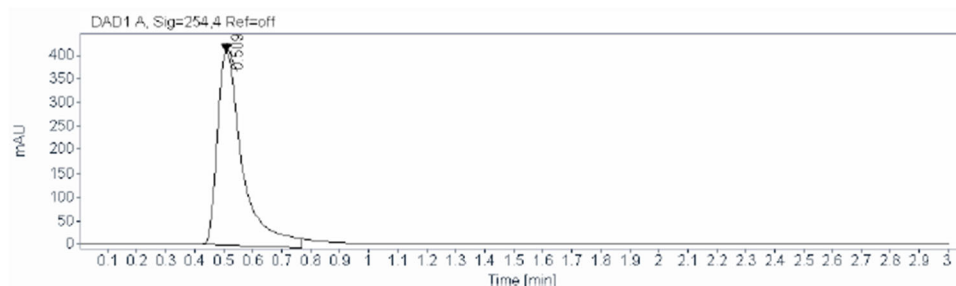


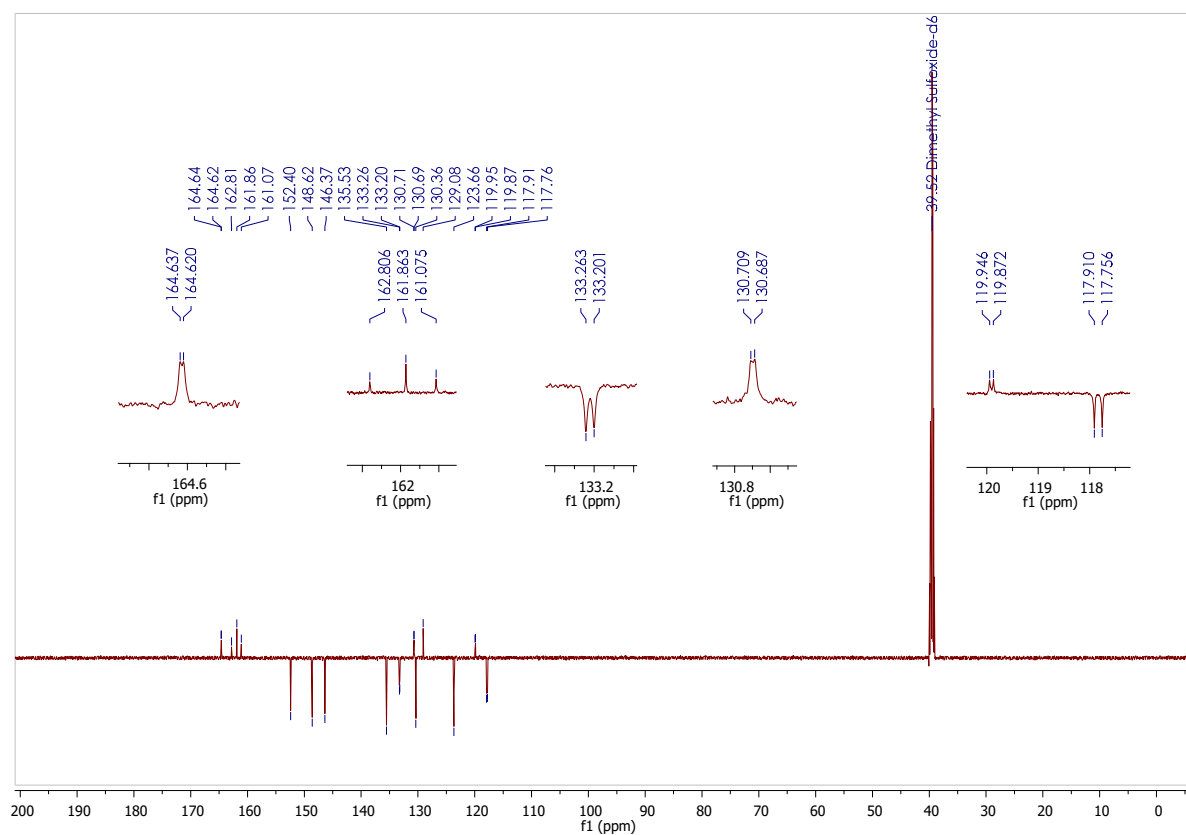
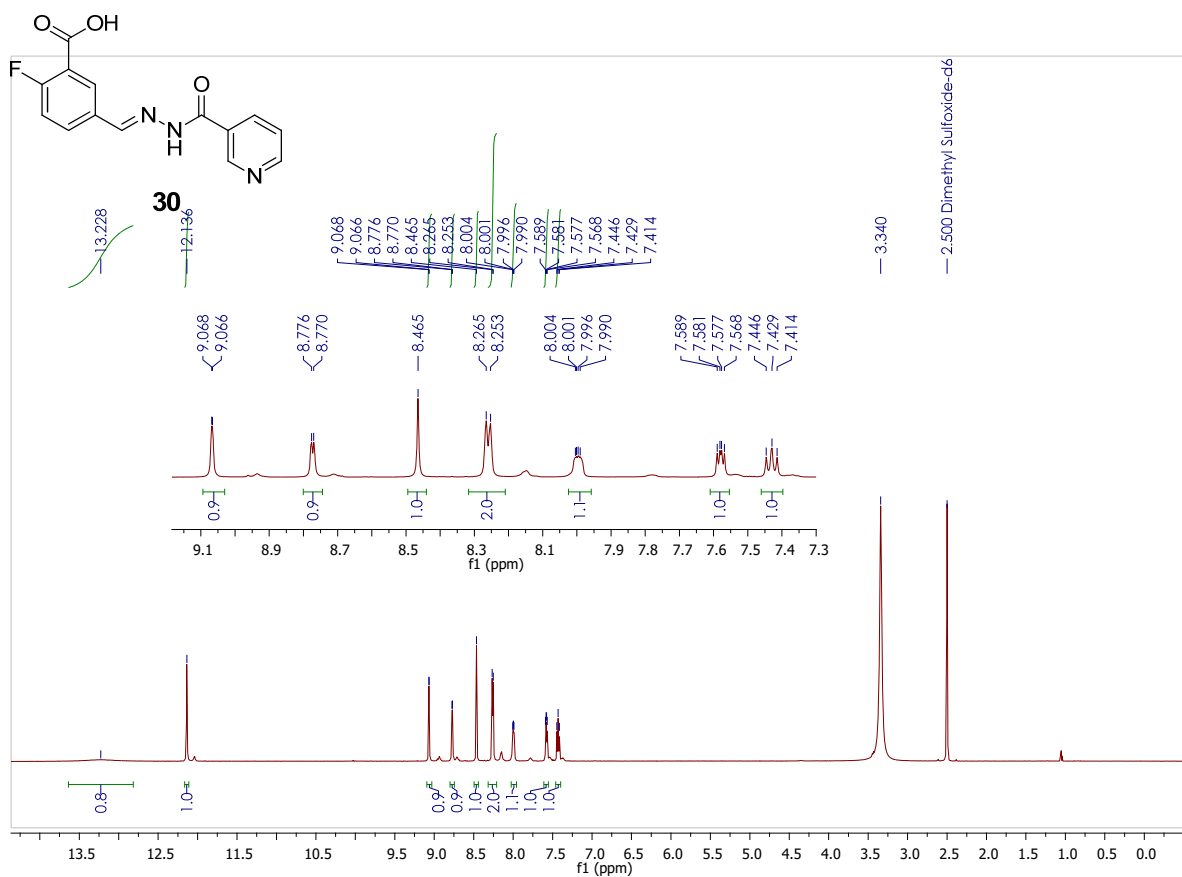
Data file: D:\Chem32\1\Data\JRB\JRB3066 3157 3158 3160 2023-07-24 12-35-44\003-99-JRB3157.D
Sample name: JRB3157
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Location: 99
Injection date: 7/24/2023 12:47:12 PM
Injection: 1 of 1
Acq. method: LCMS ISOCRATIC 80%
Injection volume: 2.000
B_3 MINS.M
Analysis method: LCMS ISOCRATIC
Acq. operator: SYSTEM
80%B_3 MINS.M
Last changed: 11/26/2021 9:20:48 AM

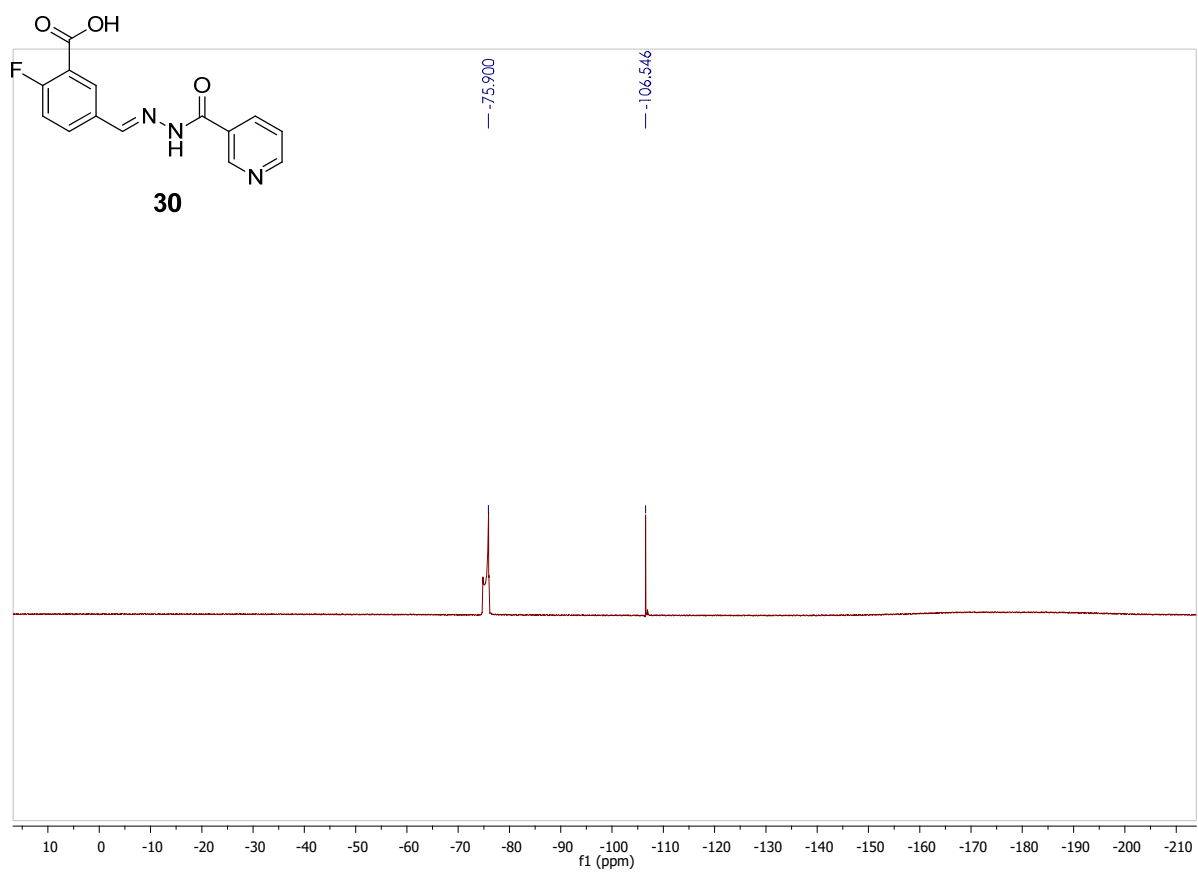


Molecular Weight: 285.255

29

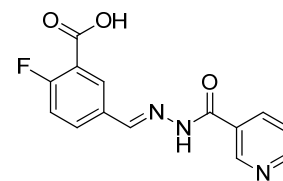






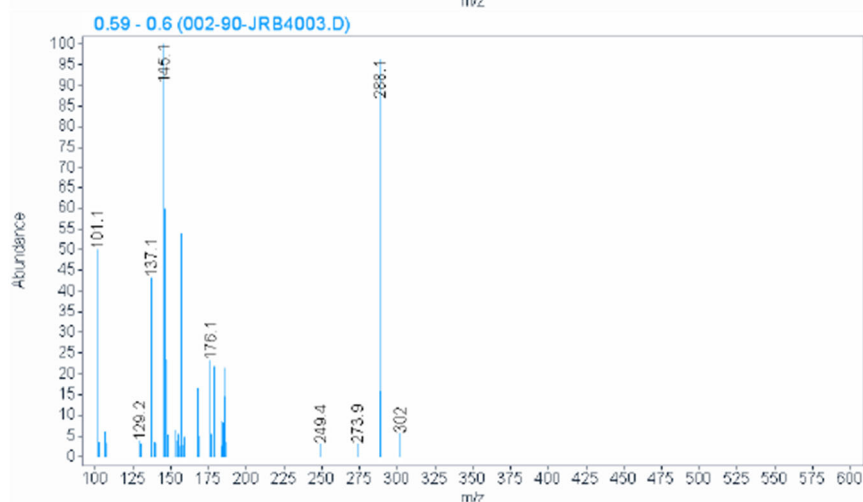
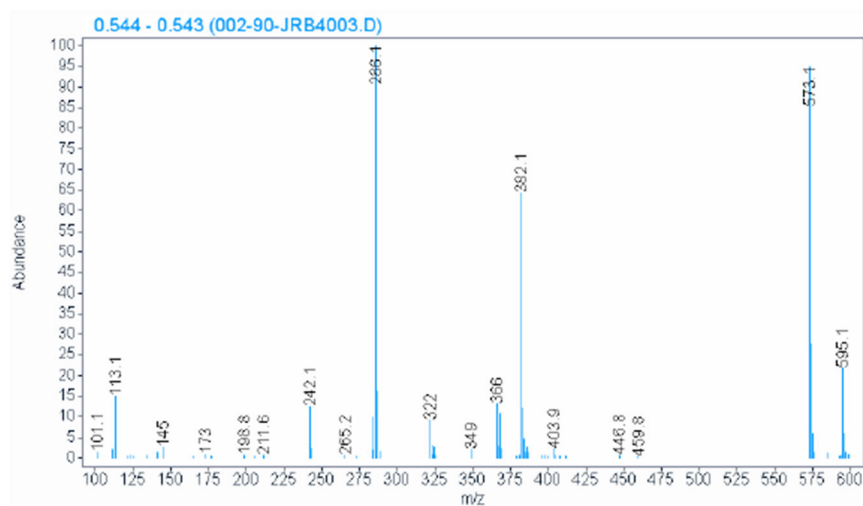
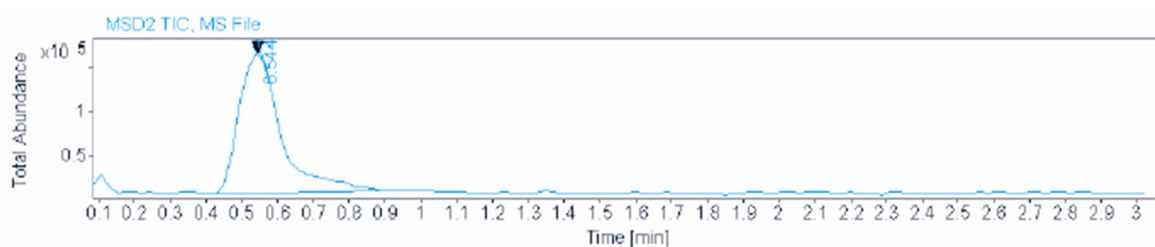


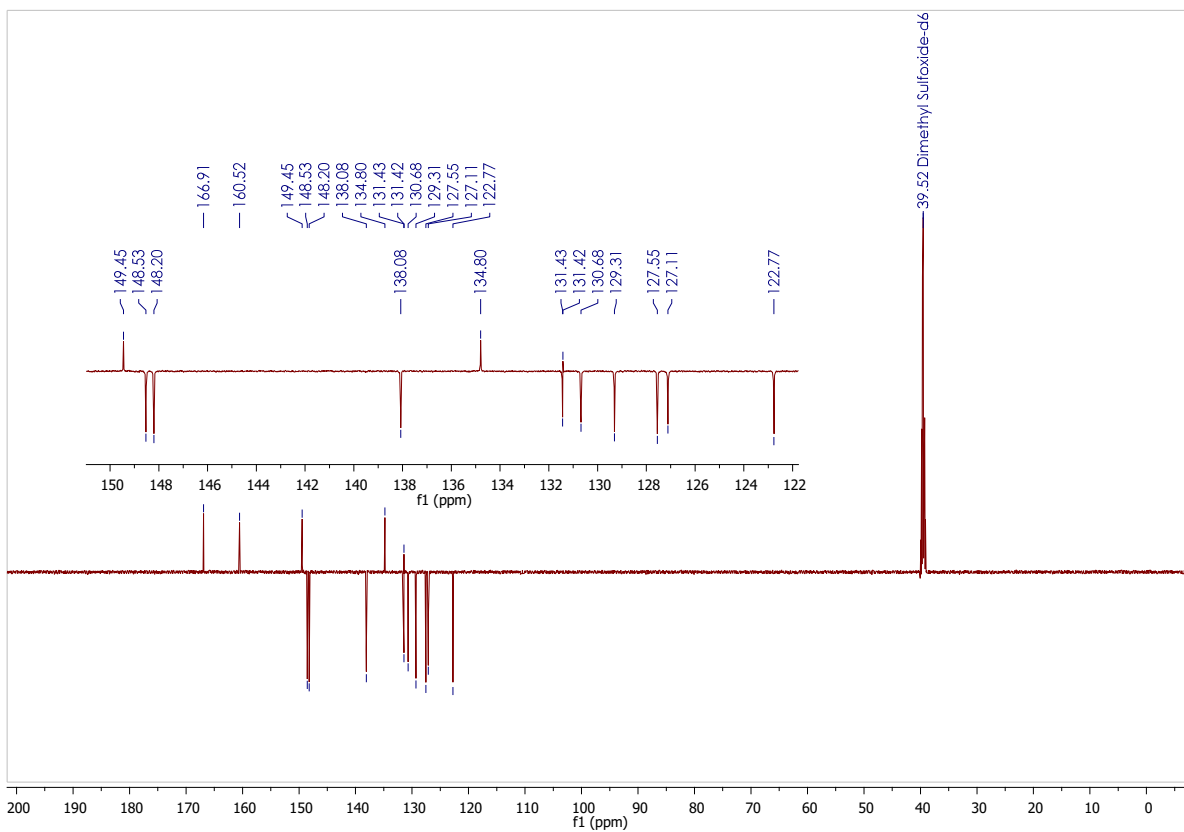
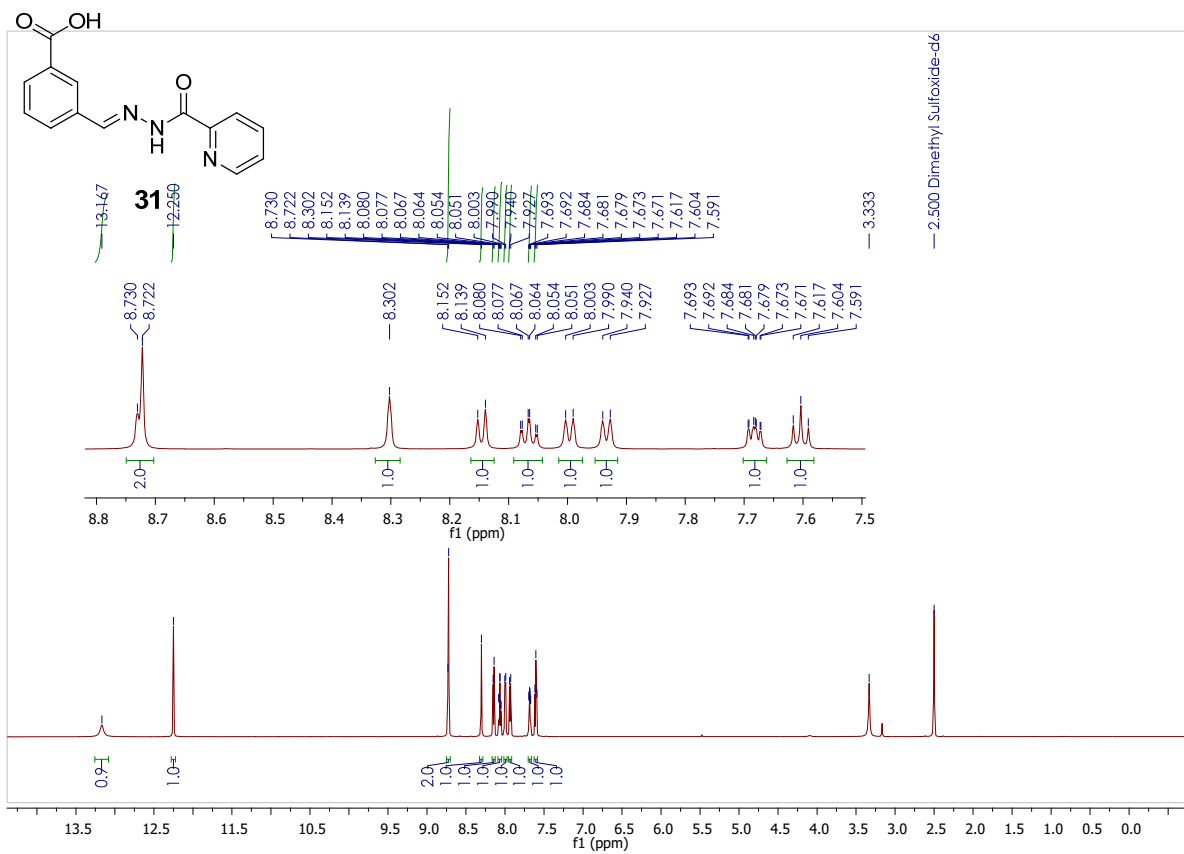
Data file: D:\Chem32\1\Data\JRB\JRB4003 4007-4009 2023-07-24 14-06-38\002-90-JRB4003.D
Sample name: JRB4003
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Injection date: 7/24/2023 2:13:12 PM
Acq. method: LCMS ISOCRATIC 80%
B_3 MINS.M
Location: 90
Injection: 1 of 1
Injection volume: 2.000
Analysis method: LCMS ISOCRATIC
80%B_3 MINS.M
Acq. operator: SYSTEM
Last changed: 11/26/2021 9:20:48 AM



Molecular Weight: 287.246

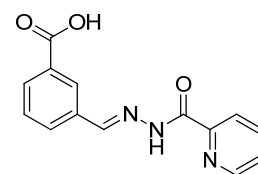
30



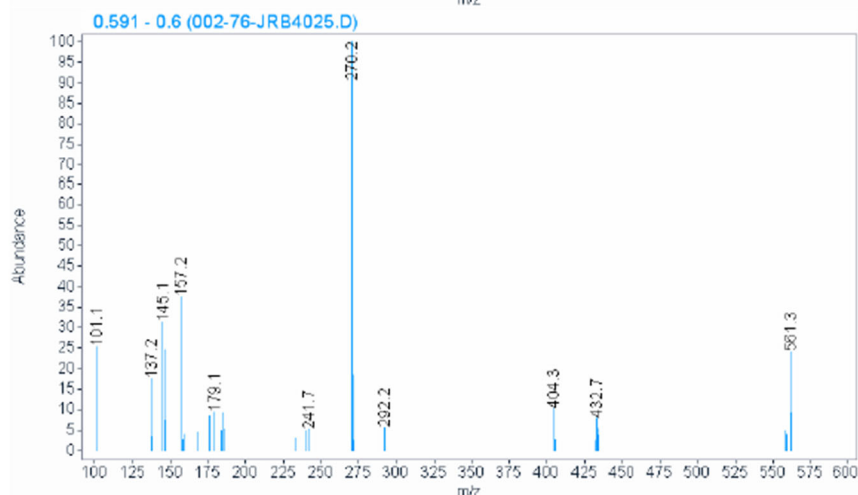
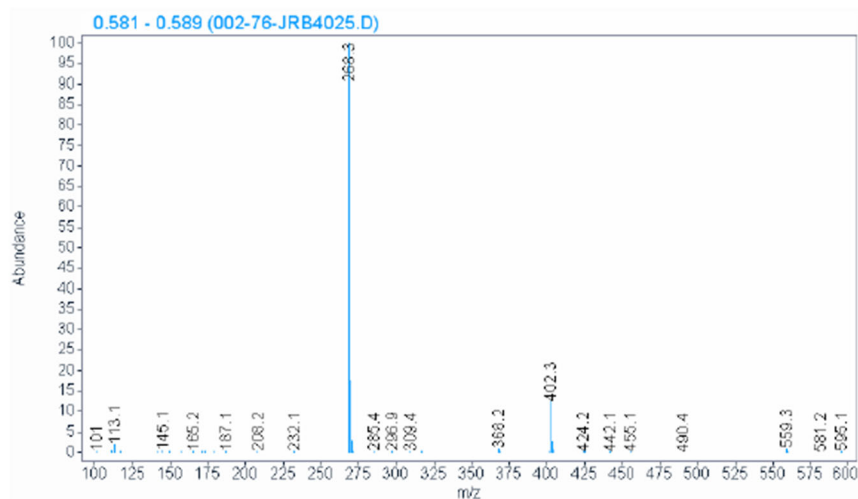
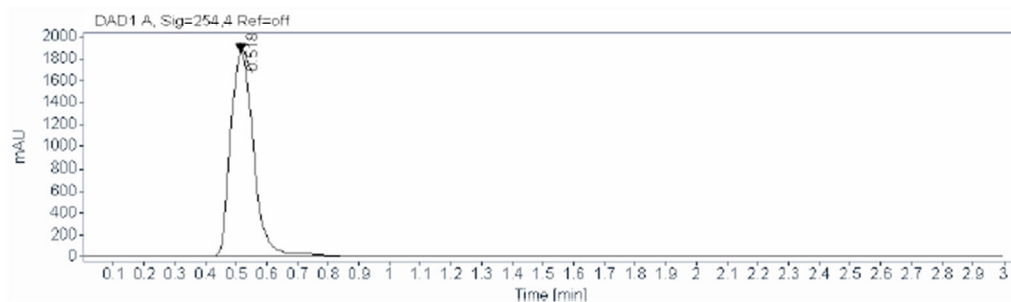


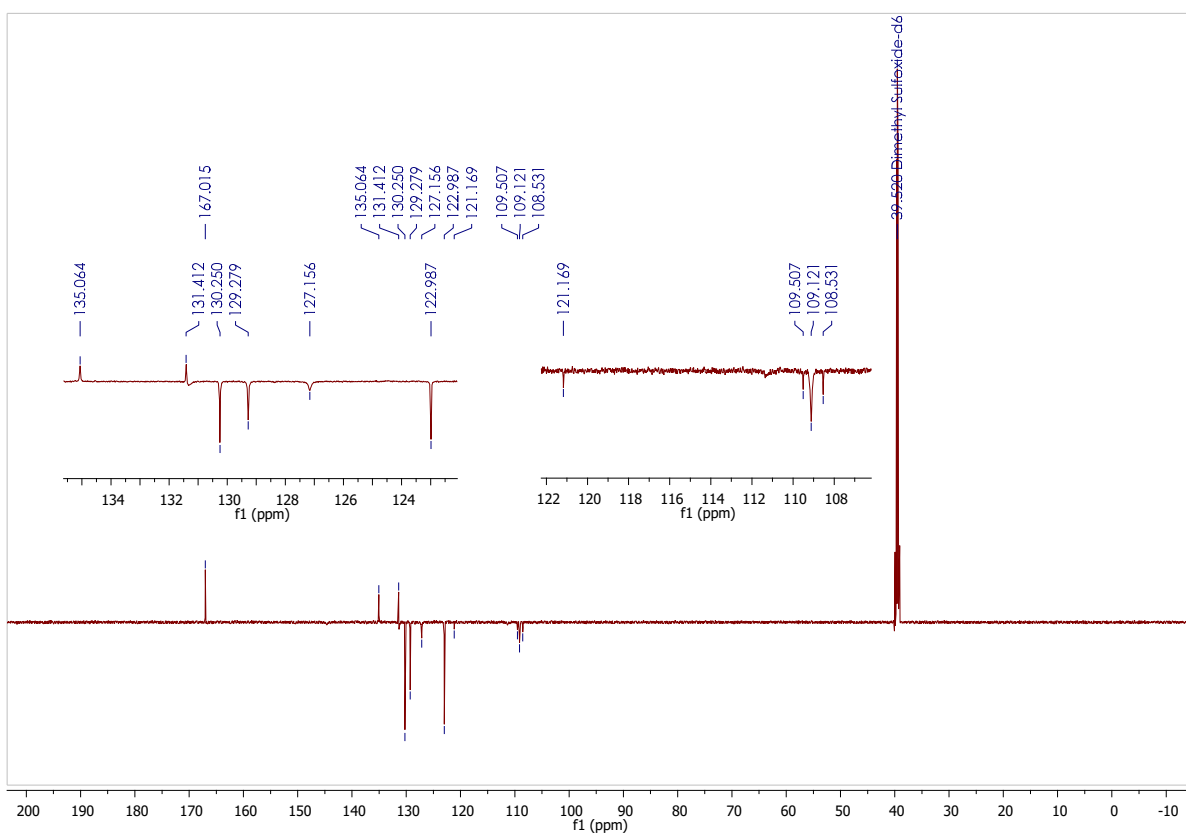
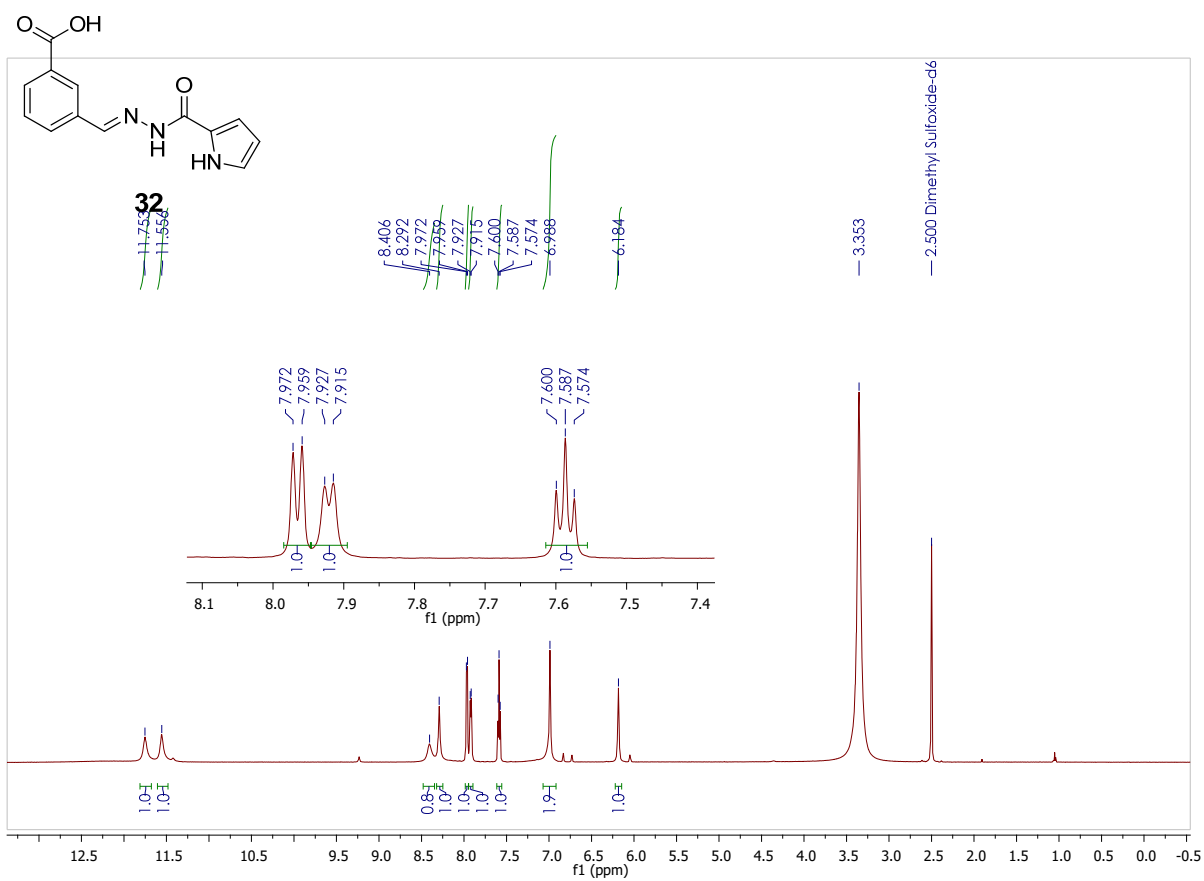


Data file: D:\Chem321\Data\JRB\JRB4025-4027-2 2023-07-24 15-27-22\002-76-JRB4025.D
 Sample name: JRB4025
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 76
 Injection date: 7/24/2023 3:35:33 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 Injection volume: 2.000
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 80%B_3 MINS.M
 Last changed: 11/26/2021 9:20:48 AM



Molecular Weight: 269.255
31



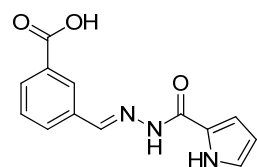


LCMS Report

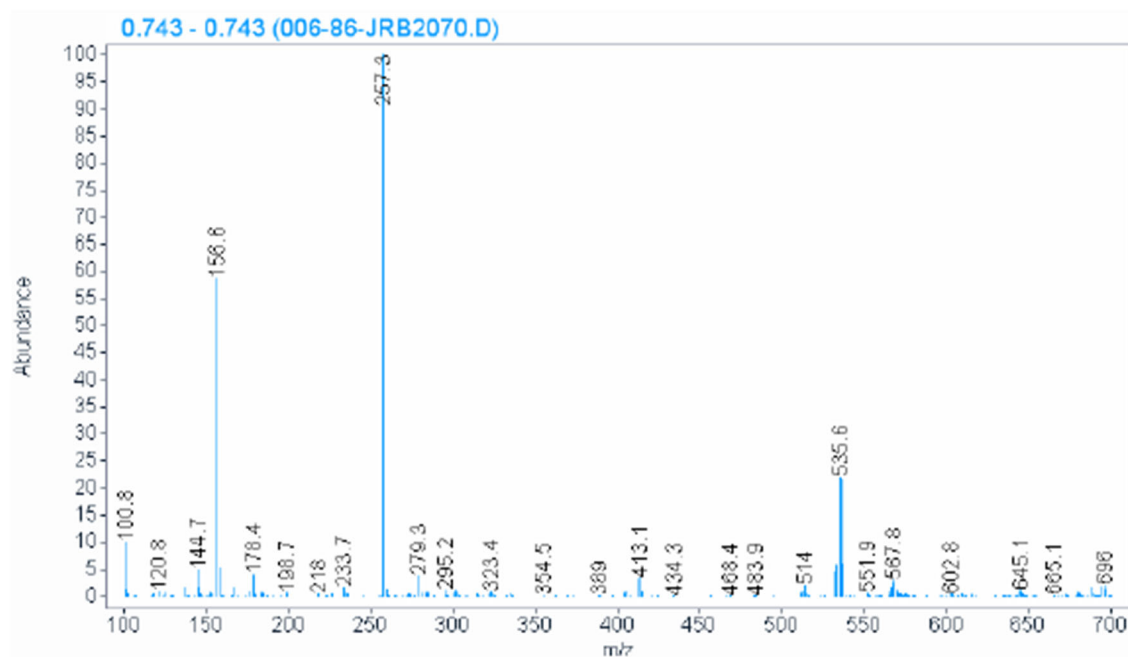
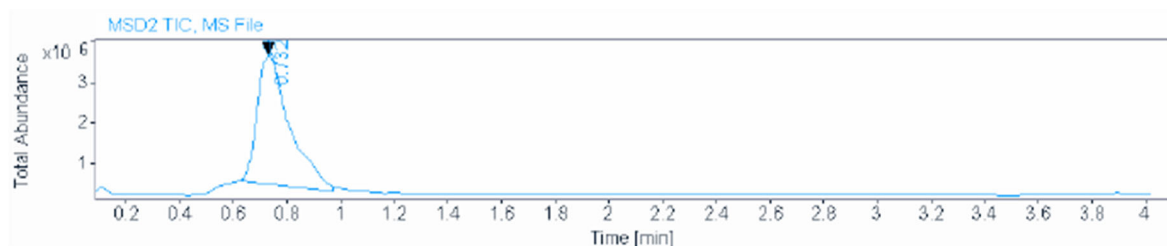
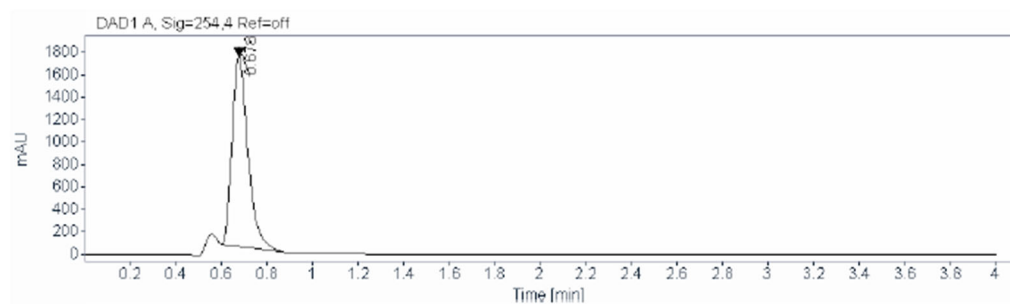


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Data file: D:\Chem32\11\Data\JRB\JRB2072 2080 2084 2081 2070 2022-01-31 15-09-41\006
Sample name: -86-JRB2070.D
Description: JRB2070
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Location: 86
Injection date: 1/31/2022 3:38:49 PM
Injection: 1 of 1
Acq. method: LCMS ISOCRATIC_50%
Injection volume: 2.000
Analysis method: LCMS
Acq. operator: SYSTEM
**ISOCRATIC_50%
 B_0.4MLMIN-
 1_4MINS.M**
Last changed: 7/14/2016 12:06:24 PM

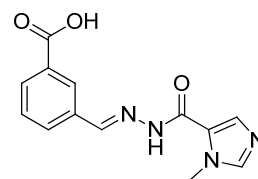


Molecular Weight: 257.245
32



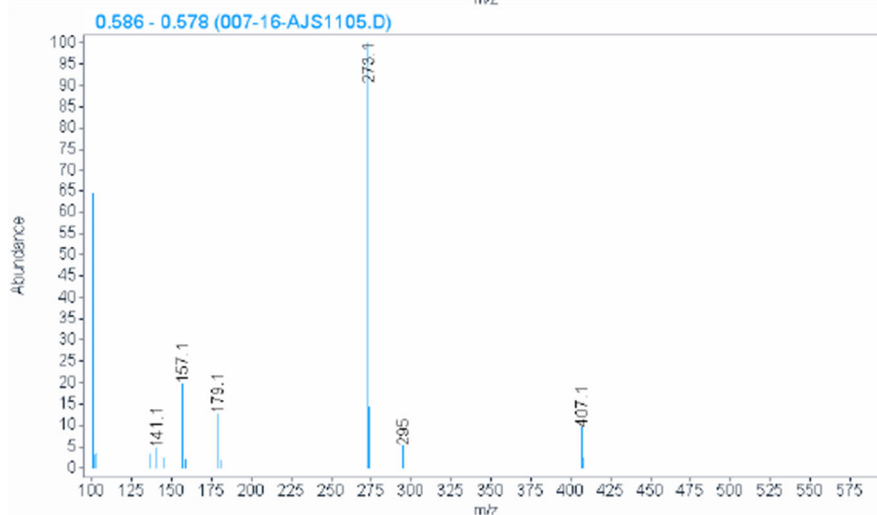
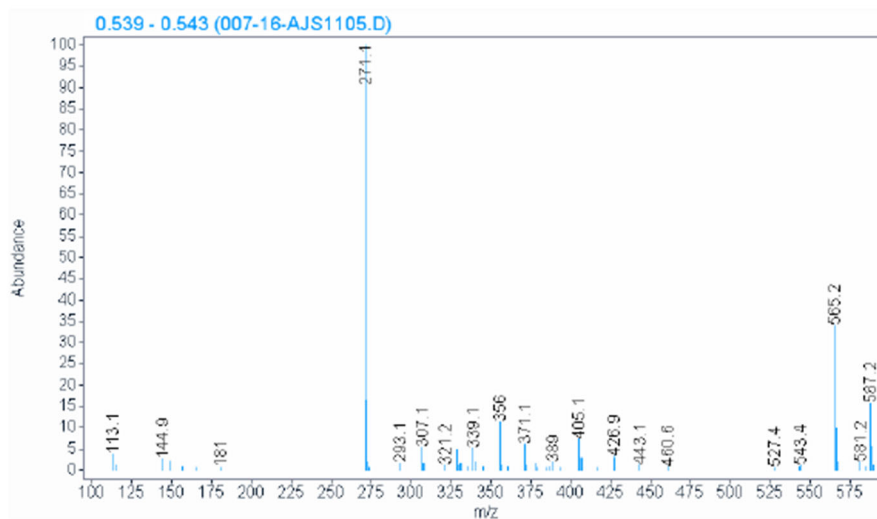


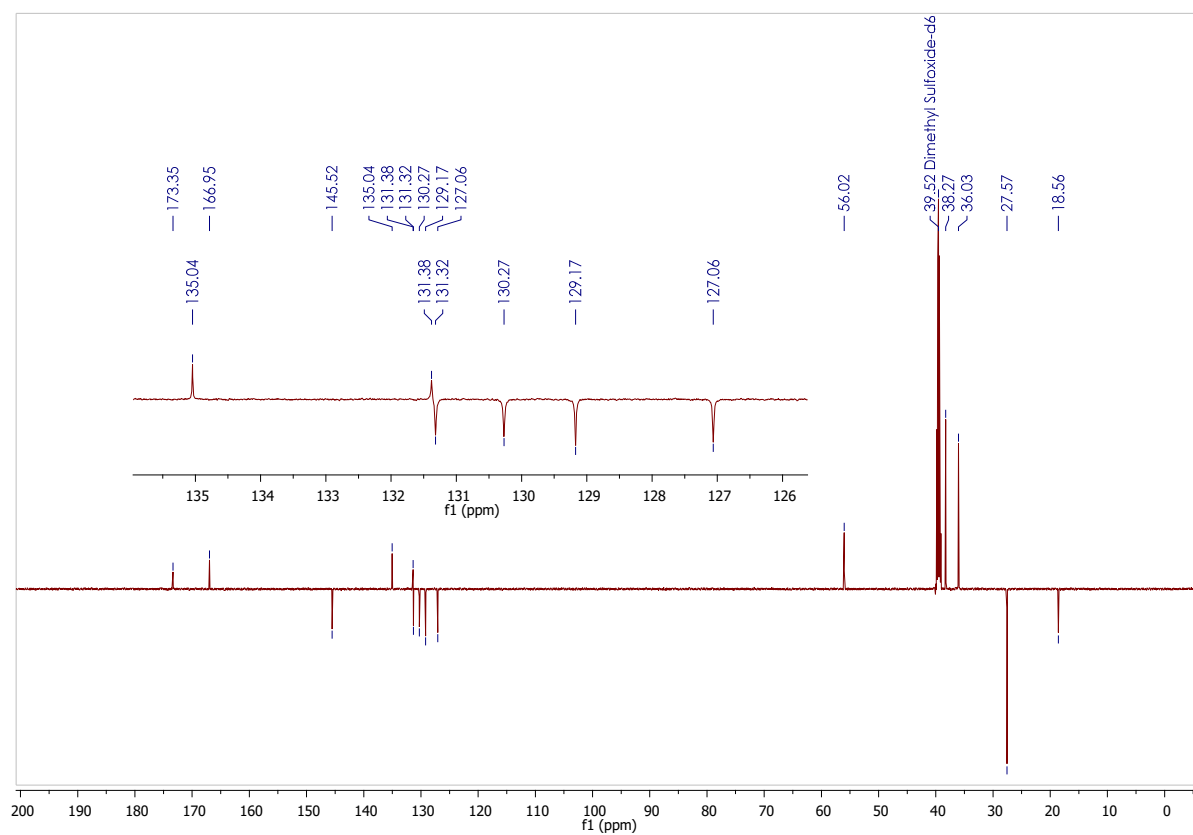
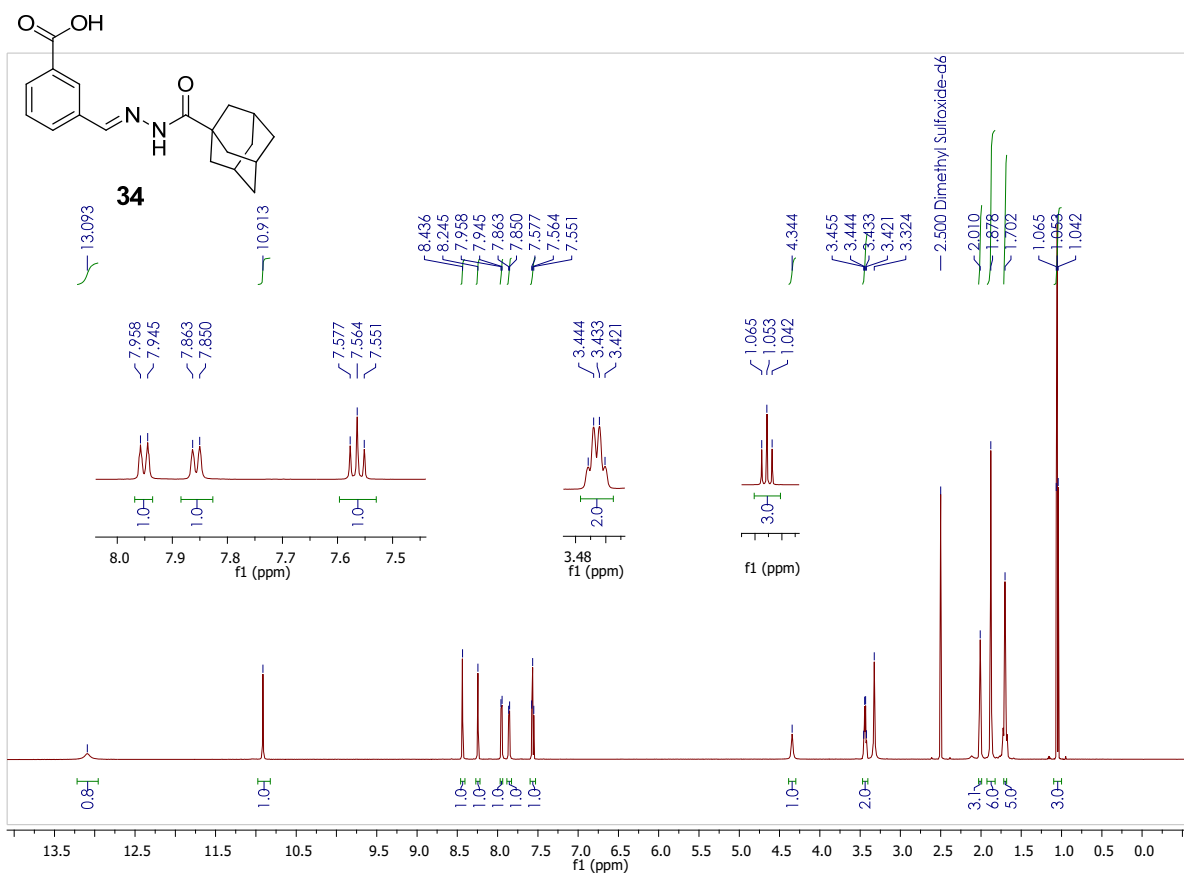
Data file: D:\Chem32\1\Data\AJS\AJS Table1 2023-07-25 14-45-29\007-16-AJS1105.D
 Sample name: AJS1105
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 16
 Injection date: 7/25/2023 3:14:09 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 B_3 MINS.M
 Injection volume: 2.000
 Analysis method: LCMS ISOCRATIC
 80%B_3 MINS.M
 Acq. operator: SYSTEM
 Last changed: 11/26/2021 9:20:48 AM



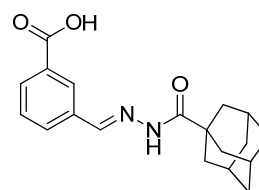
Molecular Weight: 272.259

33

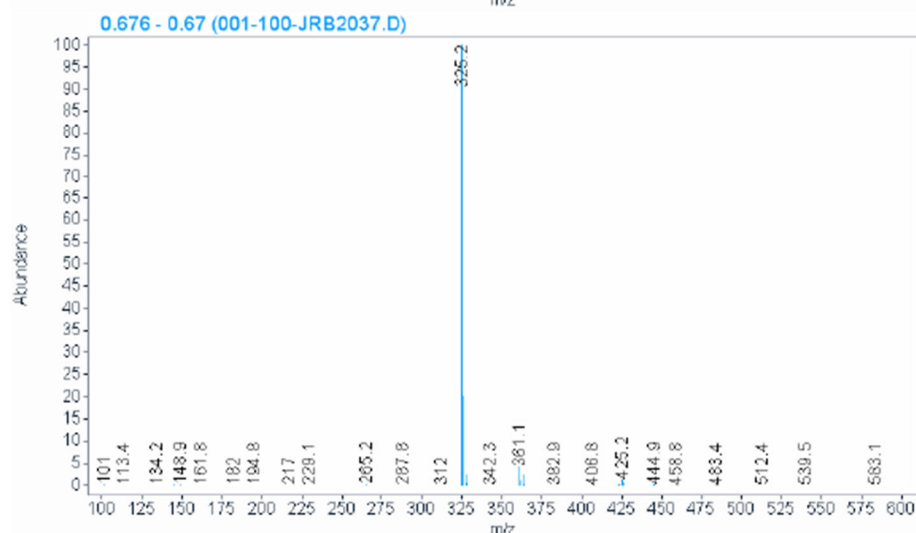
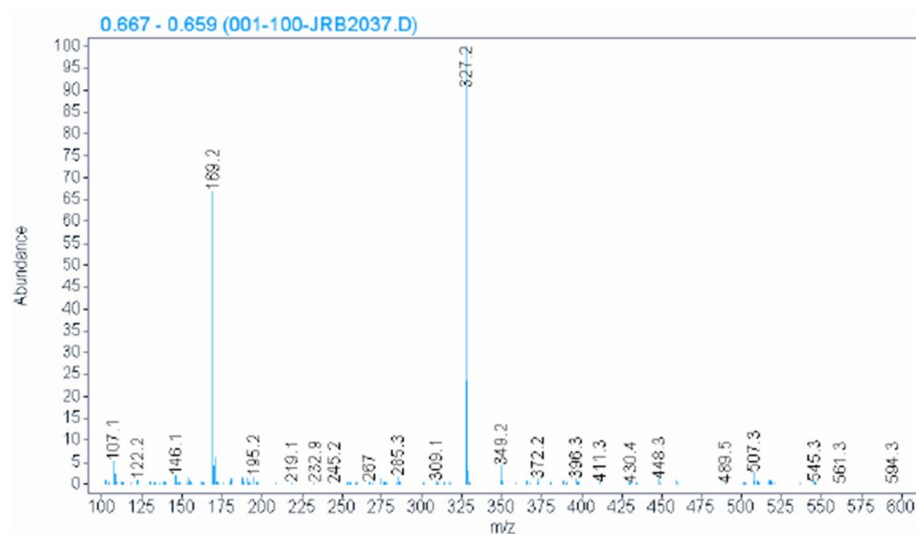
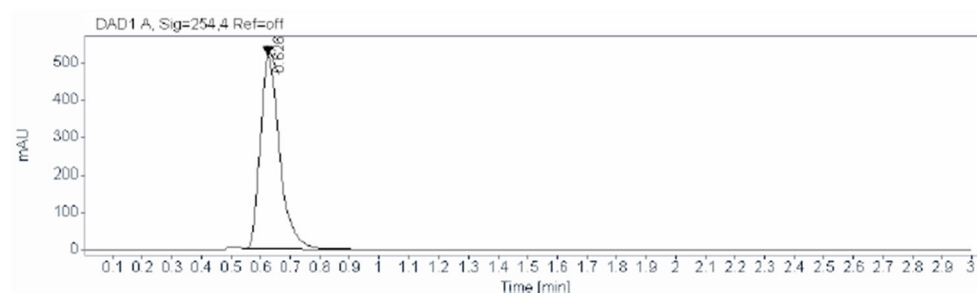


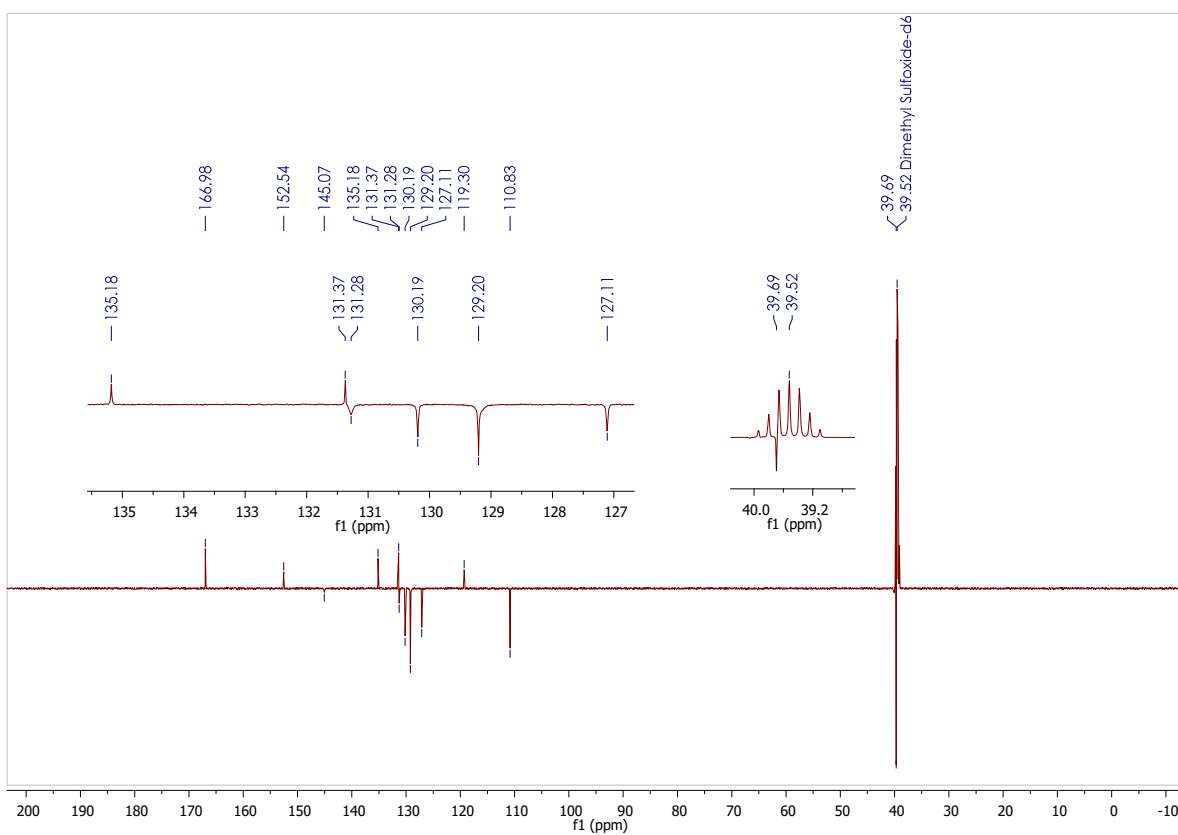
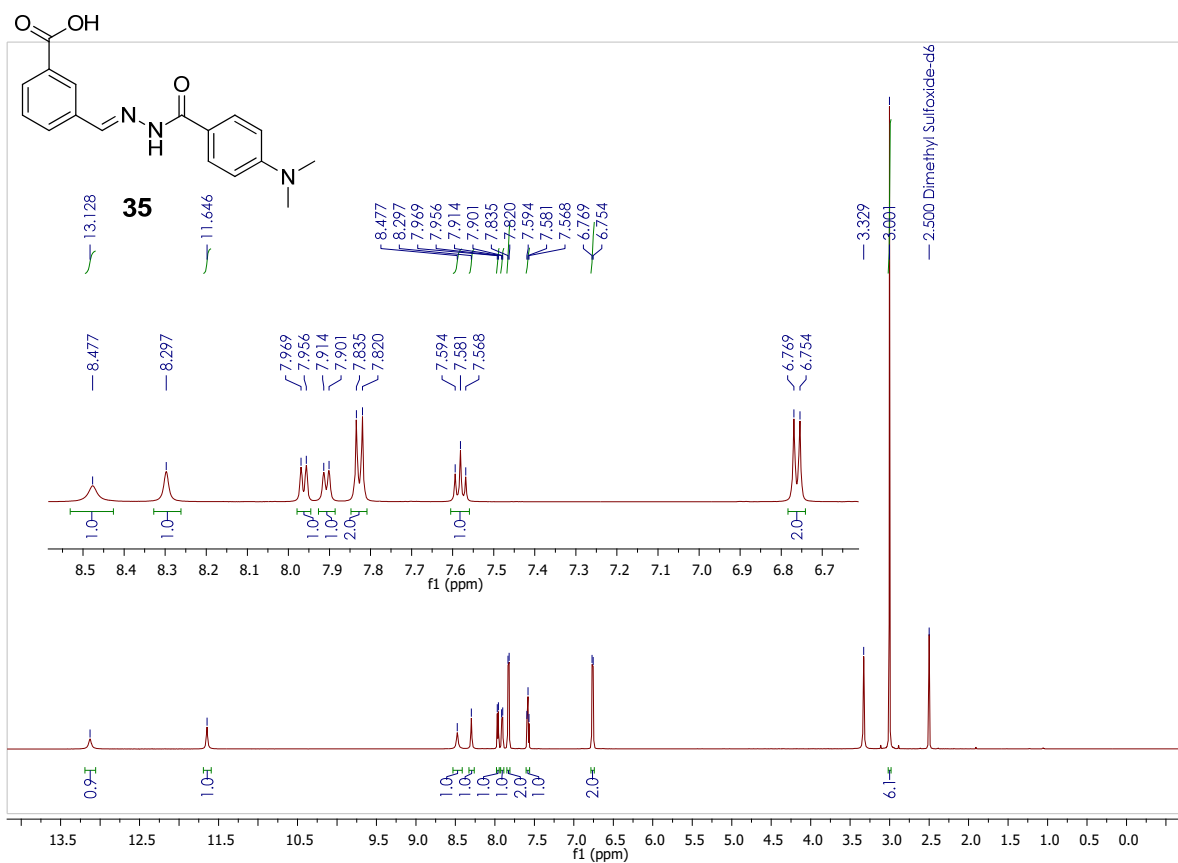


Data file: D:\Chem32\1\Data\JRB\JRB2037 2021-11-26 12-45-35\001-100-JRB2037.D
 Sample name: JRB2037
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 100
 Injection date: 11/26/2021 12:47:21 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 Injection volume: 2.000
 B_3 MINS.M
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 80%B_3 MINS.M
 Last changed: 11/26/2021 9:20:48 AM

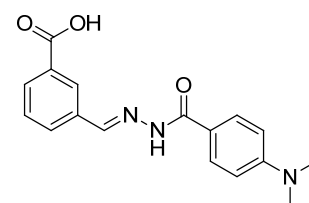


Molecular Weight: 326.390

34

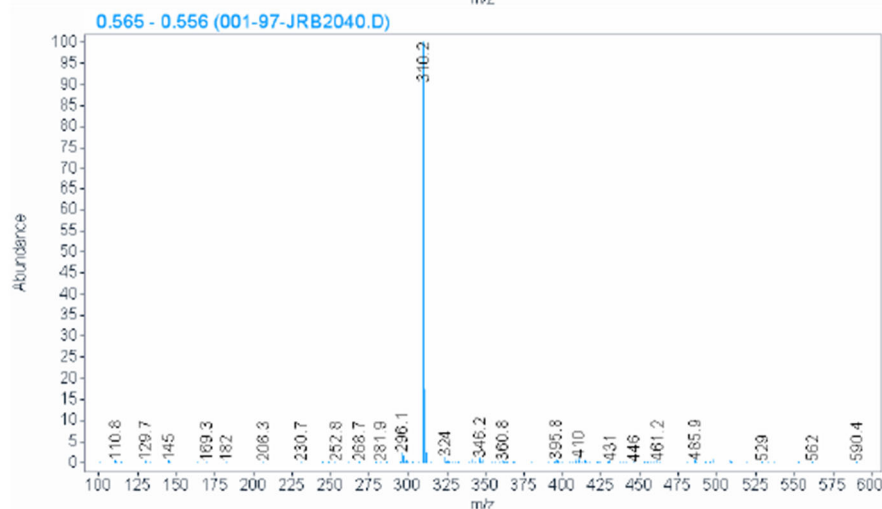
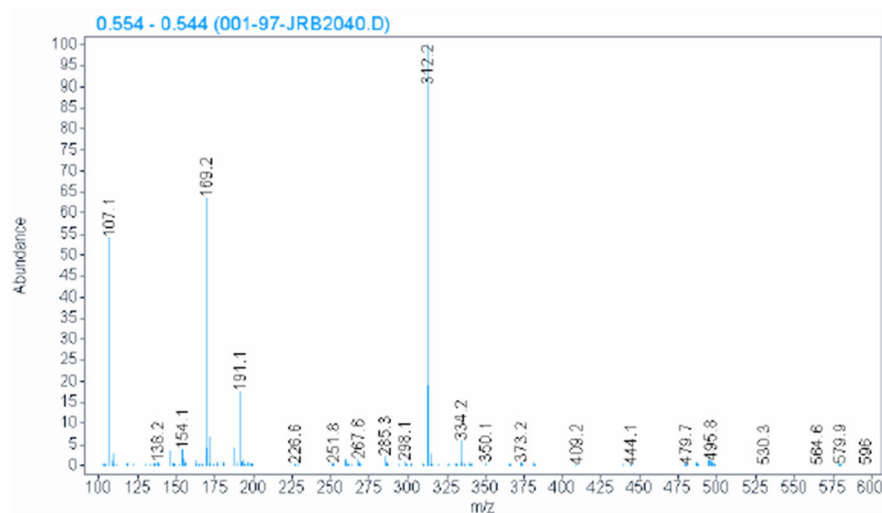
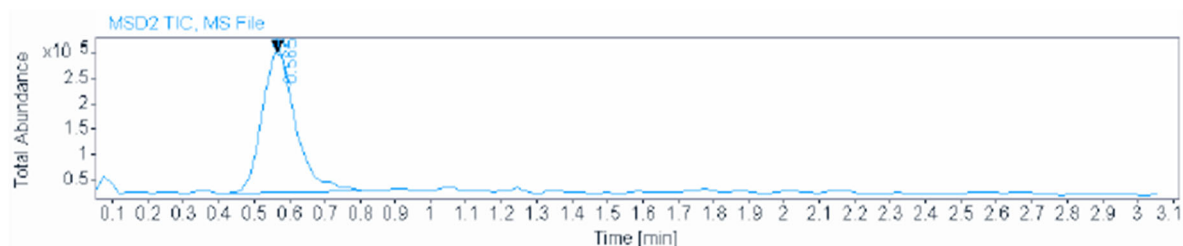


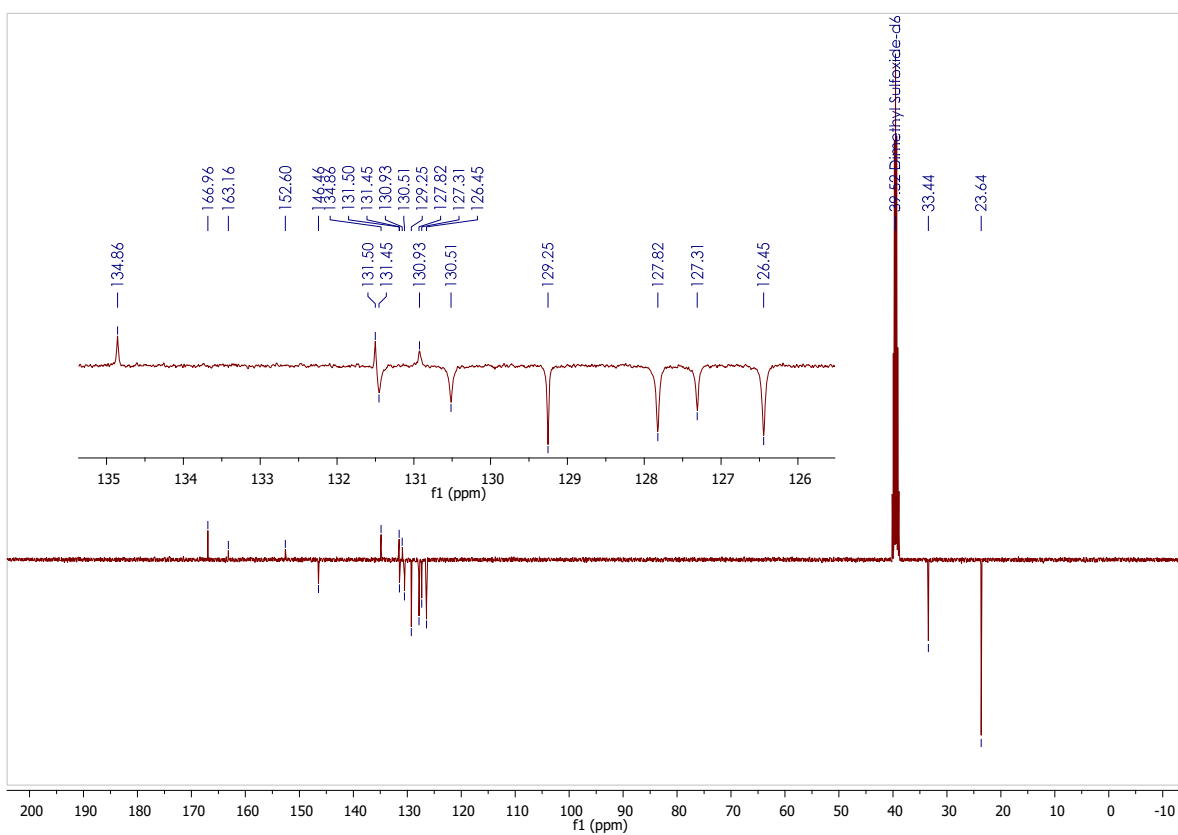
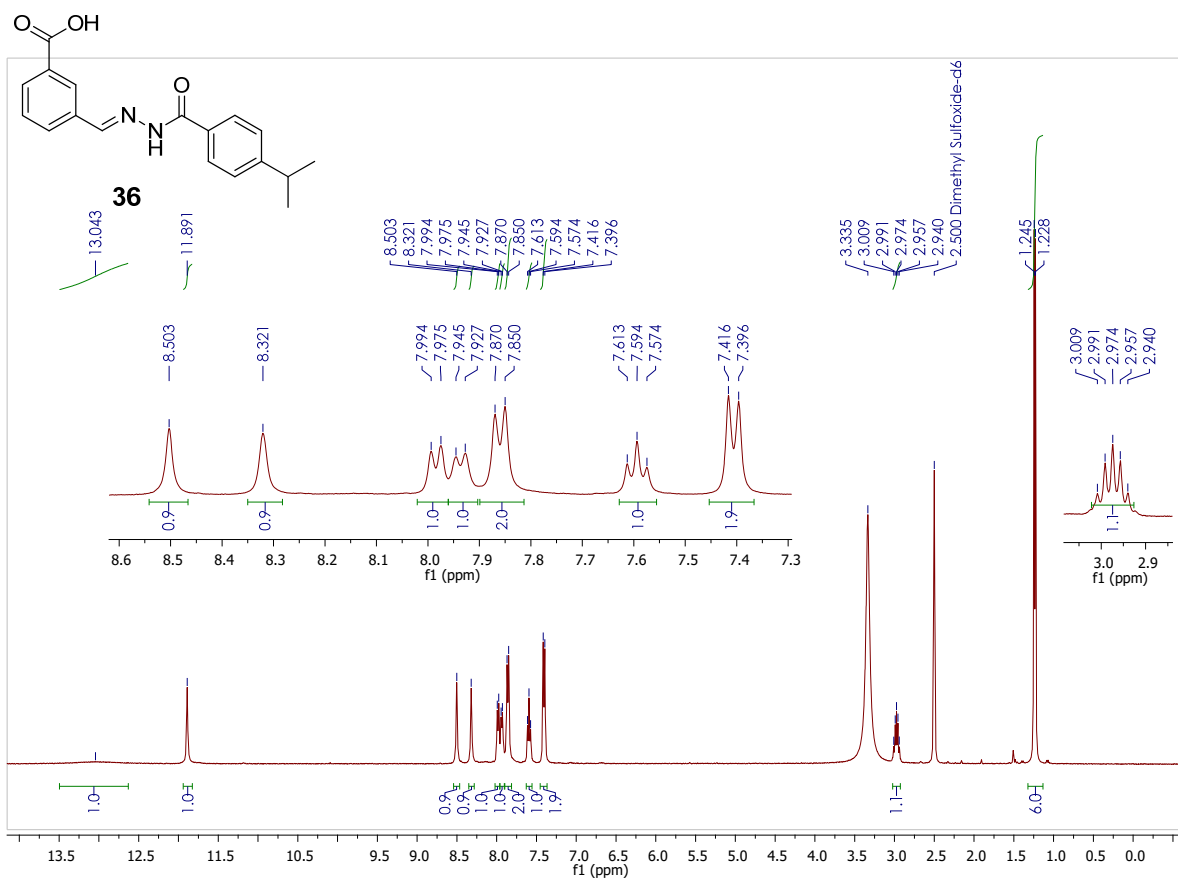
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Sample name: JRB2040
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Location: 97
Injection date: 11/26/2021 4:40:04 PM
Injection: 1 of 1
Acq. method: LCMS ISOCRATIC 80%
Injection volume: 2.000
Analysis method: LCMS ISOCRATIC
Acq. operator: SYSTEM
Last changed: 11/26/2021 9:20:48 AM



Molecular Weight: 311.335

35





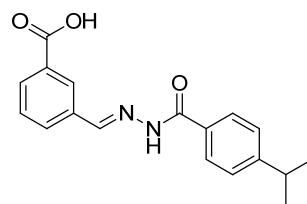
LCMS Report



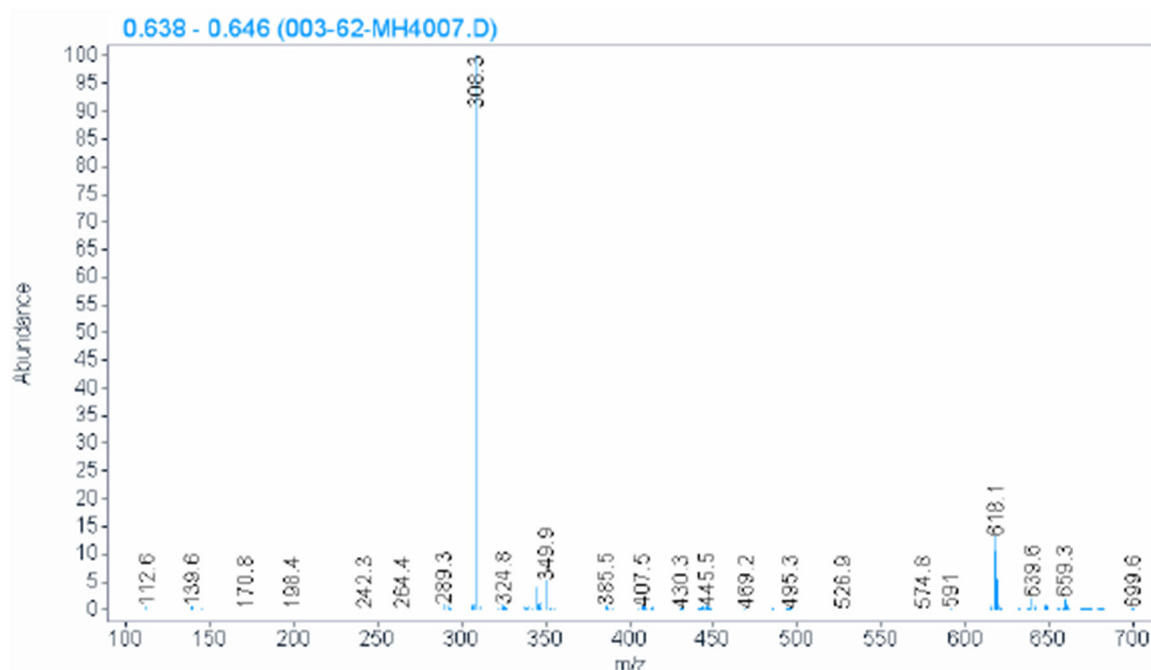
Agilent Technologies

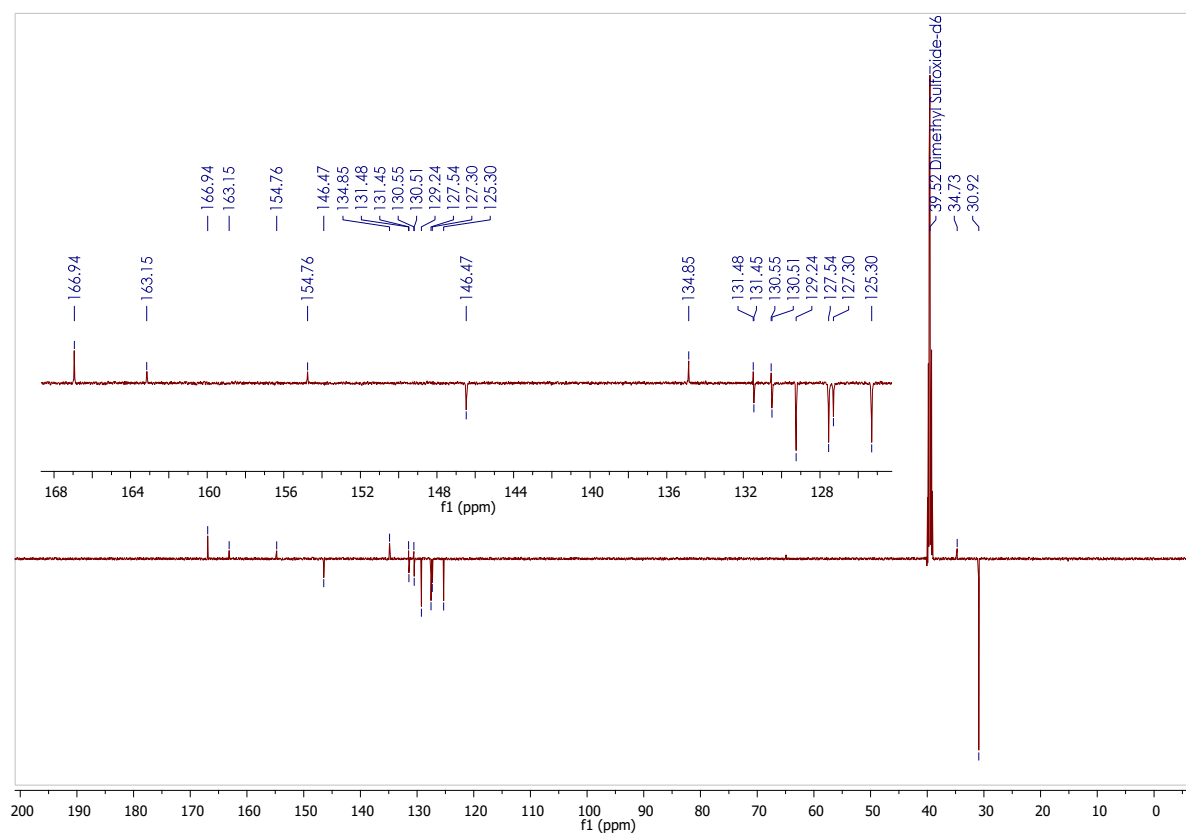
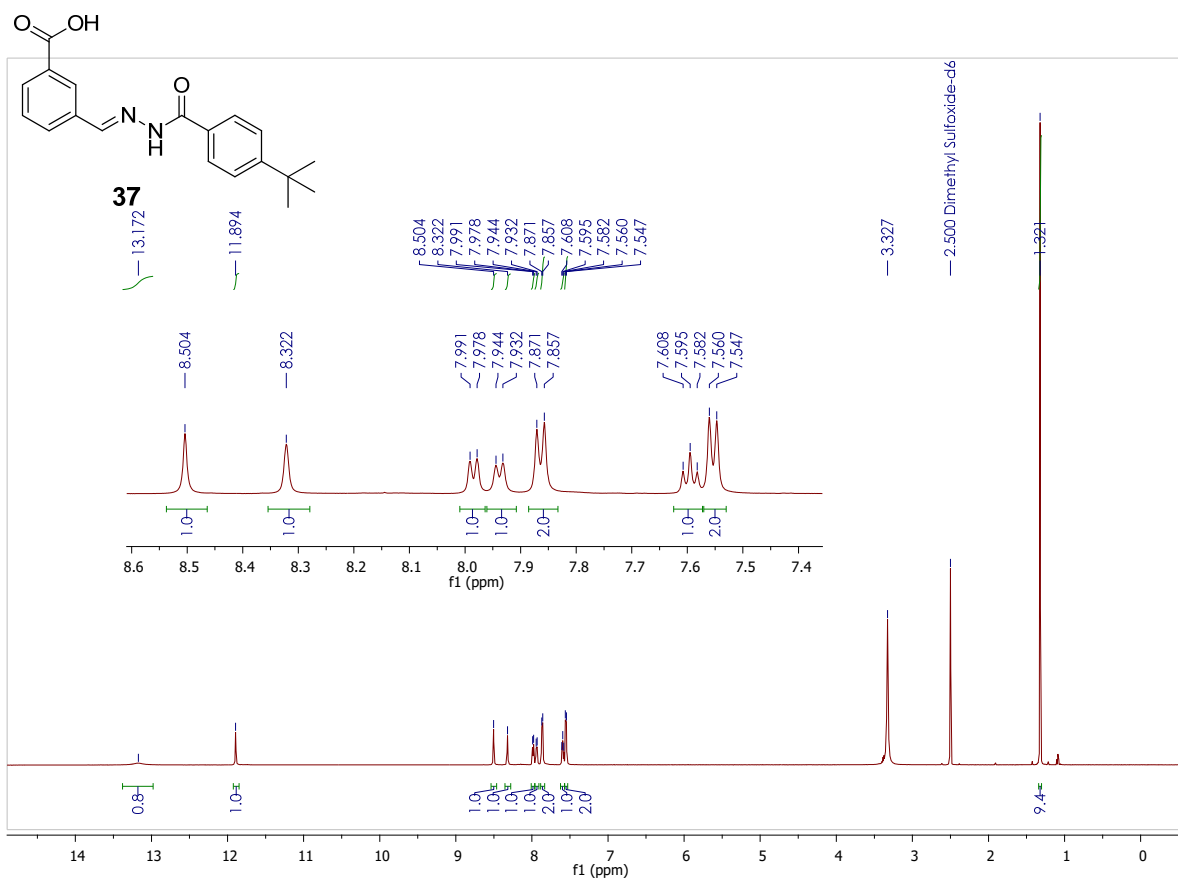
Data file: D:\Chem32\11\Data\MH4006-4010 and MH4014 2022-03-01 12-11-51\003-62-MH4007.D
Sample name: MH4007
Description:
Sample amount: 0.000
Instrument: LCMS
Injection date: 3/1/2022 12:23:47 PM
Acq. method: LCMS ISOCRATIC_80%
 B_0.4MLMIN-
 1_4MINS.M
Analysis method: LCMS
 ISOCRATIC_80%
 B_0.4MLMIN-
 1_4MINS.M
Last changed: 7/13/2021 10:05:44 AM

Sample type: Sample
Location: 62
Injection: 1 of 1
Injection volume: 2.000
Acq. operator: SYSTEM



Molecular Weight: 310.347
36



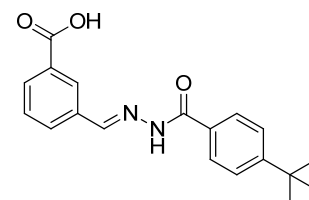


LCMS Report



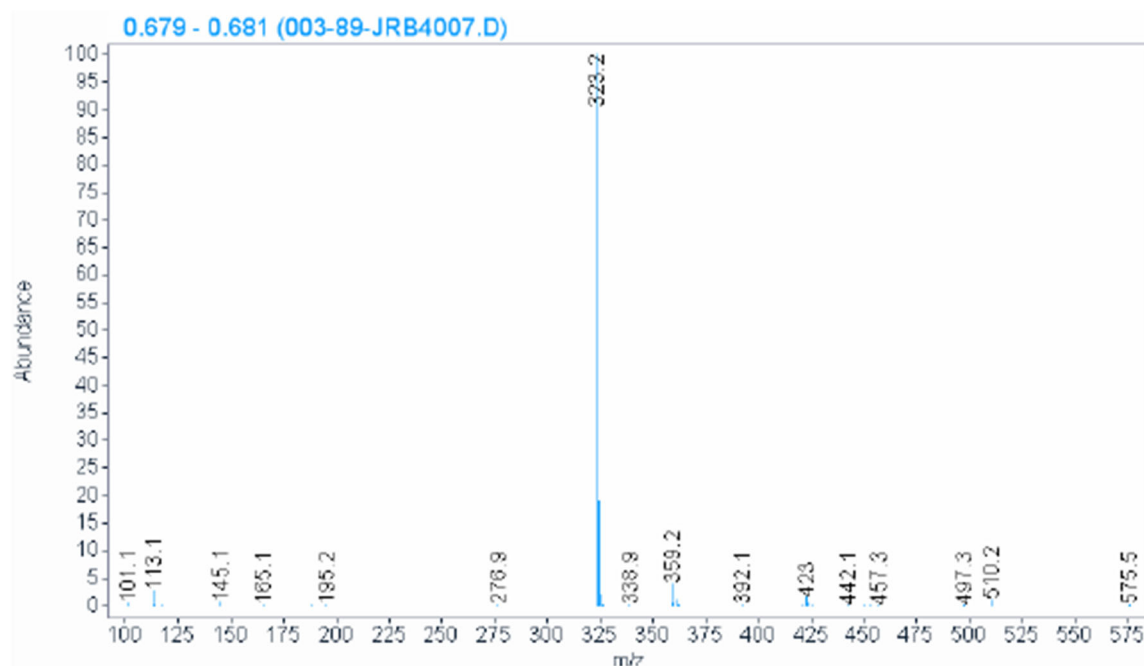
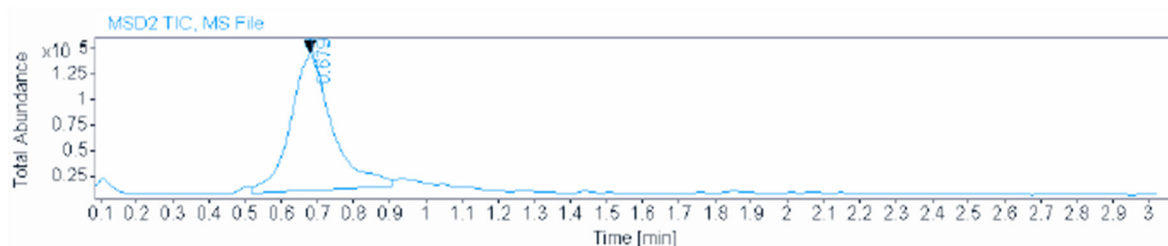
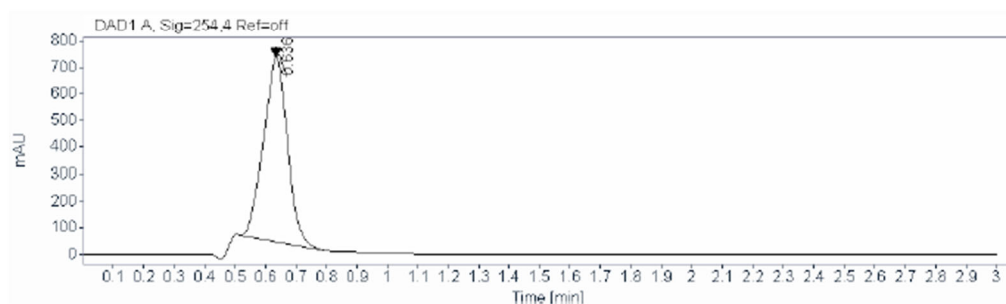
Agilent Technologies

