Supplementary Material

Solvent-assisted one-pot green and diastereoselective synthesis of 1,4-oxazines and 1,4-thioxazines under metal-free conditions

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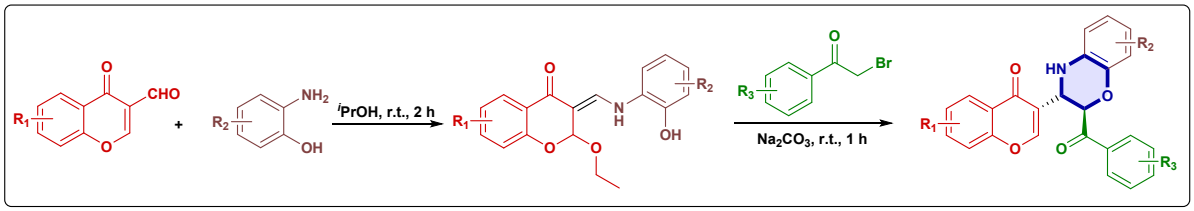
Experimental



General procedure: 3.0 ml of isopropanol was added to a round-bottom flask containing 0.5 mmol of formyl chromone (**1**) and 0.5 mmol of 2-aminophenol (**2**) or 2-aminothiophenol (**2'**), and the resulting mixture was stirred for 2 hours at room temperature, followed by the addition of 0.5 mmol 2-bromoacetophenone (**3**) and 1.5 mmol of Na_2CO_3, and stirred at same temperature for 1 hour. After completion of the reaction, 20.0 ml of ice-cold water was added to the reaction mixture to afford precipitates, which were filtered and recrystallised to get the desired product.

3-(2-benzoyl-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)-4H-chromen-4-one (4a): Yield 92%; Off-white solid; mp. 176-178 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.27 – 8.21 (m, 3H), 7.87 (s, 1H), 7.66 (td, *J* = 7.8, 1.7 Hz, 1H), 7.57 (t, *J* = 7.3 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 2H), 7.42 (t, *J* = 7.7 Hz, 2H), 6.91 – 6.77 (m, 2H), 6.72 (td, *J* = 7.7, 1.6 Hz, 1H), 6.66 (dd, *J* = 7.8, 1.6 Hz, 1H), 5.96 (d, *J* = 1.8 Hz, 1H), 5.24 (d, *J* = 5.0 Hz, 1H), 4.23 (d, *J* = 5.1 Hz, 1H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 195.31, 177.86, 156.52, 154.64, 142.36, 134.36, 134.05, 133.72, 130.69, 129.20, 128.82, 125.64, 125.47, 123.83, 123.05, 122.13, 120.08, 118.34, 116.95, 115.93, 75.57, 48.34. HRMS-ESI (m/z) calculated for $C_{24}H_{17}NO_4$ $(M+H)^+$: 384.1238, Experimental: $(M+H)^+$ = 384.1234. (Mass Error = 1.04 ppm)

3-(2-(4-bromobenzoyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)-4H-chromen-4-one (4b): Yield 89%; Off-white solid; mp. 182-184 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.23 (dd, *J* = 8.4, 1.7 Hz, 1H), 8.15 – 8.09 (m, 2H), 7.85 (d, *J* = 1.2 Hz, 1H), 7.67 (ddd, *J* = 8.9, 7.4, 1.7 Hz, 1H), 7.66 – 7.55 (m, 2H), 7.50 – 7.39 (m, 2H), 6.85 – 6.78 (m, 2H), 6.71 (td, *J* = 7.5, 1.6 Hz, 1H), 6.66 (dd, *J* = 8.1, 1.6 Hz, 1H), 5.88 (d, *J* = 1.7 Hz, 1H), 5.22 (dt, *J* = 5.3, 1.5 Hz, 1H), 4.22 (d, *J* = 5.2 Hz, 1H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 194.61, 177.85, 156.54, 154.68, 142.07, 134.13, 133.08, 132.16, 130.76, 130.64, 129.07, 125.61, 125.54, 123.76, 122.94, 122.31, 120.12, 118.36, 117.01, 115.90, 75.52, 48.25 HRMS-ESI (m/z) calculated for $C_{24}H_{16}BrNO_4$ $(M+H)^+$: 462.0341, Experimental: $(M+H)^+$ = 462.0338.

3-(2-(4-methoxybenzoyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)-4H-chromen-4-one (4c): Yield 93%; White solid; mp. 188-190 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.31 – 8.20 (m, 3H), 7.86 (d, *J* = 1.2 Hz, 1H), 7.66 (ddd, *J* = 8.7, 7.1, 1.7 Hz, 1H), 7.46 – 7.38 (m, 2H), 7.04 – 6.92 (m, 2H), 6.88 – 6.77 (m, 2H), 6.72 (td, *J* = 7.6, 1.6 Hz, 1H), 6.66 (dd, *J* = 7.8, 1.6 Hz, 1H), 5.90 (dd, *J* = 1.9, 0.8 Hz, 1H), 5.21 (dt, *J* = 5.3, 1.6 Hz, 1H), 4.23 (d, *J* = 5.2 Hz, 1H), 3.85 (s, 3H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 193.66, 177.89, 164.02, 156.52, 154.68, 142.61, 134.03, 131.61, 130.69, 127.23, 125.63, 125.44, 123.84, 123.21, 122.02, 120.08, 118.34, 116.86, 115.99, 114.07, 75.23, 55.58, 48.56 HRMS-ESI (m/z) calculated for $C_{25}H_{19}NO_5$ $(M+H)^+$: 414.1332, Experimental: $(M+H)^+$ = 414.1326.

3-(2-(4-methoxybenzoyl)-6-nitro-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)-4H-chromen-4-one (4d): Yield 84%; Pale-yellow solid; mp. 240-242 °C. ^{1}H NMR (700 MHz, $CDCl_3$) δ 8.33 (t, *J* = 6.9 Hz, 2H), 8.28 (t, *J* = 6.6 Hz, 1H), 7.80 (d, *J* = 4.9 Hz, 1H), 7.71 (dd, *J* = 15.4, 7.0 Hz, 2H), 7.59 (d, *J* = 4.8 Hz, 1H), 7.47 (t, *J* = 7.0 Hz, 2H), 7.04 (t, *J* = 6.4 Hz, 2H), 6.97 (t, *J* = 7.1 Hz, 1H), 6.13 (d, *J* = 4.8 Hz, 1H), 5.24 (d, *J* = 5.6 Hz, 1H), 4.63 (d, *J* = 5.8 Hz, 1H), 3.89 (d, *J* = 4.8 Hz, 3H). ^{13}C NMR (176 MHz, $CDCl_3$) δ 192.15, 177.77, 164.40, 156.45, 154.10, 148.15, 142.27, 134.33, 131.56, 130.78, 126.24, 125.69, 125.53, 123.59, 122.33, 118.37, 116.55, 116.09, 114.32, 110.29, 75.48, 55.59, 48.43. HRMS-ESI (m/z) calculated for $C_{25}H_{18}N_2O_7$ $(M+H)^+$: 459.1181, Experimental: $(M+H)^+$ = 459.1176.

3-(2-(4-chlorobenzoyl)-6-methyl-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)-4H-chromen-4-one (4e): Yield 90%; Off-white solid; mp. 188-190 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.22 (td, *J* = 7.7, 6.9, 1.9 Hz, 3H), 7.85 (d, *J* = 1.2 Hz, 1H), 7.67 (ddd, *J* = 8.6, 7.4, 1.7 Hz, 1H), 7.50 – 7.44 (m, 2H), 7.46 – 7.39 (m, 2H), 6.68 – 6.60 (m, 2H), 6.58 (d, *J* = 8.0 Hz, 1H), 5.89 (d, *J* = 1.9 Hz, 1H), 5.17 (dt, *J* = 5.4, 1.6 Hz, 1H), 4.09 (d, *J* = 5.2 Hz, 1H), 2.21 (s, 3H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 194.46, 177.91, 156.53, 154.74, 142.14, 140.23, 134.09, 132.67,

130.71, 130.09, 129.19, 127.80, 125.61, 125.51, 123.78, 122.94, 122.90, 118.34, 117.37, 116.18, 75.49, 48.34, 20.79. HRMS-ESI (m/z) calculated for $C_{25}H_{18}ClNO_4$ $(M+H)^+$: 432.0985, Experimental: $(M+H)^+$ = 432.0982.

3-(2-(4-methylbenzoyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)-4H-chromen-4-one (4f): Yield 90%; Off-white solid; mp. 186-188 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.27 – 8.21 (m, 1H), 8.17 – 8.11 (m, 2H), 7.87 (d, *J* = 1.2 Hz, 1H), 7.66 (ddd, *J* = 8.8, 7.2, 1.7 Hz, 1H), 7.46 – 7.39 (m, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 6.88 – 6.77 (m, 2H), 6.72 (td, *J* = 7.7, 1.6 Hz, 1H), 6.66 (dd, *J* = 7.8, 1.6 Hz, 1H), 5.92 (dd, *J* = 1.9, 0.9 Hz, 1H), 5.22 (dt, *J* = 5.2, 1.5 Hz, 1H), 4.22 (d, *J* = 5.1 Hz, 1H), 2.40 (s, 3H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 194.87, 177.85, 156.52, 154.63, 144.67, 142.48, 134.04, 131.80, 130.70, 129.54, 129.33, 125.65, 125.45, 123.84, 123.12, 122.06, 120.07, 118.33, 116.91, 115.98, 75.47, 48.40, 21.86. HRMS-ESI (m/z) calculated for $C_{25}H_{19}NO_4$ $(M+H)^+$:398.1403, Experimental: $(M+H)^+$ = 398.1398.

3-(6-chloro-2-(4-methoxybenzoyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)-4H-chromen-4-one (4g): Yield 89%; Pale-brown solid; mp. 192-194 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.31 – 8.19 (m, 3H), 7.81 (d, *J* = 1.1 Hz, 1H), 7.67 (ddd, *J* = 8.7, 7.2, 1.7 Hz, 1H), 7.46 – 7.39 (m, 2H), 7.03 – 6.93 (m, 2H), 6.87 (d, *J* = 2.3 Hz, 1H), 6.77 (dd, *J* = 8.4, 2.3 Hz, 1H), 6.58 (d, *J* = 8.4 Hz, 1H), 5.92 (d, *J* = 1.7 Hz, 1H), 5.17 (dt, *J* = 5.2, 1.5 Hz, 1H), 4.27 (d, *J* = 5.2 Hz, 1H), 3.86 (s, 3H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 193.17, 177.86, 164.19, 156.51, 154.51, 143.08, 134.16, 131.61, 129.39, 126.89, 125.61, 125.55, 124.36, 123.76, 122.84, 121.92, 118.38, 116.99, 116.54, 114.19, 75.06, 55.61, 48.44. HRMS-ESI (m/z) calculated for $C_{25}H_{18}ClNO_5$ $(M+H)^+$: 448.0963, Experimental: $(M+H)^+$ = 448.0959.