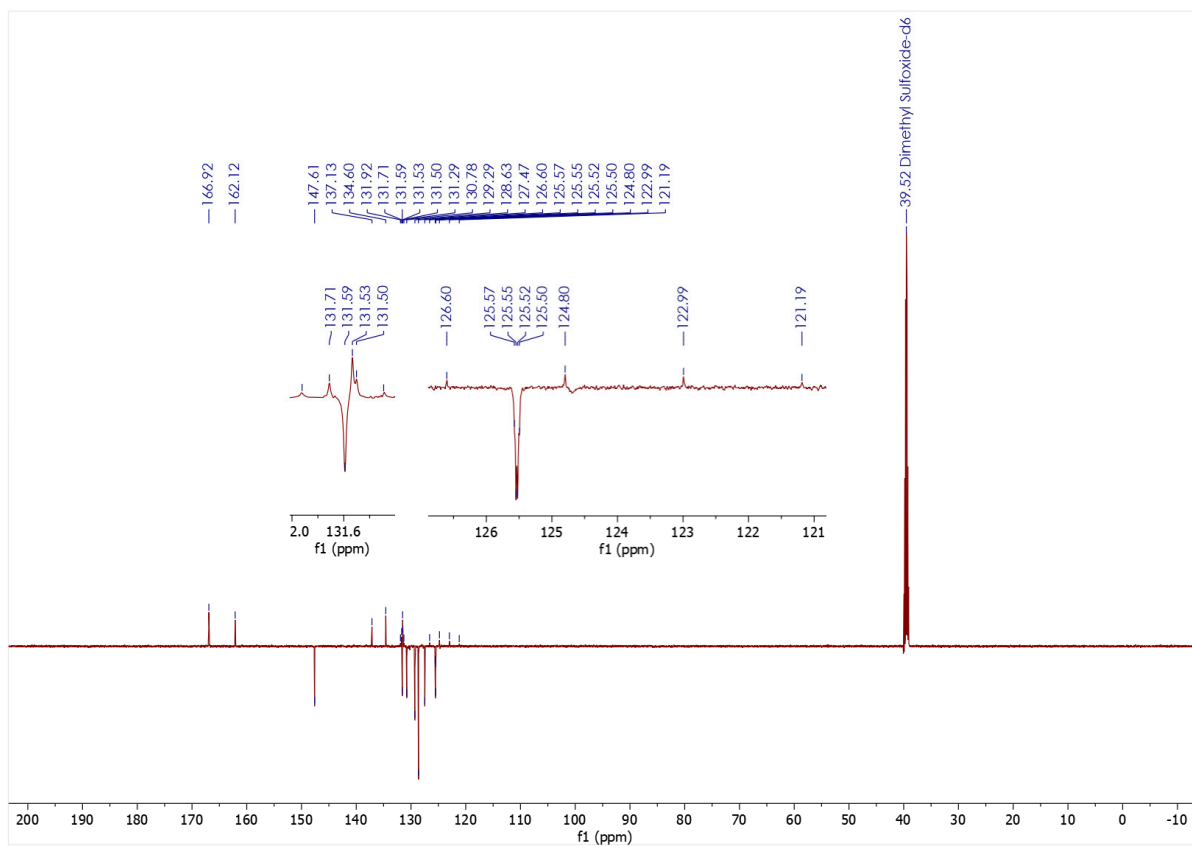
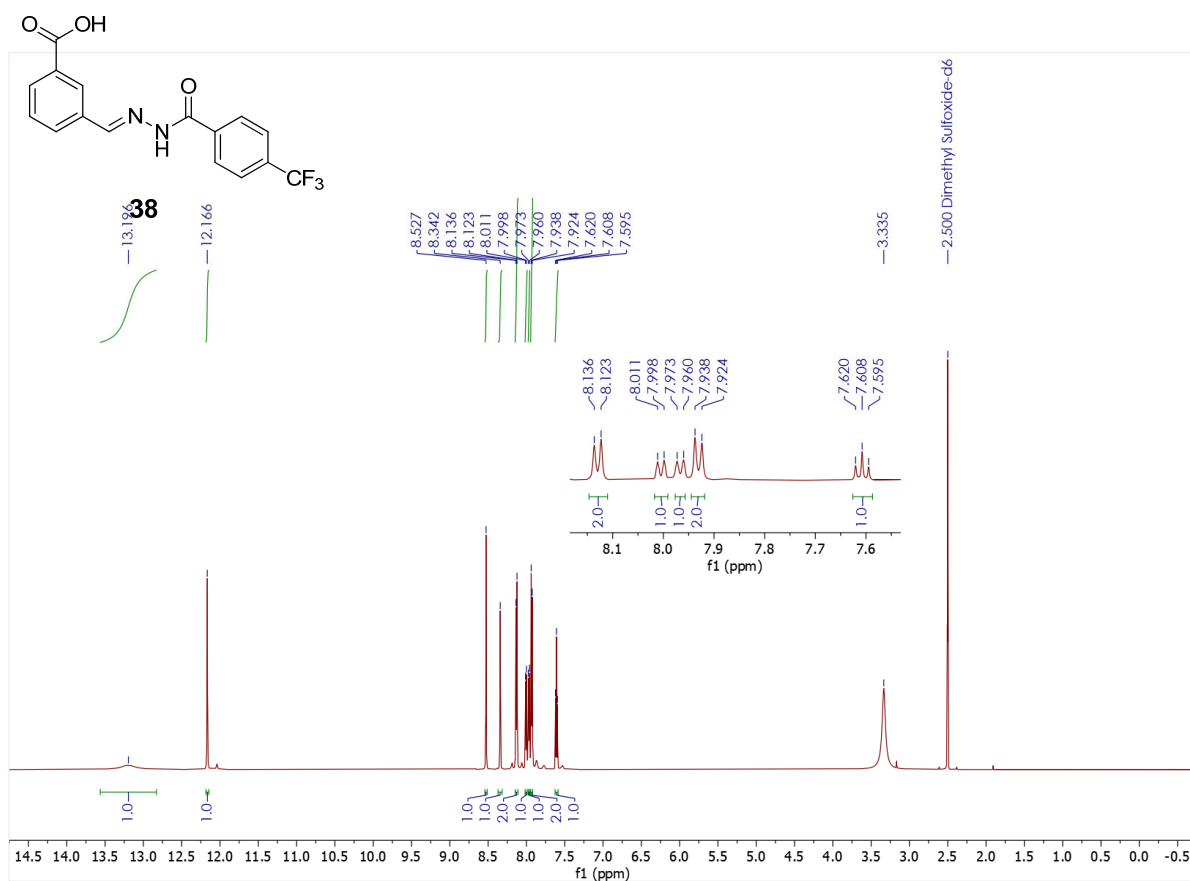
Data file: D:\Chem32\1\Data\JRB\JRB4003 4007-4009 2023-07-24 14-06-38\003-89-JRB4007.D
 Sample name: JRB4007
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 89
 Injection date: 7/24/2023 2:17:57 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 Injection volume: 2.000
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 80%B_3 MINS.M
 Last changed: 11/26/2021 9:20:48 AM

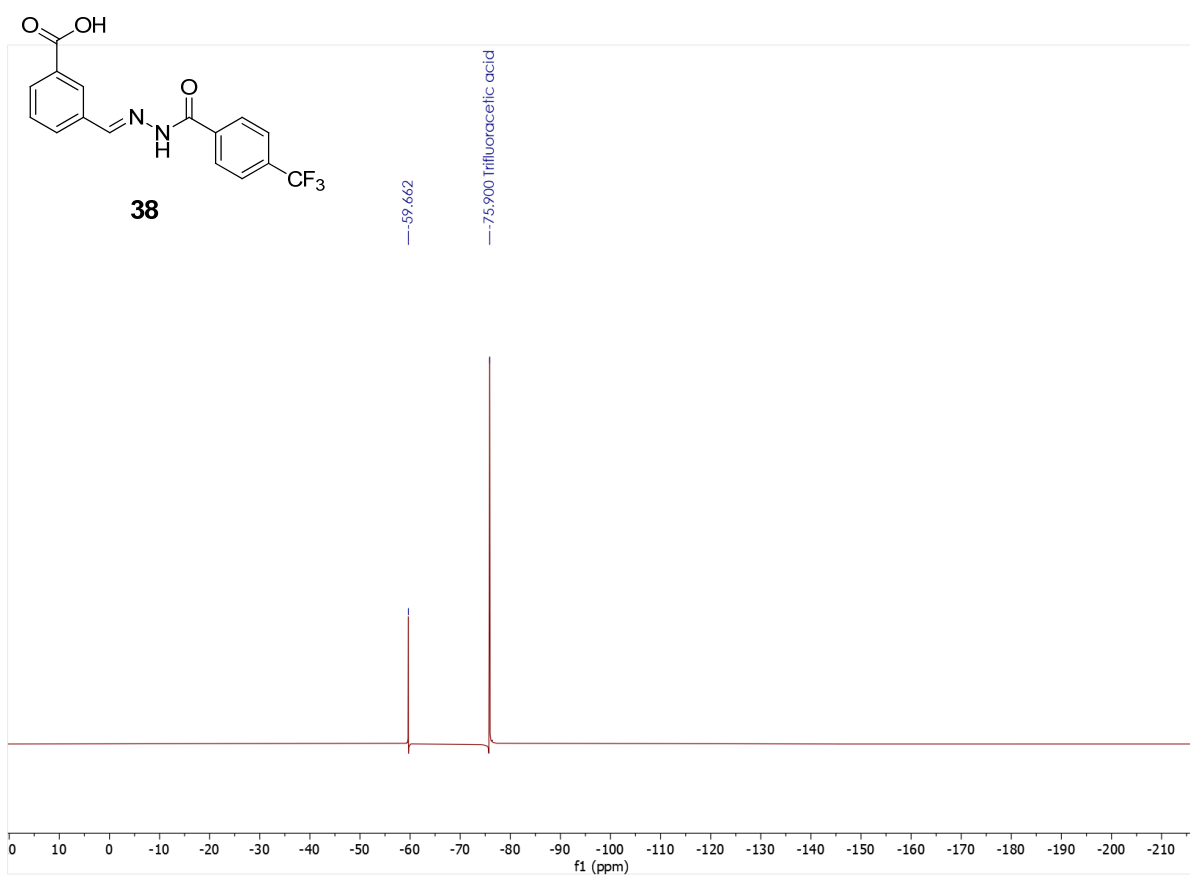


Molecular Weight: 324.374

37





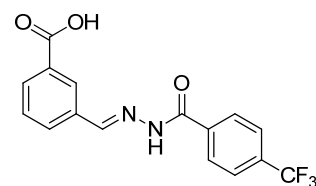


LCMS Report



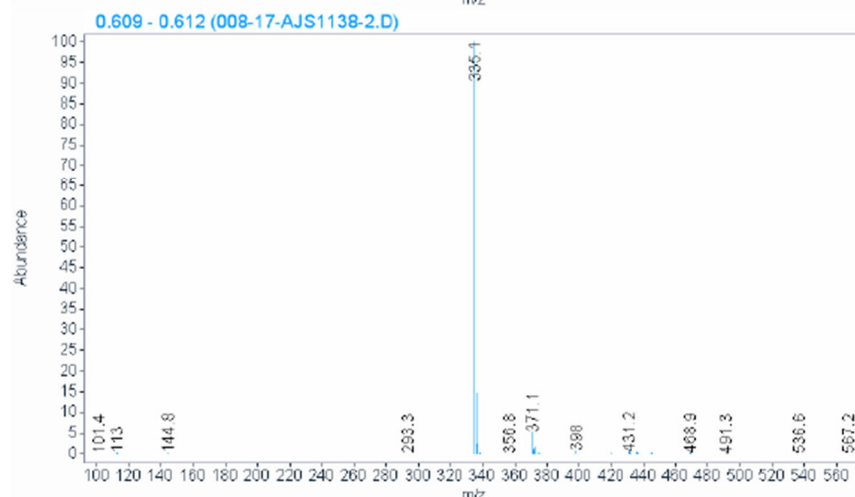
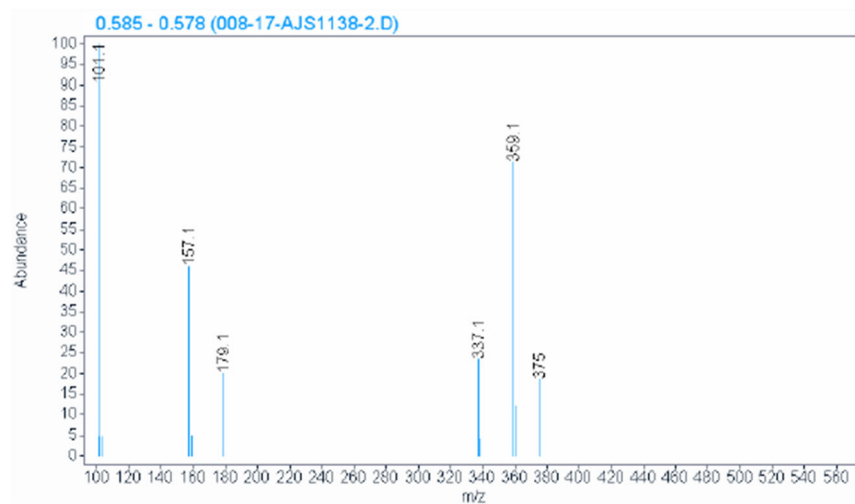
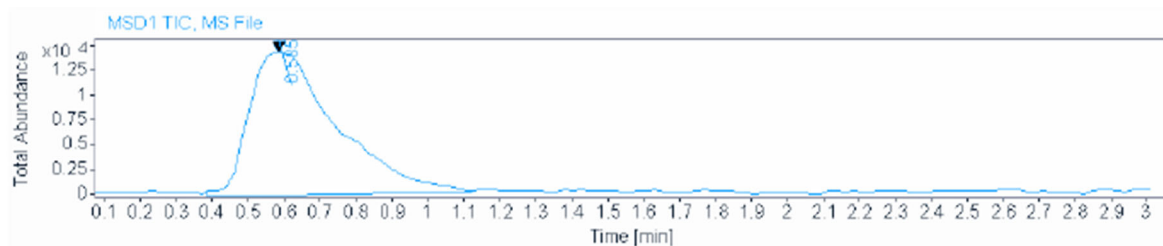
Agilent Technologies

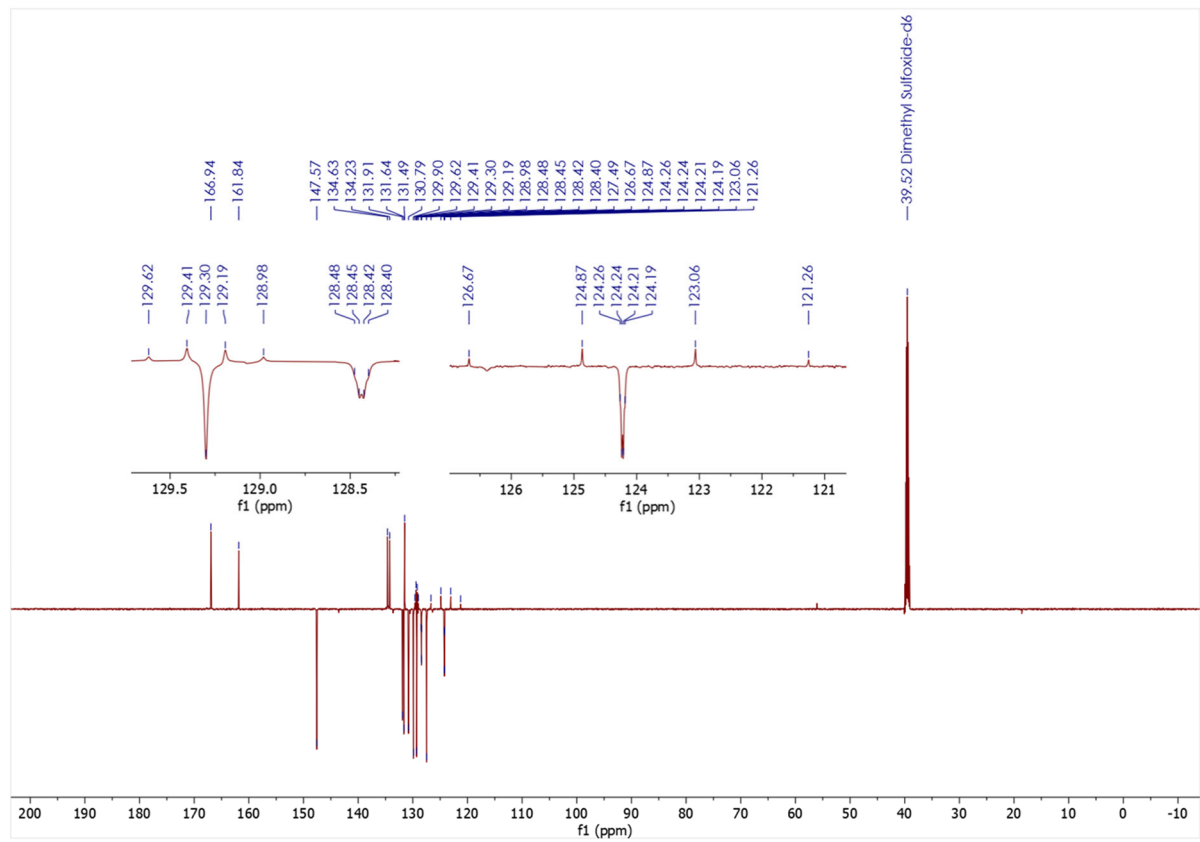
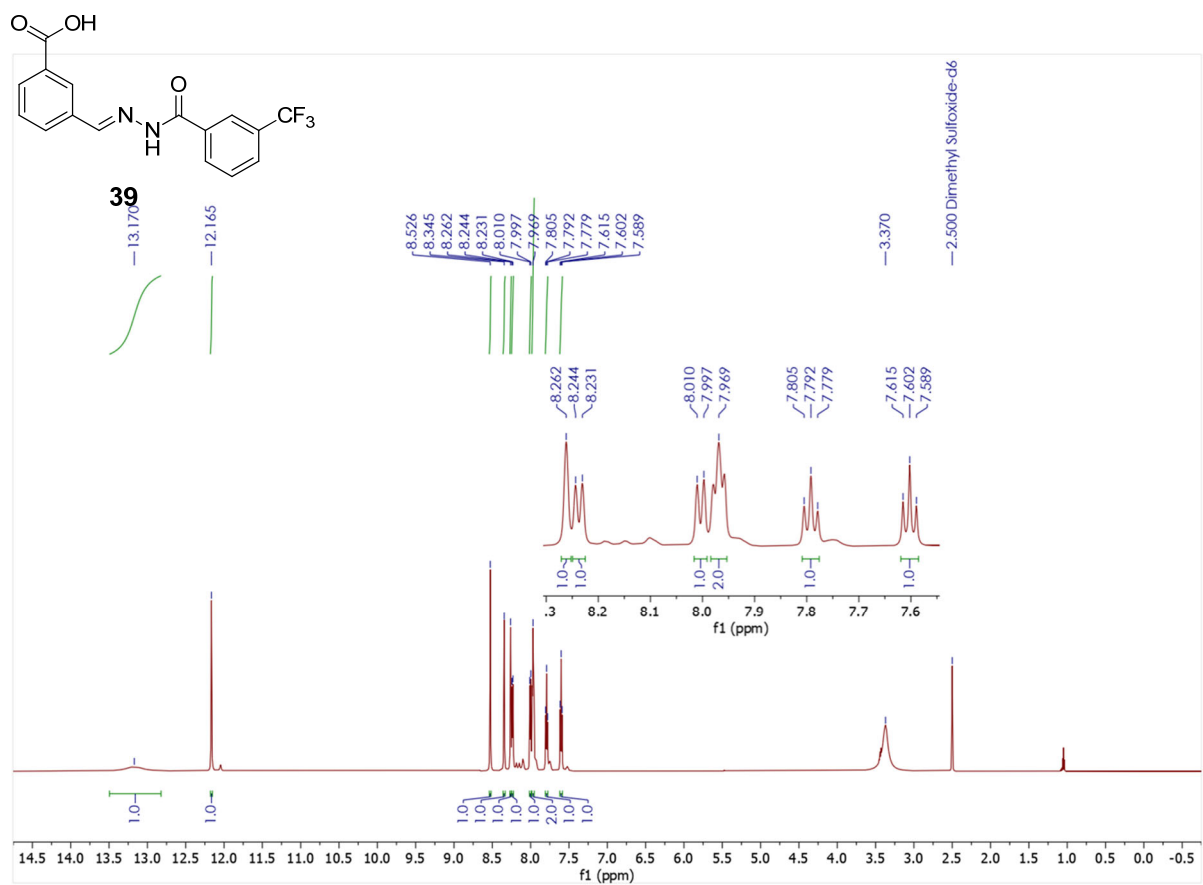
Data file: D:\Chem32\1\Data\AJS\AJS Table1 2023-07-25 14-45-29\008-17-AJS1138-2.D
 Sample name: AJS1138-2
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 17
 Injection date: 7/25/2023 3:18:49 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 B_3 MINS.M
 Injection volume: 2.000
 Analysis method: LCMS ISOCRATIC
 80%B_3 MINS.M
 Acq. operator: SYSTEM
 Last changed: 11/26/2021 9:20:48 AM

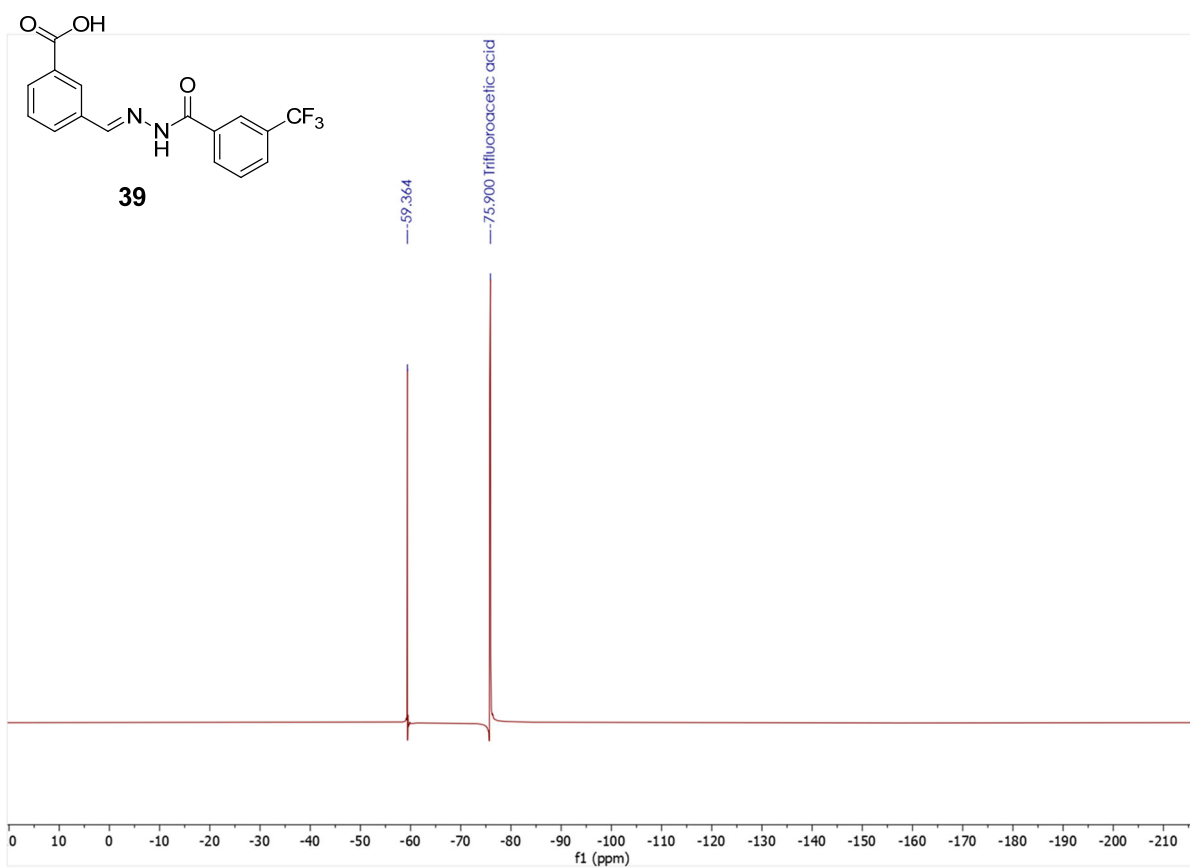


Molecular Weight: 336.265

38



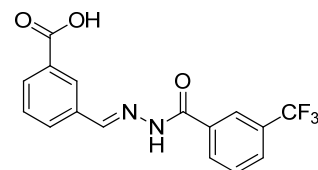




LCMS Report

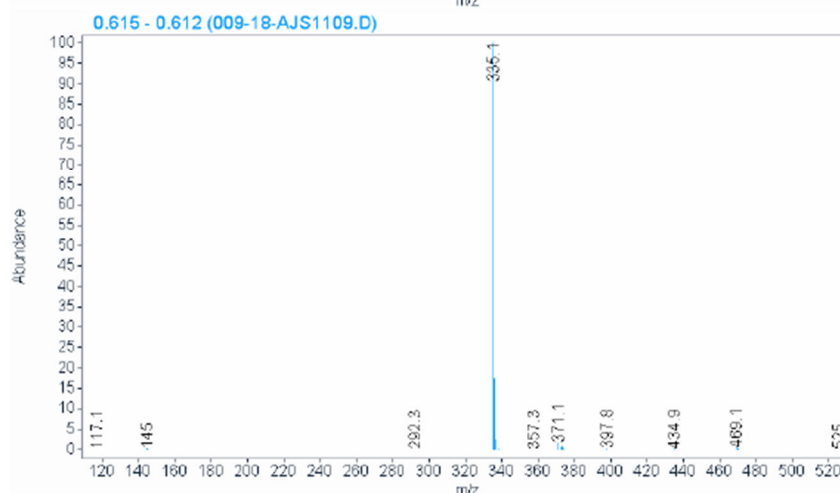
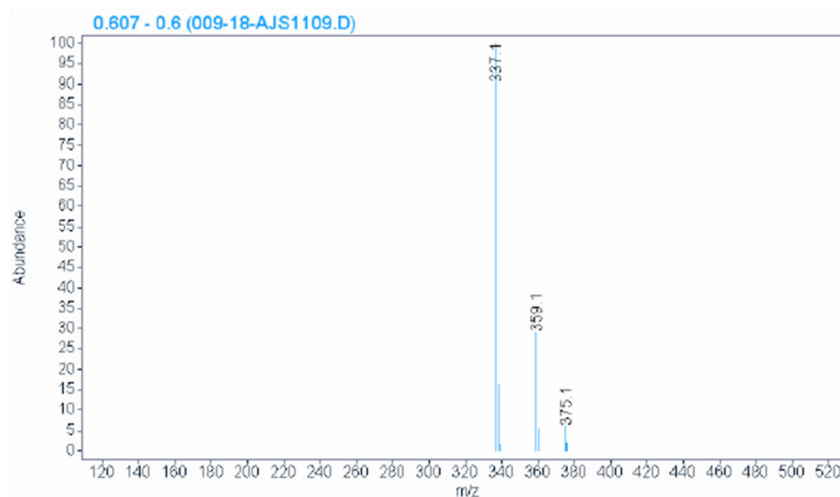
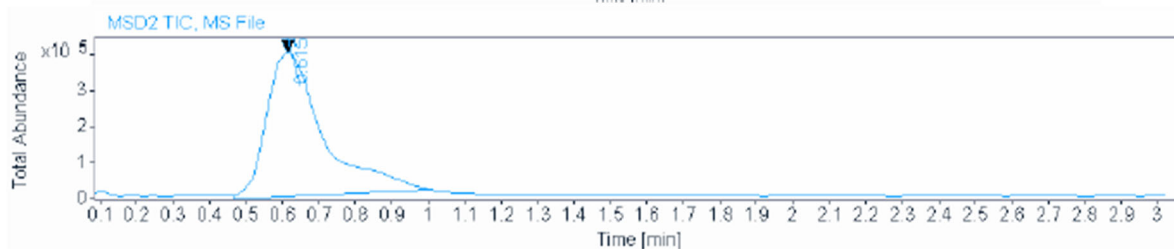


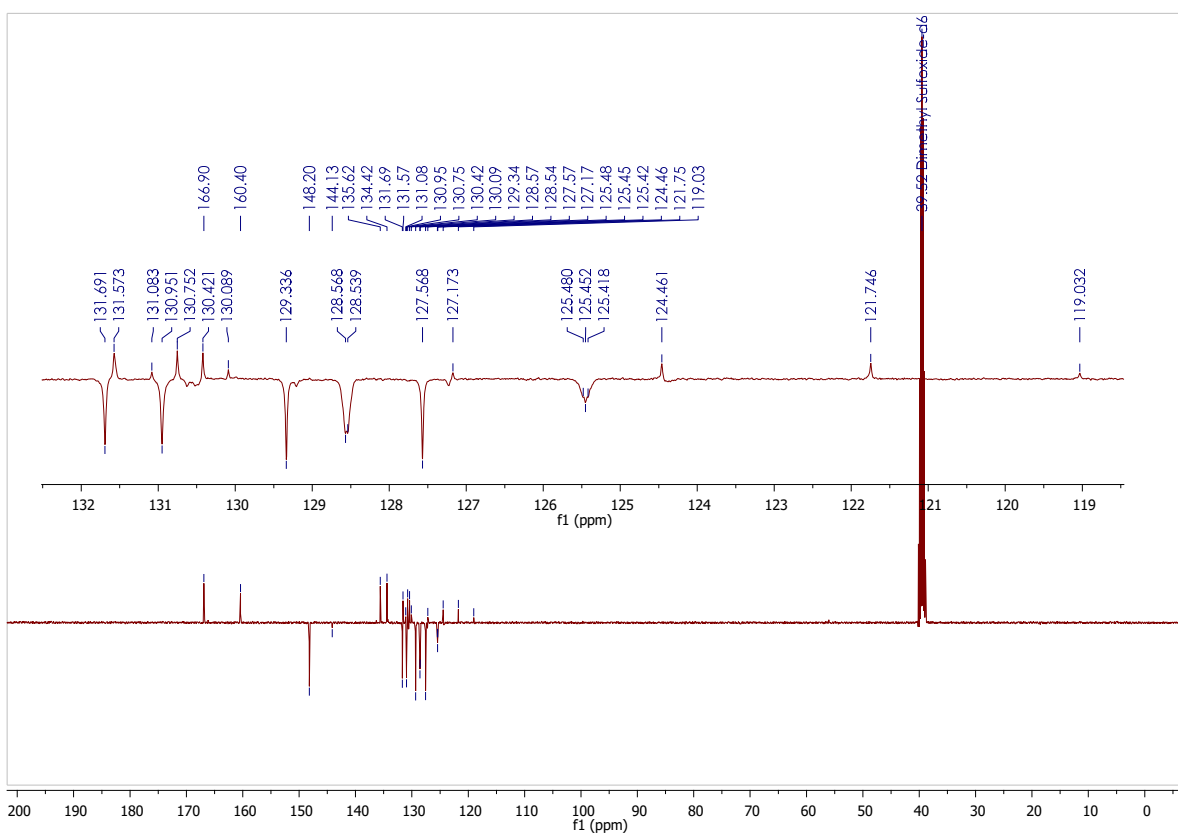
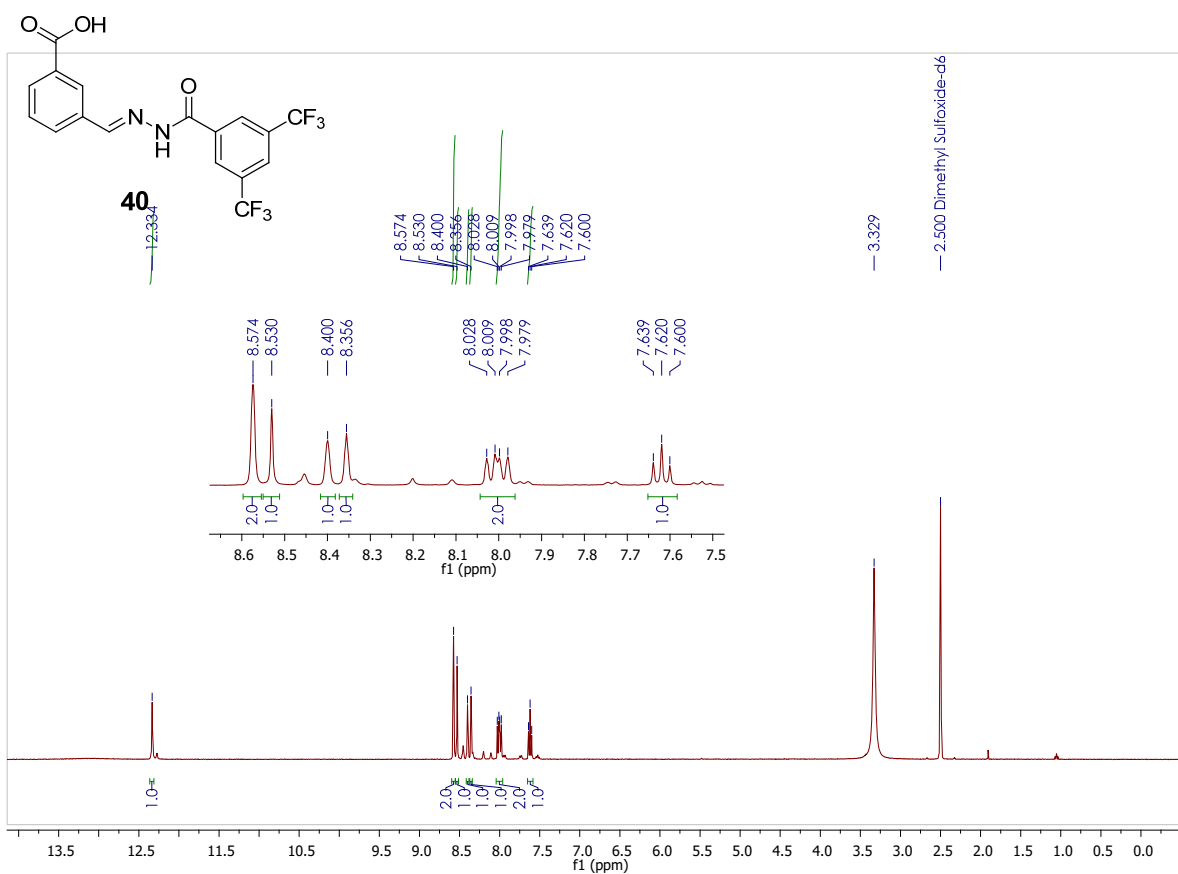
Data file: D:\Chem3211\Data\AJS\AJS Table1 2023-07-25 14-45-29\009-18-AJS1109.D
Sample name: AJS1109
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Location: 18
Injection date: 7/25/2023 3:23:33 PM
Injection: 1 of 1
Acq. method: LCMS ISOCRATIC 80%
Injection volume: 2.000
Analysis method: LCMS ISOCRATIC
Acq. operator: SYSTEM
80%B_3 MINS.M
Last changed: 11/26/2021 9:20:48 AM

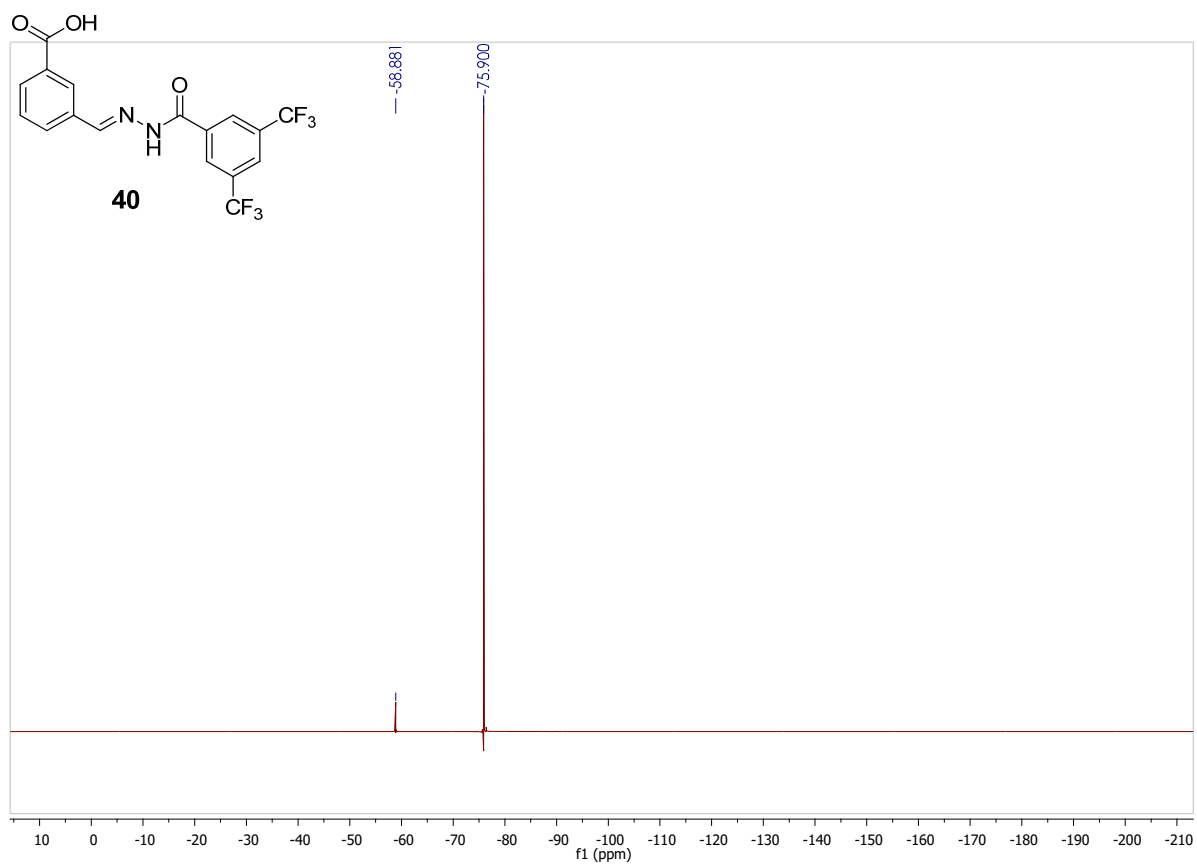


Molecular Weight: 336.265

39







Data file:	D:\Chem32\1\Data\MH\mh40222-4026 2022-03-04 12-44-11\006-71-MH4026.D
Sample name:	MH4026
Description:	
Sample amount:	0.000
Instrument:	LCMS
Injection date:	3/4/2022 1:09:15 PM
Acq. method:	LCMS ISOCRATIC 80% B_3 MINS.M
Analysis method:	LCMS ISOCRATIC 80%B_3 MINS.M
Last changed:	11/26/2021 9:20:48 AM

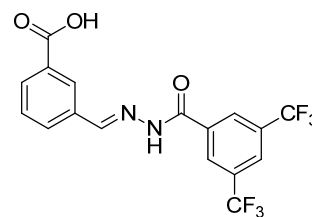
Sample type: Sample

Location: 71

Injection: 1 of 1

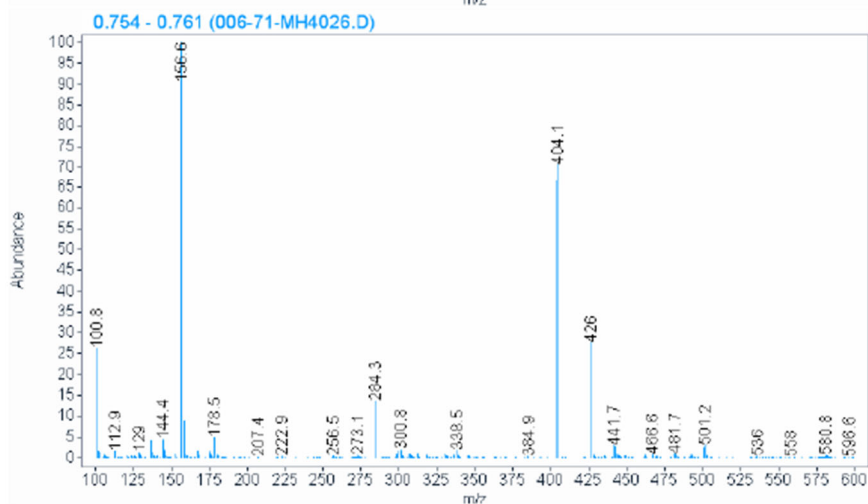
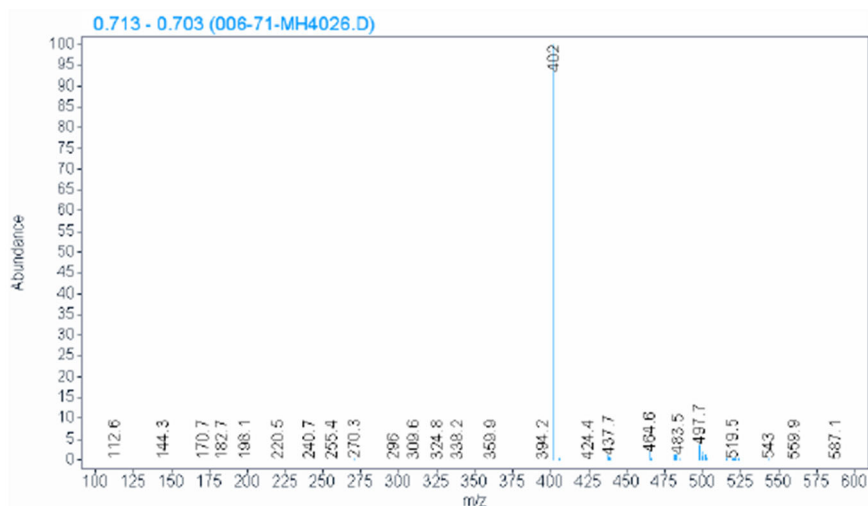
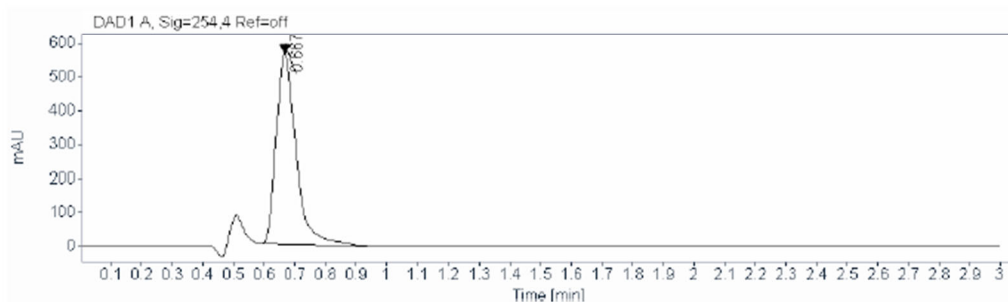
Injection volume: 2.000

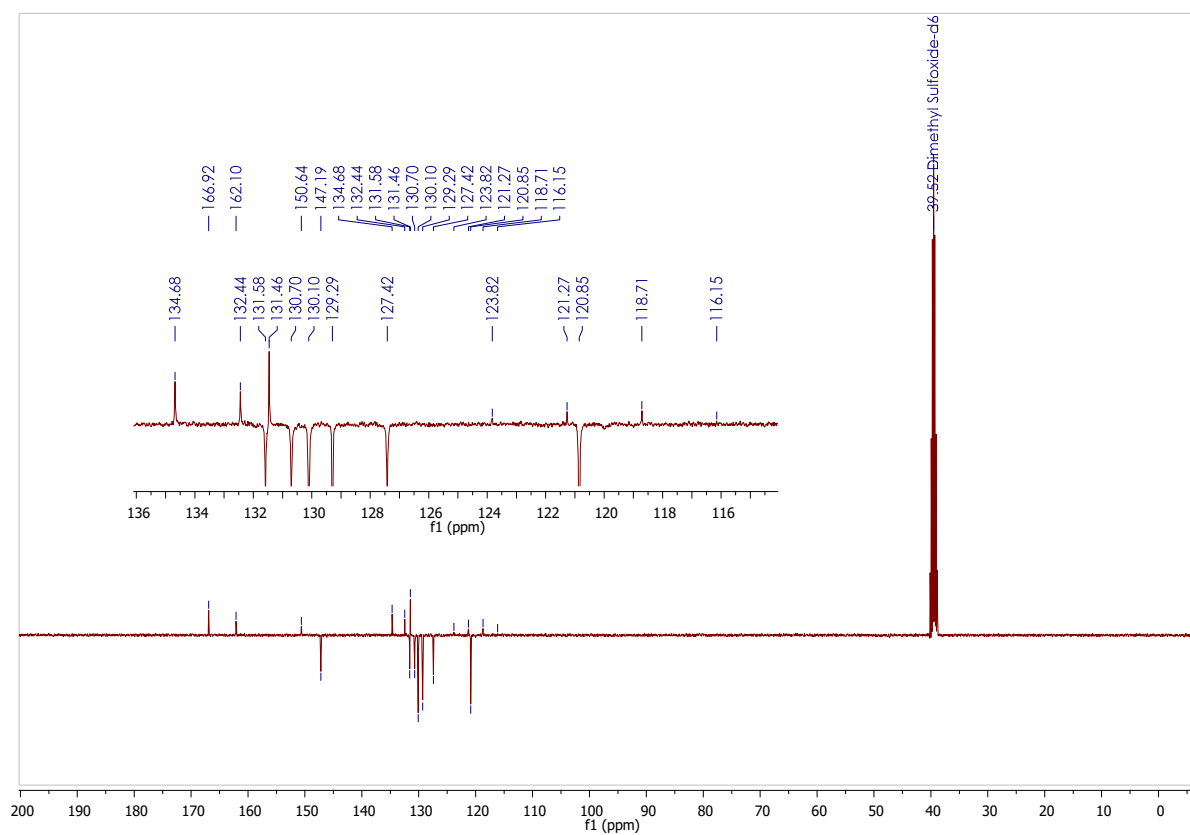
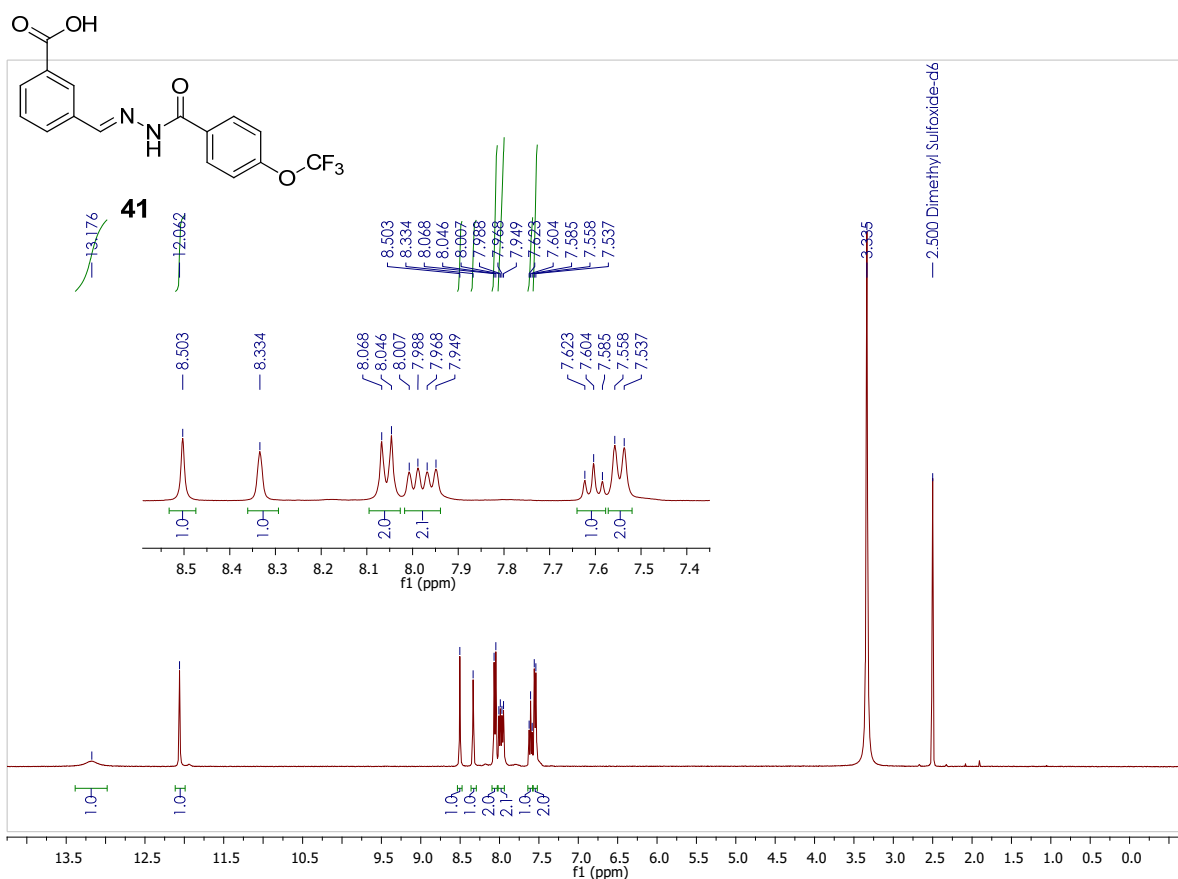
Acq. operator: SYSTEM

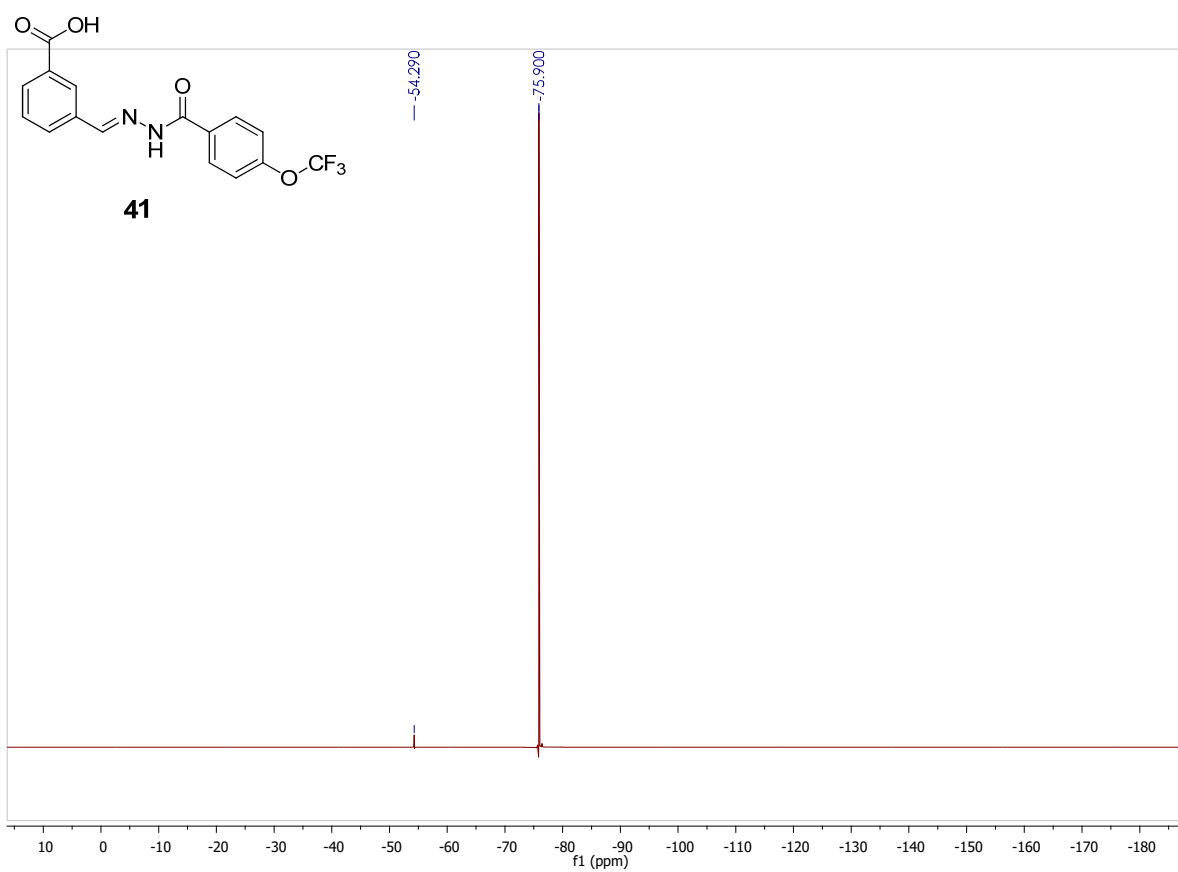


Molecular Weight: 404.263

40

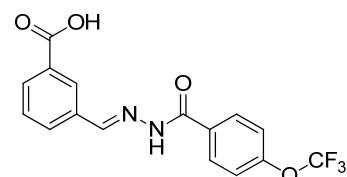






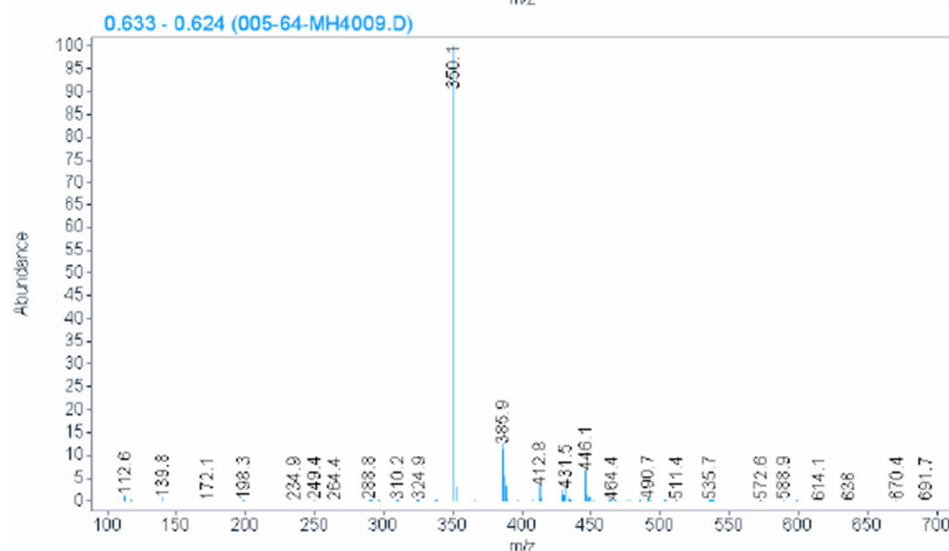
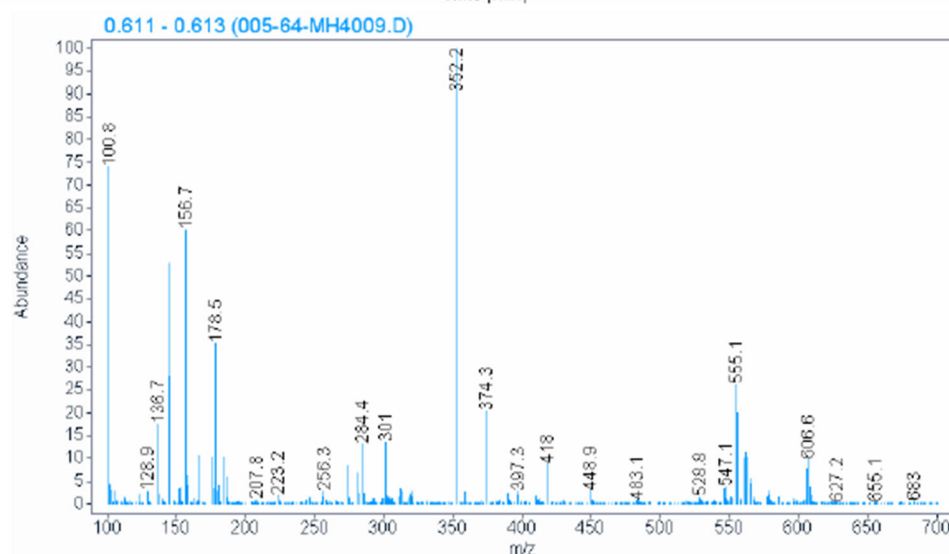
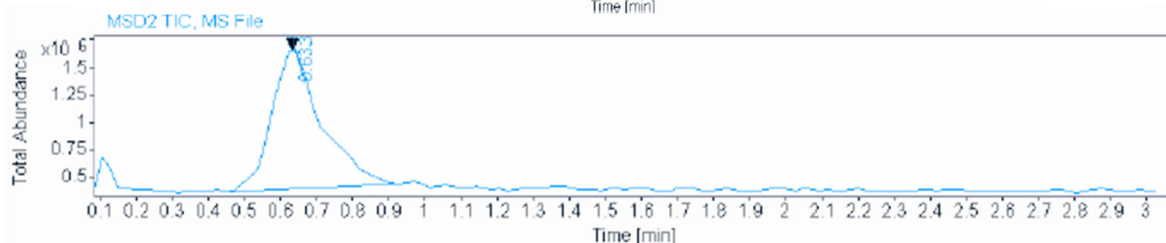
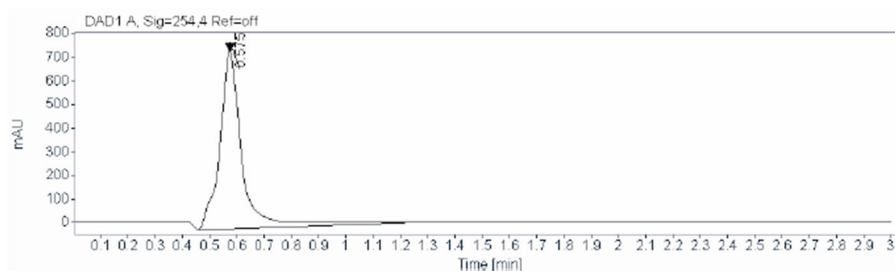


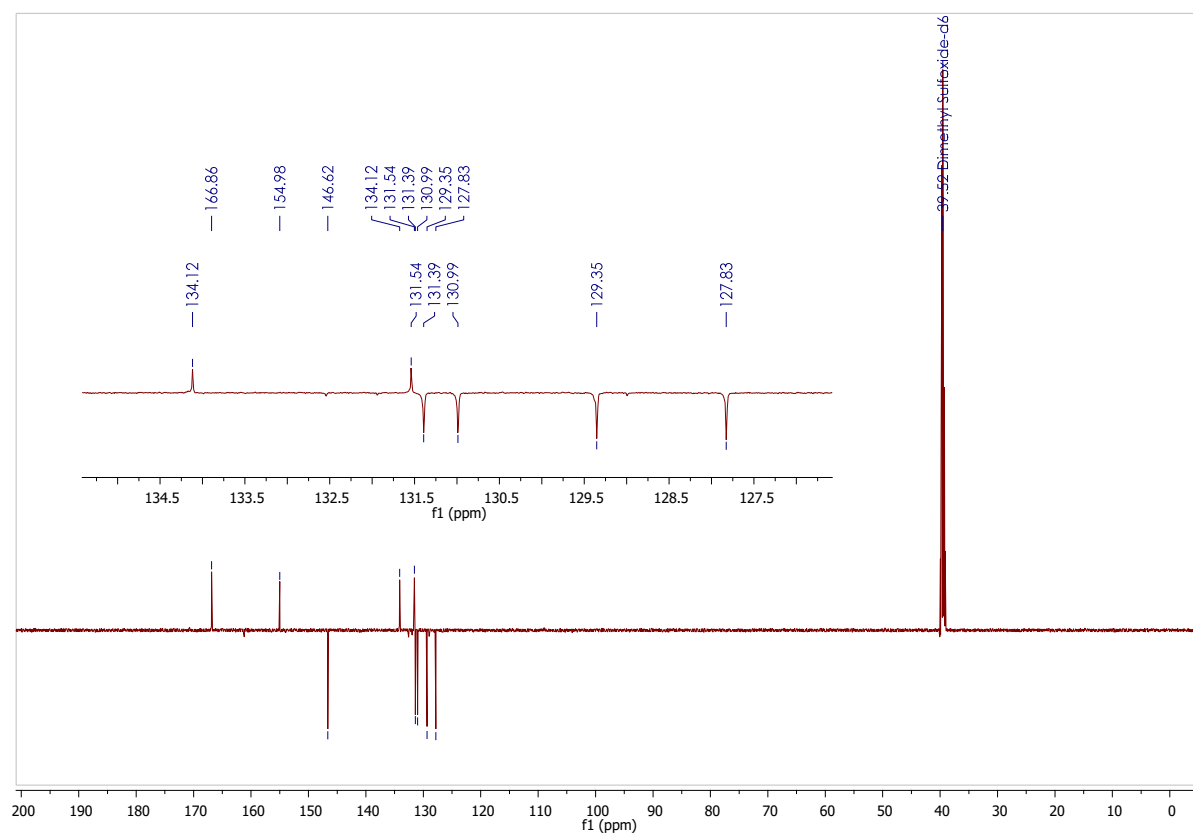
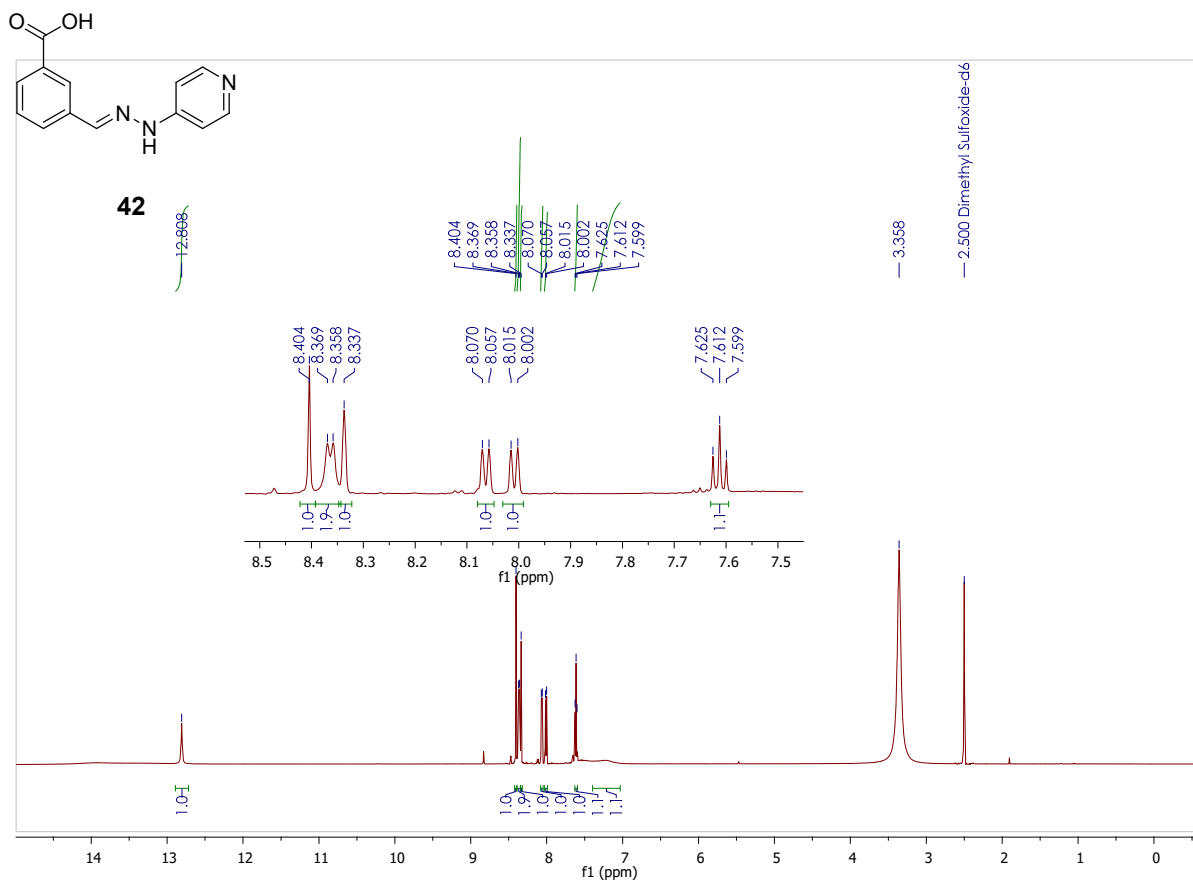
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Sample name: MH4009
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Location: 64
Injection date: 3/1/2022 12:33:03 PM
Injection: 1 of 1
Acq. method: LCMS ISOCRATIC_80%
Injection volume: 2.000
Analysis method: LCMS ISOCRATIC_80%
Acq. operator: SYSTEM
Last changed: 7/13/2021 10:05:44 AM



Molecular Weight: 352.265

41



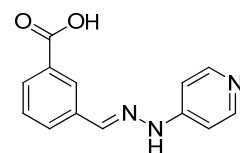


LCMS Report



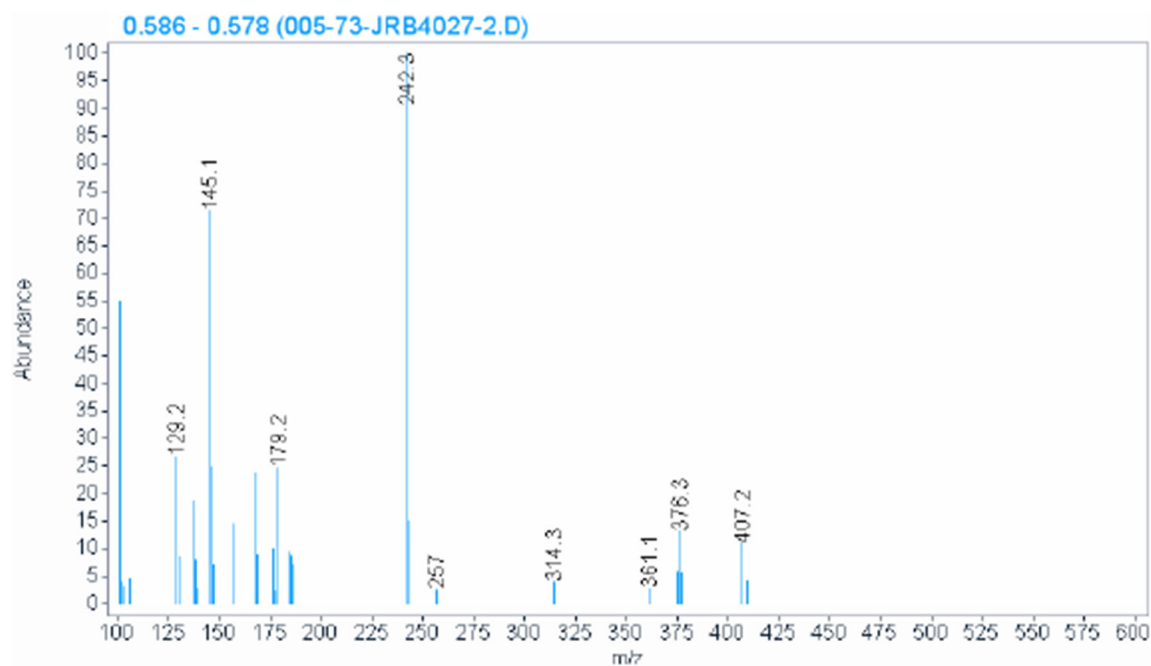
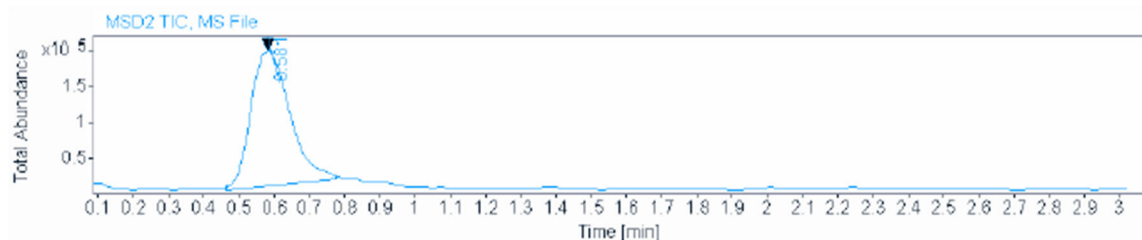
Agilent Technologies

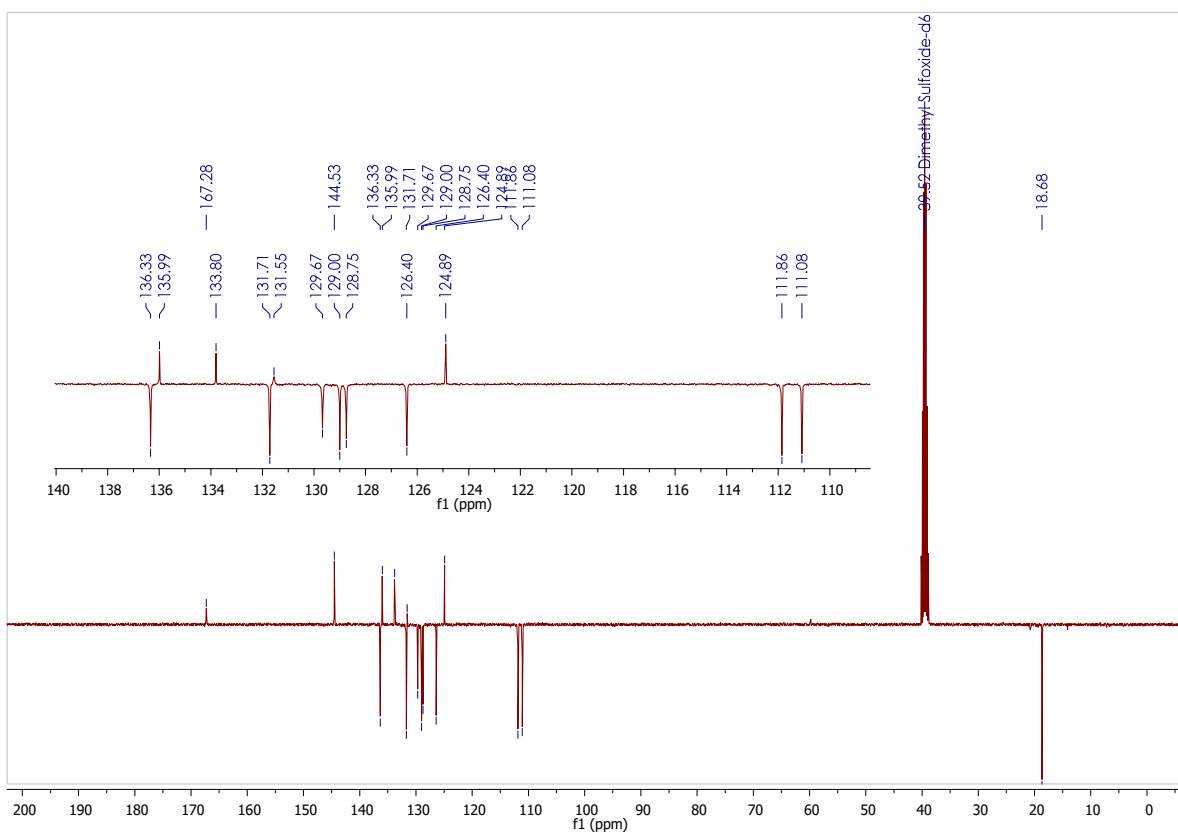
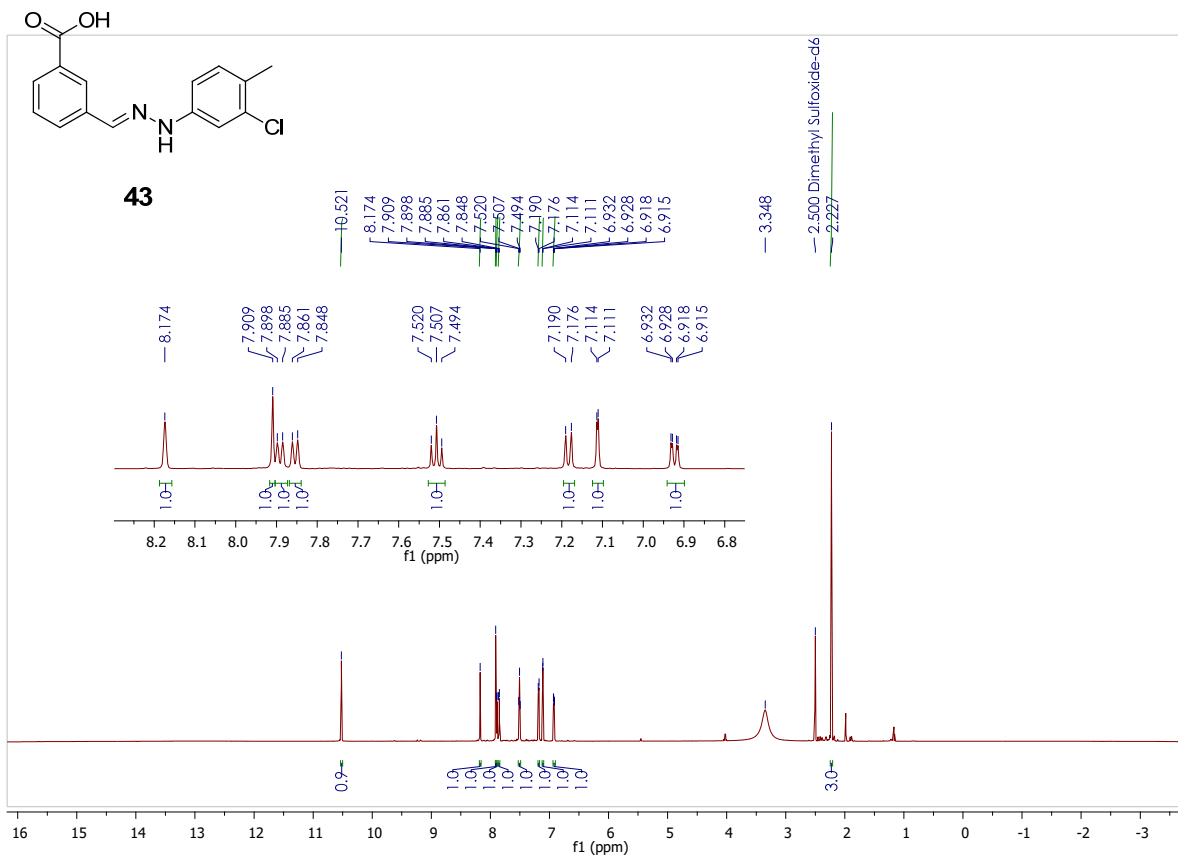
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 Sample name: JRB4027-2
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 73
 Injection date: 7/24/2023 3:49:41 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80% B_3 MINS.M
 Injection volume: 2.000
 Analysis method: LCMS ISOCRATIC 80%B_3 MINS.M
 Acq. operator: SYSTEM
 Last changed: 11/26/2021 9:20:48 AM



Molecular Weight: 241.245

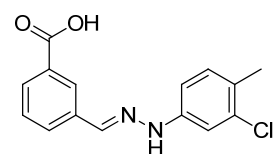
42





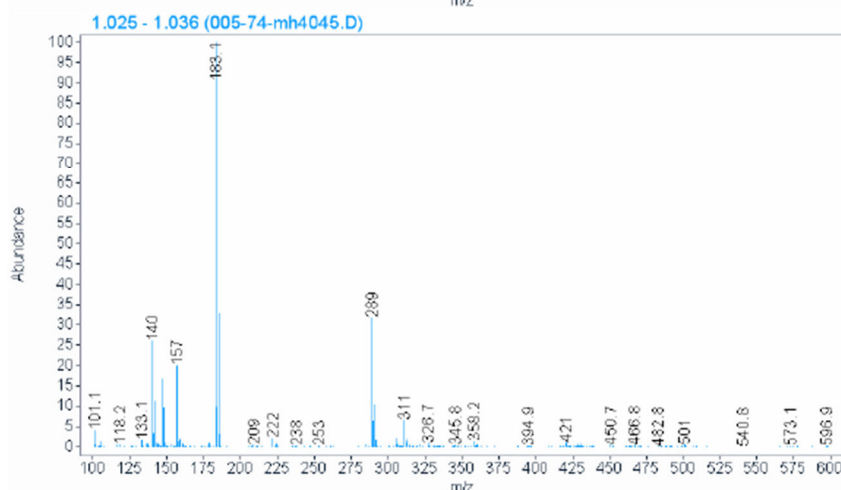
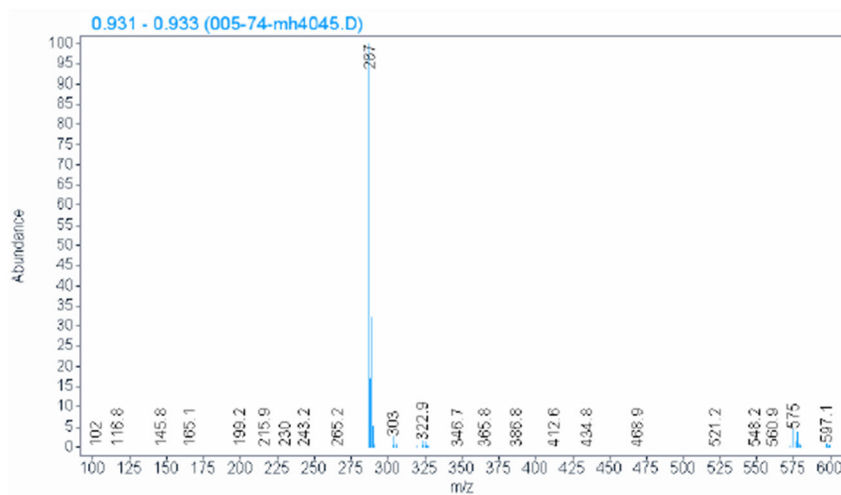
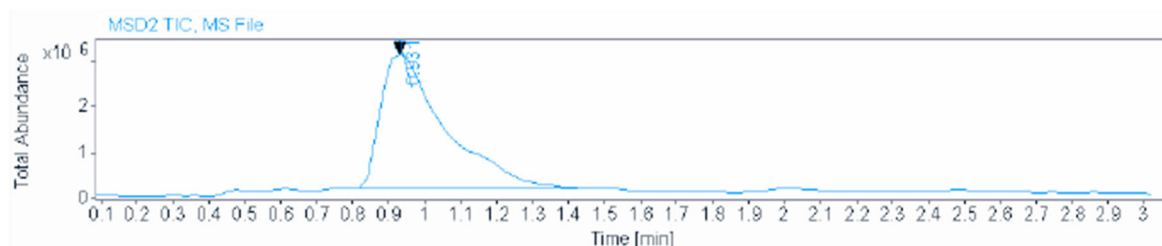
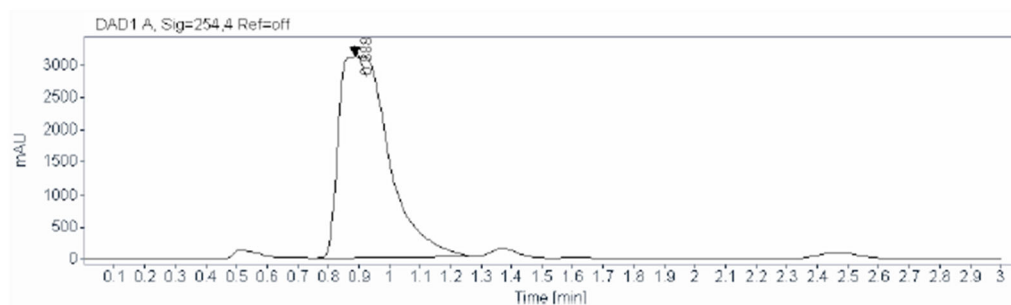


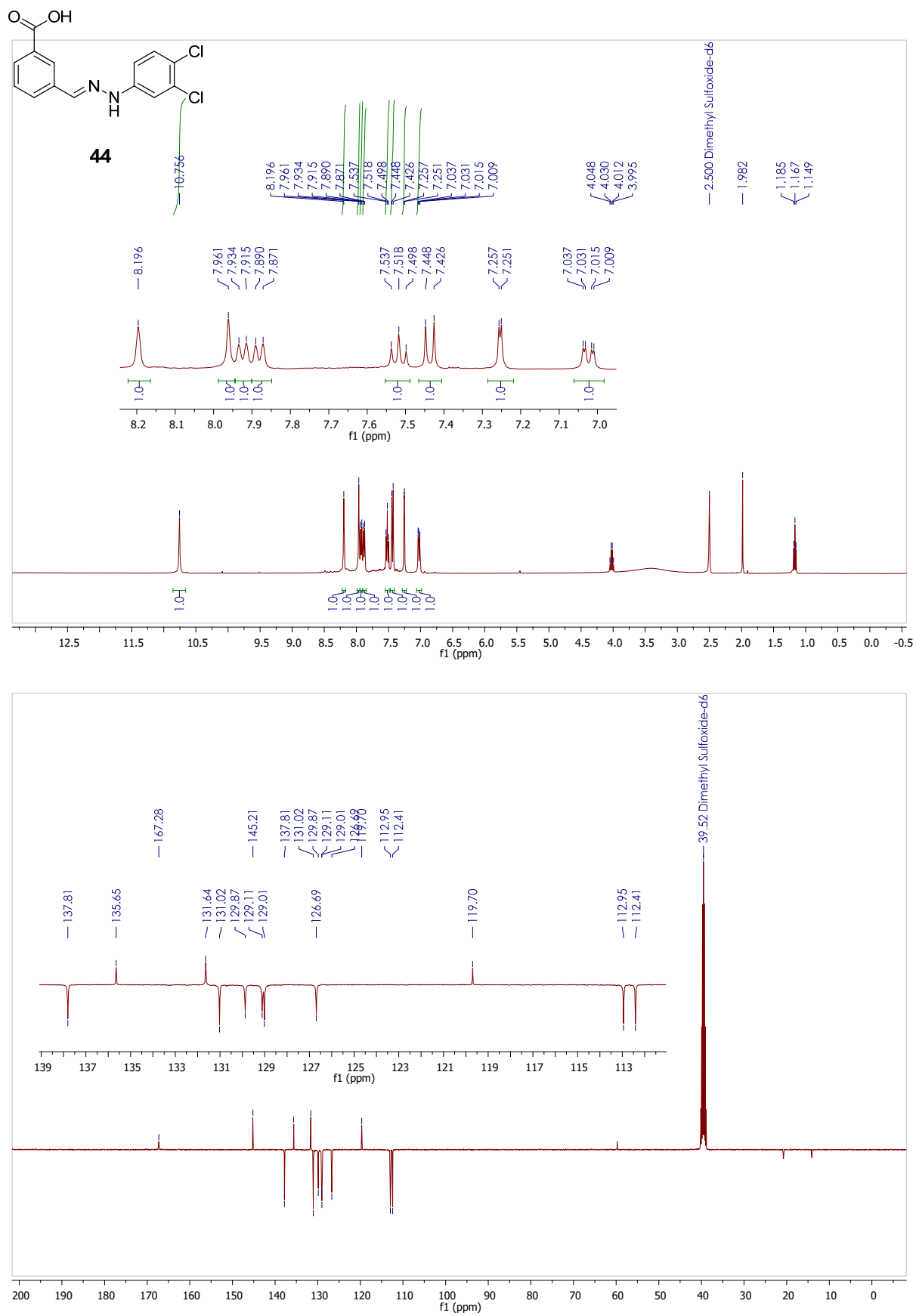
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 Sample name: mh4045
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 74
 Injection date: 3/23/2022 12:11:39 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 Injection volume: 2.000
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 80%B_3 MINS.M
 Last changed: 11/26/2021 9:20:48 AM



Molecular Weight: 288.729

43



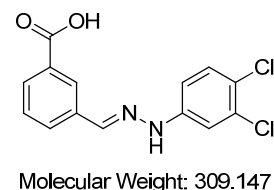


LCMS Report

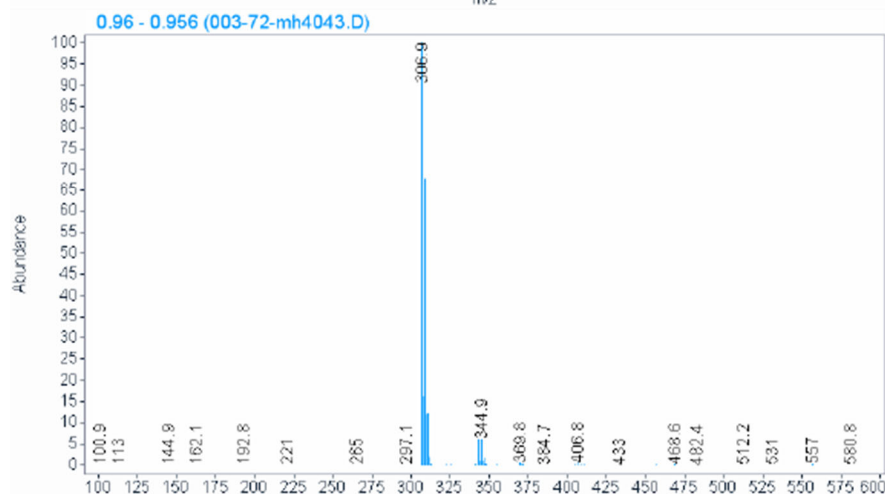
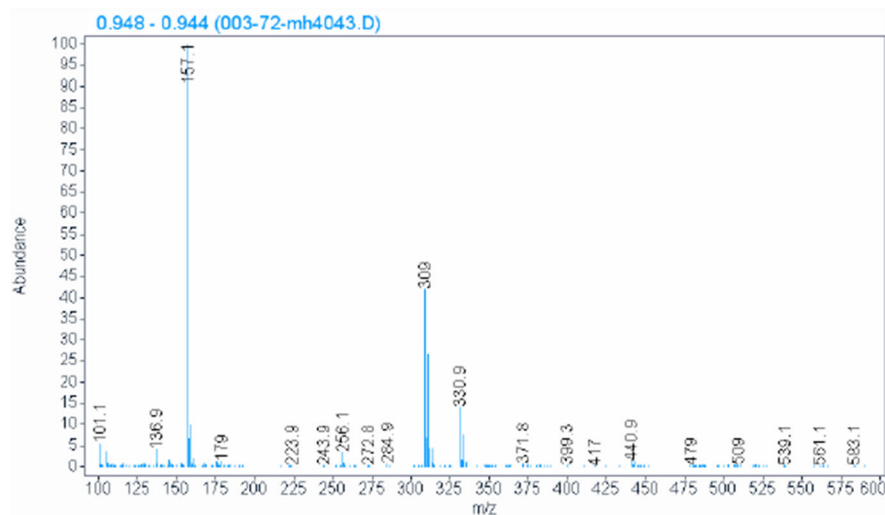
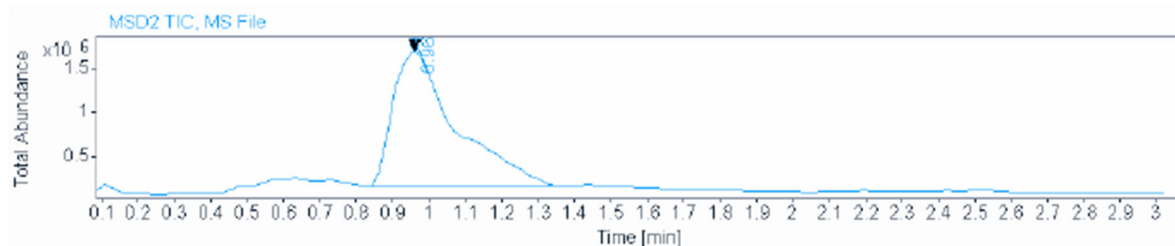
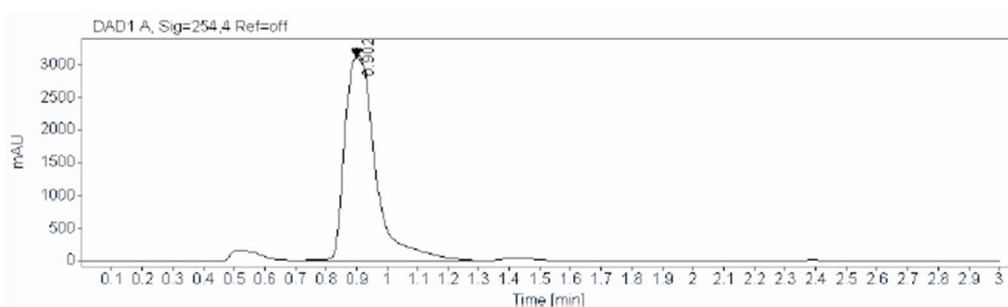


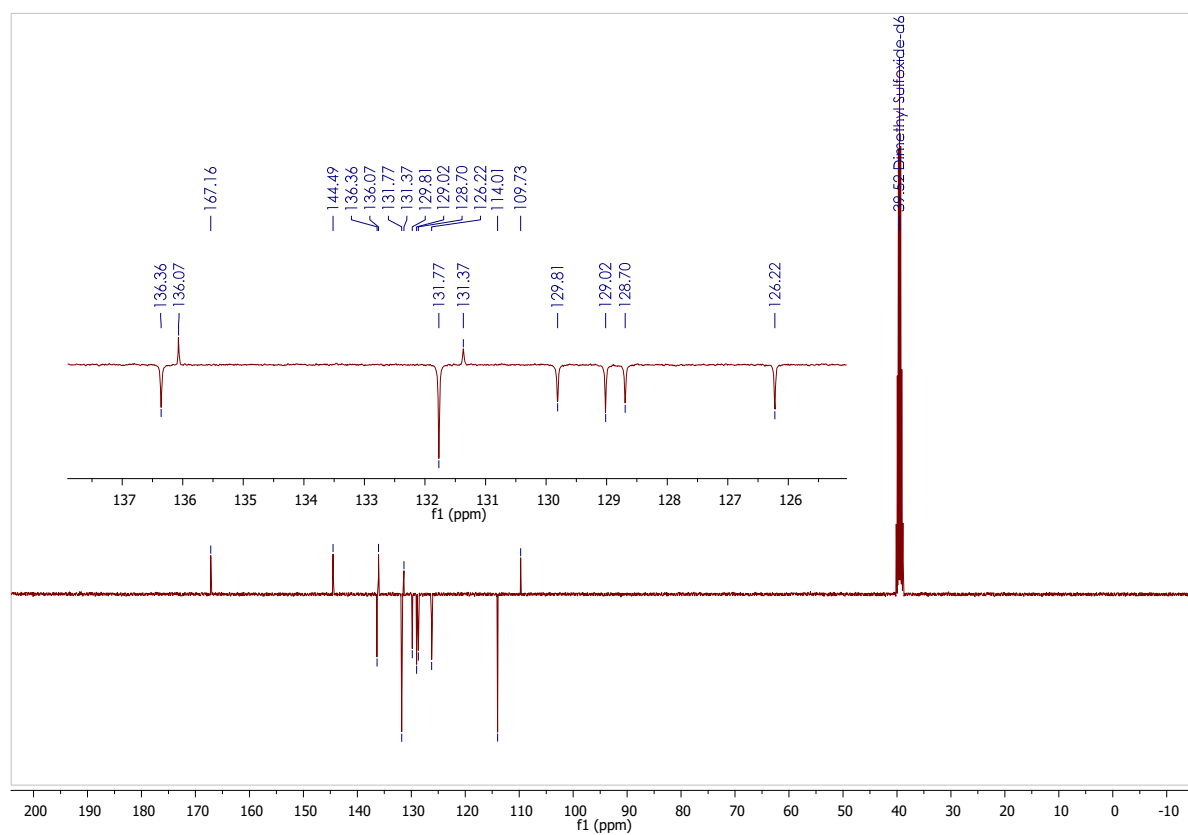
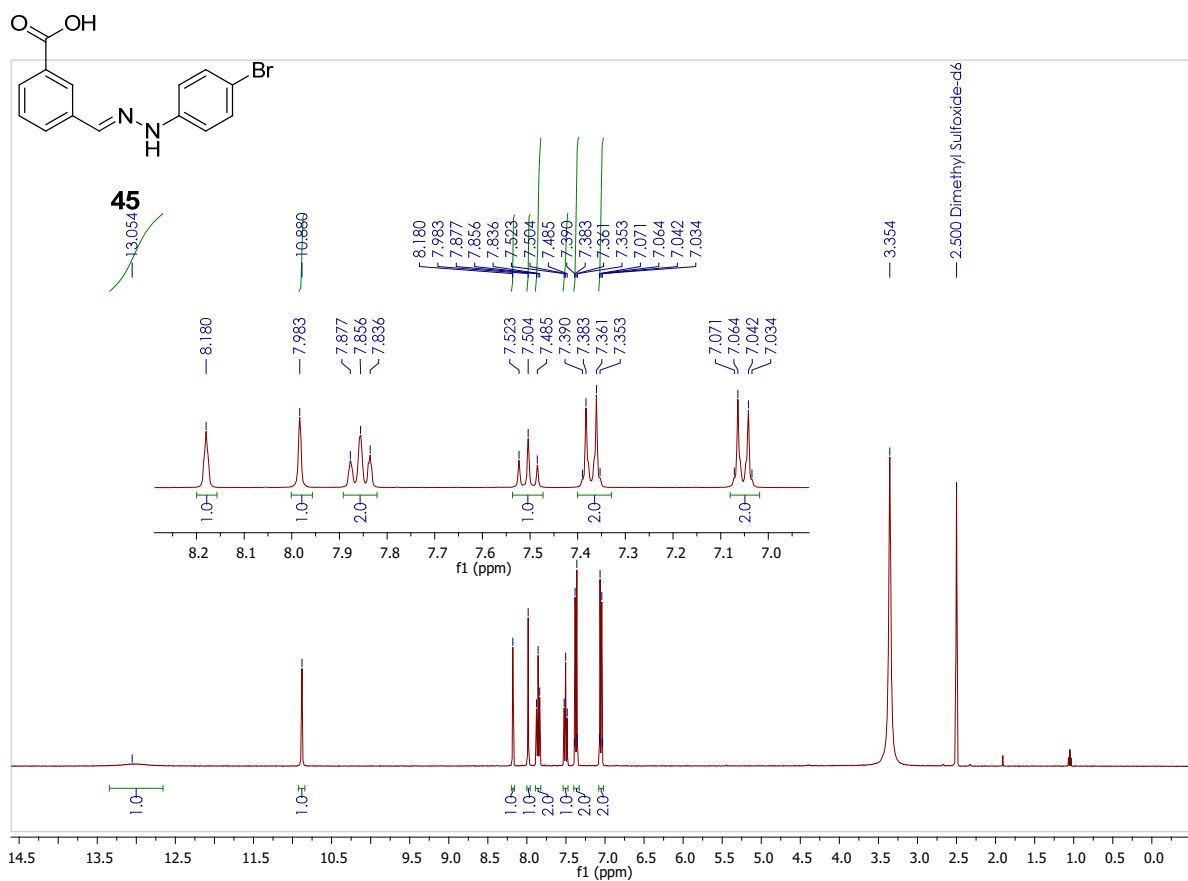
Agilent Technologies

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 Sample name: mh4043
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 72
 Injection date: 3/23/2022 12:02:24 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 Injection volume: 2.000
 B_3 MINS.M
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 80%B_3 MINS.M
 Last changed: 11/26/2021 9:20:48 AM



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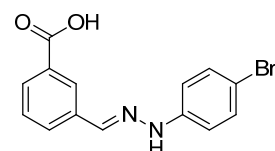


LCMS Report



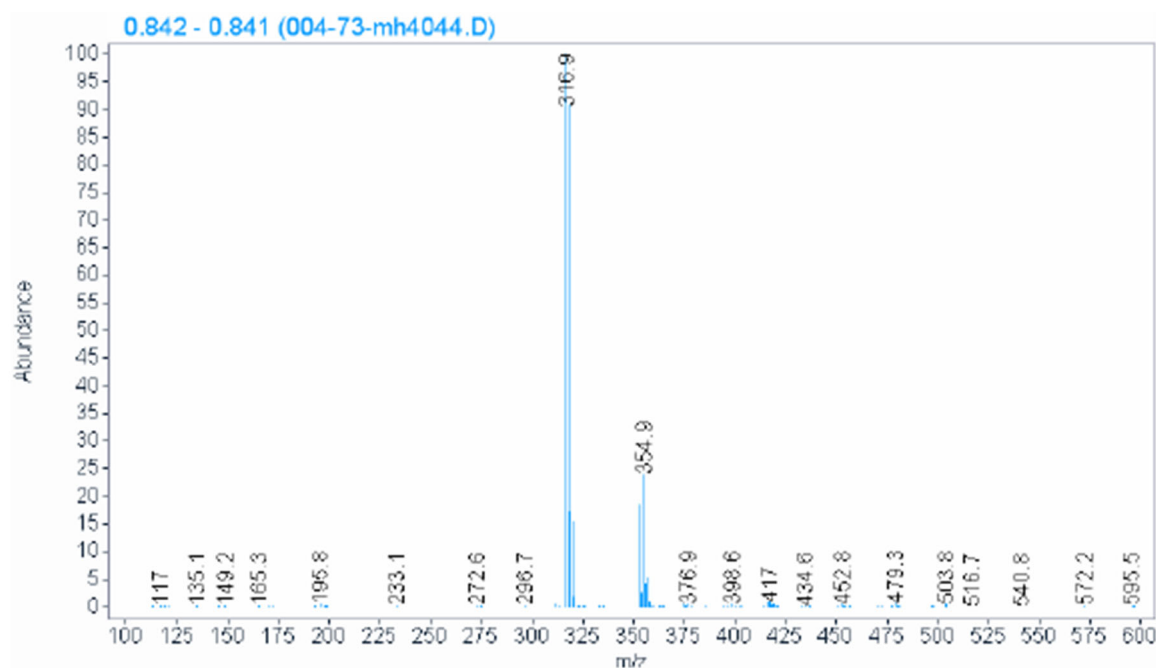
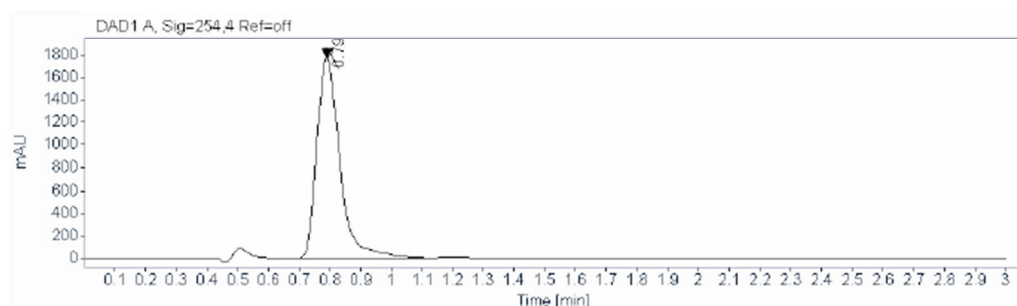
Agilent Technologies

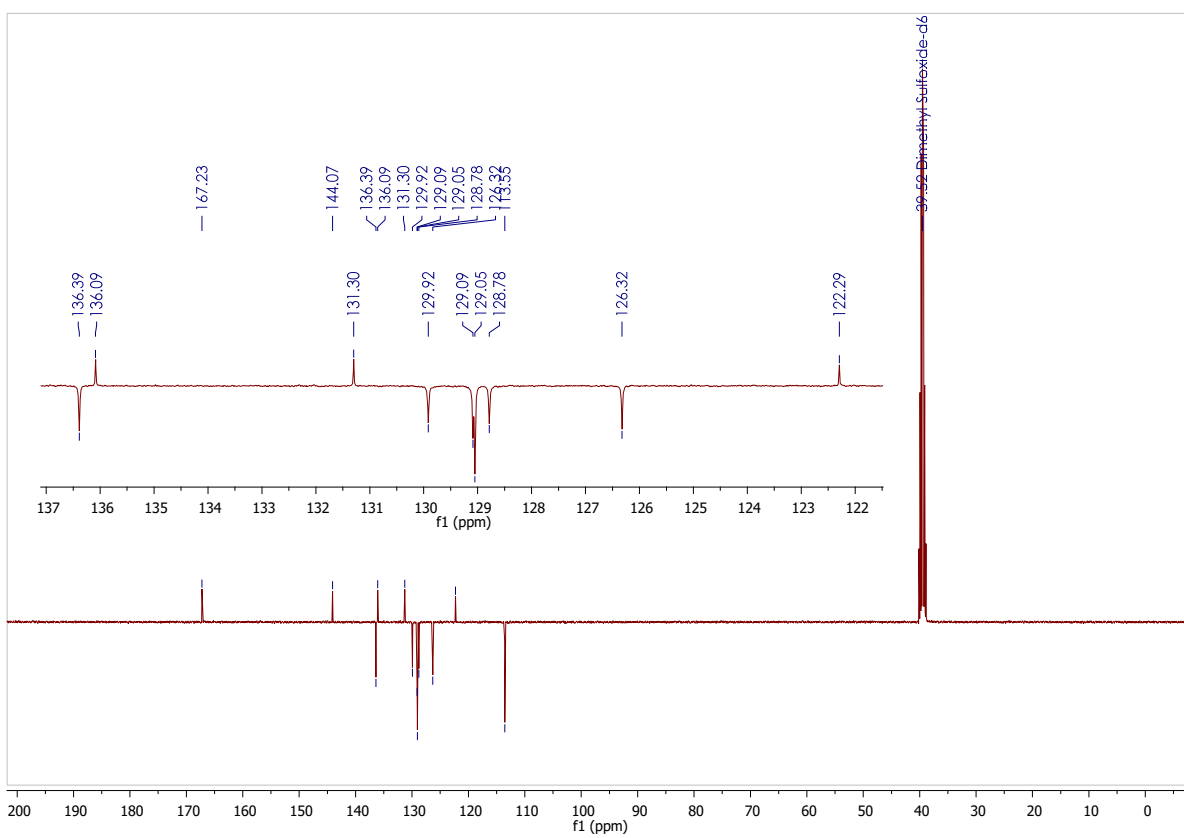
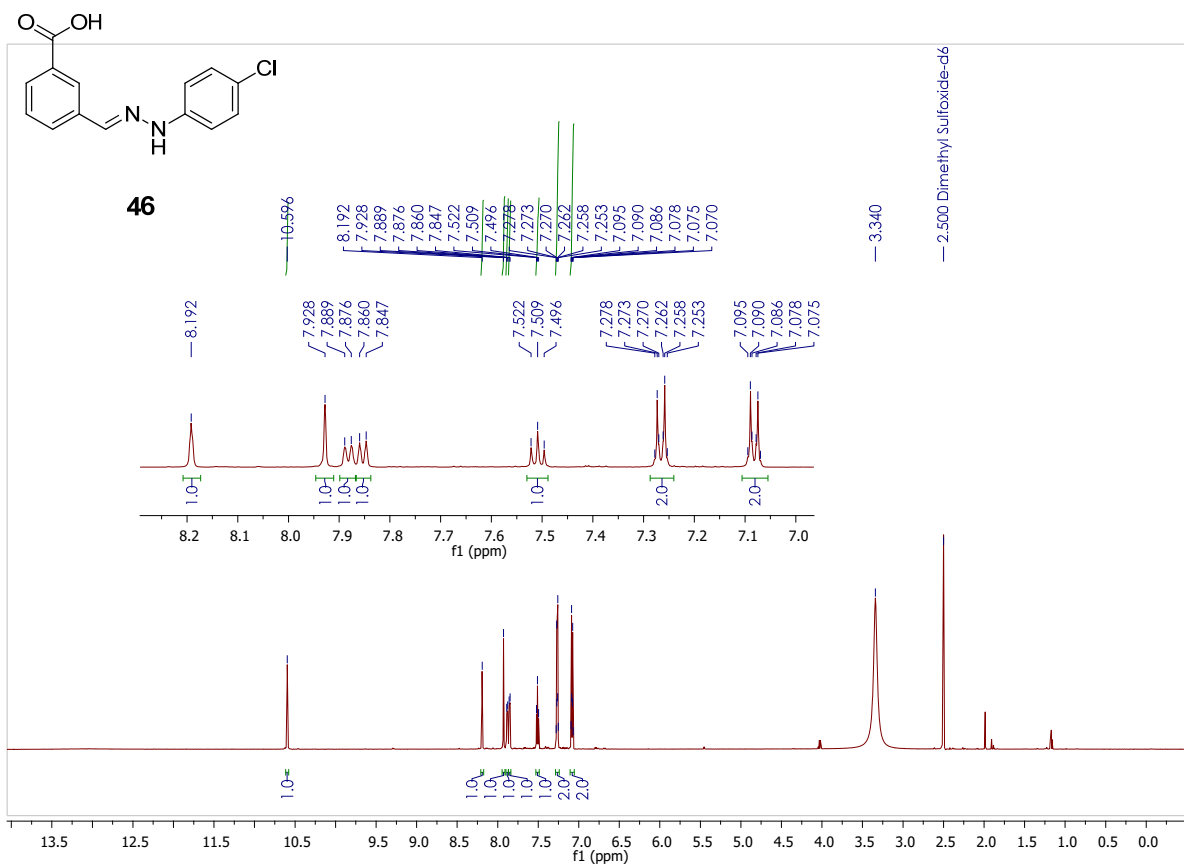
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 Sample name: mh4044
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 73
 Injection date: 3/23/2022 12:06:54 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 Injection volume: 2.000
 B_3 MINS.M
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 80%B_3 MINS.M
 Last changed: 11/26/2021 9:20:48 AM



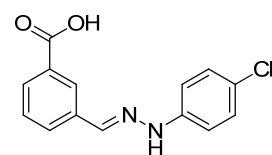
Molecular Weight: 319.153

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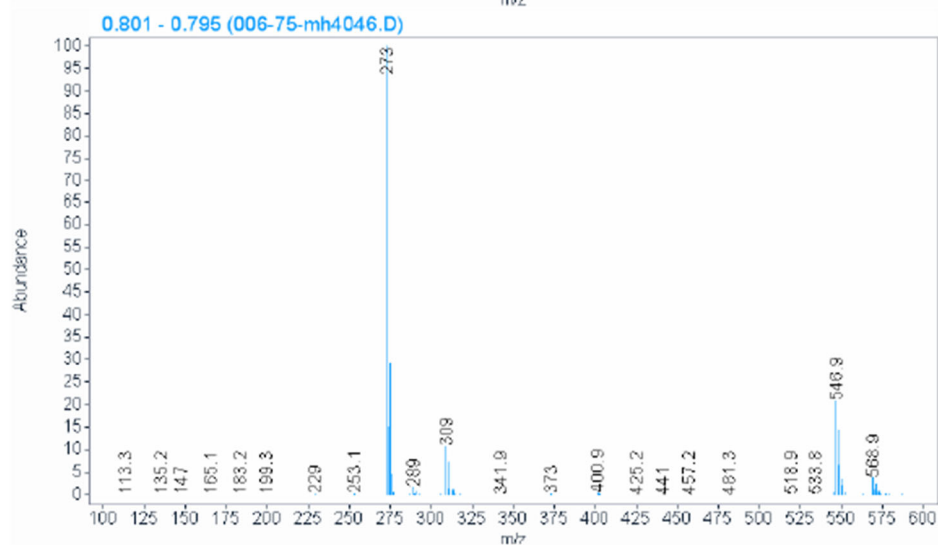
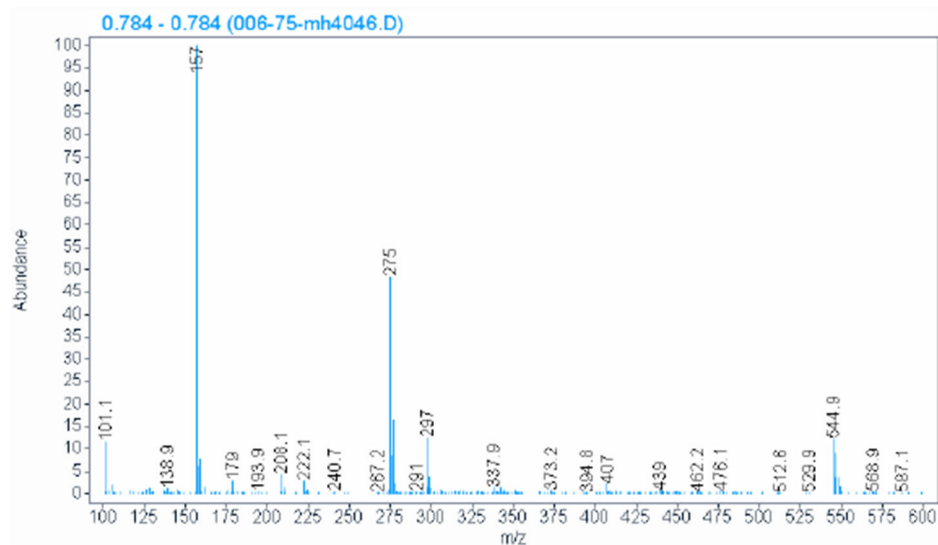
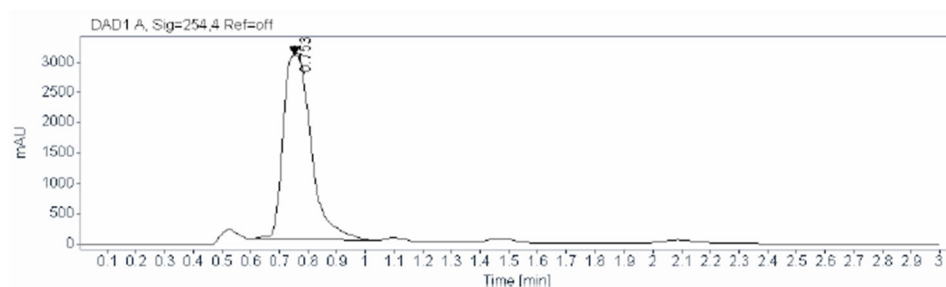


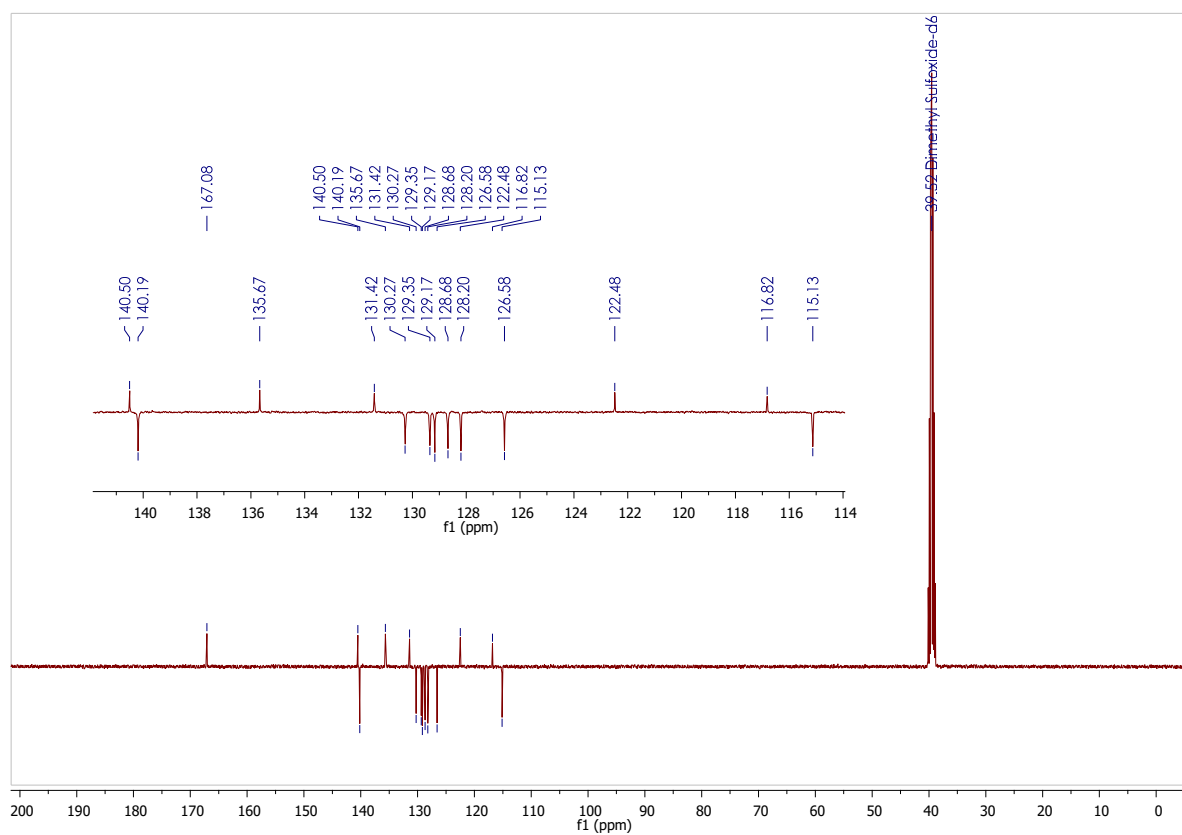
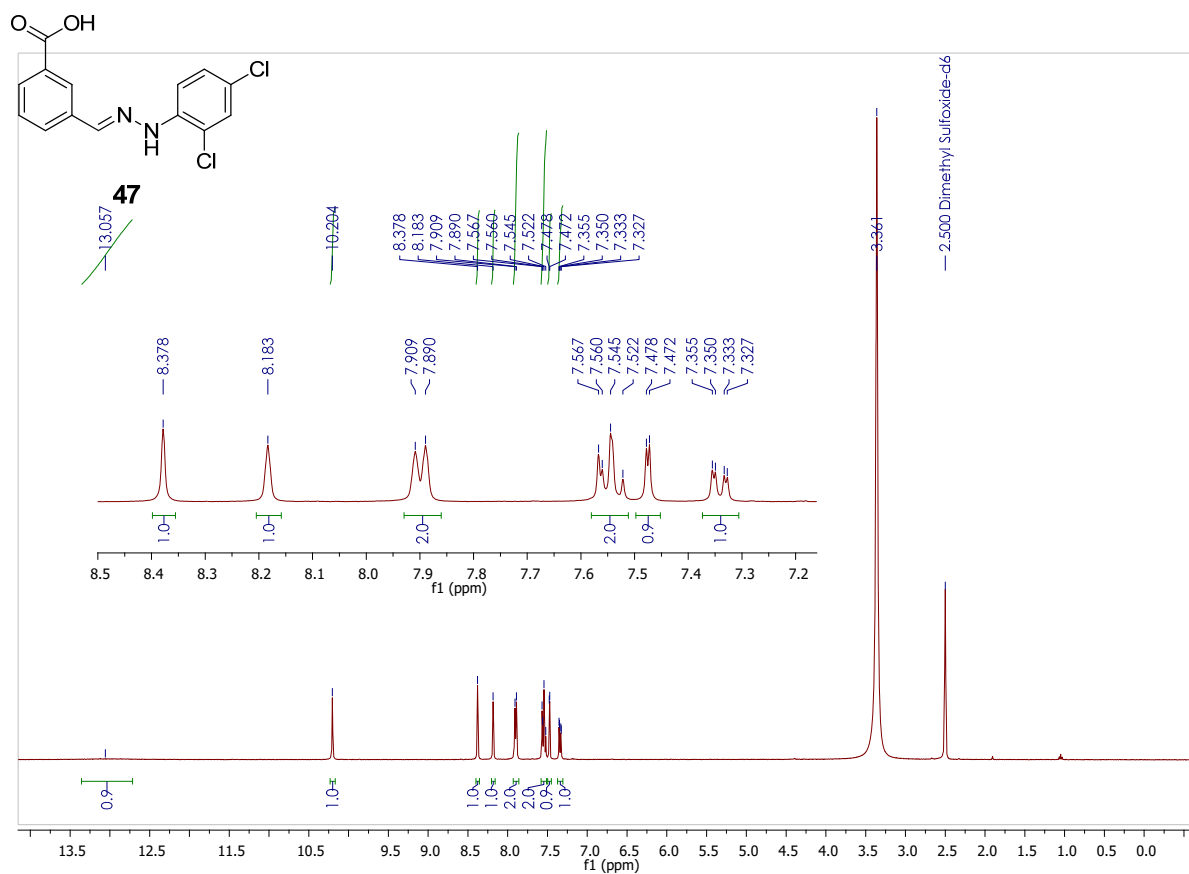
Data file: D:\Chem321\1\Data\MH\mh4042-47 2022-03-23 11-51-40\006-75-mh4046.D
 Sample name: mh4046
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 75
 Injection date: 3/23/2022 12:16:23 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 B_3 MINS.M
 Injection volume: 2.000
 Analysis method: LCMS ISOCRATIC
 80%B_3 MINS.M
 Acq. operator: SYSTEM
 Last changed: 11/26/2021 9:20:48 AM



Molecular Weight: 274.702

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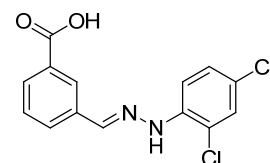


LCMS Report



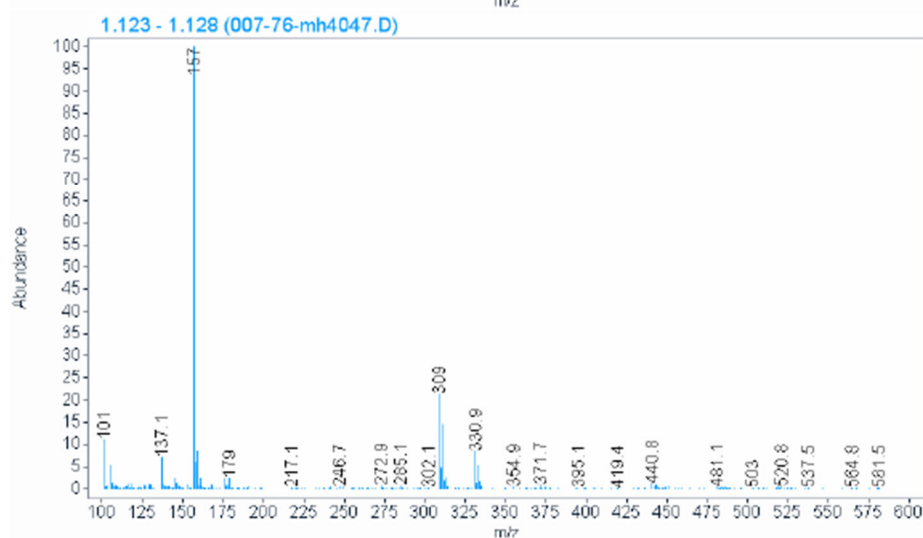
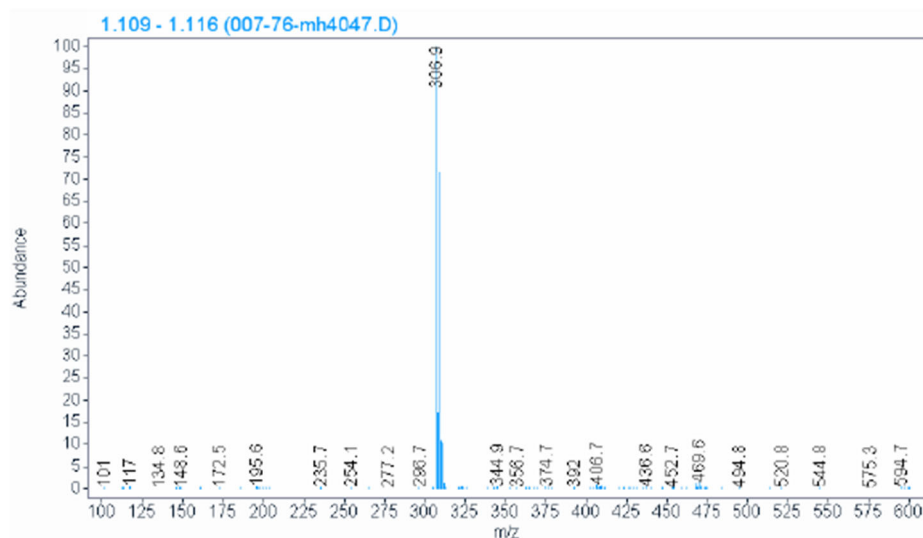
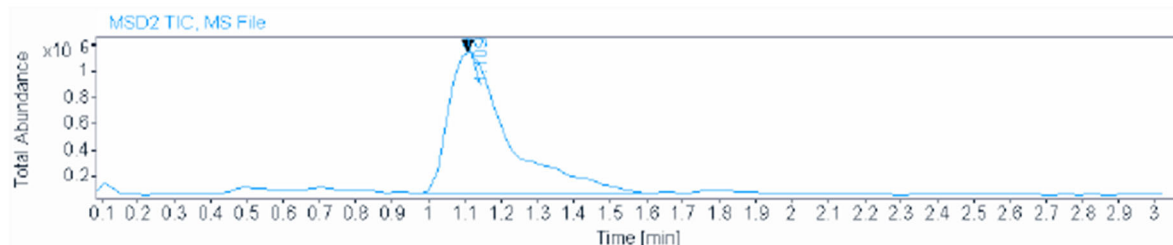
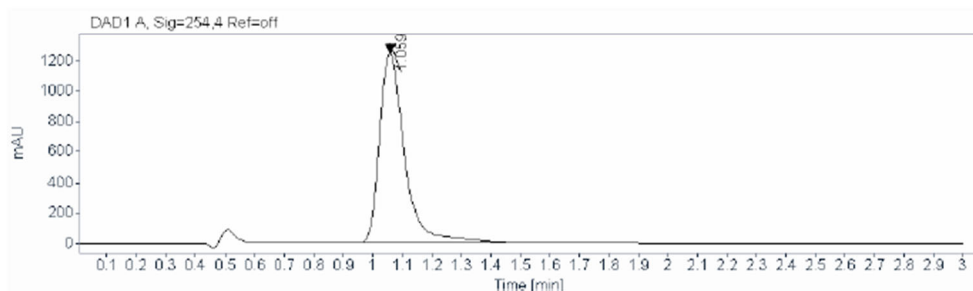
Agilent Technologies

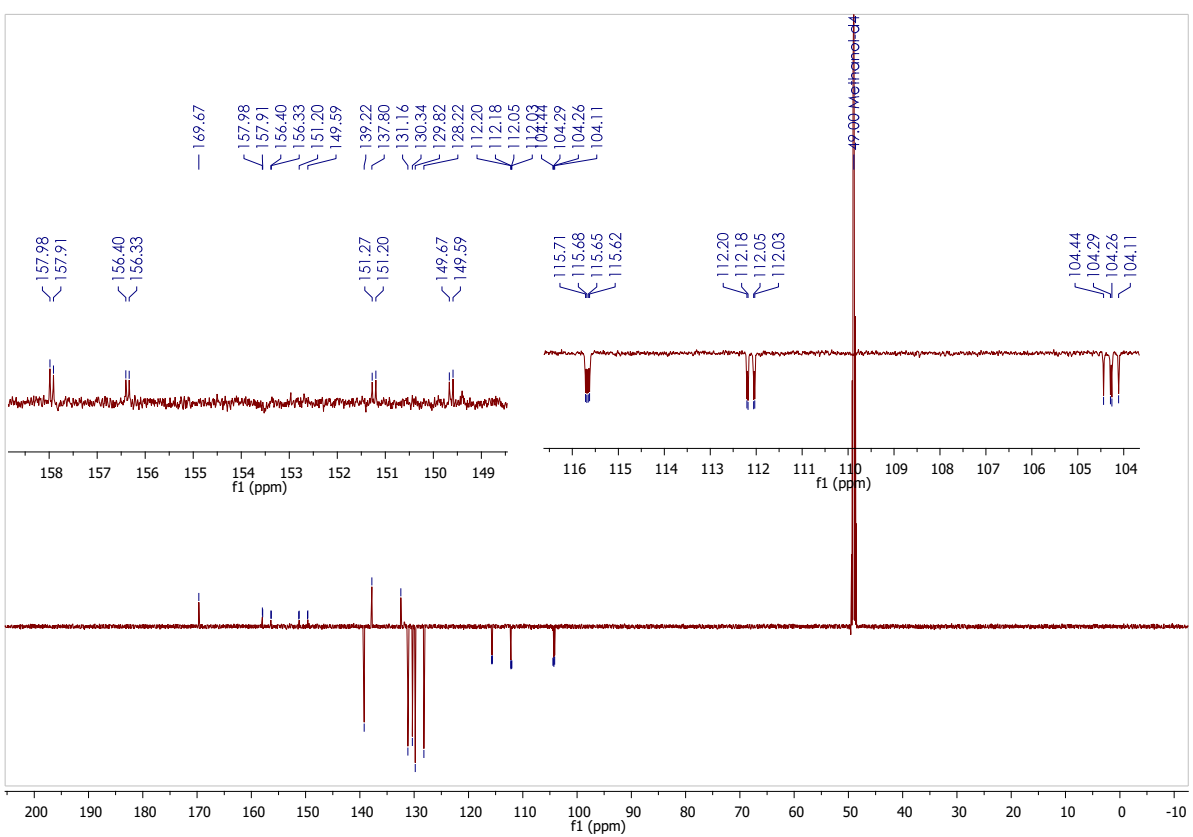
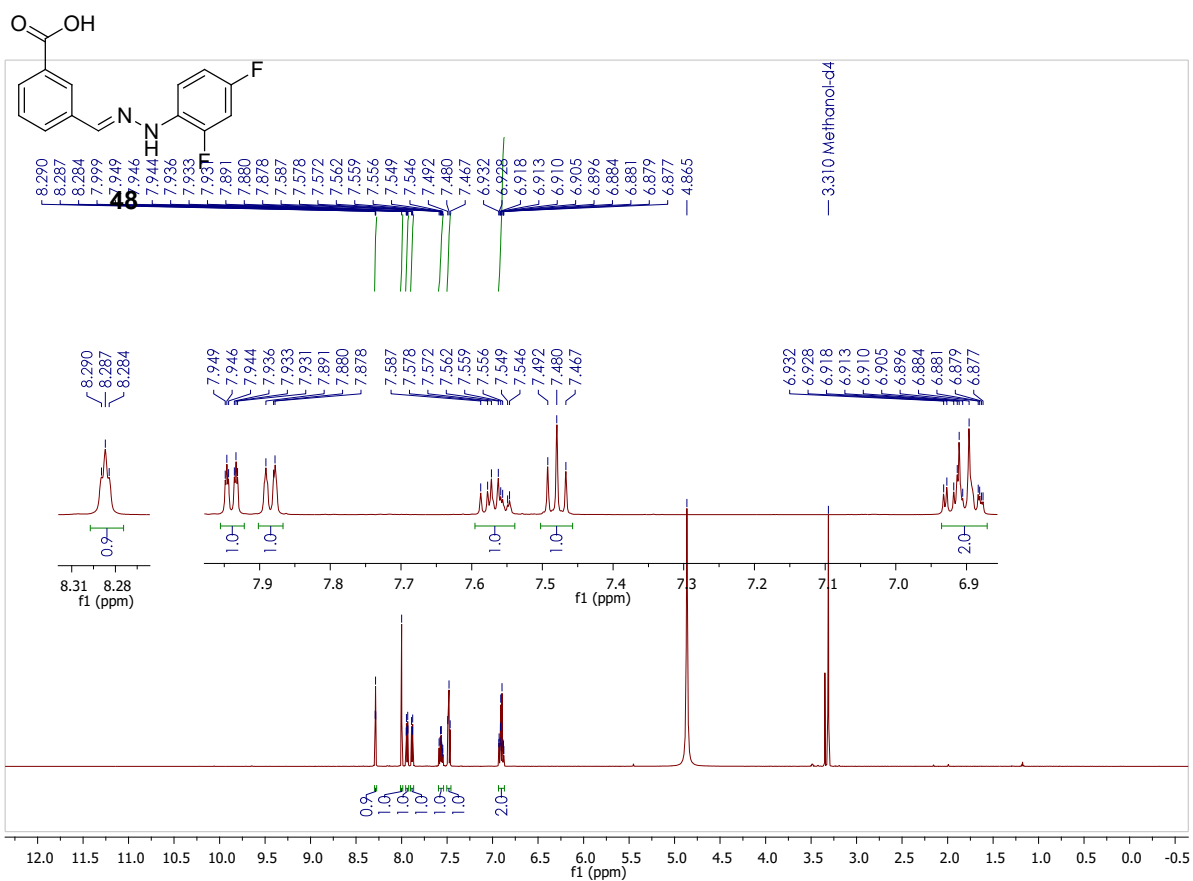
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Sample name: mh4047
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Injection date: 3/23/2022 12:21:03 PM
Acq. method: LCMS ISOCRATIC 80%
B_3 MINS.M
Analysis method: LCMS ISOCRATIC
80%B_3 MINS.M
Last changed: 11/26/2021 9:20:48 AM
Location: 76
Injection: 1 of 1
Injection volume: 2.000
Acq. operator: SYSTEM

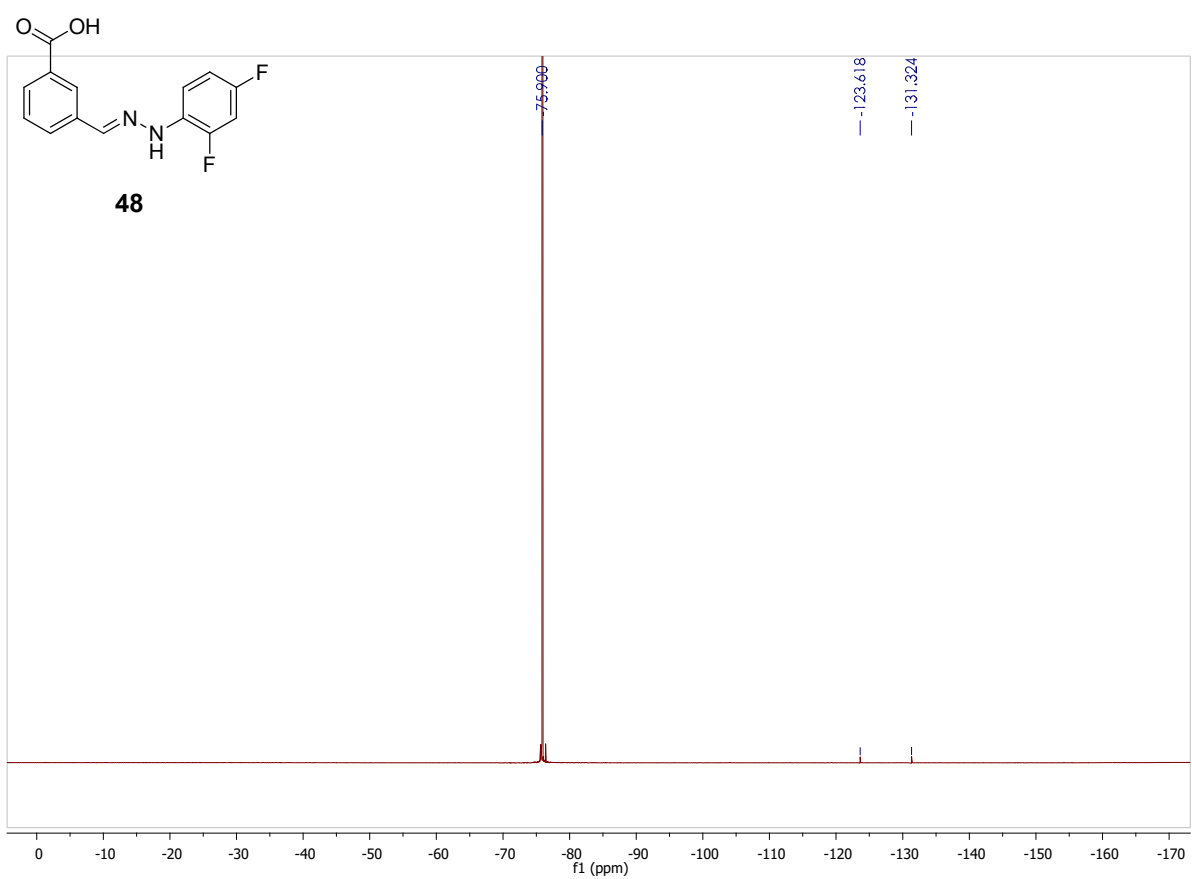


Molecular Weight: 309.147

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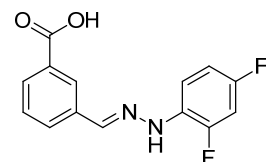


LCMS Report



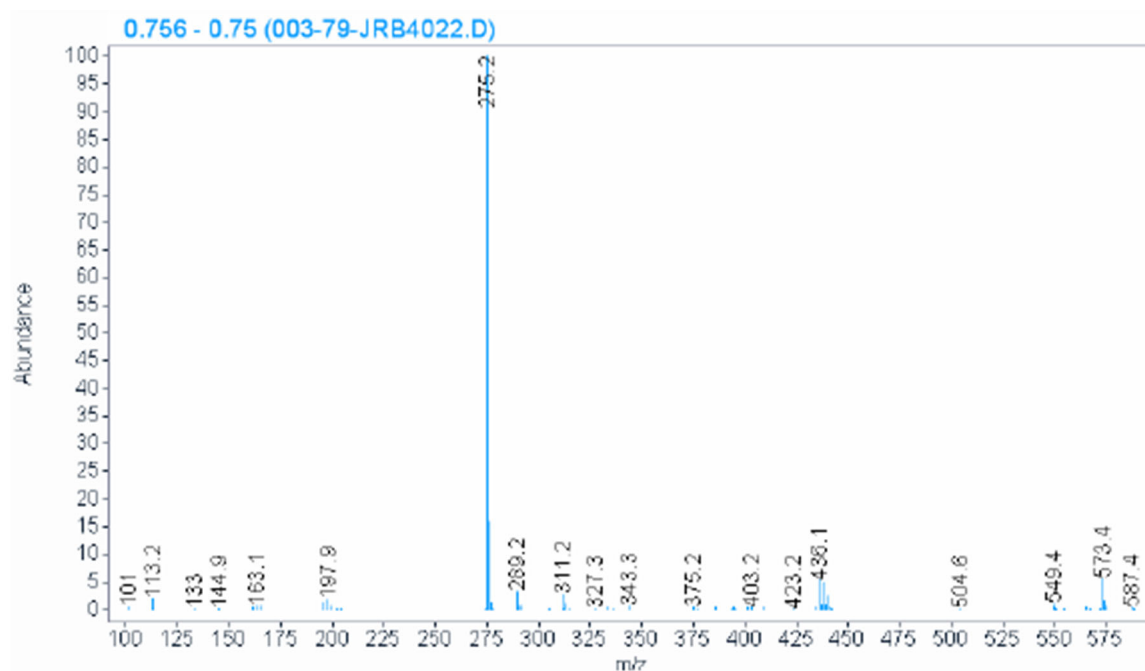
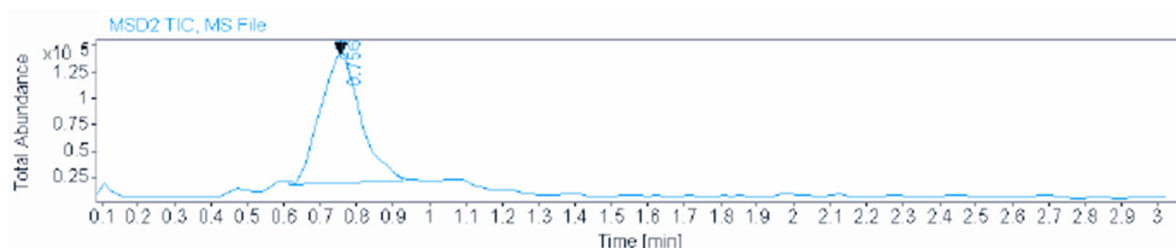
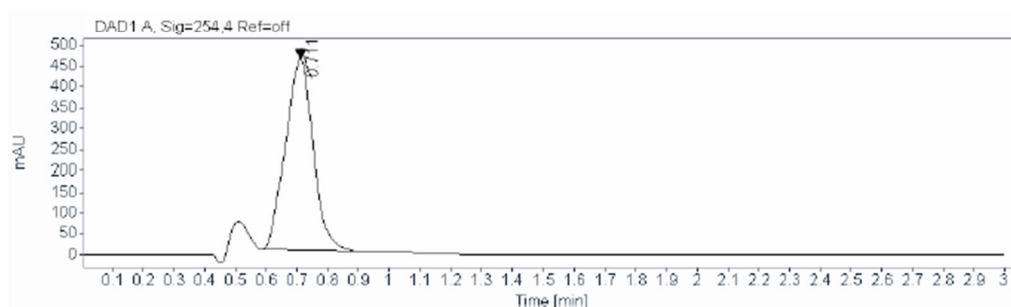
Agilent Technologies

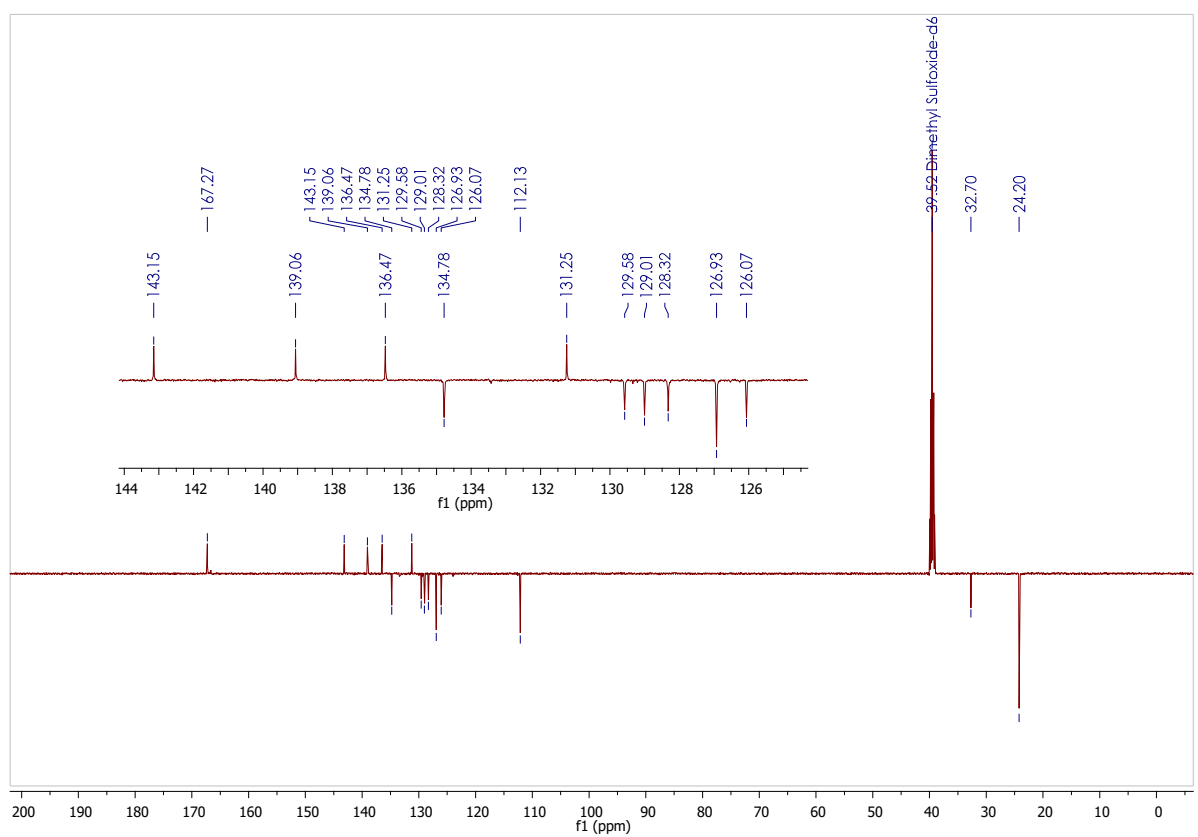
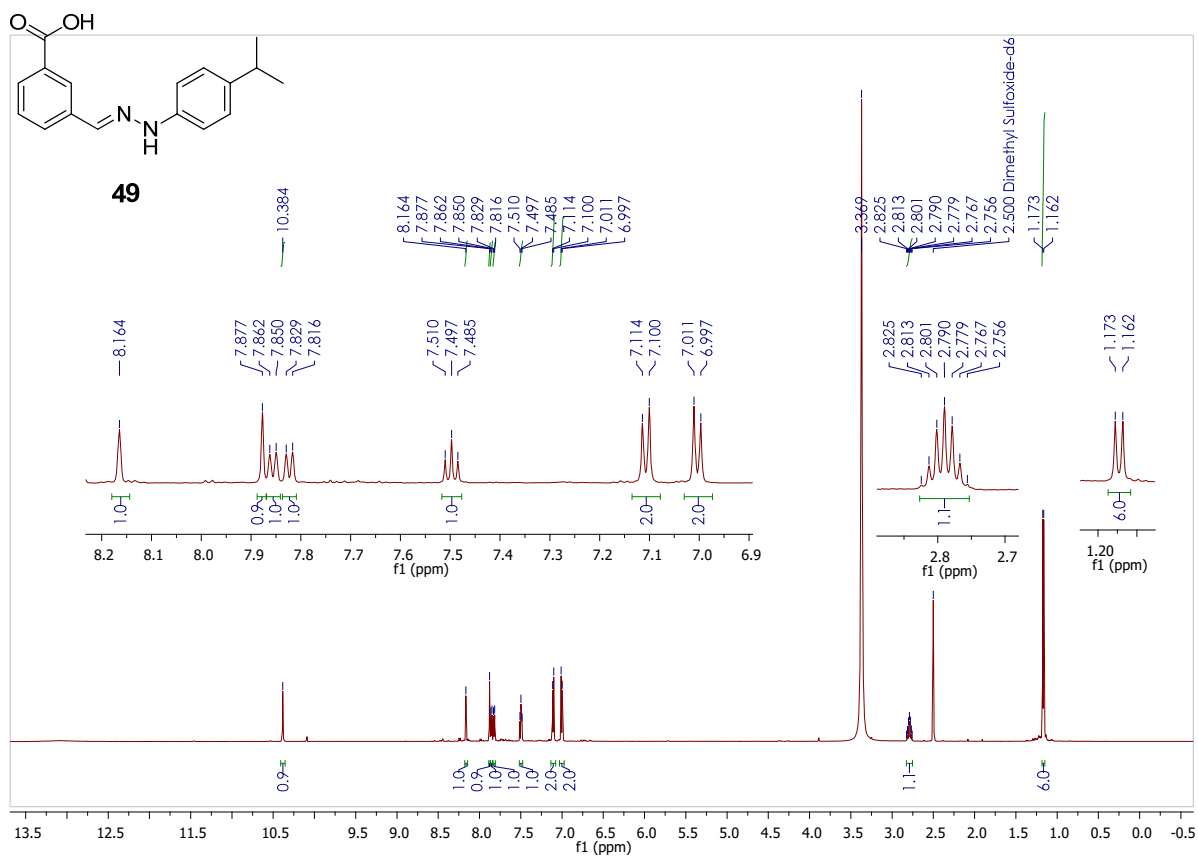
Data file: D:\Chem32\1\Data\JRB\JRB4019 4022 4023B 4024 2023-07-24 14-54-21\003-79-JRB4022.D
Sample name: JRB4022
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Injection date: 7/24/2023 3:05:49 PM
Acq. method: LCMS ISOCRATIC 80%
B_3 MINS.M
Analysis method: LCMS ISOCRATIC
80%B_3 MINS.M
Last changed: 11/26/2021 9:20:48 AM
Location: 79
Injection: 1 of 1
Injection volume: 2.000
Acq. operator: SYSTEM



Molecular Weight: 276.238

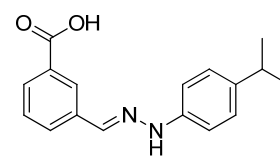
48





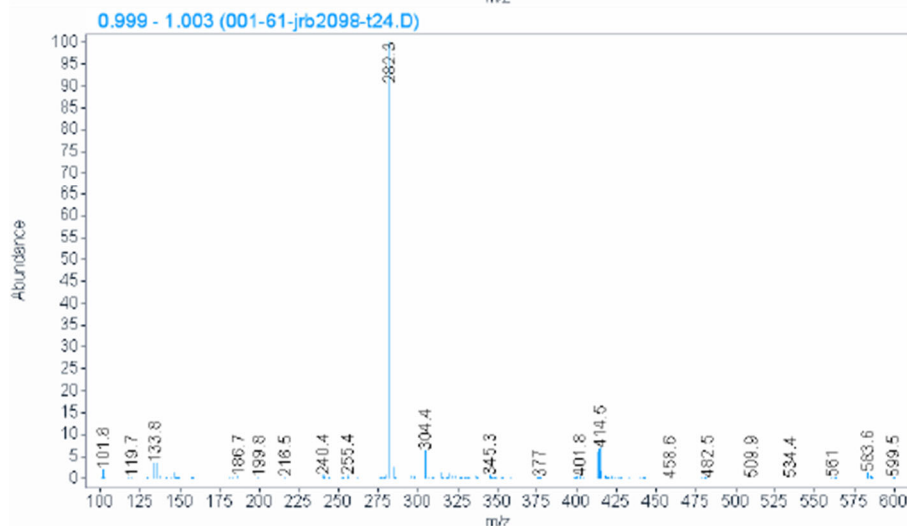
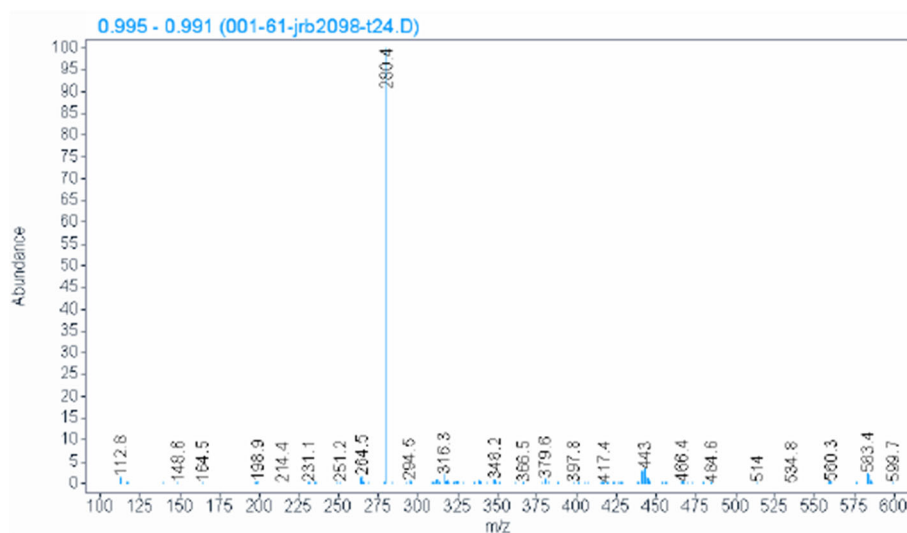
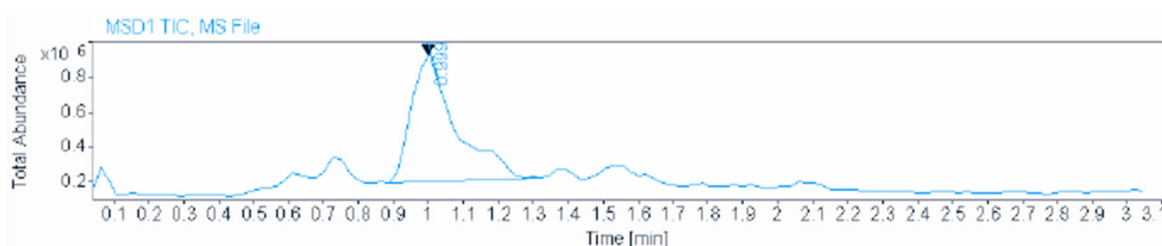
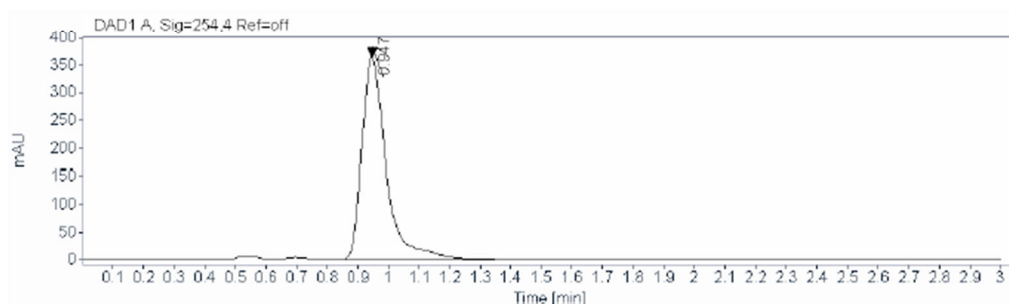


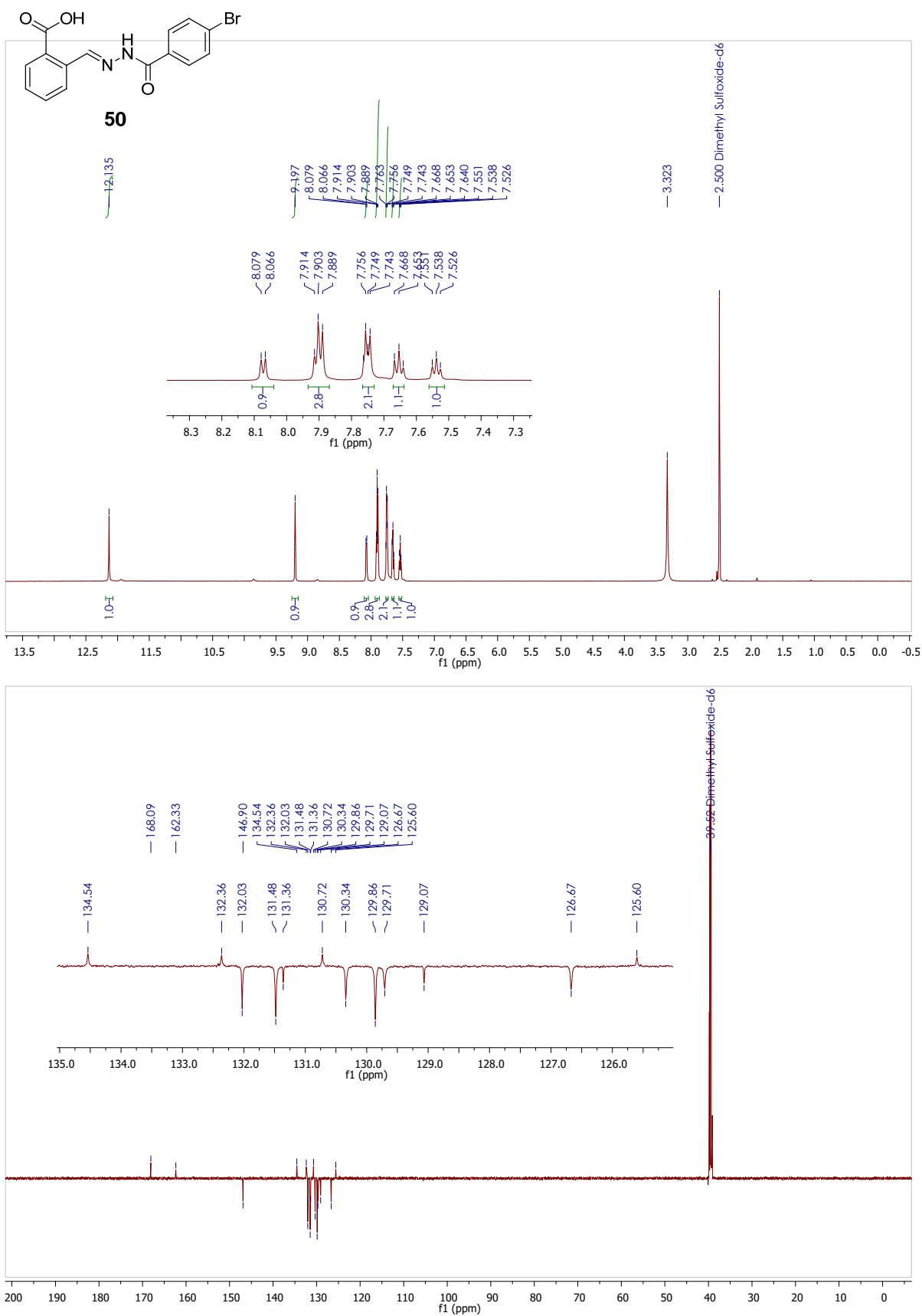
Data file: D:\Chem32\1\Data\JRB\Pre-April 2022\JRB2098-T24 2022-02-11 11:45-51\001-61-jrb2098-t24.D
 Sample name: jrb2098-t24
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 61
 Injection date: 2/11/2022 11:47:32 AM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80% B_3 MINS.M
 Injection volume: 2.000
 Analysis method: LCMS ISOCRATIC 80%B_3 MINS.M
 Acq. operator: SYSTEM
 Last changed: 11/26/2021 9:20:48 AM



Molecular Weight: 282.337

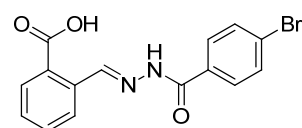
49





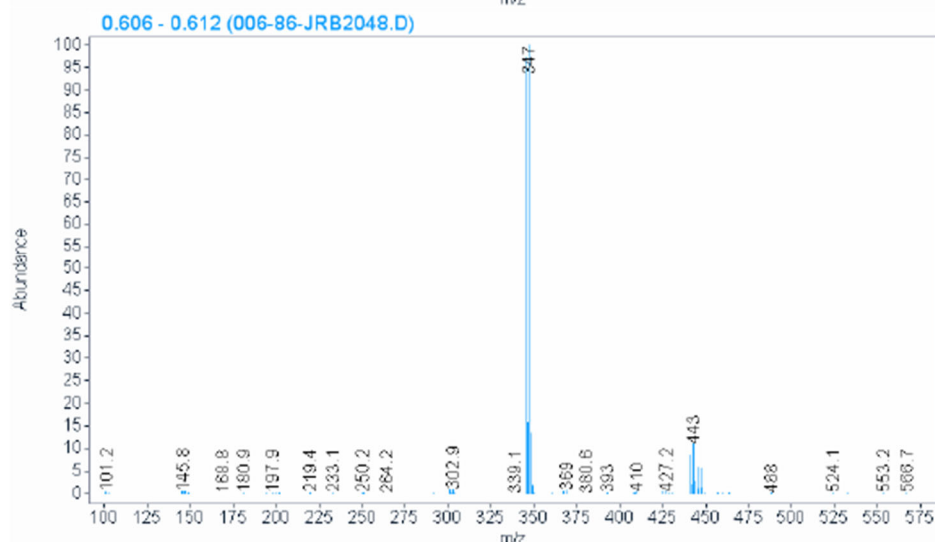
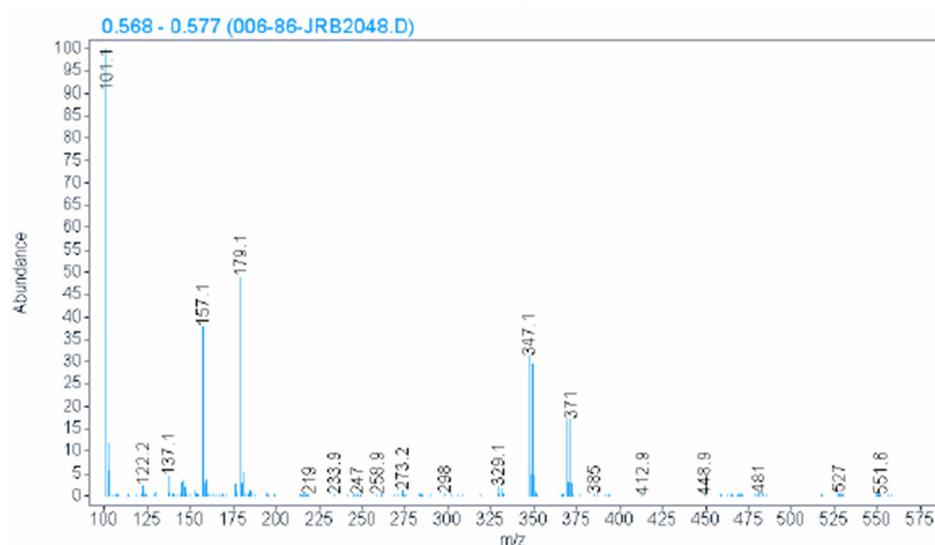
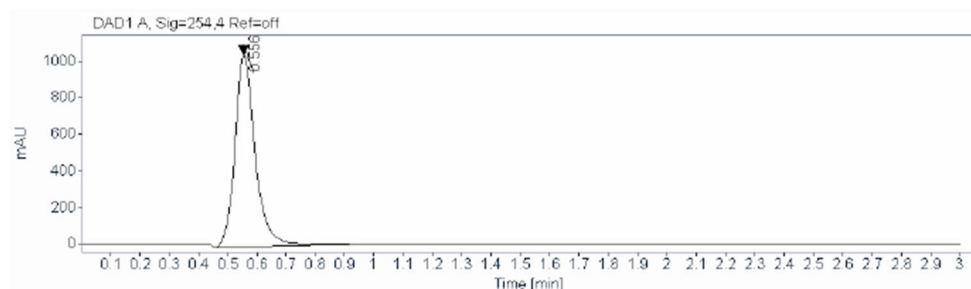


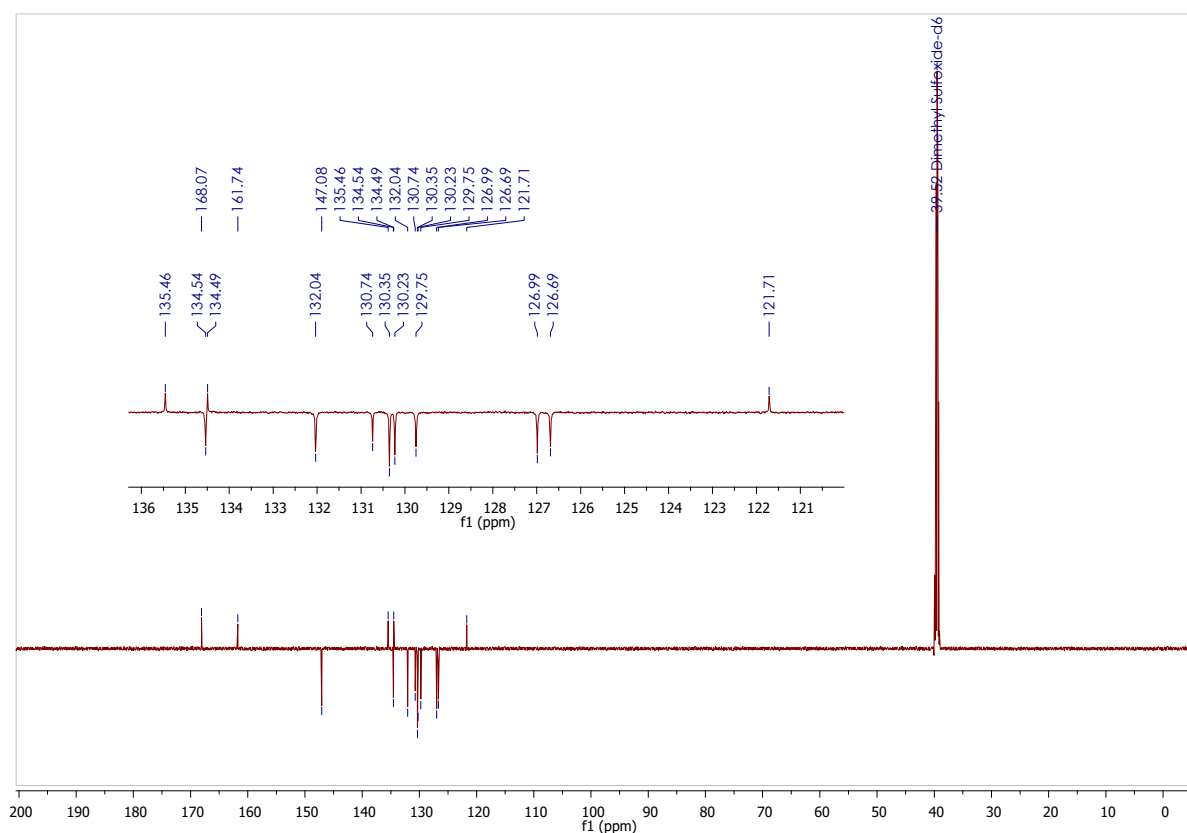
Data file: D:\Chem32\1\Data\JRB\JRB2030 2035 2048_AJS1017 2021-12-03 09-05-12\006-86-JRB2048.D
Sample name: JRB2048
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Location: 86
Injection date: 12/3/2021 9:30:05 AM
Injection: 1 of 1
Acq. method: LCMS ISOCRATIC 80%
Injection volume: 2.000
B_3 MINS.M
Analysis method: LCMS ISOCRATIC
Acq. operator: SYSTEM
80%B_3 MINS.M
Last changed: 11/26/2021 9:20:48 AM



Molecular Weight: 347.163

50





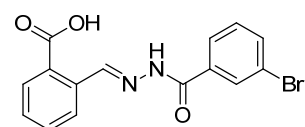
LCMS Report



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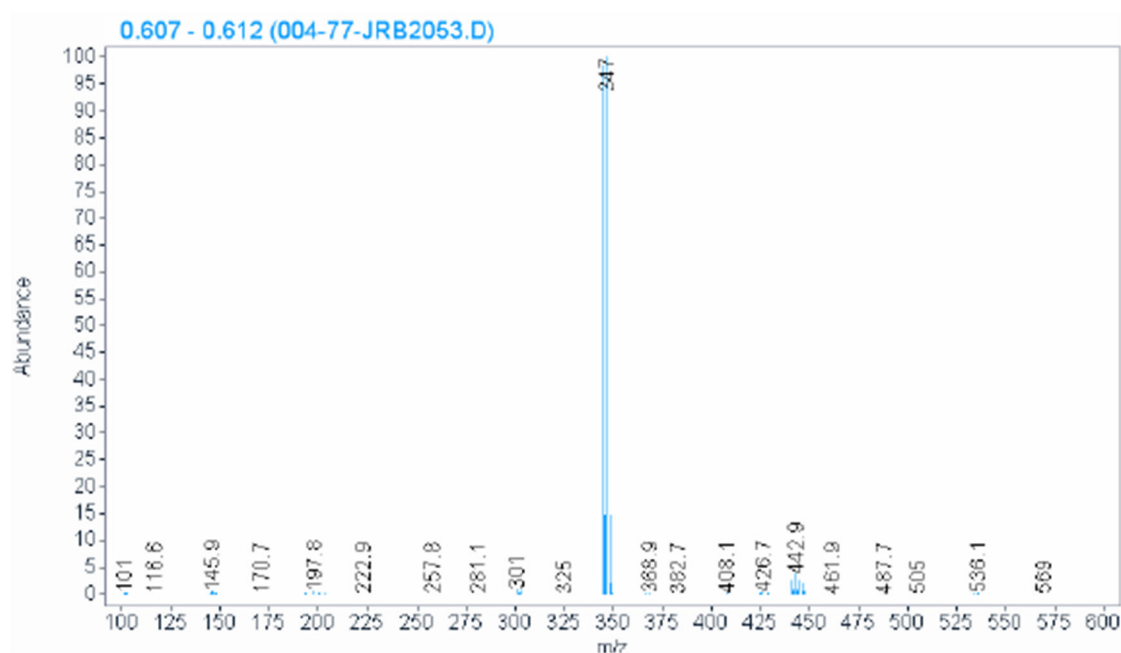
Data file: D:\Chem32\1\Data\JRB\JRB2050-2055 2021-12-03 09-45-10\004-77-JRB2053.D
 Sample name: JRB2053
 Description:
 Sample amount: 0.000
 Instrument: LCMS
 Injection date: 12/3/2021 10:01:06 AM
 Acq. method: LCMS ISOCRATIC 80%
 B_3 MINS.M
 Analysis method: LCMS ISOCRATIC
 80%B_3 MINS.M
 Last changed: 11/26/2021 9:20:48 AM

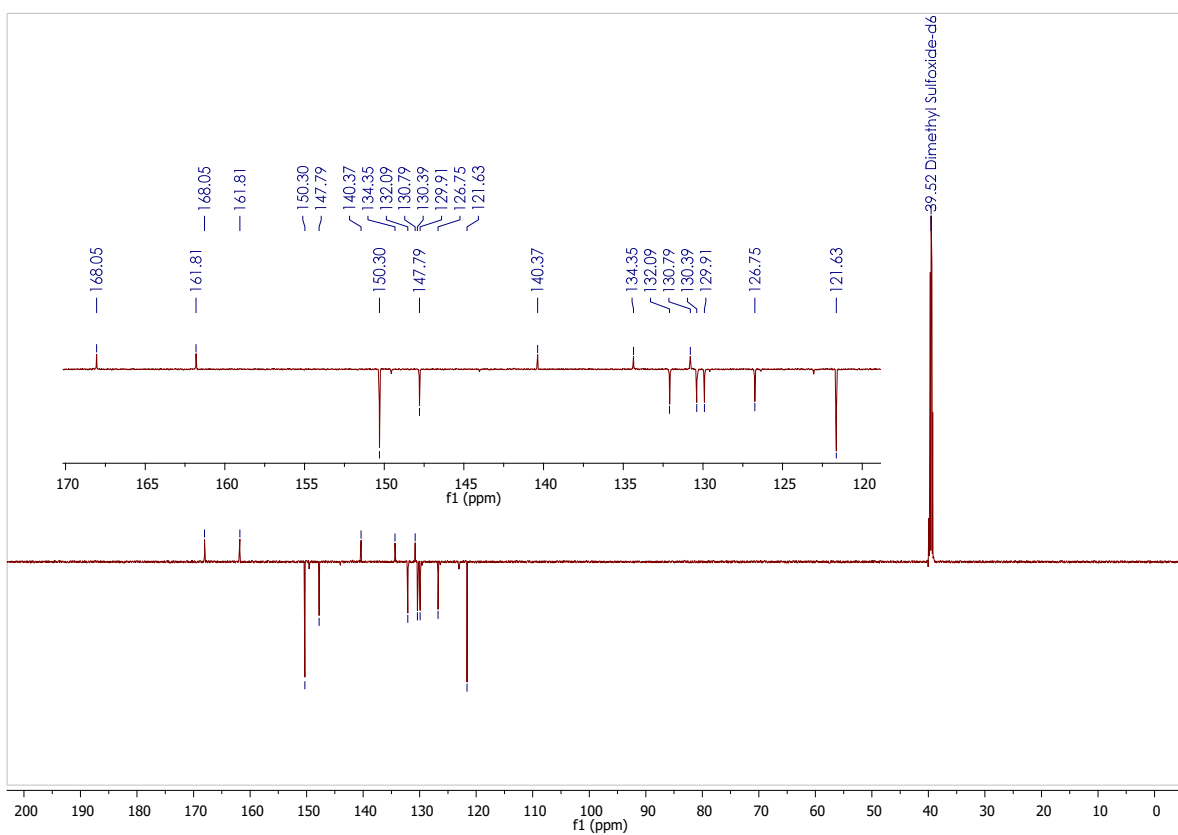
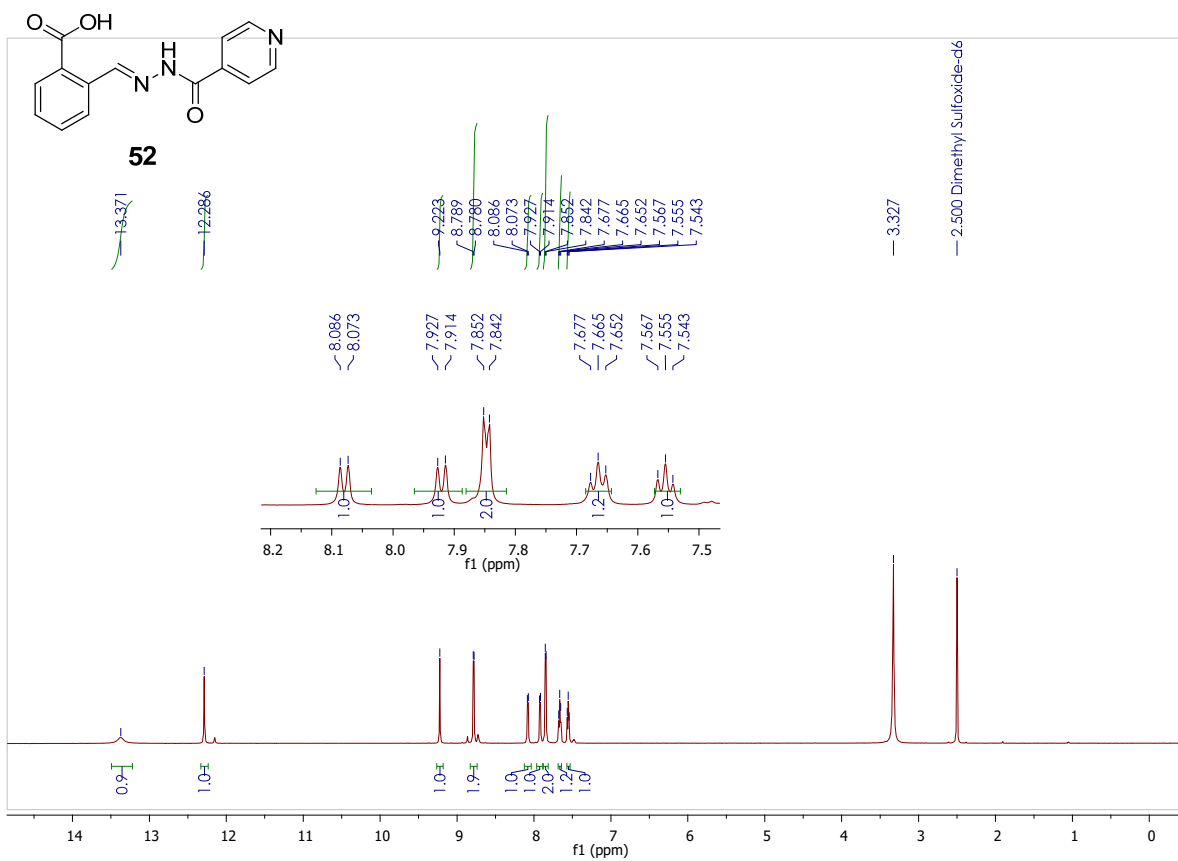
Sample type: Sample
 Location: 77
 Injection: 1 of 1
 Injection volume: 2.000
 Acq. operator: SYSTEM



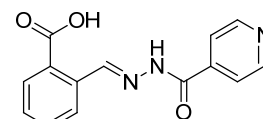
Molecular Weight: 347.163

51



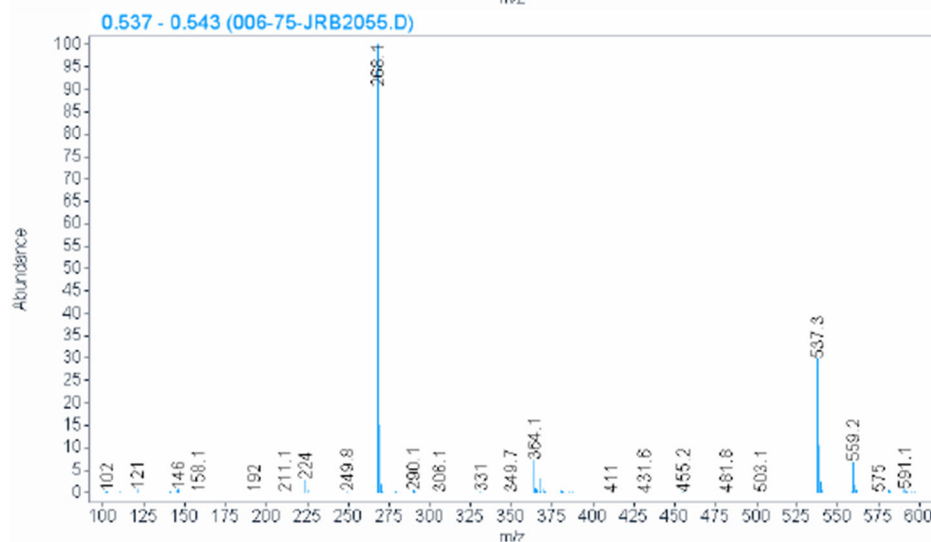
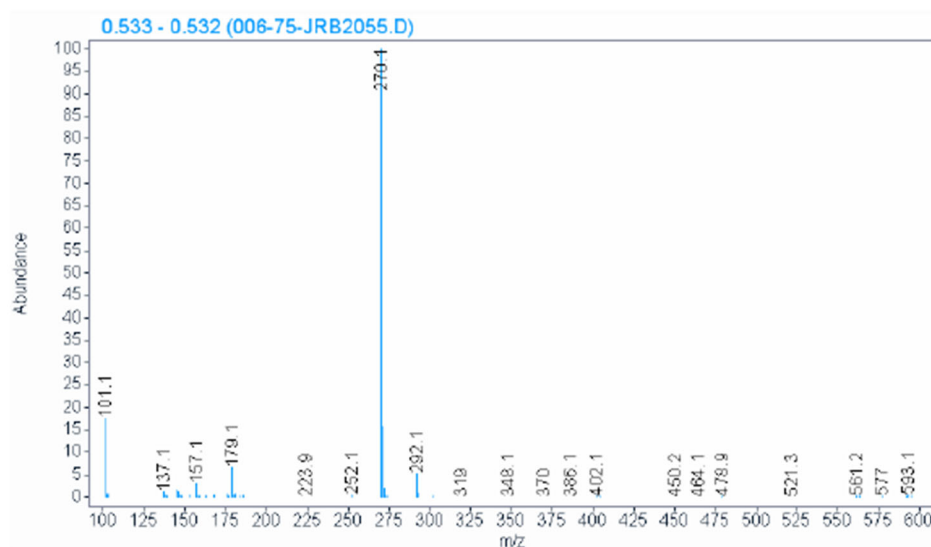
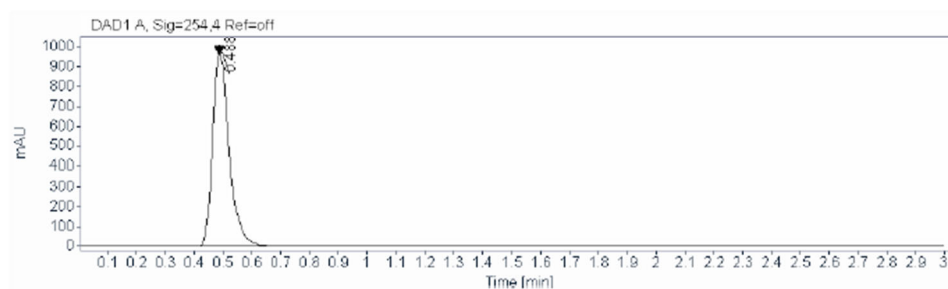