3-(2-(4-bromobenzoyl)-6-nitro-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)-4H-chromen-4-one (4h): Yield 81%; Yellow solid; mp. 244-246 °C. ^{1}H NMR (500 MHz, DMSO-D_6) δ 8.14 (ddt, *J* = 12.8, 10.9, 2.9 Hz, 3H), 7.91 (s, 1H), 7.86 – 7.71 (m, 3H), 7.64 – 7.43 (m, 4H), 7.00 – 6.91 (m, 2H), 6.33 – 6.27 (m, 1H), 5.03 (dd, *J* = 4.0, 2.0 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-D_6) δ 189.47, 182.04, 161.10, 159.73, 152.62, 146.89, 140.08, 137.78. 137.63, 137.37, 136.13, 123.81, 121.17, 114.47, 81.30, 52.28. HRMS-ESI (m/z) calculated for $C_{24}H_{15}BrN_2O_6$ $(M+H)^+$: 507.0186, Experimental: $(M+H)^+$ = 507.0182.

3-(6-chloro-2-(4-chlorobenzoyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)-4H-chromen-4-one (4i): Yield 83%; Pale-brown solid; mp. 186-188 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.26 – 8.18 (m, 3H), 7.81 (d, *J* = 1.2 Hz, 1H), 7.69 (ddd, *J* = 8.7, 7.1, 1.7 Hz, 1H), 7.52 – 7.39 (m, 4H), 6.86 (d, *J* = 2.4 Hz, 1H), 6.79 (dd, *J* = 8.5, 2.3 Hz, 1H), 6.59 (d, *J* = 8.4 Hz, 1H), 5.92 (d, *J* = 1.7 Hz, 1H), 5.18 (dt, *J* = 5.2, 1.4 Hz, 1H), 4.24 (d, *J* = 5.1 Hz, 1H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 193.80, 177.83, 156.53, 154.50, 142.61, 140.54, 134.26, 132.33, 130.67, 129.32, 129.27, 125.65, 125.61, 124.47, 123.71, 122.58, 122.20, 118.40, 117.13, 116.49, 75.33, 48.15. HRMS-ESI (m/z) calculated for $C_{24}H_{15}Cl_2NO_4$ $(M+H)^+$: 452.0467, Experimental: $(M+H)^+$ = 452.0465.

3-(6-chloro-2-(4-methylbenzoyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)-4H-chromen-4-one (4j): Yield 88%; Light-pink solid; mp. 188-190 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.24 (dd, *J* = 8.2, 1.7 Hz, 1H), 8.17 – 8.12 (m, 2H), 7.82 (d, *J* = 1.1 Hz, 1H), 7.68 (ddd, *J* = 8.7, 7.1, 1.7 Hz, 1H), 7.46 – 7.39 (m, 2H), 7.30 (d, *J* = 7.9 Hz, 2H), 6.87 (d, *J* = 2.3 Hz, 1H), 6.78 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.58 (d, *J* = 8.4 Hz, 1H), 5.95 (d, *J* = 1.8 Hz, 1H), 5.18 (dt, *J* = 5.2, 1.5 Hz, 1H), 4.25 (d, *J* = 5.1 Hz, 1H), 2.41 (s, 3H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 194.34, 177.80, 156.51, 154.45, 144.96, 142.96, 134.16, 131.48, 129.66, 129.37, 129.31, 125.64, 125.55, 124.38, 123.77, 122.75, 121.97, 118.37, 117.06, 116.55, 75.31, 48.28, 21.88. HRMS-ESI (m/z) calculated for $C_{25}H_{18}ClNO_4$ $(M+H)^+$: 432.1013, Experimental: $(M+H)^+$ = 432.1009.

7-bromo-3-(2-(4-bromobenzoyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)-4H-chromen-4-one (4k): Yield 85%; Yellow solid; mp. 190-192 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.29 (d, *J* = 2.4 Hz, 1H), 8.15 – 8.04 (m, 2H), 7.79 (d, *J* = 1.2 Hz, 1H), 7.70 (dd, *J* = 8.9, 2.4 Hz, 1H), 7.67 – 7.56 (m, 2H), 7.28 (d, *J* = 8.9 Hz, 1H), 6.76 (ddd, *J* = 8.9, 7.5, 1.5 Hz, 2H), 6.64 (t, *J* = 7.8 Hz, 2H), 5.83 – 5.77 (m, 1H), 5.15 (dt, *J* = 5.1, 1.5 Hz, 1H), 4.64 (d, *J* = 5.1 Hz, 1H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 194.43, 176.59, 155.24, 154.97, 141.79, 137.03, 132.99, 132.12, 130.75, 130.70, 129.01, 128.13, 124.98, 123.24, 122.27, 120.34, 119.75, 118.89, 116.84, 115.69, 75.36, 48.08. HRMS-ESI (m/z) calculated for $C_{24}H_{15}Br_2NO_4$ $(M+H)^+$: 539.9452, Experimental: $(M+H)^+$ = 539.9447.

7-bromo-3-(2-(4-chlorobenzoyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)-4H-chromen-4-one (4l): Yield 84%; Off-white solid; mp. 218-220 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.35 (d, *J* = 2.5 Hz, 1H), 8.19 – 8.14 (m, 2H), 7.86 – 7.82 (m, 1H), 7.74 (dd, *J* = 8.9, 2.5 Hz, 1H), 7.48 – 7.42 (m, 2H), 7.31 (d, *J* = 8.9 Hz, 1H), 6.81 (t, *J* = 7.8 Hz, 2H), 6.70 (td, *J* = 7.6, 7.0, 1.6 Hz, 1H), 6.66 (dd, *J* = 7.8, 1.5 Hz, 1H), 5.83 (d, *J* = 1.9 Hz, 1H), 5.21 (dt, *J* = 5.5,

1.5 Hz, 1H), 4.23 (d, *J* = 5.4 Hz, 1H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 194.32, 176.52, 155.28, 154.92, 141.98, 140.31, 137.08, 132.64, 130.66, 130.53, 129.17, 128.27, 125.03, 123.30, 122.41, 120.30, 120.19, 118.99, 117.09, 116.02, 75.35, 48.17. HRMS-ESI (m/z) calculated for of $C_{24}H_{15}BrClNO_4$ $(M+H)^+$: 495.9958, Experimental: $(M+H)^+$ = 495.9954.

7-bromo-3-(2-(4-methoxybenzoyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)-4H-chromen-4-one (4m): Yield 87%; Brown solid; mp. 164-166 °C. ^{1}H NMR (700 MHz, $CDCl_3$) δ 8.37 (d, *J* = 4.9 Hz, 1H), 8.25 (t, *J* = 6.7 Hz, 2H), 7.86 (d, *J* = 4.9 Hz, 1H), 7.74 (t, *J* = 6.6 Hz, 1H), 7.32 (t, *J* = 7.1 Hz, 1H), 6.97 (t, *J* = 6.6 Hz, 2H), 6.85 (t, *J* = 6.6 Hz, 1H), 6.81 (t, *J* = 6.9 Hz, 1H), 6.73 (d, *J* = 7.0 Hz, 1H), 6.68 (t, *J* = 6.5 Hz, 1H), 5.86 (d, *J* = 4.8 Hz, 1H), 5.20 (d, *J* = 5.9 Hz, 1H), 4.25 (d, *J* = 5.9 Hz, 1H), 3.87 (d, *J* = 4.9 Hz, 3H). ^{13}C NMR (176 MHz, $CDCl_3$) δ 193.51, 176.49, 163.98, 155.18, 154.83, 142.41, 136.92, 131.52, 130.48, 128.21, 127.09, 125.01, 123.47, 122.04, 120.21, 118.82, 116.86, 116.00, 113.99, 74.98, 55.52, 48.40. HRMS-ESI (m/z) calculated for $C_{25}H_{18}BrNO_5$ $(M+H)^+$: 492.0454, Experimental: $(M+H)^+$ = 492.0451.

7-bromo-3-(2-(4-methoxybenzoyl)-7-nitro-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)-4H-chromen-4-one (4n): Yield 84%; Dark-brown solid; mp. 246-248 °C. ^{1}H NMR (700 MHz, DMSO) δ 8.24 (d, *J* = 6.6 Hz, 3H), 7.72 – 7.67 (m, 2H), 7.55 – 7.50 (m, 2H), 7.46 (d, *J* = 8.8 Hz, 1H), 7.30 (t, *J* = 6.2 Hz, 1H), 6.93 (t, *J* = 6.2 Hz, 2H), 6.79 (t, *J* = 6.2 Hz, 1H), 6.49 (s, 1H), 6.05 (s, 1H), 5.03 (d, *J* = 4.3 Hz, 1H), 3.79 (d, *J* = 4.5 Hz, 3H). ^{13}C NMR (126 MHz, DMSO-D_6) δ 192.13, 176.58, 164.25, 155.18, 154.74, 147.86, 142.08, 137.13, 131.45, 127.88, 124.86, 122.67, 120.58, 118.79, 115.92, 114.56, 114.26, 109.54, 75.44, 55.64, 48.13. HRMS-ESI (m/z) calculated for $C_{25}H_{17}BrN_2O_7$ $(M+H)^+$: 537.0302, Experimental: $(M+H)^+$ = 537.0297.

7-bromo-3-(2-(4-bromobenzoyl)-6-nitro-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)-4H-chromen-4-one (4o): Yield 80%; Yellow solid; mp. 232-234 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.14 (d, *J* = 2.4 Hz, 1H), 8.06 – 8.00 (m, 2H), 7.63 – 7.56 (m, 2H), 7.56 – 7.47 (m, 2H), 7.45 (d, *J* = 2.7 Hz, 1H), 7.39 (dd, *J* = 8.8, 2.7 Hz, 1H), 7.18 (d, *J* = 8.9 Hz, 1H), 6.69 (d, *J* = 8.8 Hz, 1H), 6.23 (d, *J* = 4.4 Hz, 1H), 5.95 (d, *J* = 1.3 Hz, 1H), 4.92 (dt, *J* = 4.5, 1.5 Hz, 1H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 192.94, 176.61, 154.67, 137.15, 132.27, 132.13, 131.74, 130.60, 129.34, 127.89, 124.75, 122.32, 120.41, 116.10, 114.80, 109.71, 75.56, 47.82. HRMS-ESI (m/z) calculated for $C_{24}H_{14}Br_2N_2O_6$ $(M+H)^+$: 584.9300, Experimental: $(M+H)^+$ = 584.9295.

7-bromo-3-(2-(4-chlorobenzoyl)-6-methyl-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)-4H-chromen-4-one (4p): Yield 83%; Off-white solid; mp. 196-198 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.36 (d, *J* = 2.4 Hz, 1H), 8.22 – 8.16 (m, 2H), 7.84 (d, *J* = 1.2 Hz, 1H), 7.74 (dd, *J* = 8.9, 2.5 Hz, 1H), 7.50 – 7.44 (m, 2H), 7.32 (d, *J* = 8.9 Hz, 1H), 6.64 (d, *J* = 8.0 Hz, 2H), 6.58 (d, *J* = 7.9 Hz, 1H), 5.84 (d, *J* = 1.8 Hz, 1H), 5.16 (dt, *J* = 5.5, 1.5 Hz, 1H), 4.08 (d, *J* = 5.4 Hz, 1H), 2.20 (s, 3H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 194.39, 176.59, 155.28, 154.98, 142.03, 140.31, 137.06, 132.62, 130.69, 130.22, 129.20, 128.28, 127.64, 125.05, 123.27, 123.01, 120.29, 118.97, 117.44, 116.32, 75.29, 48.25, 20.78. HRMS-ESI (m/z) calculated for $C_{25}H_{17}BrClNO_4$ $(M+H)^+$: 510.0115, Experimental: $(M+H)^+$ = 510.0111.