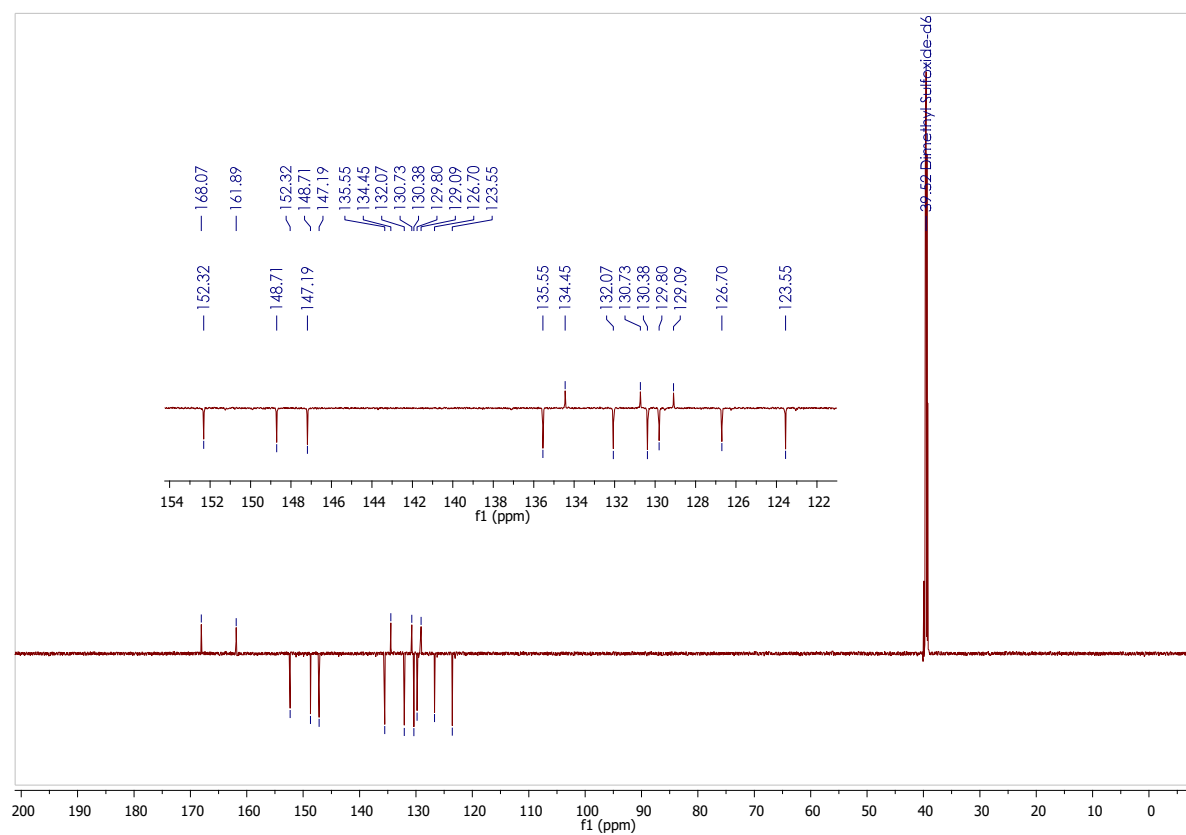
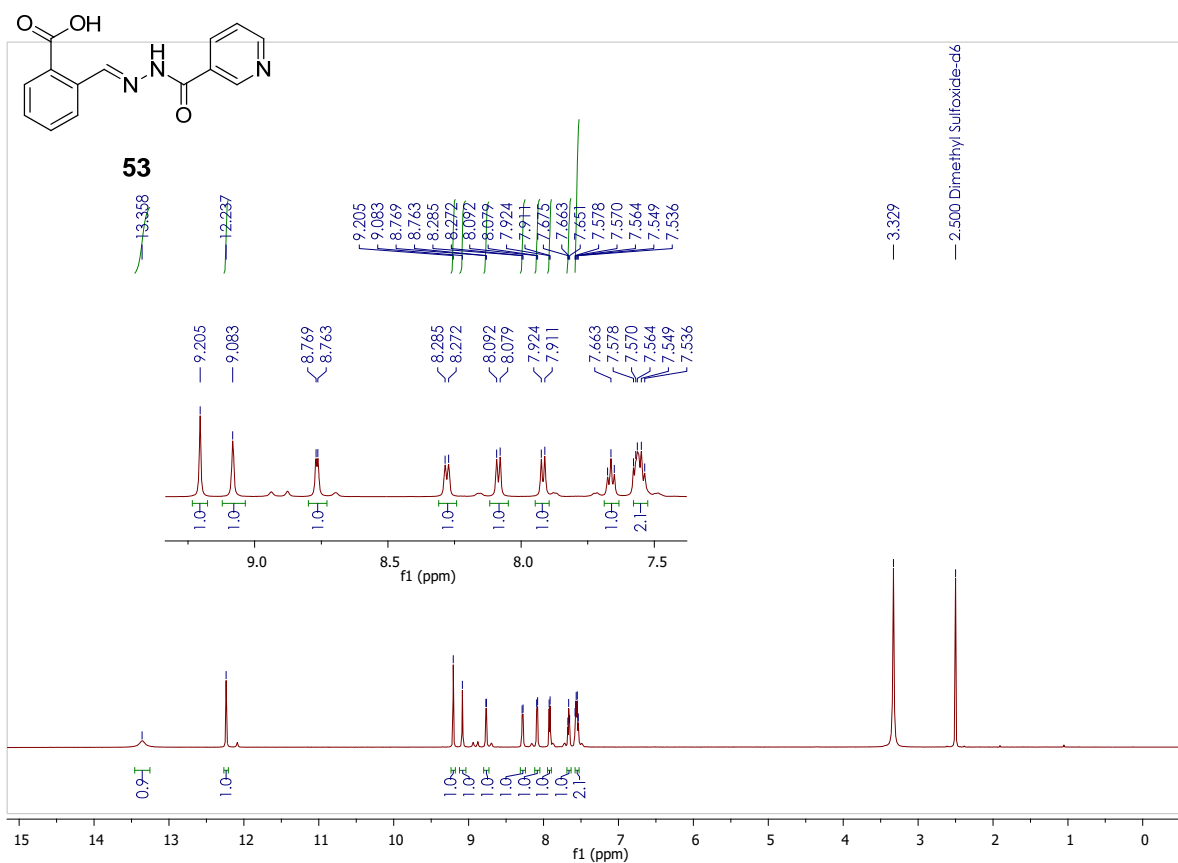
Data file: D:\Chem32\11\Data\JRB\JRB2050-2055 2021-12-03 09-45-10\006-75-JRB2055.D
Sample name: JRB2055
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Injection date: 12/3/2021 10:10:33 AM
Acq. method: LCMS ISOCRATIC 80%
B_3 MINS.M
Analysis method: LCMS ISOCRATIC
80%B_3 MINS.M
Last changed: 11/26/2021 9:20:48 AM
Location: 75
Injection: 1 of 1
Injection volume: 2.000
Acq. operator: SYSTEM



Molecular Weight: 269.255

52



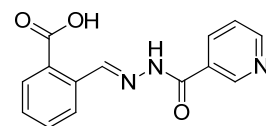


LCMS Report



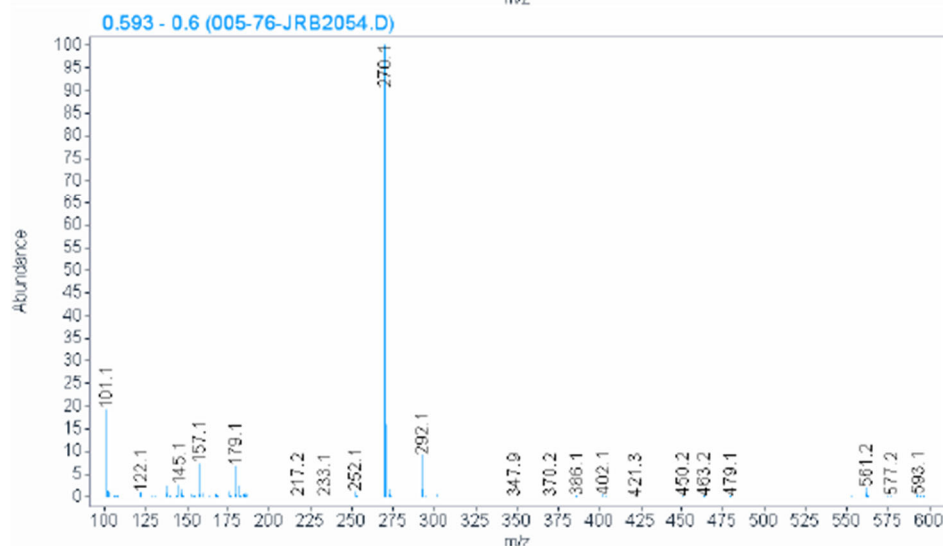
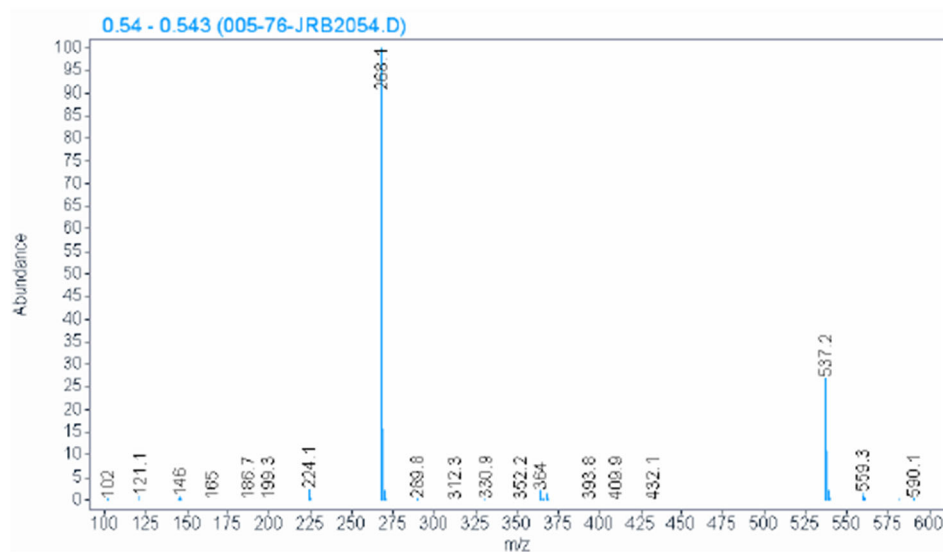
Agilent Technologies

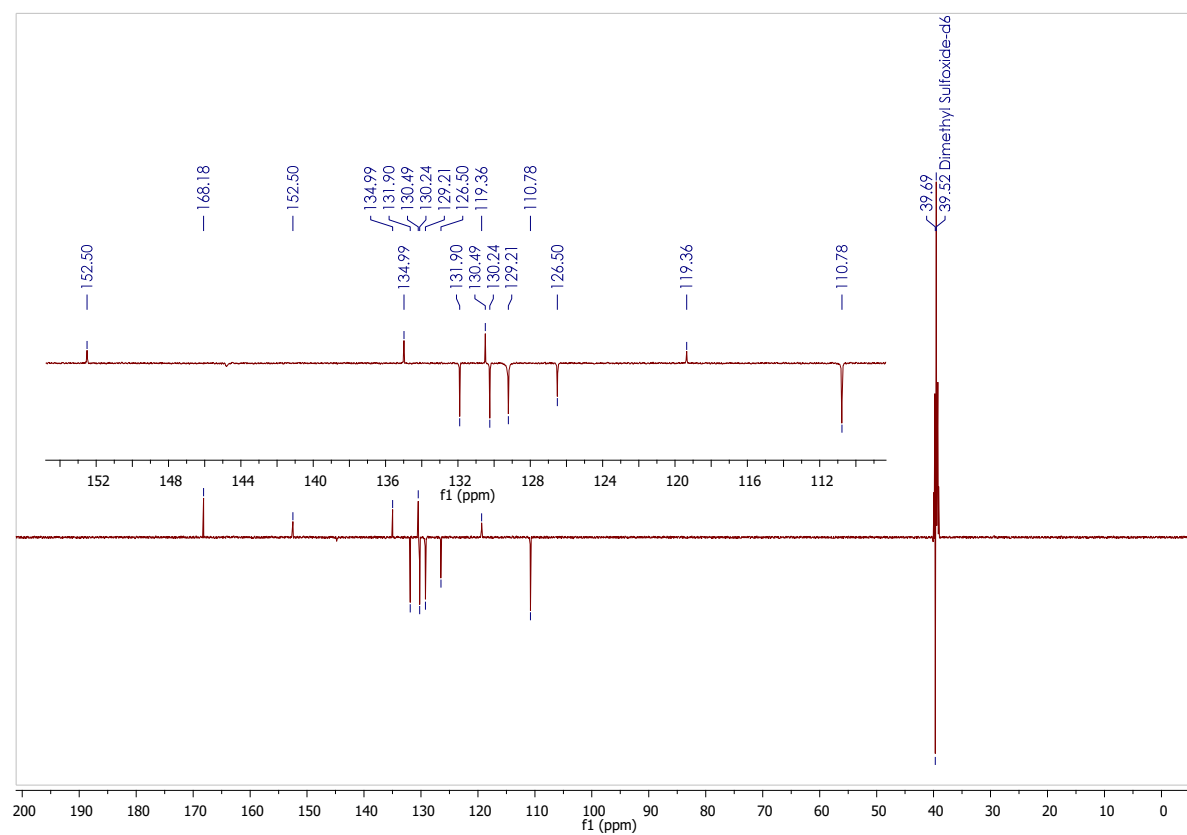
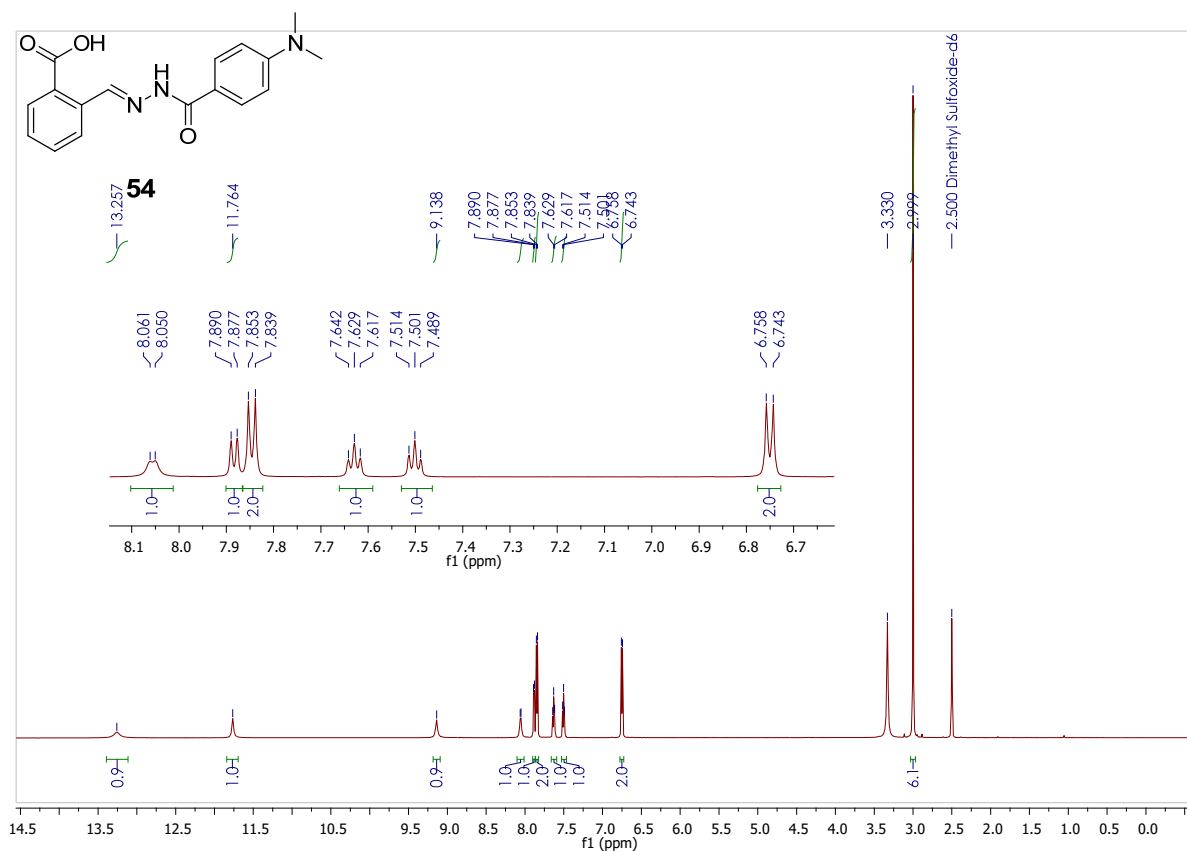
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 Sample name: JRB2054
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 76
 Injection date: 12/3/2021 10:05:48 AM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 Injection volume: 2.000
 B 3 MINS.M
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 80%B_3 MINS.M
 Last changed: 11/26/2021 9:20:48 AM



Molecular Weight: 269.255

53

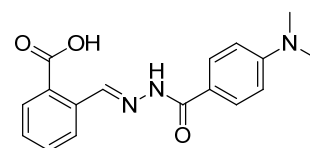




LCMS Report

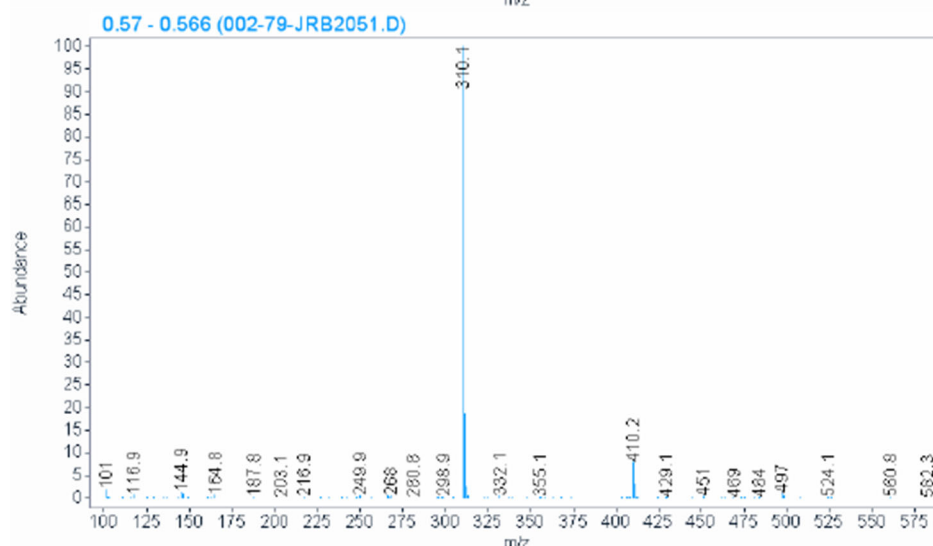
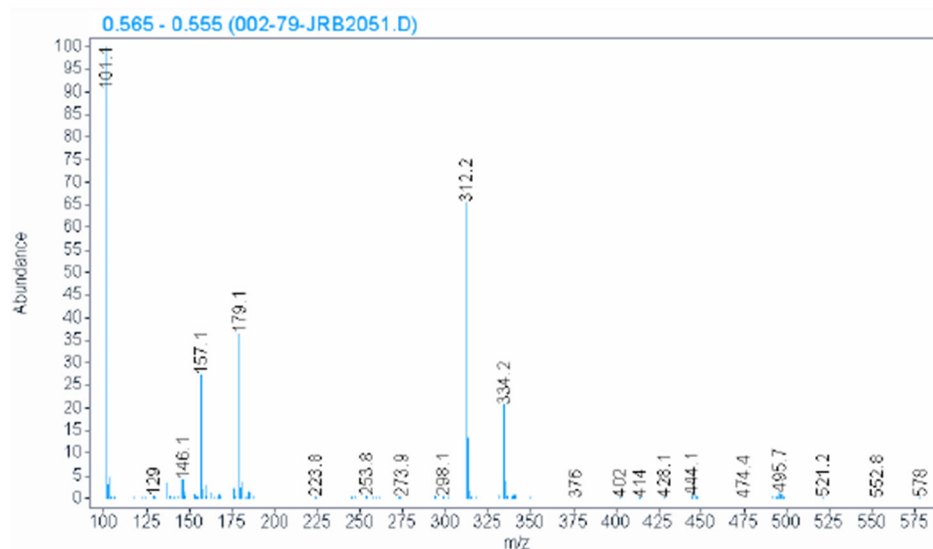
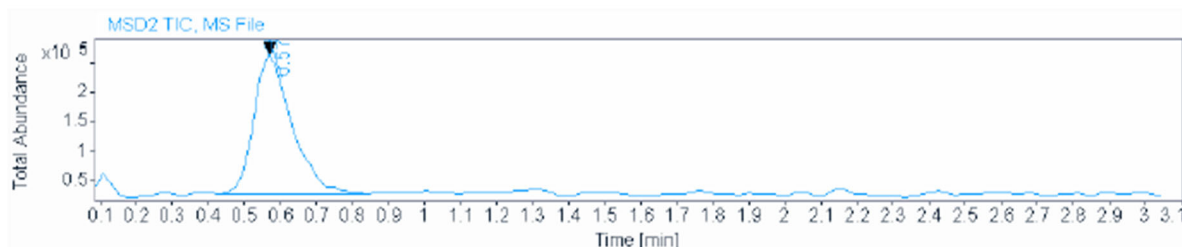
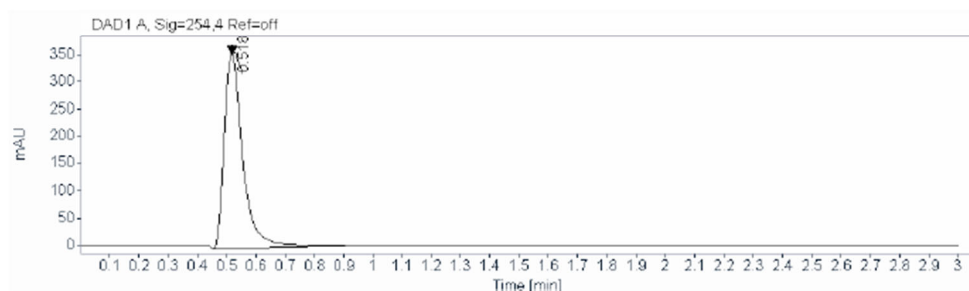


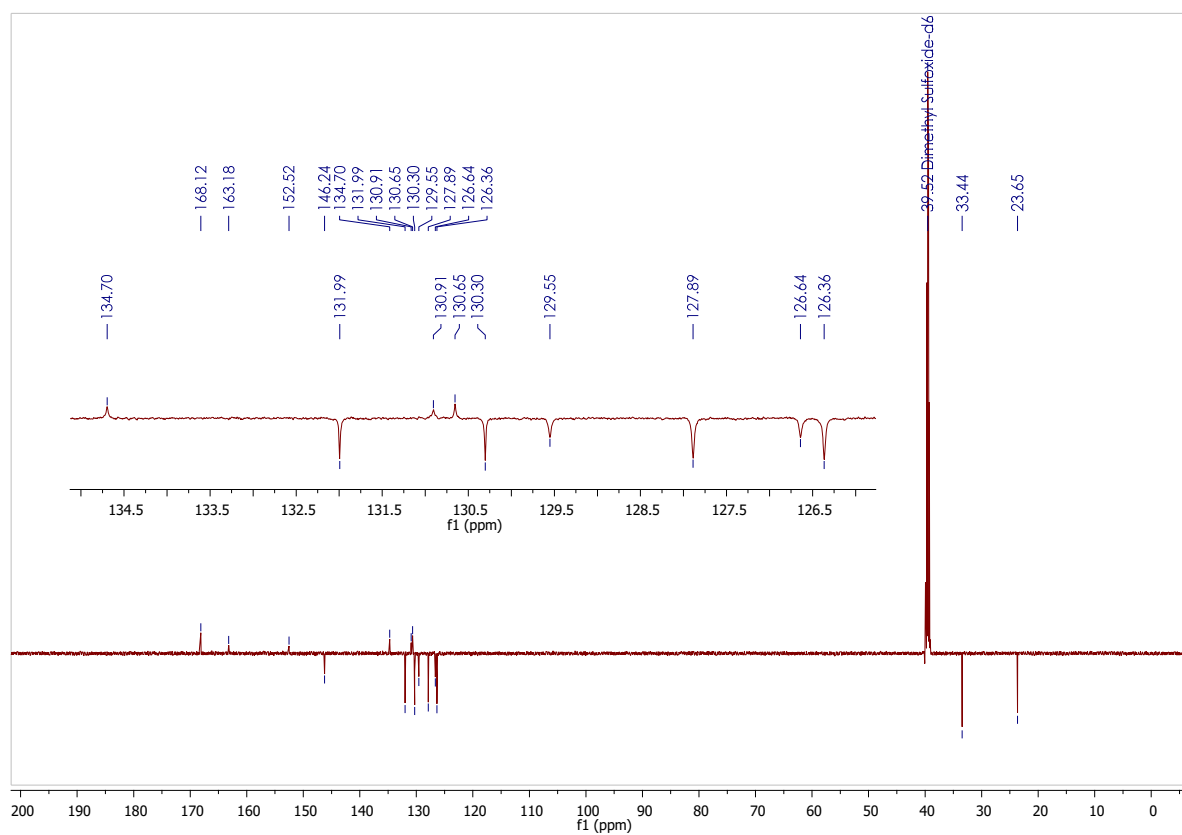
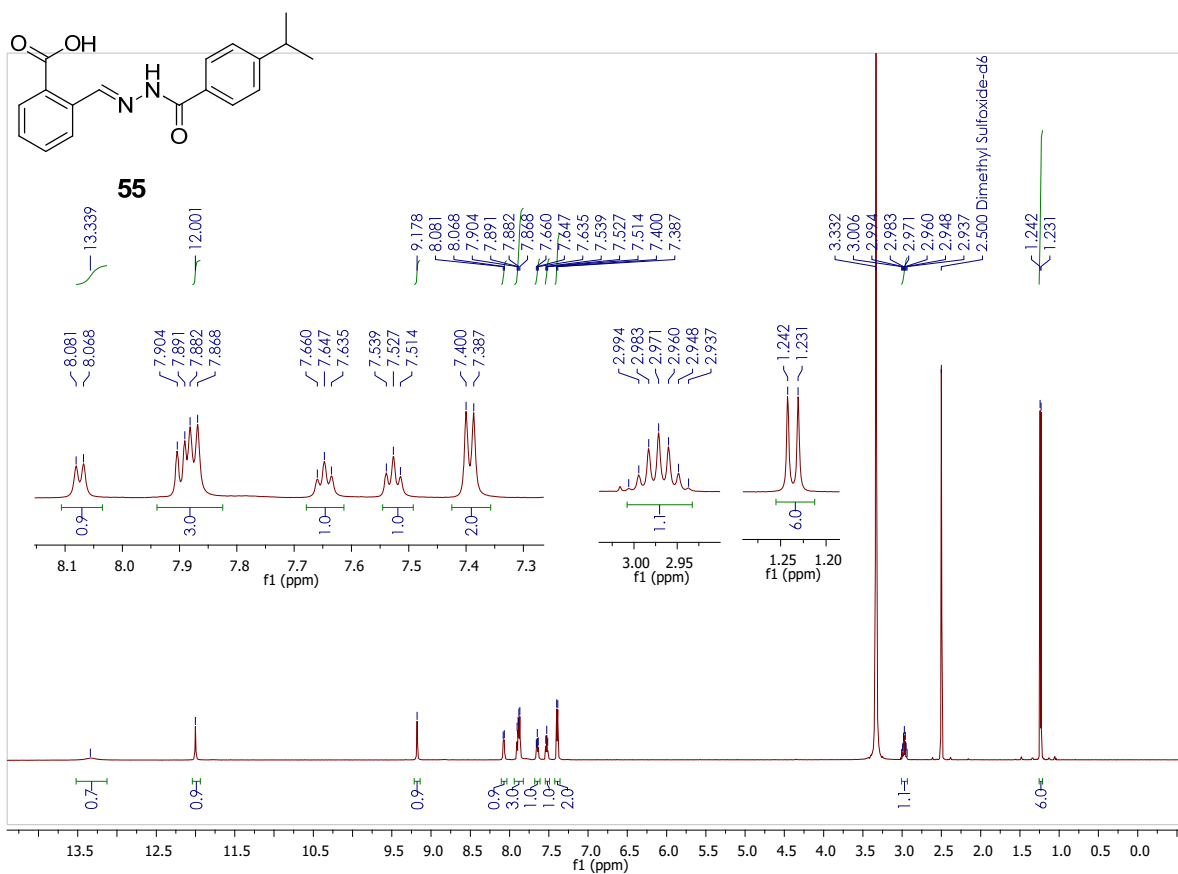
Data file: D:\Chem32\1\Data\JRB\JRB2050-2055 2021-12-03 09-45-10\002-79-JRB2051.D
Sample name: JRB2051
Description:
Sample amount: 0.000
Instrument: LCMS
Injection date: 12/3/2021 9:51:41 AM
Acq. method: LCMS ISOCRATIC 80%
Analysis method: B_3 MINS.M
Last changed: 11/26/2021 9:20:48 AM
Sample type: Sample
Location: 79
Injection: 1 of 1
Injection volume: 2.000
Acq. operator: SYSTEM



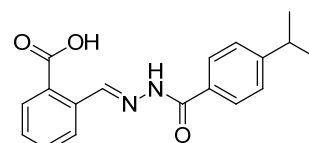
Molecular Weight: 311.335

54



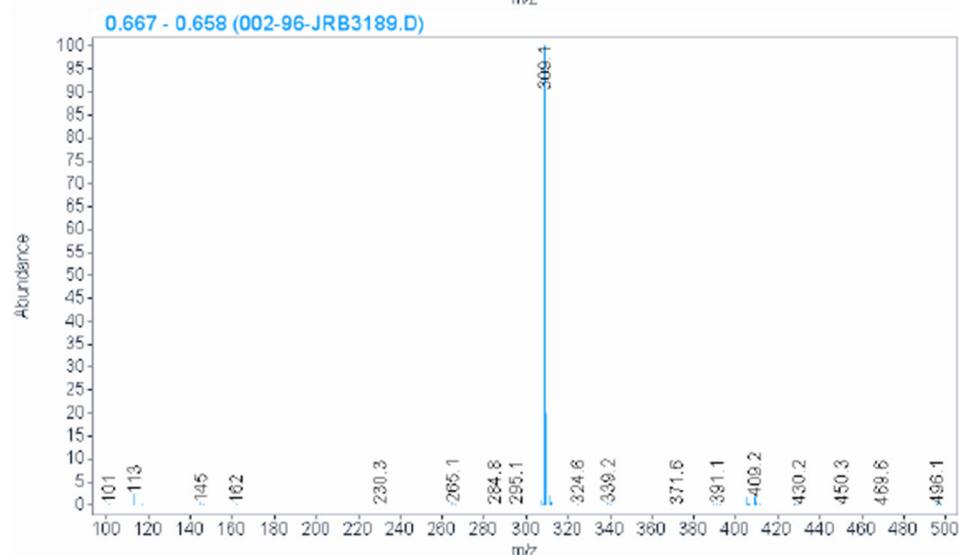
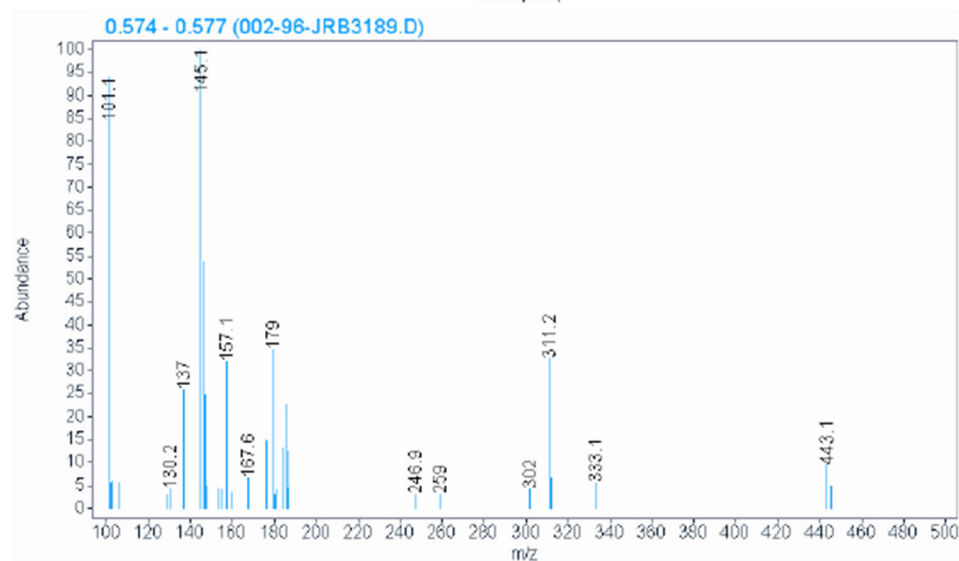
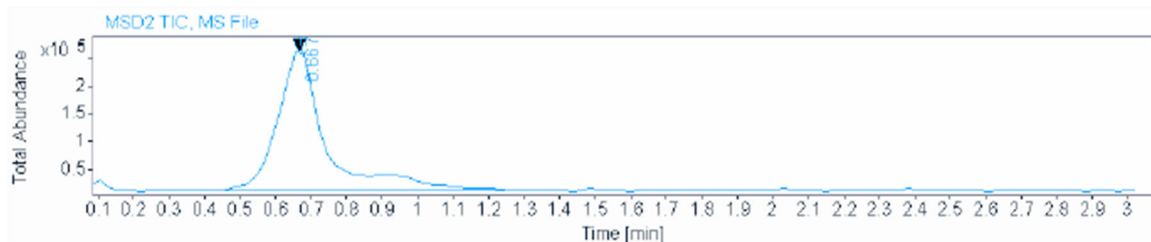
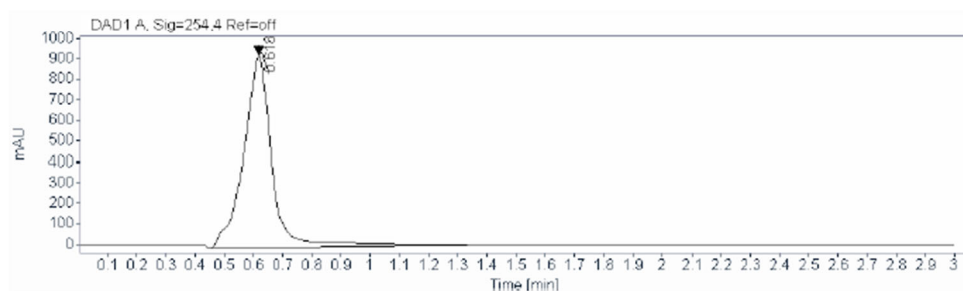


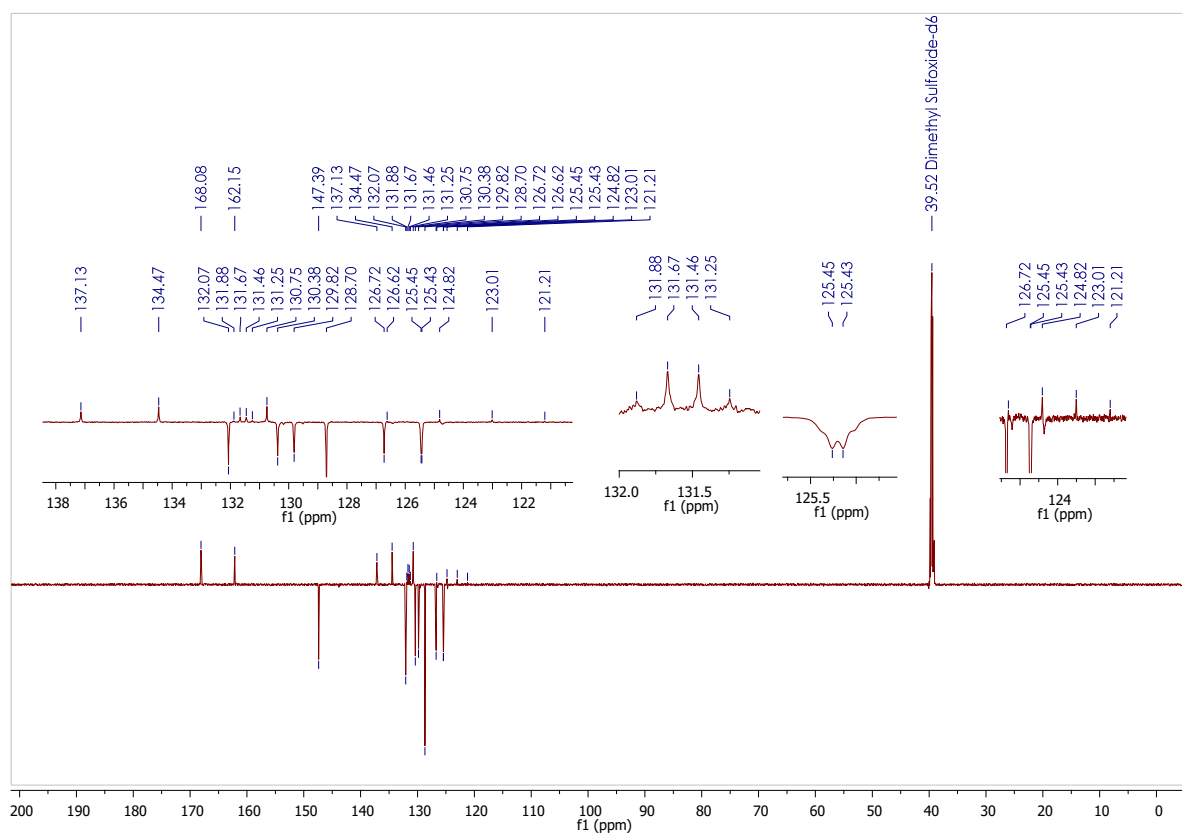
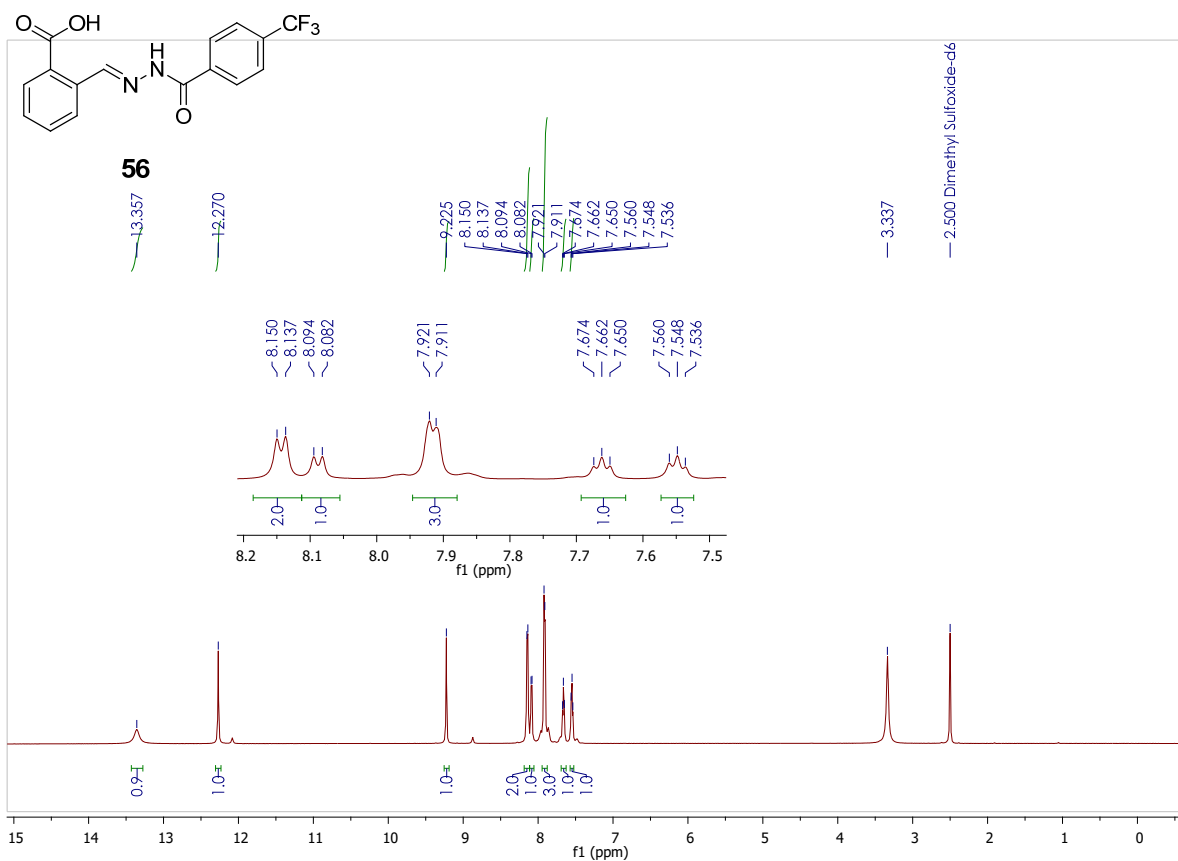
Data file: D:\Chem32\1\Data\JRB\JRB3189 3196 4001 4002 2023-07-24 12-59-52\002-96-JRB3189.D
Sample name: JRB3189
Description:
Sample amount: 0.000
Instrument: LCMS
Injection date: 7/24/2023 1:06:20 PM
Acq. method: LCMS ISOCRATIC 80%
Analysis method: B_3 MINS.M
Last changed: 11/26/2021 9:20:48 AM
Sample type: Sample
Location: 96
Injection: 1 of 1
Injection volume: 2.000
Acq. operator: SYSTEM

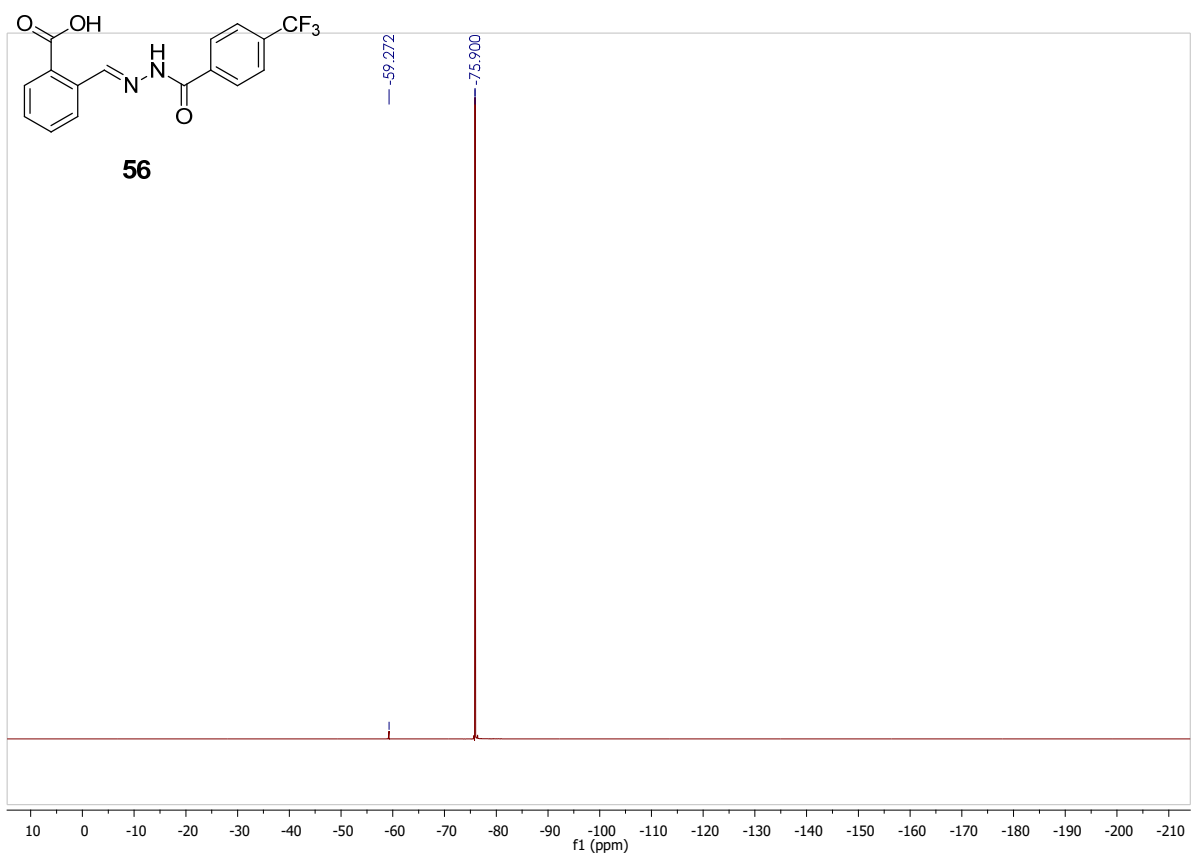


Molecular Weight: 310.347

55





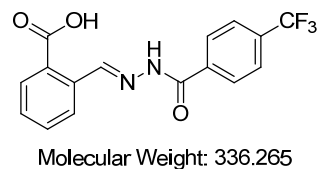


LCMS Report

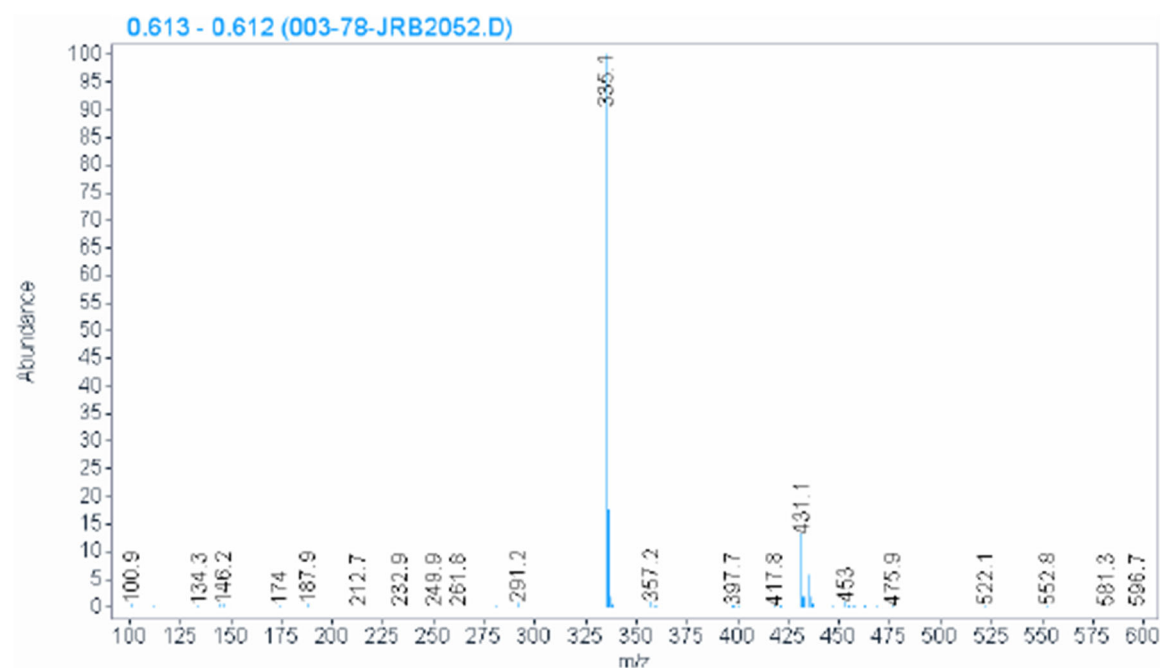
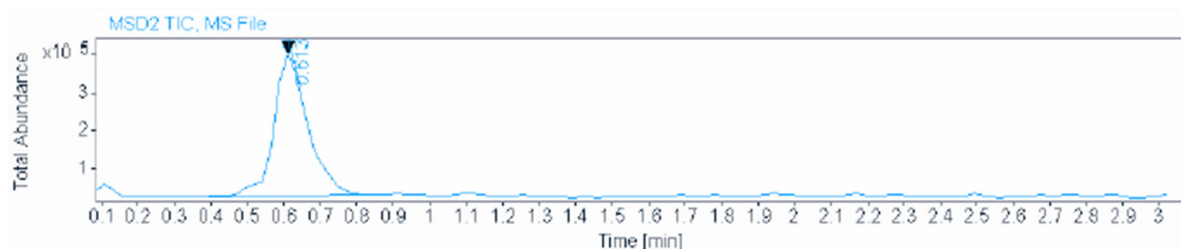
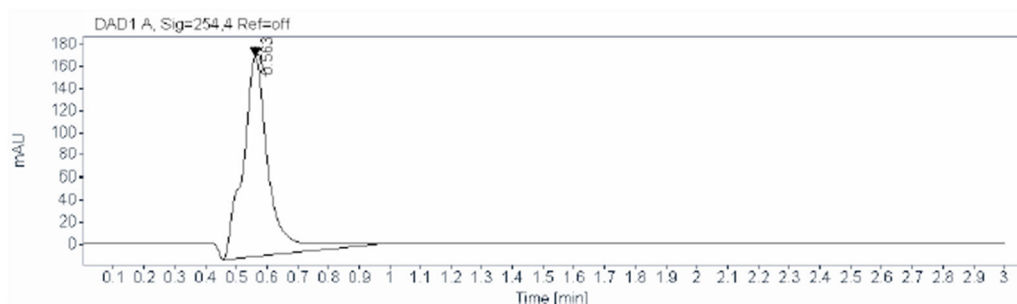


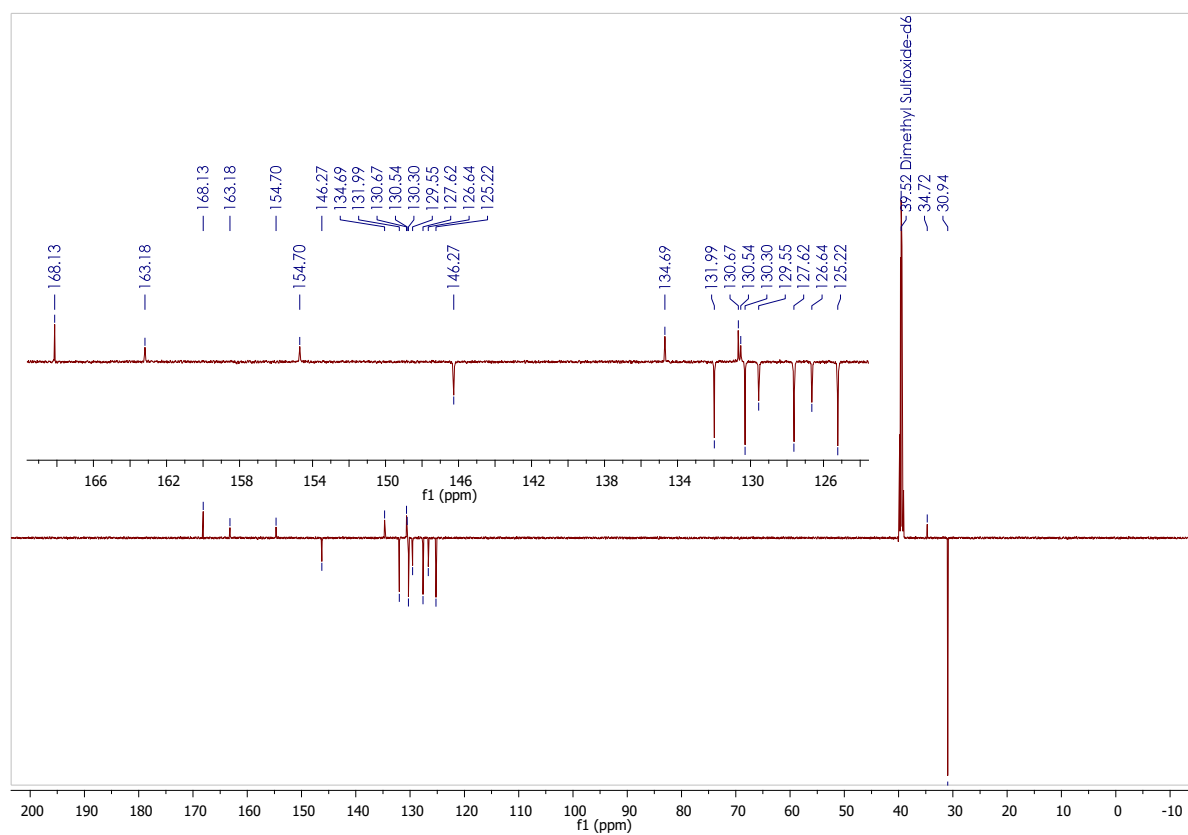
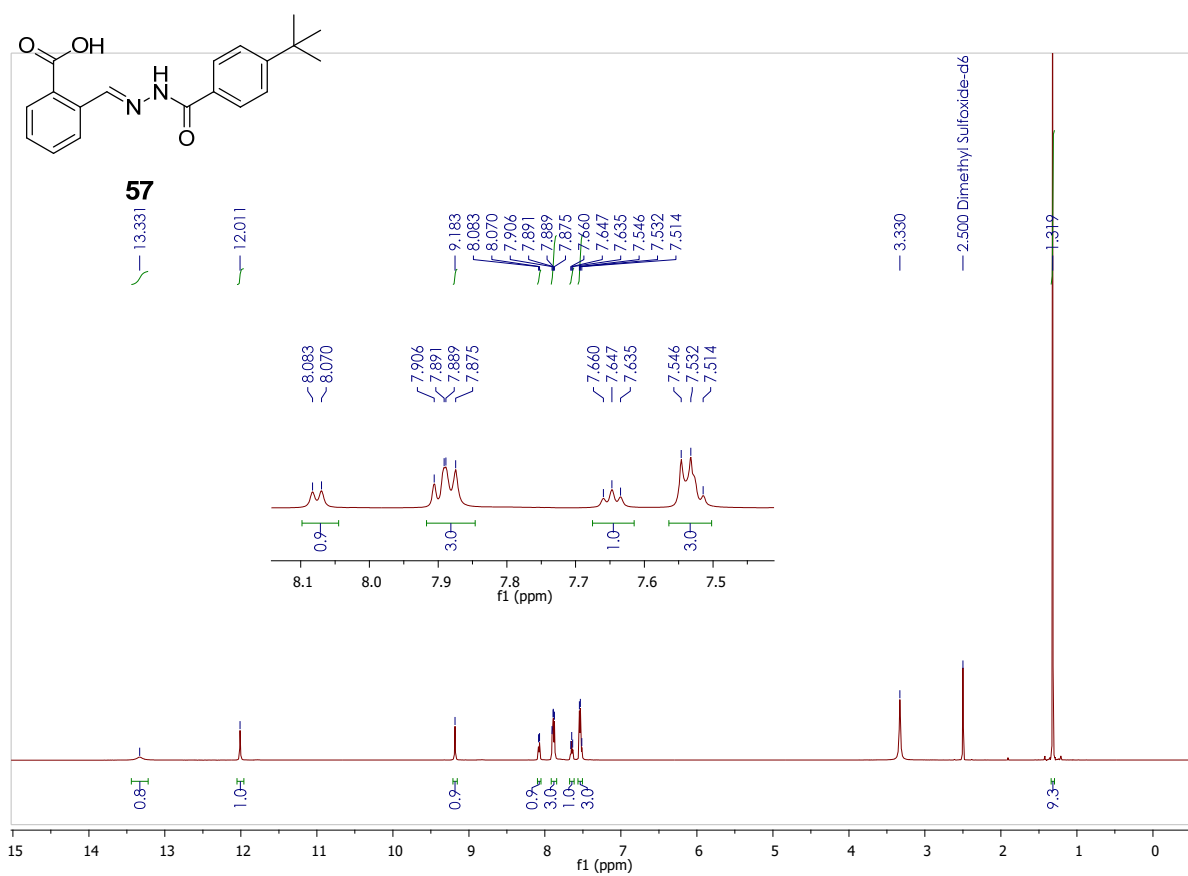
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Data file: D:\Chem32\11\Data\JRB\JRB2050-2055 2021-12-03 09-45-10\003-78-JRB2052.D
 Sample name: JRB2052
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 78
 Injection date: 12/3/2021 9:56:23 AM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 Injection volume: 2.000
 B_3 MINS.M
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 80%B_3 MINS.M
 Last changed: 11/26/2021 9:20:48 AM



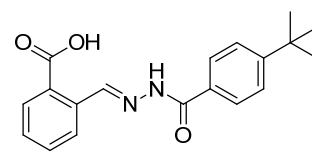
56





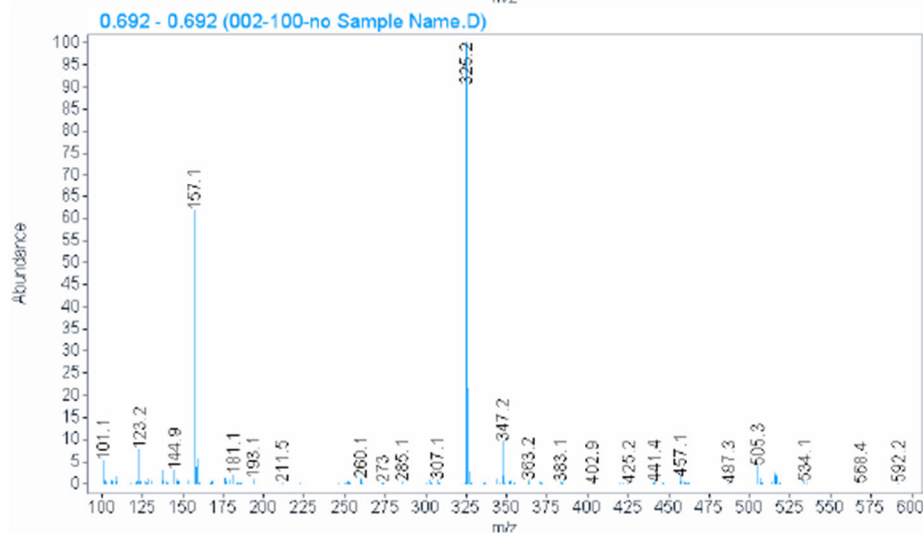
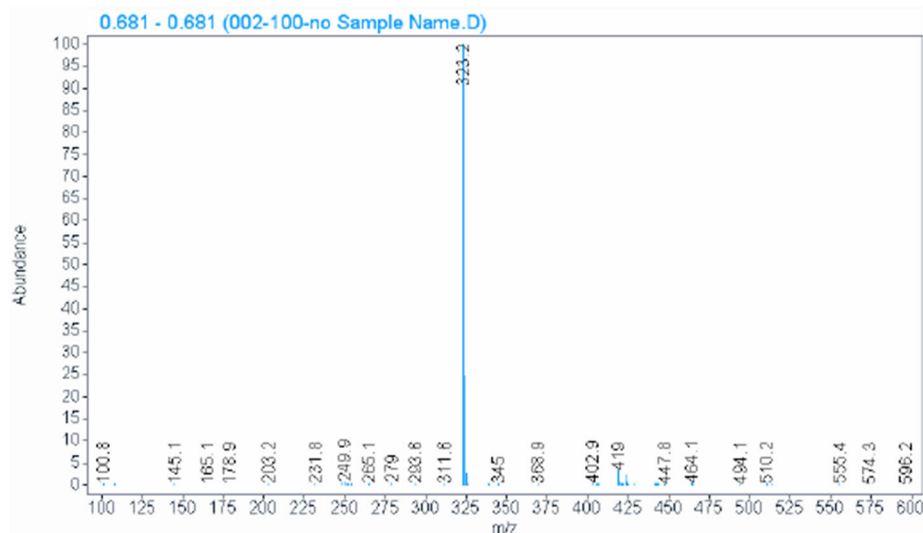
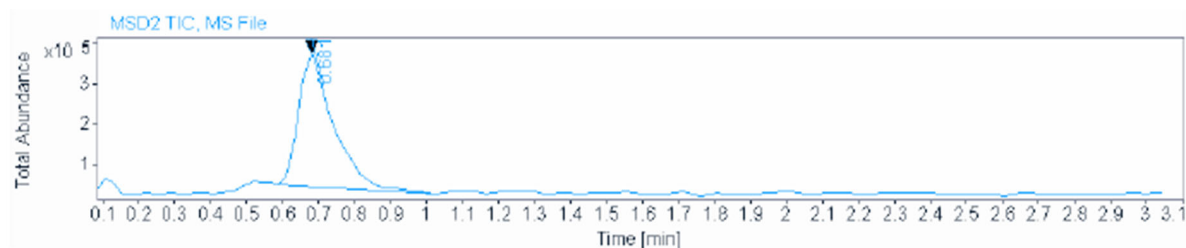
Data file: D:\Chem32\1\Data\JRB\JRB2057 2059 2060 2061 2021-12-09 12-15-05\002-100-no Sample Name.D
 Sample name: JRB2057
 Description: JRB2057
 Sample amount: 0.000
 Instrument: LCMS
 Injection date: 12/9/2021 12:21:32 PM
 Acq. method: LCMS ISOCRATIC 80% B_3 MINS.M
 Analysis method: LCMS ISOCRATIC 80%B_3 MINS.M
 Last changed: 11/26/2021 9:20:48 AM

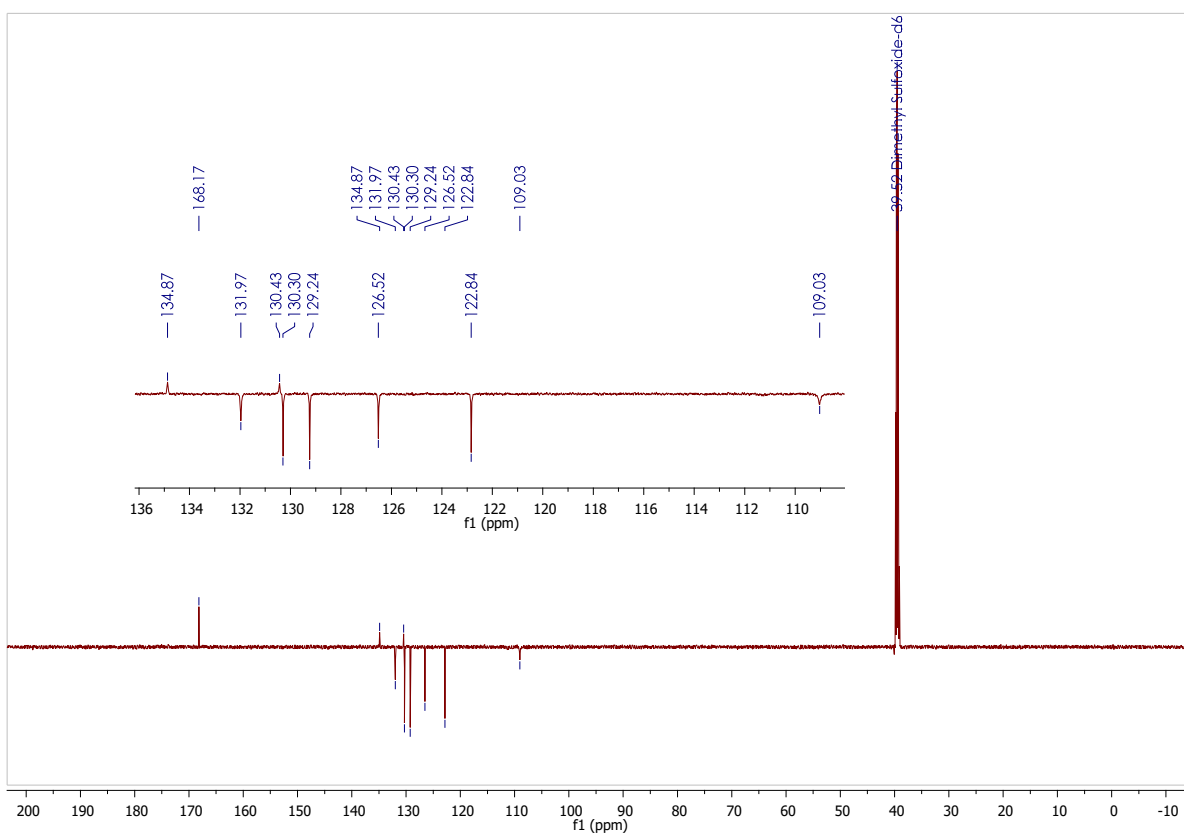
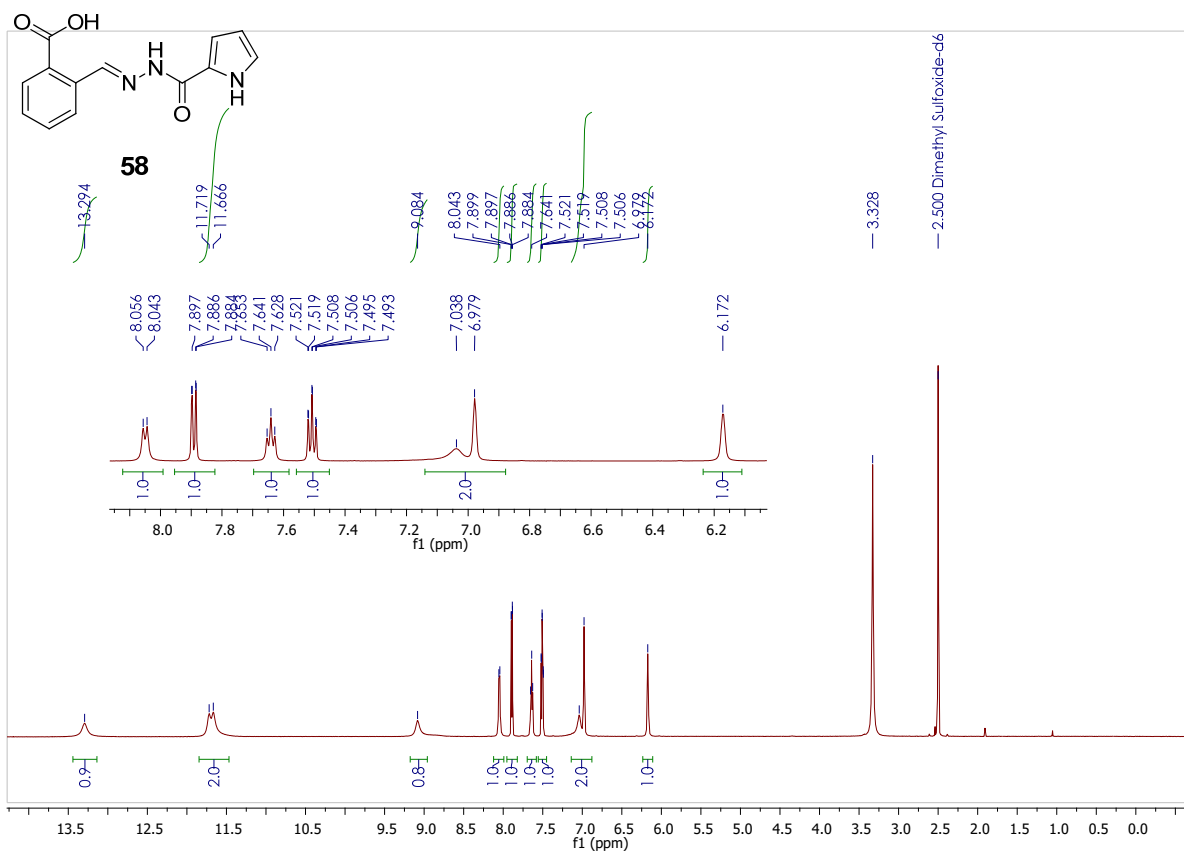
Sample type: Sample
 Location: 100
 Injection: 1 of 1
 Injection volume: 2.000
 Acq. operator: SYSTEM



Molecular Weight: 324.374

57





Data file: D:\Chem32\11\Data\JRB\JRB2057 2059 2060 2061 2021-12-09 12-15-05\005-97-no Sample Name.D

Sample name:

Description:

Sample amount:

JRB2061

0.000

Sample type:

Sample

Instrument:

LCMS

Location:

97

Injection date:

12/9/2021 12:35:28 PM

Injection:

1 of 1

Acq. method:

LCMS ISOCRATIC 80%
B_3 MINS.M

Injection volume:

2.000

Analysis method:

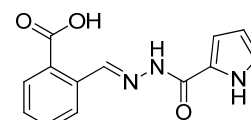
LCMS ISOCRATIC
80%B_3 MINS.M

Acq. operator:

SYSTEM

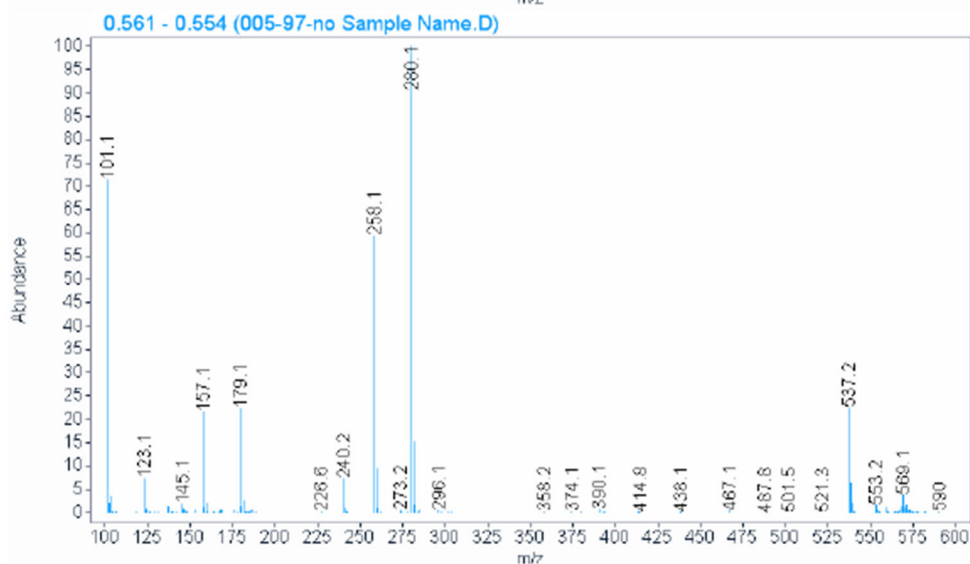
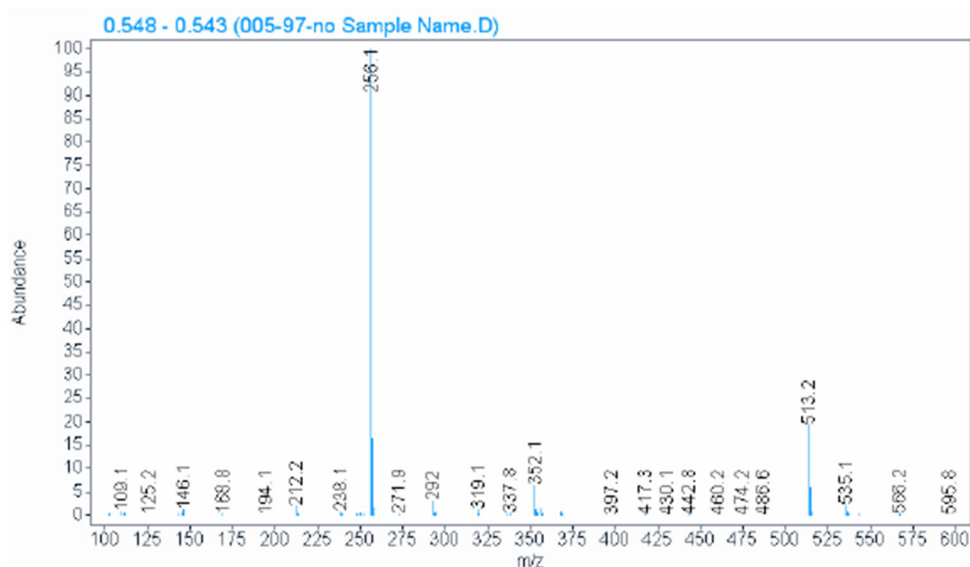
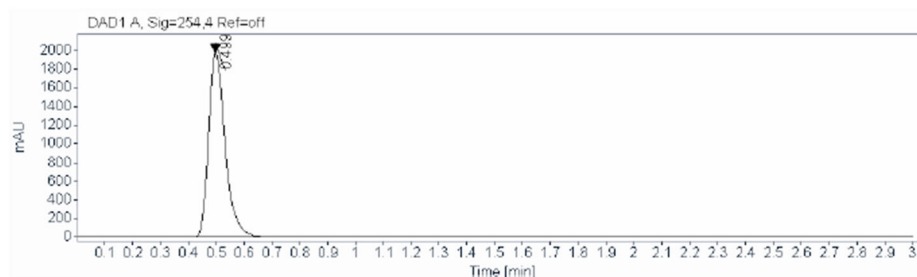
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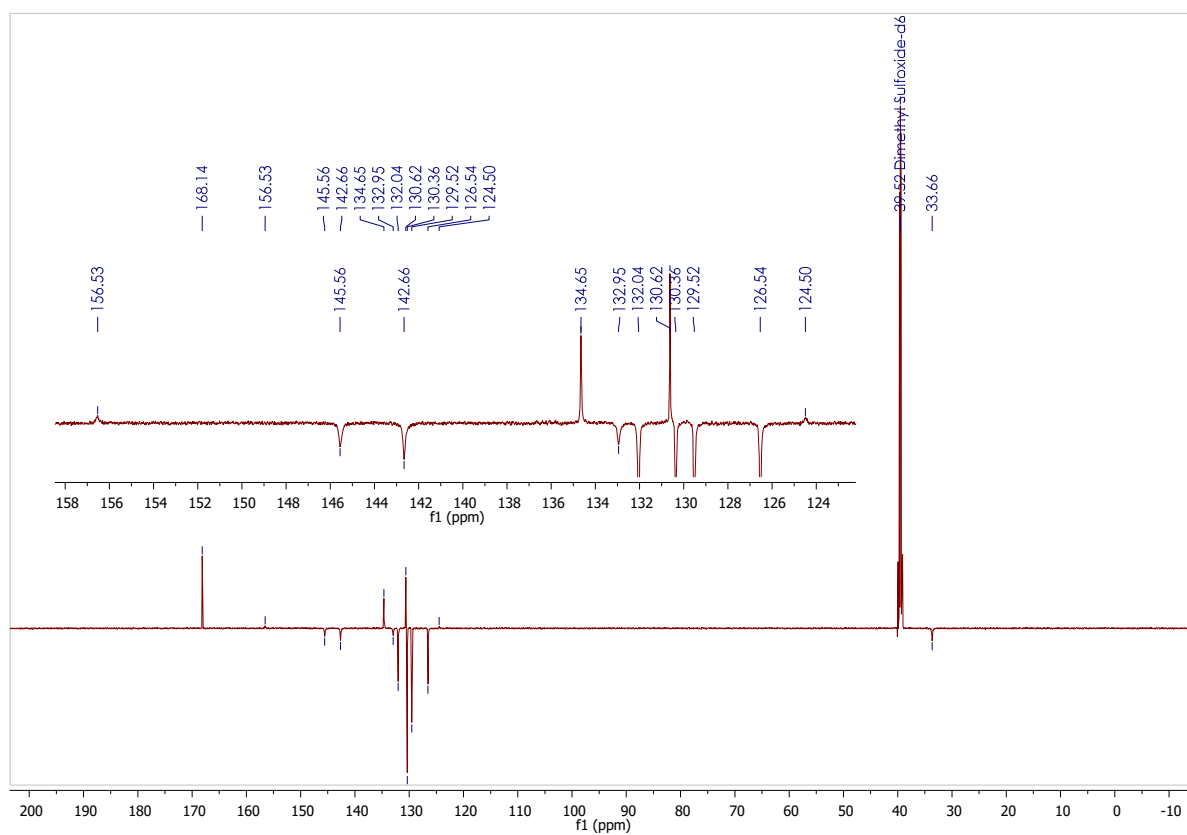
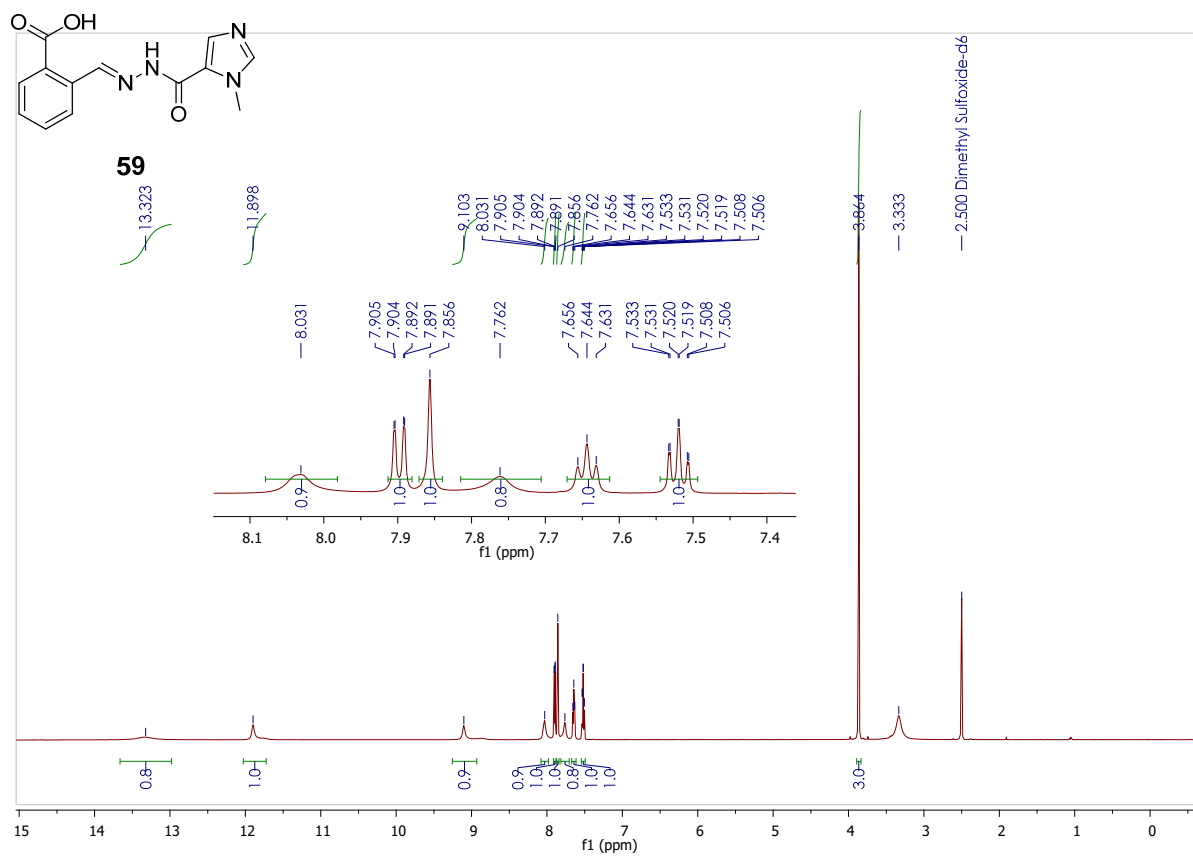
11/26/2021 9:20:48 AM



Molecular Weight: 257.245

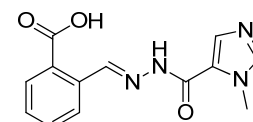
58





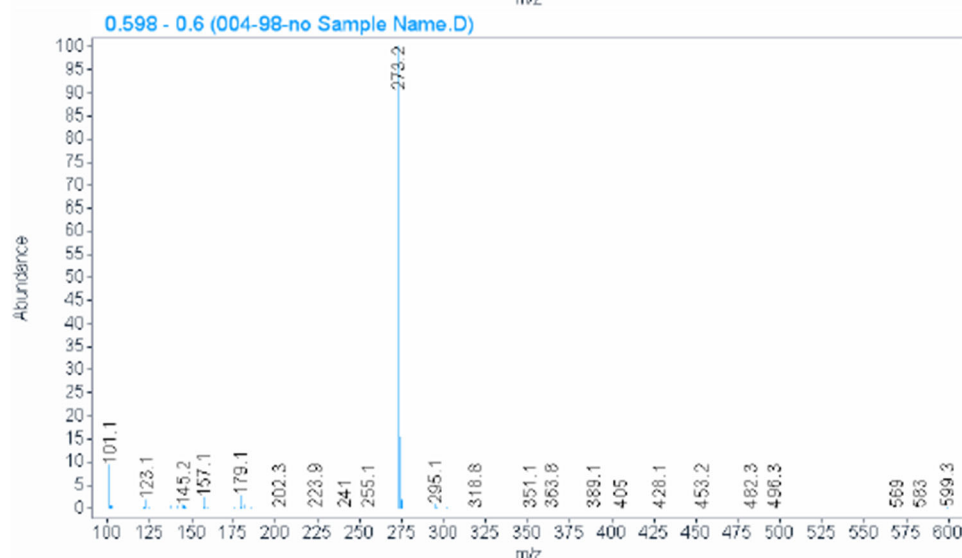
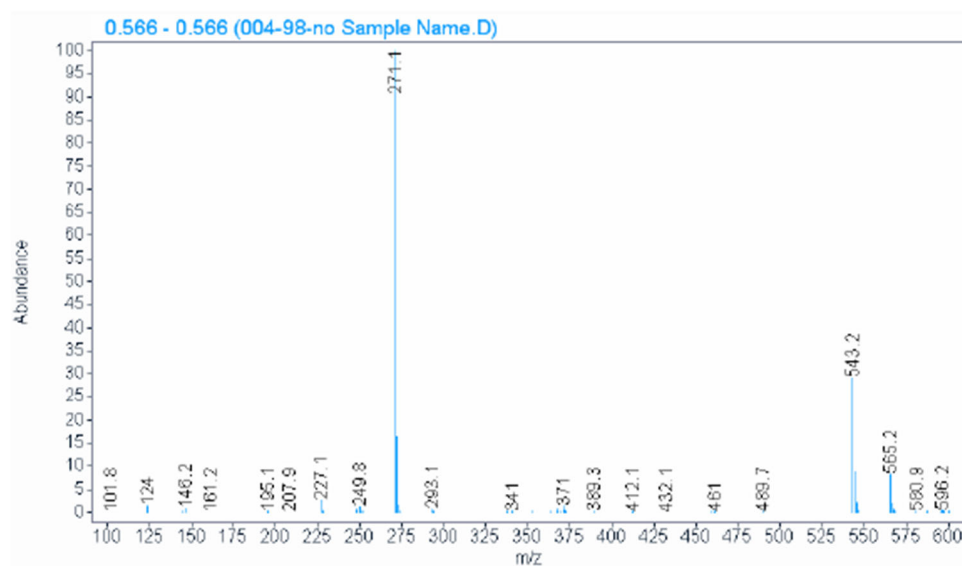
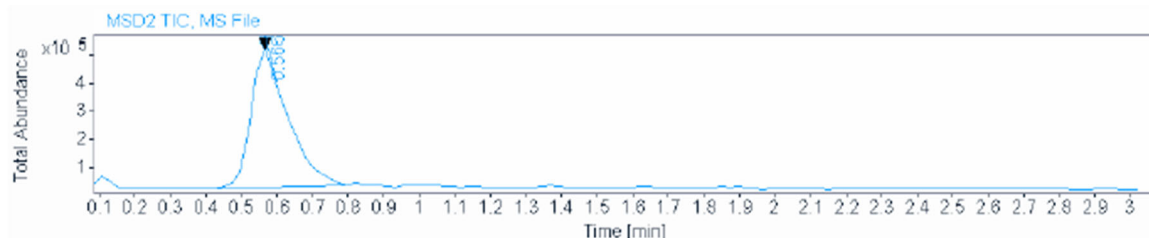


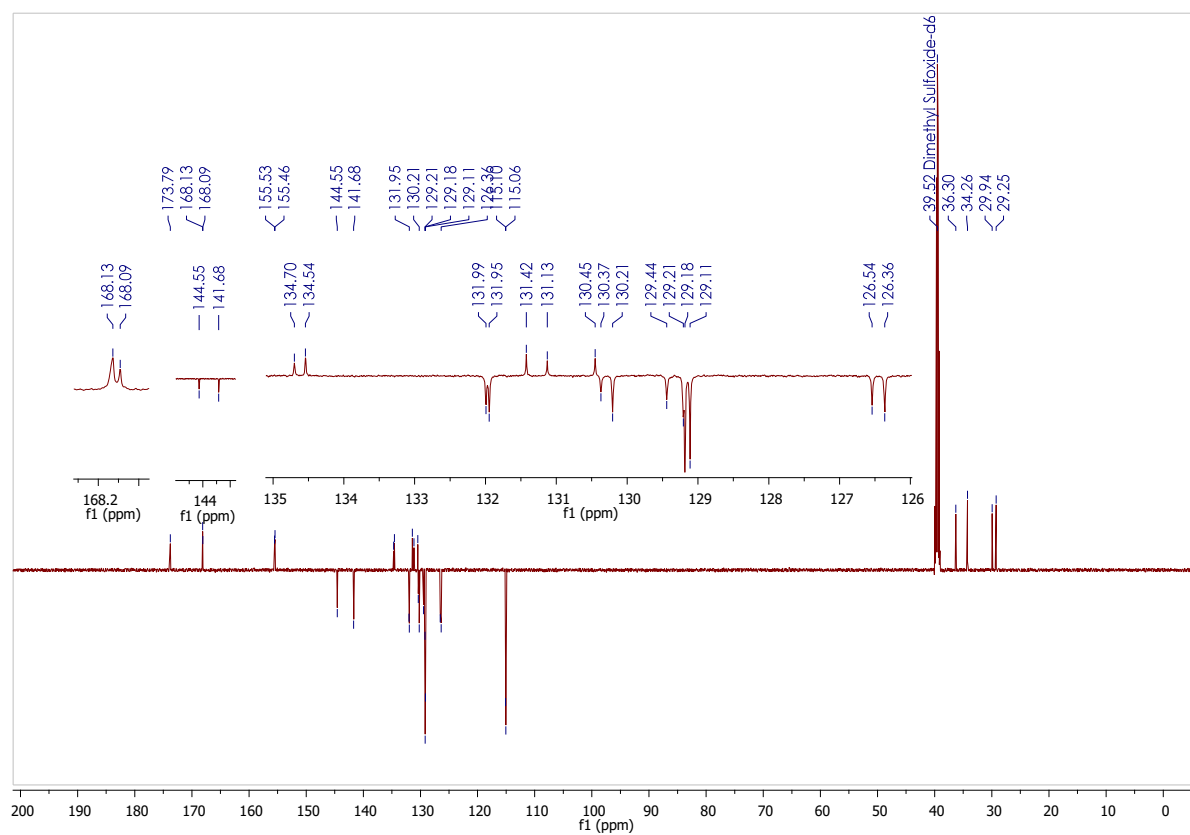
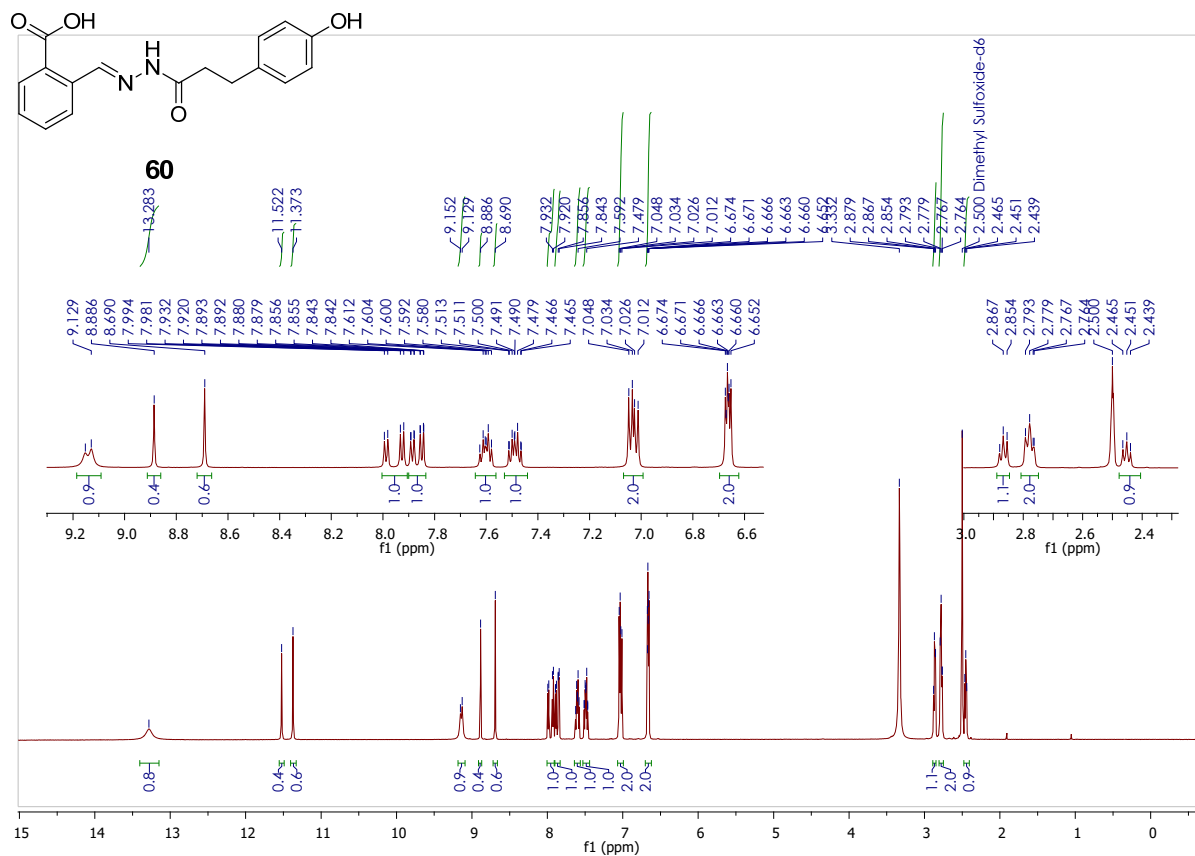
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 Sample name: JRB2060
 Description: JRB2060
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 98
 Injection date: 12/9/2021 12:30:50 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 Injection volume: 2.000
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 Last changed: 11/26/2021 9:20:48 AM