3-(2-(4-chlorobenzoyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)-7-methyl-4H-chromen-4-one (4q): Yield 88%; White solid; mp. 190-192 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.20 (td, *J* = 8.0, 3.8 Hz, 2H), 7.99 (d, *J* = 4.8 Hz, 1H), 7.82 (t, *J* = 5.8 Hz, 1H), 7.52 – 7.41 (m, 3H), 7.30 (dd, *J* = 9.0, 5.4 Hz, 1H), 6.81 (tq, *J* = 10.2, 6.4, 5.4 Hz, 2H), 6.71 (t, *J* = 6.8 Hz, 1H), 6.65 (t, *J* = 6.6 Hz, 1H), 5.87 (d, *J* = 5.3 Hz, 1H), 5.20 (q, *J* = 9.5, 5.4 Hz, 1H), 4.23 (dd, *J* = 8.0, 4.6 Hz, 1H), 2.45 (t, *J* = 5.8 Hz, 3H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 194.38, 177.90, 154.83, 154.53, 142.15, 140.21, 135.59, 135.41, 132.67, 130.68, 129.16, 124.82, 123.42, 122.73, 122.24, 120.05, 118.09, 116.94, 115.82, 75.59, 48.29, 21.06. HRMS-ESI (m/z) calculated for $C_{25}H_{18}ClNO_4$ $(M+H)^+$: 432.1008, Experimental: $(M+H)^+$ = 432.1004.

3-(2-(4-bromobenzoyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)-7-methyl-4H-chromen-4-one (4r): Yield 88%; Yellow solid; mp. 192-194 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.19 – 8.10 (m, 2H), 8.00 (dd, *J* = 2.2, 1.0 Hz, 1H), 7.82 (d, *J* = 1.1 Hz, 1H), 7.69 – 7.58 (m, 2H), 7.48 (dd, *J* = 8.6, 2.3 Hz, 1H), 7.31 (d, *J* = 8.6 Hz, 1H), 6.85 – 6.76 (m, 2H), 6.71 (td, *J* = 7.7, 1.6 Hz, 1H), 6.66 (dd, *J* = 7.7, 1.6 Hz, 1H), 5.88 (dd, *J* = 1.9, 0.9 Hz, 1H), 5.20 (dt, *J* = 5.1, 1.5 Hz, 1H), 4.22 (d, *J* = 5.1 Hz, 1H), 2.45 (s, 3H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 194.59, 177.92, 154.84, 154.53, 142.13, 135.60, 135.43, 133.06, 132.16, 130.76, 130.67, 129.05, 124.82, 123.41, 122.71, 122.26, 120.08, 118.10, 116.95, 115.82, 75.58, 48.28, 21.08. HRMS-ESI (m/z) calculated for $C_{25}H_{18}BrNO_4$ $(M+H)^+$: 476.0507, Experimental: $(M+H)^+$ = 476.0504.

3-(2-(4-methoxybenzoyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)-7-methyl-4H-chromen-4-one (4s): Yield 94%; Pale yellow solid; mp. 194-196 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.33 – 8.23 (m, 2H), 8.04 – 8.00 (m, 1H), 7.83 (d, *J* = 1.1 Hz, 1H), 7.47 (dd, *J* = 8.6, 2.2 Hz, 1H), 7.31 (d, *J* = 8.6 Hz, 1H), 7.05 – 6.92 (m, 2H), 6.86 (dd, *J* = 8.0, 1.5 Hz, 1H), 6.81 (td, *J* = 7.6, 1.5 Hz, 1H), 6.72 (td, *J* = 7.7, 1.6 Hz, 1H), 6.66 (dd, *J* = 7.8, 1.6 Hz, 1H), 5.90 (d, *J* = 1.8 Hz, 1H), 5.23 – 5.15 (m, 1H), 4.21 (d, *J* = 5.1 Hz, 1H), 3.86 (s, 3H), 2.45 (s, 3H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 193.68, 177.97, 164.00, 154.83, 154.53, 142.66, 135.49, 135.34, 131.62, 130.71, 127.21, 124.85, 123.49, 122.99, 121.97, 120.05, 118.09, 116.81, 115.90, 114.07, 75.28, 55.58, 48.59, 21.07. HRMS-ESI (m/z) calculated for $C_{26}H_{21}NO_5$ $(M+H)^+$: 428.1505, Experimental: $(M+H)^+$ = 428.1500.

3-(2-(4-methoxybenzoyl)-6-nitro-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)-7-methyl-4H-chromen-4-one (4t): Yield 85%; Orange solid; mp. 234-236 °C. ^{1}H NMR (500 MHz, DMSO-D_6) δ 8.32 – 8.22 (m, 2H), 7.90 (dd, *J* = 15.5, 1.7 Hz, 2H), 7.62 (dd, *J* = 8.7, 2.1 Hz, 1H), 7.54 (d, *J* = 2.8 Hz, 1H), 7.53 – 7.47 (m, 2H), 7.15 – 7.06 (m, 2H), 6.98 – 6.89 (m, 2H), 6.22 (t, *J* = 1.4 Hz, 1H), 5.03 (dt, *J* = 3.5, 1.5 Hz, 1H), 3.83 (s, 3H), 2.41 (s, 3H). ^{13}C NMR (126 MHz, DMSO-D_6) δ 192.54, 177.24, 164.38, 154.79, 154.67, 148.25, 142.01, 136.34, 136.02, 133.14, 131.81, 126.55, 124.69, 123.19, 122.47, 118.81, 116.25, 114.80, 114.30, 109.48, 76.17, 56.22, 47.90, 21.03. HRMS-ESI (m/z) calculated for $C_{26}H_{20}N_2O_7$ $(M+H)^+$: 473.1360, Experimental: $(M+H)^+$ = 473.1353.

3-(2-(4-bromobenzoyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)-7-methoxy-4H-chromen-4-one (4u): Yield 83%; White solid; mp. 180-182 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.17 – 8.11 (m, 2H), 7.84 (d, *J* = 1.1 Hz, 1H), 7.68 – 7.60 (m, 2H), 7.57 (d, *J* = 3.1 Hz, 1H), 7.36 (d, *J* = 9.1 Hz, 1H), 7.27 (dd, *J* = 9.2, 3.1 Hz, 1H), 6.86 – 6.79 (m, 2H), 6.72 (td, *J* = 7.8, 1.6 Hz, 1H), 6.67 (dd, *J* = 7.9, 1.4 Hz, 1H), 5.89 (dd, *J* = 1.9, 0.9 Hz, 1H), 5.23 (dt, *J* = 5.2, 1.5 Hz, 1H), 4.18 (d, *J* = 5.1 Hz, 1H), 3.91 (s, 3H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 194.55, 177.63, 157.25, 154.40, 151.49, 142.13, 133.07, 132.18, 130.77, 130.62, 129.07, 124.45, 124.36, 122.28, 122.13, 120.15, 119.80, 116.99, 115.84, 104.37, 75.59, 56.06, 48.33. HRMS-ESI (m/z) calculated for $C_{25}H_{18}BrNO_5(M+H)^+$: 492.0444, Experimental: $(M+H)^+$ = 492.0440.

7-methoxy-3-(2-(4-methoxybenzoyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)-4H-chromen-4-one (4v): Yield 93%; Pale-brown solid; mp. 182-184 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.33 – 8.23 (m, 2H), 7.85 (d, *J* = 1.1 Hz, 1H), 7.58 (d, *J* = 3.1 Hz, 1H), 7.35 (d, *J* = 9.2 Hz, 1H), 7.32 – 7.23 (m, 1H), 6.99 (d, *J* = 2.0 Hz, 1H), 6.97 (s, 1H), 6.88 – 6.78 (m, 2H), 6.76 – 6.60 (m, 2H), 5.91 (d, *J* = 1.8 Hz, 1H), 5.22 (dt, *J* = 5.2, 1.4 Hz, 1H), 4.21 (d, *J* = 5.1 Hz, 1H), 3.90 (s, 3H), 3.86 (s, 3H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 193.66, 177.68, 164.01, 157.19, 154.43, 151.47, 142.65, 131.61, 130.70, 127.22, 124.34, 122.41, 122.00, 120.09, 119.77, 116.84, 115.92, 114.07, 104.43, 75.31, 56.05, 55.58, 48.63. HRMS-ESI (m/z) calculated for $C_{26}H_{21}NO_6$ $(M+H)^+$: 444.1454, Experimental: $(M+H)^+$ = 444.1449.

3-(2-(4-bromobenzoyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-3-yl)-7-hydroxy-4H-chromen-4-one (4w): Yield 80%; Orange solid; mp. 210-212 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.36 (d, *J* = 2.4 Hz, 1H), 8.16 – 8.01 (m, 2H), 7.85 (d, *J* = 1.2 Hz, 1H), 7.75 (dd, *J* = 8.9, 2.5 Hz, 1H), 7.70 – 7.60 (m, 2H), 7.33 (d, *J* = 8.9 Hz, 1H), 6.86 – 6.78 (m, 2H), 6.71 (ddd, *J* = 8.3, 7.3, 1.5 Hz, 1H), 6.67 (dd, *J* = 7.8, 1.5 Hz, 1H), 5.83 (d, *J* = 1.8 Hz, 1H), 5.24 – 5.20 (m, 1H), 4.20 (s, 1H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 194.52, 176.52, 155.30, 154.92, 141.97, 137.10, 133.07, 132.17, 130.74, 130.49, 129.13, 128.30, 125.05, 123.28, 122.42, 120.29, 120.25, 119.00, 117.12, 116.06, 75.33, 48.17. HRMS-ESI (m/z) calculated for $C_{24}H_{16}BrNO_5$ $(M)^+$: 477.0158, Experimental: M^+ = 477.0110.

3-(2-benzoyl-3,4-dihydro-2H-benzo[b][1,4]thiazin-3-yl)-4H-chromen-4-one (5a): Yield 94%; White solid; mp. 182-184 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.24 (d, *J* = 7.9 Hz, 1H), 8.02 – 7.90 (m, 3H), 7.67 (t, *J* = 8.0 Hz, 1H), 7.56 – 7.41 (m, 5H), 7.03 (t, *J* = 7.9 Hz, 1H), 6.96 (d, *J* = 7.7 Hz, 1H), 6.72 – 6.62 (m, 2H), 5.44 (d, *J* = 6.2 Hz, 1H), 4.96 (s, 1H), 4.59 (d, *J* = 6.4 Hz, 1H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 193.60, 177.03, 156.50, 156.05, 140.61, 135.27, 133.96, 133.20, 128.90, 128.75, 128.67, 127.22, 125.95, 125.76, 125.41, 123.91, 118.60, 118.41, 115.63, 111.34, 49.36, 41.67. HRMS-ESI (m/z) calculated for $C_{24}H_{17}NO_3S$ $(M+H)^+$: 400.1011, Experimental: $(M+H)^+$ = 400.1006.

3-(2-(4-bromobenzoyl)-3,4-dihydro-2H-benzo[b][1,4]thiazin-3-yl)-4H-chromen-4-one (5b): Yield 85%; Off-white solid; mp. 210-212 °C. ^{1}H NMR (500 MHz, DMSO-D_6) δ 8.08 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.99 (s, 1H), 7.93 (d, *J* = 8.2 Hz, 2H), 7.78 (d, *J* = 8.7 Hz, 1H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.62 (d, *J* = 8.4 Hz, 1H), 7.49 (t, *J* = 7.5 Hz, 1H), 6.93 (t, *J* = 8.3 Hz, 1H), 6.83 (d, *J* = 7.6 Hz, 1H), 6.68 (d, *J* = 8.2 Hz, 1H), 6.66 (d, *J* = 5.3 Hz, 1H), 6.46 (t, *J* = 7.5 Hz, 1H), 5.23 (d, *J* = 5.4 Hz, 1H), 5.06 (d, *J* = 2.0 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-D_6) δ 192.89, 176.27, 156.28, 155.80, 142.99, 134.96, 134.12, 132.29, 131.20, 128.61, 127.99, 127.44, 126.77, 126.13, 125.67, 123.68, 118.99, 117.07,

115.14, 110.73, 48.56, 43.03. HRMS-ESI (m/z) calculated for $C_{24}H_{16}BrNO_3S$ $(M+H)^+$: 478.0112, Experimental: $(M+H)^+$ = 488.0110.

3-(2-(4-methylbenzoyl)-3,4-dihydro-2H-benzo[b][1,4]thiazin-3-yl)-4H-chromen-4-one (5c): Yield 94%; Off-white solid; mp. 180-182 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.24 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.93 – 7.87 (m, 3H), 7.67 (ddd, *J* = 8.7, 7.1, 1.7 Hz, 1H), 7.48 – 7.34 (m, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.02 (ddd, *J* = 8.5, 7.2, 1.5 Hz, 1H), 6.96 (dd, *J* = 7.8, 1.5 Hz, 1H), 6.72 – 6.62 (m, 2H), 5.42 (ddd, *J* = 6.4, 2.3, 1.2 Hz, 1H), 4.93 (d, *J* = 2.1 Hz, 1H), 4.58 (d, *J* = 6.4 Hz, 1H), 2.38 (s, 3H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 193.38, 177.01, 156.50, 156.02, 144.04, 140.59, 133.92, 132.72, 129.36, 129.02, 128.68, 127.12, 125.99, 125.77, 125.37, 123.94, 118.56, 118.39, 115.65, 111.56, 49.40, 41.62, 21.76. HRMS-ESI (m/z) calculated for $C_{25}H_{19}NO_3S$ $(M+H)^+$: 414.1163, Experimental: $(M+H)^+$ = 414.1158.

3-(2-(4-methoxybenzoyl)-3,4-dihydro-2H-benzo[b][1,4]thiazin-3-yl)-4H-chromen-4-one (5d): Yield 95%; Pale-yellow solid; mp. 182-184 °C.^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.23 (d, *J* = 7.8 Hz, 1H), 8.02 (d, *J* = 8.2 Hz, 2H), 7.89 (s, 1H), 7.66 (t, *J* = 8.3 Hz, 1H), 7.42 (dd, *J* = 20.5, 9.2 Hz, 2H), 7.00 (dd, *J* = 21.2, 8.8 Hz, 2H), 6.90 (d, *J* = 8.1 Hz, 2H), 6.70 – 6.62 (m, 2H), 5.39 (s, 1H), 4.93 (s, 1H), 4.58 (s, 1H), 3.83 (s, 3H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 192.47, 163.64, 156.49, 155.97, 140.51, 133.93, 131.30, 128.58, 128.11, 127.03, 125.98, 125.75, 125.38, 123.93, 118.57, 118.40, 115.63, 113.88, 111.80, 55.56, 49.53, 41.56. HRMS-ESI (m/z) calculated for $C_{25}H_{19}NO_4S$ $(M+H)^+$: 418.1096, Experimental: $(M+H)^+$ = 418.1082.

7-bromo-3-(2-(4-methoxybenzoyl)-3,4-dihydro-2H-benzo[b][1,4]thiazin-3-yl)-4H-chromen-4-one (5e): Yield 88%; White solid; mp. 180-192 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.35 (d, *J* = 2.5 Hz, 1H), 8.00 (d, *J* = 8.7 Hz, 2H), 7.90 (s, 1H), 7.74 (dd, *J* = 8.9, 2.5 Hz, 1H), 7.35 (d, *J* = 8.9 Hz, 1H), 7.05 – 6.99 (m, 1H), 6.99 – 6.95 (m, 1H), 6.95 – 6.88 (m, 2H), 6.71 – 6.63 (m, 2H), 5.38 (dd, *J* = 6.6, 2.3 Hz, 1H), 4.88 (d, *J* = 2.3 Hz, 1H), 4.57 (d, *J* = 6.5 Hz, 1H), 3.84 (s, 3H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 192.33, 175.76, 163.68, 156.20, 155.24, 140.38, 136.91, 131.27, 128.64, 128.42, 128.02, 127.11, 126.30, 125.22, 120.35, 118.85, 118.70, 115.71, 113.89, 111.68, 55.58, 49.50, 41.26. HRMS-ESI (m/z) calculated for $C_{25}H_{18}BrNO_4S$ $(M+Na)^+$:520.0028, Experimental: $(M+Na)^+$ = 519.0074.

7-methyl-3-(2-(4-methylbenzoyl)-3,4-dihydro-2H-benzo[b][1,4]thiazin-3-yl)-4H-chromen-4-one (5f): Yield 90%; Light-yellow solid; mp. 198-200 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.35 (d, *J* = 2.5 Hz, 1H), 8.30 – 8.22 (m, 2H), 7.86 – 7.82 (m, 1H), 7.72 (dd, *J* = 8.9, 2.5 Hz, 1H), 7.30 (d, *J* = 8.9 Hz, 1H), 7.01 – 6.93 (m, 2H), 6.68 (d, *J* = 1.9 Hz, 1H), 6.62 (dd, *J* = 7.9, 1.9 Hz, 1H), 6.57 (d, *J* = 8.0 Hz, 1H), 5.85 (d, *J* = 1.8 Hz, 1H), 5.13 (dt, *J* = 5.5, 1.5 Hz, 1H), 4.10 (d, *J* = 5.5 Hz, 1H), 3.86 (s, 3H), 2.20 (s, 3H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 193.68, 176.62, 164.05, 155.25, 154.97, 142.54, 136.95, 131.61, 130.12, 128.27, 127.70, 127.16, 125.09, 123.52, 122.71, 120.27, 118.86, 117.31, 116.37, 114.08, 75.01, 55.59, 48.57, 20.81. HRMS-ESI (m/z) calculated for $C_{26}H_{20}BrNO_4S$ $(M+Na)^+$: 544.0153, Experimental: $(M+Na)^+$ = 544.0145.

7-bromo-3-(2-(4-methoxybenzoyl)-6-methyl-3,4-dihydro-2H-benzo[b][1,4]thiazin-3-yl)-4H-chromen-4-one (5g): Yield 86%; Pale-yellow solid; mp. 192-194 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.34 (d, *J* = 2.5 Hz, 1H), 7.98 – 7.89 (m, 3H), 7.76 (dd, *J* = 8.9, 2.4 Hz, 1H), 7.40 (s, 1H), 7.42 – 7.33 (m, 2H), 7.08 – 7.01 (m, 1H), 6.95 (dd, *J* = 7.8, 1.5 Hz, 1H), 6.73 – 6.63 (m, 2H), 5.41 (dt, *J* = 6.6, 1.6 Hz, 1H), 4.84 (d, *J* = 2.1 Hz, 1H), 4.57 (d, *J* = 6.6 Hz, 1H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 192.29, 175.78, 156.35, 155.24, 140.43, 139.68, 137.02, 133.44, 130.30, 129.00, 128.83, 128.38, 127.45, 126.15, 125.13, 120.38, 118.95, 118.80, 115.68, 110.89, 49.33, 41.40. HRMS-ESI (m/z) calculated for $C_{24}H_{15}BrClNO_3S$ $(M+H)^+$: 511.9723, Experimental: $(M+H)^+$ = 511.9719.

7-bromo-3-(2-(4-chlorobenzoyl)-3,4-dihydro-2H-benzo[b][1,4]thiazin-3-yl)-4H-chromen-4-one (5h): Yield 87%; Off-white solid; mp. 196-198 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.36 (d, *J* = 2.5 Hz, 1H), 7.94 – 7.85 (m, 3H), 7.75 (dd, *J* = 8.9, 2.4 Hz, 1H), 7.36 (d, *J* = 8.9 Hz, 1H), 7.23 (d, *J* = 7.9 Hz, 2H), 7.03 (ddd, *J* = 8.5, 7.3, 1.5 Hz, 1H), 6.95 (dd, *J* = 7.8, 1.5 Hz, 1H), 6.73 – 6.62 (m, 2H), 5.40 (dt, *J* = 6.5, 1.6 Hz, 1H), 4.88 (d, *J* = 2.2 Hz, 1H), 4.57 (d, *J* = 6.6 Hz, 1H), 2.39 (s, 3H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 193.21, 175.74, 156.26, 155.24, 144.17, 140.44, 136.92, 132.59, 129.40, 129.00, 128.75, 128.43, 127.22, 126.31, 125.21, 120.36, 118.86, 118.69, 115.71, 111.39, 49.36, 41.29, 21.80. HRMS-ESI (m/z) calculated for $C_{25}H_{18}BrNO_3S$ $(M+H)^+$: 492.0267, Experimental: $(M+H)^+$ = 492.0263.

7-bromo-3-(2-(4-methylbenzoyl)-3,4-dihydro-2H-benzo[b][1,4]thiazin-3-yl)-4H-chromen-4-one (5i): Yield 94%; White solid; mp. 192-194 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.02 (d, *J* = 2.3 Hz, 1H), 7.93 – 7.87 (m, 3H),

7.48 (dd, *J* = 8.6, 2.3 Hz, 1H), 7.36 (d, *J* = 8.6 Hz, 1H), 7.23 (d, *J* = 7.9 Hz, 2H), 7.06 – 6.99 (m, 1H), 6.96 (dd, *J* = 7.8, 1.4 Hz, 1H), 6.71 – 6.62 (m, 2H), 5.41 (dd, *J* = 6.6, 2.4 Hz, 1H), 4.94 (d, *J* = 2.3 Hz, 1H), 4.55 (d, *J* = 6.4 Hz, 1H), 2.46 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 193.39, 177.08, 155.89, 154.81, 144.05, 140.56, 135.40, 135.23, 132.71, 129.37, 129.03, 128.68, 127.10, 125.73, 125.00, 123.59, 118.54, 118.15, 115.61, 111.56, 49.39, 41.59, 21.79, 21.08. HRMS-ESI (m/z) calculated for $C_{26}H_{21}NO_3S$ $(M+H)^+$: 428.1327, Experimental: $(M+H)^+$ = 428.1322.

3-(2-(4-methoxybenzoyl)-3,4-dihydro-2H-benzo[b][1,4]thiazin-3-yl)-7-methyl-4H-chromen-4-one (5j): Yield 95%; White solid; mp. 194-196 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.06 – 7.99 (m, 3H), 7.87 (d, *J* = 2.7 Hz, 1H), 7.50 – 7.44 (m, 1H), 7.34 (dd, *J* = 8.9, 3.9 Hz, 1H), 6.99 (dd, *J* = 18.5, 7.9 Hz, 2H), 6.90 (dd, *J* = 8.9, 3.0 Hz, 2H), 6.70 – 6.62 (m, 2H), 5.40 – 5.35 (m, 1H), 4.94 (d, *J* = 2.3 Hz, 1H), 4.58 (dt, *J* = 10.2, 5.7 Hz, 1H), 3.84 (d, *J* = 2.7 Hz, 3H), 2.45 (d, *J* = 2.4 Hz, 3H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 192.54, 177.09, 163.62, 155.82, 154.79, 140.52, 135.38, 135.20, 131.30, 128.54, 128.14, 126.97, 125.73, 124.97, 123.59, 118.52, 118.13, 115.60, 113.87, 111.87, 55.55, 49.55, 41.63, 21.05. HRMS-ESI (m/z) calculated for $C_{26}H_{21}NO_4S$ $(M+H)^+$: 443.1190, Experimental: $(M+H)^+$ = 444.1268.