Molecular Weight: 272.259

59

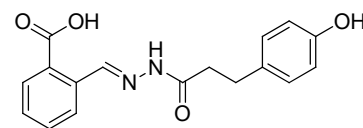




LCMS Report

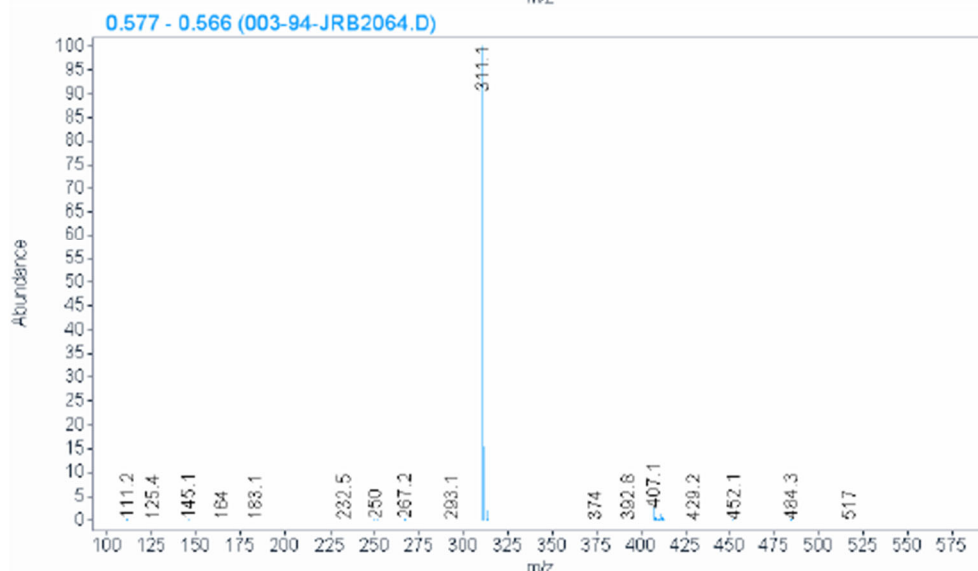
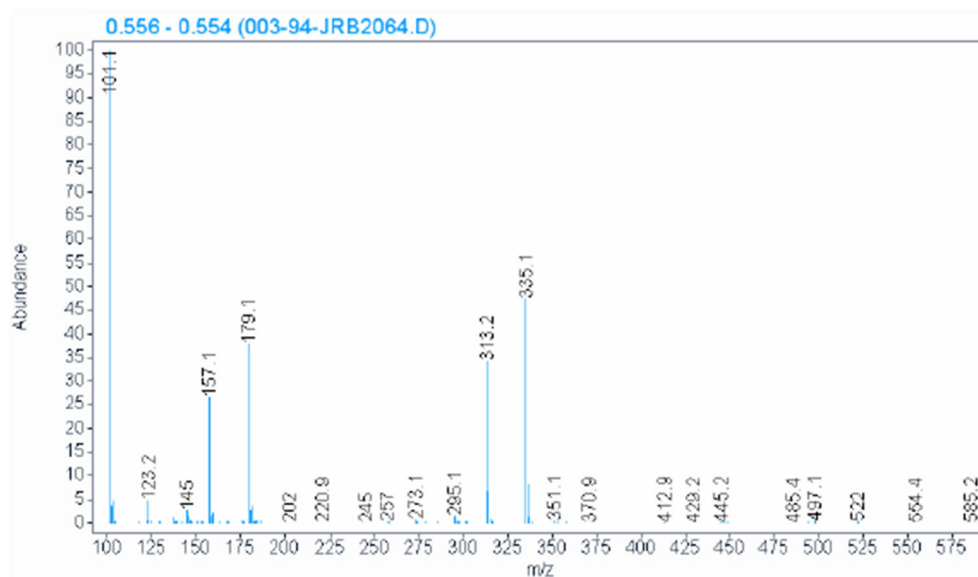
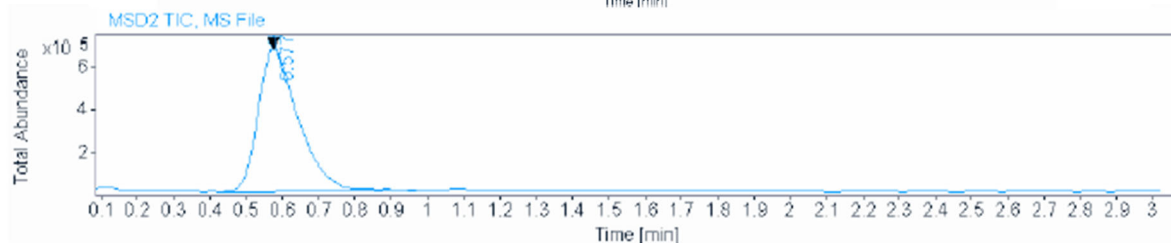


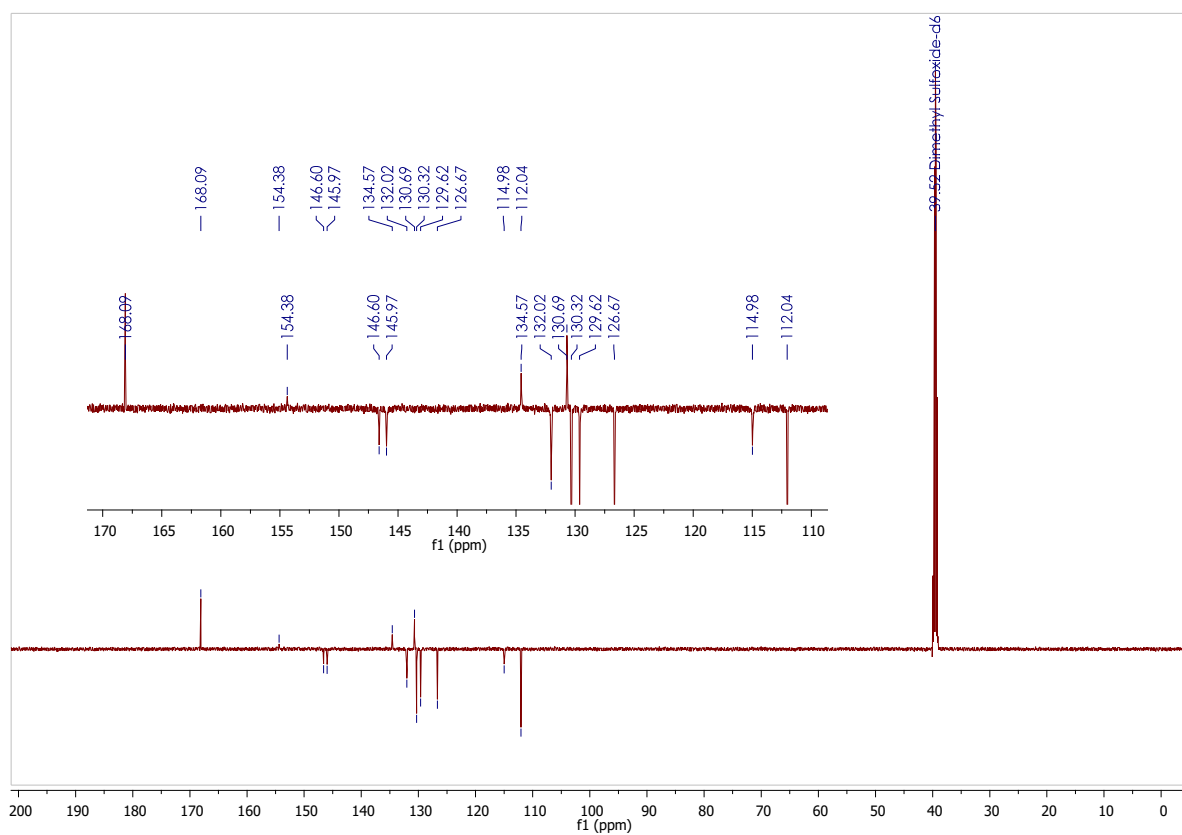
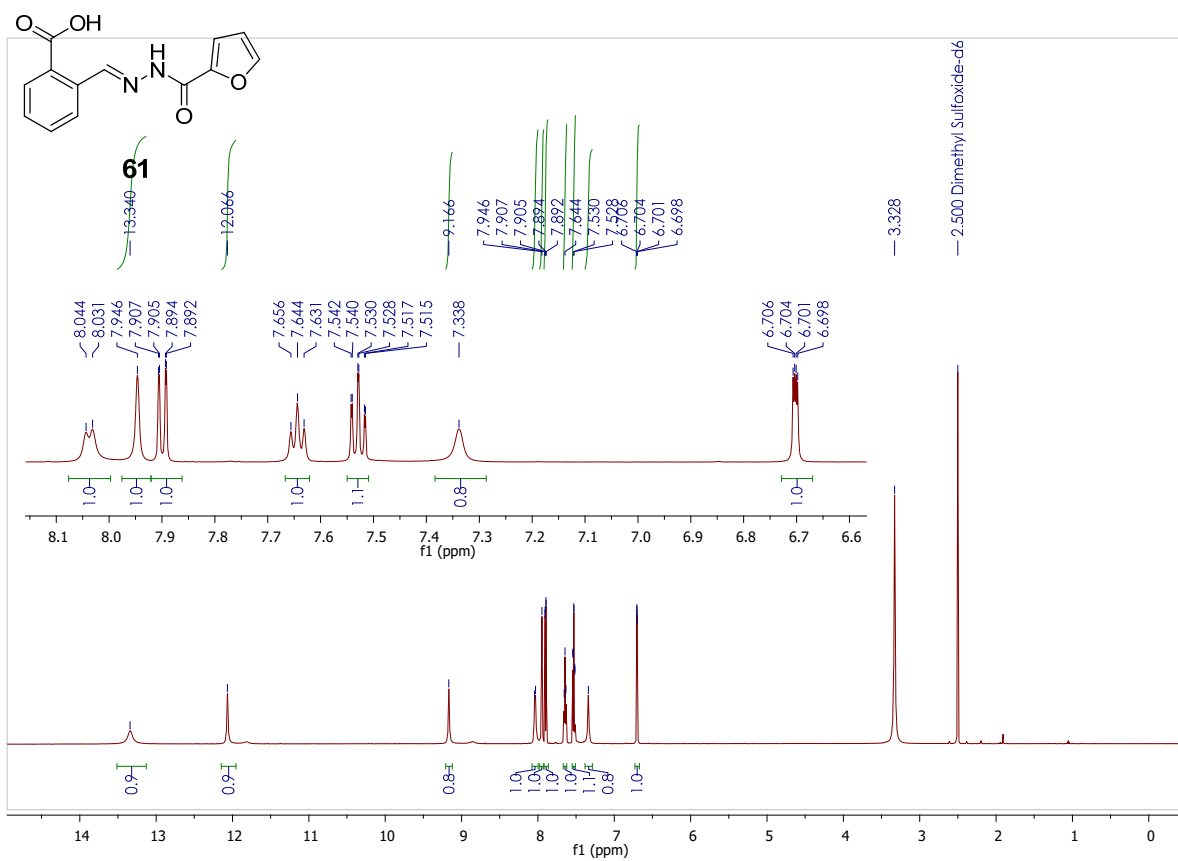
Data file: D:\Chem32\1\Data\JRB\JRB2063 2064 2021-12-09 13-07-22\003-94-JRB2064.D
Sample name: JRB2064
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Location: 94
Injection date: 12/9/2021 1:18:20 PM
Injection: 1 of 1
Acq. method: LCMS ISOCRATIC 70%
Injection volume: 2.000
 B_3MINS.M
Analysis method: LCMS ISOCRATIC
Acq. operator: SYSTEM
 70%B_3MINS.M
Last changed: 5/19/2016 3:53:37 PM



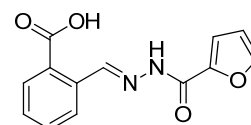
Molecular Weight: 312.320

60



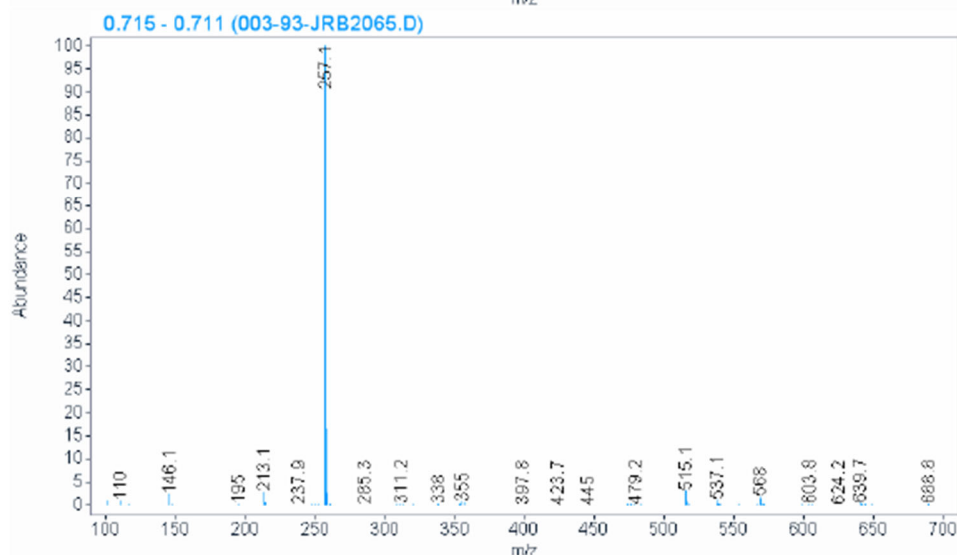
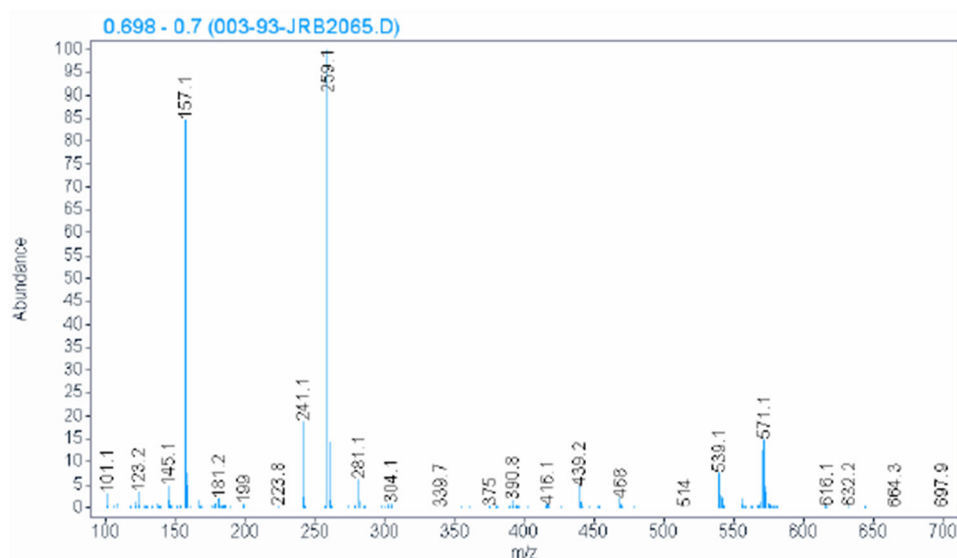
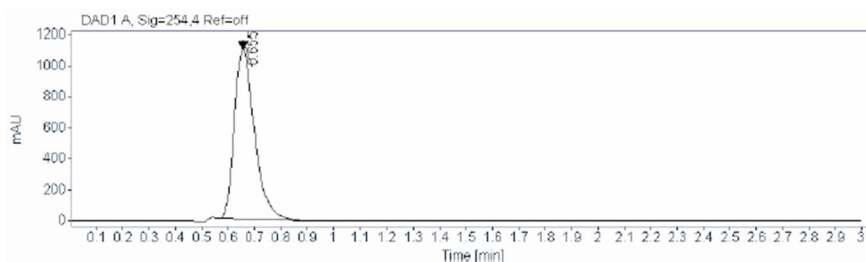


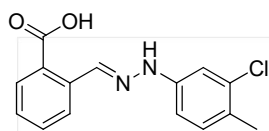
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 Sample name: JRB2065
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 93
 Injection date: 12/9/2021 1:04:09 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC_50%
 Injection volume: 2.000
 B_0.4MLMIN-1_3MINS.M
 Analysis method: LCMS
 Acq. operator: SYSTEM
 ISOCRATIC_50%
 B_0.4MLMIN-1_3MINS.M
 Last changed: 11/11/2021 3:05:21 PM



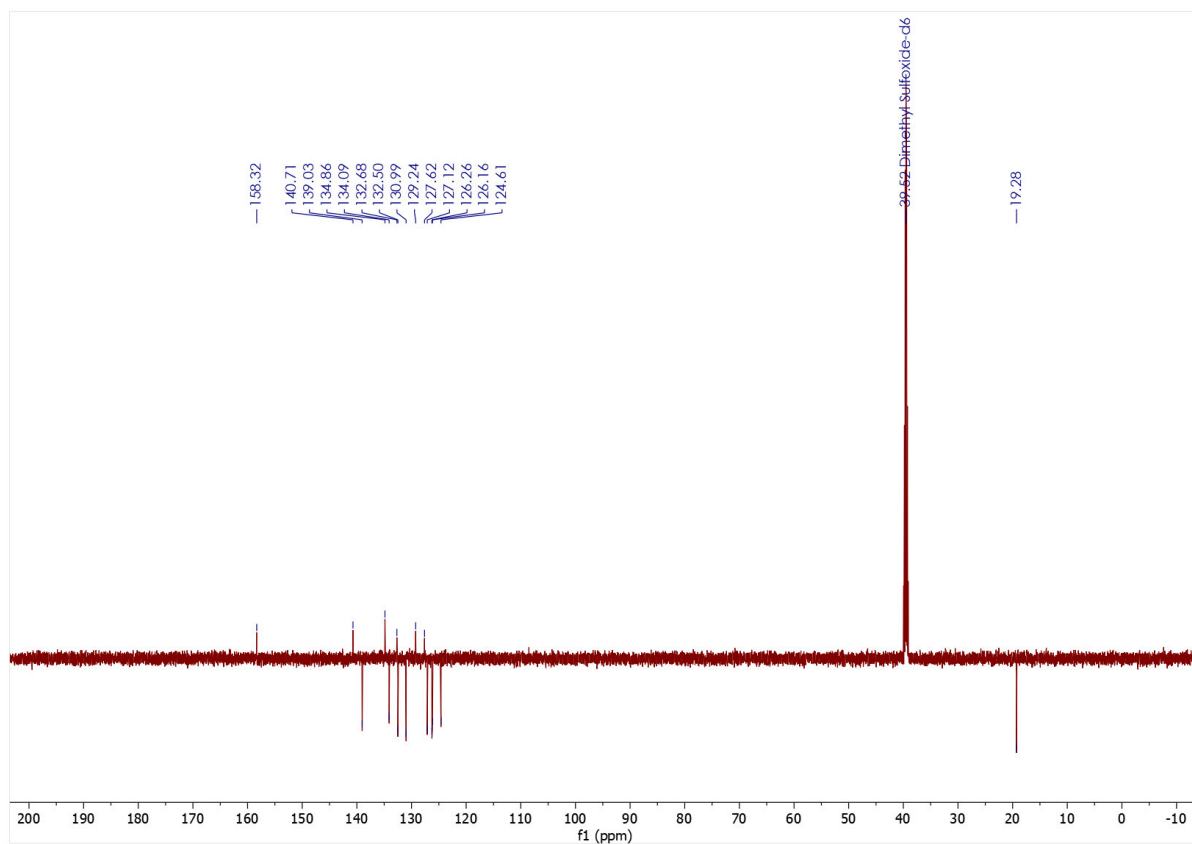
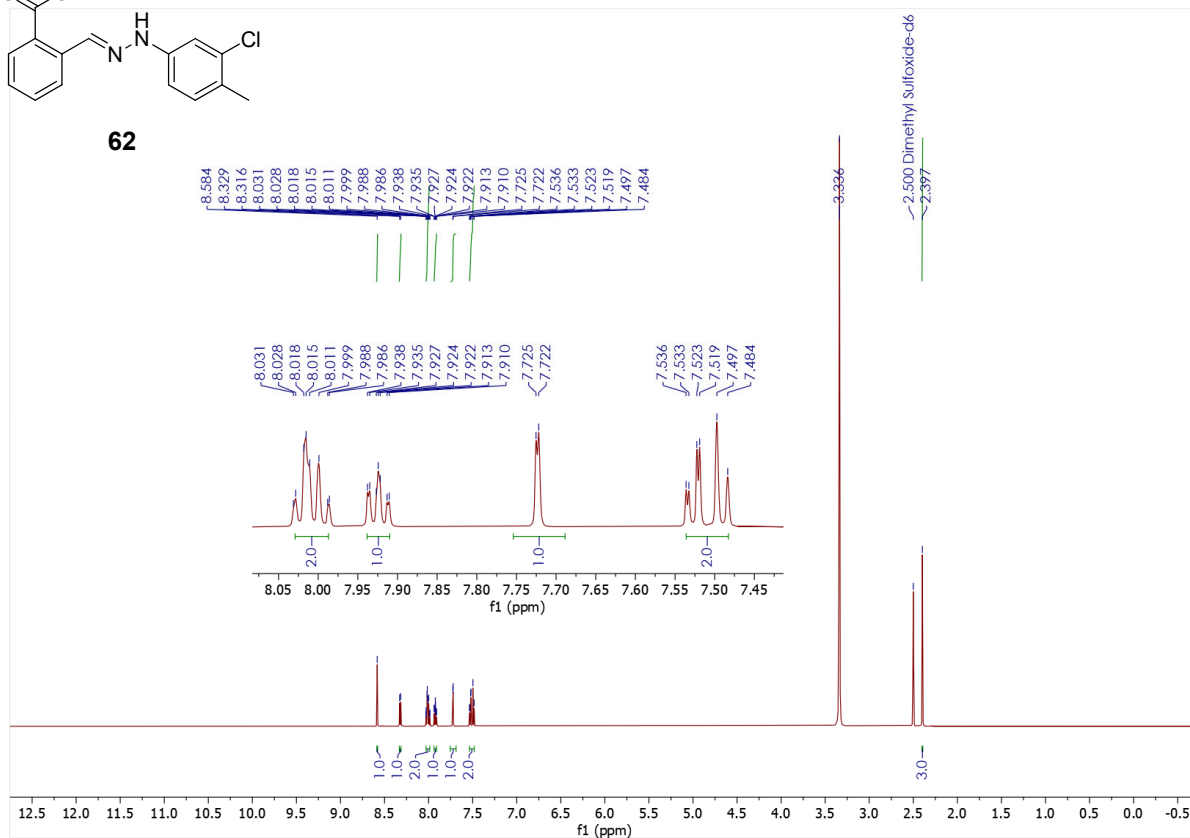
Molecular Weight: 258.229

61

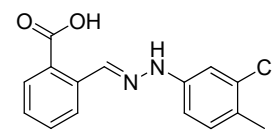




62

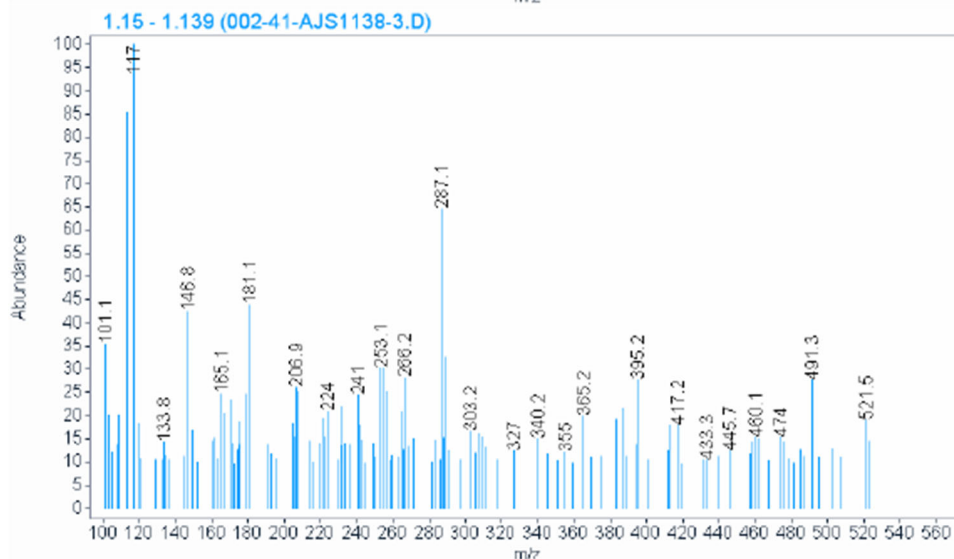
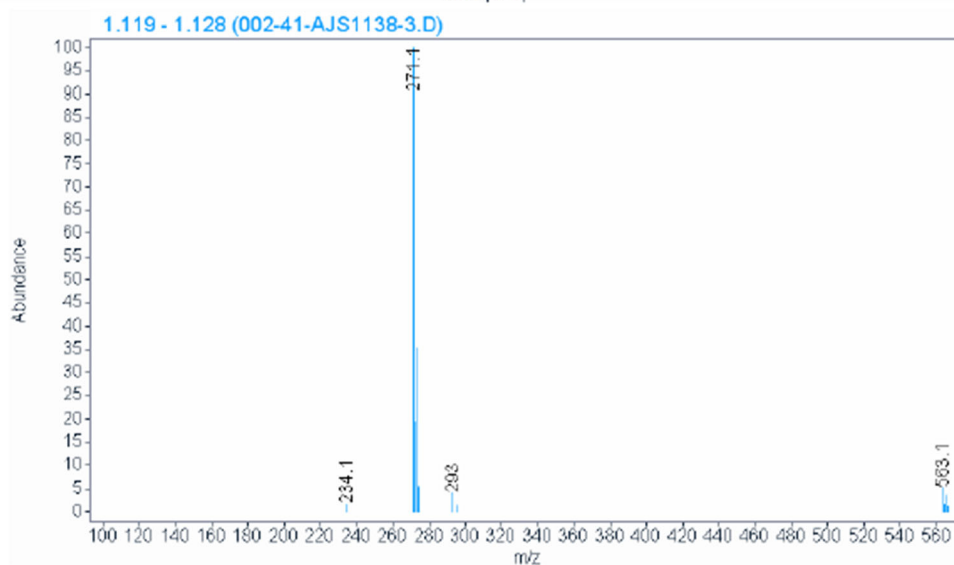
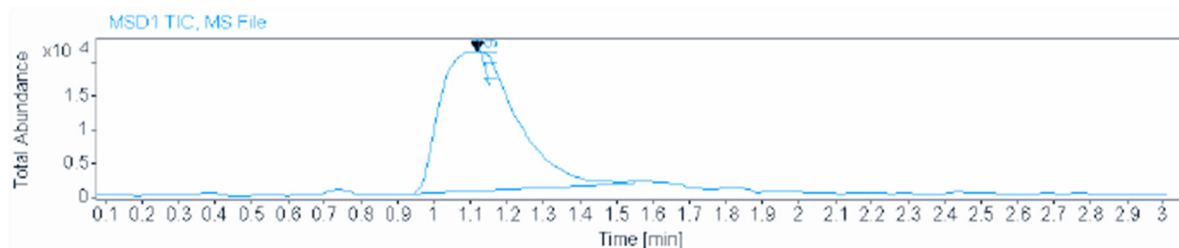
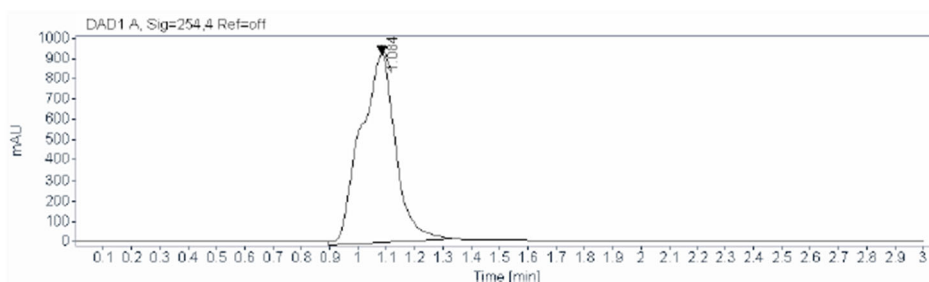


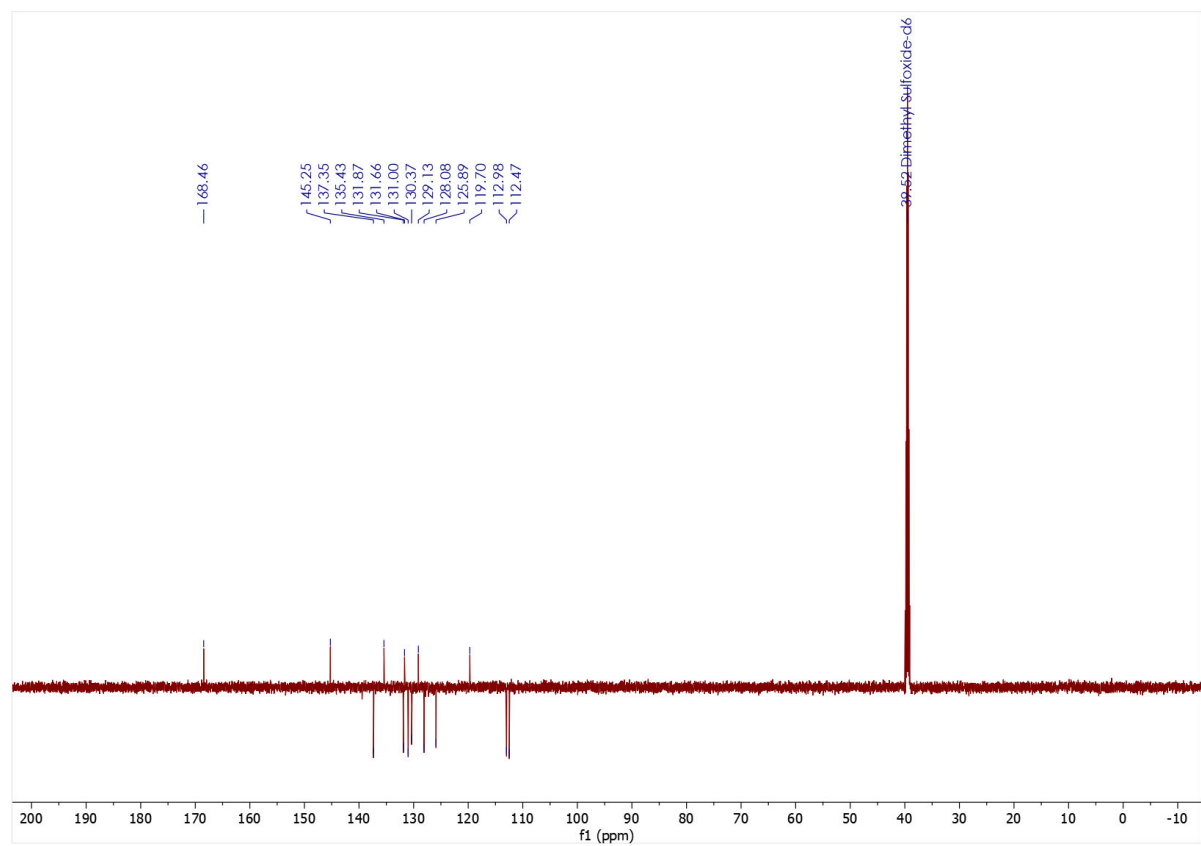
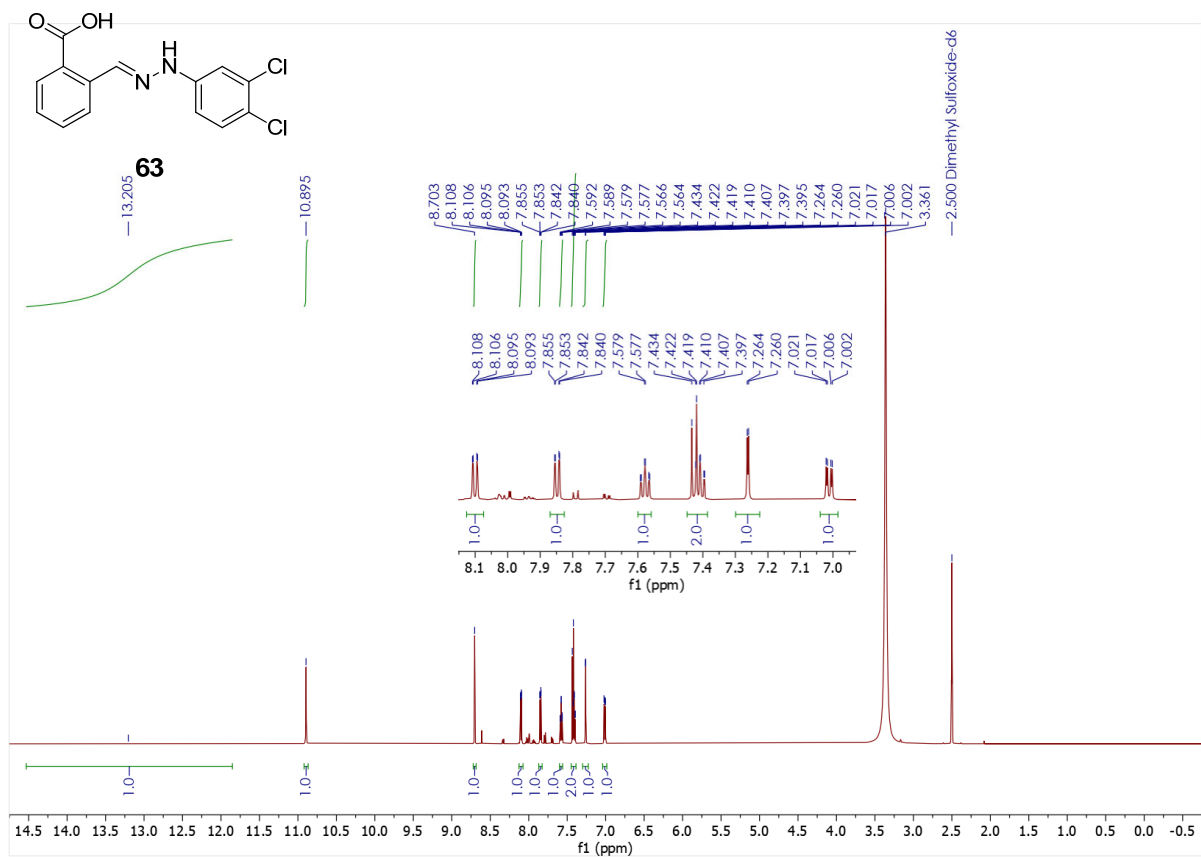
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 Sample name: AJS1138-3
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 41
 Injection date: 7/31/2023 12:59:10 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 B_3 MINS.M
 Injection volume: 2.000
 Analysis method: LCMS ISOCRATIC
 80%B_3 MINS.M
 Acq. operator: SYSTEM
 Last changed: 11/26/2021 9:20:48 AM



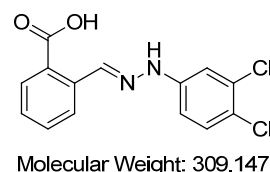
Molecular Weight: 288.729

62

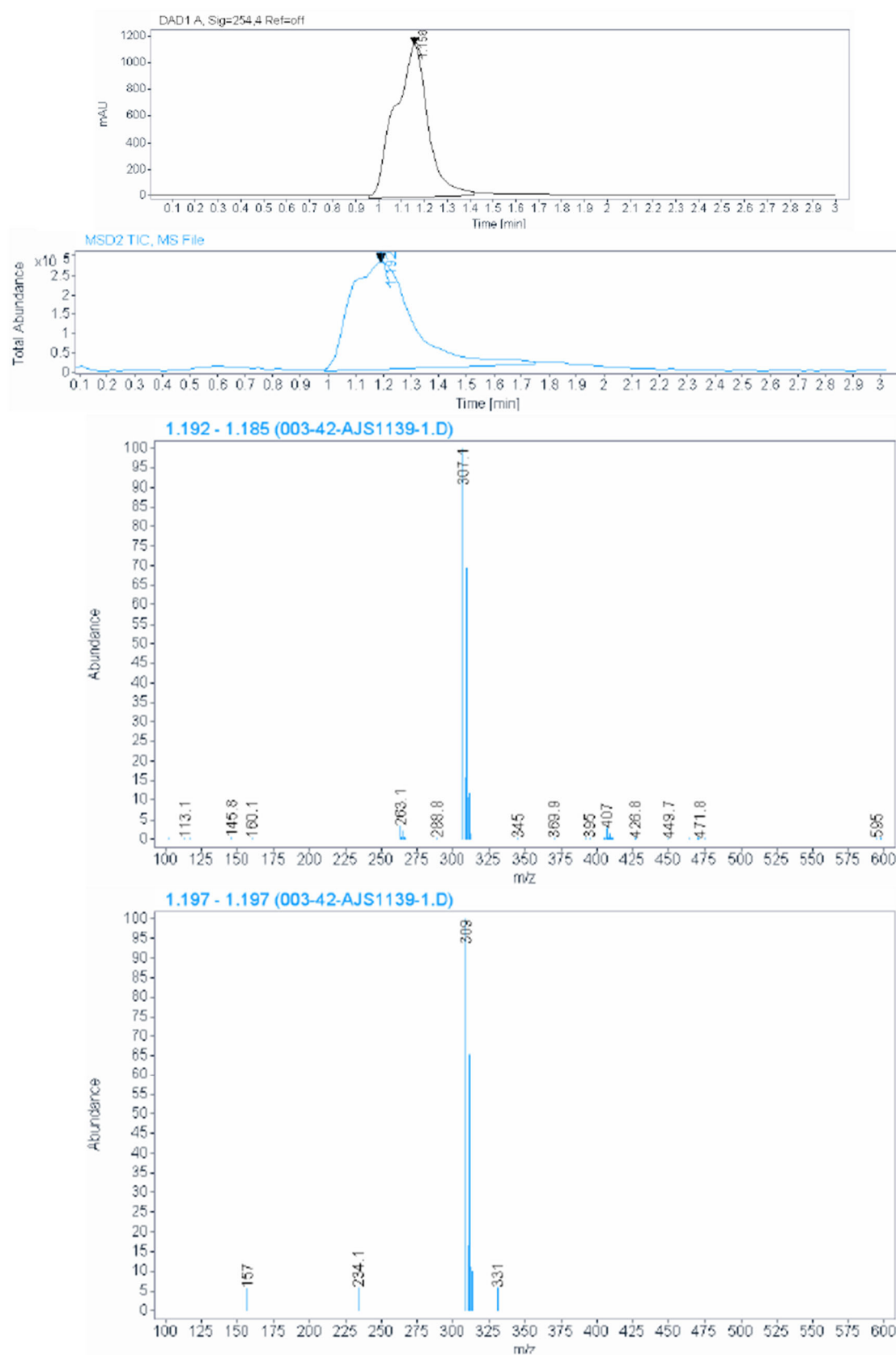


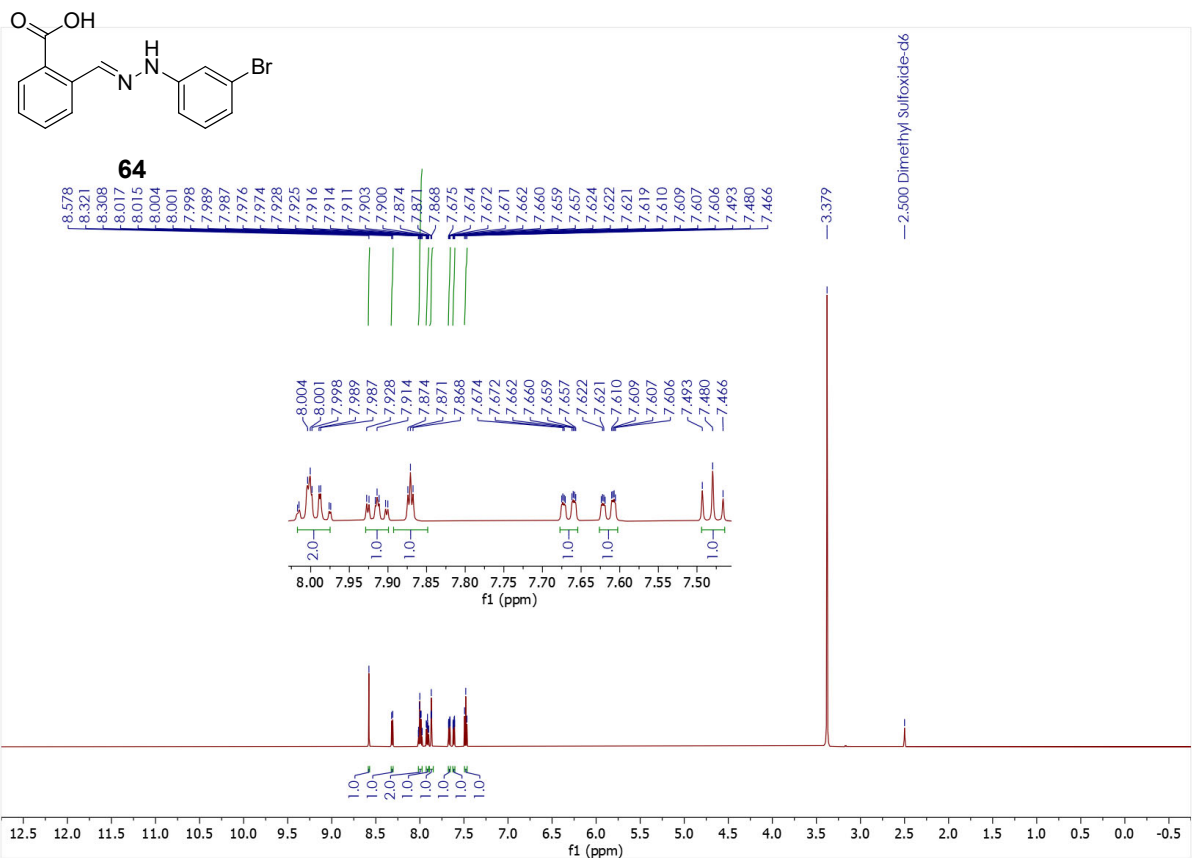


Data file: D:\Chem32\1\Data\AJSAJS Table4+ 2023-07-31 12-52-45\003-42-AJS1139-1.D
 Sample name: AJS1139-1
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Injection date: 7/31/2023 1:03:52 PM
 Location: 42
 Acq. method: LCMS ISOCRATIC 80%
 Injection: 1 of 1
 B_3 MINS.M
 Injection volume: 2.000
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 80%B_3 MINS.M
 Last changed: 11/26/2021 9:20:48 AM



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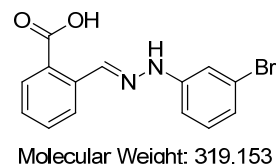


LCMS Report

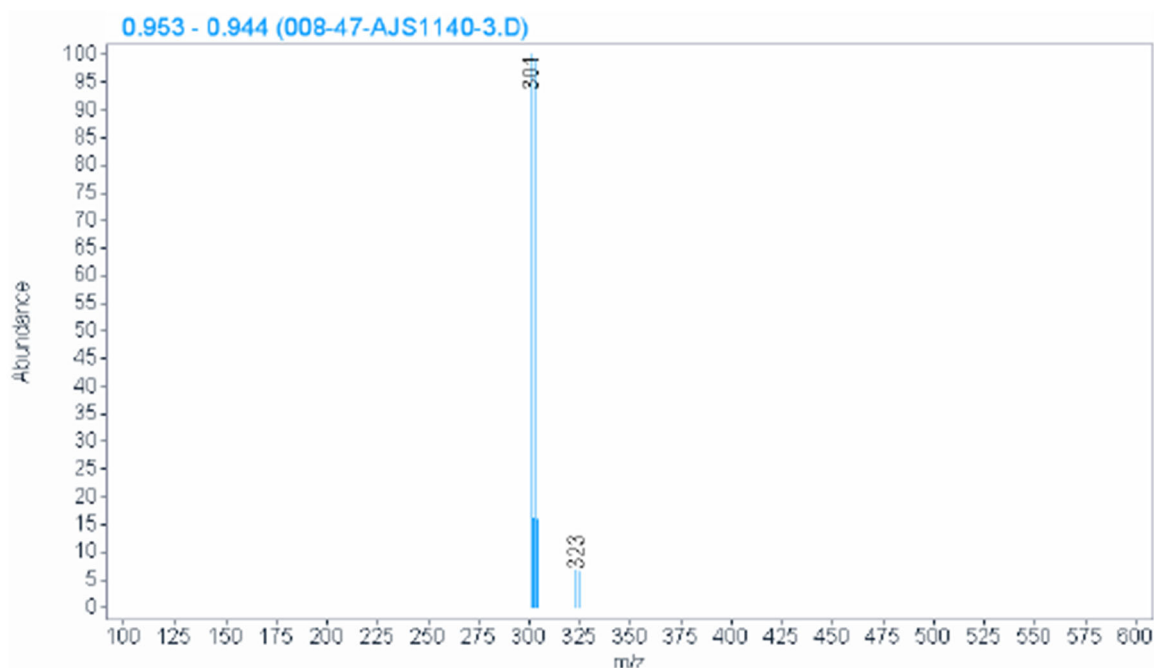
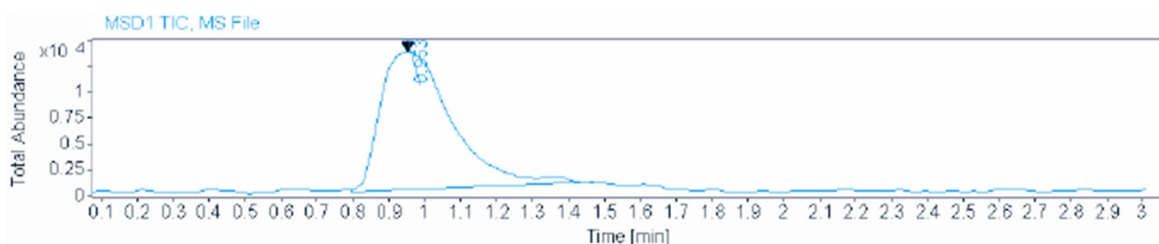
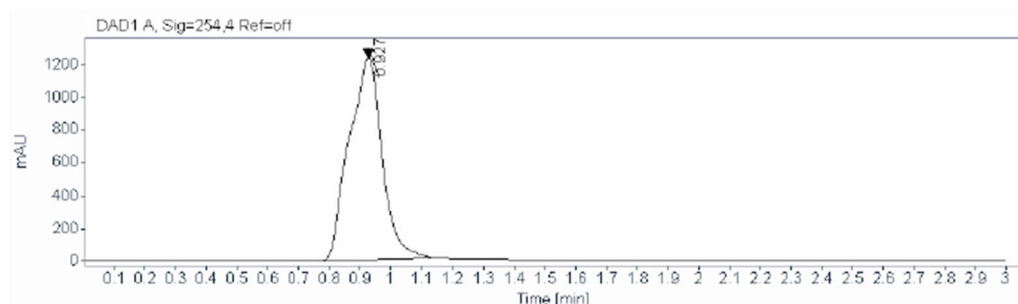


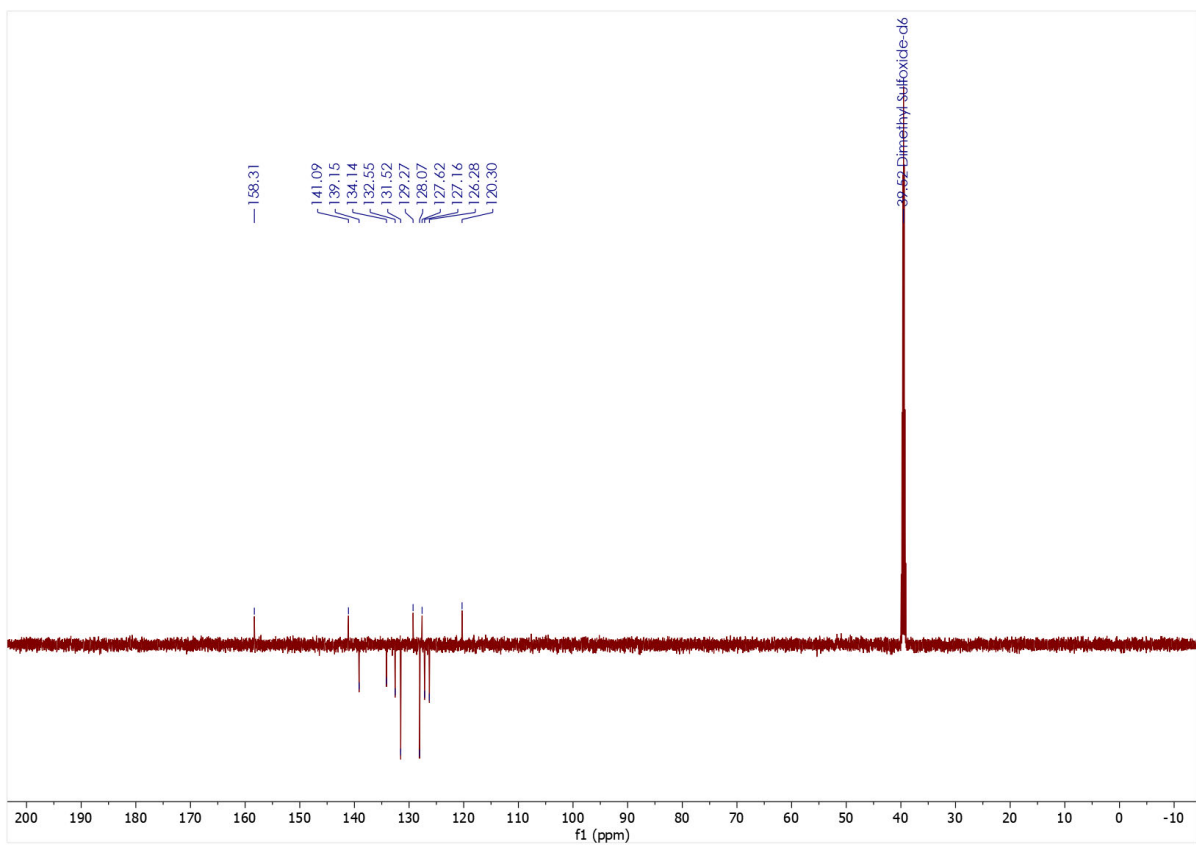
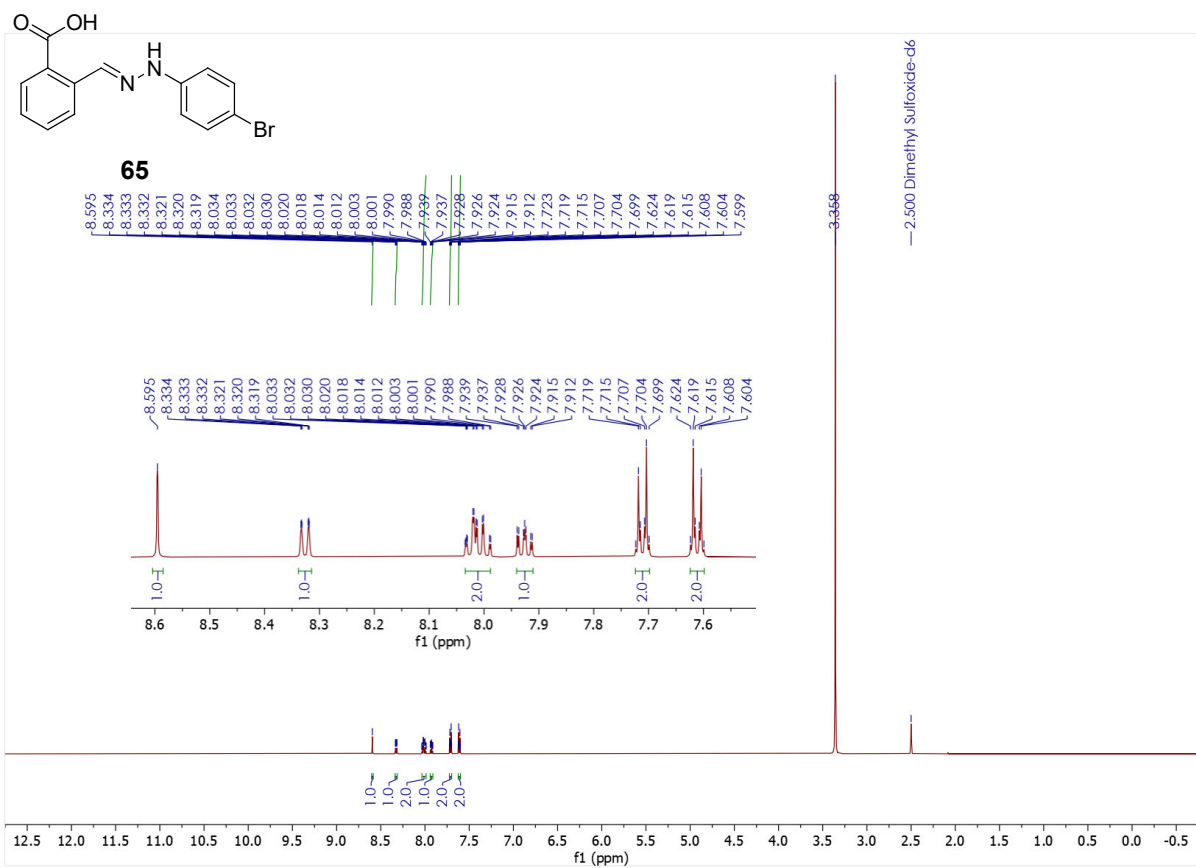
Agilent Technologies

Data file: D:\Chem32\1\Data\AJS\AJS Table4+ 2023-07-31 12-52-45\008-47-AJS1140-3.D
Sample name: AJS1140-3
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Location: 47
Injection date: 7/31/2023 1:27:25 PM
Injection: 1 of 1
Acq. method: LCMS ISOCRATIC 80%
Injection volume: 2.000
B_3 MINS.M
Analysis method: LCMS ISOCRATIC
Acq. operator: SYSTEM
80%B_3 MINS.M
Last changed: 11/26/2021 9:20:48 AM



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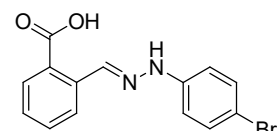


LCMS Report



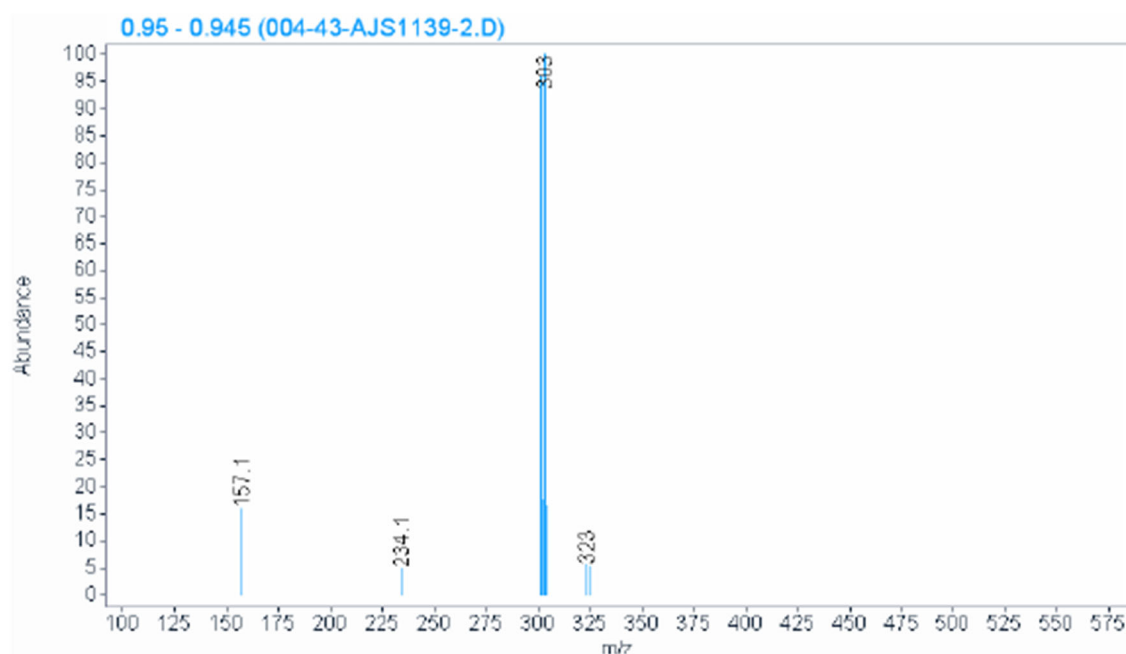
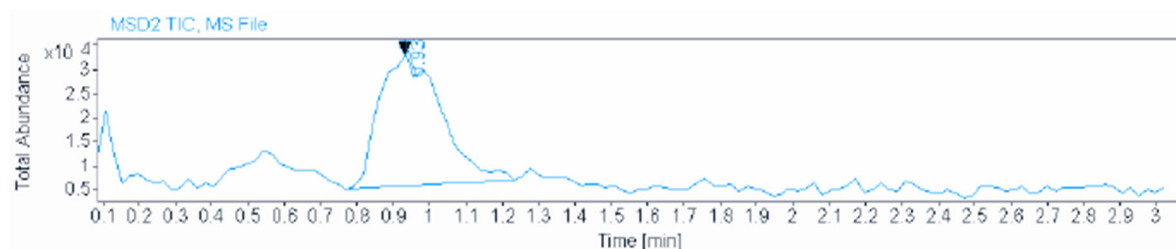
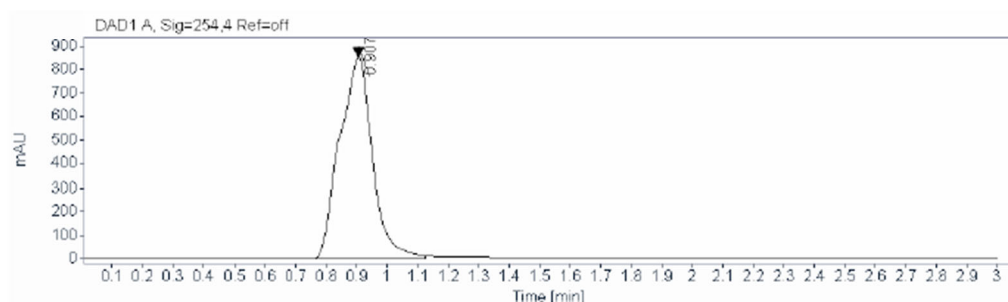
Agilent Technologies

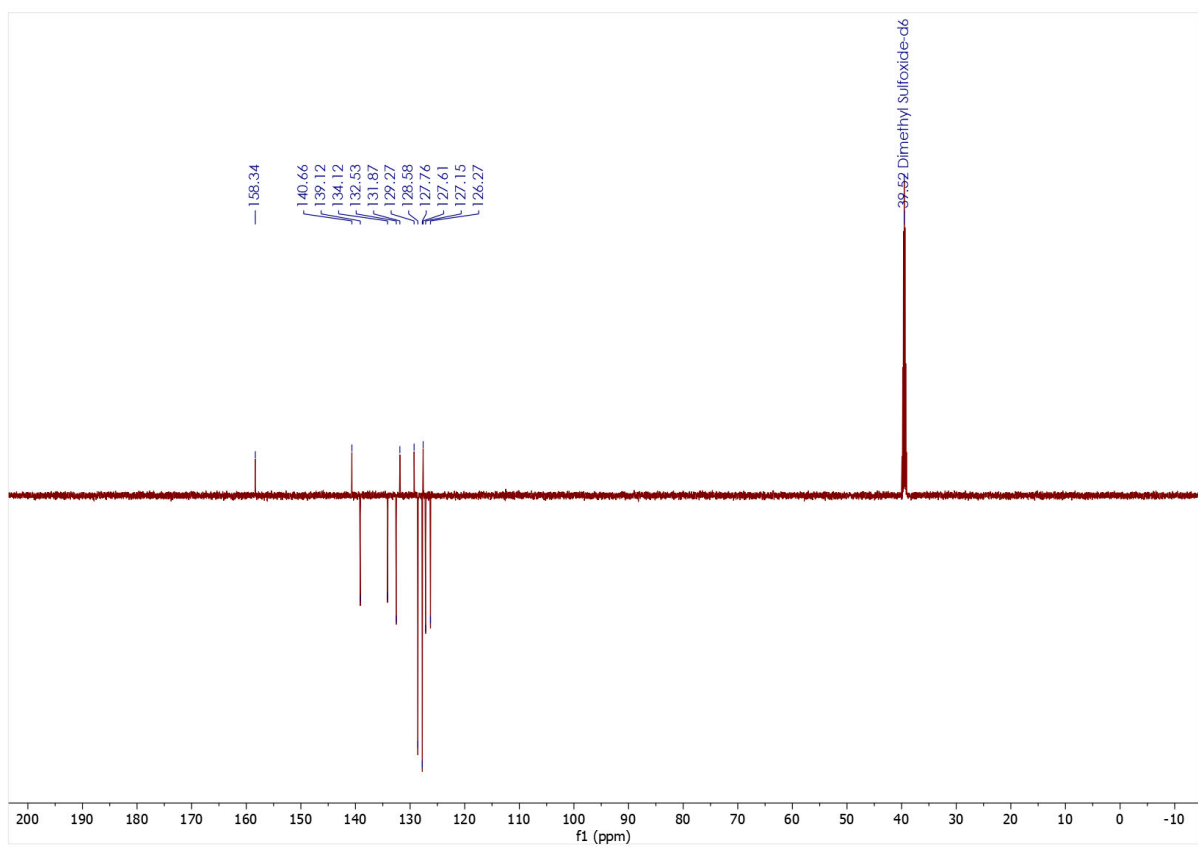
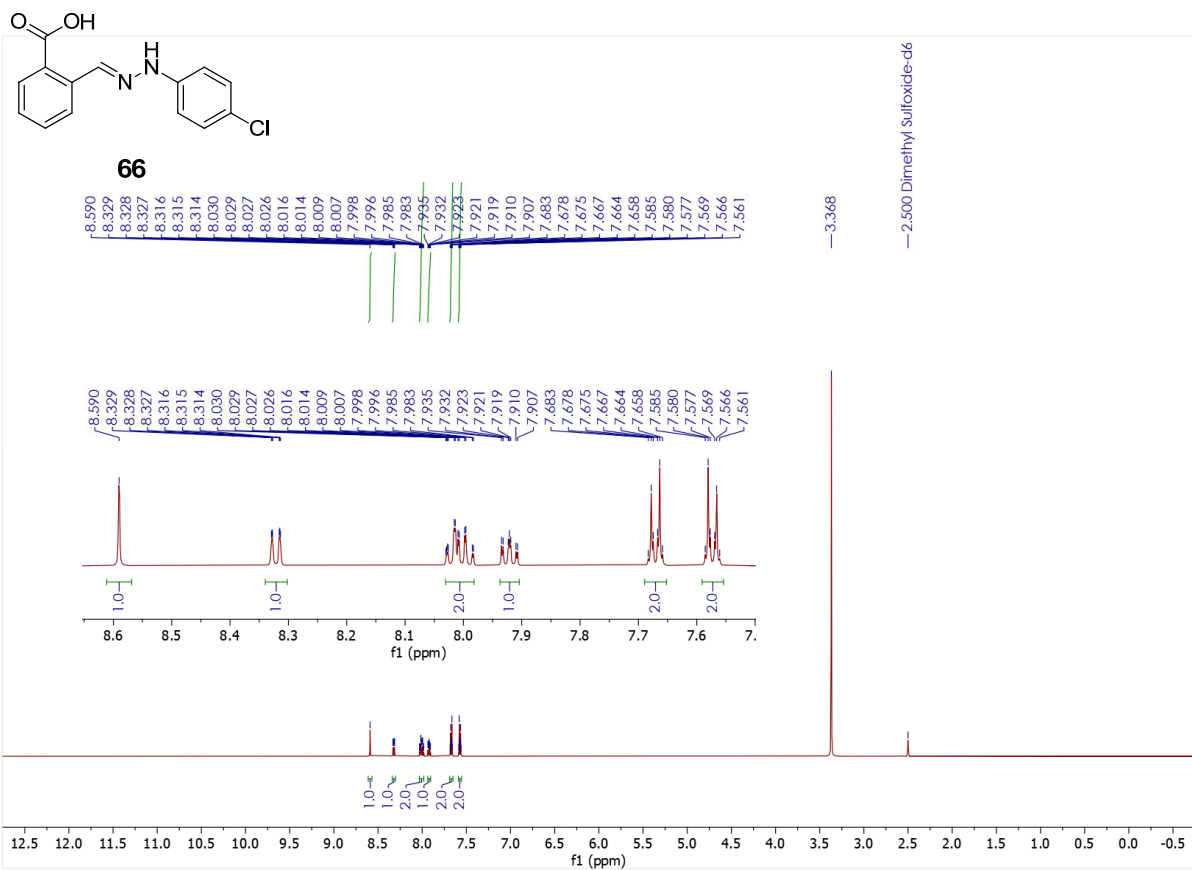
Data file: D:\Chem32\11\Data\AJSAJS Table4+ 2023-07-31 12:52:45\004-43-AJS1139-2.D
 Sample name: AJS1139-2
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Injection date: 7/31/2023 1:08:37 PM
 Location: 43
 Acq. method: LCMS ISOCRATIC 80%
 Injection: 1 of 1
 B_3 MINS.M
 Injection volume: 2.000
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 80%B_3 MINS.M
 Last changed: 11/26/2021 9:20:48 AM



Molecular Weight: 319.153

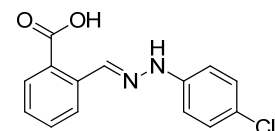
65





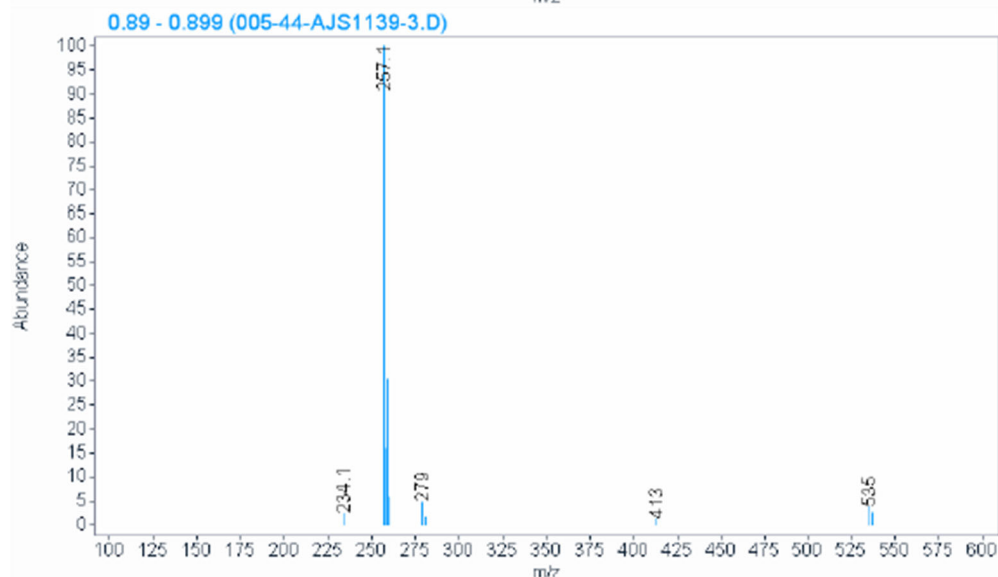
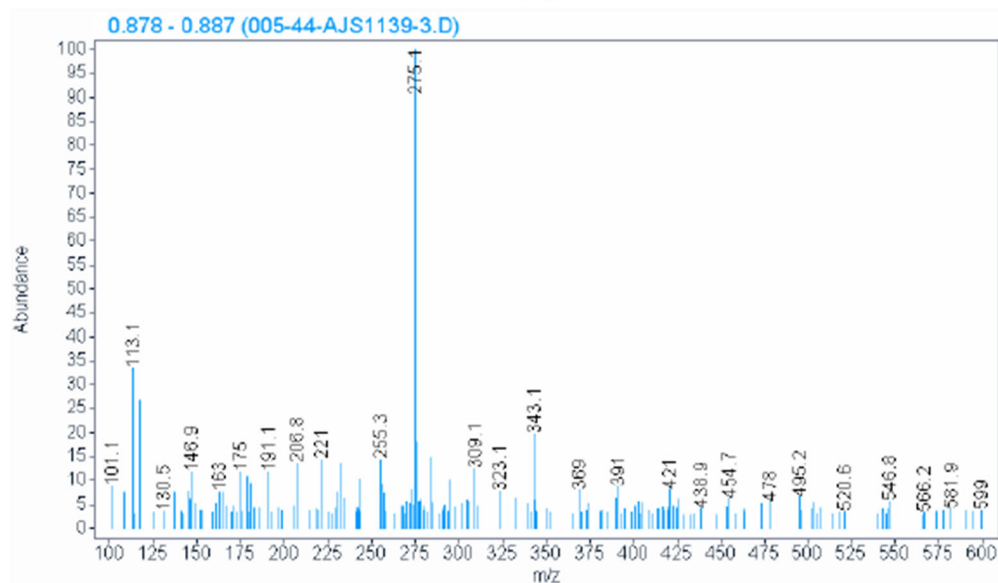
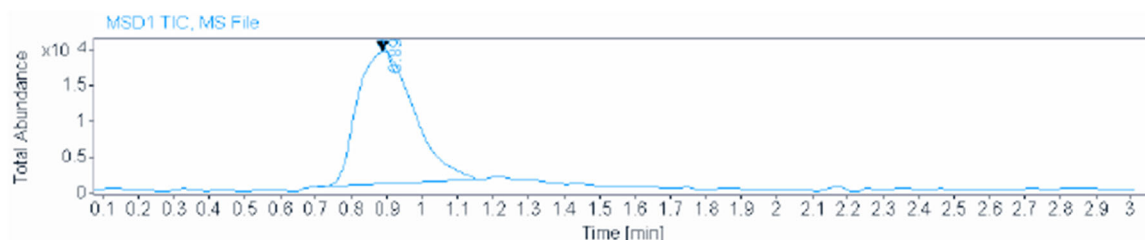
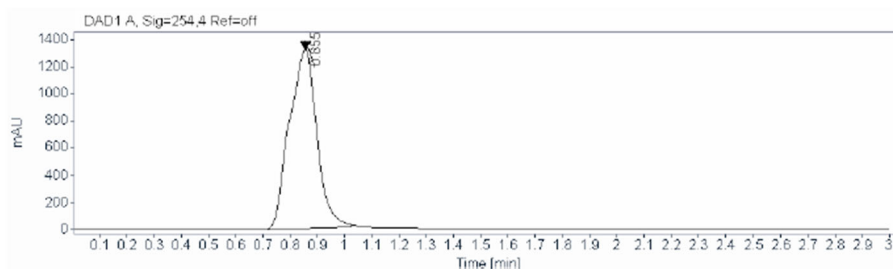


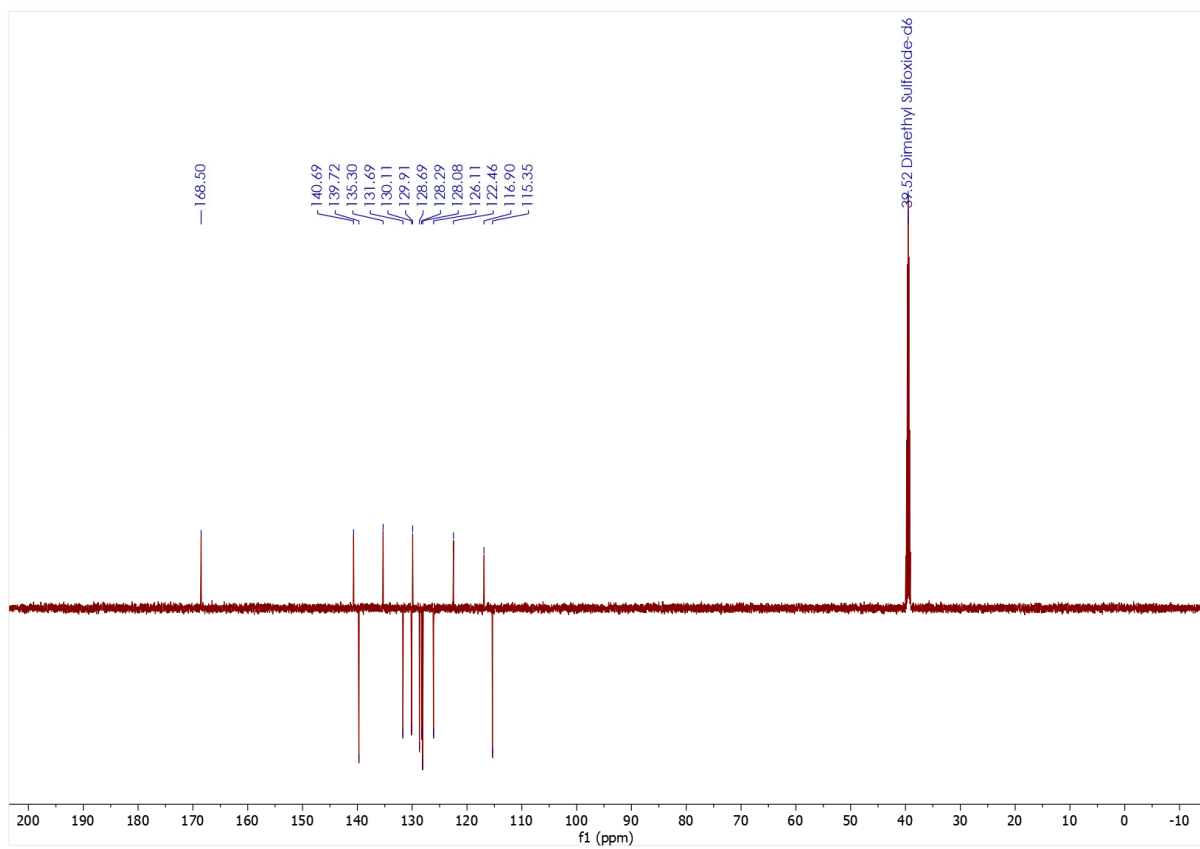
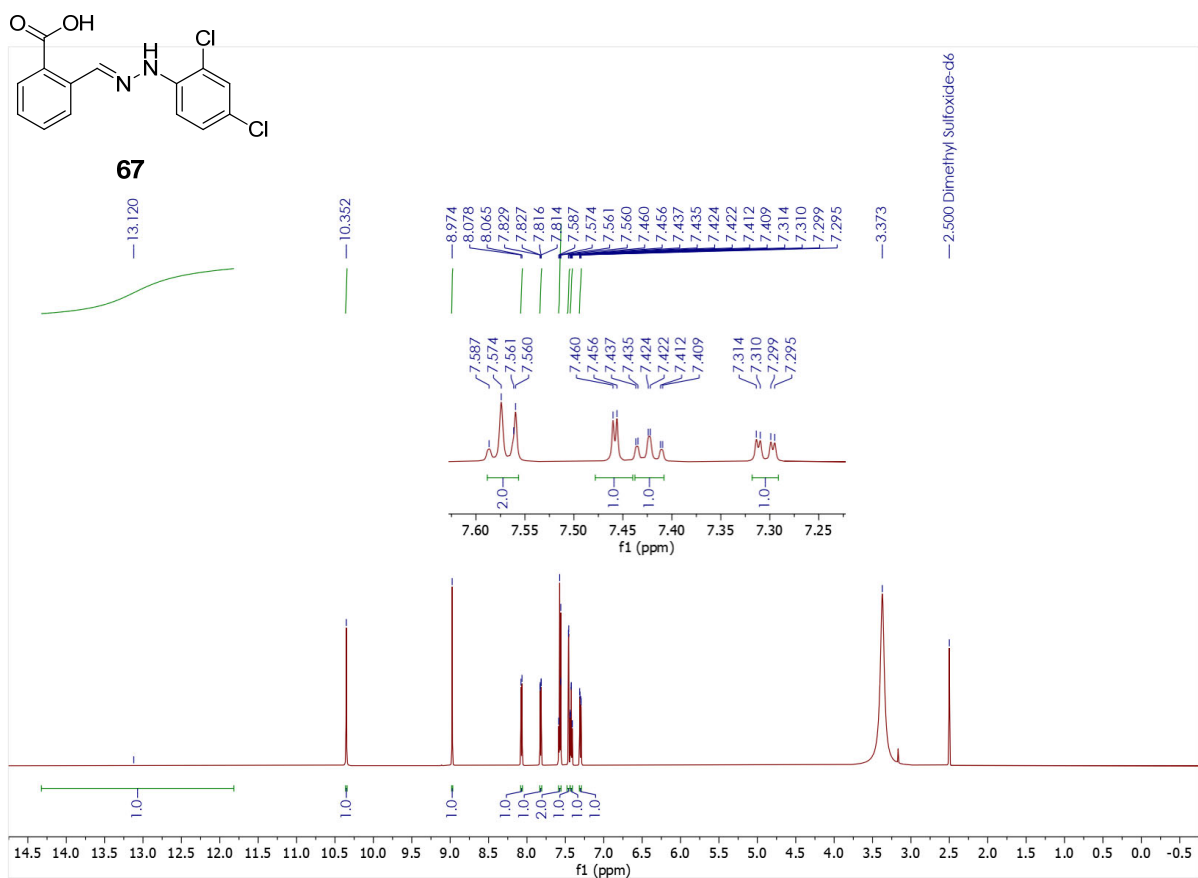
Data file: D:\Chem32\1\Data\AJS\AJS Table4+ 2023-07-31 12:52:45\005-44-AJS1139-3.D
Sample name: AJS1139-3
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Injection date: 7/31/2023 1:13:18 PM
Injection: 1 of 1
Acq. method: LCMS ISOCRATIC 80%
Injection volume: 2.000
Analysis method: LCMS ISOCRATIC
Acq. operator: SYSTEM
80%B_3 MINS.M
Last changed: 11/26/2021 9:20:48 AM



Molecular Weight: 274.702

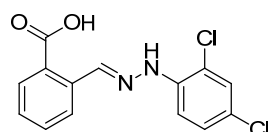
66





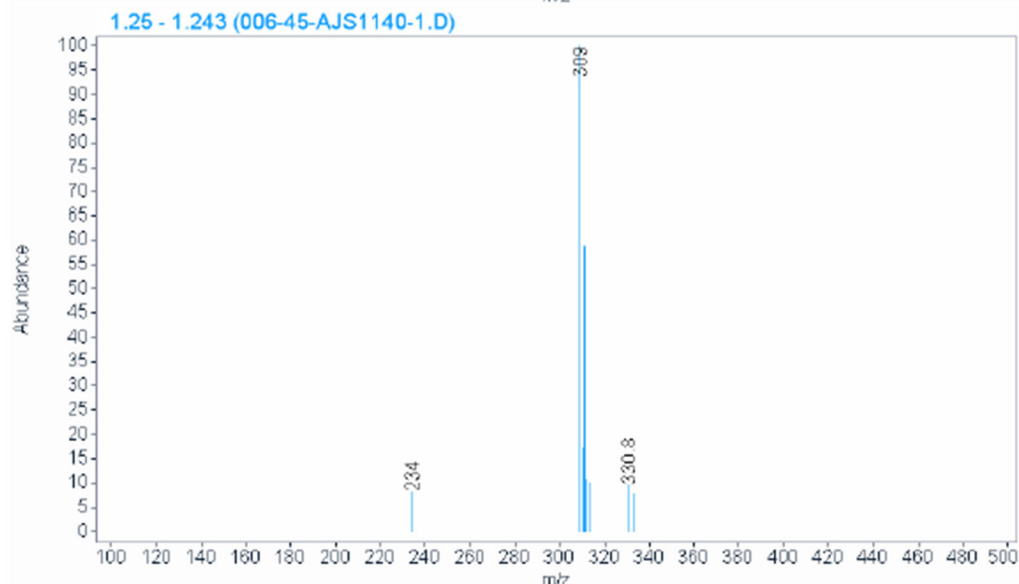
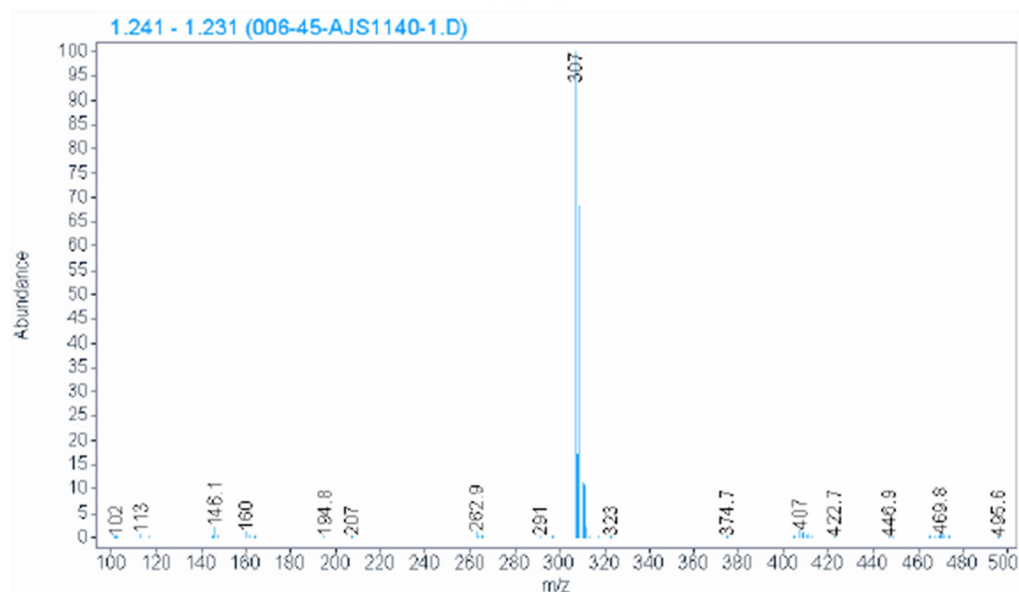
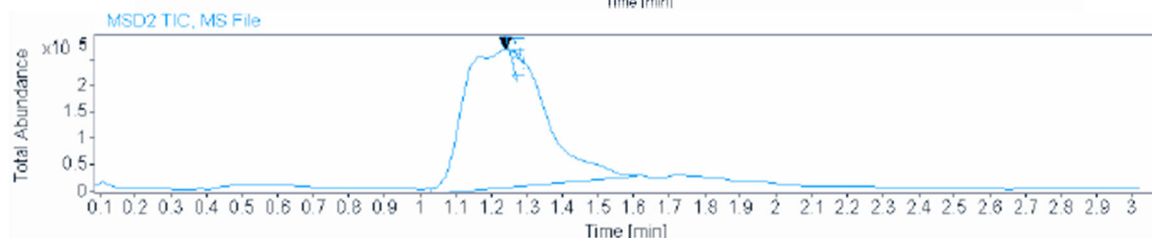
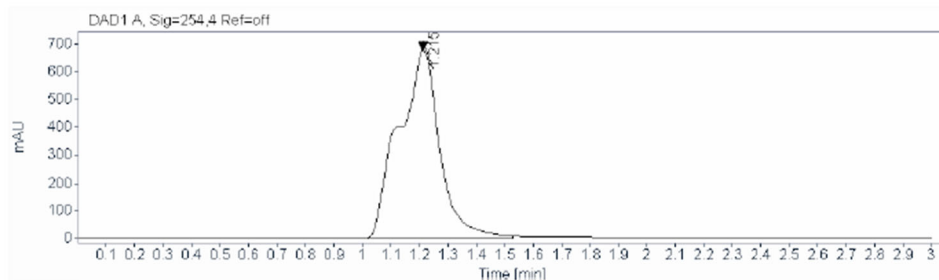


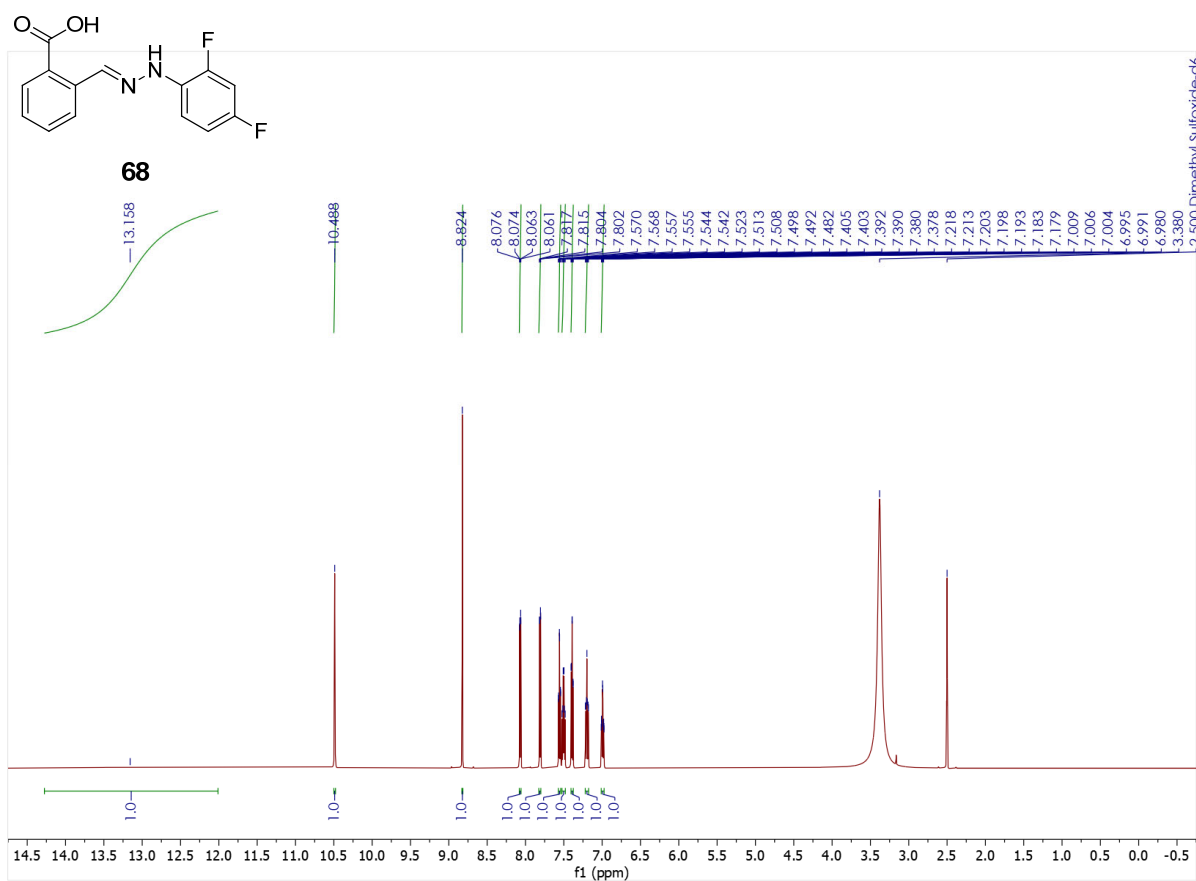
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 Sample name: AJS1140-1
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 45
 Injection date: 7/31/2023 1:17:58 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 Injection volume: 2.000
 B_3 MINS.M
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 80%B_3 MINS.M
 Last changed: 11/26/2021 9:20:48 AM