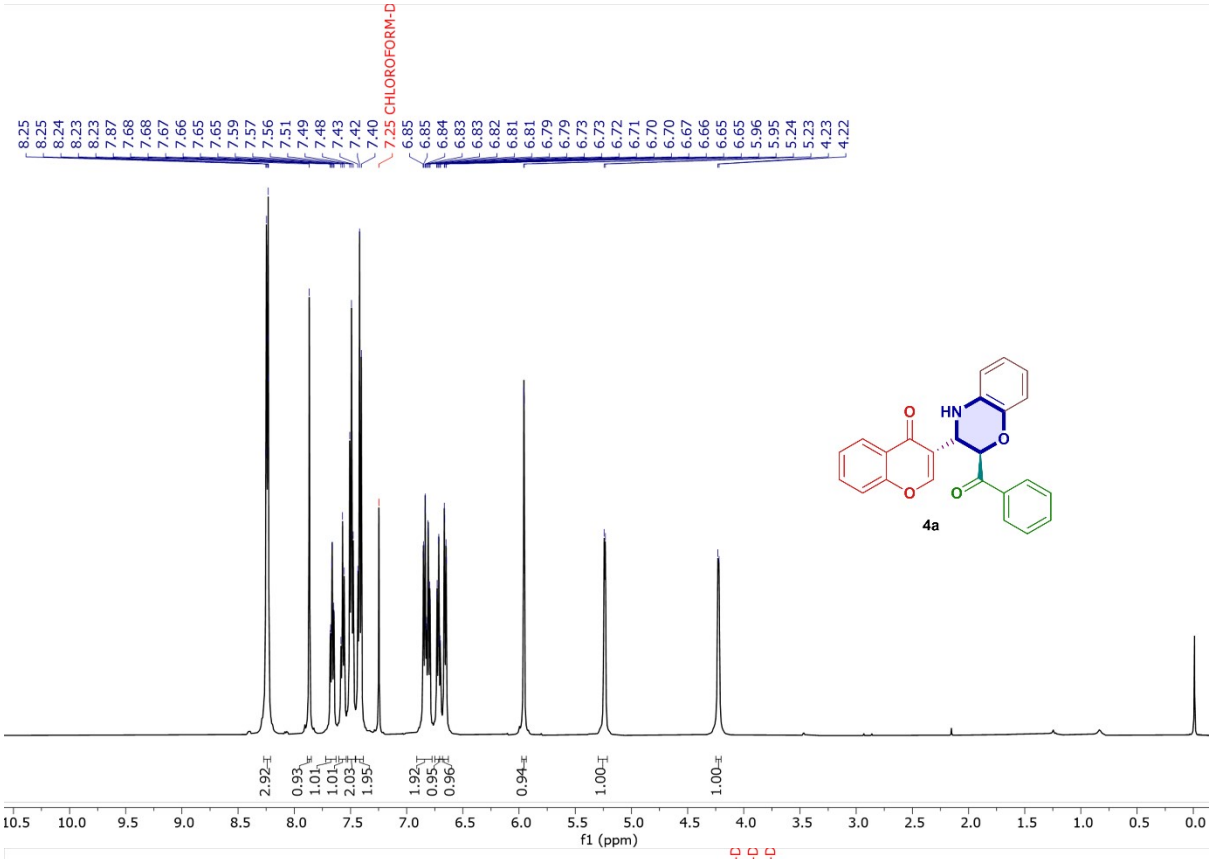
3-(2-(4-chlorobenzoyl)-3,4-dihydro-2H-benzo[b][1,4]thiazin-3-yl)-7-methyl-4H-chromen-4-one (5k): Yield 90%; Yellow solid; mp. 194-196 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.00 (d, *J* = 2.3 Hz, 1H), 7.97 – 7.91 (m, 2H), 7.89 (d, *J* = 1.1 Hz, 1H), 7.48 (dd, *J* = 8.6, 2.2 Hz, 1H), 7.46 – 7.36 (m, 2H), 7.35 (d, *J* = 8.5 Hz, 1H), 7.03 (ddd, *J* = 8.4, 7.3, 1.5 Hz, 1H), 6.95 (dd, *J* = 7.8, 1.5 Hz, 1H), 6.72 – 6.62 (m, 2H), 5.44 – 5.38 (m, 1H), 4.91 (d, *J* = 2.2 Hz, 1H), 4.56 (d, *J* = 6.4 Hz, 1H), 2.46 (s, 3H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 192.52, 177.10, 155.95, 154.82, 140.58, 139.58, 135.50, 135.31, 133.60, 130.33, 128.96, 128.74, 127.30, 125.57, 124.94, 123.52, 118.63, 118.16, 115.59, 111.11, 49.38, 41.76, 21.06. HRMS-ESI (m/z) calculated for $C_{25}H_{18}ClNO_3S$ $(M+H)^+$: 448.0773, Experimental: $(M+H)^+$ = 448.0769.

3-(2-(4-bromobenzoyl)-3,4-dihydro-2H-benzo[b][1,4]thiazin-3-yl)-7-methyl-4H-chromen-4-one (5l): Yield 89%; Off-white solid; mp. 200-202 °C. ^{1}H NMR (500 MHz, CHLOROFORM-*D*) δ 8.00 (s, 1H), 7.90 – 7.84 (m, 3H), 7.56 (d, *J* = 8.2 Hz, 2H), 7.49 (d, *J* = 8.7 Hz, 1H), 7.35 (d, *J* = 8.5 Hz, 1H), 7.03 (t, *J* = 7.7 Hz, 1H), 6.95 (d, *J* = 7.8 Hz, 1H), 6.72 – 6.62 (m, 2H), 5.41 (d, *J* = 6.4 Hz, 1H), 4.90 (s, 1H), 4.55 (d, *J* = 6.5 Hz, 1H), 2.46 (s, 3H). ^{13}C NMR (126 MHz, CHLOROFORM-*D*) δ 192.66, 177.11, 155.96, 154.81, 140.56, 135.51, 135.33, 133.98, 131.96, 130.44, 128.77, 128.35, 127.33, 125.56, 124.93, 123.51, 118.64, 118.17, 115.57, 111.04, 49.36, 41.70, 21.09. HRMS-ESI (m/z) calculated for $C_{25}H_{18}BrNO_3S$ $(M+H)^+$: 492.0268, Experimental: $(M+H)^+$ = 492.0263.

3-(((2-hydroxyphenyl)amino)methylene)-2-isopropoxychroman-4-one (Int-1): Yield 97%; White solid; mp. °C. ^{1}H NMR (500 MHz, DMSO-D_6) δ 11.97 (d, *J* = 12.9 Hz, 1H), 10.28 (s, 1H), 8.04 (d, *J* = 12.9 Hz, 1H), 7.80 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.50 – 7.38 (m, 2H), 7.10 – 7.03 (m, 1H), 6.99 (dd, *J* = 8.2, 1.0 Hz, 1H), 6.93 (s, 0H), 6.90 (q, *J* = 2.3 Hz, 2H), 6.83 (ddd, *J* = 8.6, 5.5, 3.3 Hz, 1H), 6.00 (s, 1H), 4.05 (h, *J* = 6.2 Hz, 1H), 1.14 (d, *J* = 6.1 Hz, 3H), 0.98 (d, *J* = 6.2 Hz, 3H). ^{13}C NMR (126 MHz, DMSO-D_6) δ 180.50, 180.21, 156.12, 146.57, 144.30, 143.50, 134.63, 128.27, 126.09, 124.73, 123.32, 122.18, 120.35, 118.46, 116.04, 114.69, 104.28, 99.41, 95.34, 70.11, 23.75, 22.64. HRMS-ESI (m/z) calculated for $C_{19}H_{19}NO_4$ $(M+Na)^+$: 348.1278, Experimental: $(M+Na)^+$ = 348.1273.

3-(((2-((4-bromobenzyl)oxy)phenyl)amino)methylene)-2-isopropoxychroman-4-one (Int-2): HRMS-ESI (m/z) calculated for $C_{27}H_{24}BrNO_5$ $(M+H)^+$: 522.0914, Experimental: $(M+H)^+$ = 522.0910.