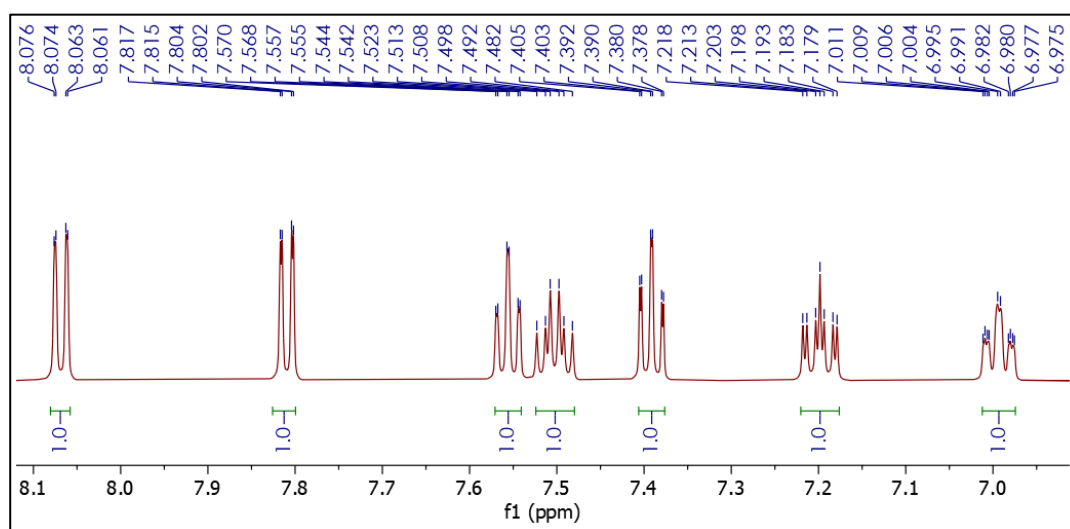
Molecular Weight: 309.147

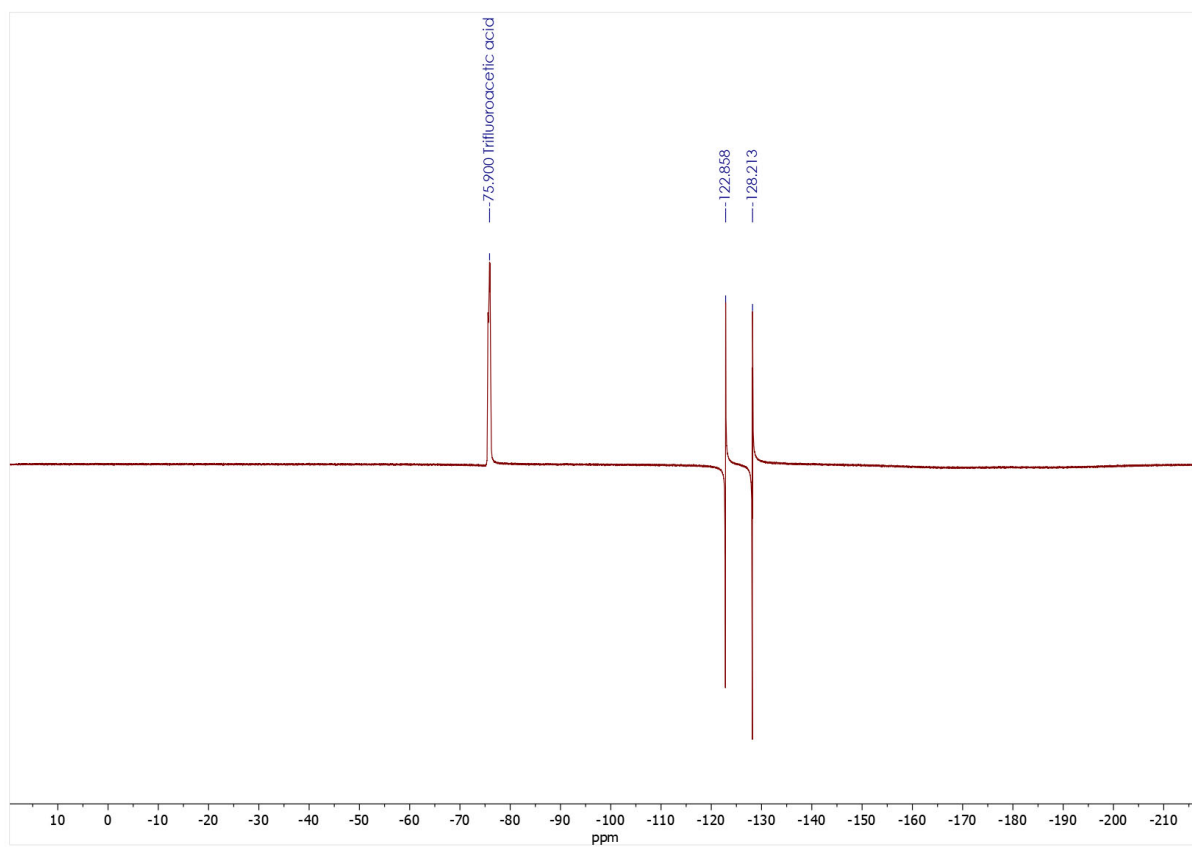
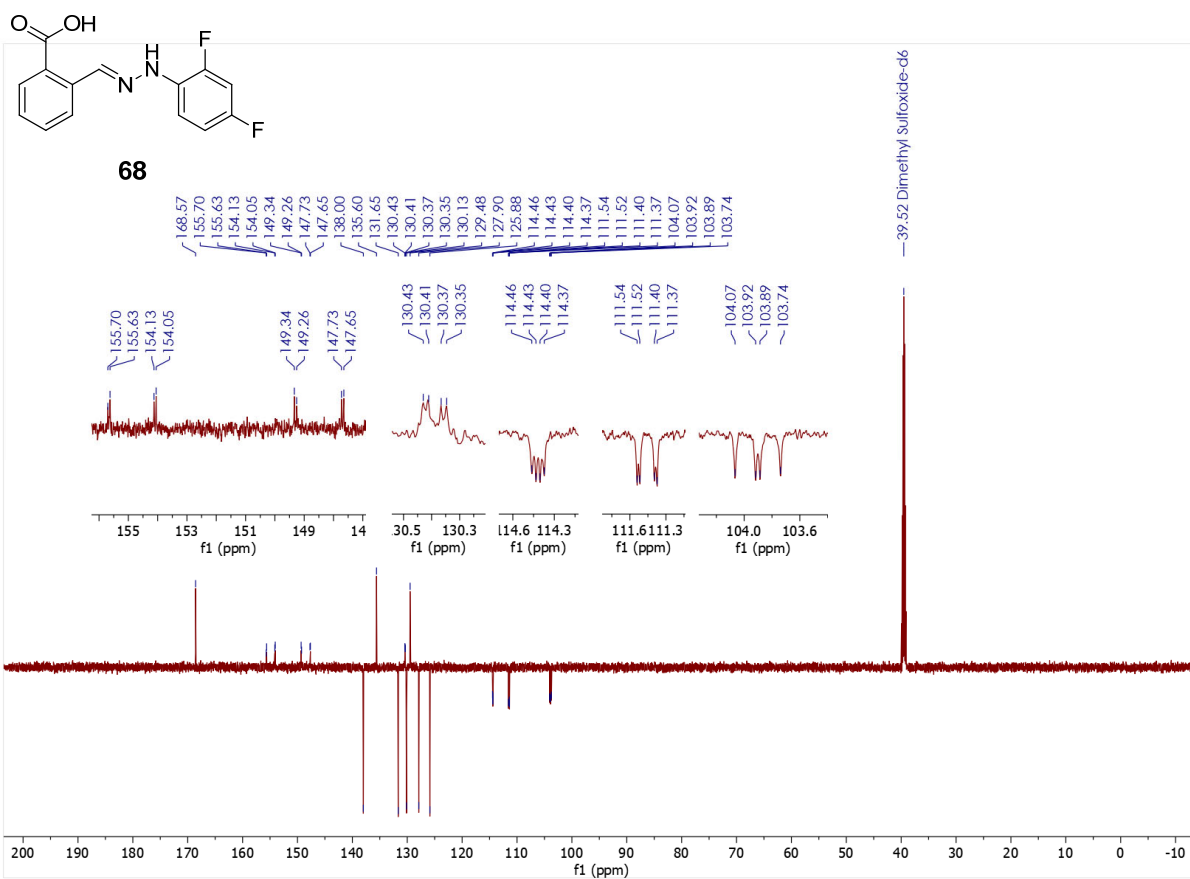
67





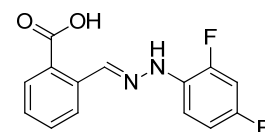
Aromatic expansion of the proton spectra:





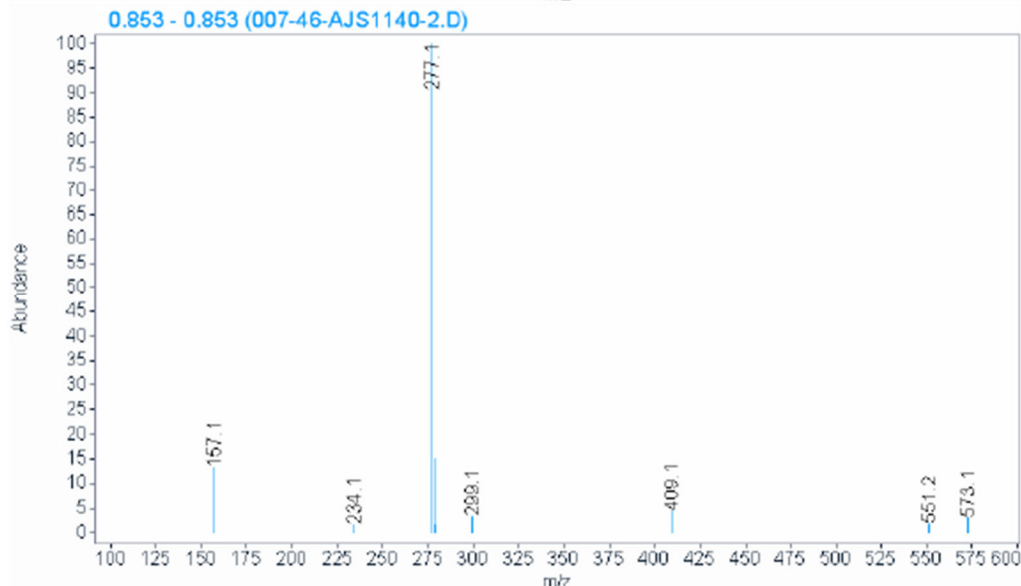
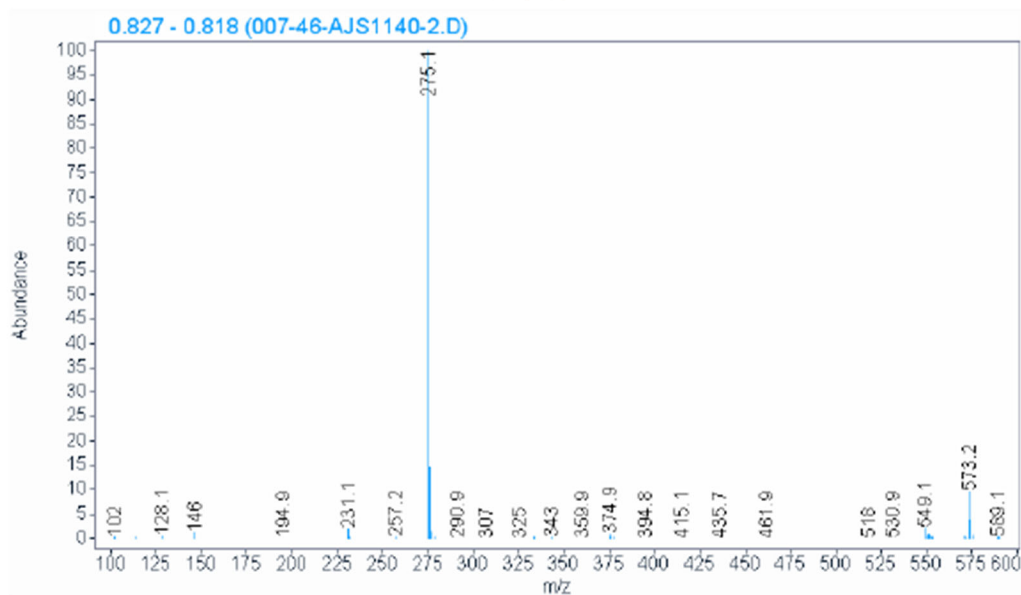
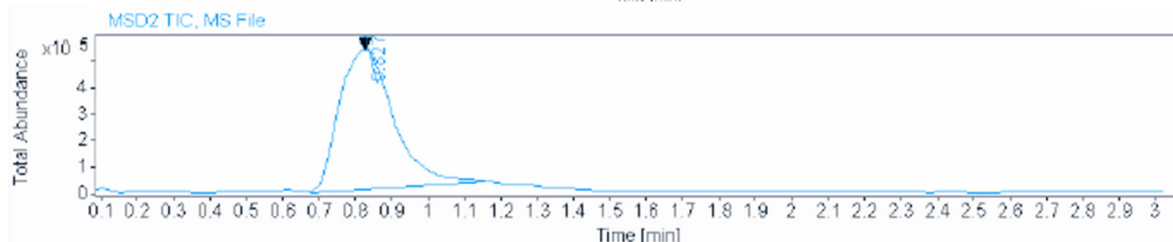
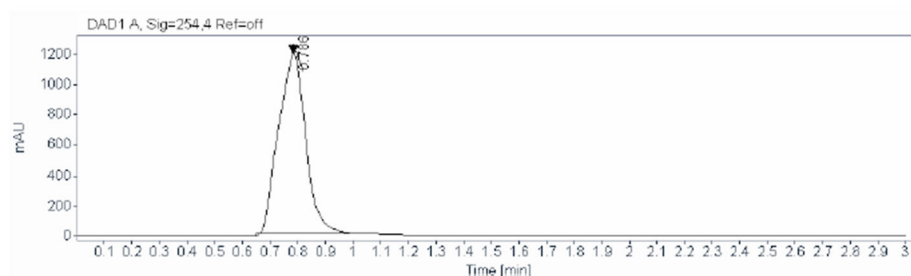


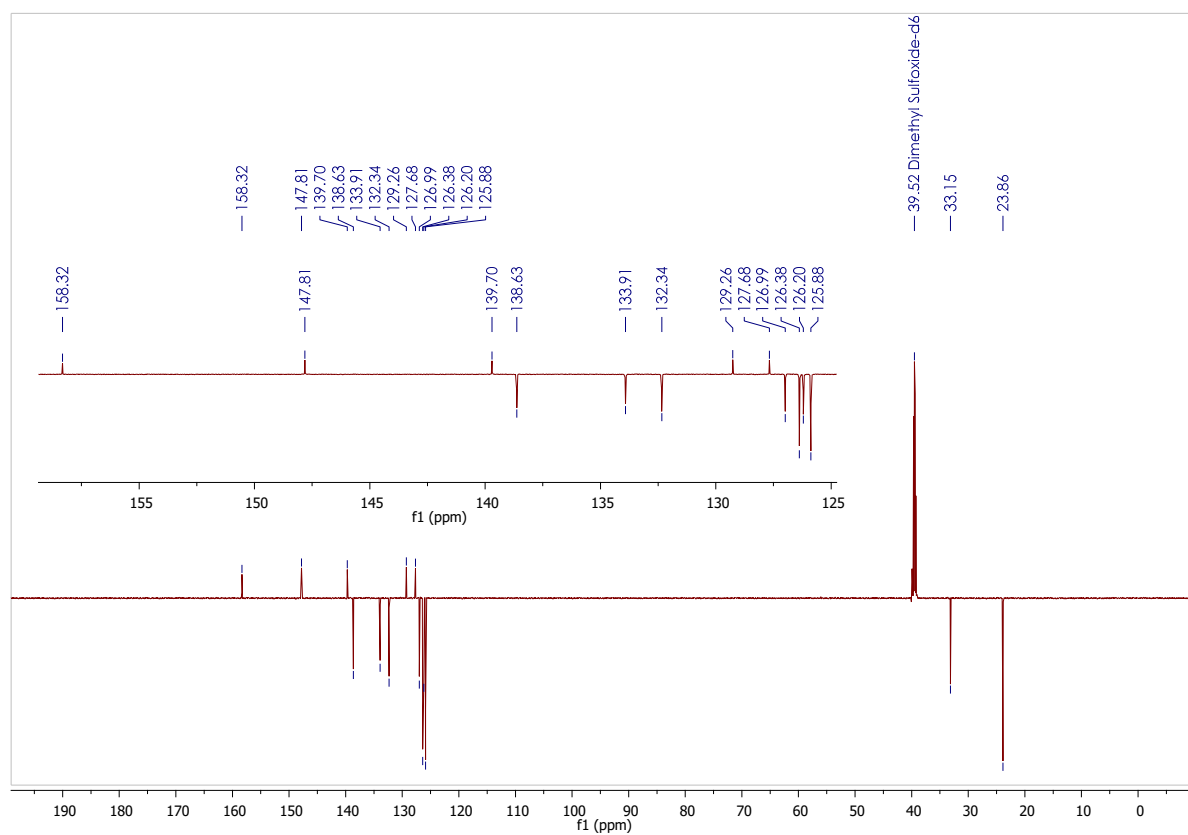
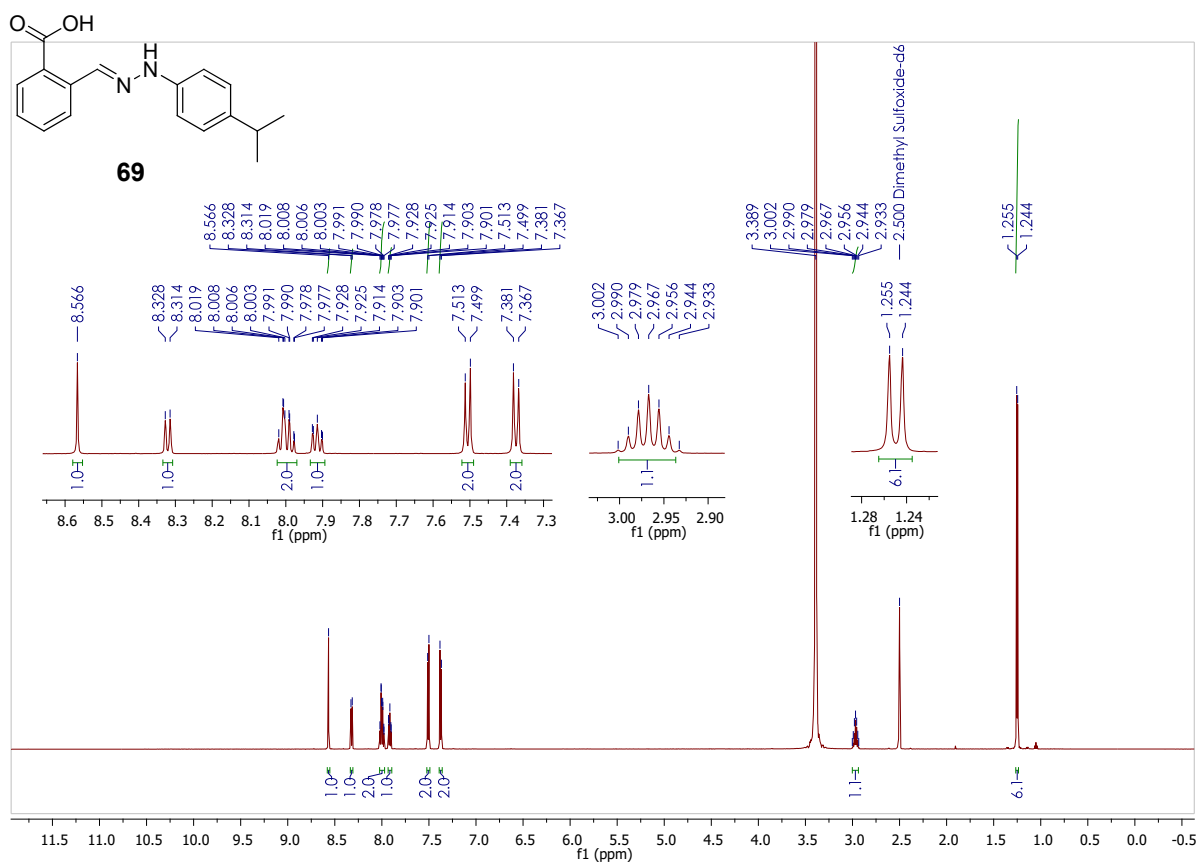
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Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Injection date: 7/31/2023 1:22:39 PM
Acq. method: LCMS ISOCRATIC 80%
B_3 MINS.M
Analysis method: LCMS ISOCRATIC
80%B_3 MINS.M
Last changed: 6/17/2024 4:15:11 PM
Location: 46
Injection: 1 of 1
Injection volume: 2.000
Acq. operator: SYSTEM



Molecular Weight: 276.238

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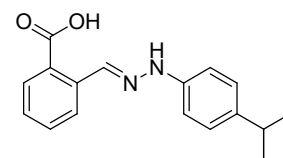


LCMS Report



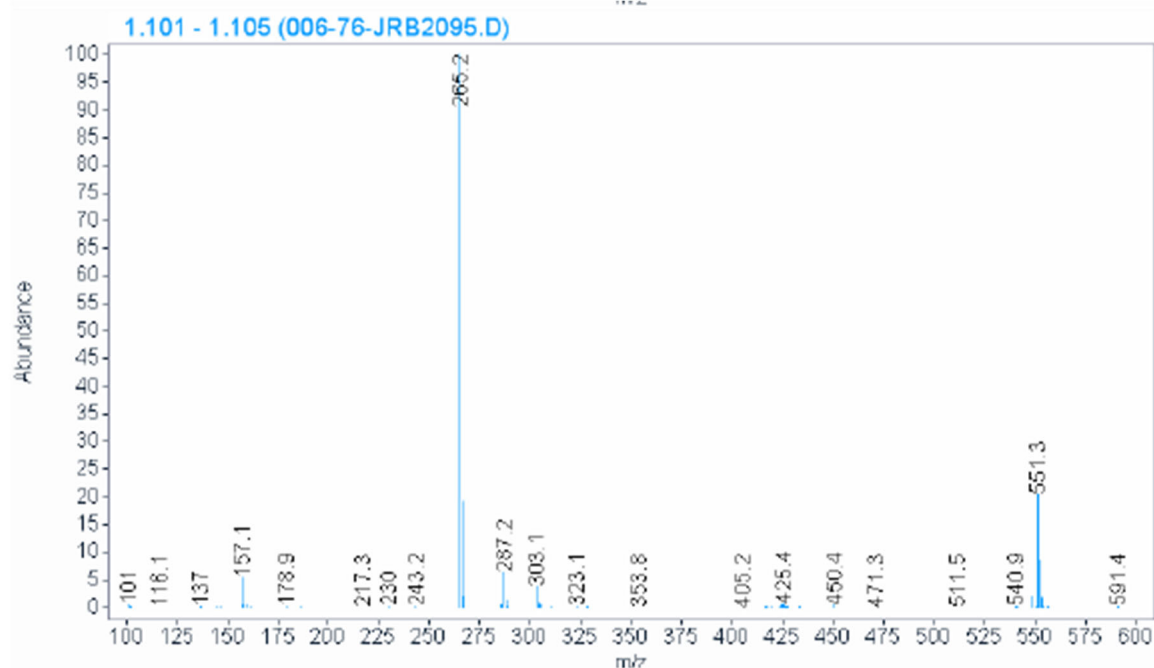
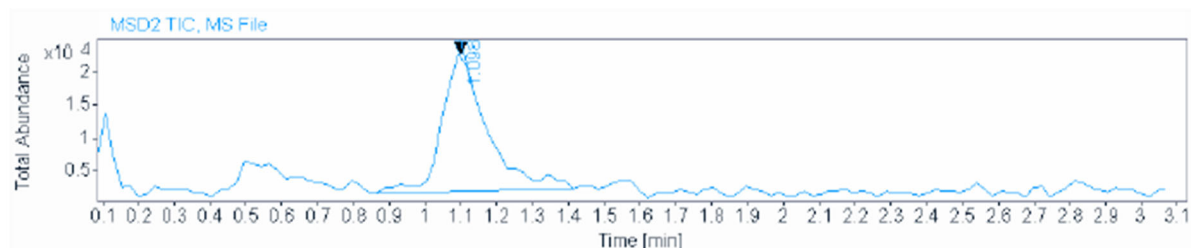
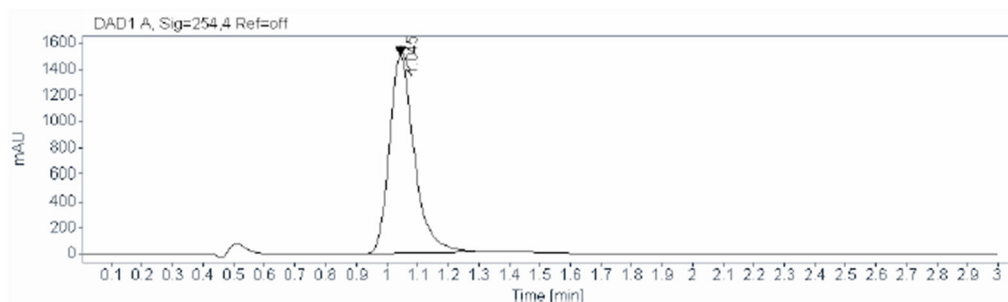
Agilent Technologies

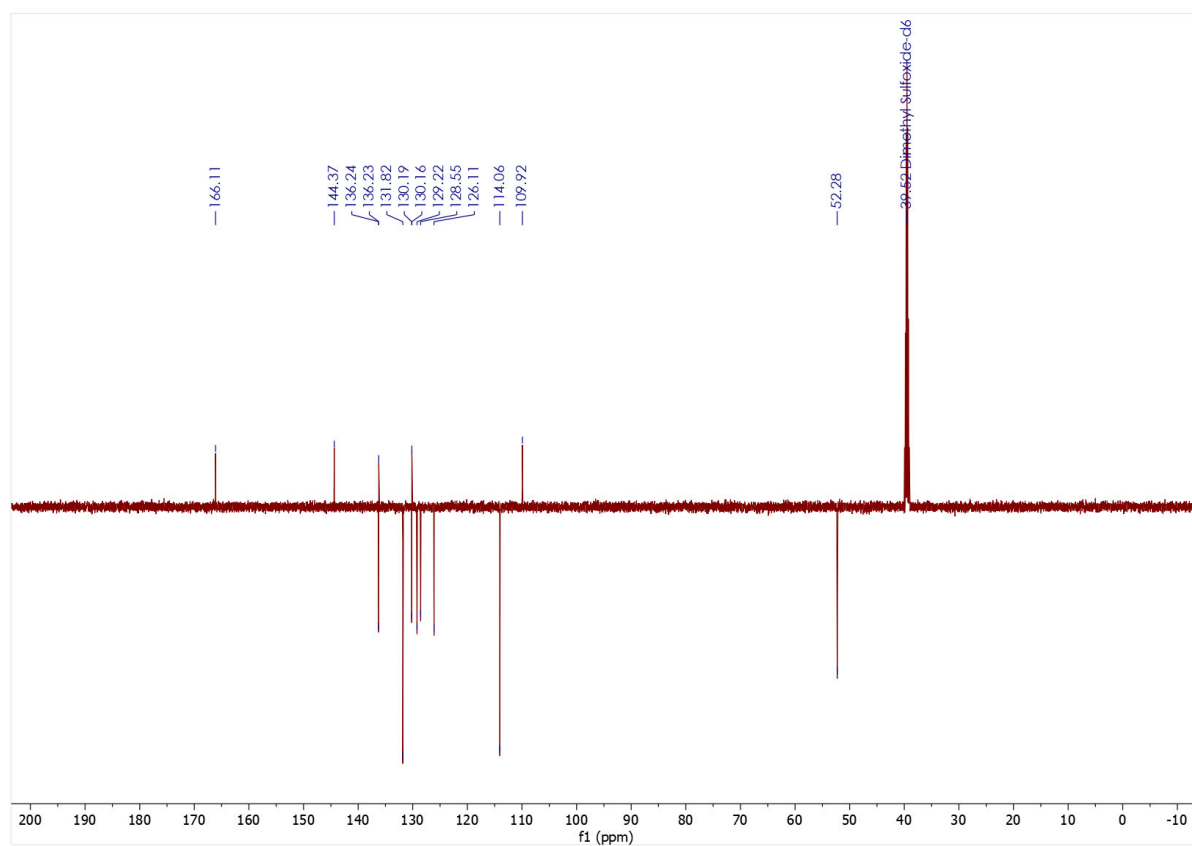
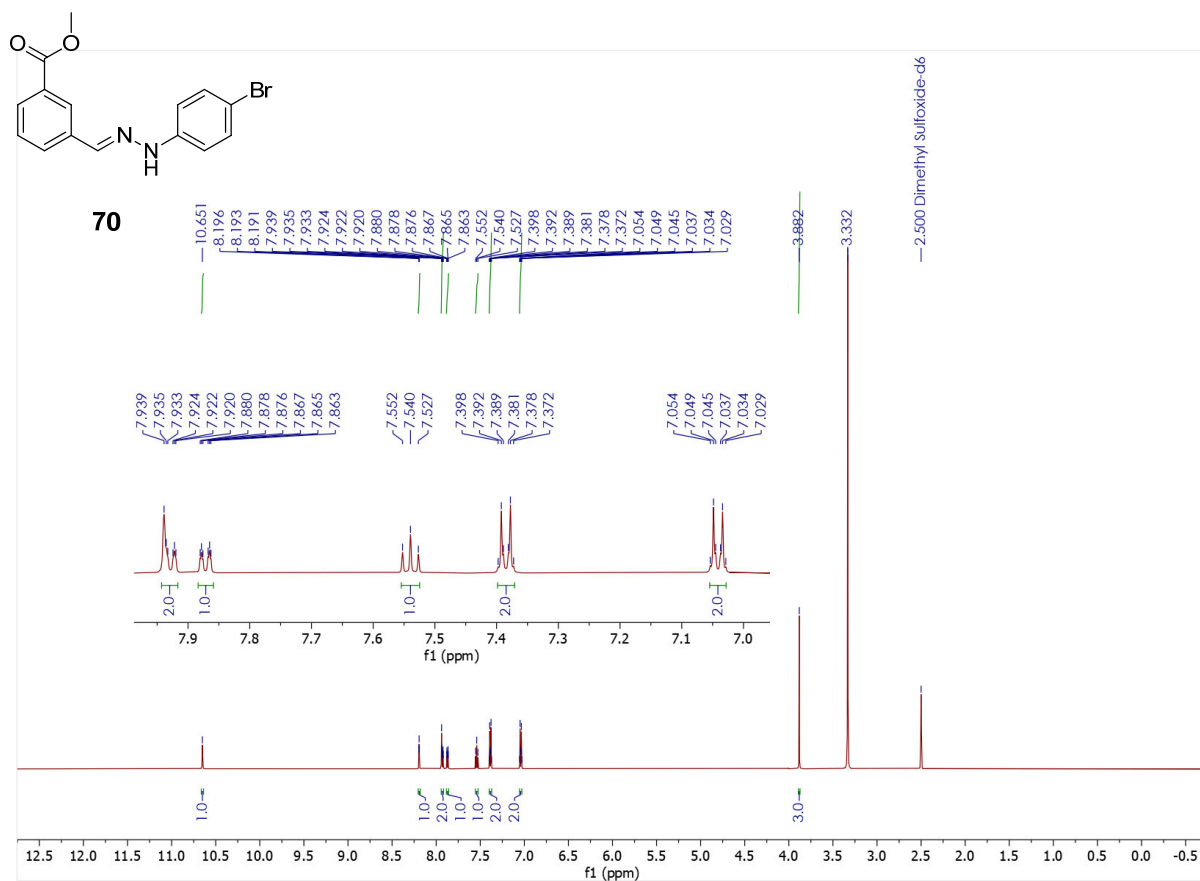
Data file: D:\Chem32\11\Data\JRB\JRB-DATA 2022-09-13 12-15-42\006-76-JRB2095.D
 Sample name: JRB2095
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 76
 Injection date: 9/13/2022 12:41:15 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 Injection volume: 2.000
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 80%B_3 MINS.M
 Last changed: 11/26/2021 9:20:48 AM



Molecular Weight: 282.337

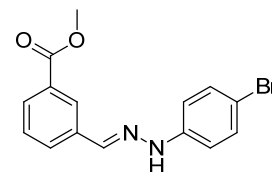
69





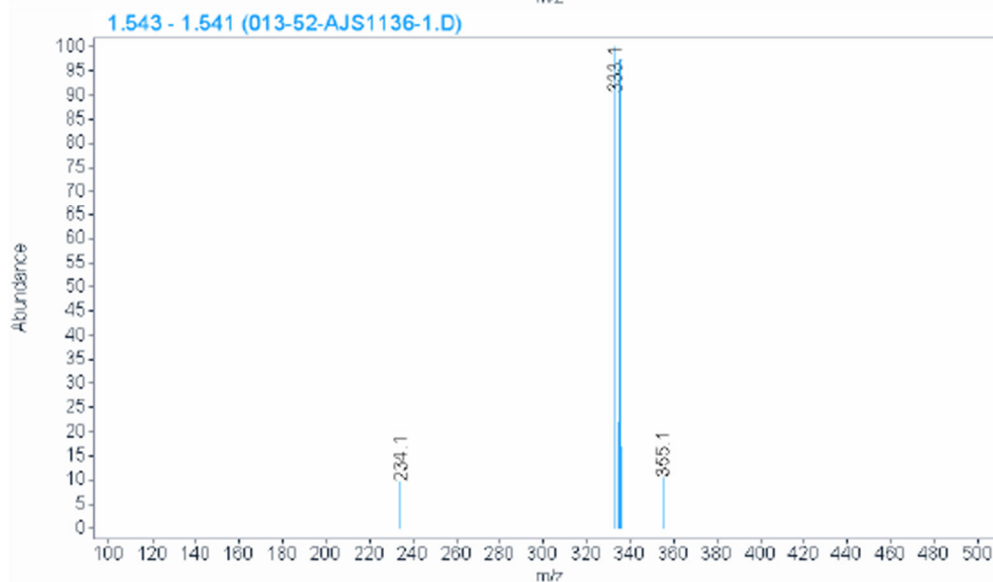
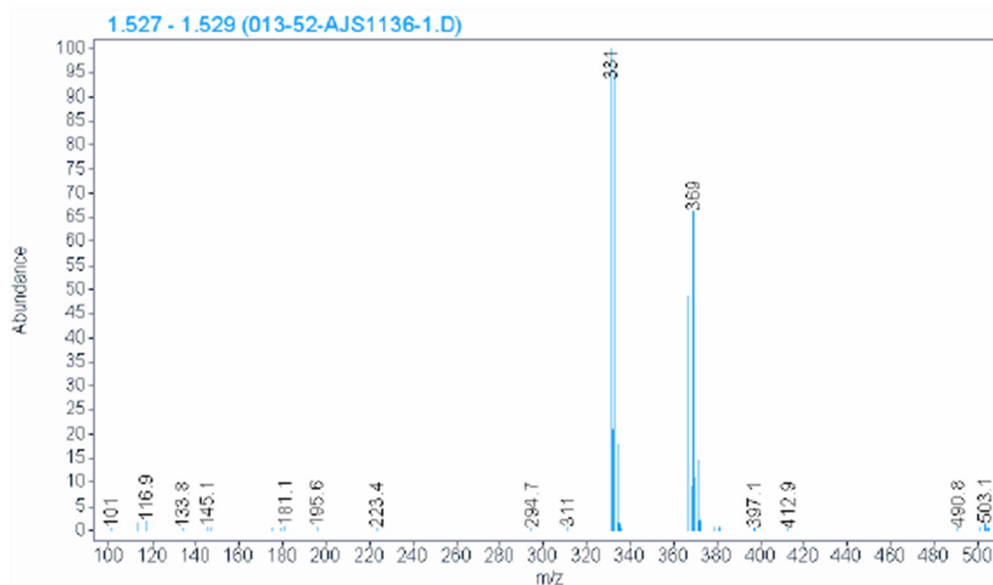
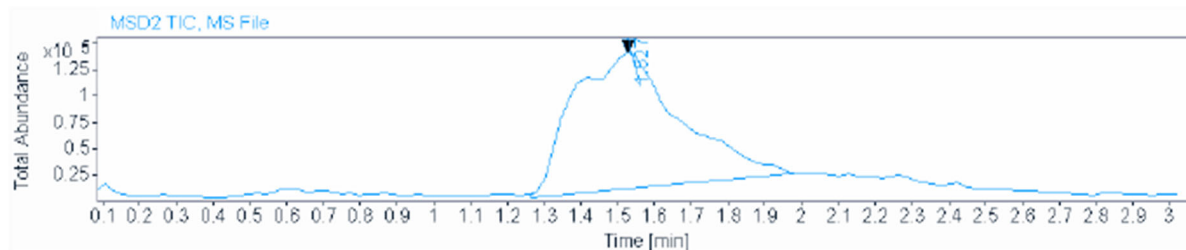
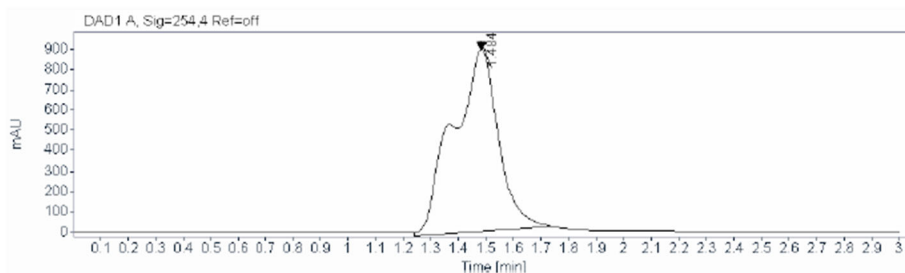
Data file: D:\Chem32\1\Data\AJS\AJS Table4+ 2023-07-31 12-52-45\013-52-AJS1136-1.D
Sample name: AJS1136-1
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Injection date: 7/31/2023 1:50:52 PM
Acq. method: LCMS ISOCRATIC 80%
B_3 MINS.M
Analysis method: LCMS ISOCRATIC
80%B_3 MINS.M
Last changed: 11/26/2021 9:20:48 AM

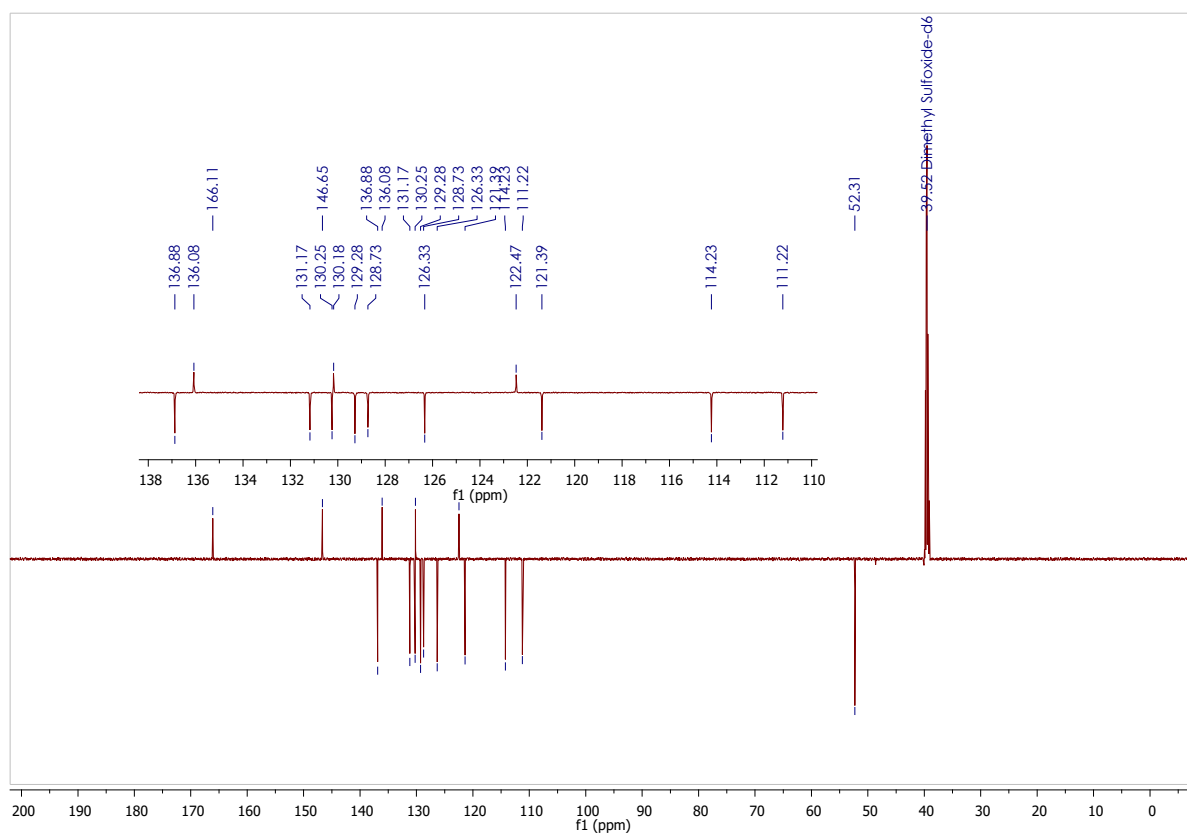
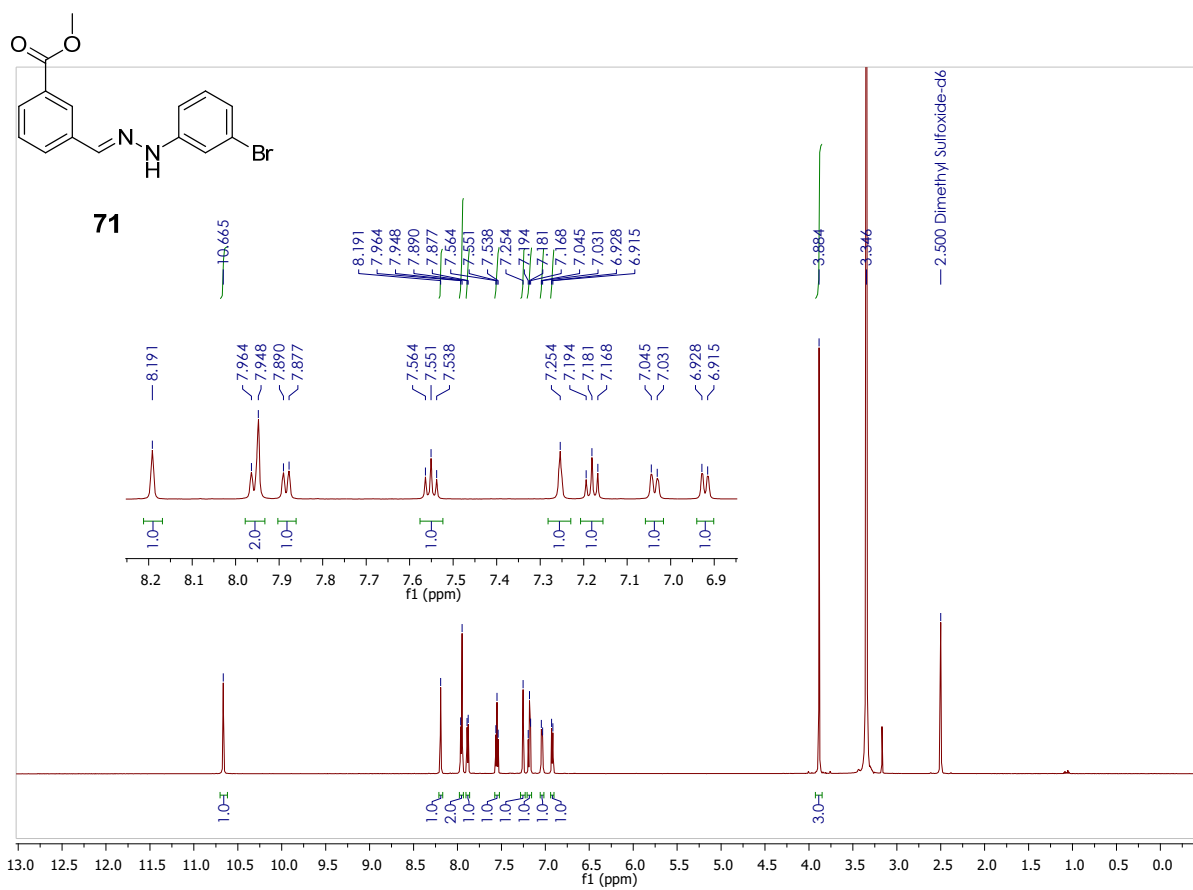
Location: 52
Injection: 1 of 1
Injection volume: 2.000
Acq. operator: SYSTEM



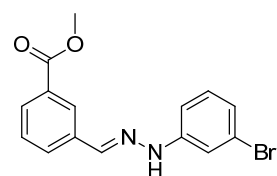
Molecular Weight: 333.180

70



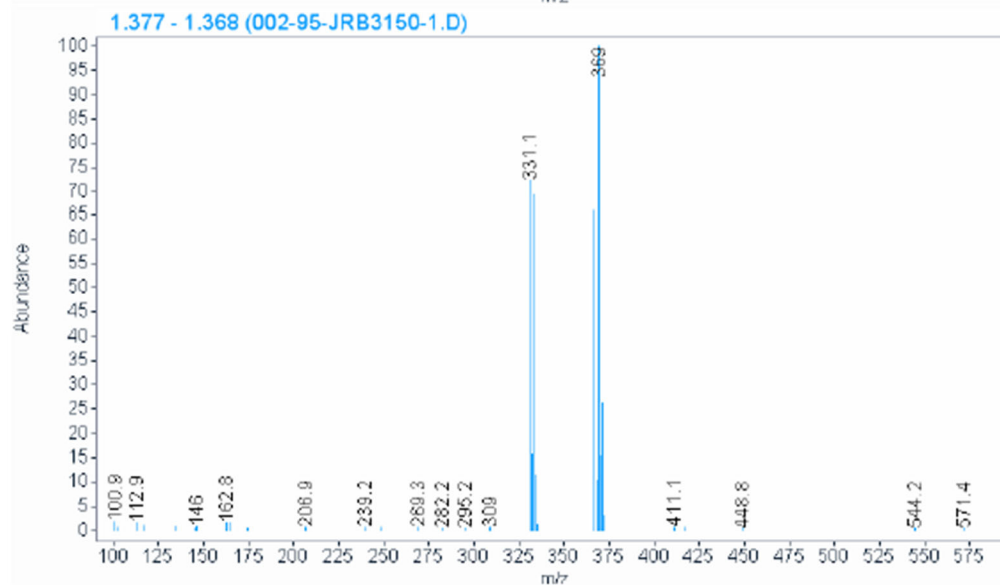
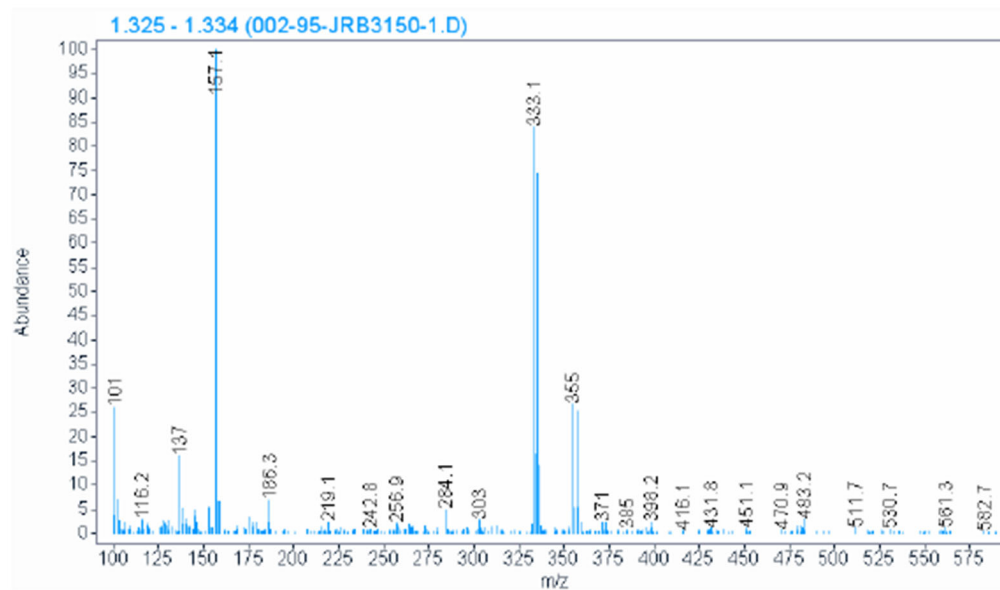
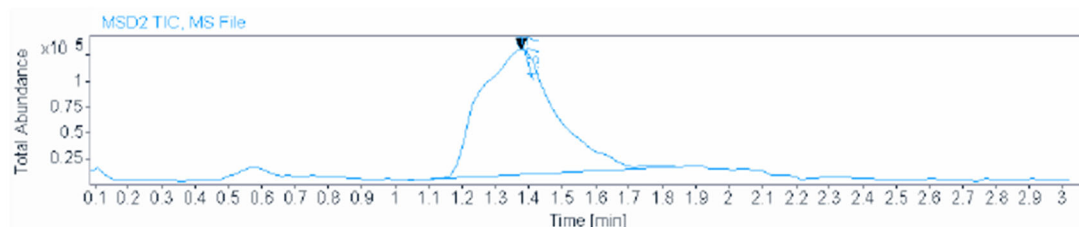
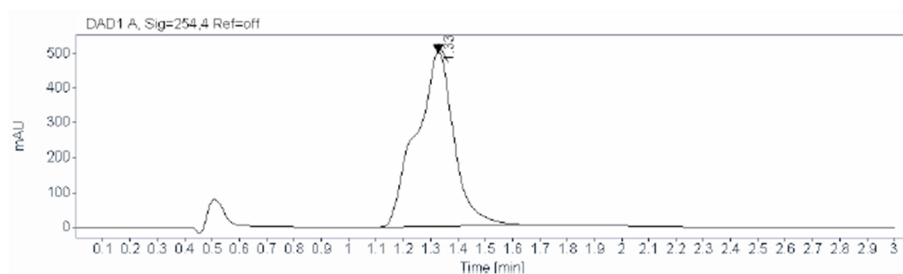


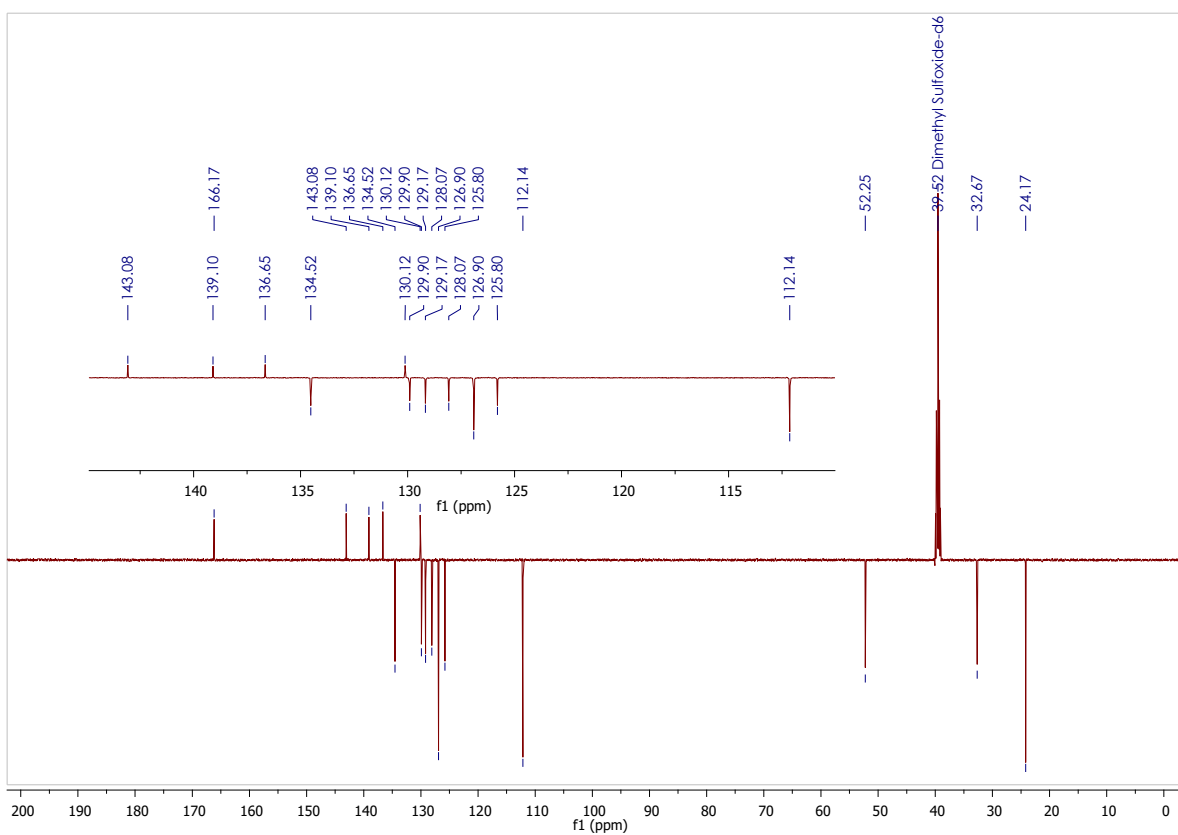
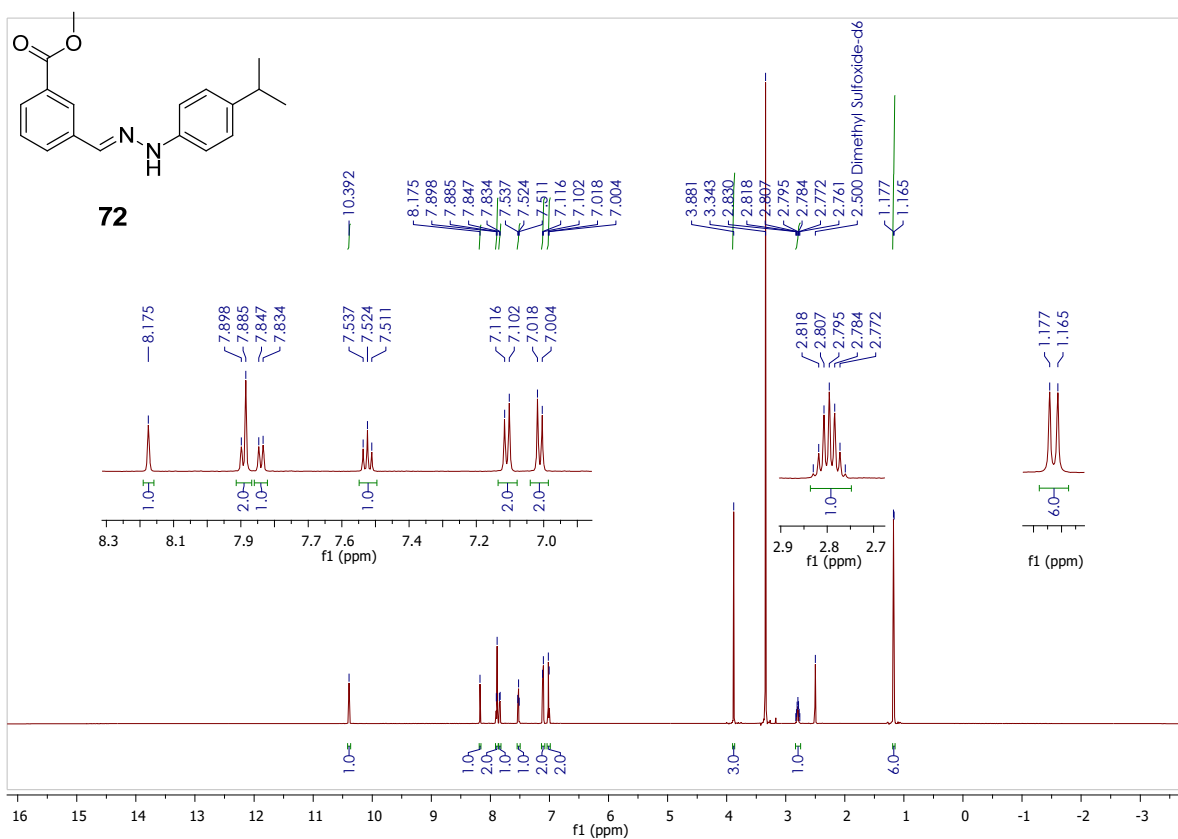
Data file: D:\Chem32\1\Data\JEN\JRB3150 3151 2023-04-28 10-07-04\002-95-JRB3150-1.D
Sample name: JRB3150-1
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Location: 95
Injection date: 4/28/2023 10:13:29 AM
Injection: 1 of 1
Acq. method: LCMS ISOCRATIC 80% B_3 MINS.M
Injection volume: 2.000
Analysis method: LCMS ISOCRATIC 80%B_3 MINS.M
Acq. operator: SYSTEM
Last changed: 11/26/2021 9:20:48 AM



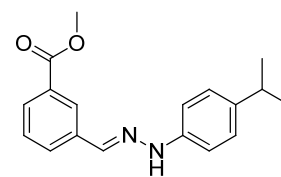
Molecular Weight: 333.180

71



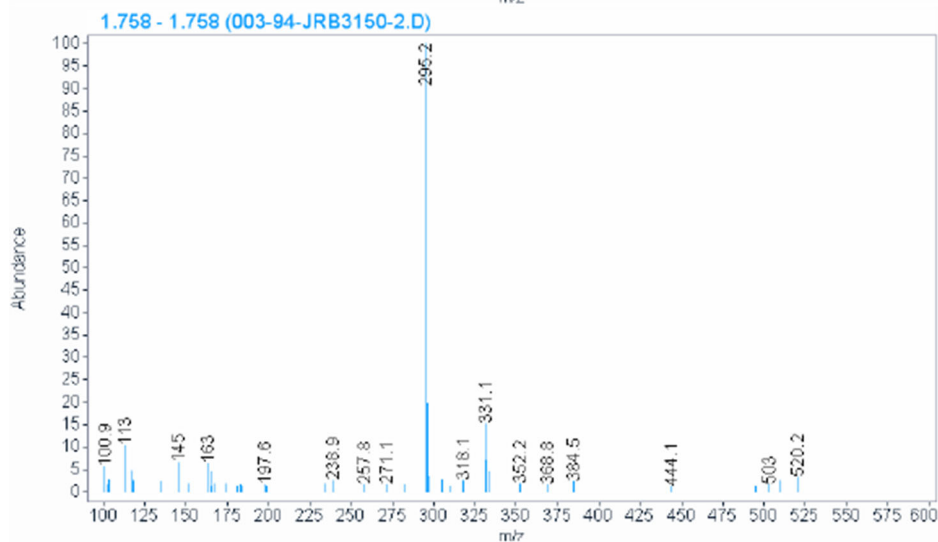
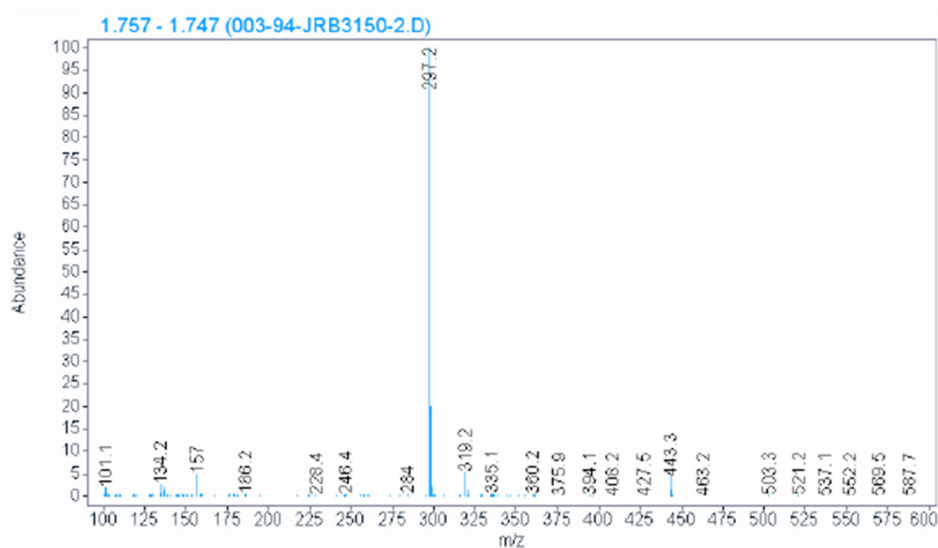
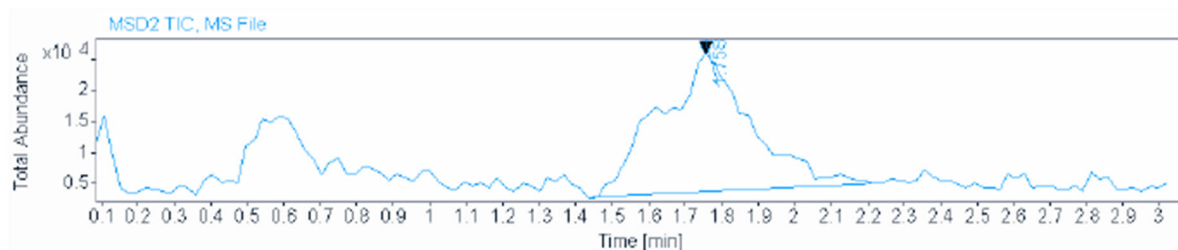
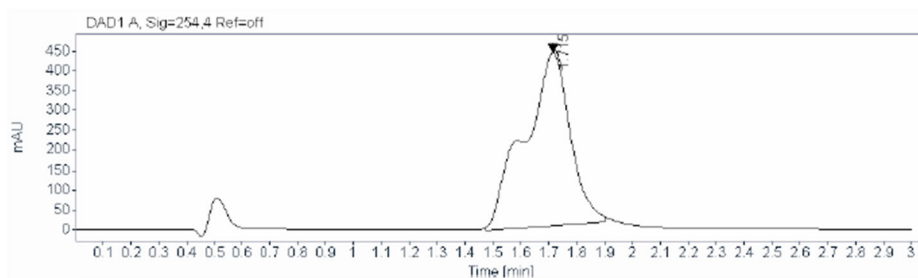


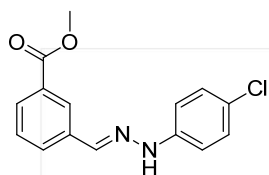
Data file: D:\Chem32\1\Data\JEN\JRB3150 3151 2023-04-28 10-07-04\003-94-JRB3150-2.D
 Sample name: JRB3150-2
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 94
 Injection date: 4/28/2023 10:18:07 AM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80% B_3 MINS.M
 Injection volume: 2.000
 Analysis method: LCMS ISOCRATIC 80%B_3 MINS.M
 Acq. operator: SYSTEM
 Last changed: 11/26/2021 9:20:48 AM



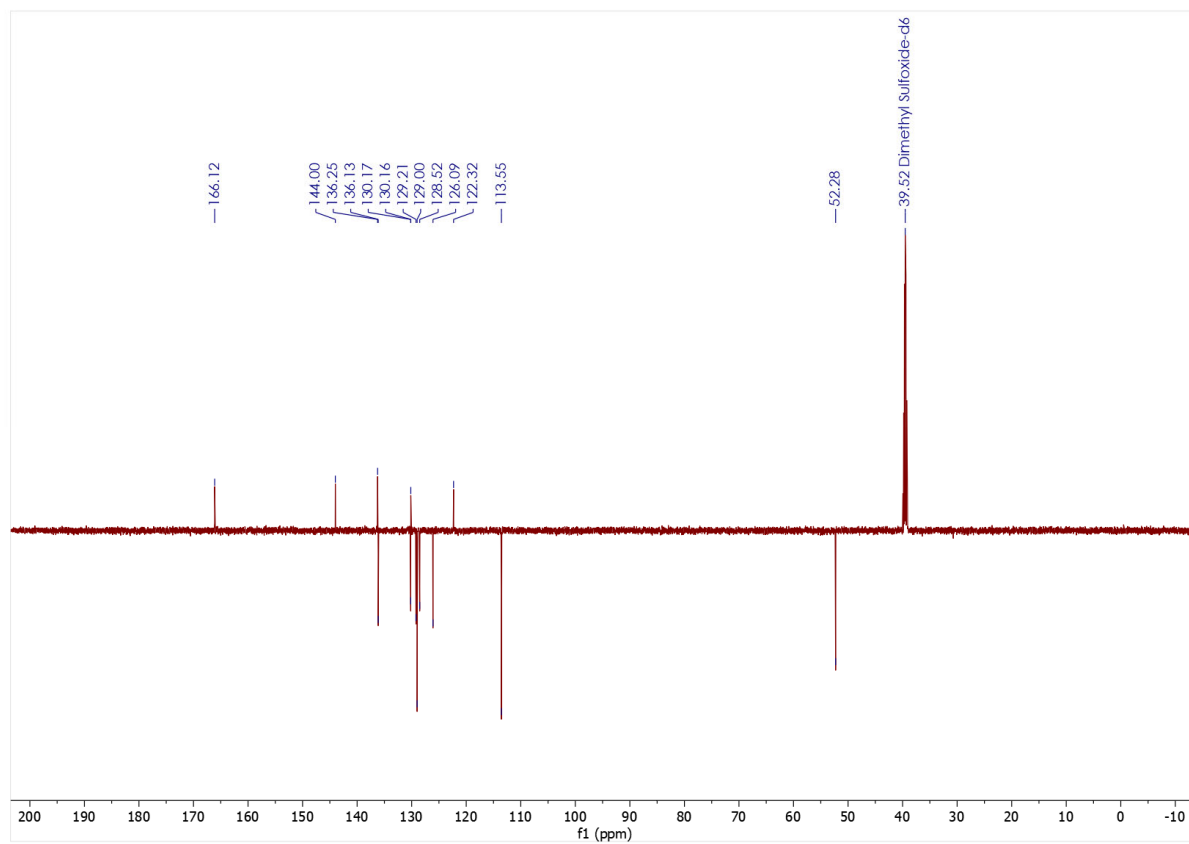
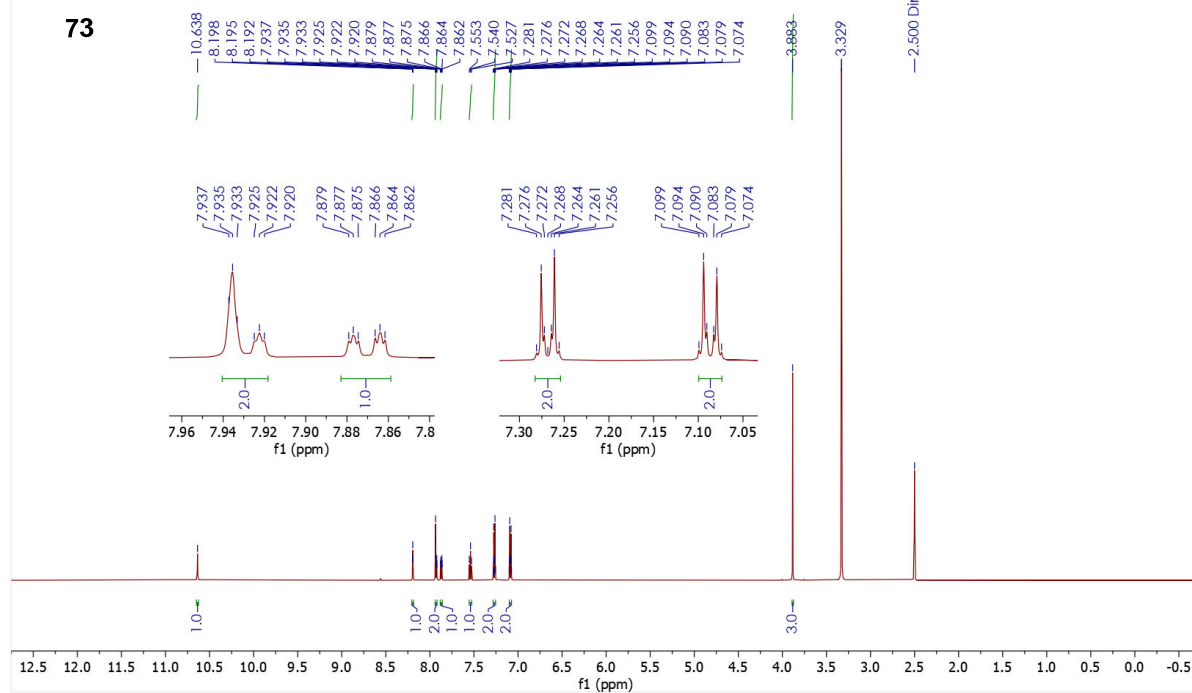
Molecular Weight: 296.364

72

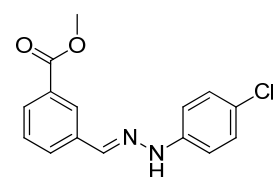




73

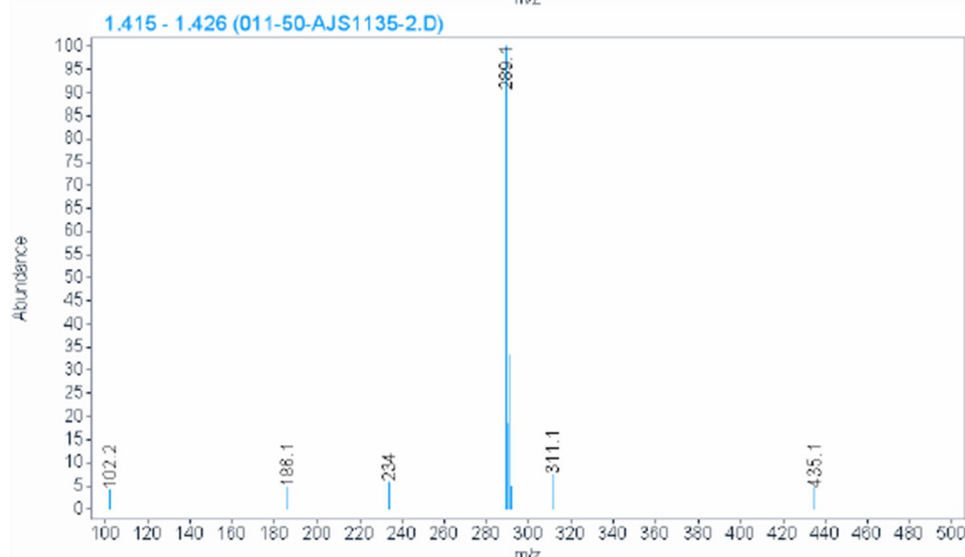
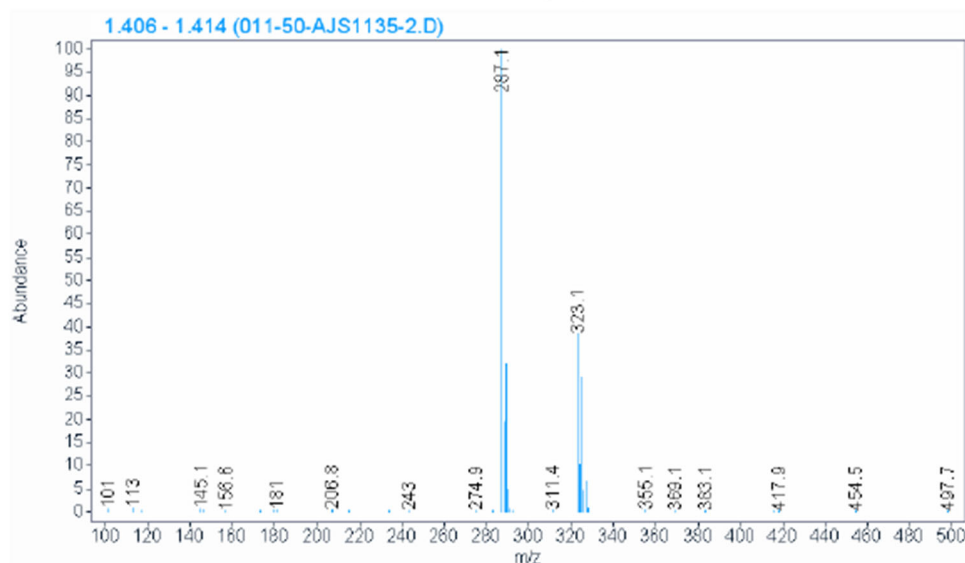
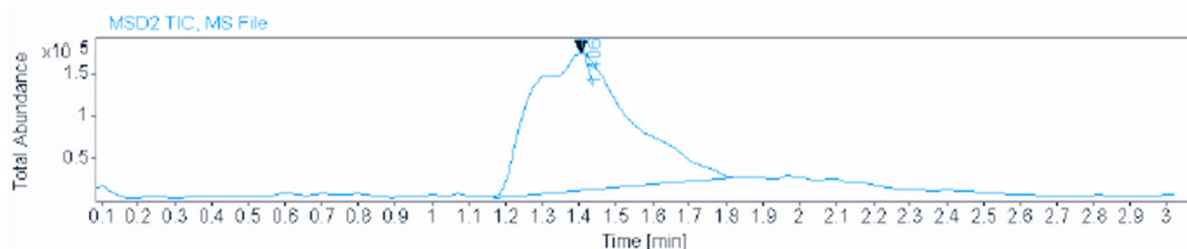
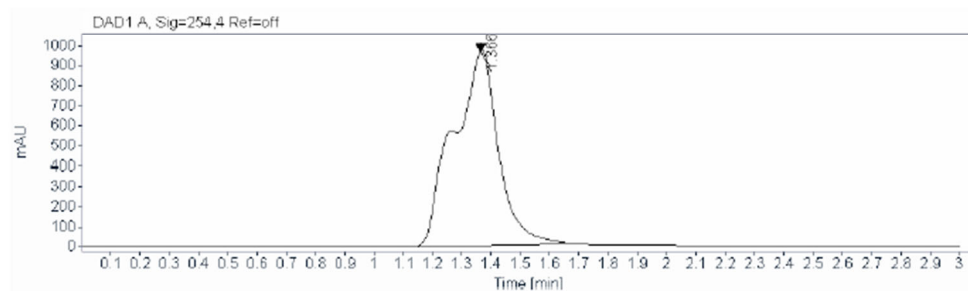


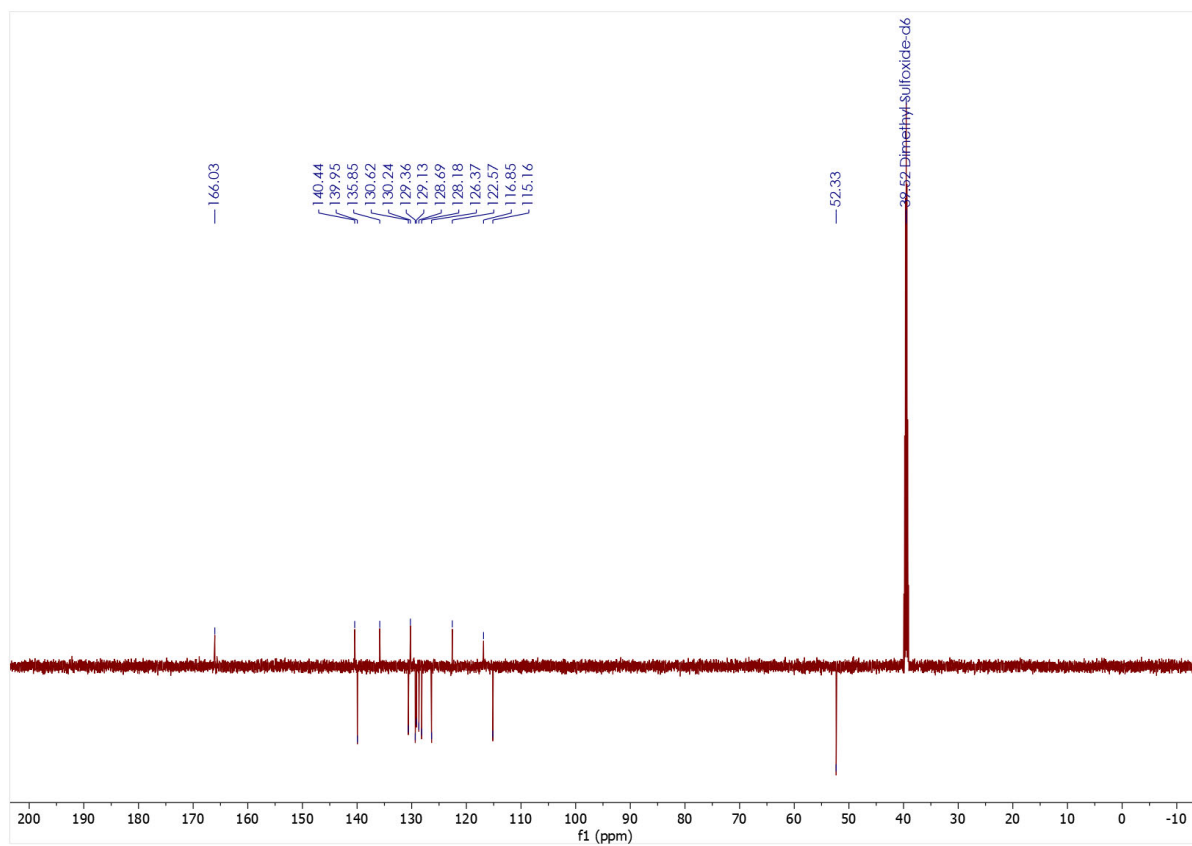
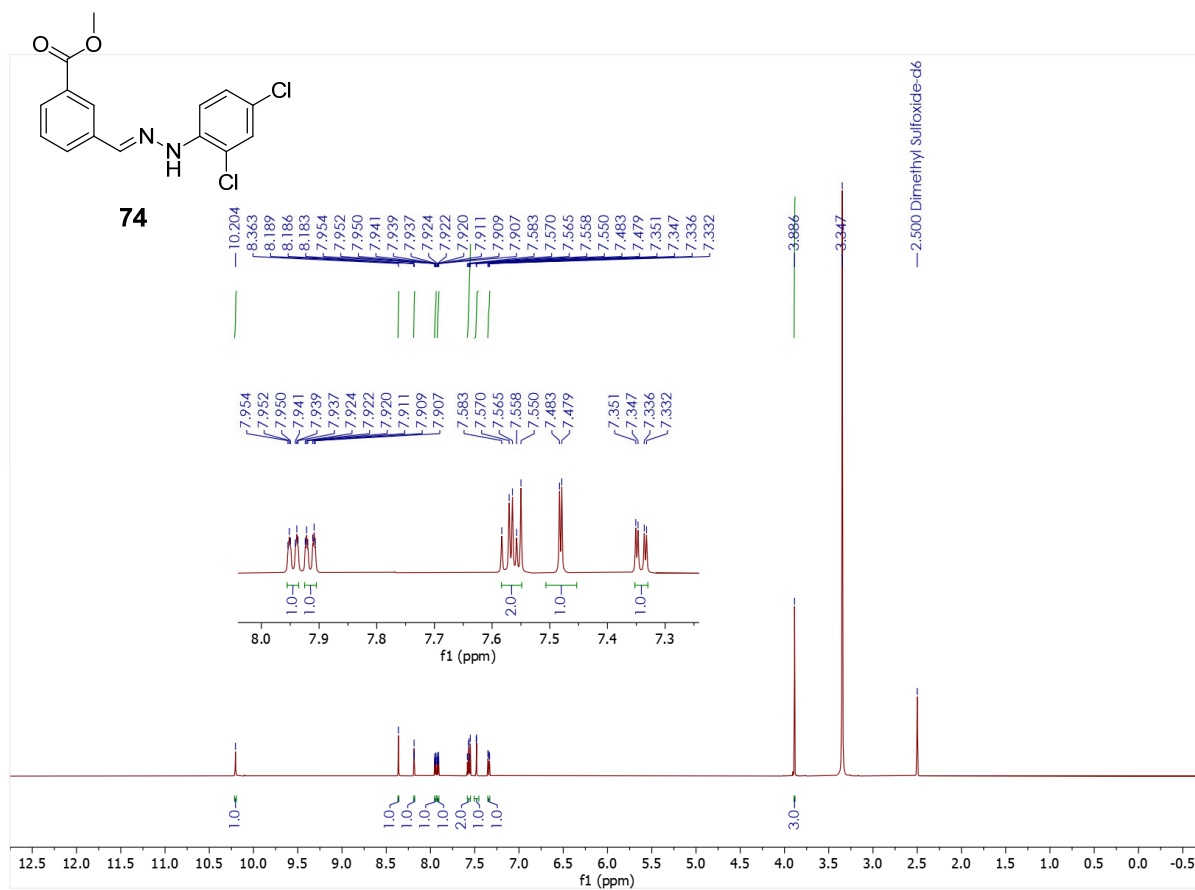
Data file: D:\Chem32\1\Data\AJS\AJS Table4+ 2023-07-31 12-52-45\011-50-AJS1135-2.D
Sample name: AJS1135-2
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Location: 50
Injection date: 7/31/2023 1:41:34 PM
Injection: 1 of 1
Acq. method: LCMS ISOCRATIC 80%
Injection volume: 2.000
Analysis method: LCMS ISOCRATIC
Acq. operator: SYSTEM
Last changed: 11/26/2021 9:20:48 AM
80%B_3 MINS.M



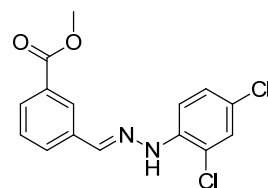
Molecular Weight: 288.729

73



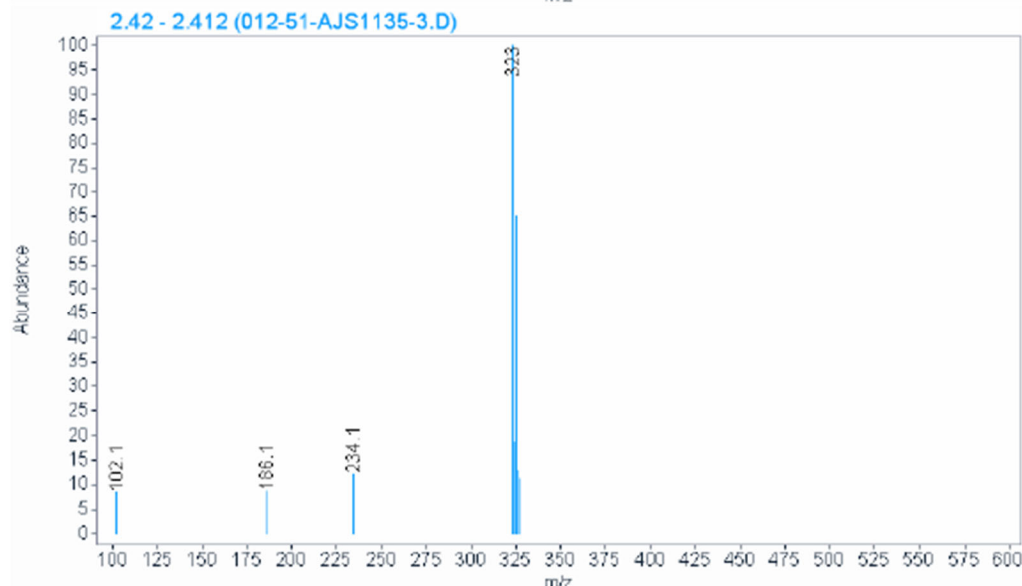
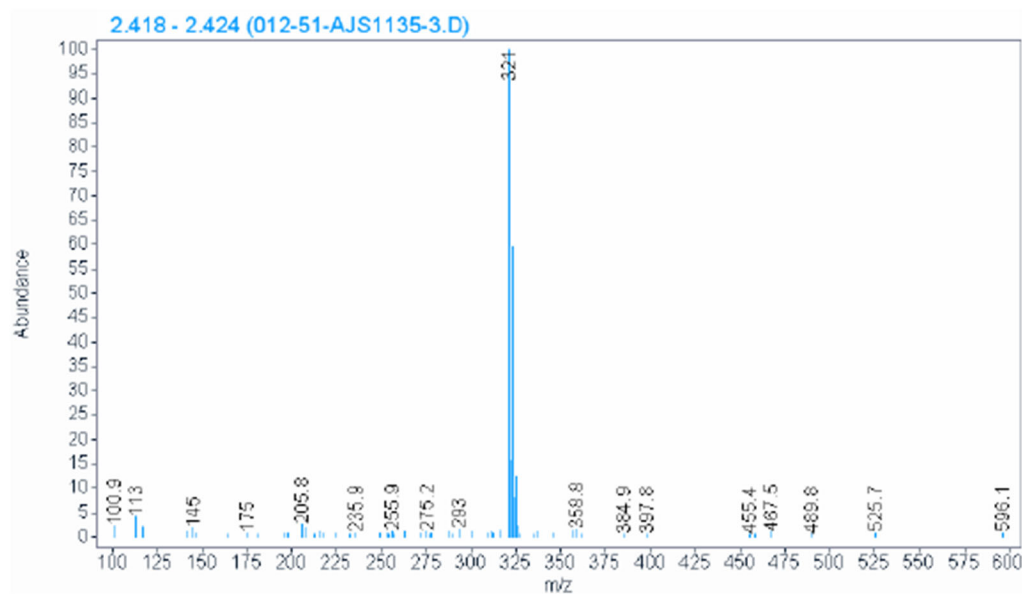


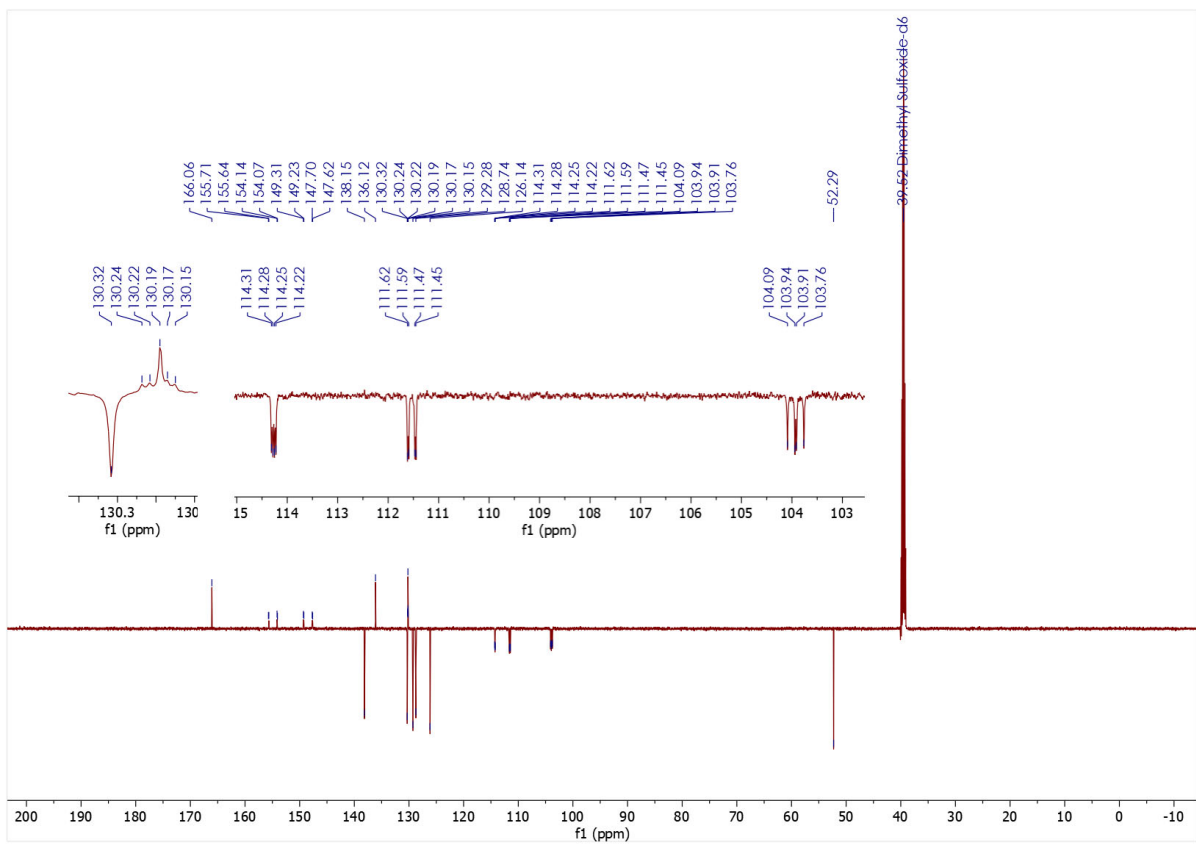
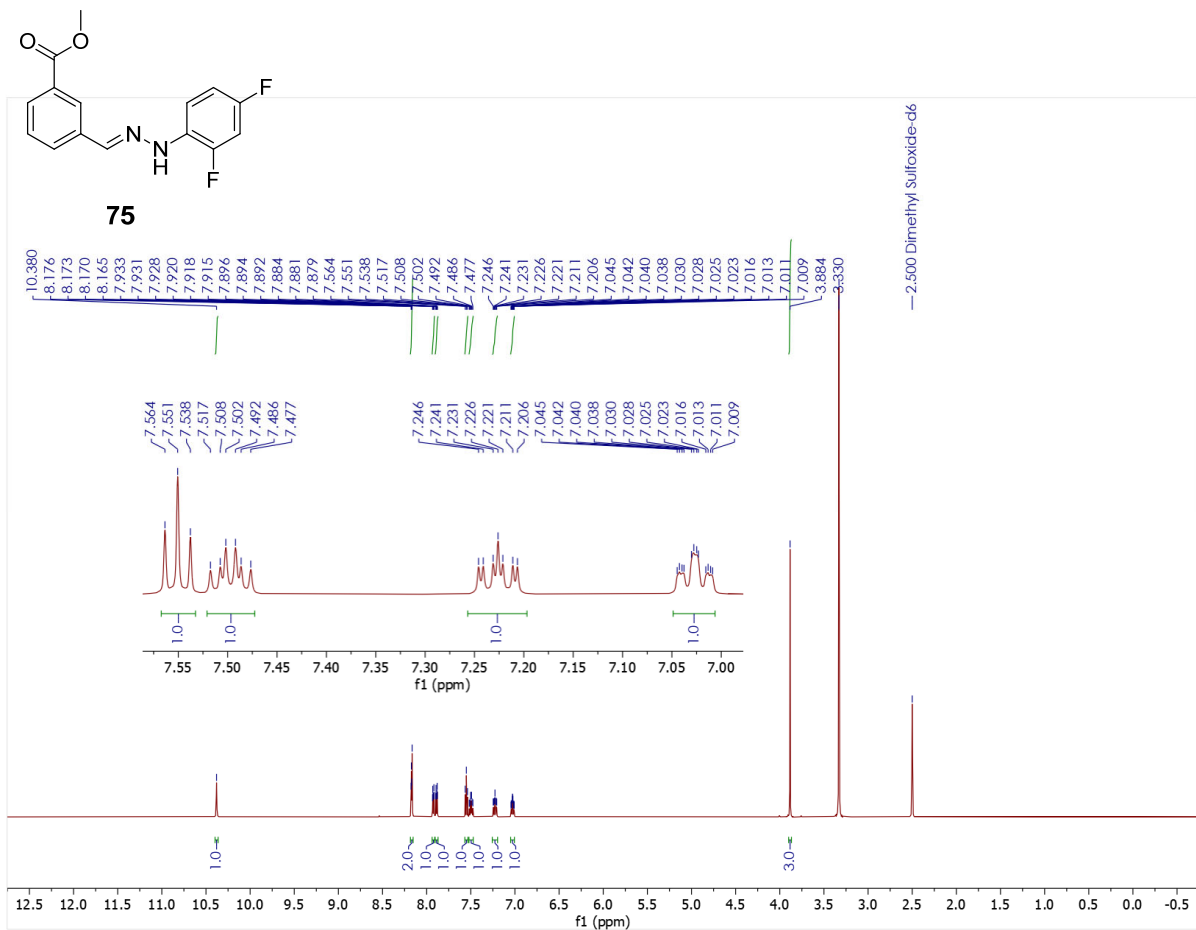
Data file: D:\Chem32\11Data\AJS\AJS Table4+ 2023-07-31 12-52-45\012-51-AJS1135-3.D
Sample name: AJS1135-3
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Location: 51
Injection date: 7/31/2023 1:46:13 PM
Injection: 1 of 1
Acq. method: LCMS ISOCRATIC 80%
B_3 MINS.M
Injection volume: 2.000
Analysis method: LCMS ISOCRATIC
80%B_3 MINS.M
Acq. operator: SYSTEM
Last changed: 11/26/2021 9:20:48 AM

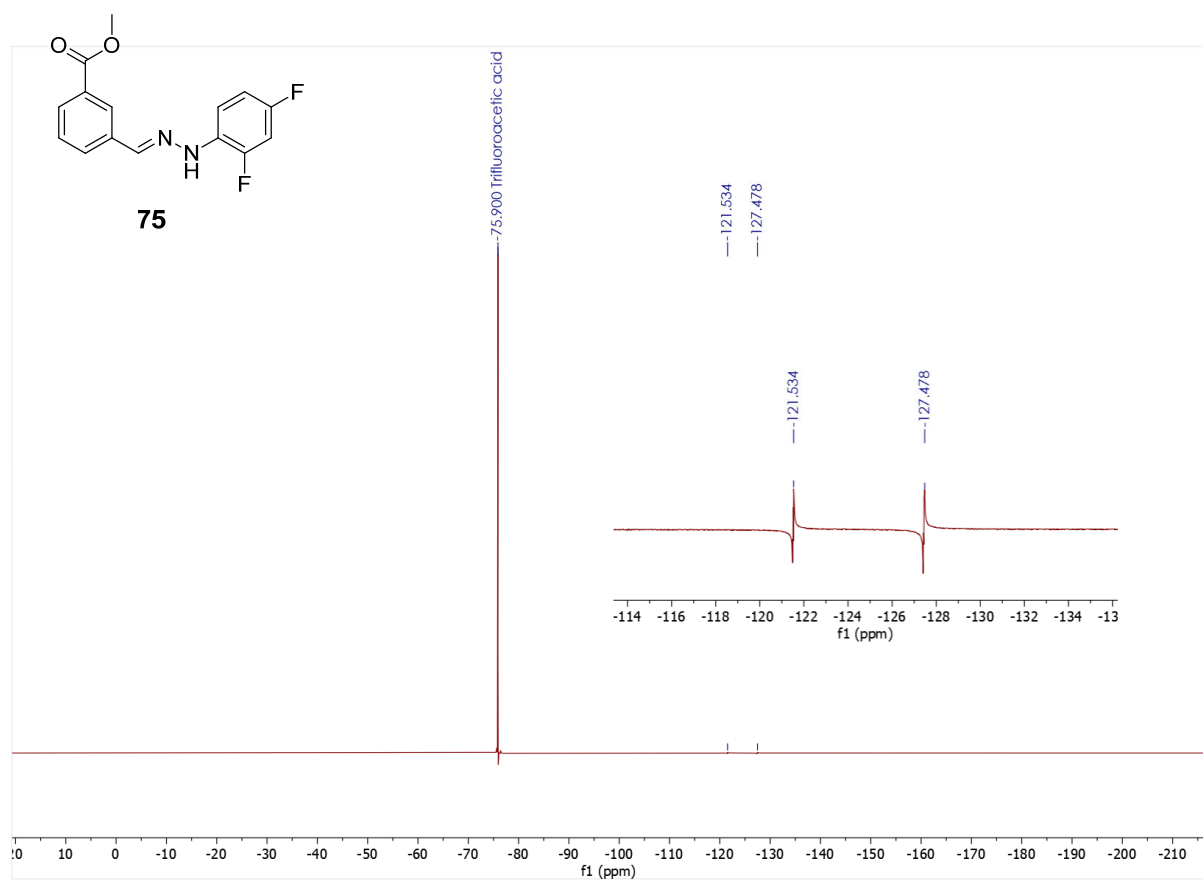


Molecular Weight: 323.174

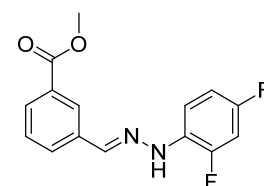
74





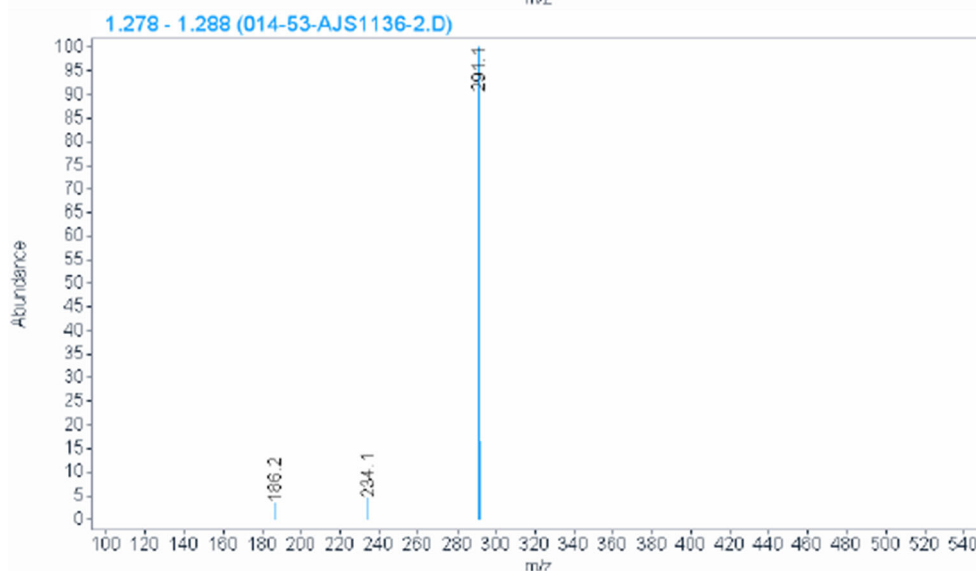
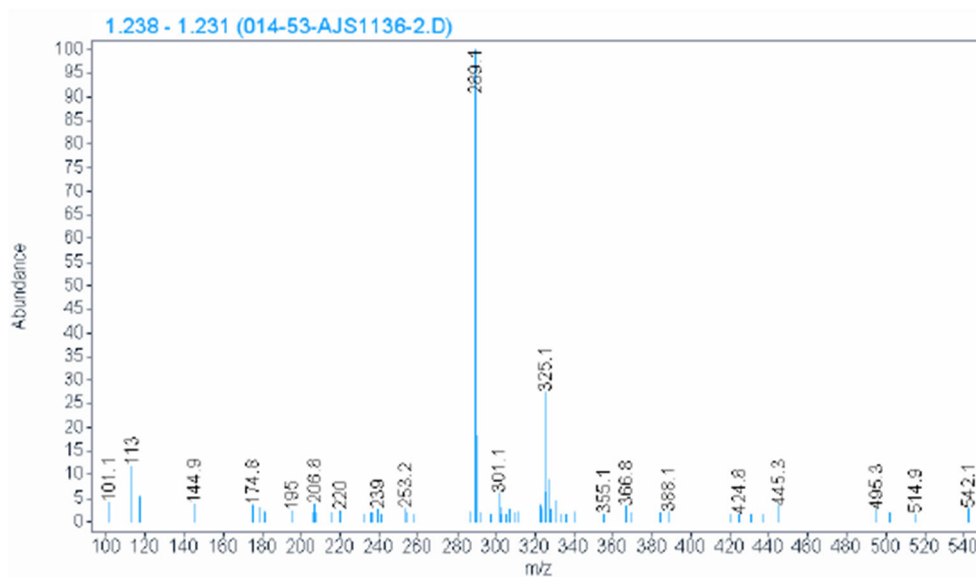
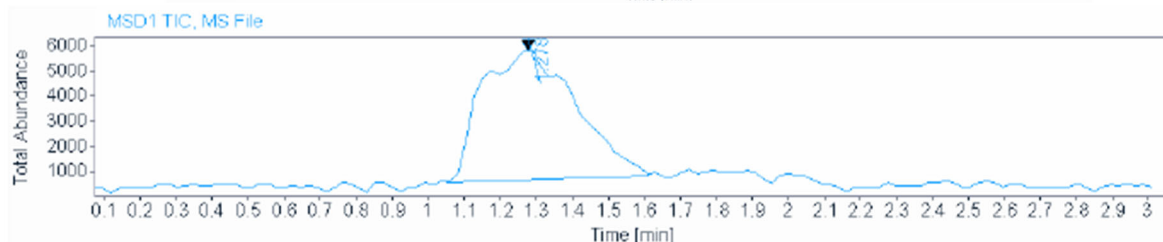
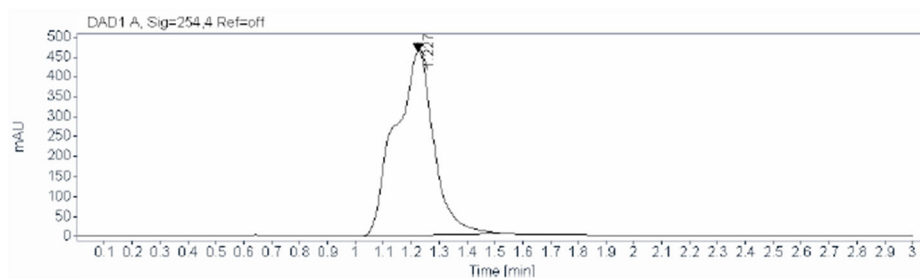


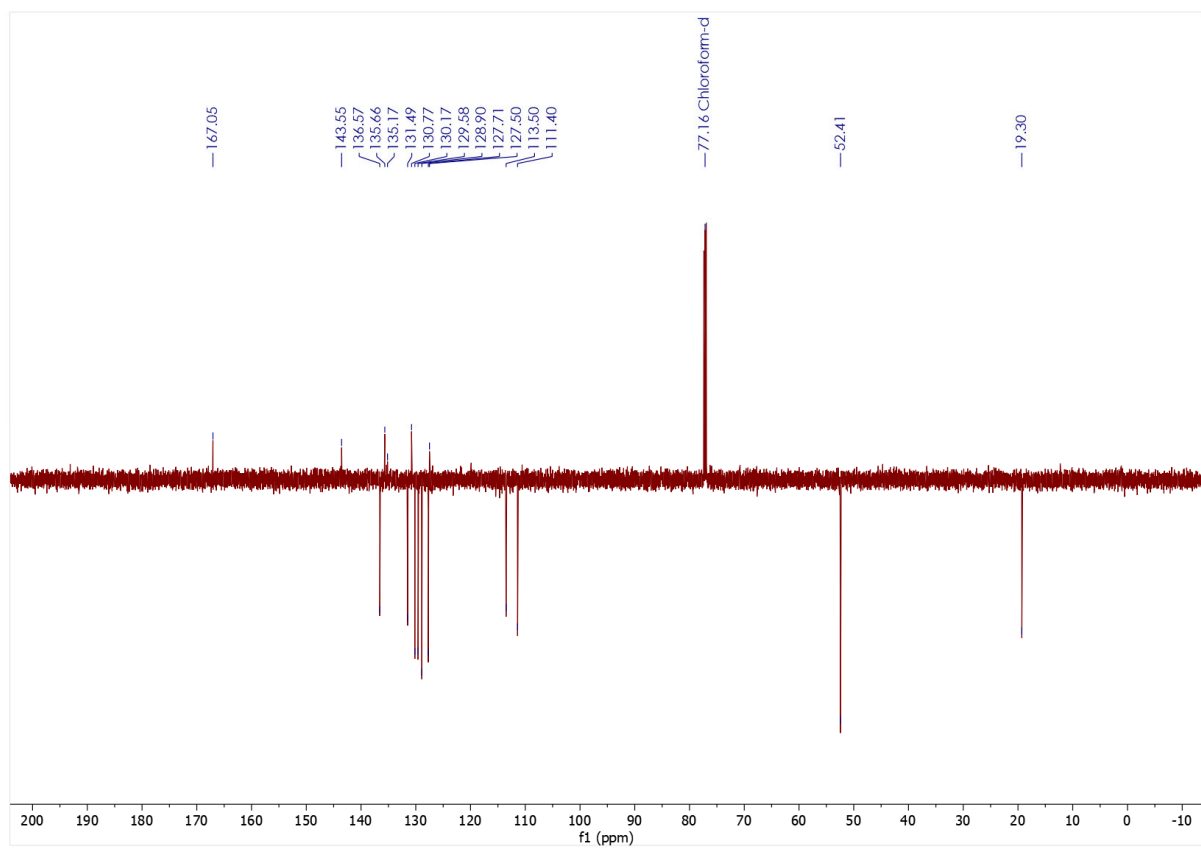
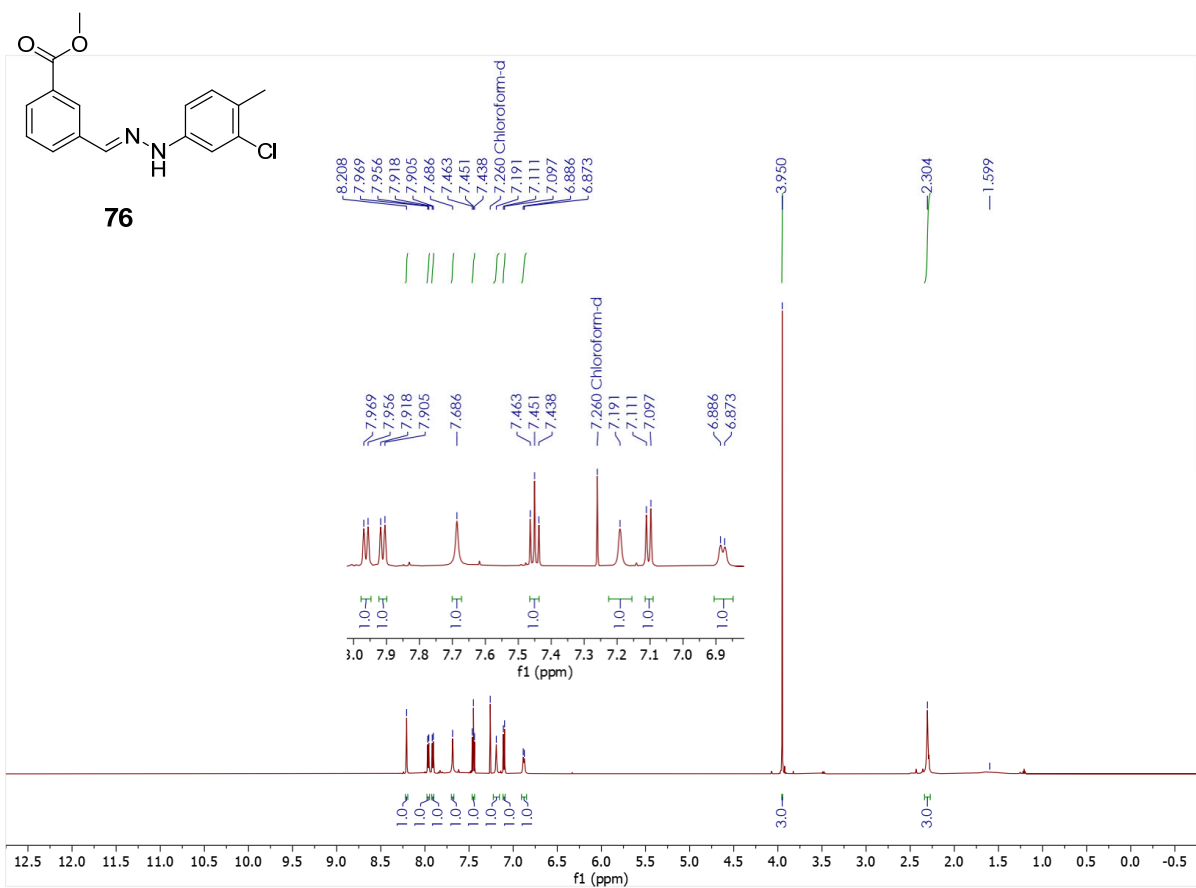
Data file: D:\Chem3211\Data\AJS\AJS Table4+ 2023-07-31 12-52-45\014-53-AJS1136-2.D
Sample name: AJS1136-2
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Injection date: 7/31/2023 1:55:33 PM
Acq. method: LCMS ISOCRATIC 80%
B_3 MINS.M
Analysis method: LCMS ISOCRATIC
80%B_3 MINS.M
Last changed: 11/26/2021 9:20:48 AM
Location: 53
Injection: 1 of 1
Injection volume: 2.000
Acq. operator: SYSTEM



Molecular Weight: 290.265

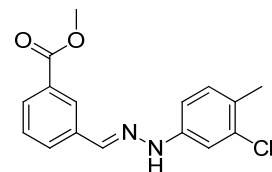
75





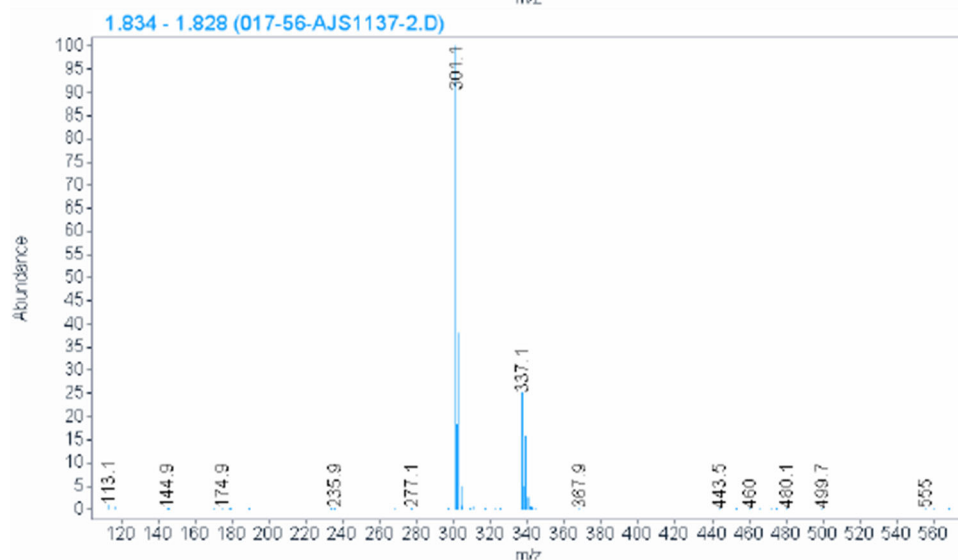
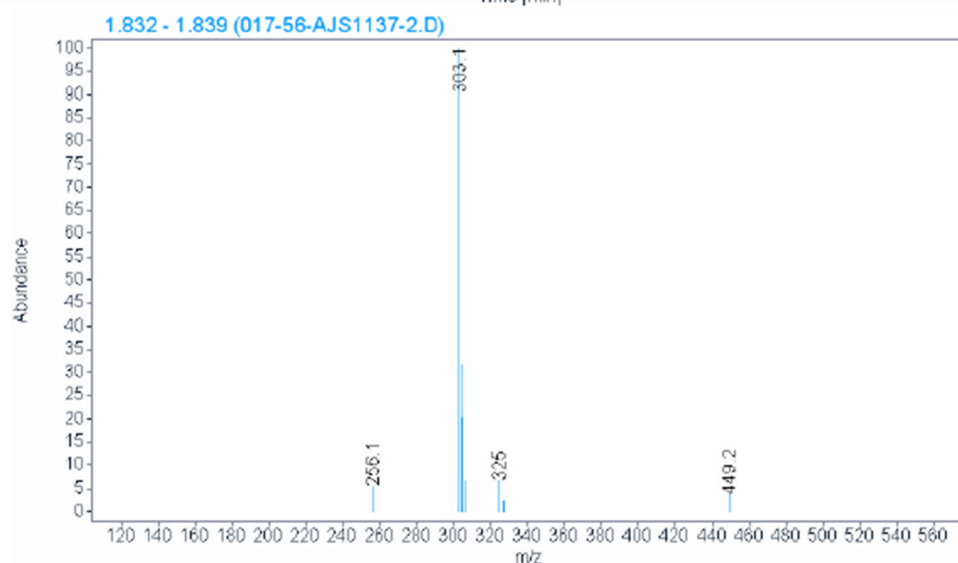
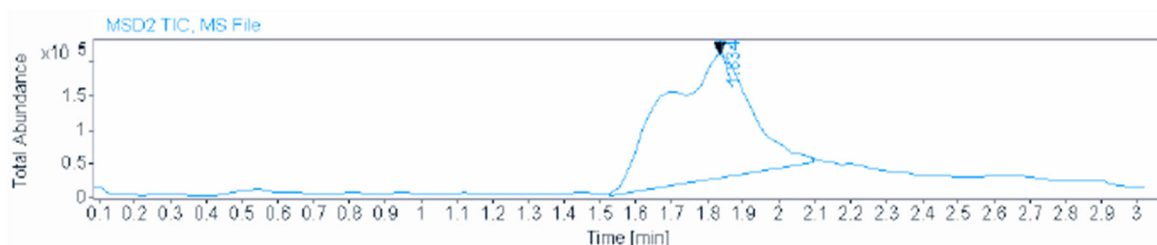
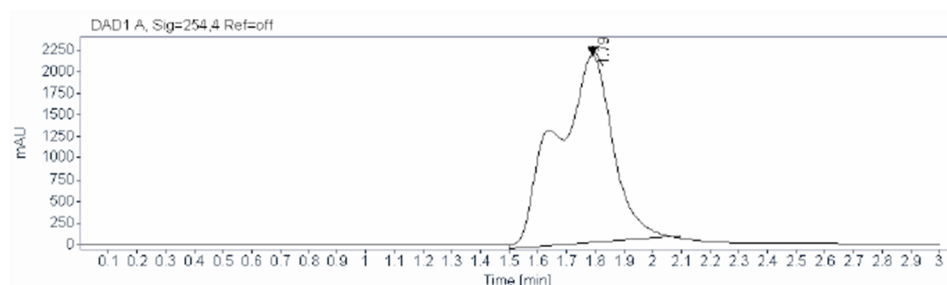


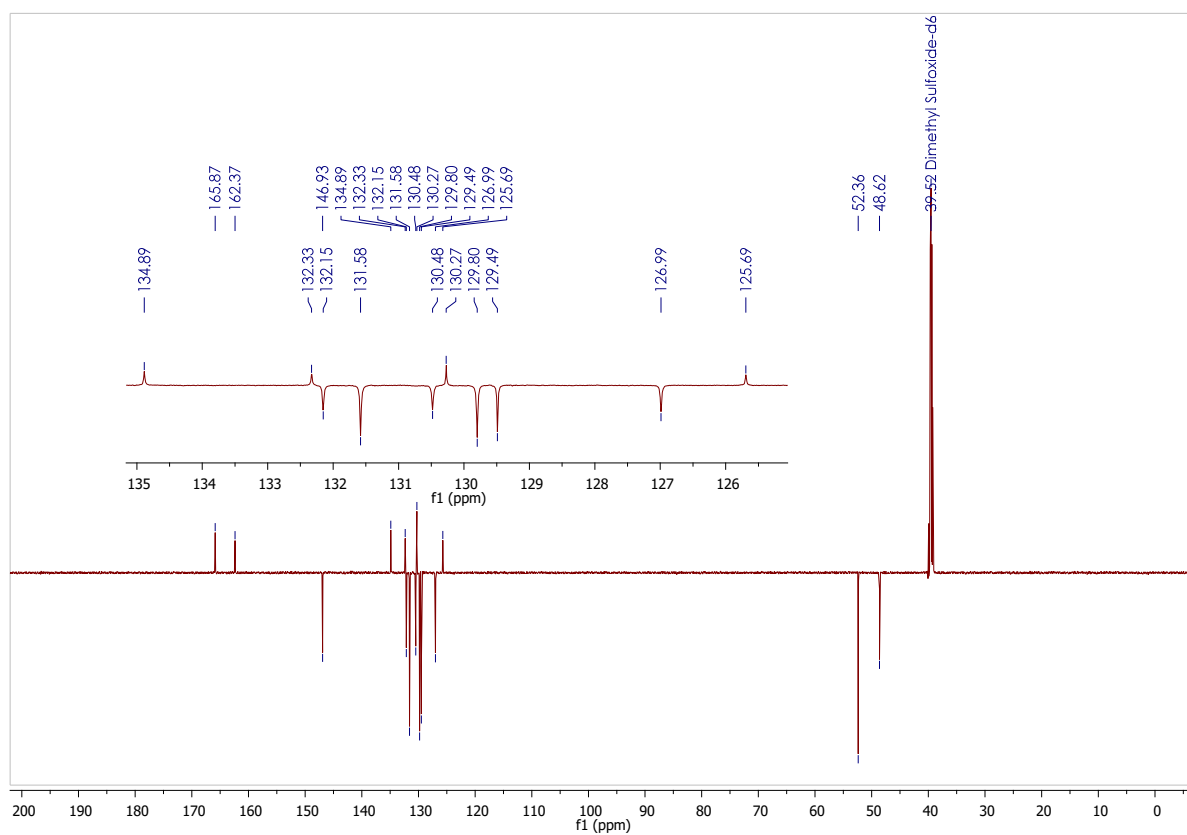
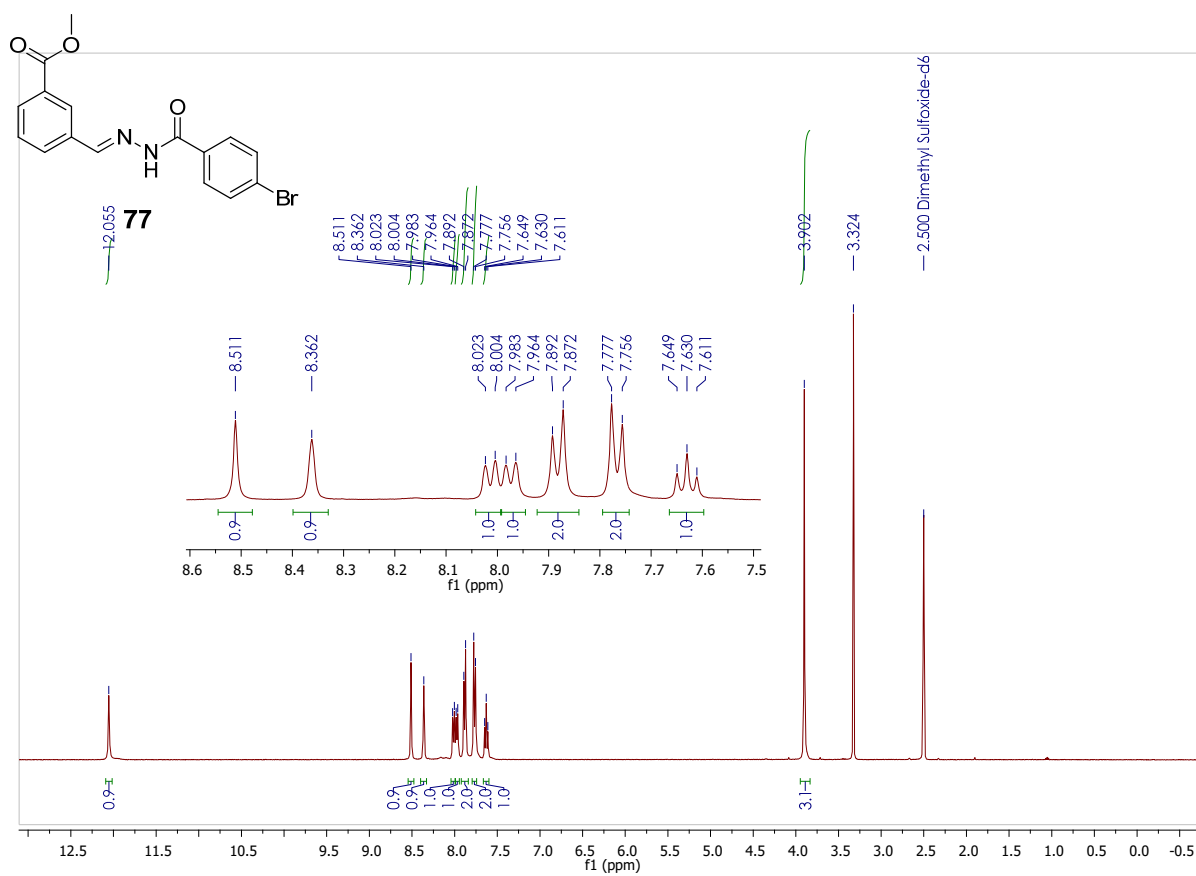
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Sample name: AJS1137-2
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Location: 56
Injection date: 7/31/2023 2:09:51 PM
Injection: 1 of 1
Acq. method: LCMS ISOCRATIC 80%
B_3 MINS.M
Injection volume: 2.000
Analysis method: LCMS ISOCRATIC
80%B_3 MINS.M
Acq. operator: SYSTEM
Last changed: 11/26/2021 9:20:48 AM



Molecular Weight: 302.756

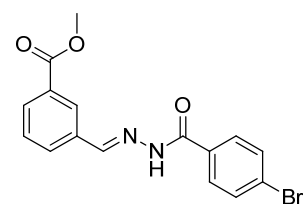
76





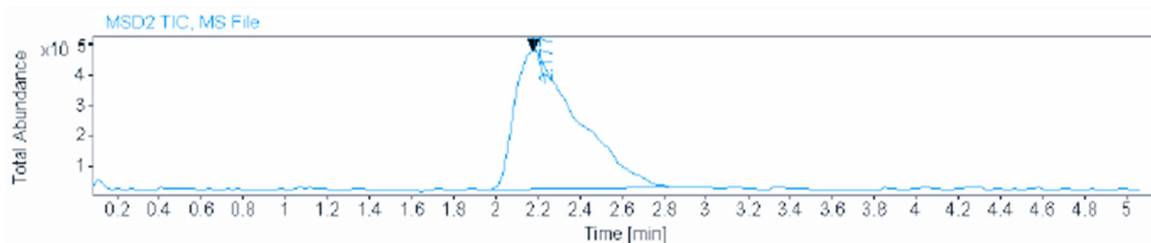
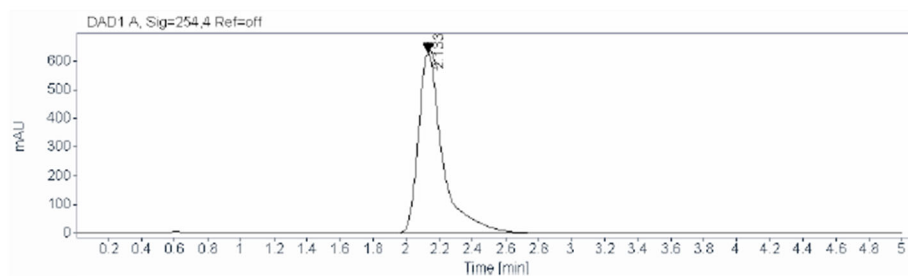


Data file: D:\Chem32\11\Data\JRB\JRB2023 2024 2021-11-23 12-21-42\003-99-JRB2024.D
Sample name: JRB2024
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Injection date: 11/23/2021 12:36:53 PM
Acq. method: LCMS ISOCRATIC 50%
B.M_REDUCED
FLOW.M
Analysis method: LCMS ISOCRATIC
50%
B.M_REDUCED
FLOW.M
Acq. operator: SYSTEM
Last changed: 5/15/2019 9:20:00 AM

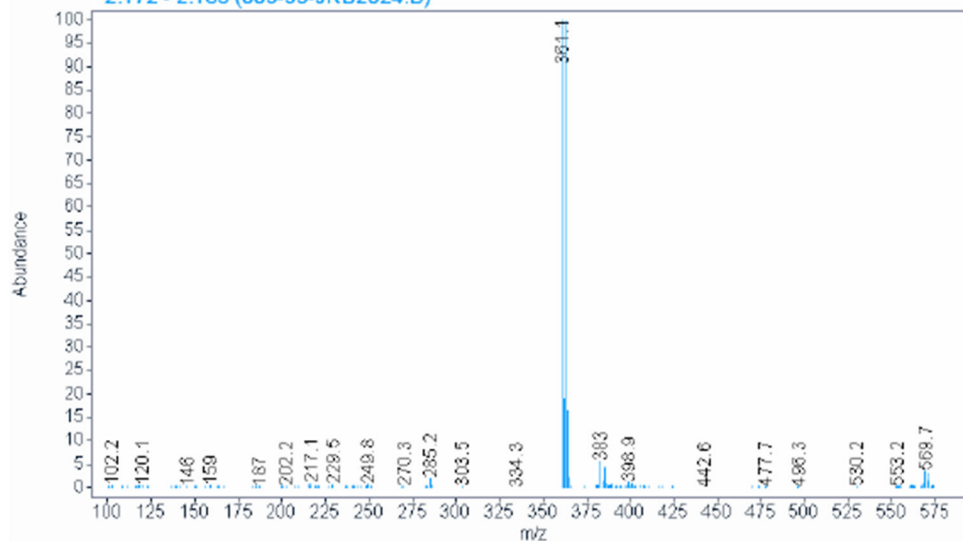


Molecular Weight: 361.190

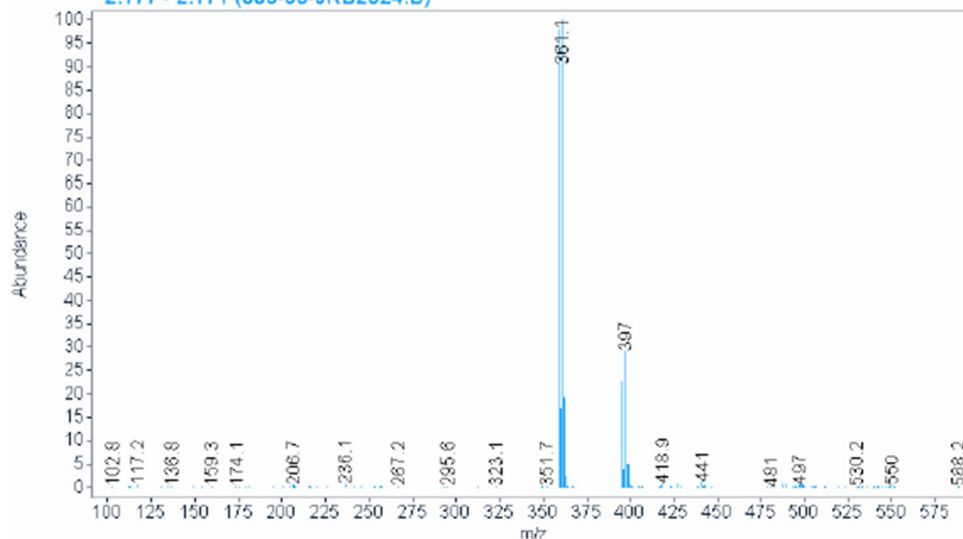
77

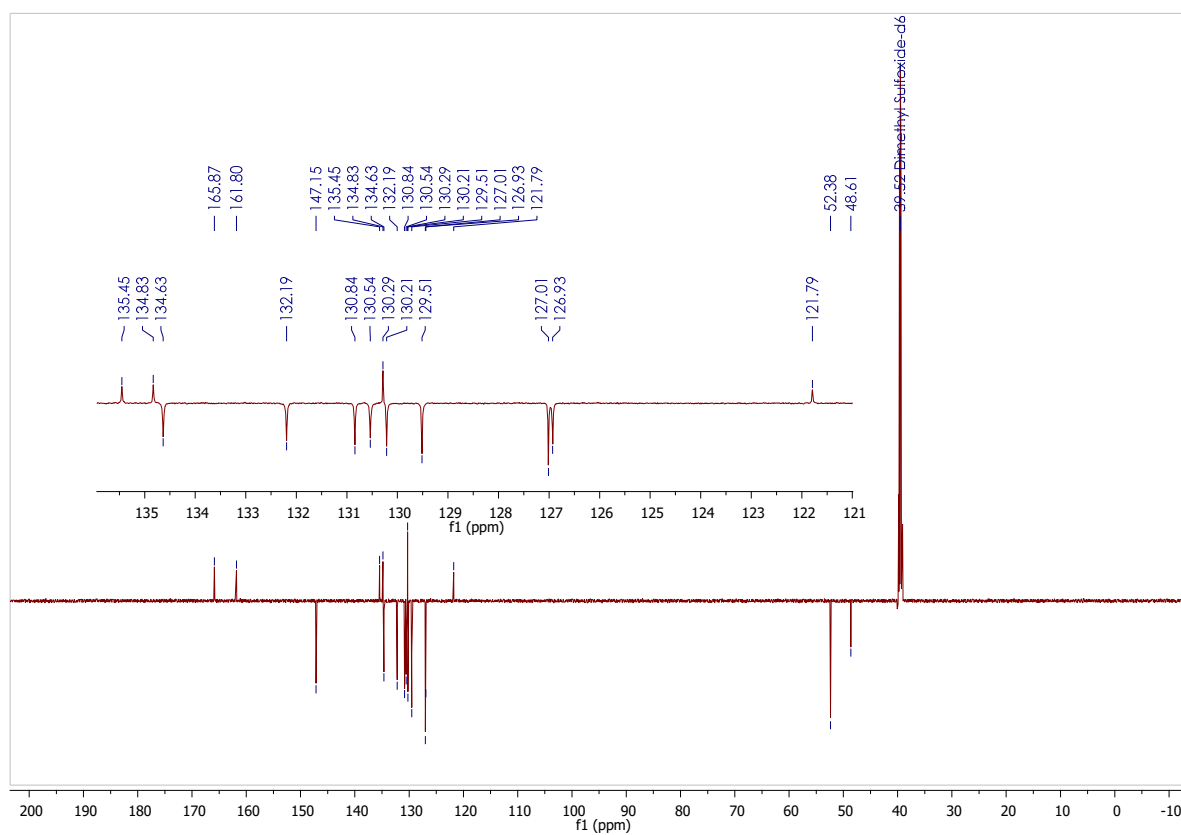
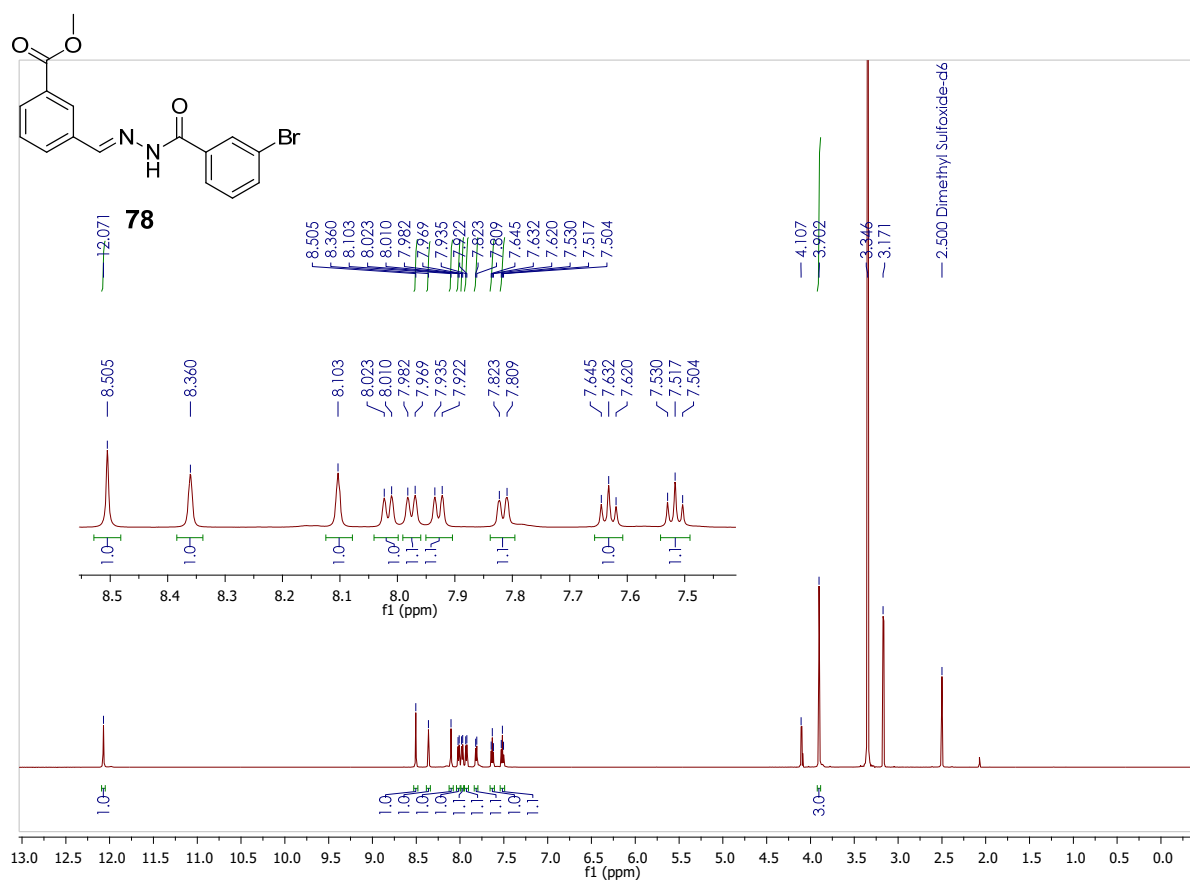


2.172 - 2.183 (003-99-JRB2024.D)



2.177 - 2.171 (003-99-JRB2024.D)



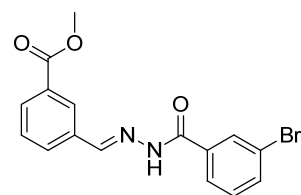


LCMS Report



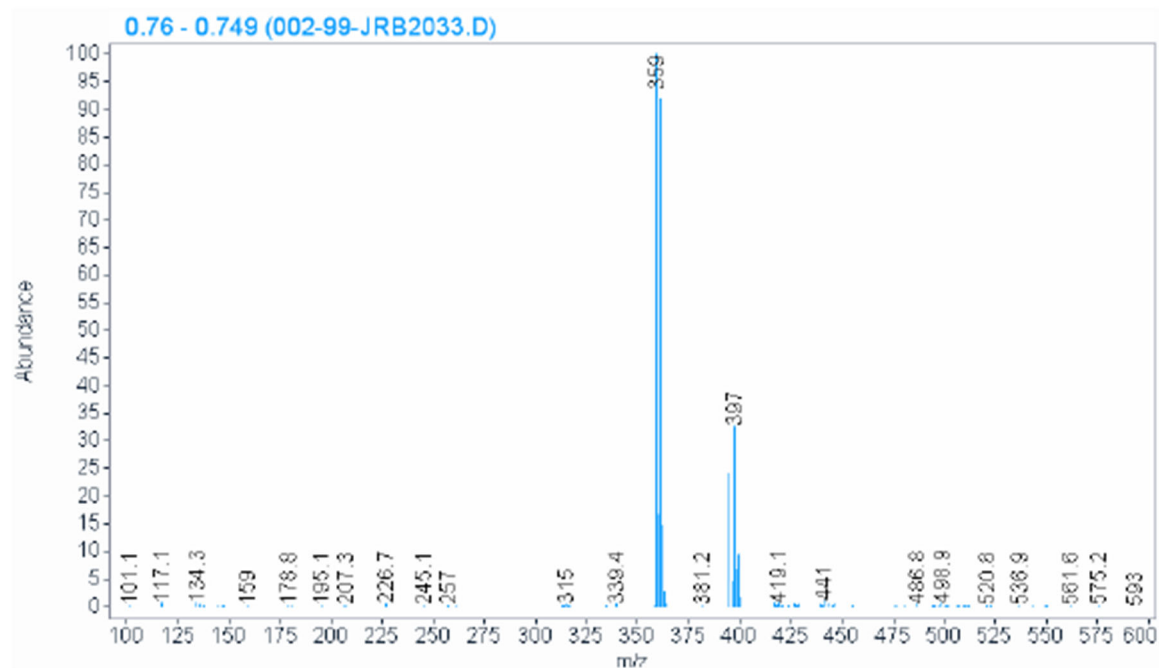
Agilent Technologies

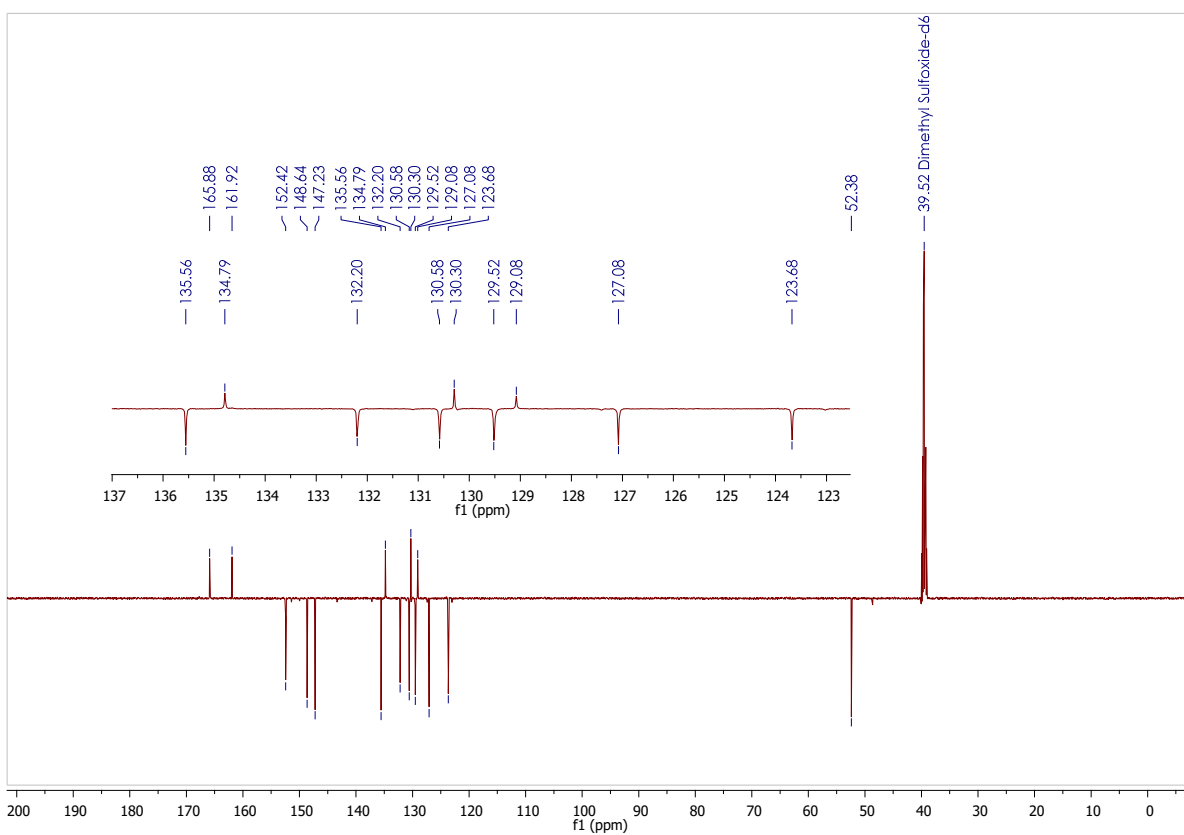
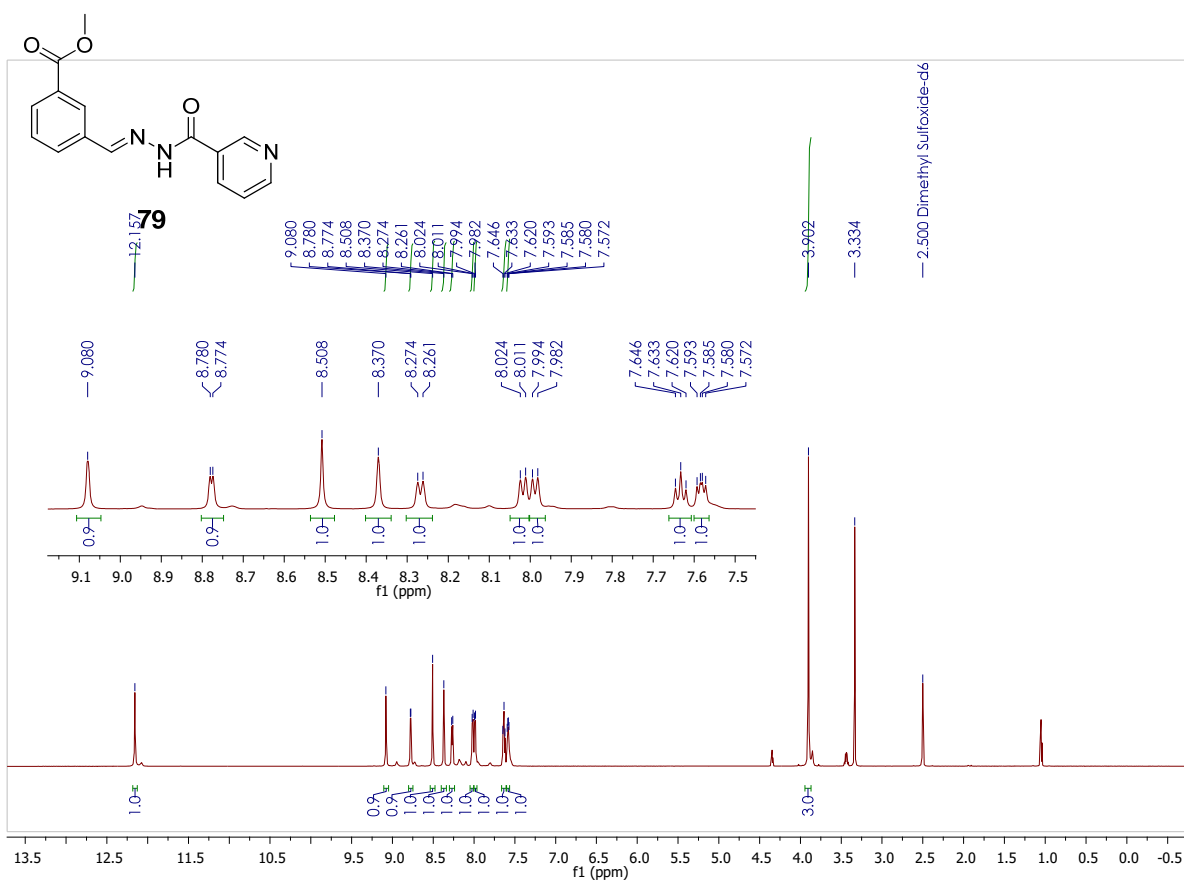
Data file: D:\Chem32\11\Data\JRB\JRB2036 2033 2021-11-26 11-46-33\002-99-JRB2033.D
 Sample name: JRB2033
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 99
 Injection date: 11/26/2021 11:53:05 AM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 Injection volume: 2.000
 B_3 MINS.M
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 80%B_3 MINS.M
 Last changed: 11/26/2021 9:20:48 AM



Molecular Weight: 361.190

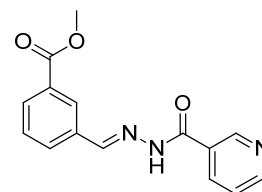
78





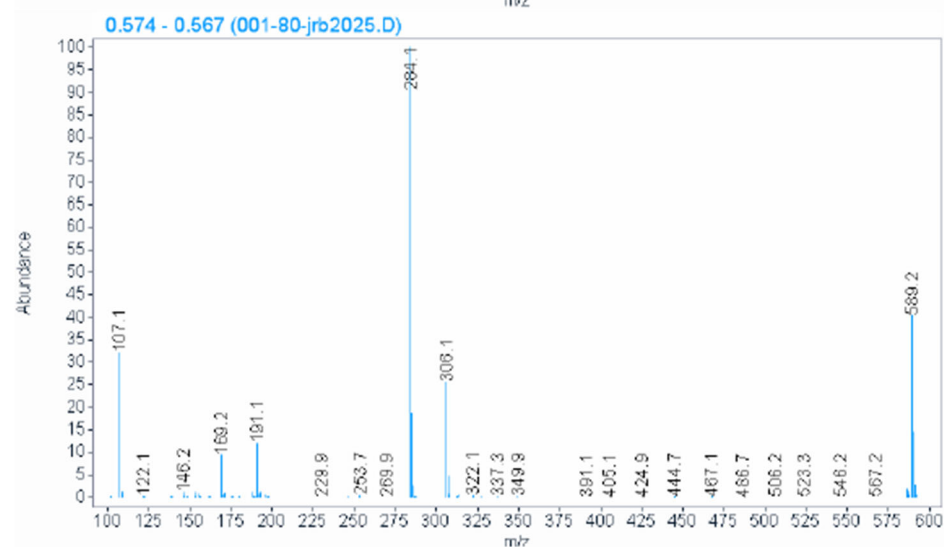
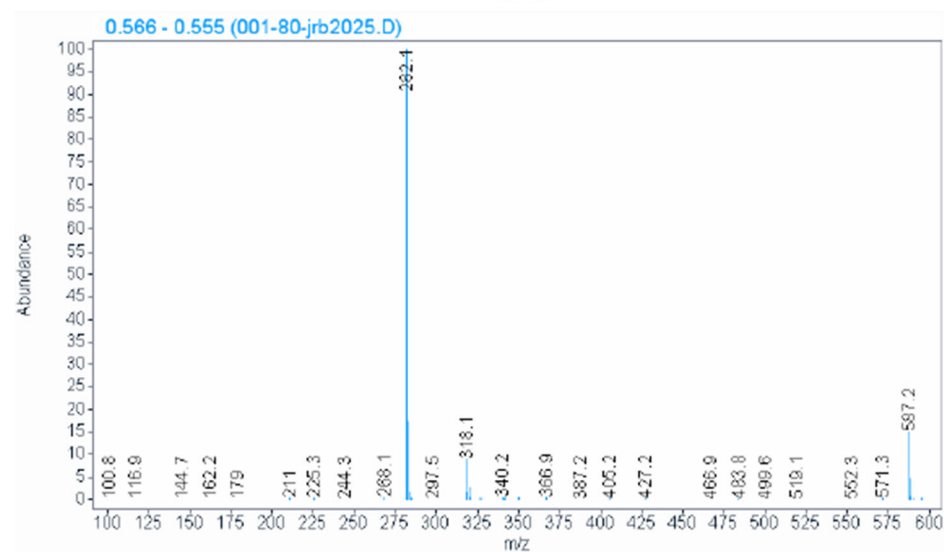


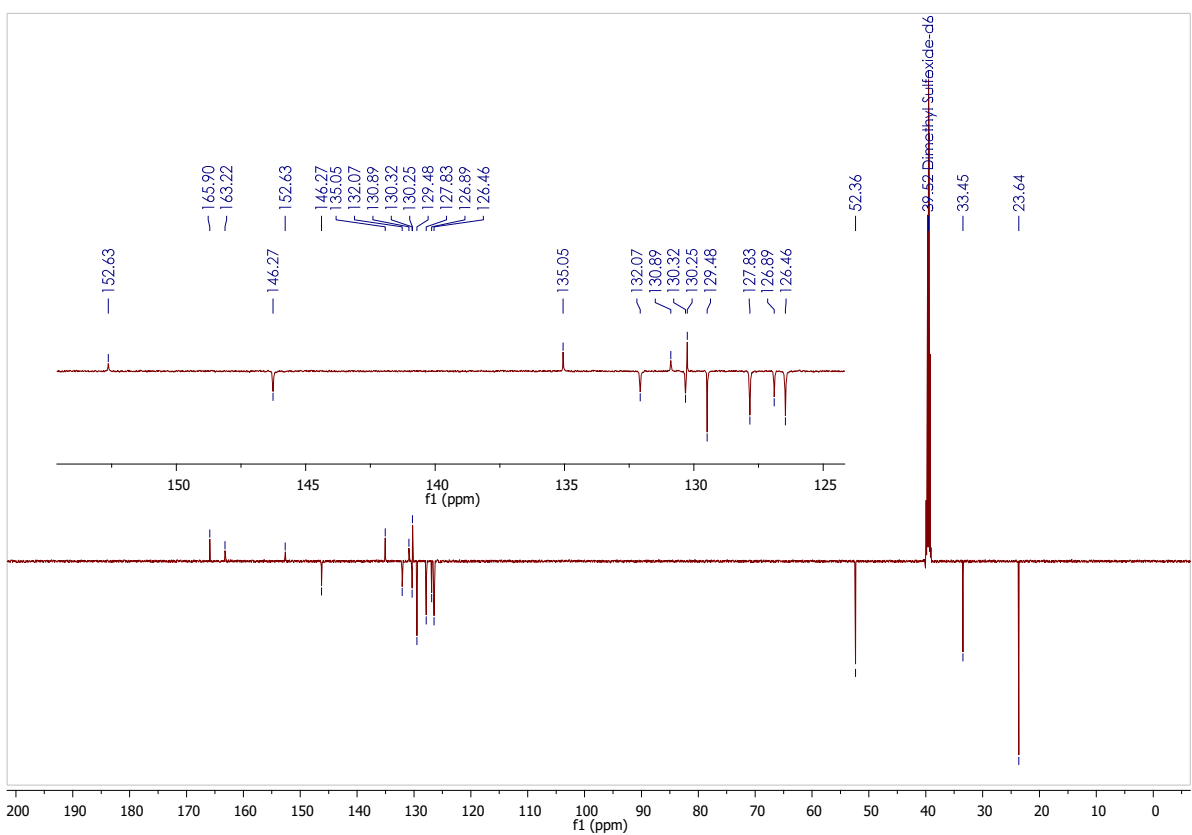
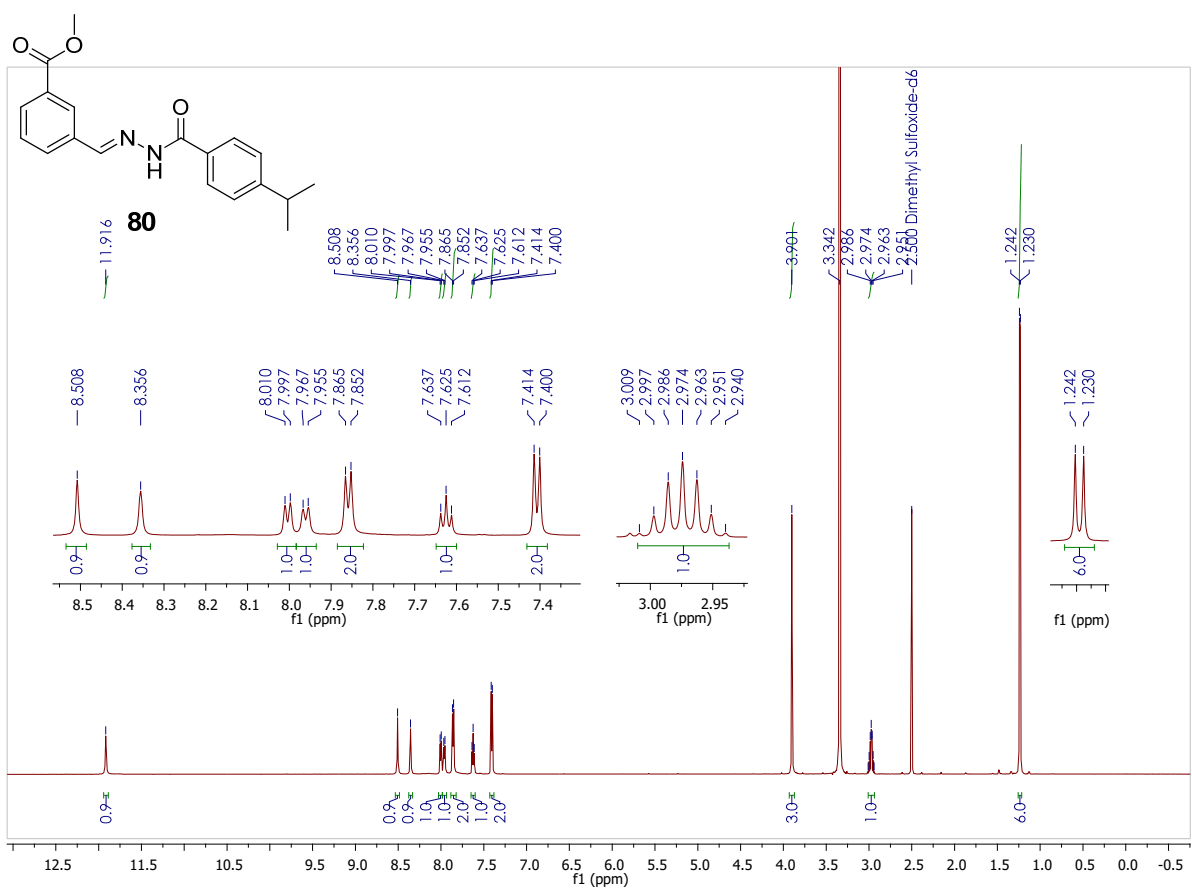
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 Sample name: jrb2025
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 80
 Injection date: 11/25/2021 5:04:00 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 Injection volume: 2.000
 B_3 MINS.M
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 80%B_3 MINS.M
 Last changed: 11/25/2021 10:50:38 AM



Molecular Weight: 283.282

79



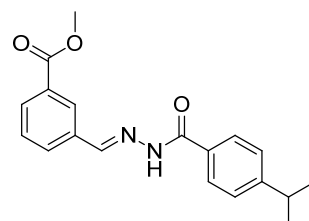


LCMS Report



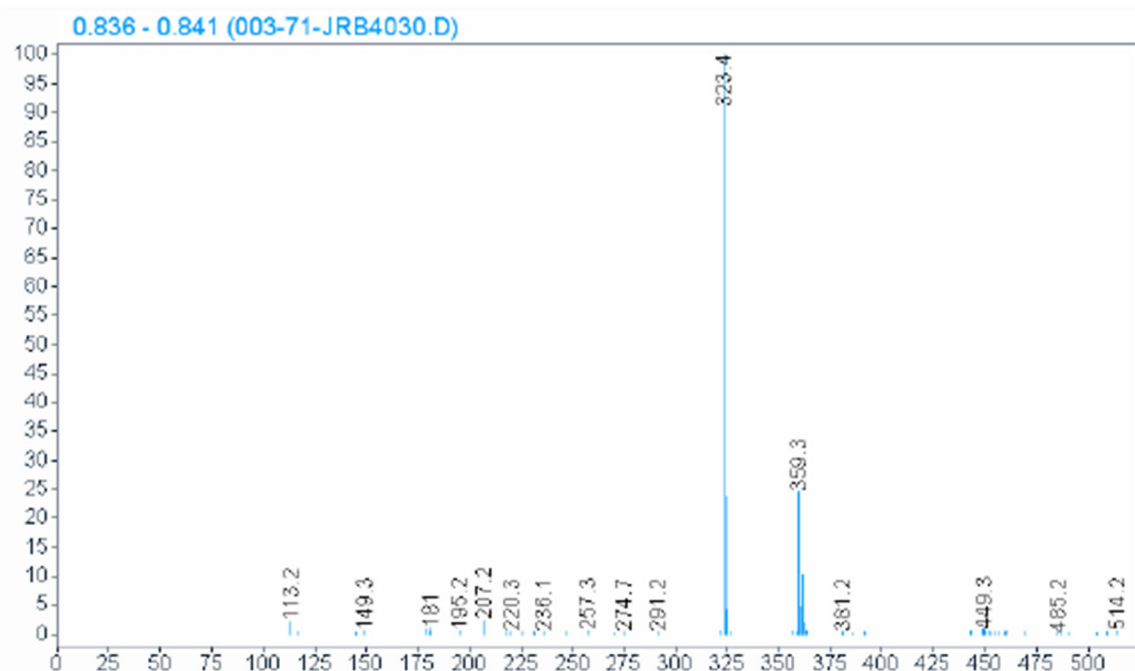
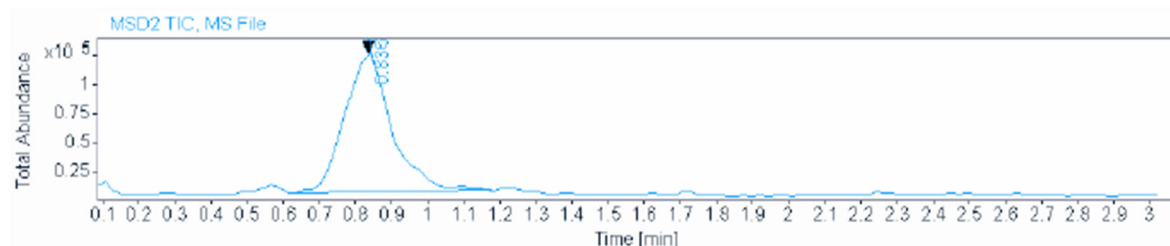
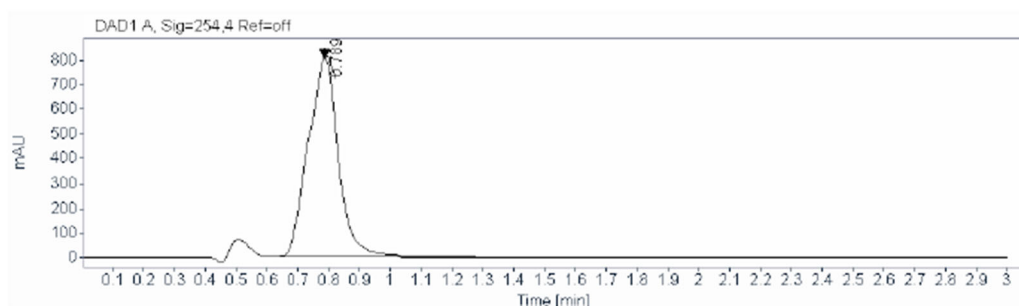
Agilent Technologies

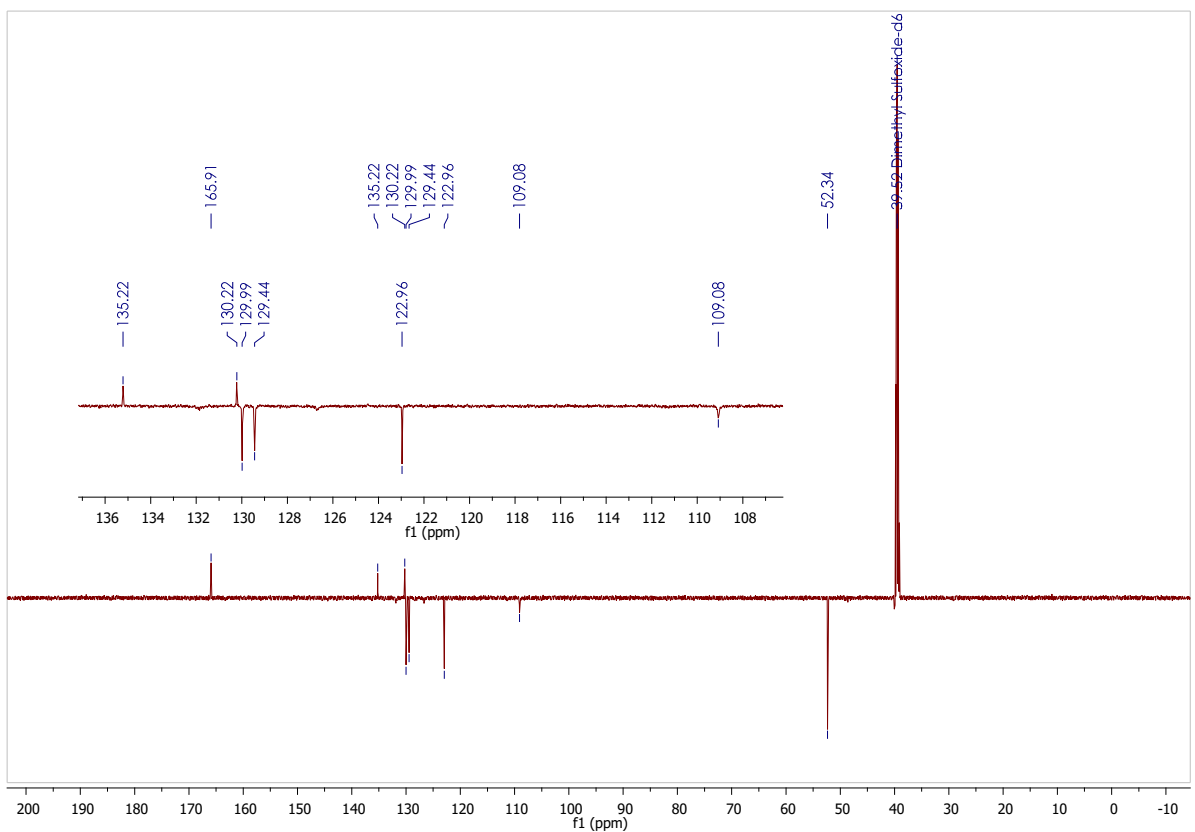
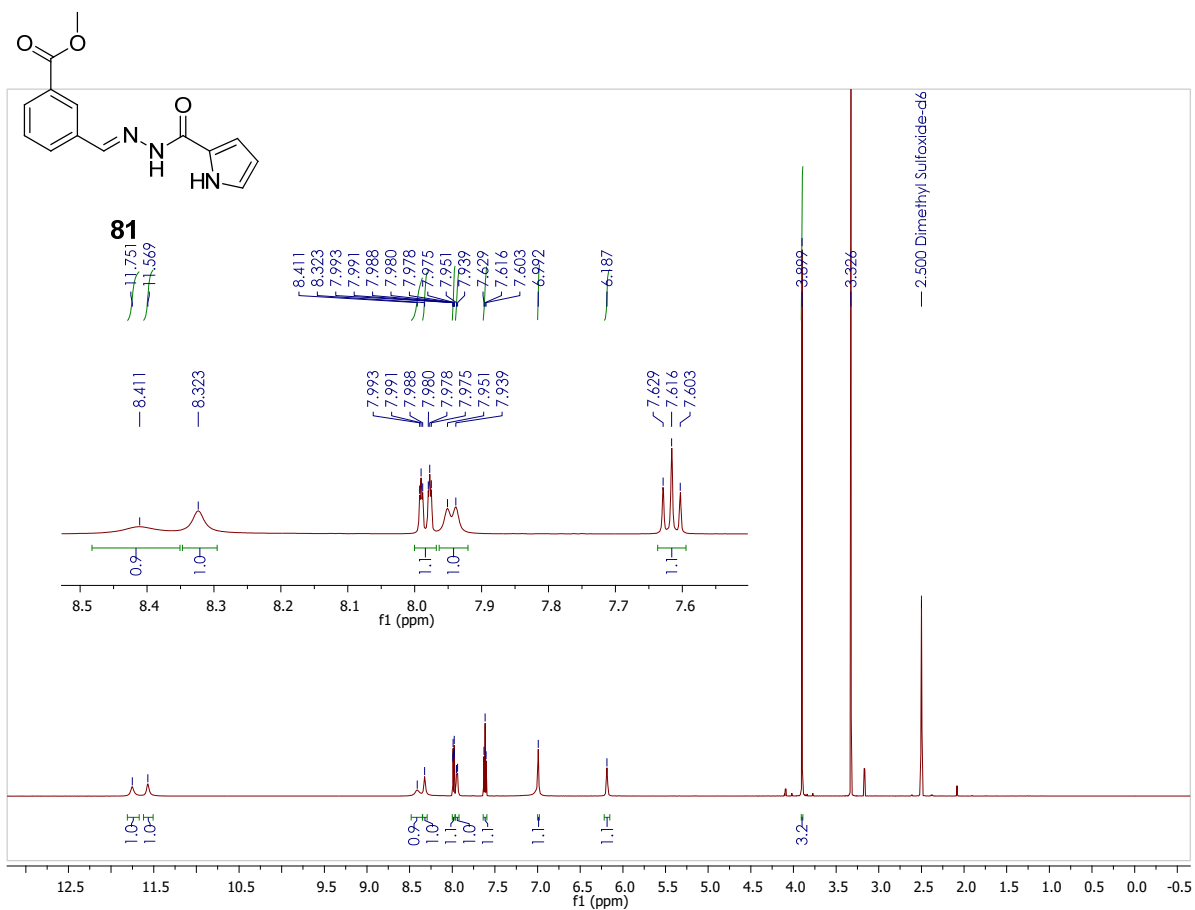
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Sample name: JRB4030
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Location: 71
Injection date: 7/24/2023 4:03:59 PM
Injection: 1 of 1
Acq. method: LCMS ISOCRATIC 80%
Injection volume: 2.000
 B_3 MINS.M
Analysis method: LCMS ISOCRATIC
Acq. operator: SYSTEM
 80%B_3 MINS.M
Last changed: 11/26/2021 9:20:48 AM



Molecular Weight: 324.374

80

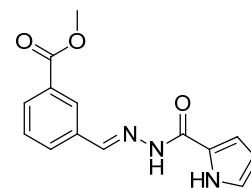




LCMS Report

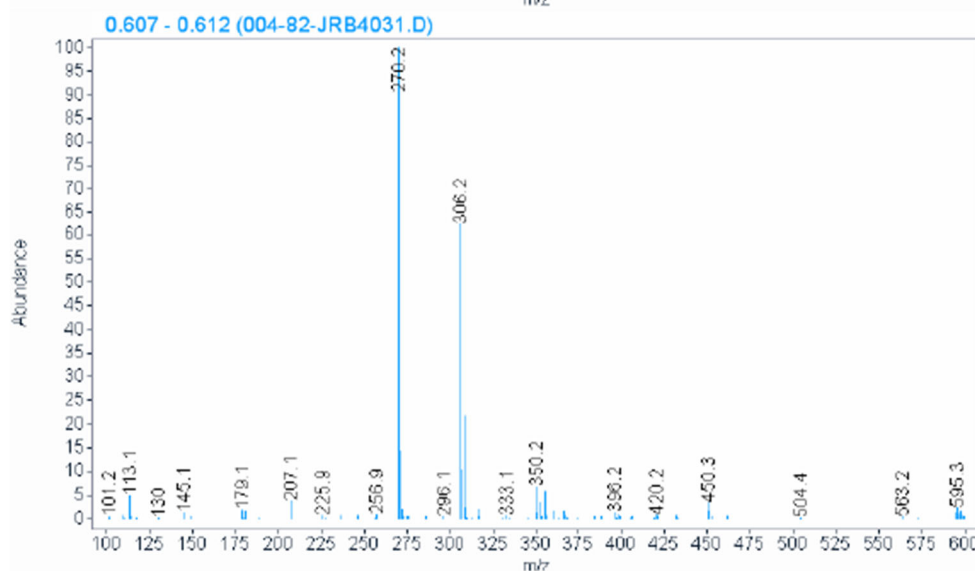
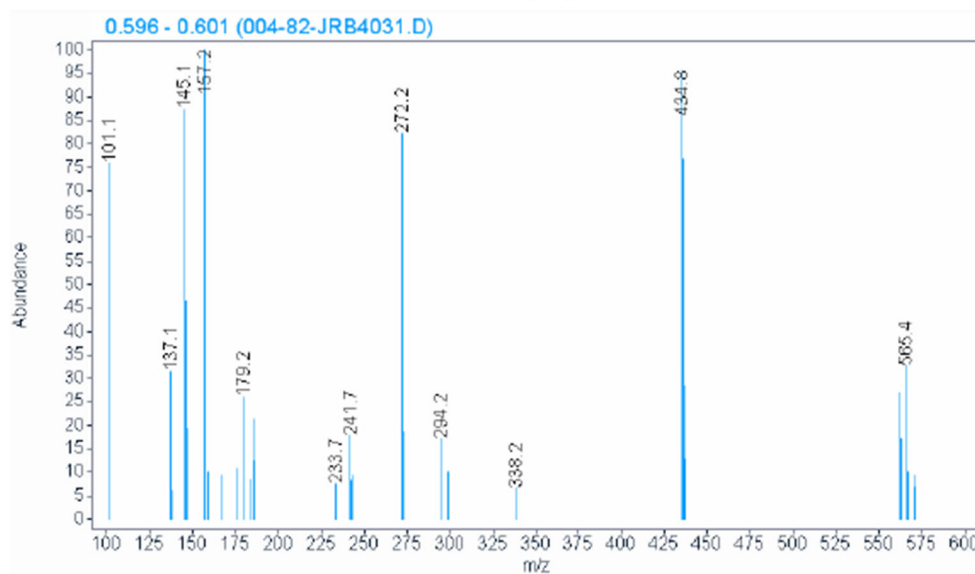
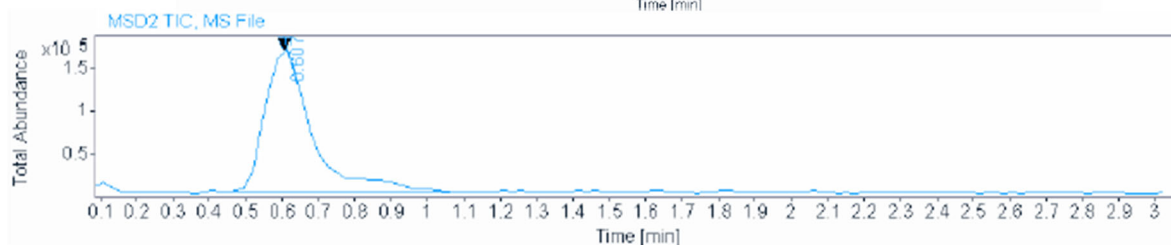
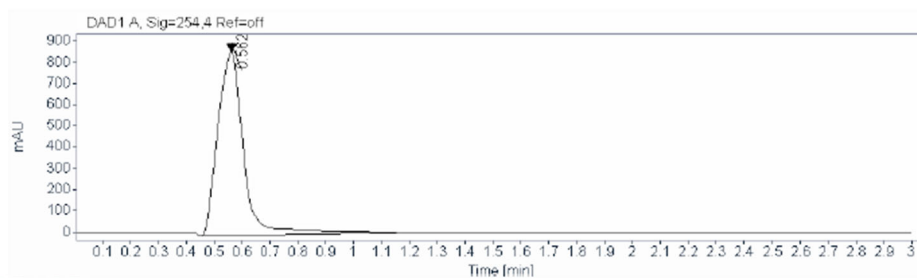


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Sample name: JRB4031
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Injection date: 7/24/2023 4:08:31 PM
Acq. method: LCMS ISOCRATIC 80%
Analysis method: B_3 MINS.M
Last changed: 11/26/2021 9:20:48 AM
Location: 82
Injection: 1 of 1
Injection volume: 2.000
Acq. operator: SYSTEM