^{1}H and 13C NMR spectra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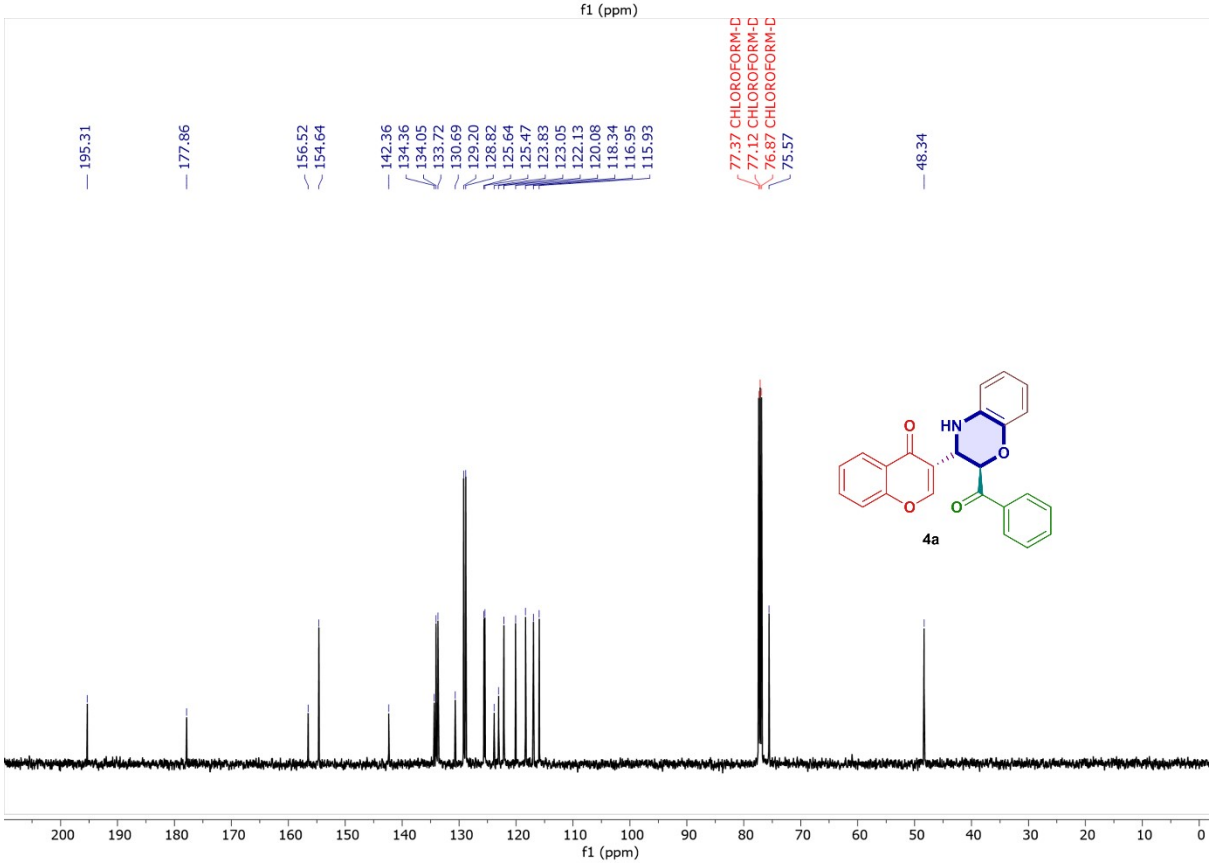
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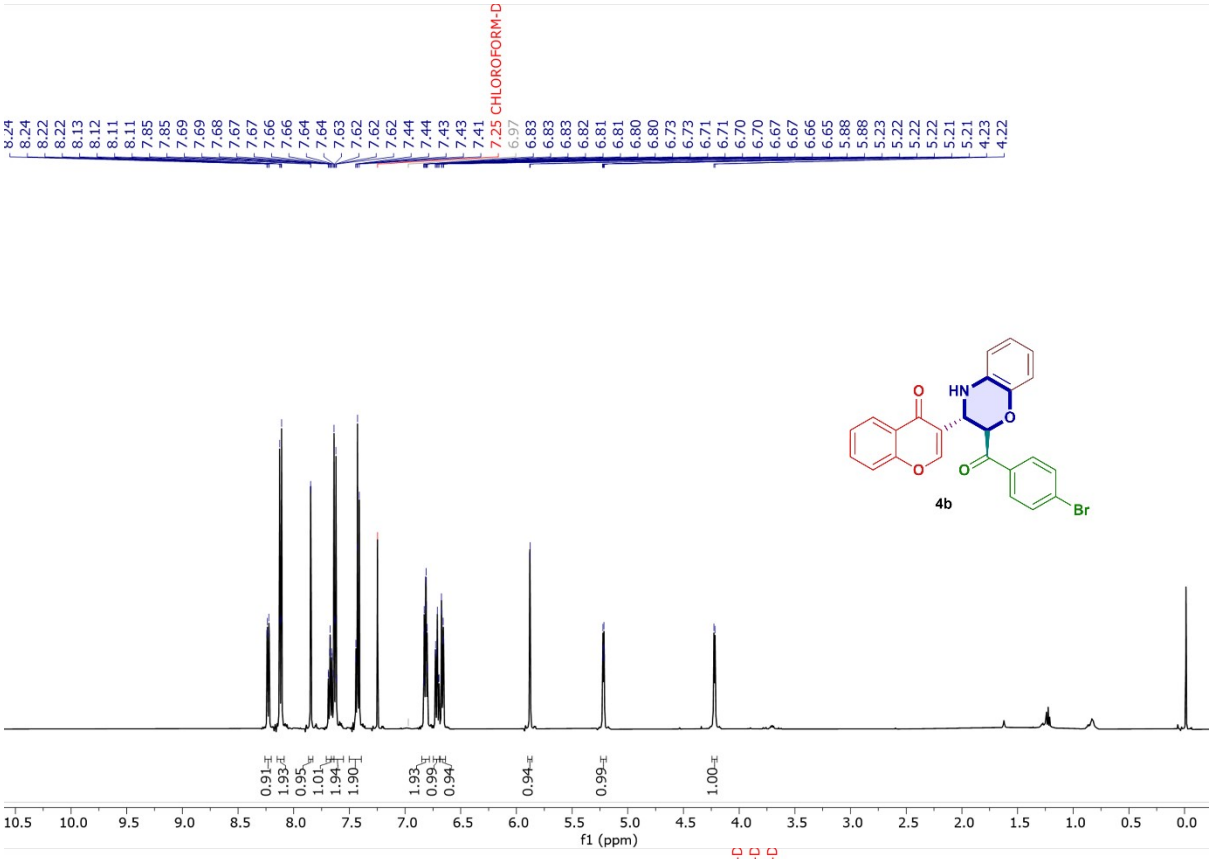
f1 (ppm)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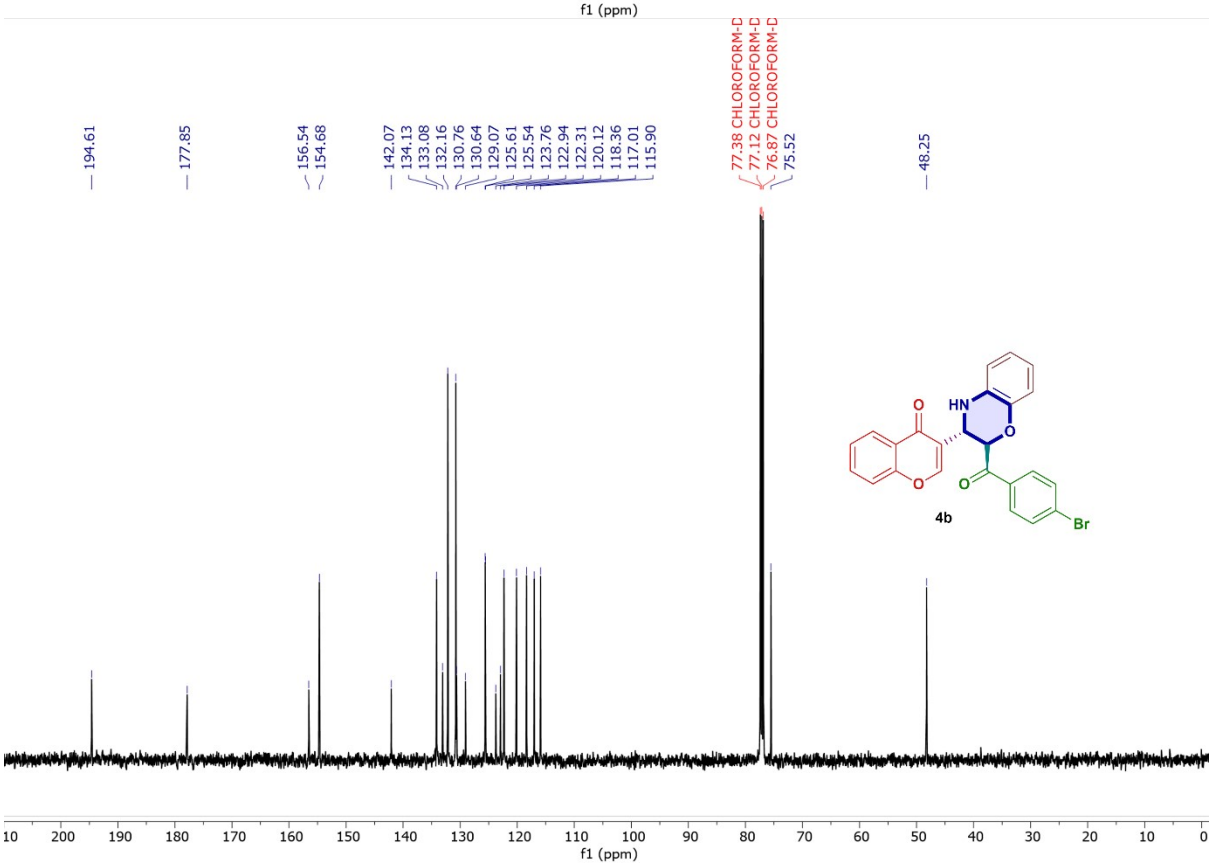
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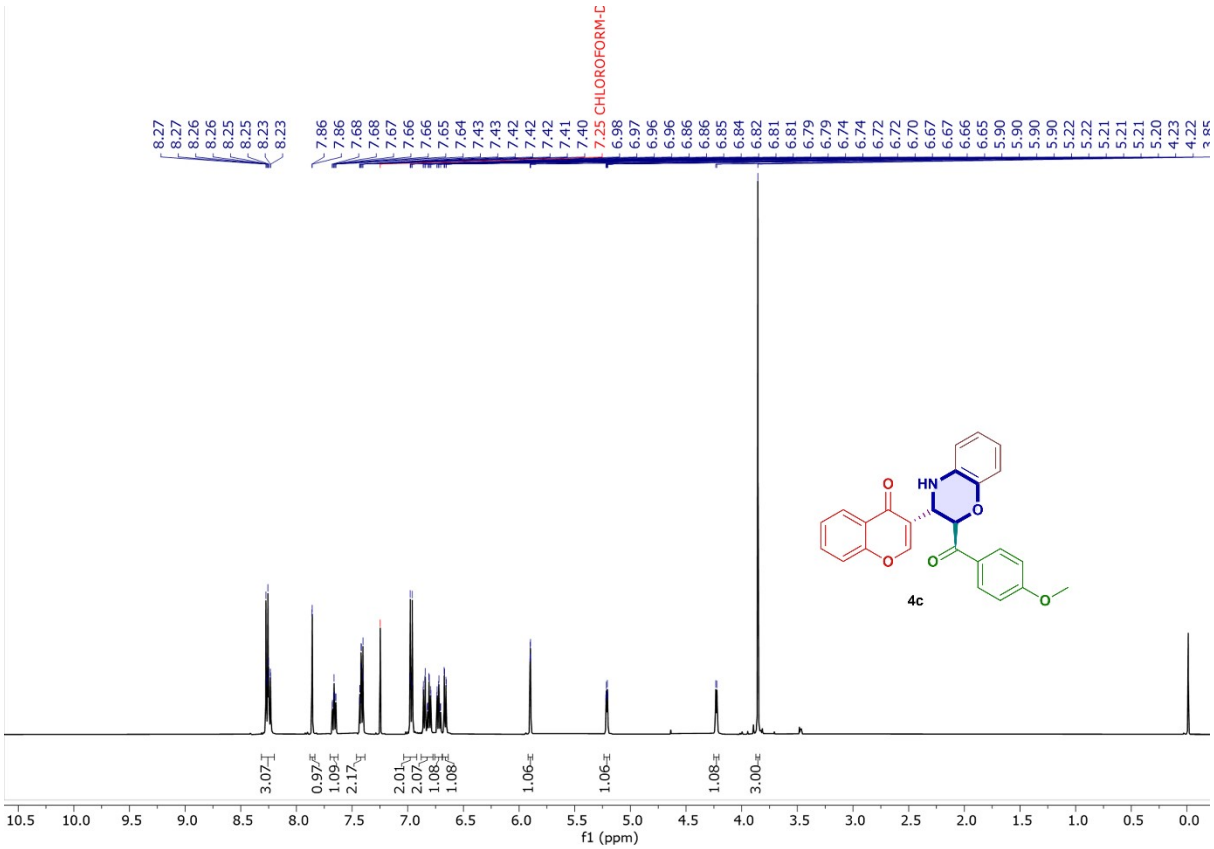