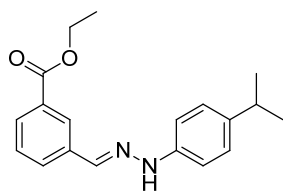


Molecular Weight: 271.271

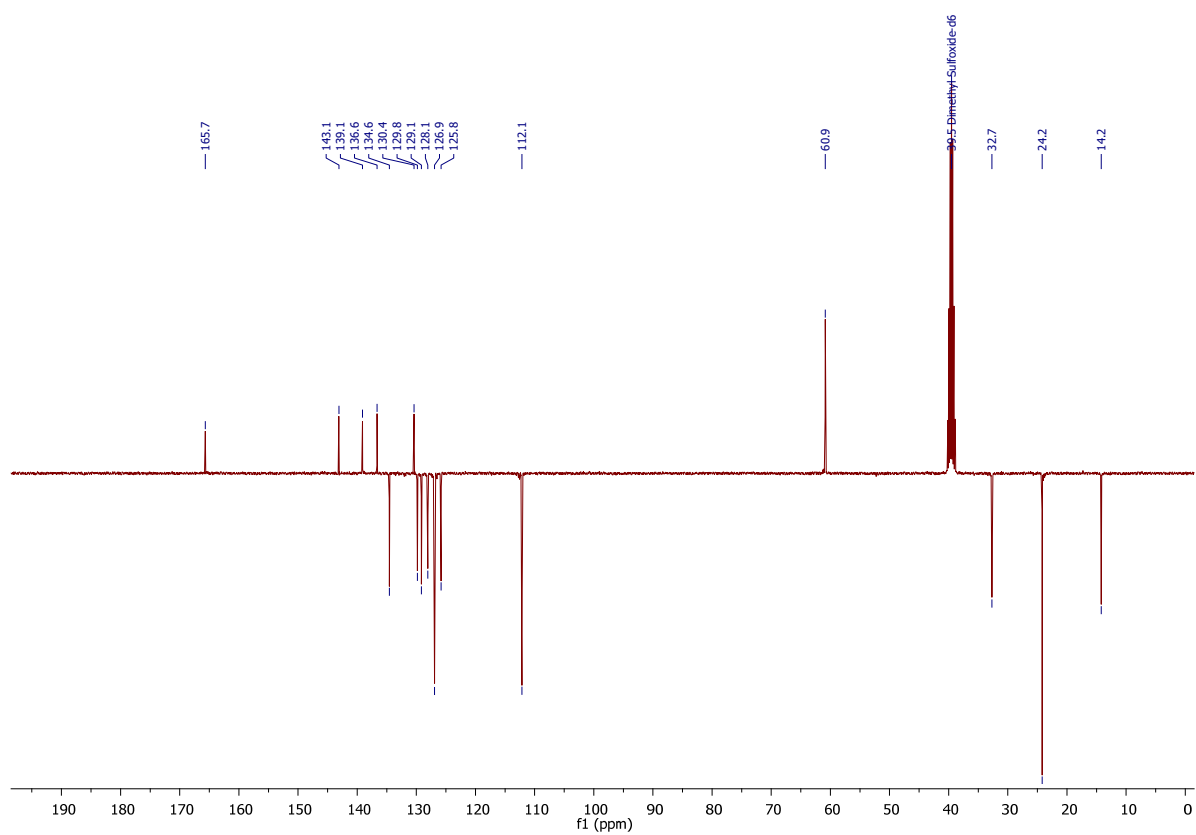
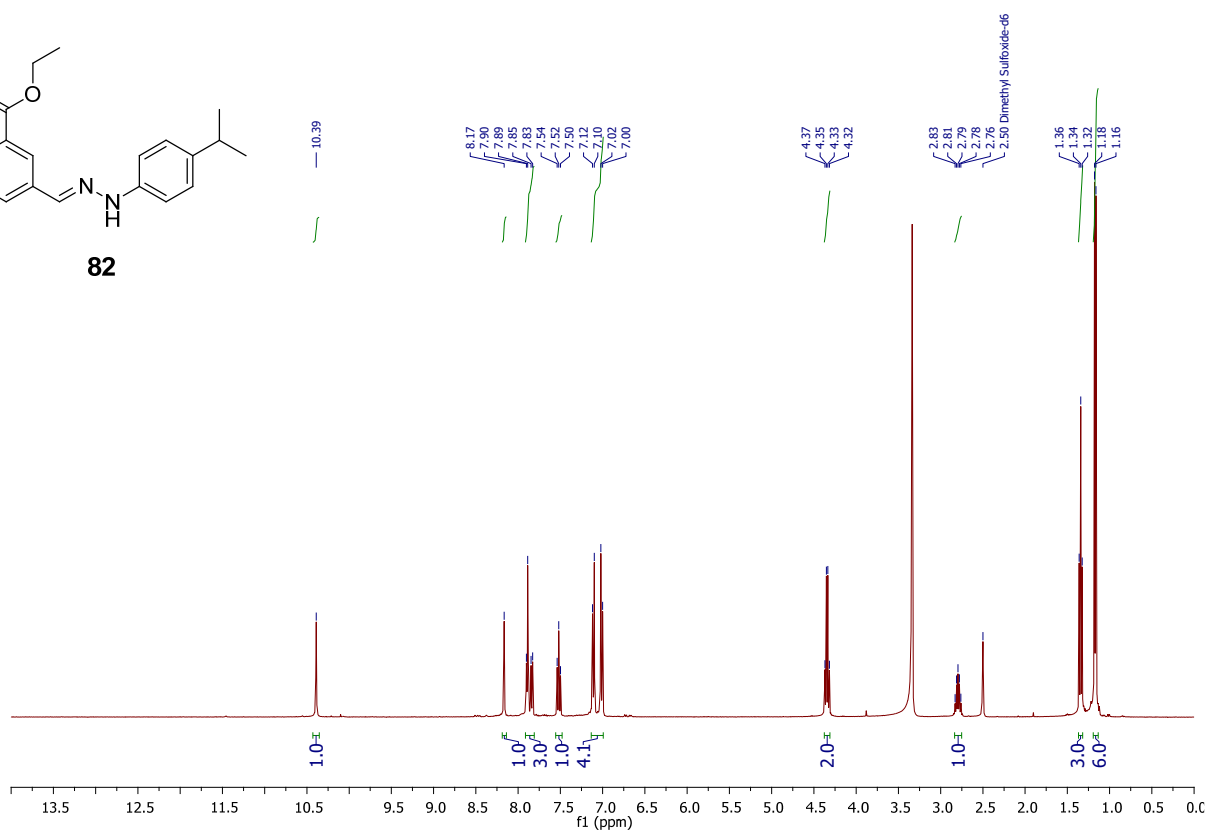
81



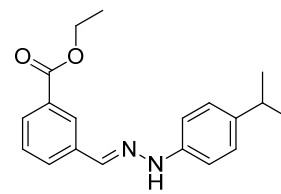
186



82

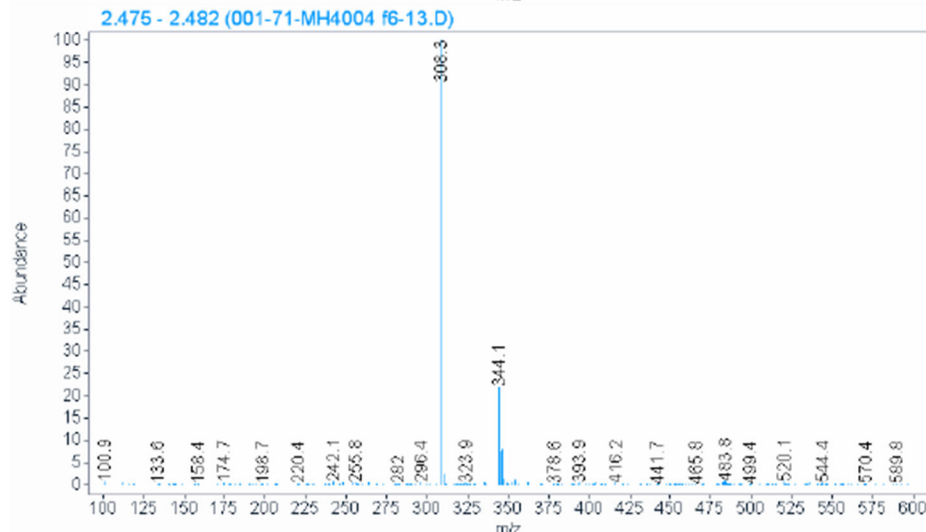
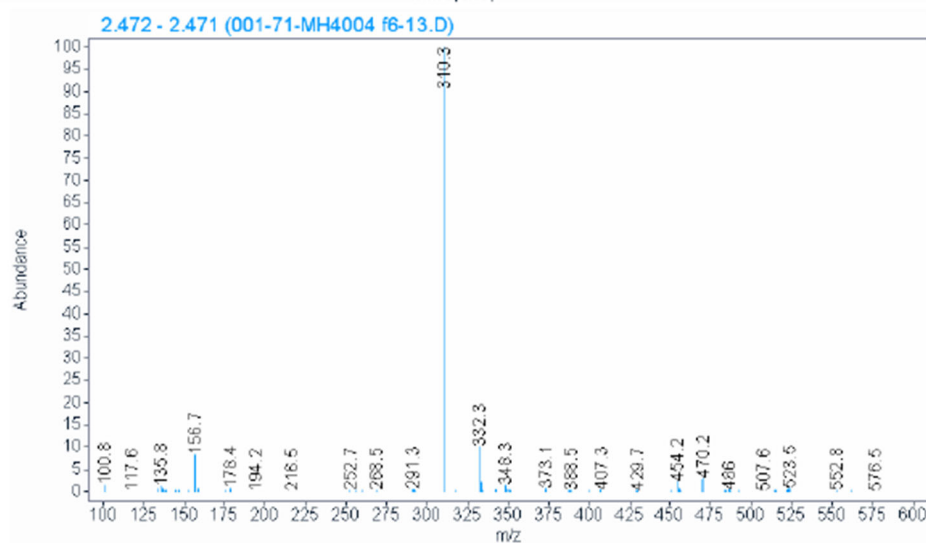
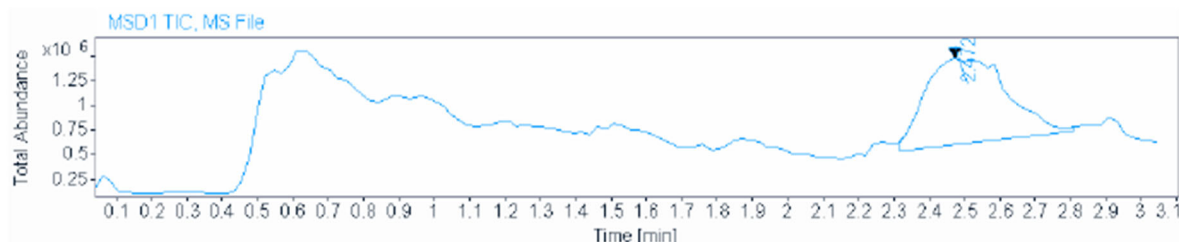
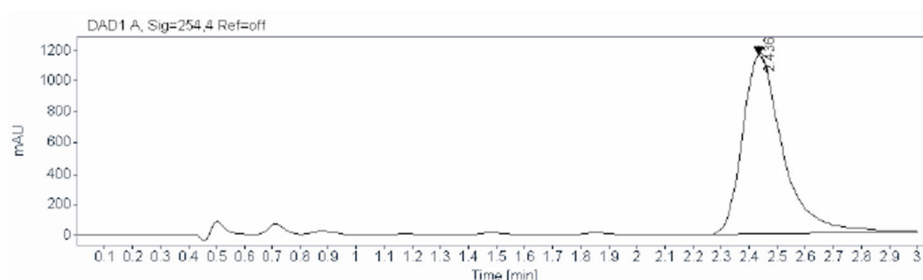


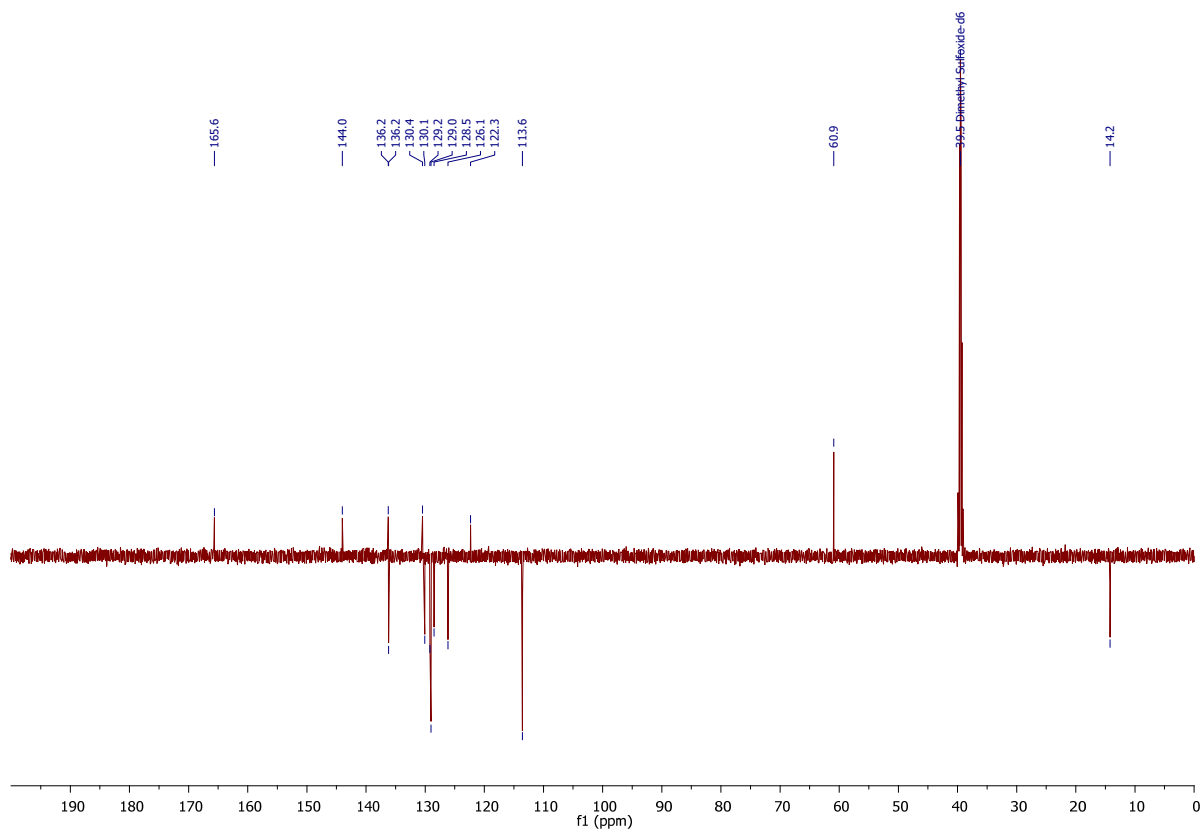
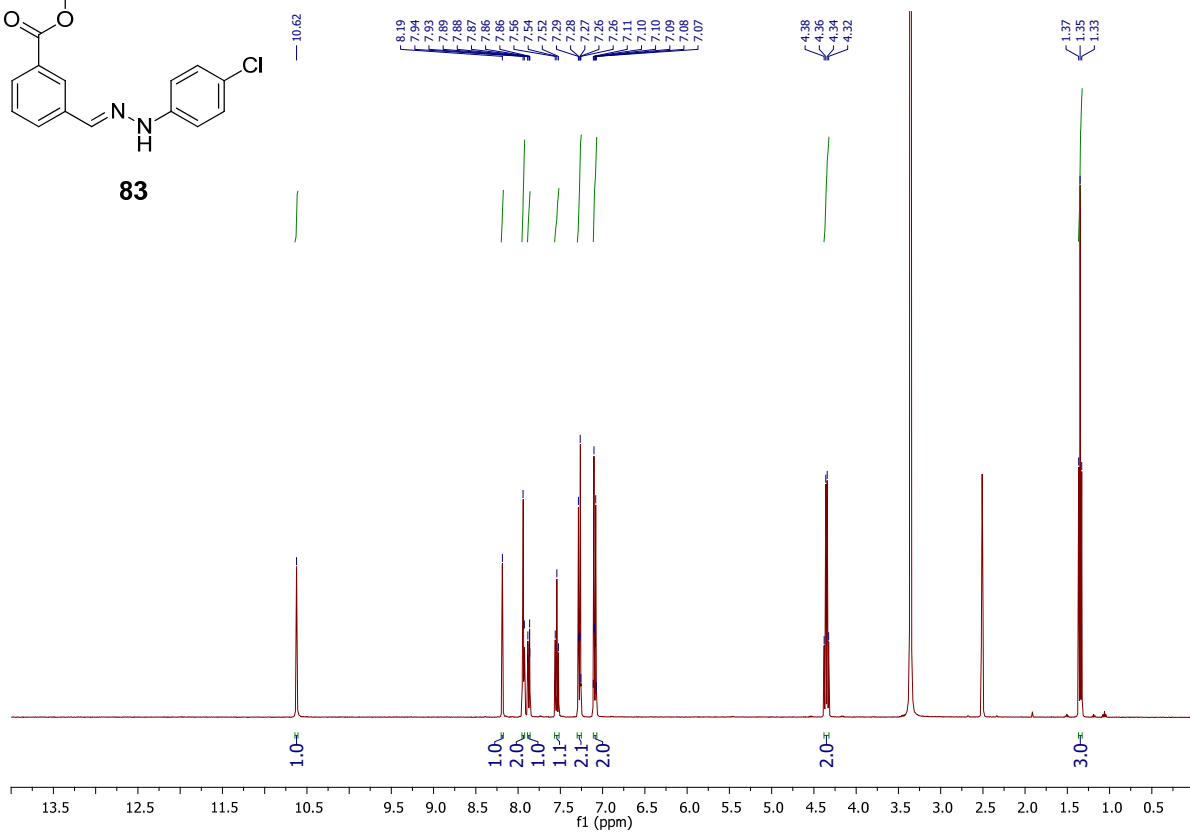
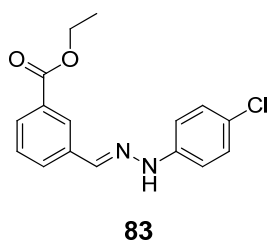
Data file: D:\Chem32\1\Data\MH4004 f6-13 and f15-58 2022-04-08 13-24-06\001-71-MH4004 f6-13.D
 Sample name: MH4004 f6-13
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 71
 Injection date: 4/8/2022 1:26:59 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 B_3 MINS.M
 Injection volume: 2.000
 Analysis method: LCMS ISOCRATIC
 80%B_3 MINS.M
 Acq. operator: SYSTEM
 Last changed: 11/26/2021 9:20:48 AM



Molecular Weight: 310.390

82



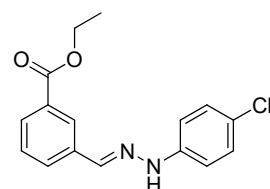


LCMS Report



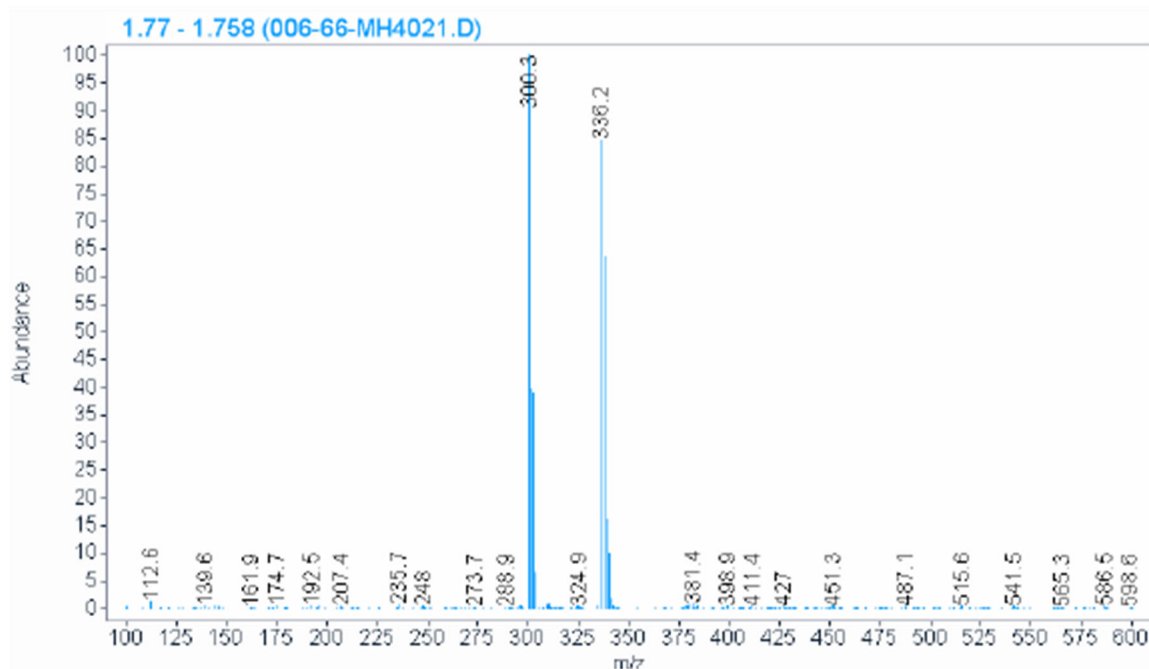
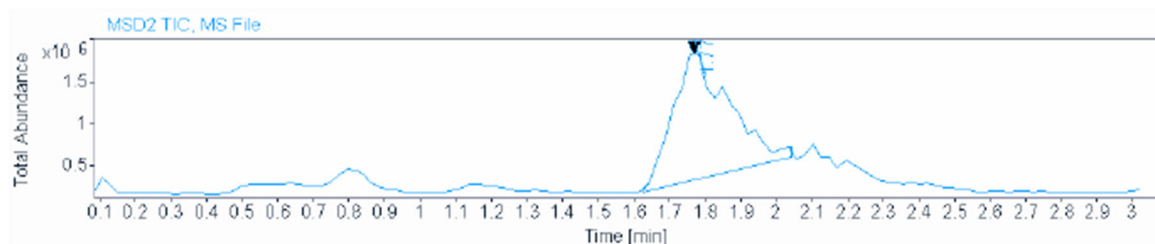
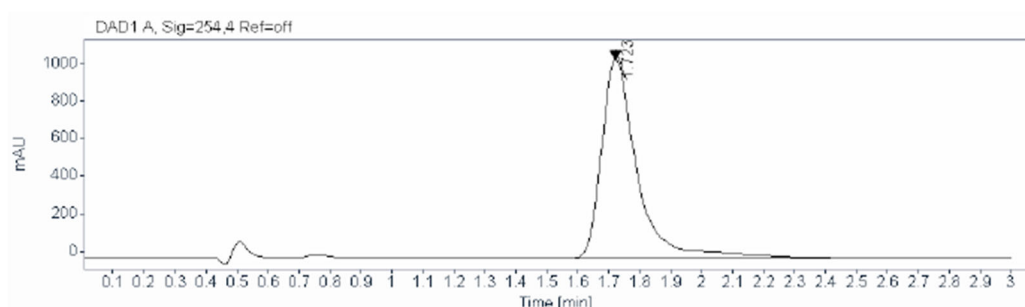
Agilent Technologies

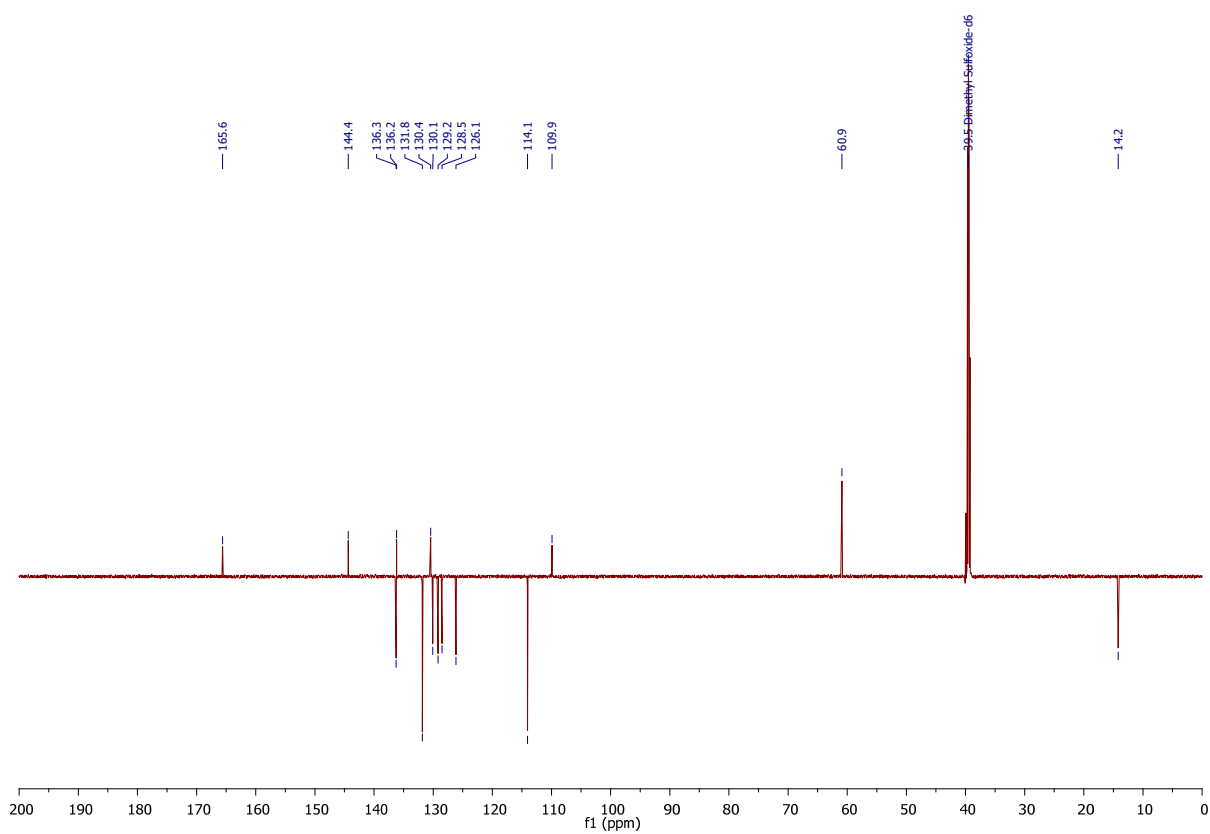
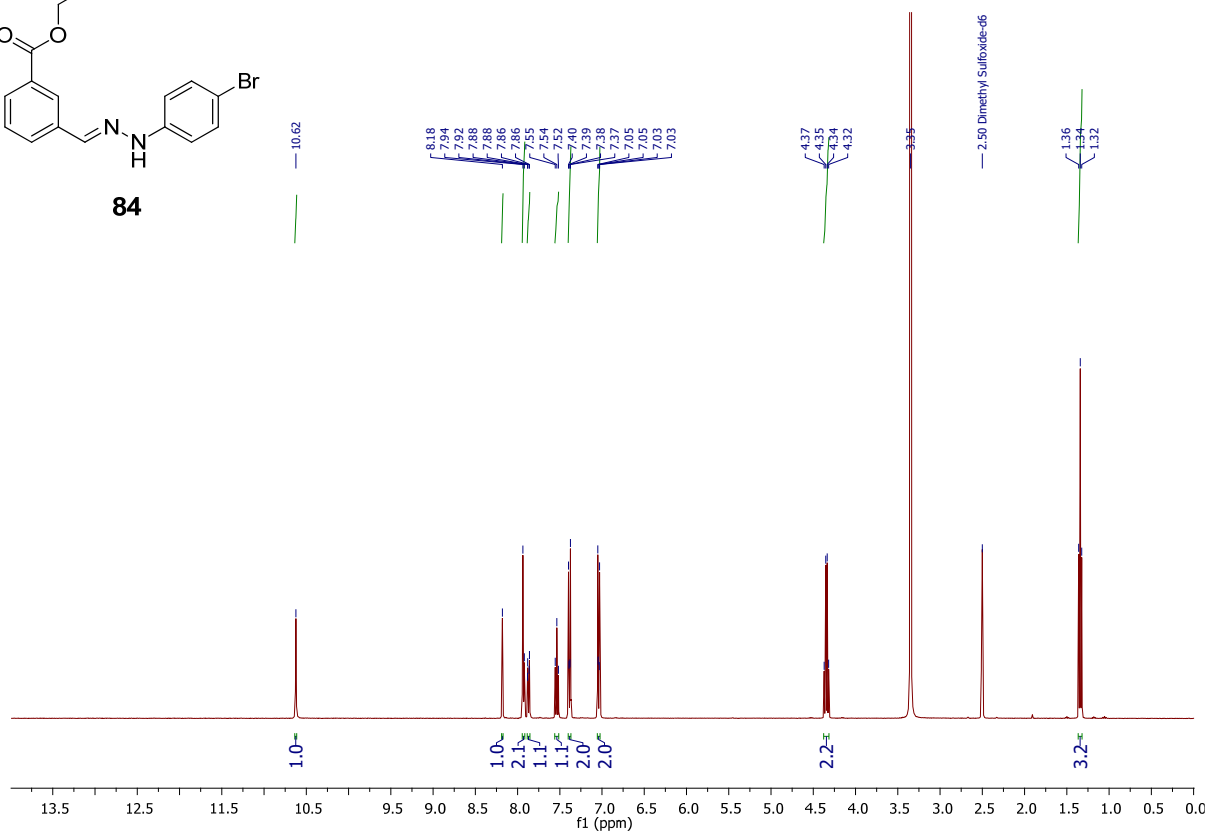
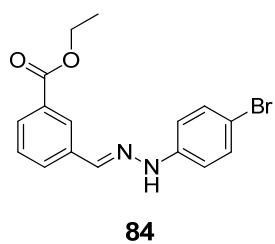
Data file: D:\Chem321\1\Data\AJS\mh4017-4021 2022-03-04 12-16-02\006-66-MH4021.D
 Sample name: MH4021
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 66
 Injection date: 3/4/2022 12:40:58 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 Injection volume: 2.000
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 80%B_3 MINS.M
 Last changed: 6/21/2024 5:34:02 PM



Molecular Weight: 302.756

83



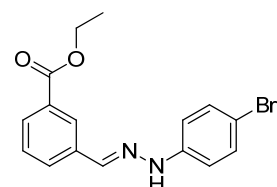


LCMS Report



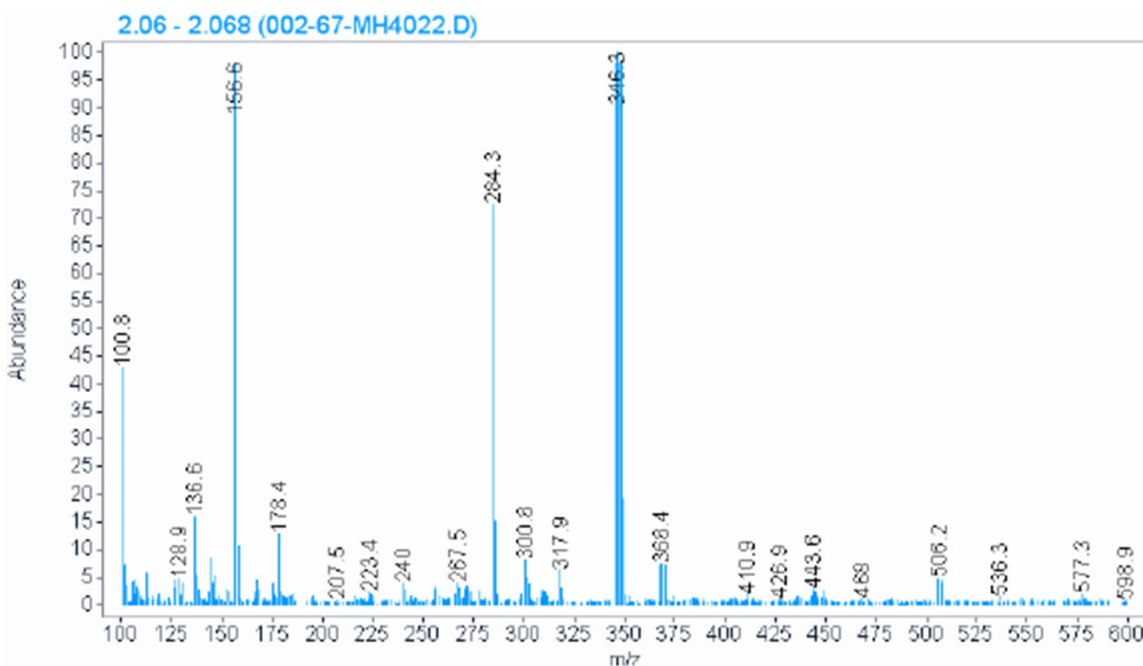
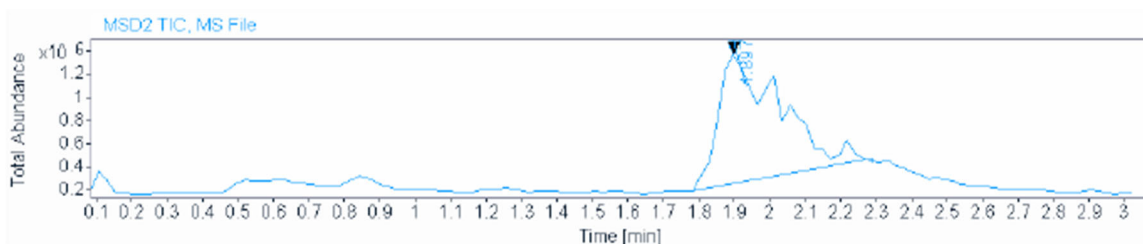
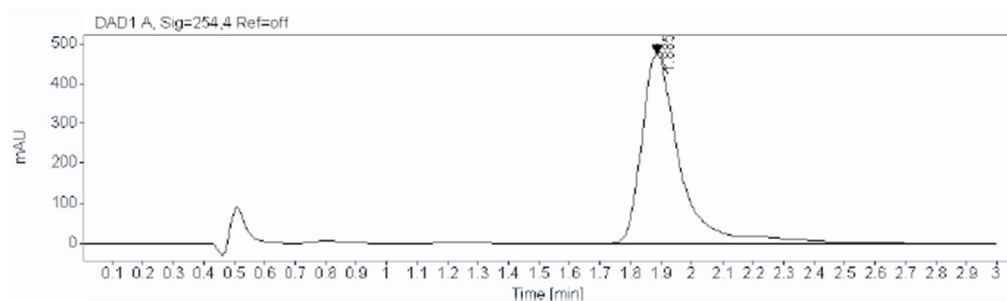
Agilent Technologies

Data file: D:\Chem32\1\Data\MH\mh40222-4026 2022-03-04 12-44-11\002-67-MH4022.D
 Sample name: MH4022
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 67
 Injection date: 3/4/2022 12:50:36 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 Injection volume: 2.000
 B_3 MINS.M
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 80%B_3 MINS.M
 Last changed: 11/26/2021 9:20:48 AM

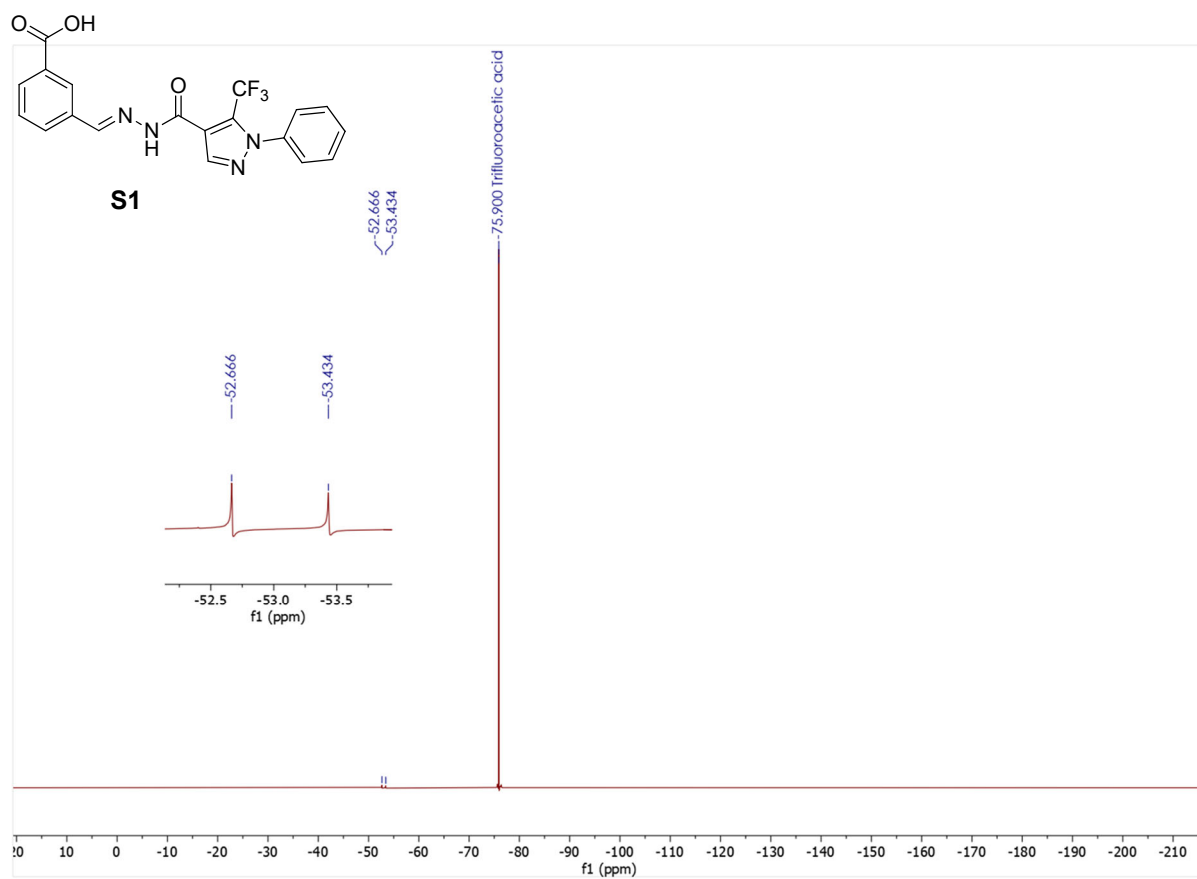


Molecular Weight: 347.207

84

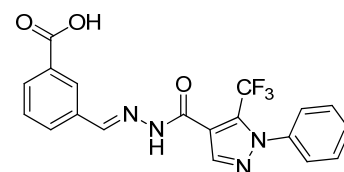






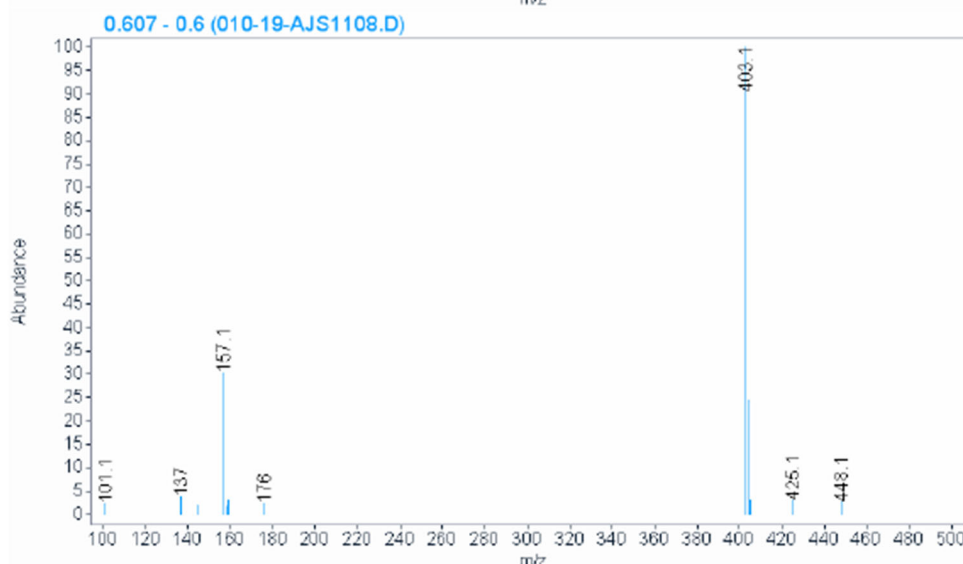
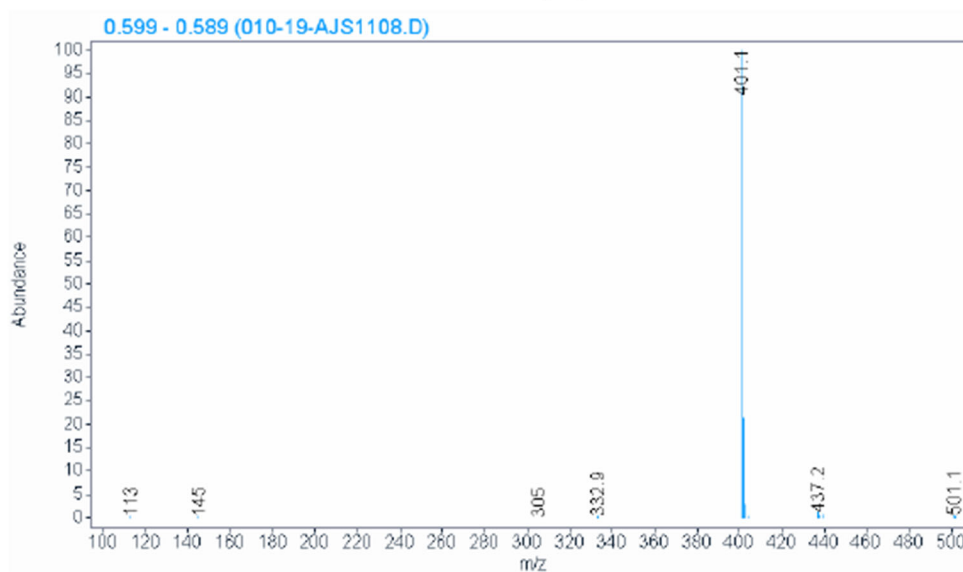
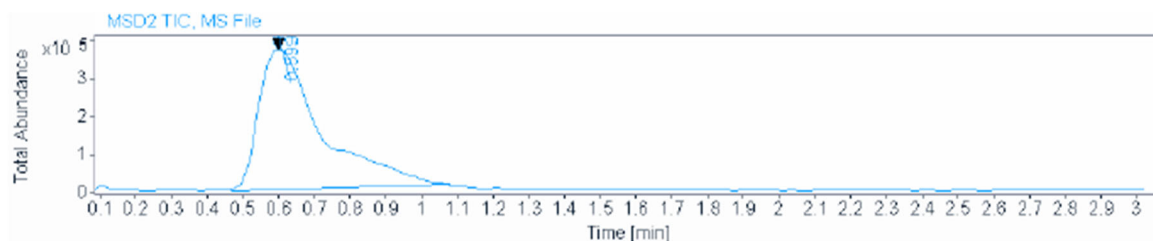
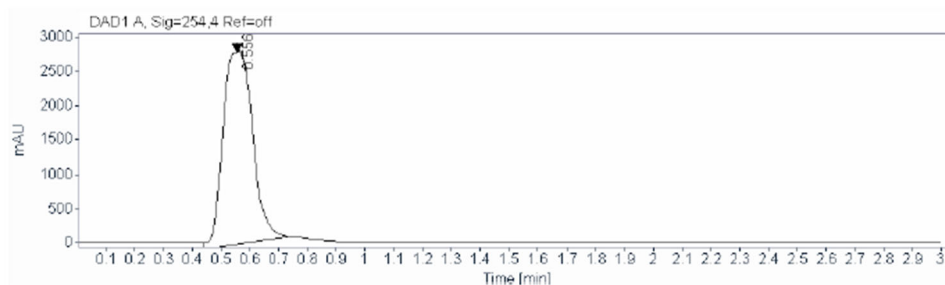


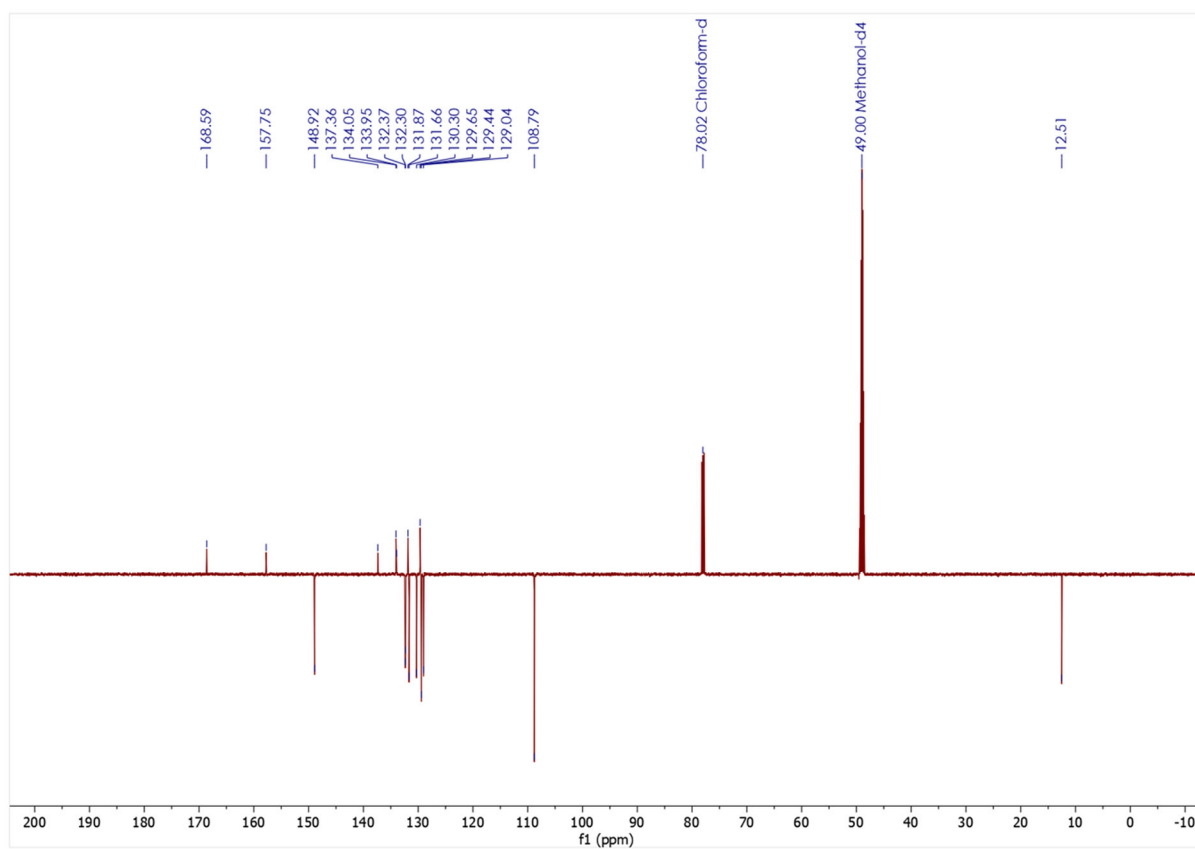
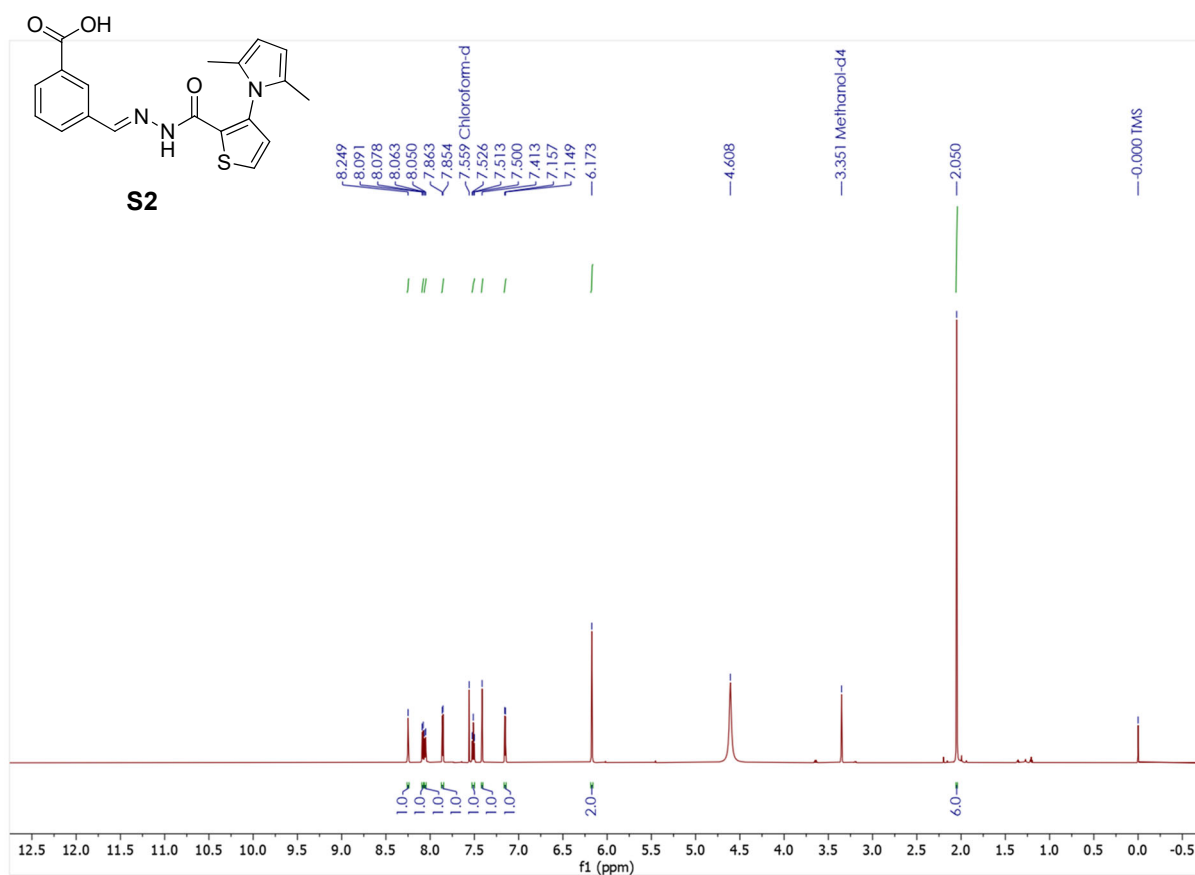
Data file: D:\Chem32\1\Data\AJS\AJS Table1 2023-07-25 14-45-29\010-19-AJS1108.D
Sample name: AJS1108
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Injection date: 7/25/2023 3:28:22 PM
Acq. method: LCMS ISOCRATIC 80%
B_3 MINS.M
Analysis method: LCMS ISOCRATIC
80%B_3 MINS.M
Last changed: 11/26/2021 9:20:48 AM
Location: 19
Injection: 1 of 1
Injection volume: 2.000
Acq. operator: SYSTEM



Molecular Weight: 402.327

S1



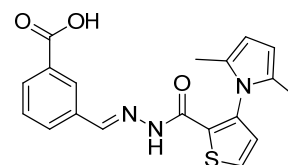


LCMS Report



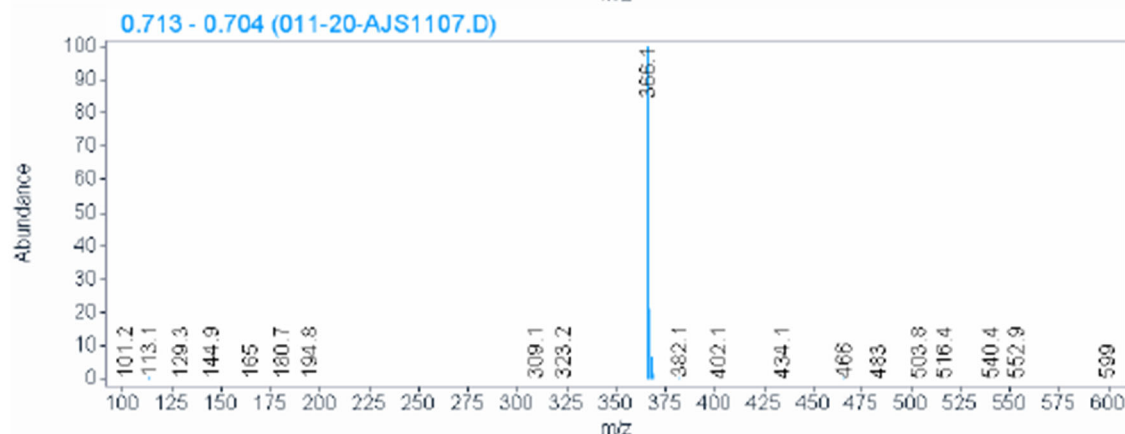
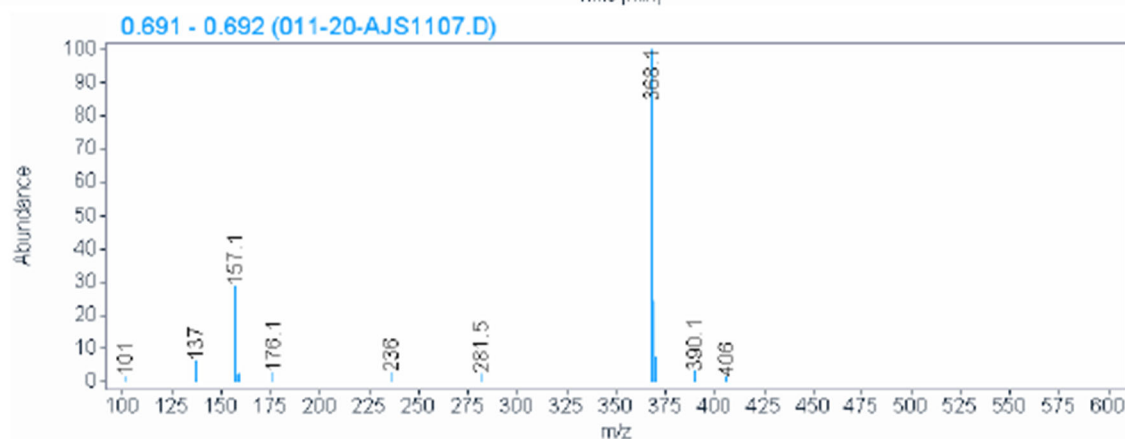
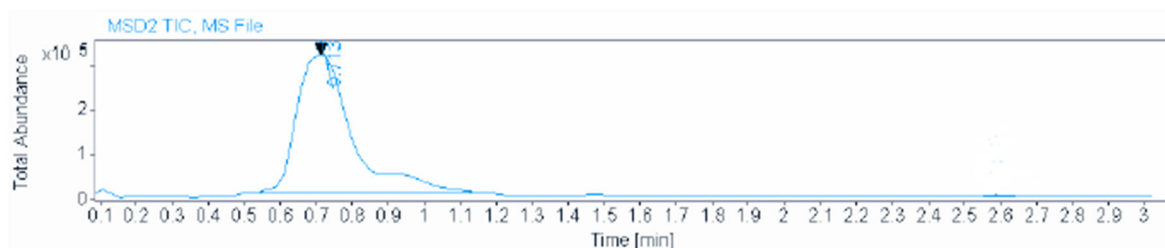
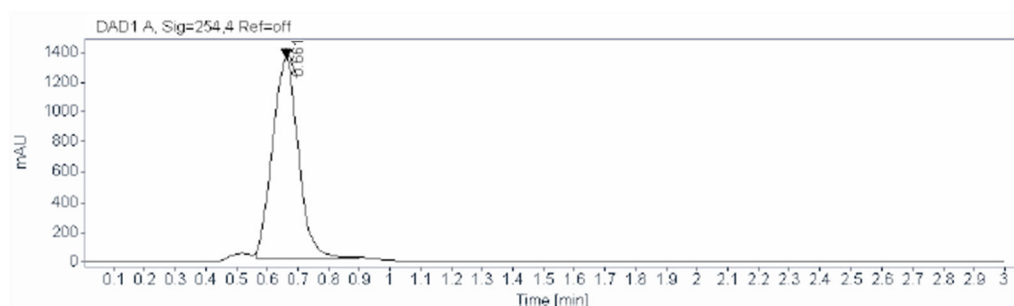
Agilent Technologies

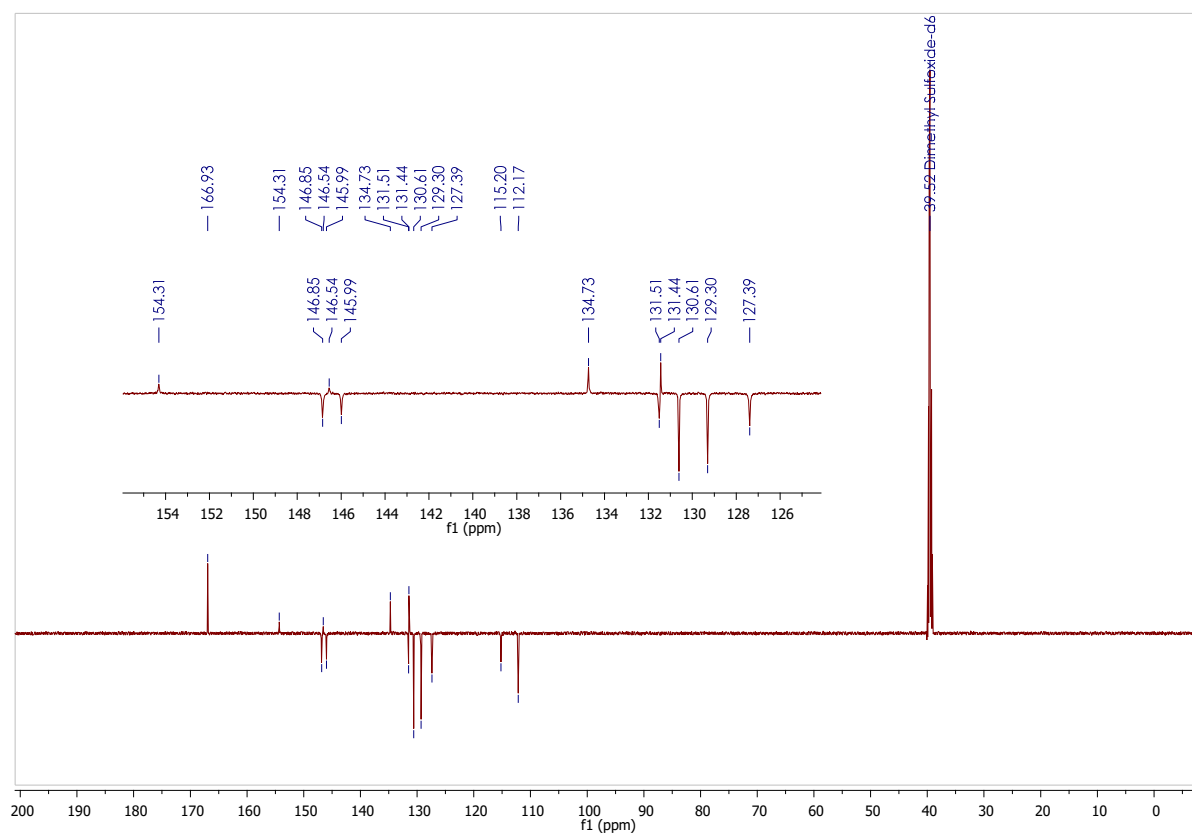
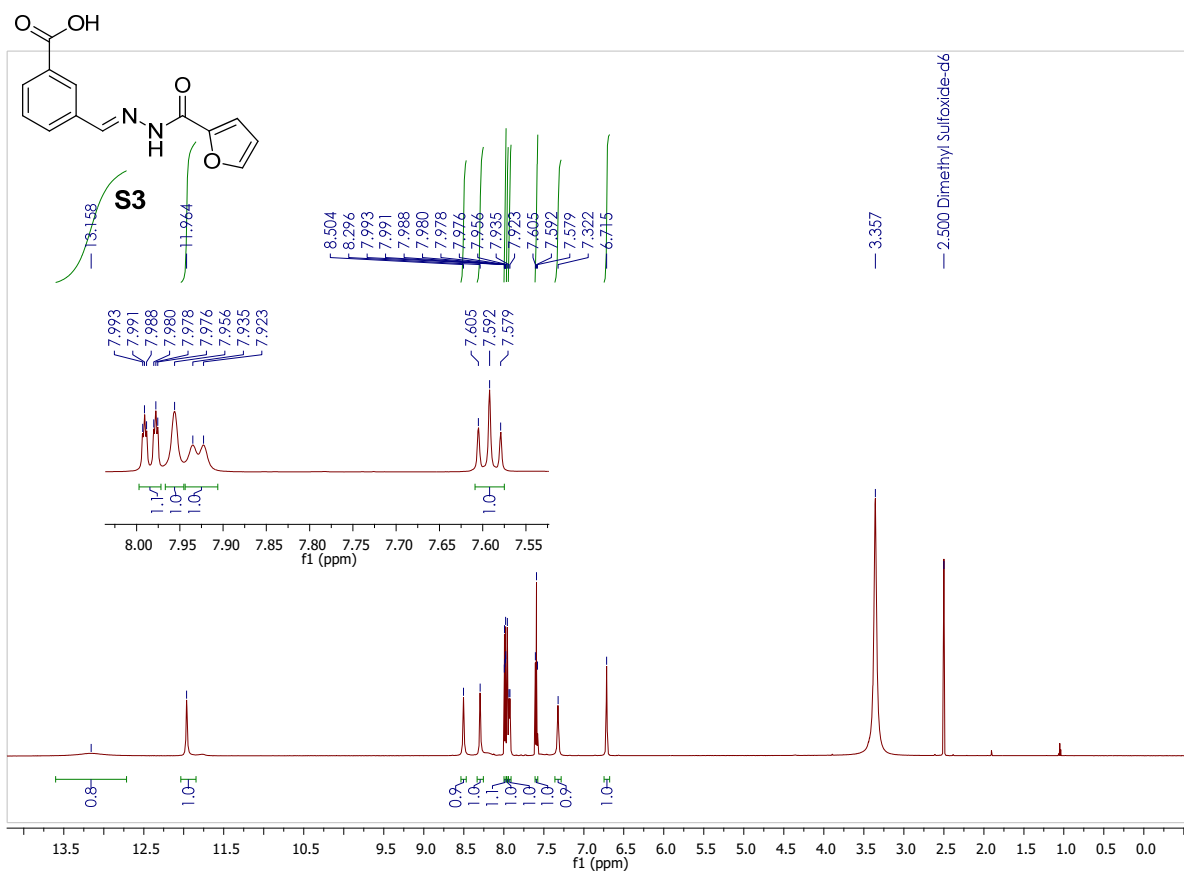
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 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 20
 Injection date: 7/25/2023 3:33:08 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 Injection volume: 2.000
 Analysis method: LCMS ISOCRATIC
 Acq. operator: SYSTEM
 80%B_3 MINS.M
 Last changed: 6/21/2024 5:37:01 PM



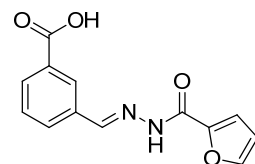
Molecular Weight: 367.422

S2



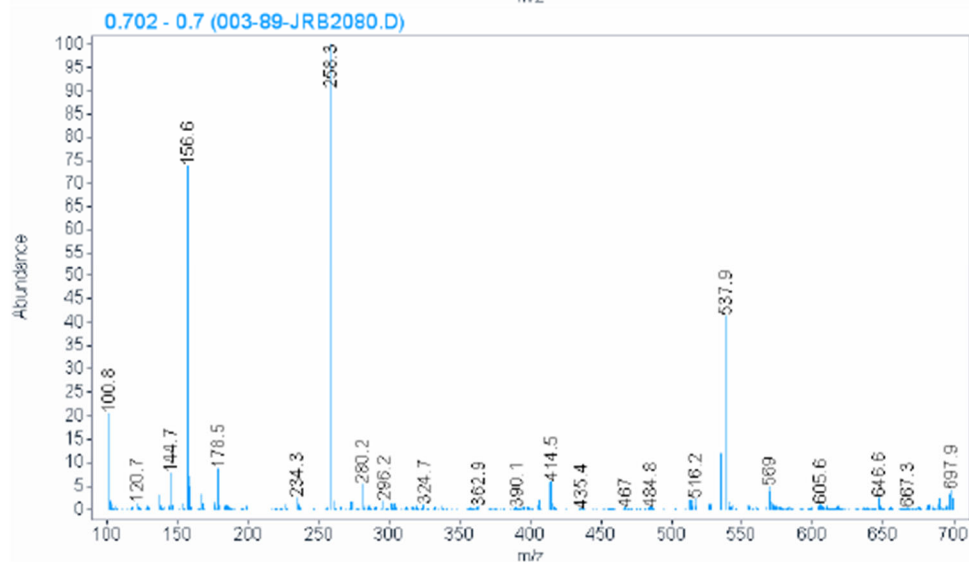
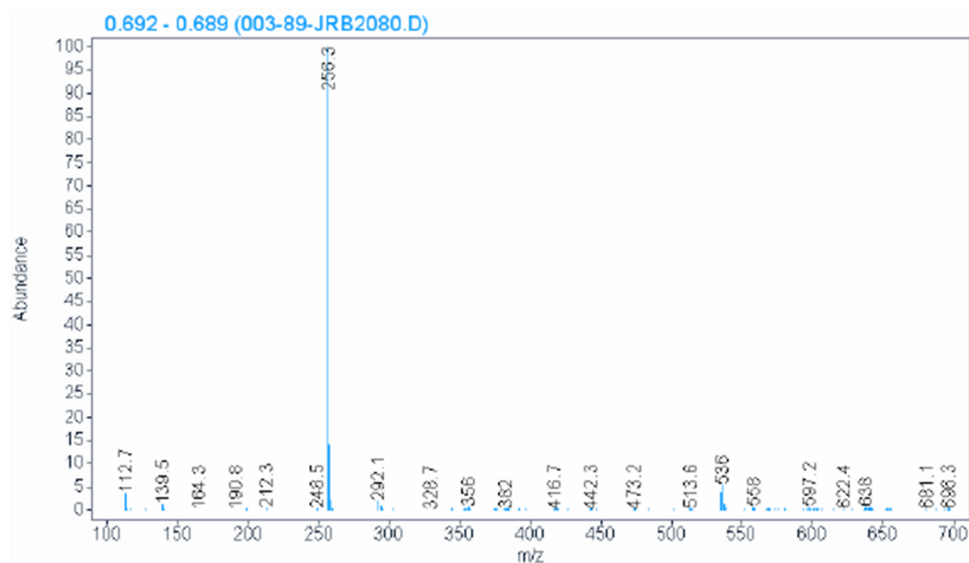
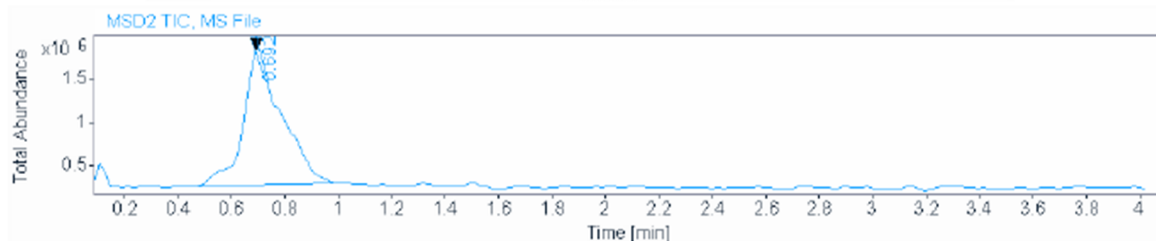
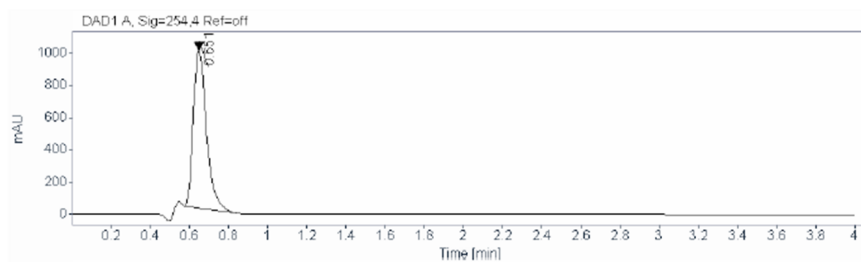


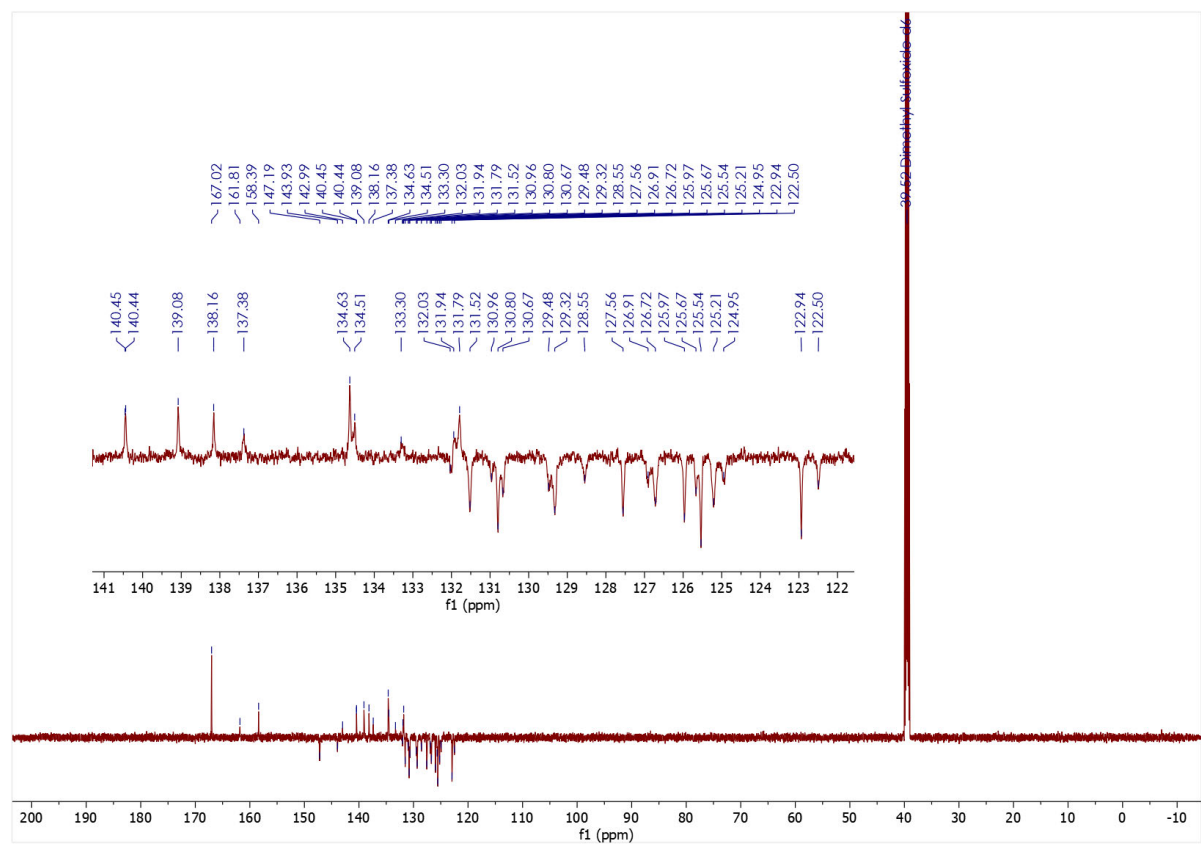
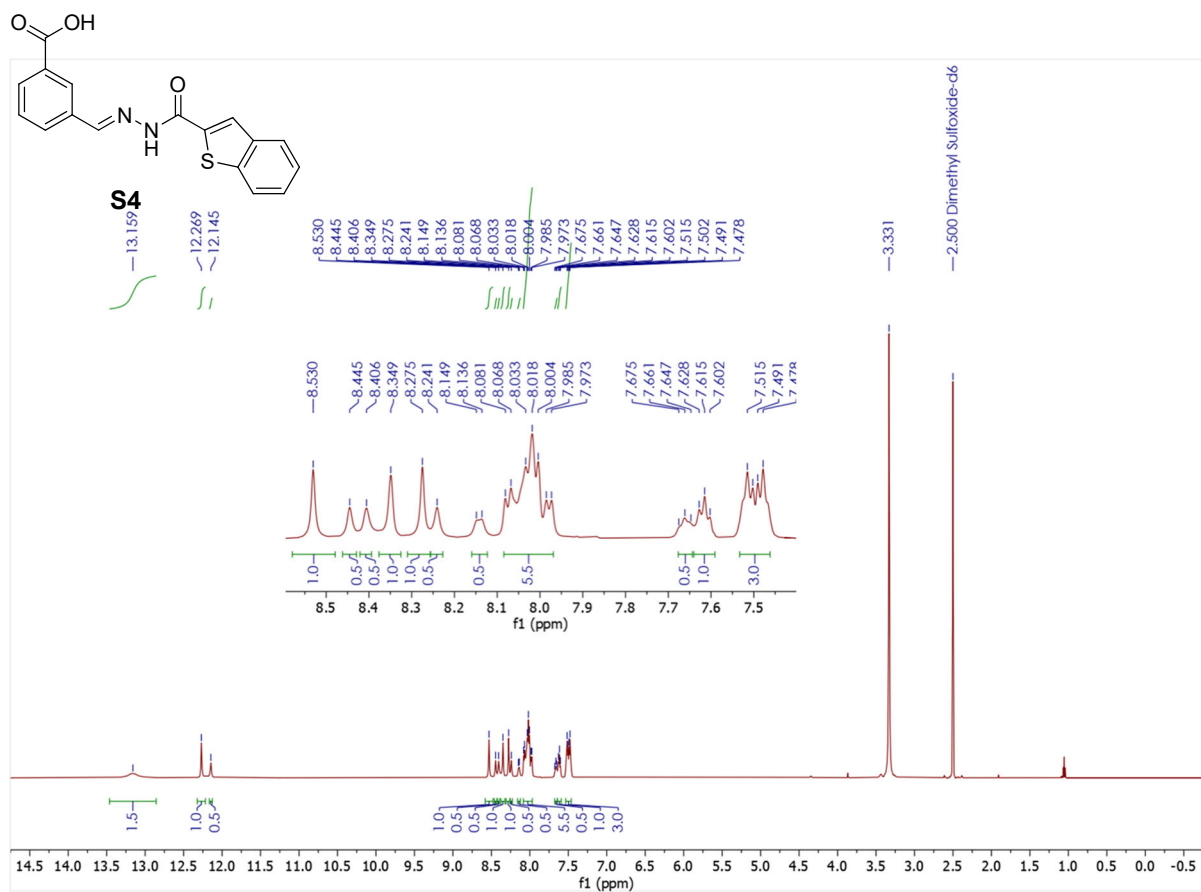
Data file: D:\Chem321\1Data\JRB\JRB2072 2080 2084 2081 2070 2022-01-31 15-09-41\003
 -89-JRB2080.D
 Sample name: JRB2080
 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Injection date: 1/31/2022 3:22:00 PM
 Location: 89
 Acq. method: LCMS ISOCRATIC_50%
 B_0.4MLMIN-
 1_4MINS.M
 Injection: 1 of 1
 Injection volume: 2.000
 Analysis method: LCMS
 ISOCRATIC_50%
 B_0.4MLMIN-
 1_4MINS.M
 Acq. operator: SYSTEM
 Last changed: 7/14/2016 12:06:24 PM



Molecular Weight: 258.229

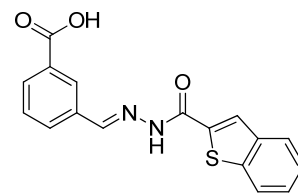
S3





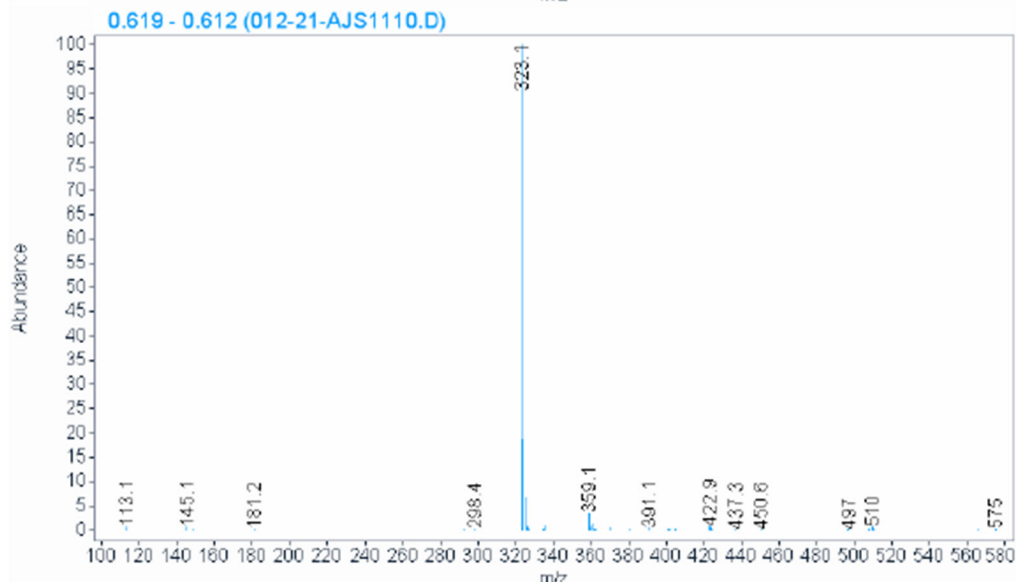
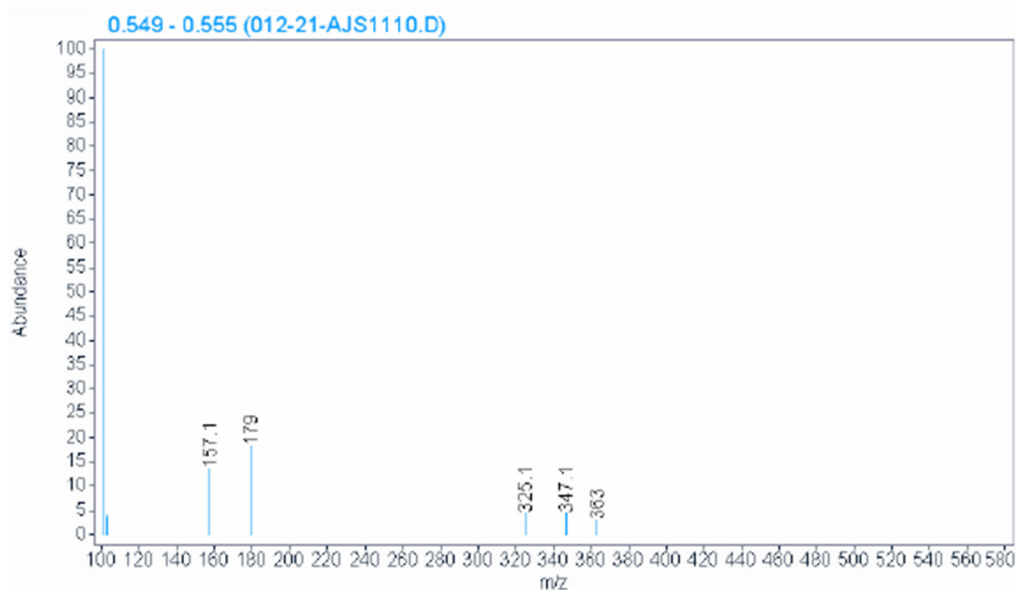
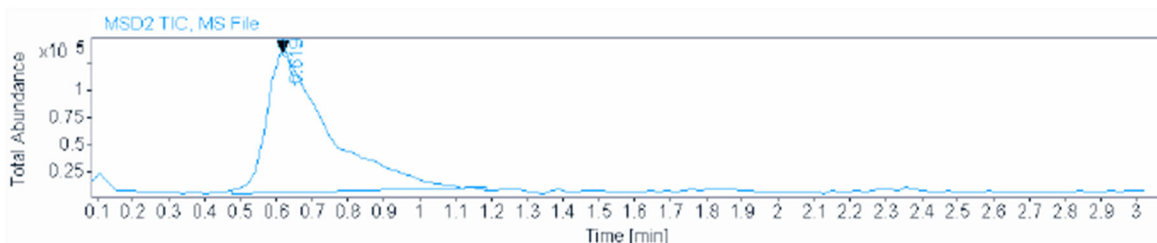
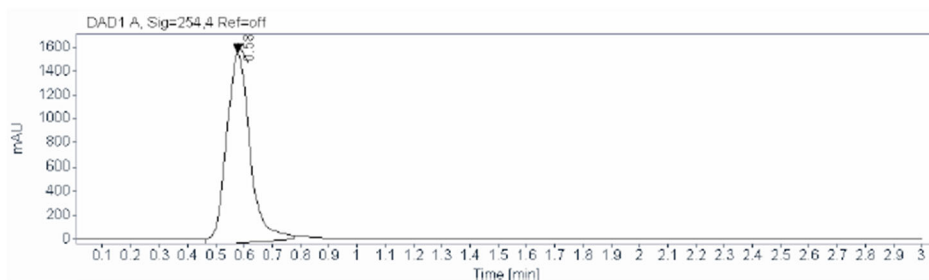


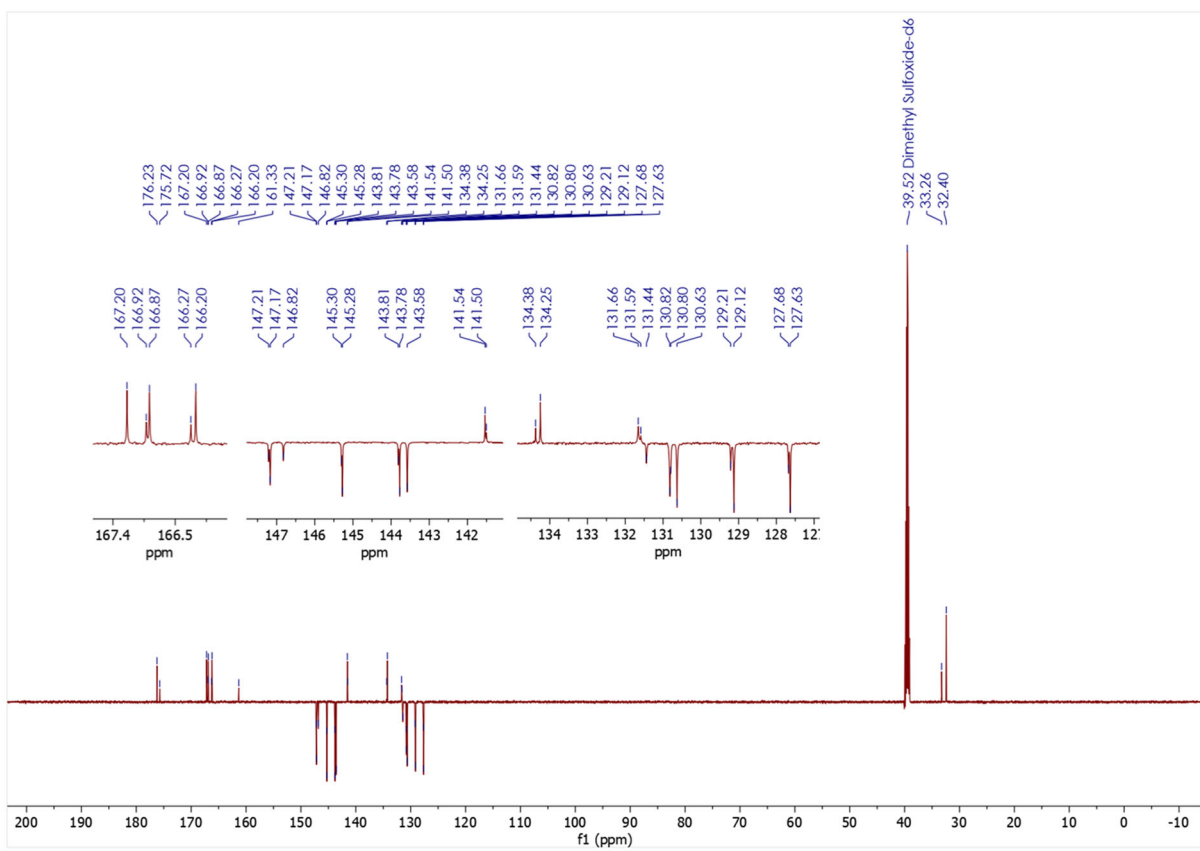
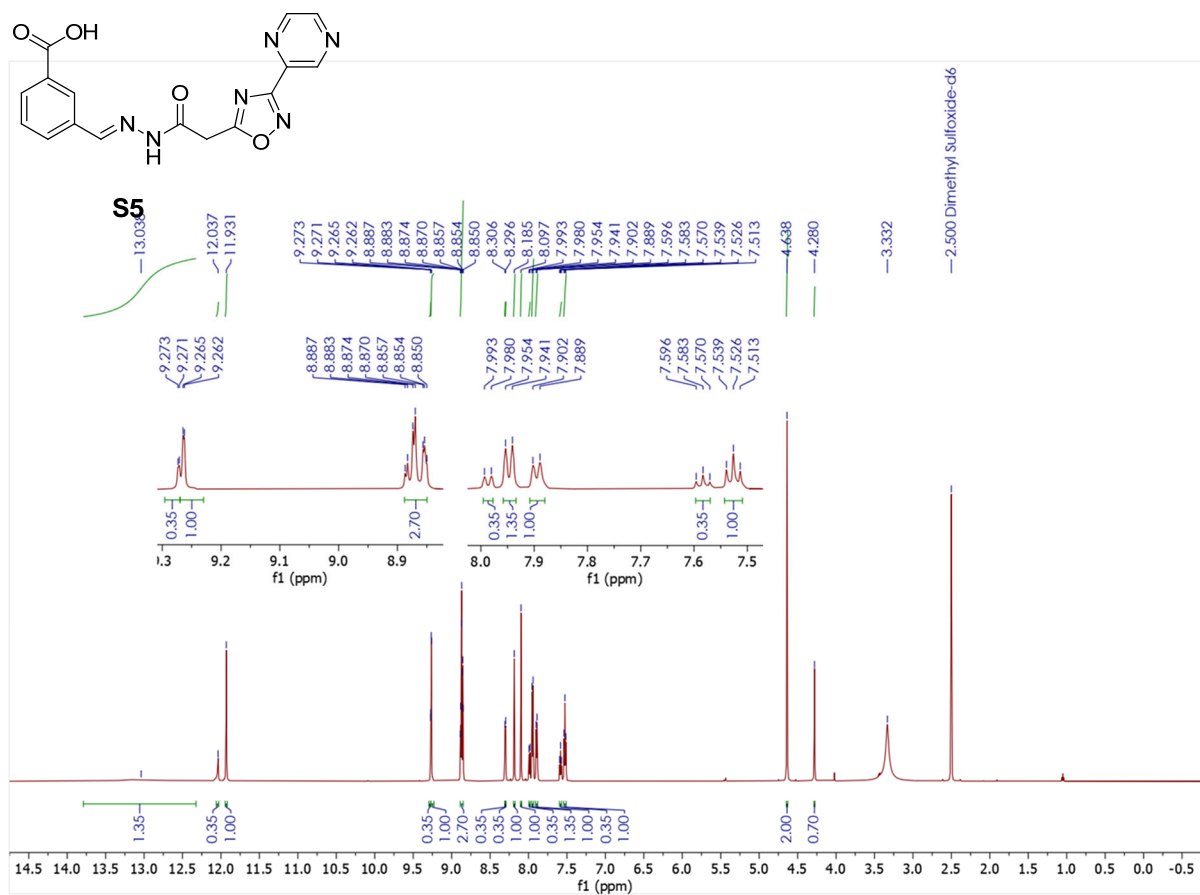
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 Description:
 Sample amount: 0.000
 Sample type: Sample
 Instrument: LCMS
 Location: 21
 Injection date: 7/25/2023 3:37:51 PM
 Injection: 1 of 1
 Acq. method: LCMS ISOCRATIC 80%
 B_3 MINS.M
 Injection volume: 2.000
 Analysis method: LCMS ISOCRATIC
 80%B_3 MINS.M
 Acq. operator: SYSTEM
 Last changed: 11/26/2021 9:20:48 AM



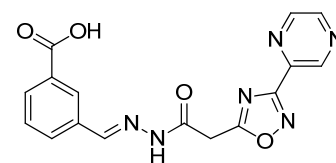
Molecular Weight: 324.354

S4





Data file: D:\Chem32\11Data\AJS\AJS Table1 2023-07-25 14-45-29\013-22-AJS1106.D
Sample name: AJS1106
Description:
Sample amount: 0.000
Sample type: Sample
Instrument: LCMS
Injection date: 7/25/2023 3:42:32 PM
Acq. method: LCMS ISOCRATIC 80%
B_3 MINS.M
Analysis method: LCMS ISOCRATIC
80%B_3 MINS.M
Last changed: 11/26/2021 9:20:48 AM
Location: 22
Injection: 1 of 1
Injection volume: 2.000
Acq. operator: SYSTEM



Molecular Weight: 352.304

S5