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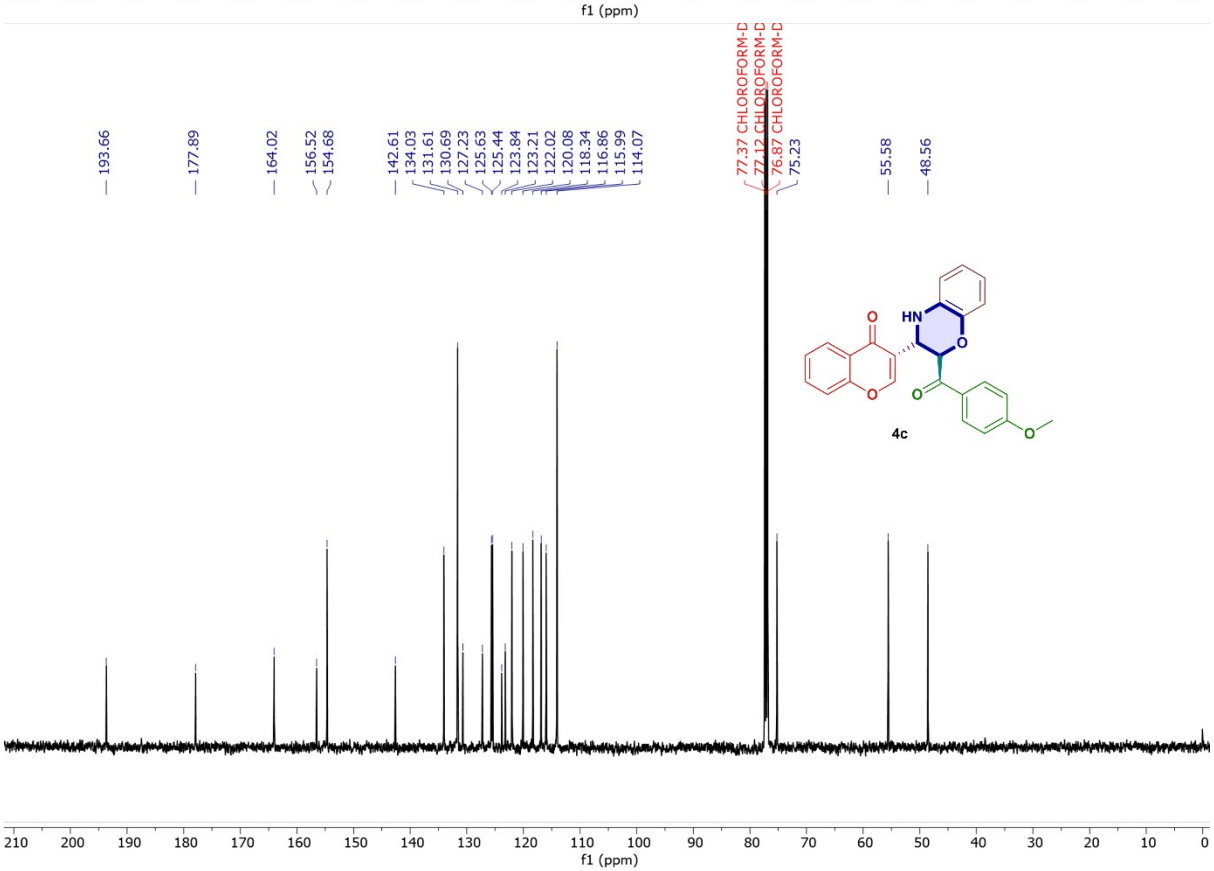
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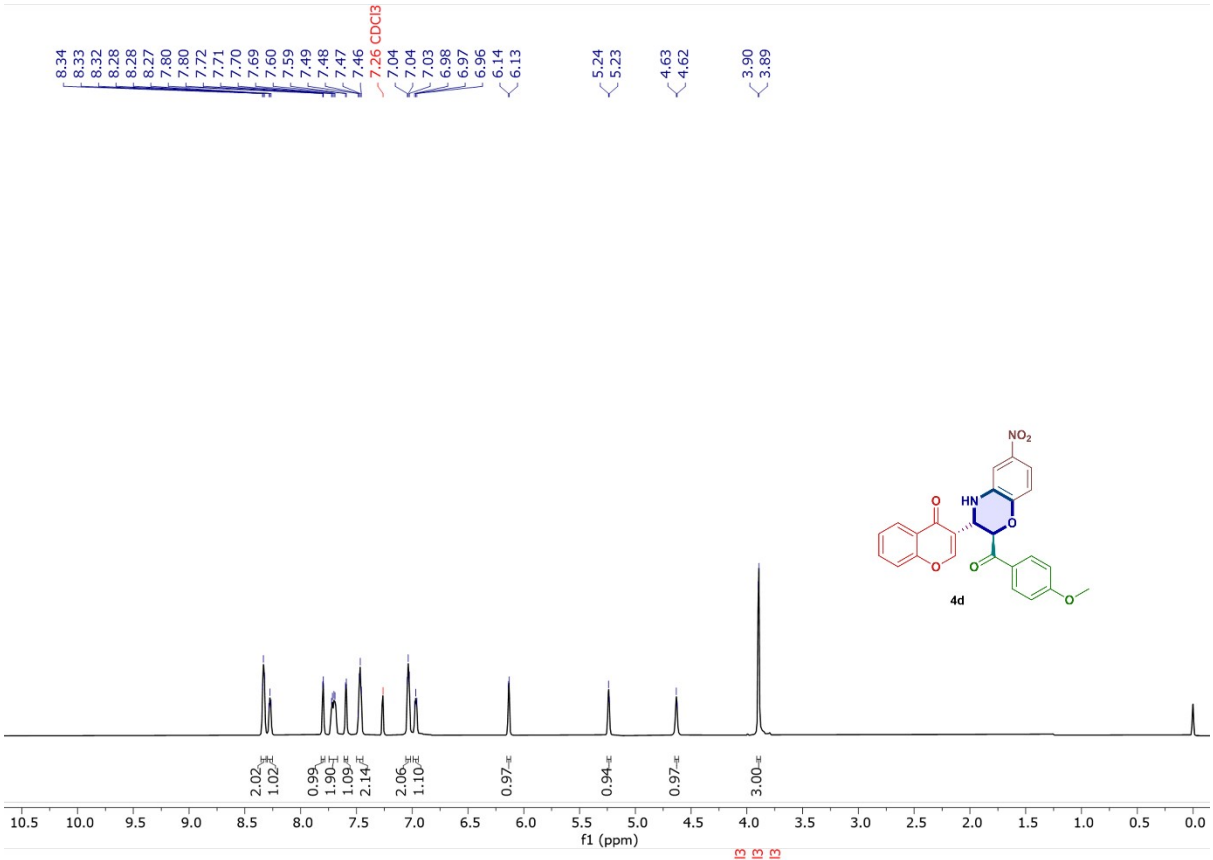
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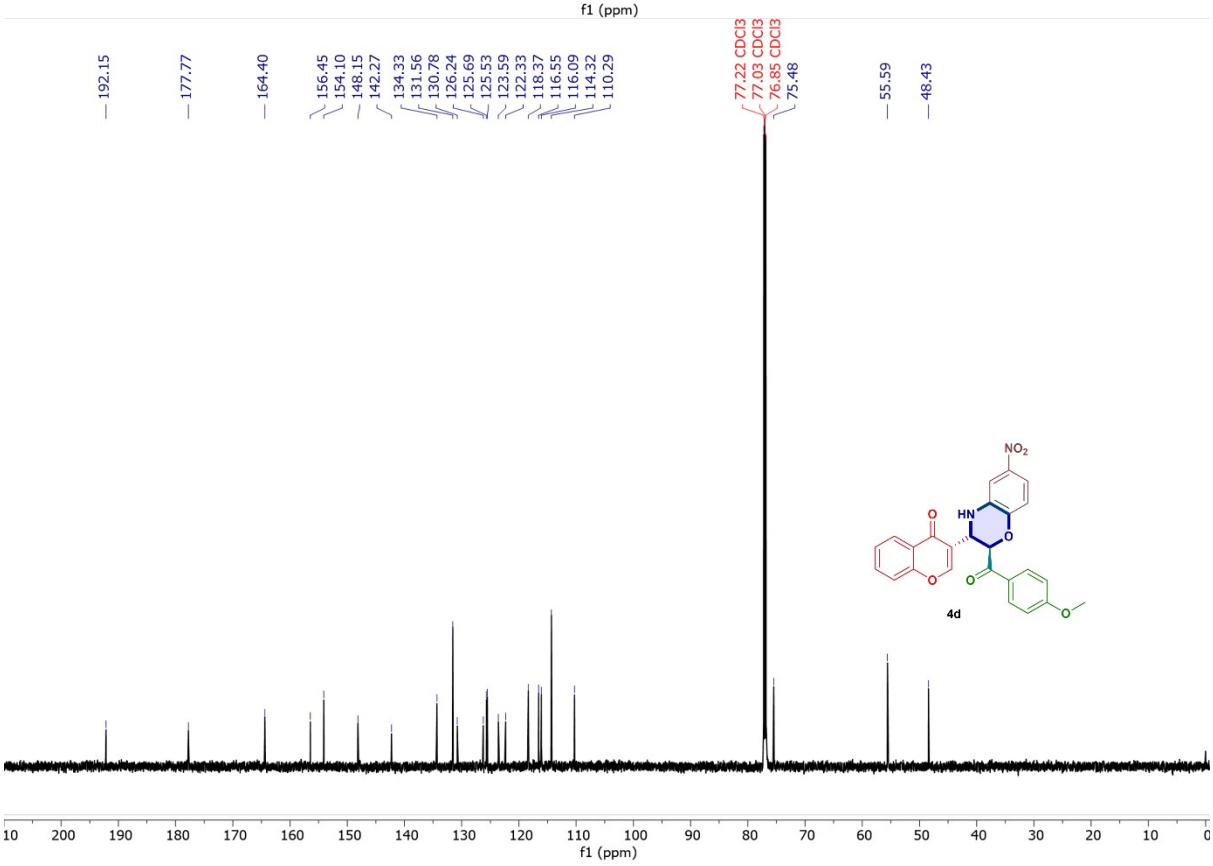
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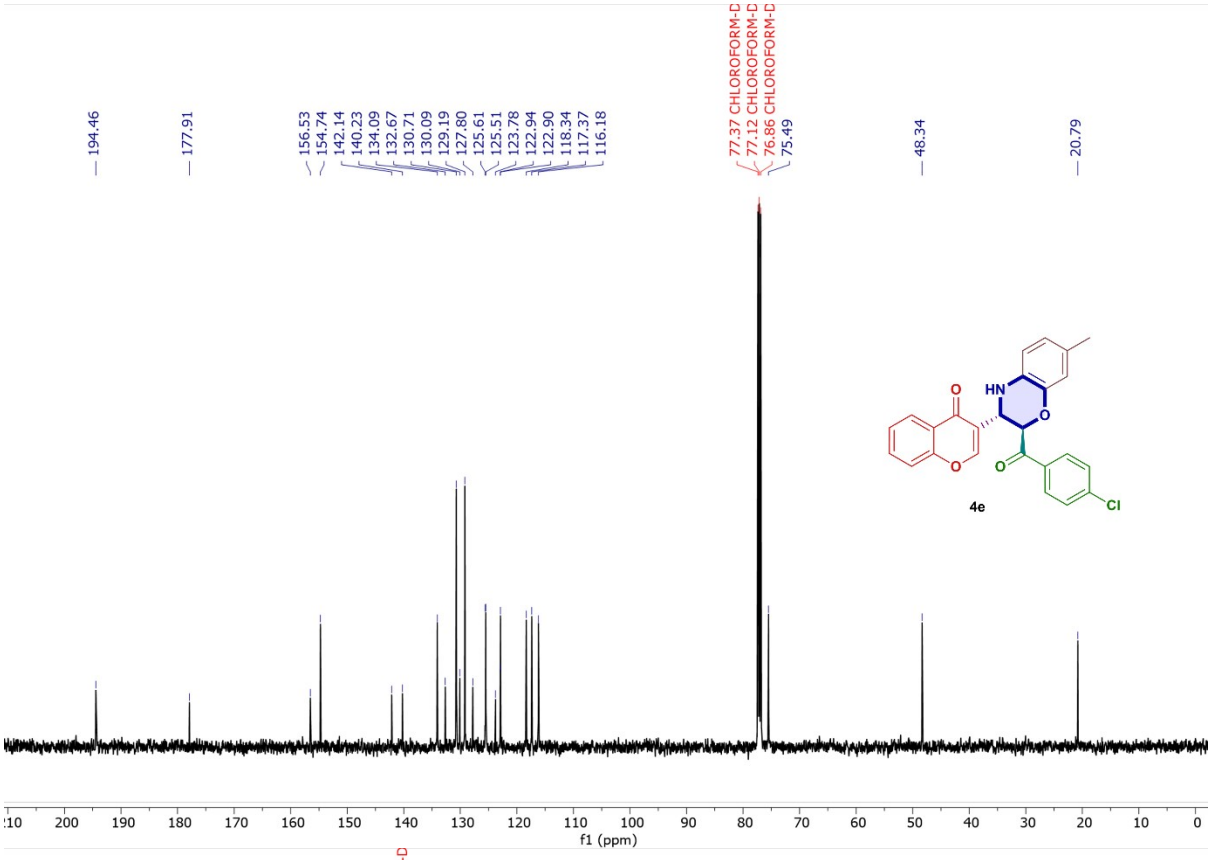
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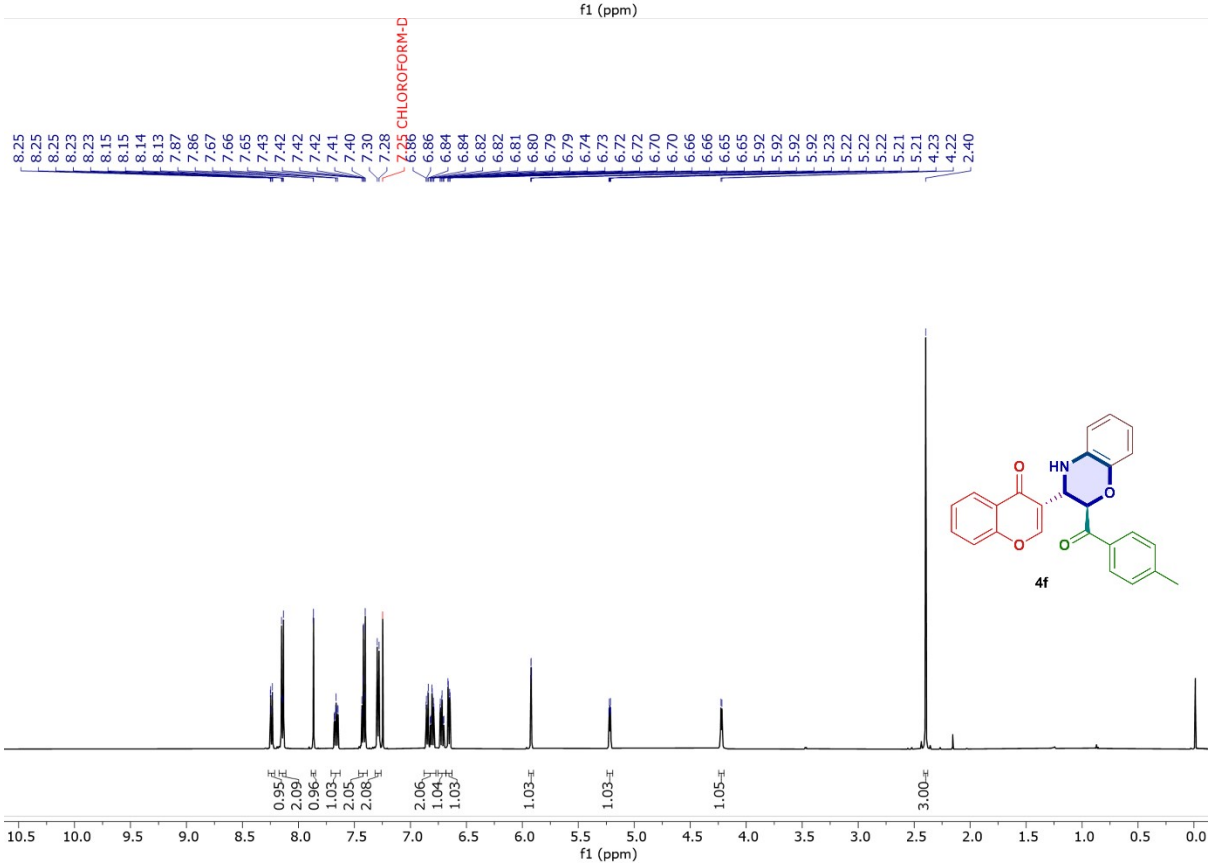
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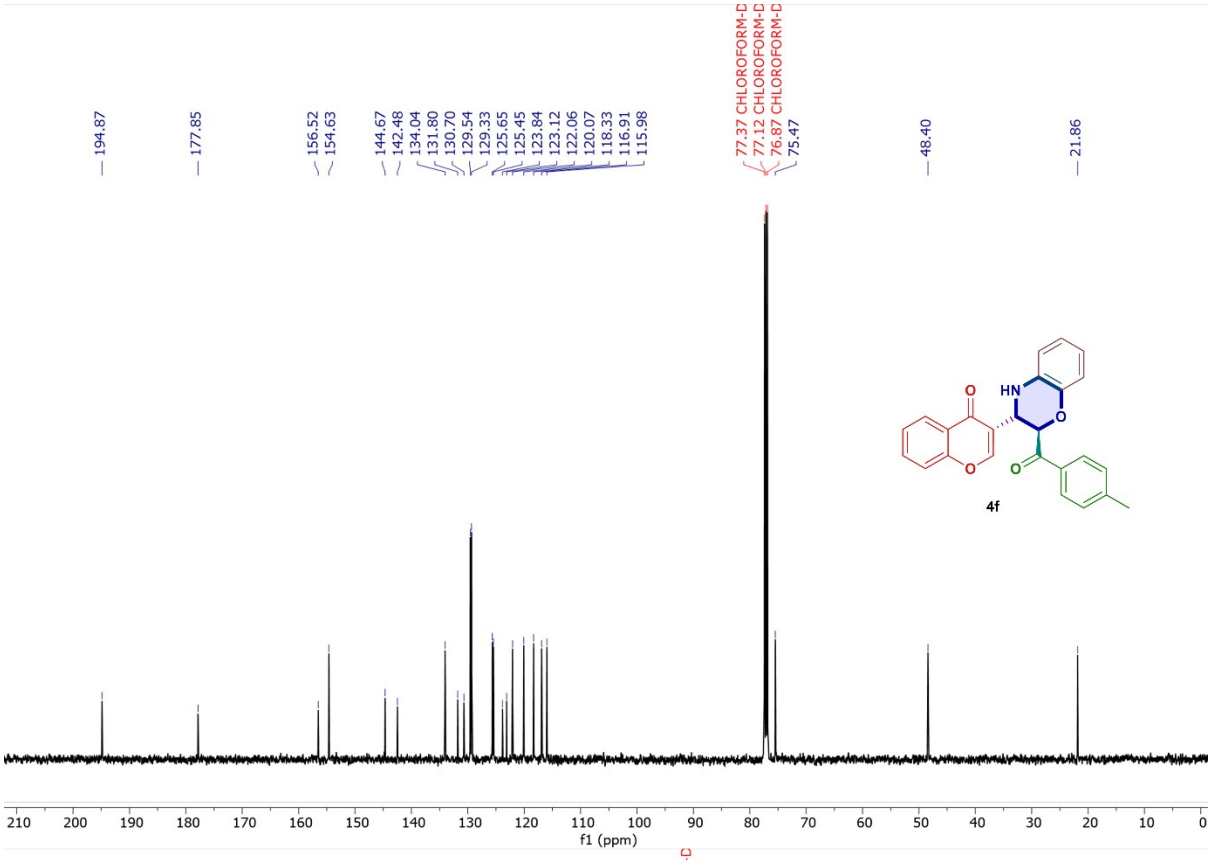
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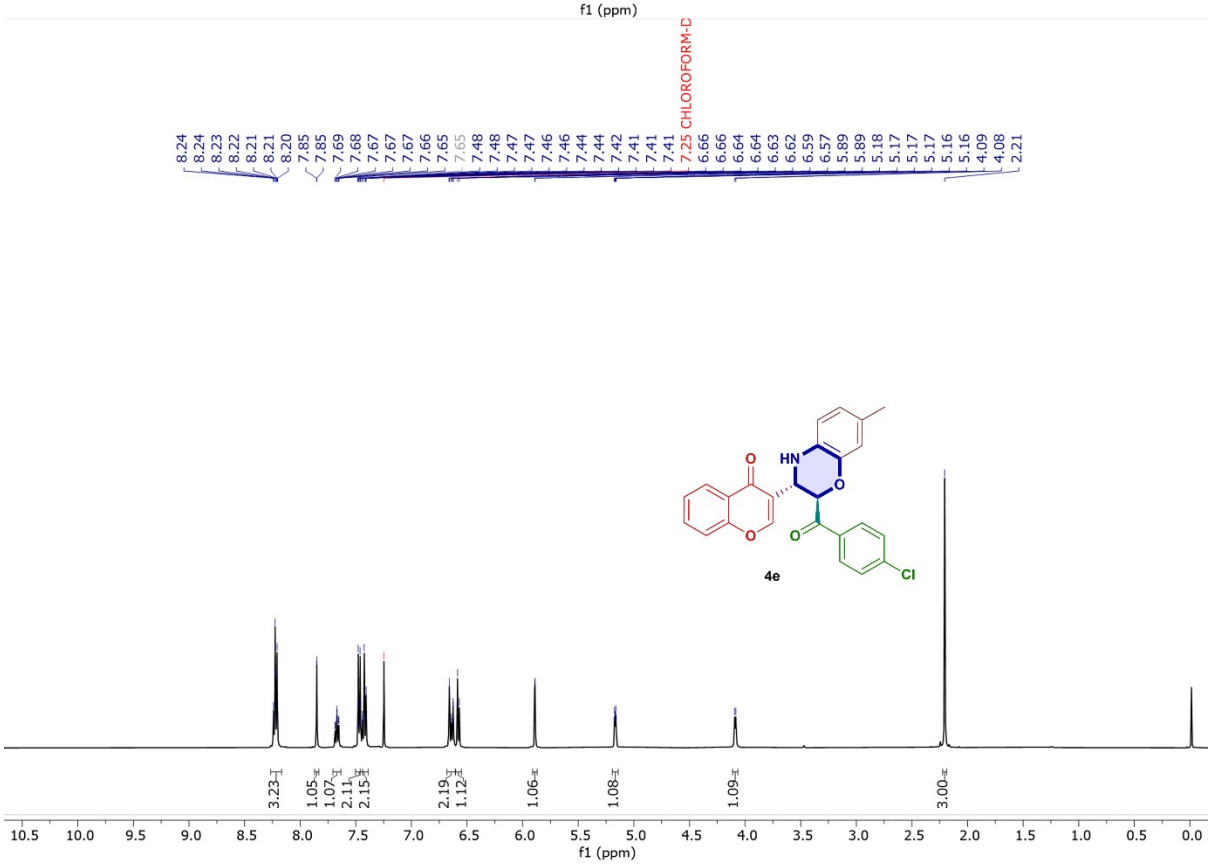
f1 (ppm)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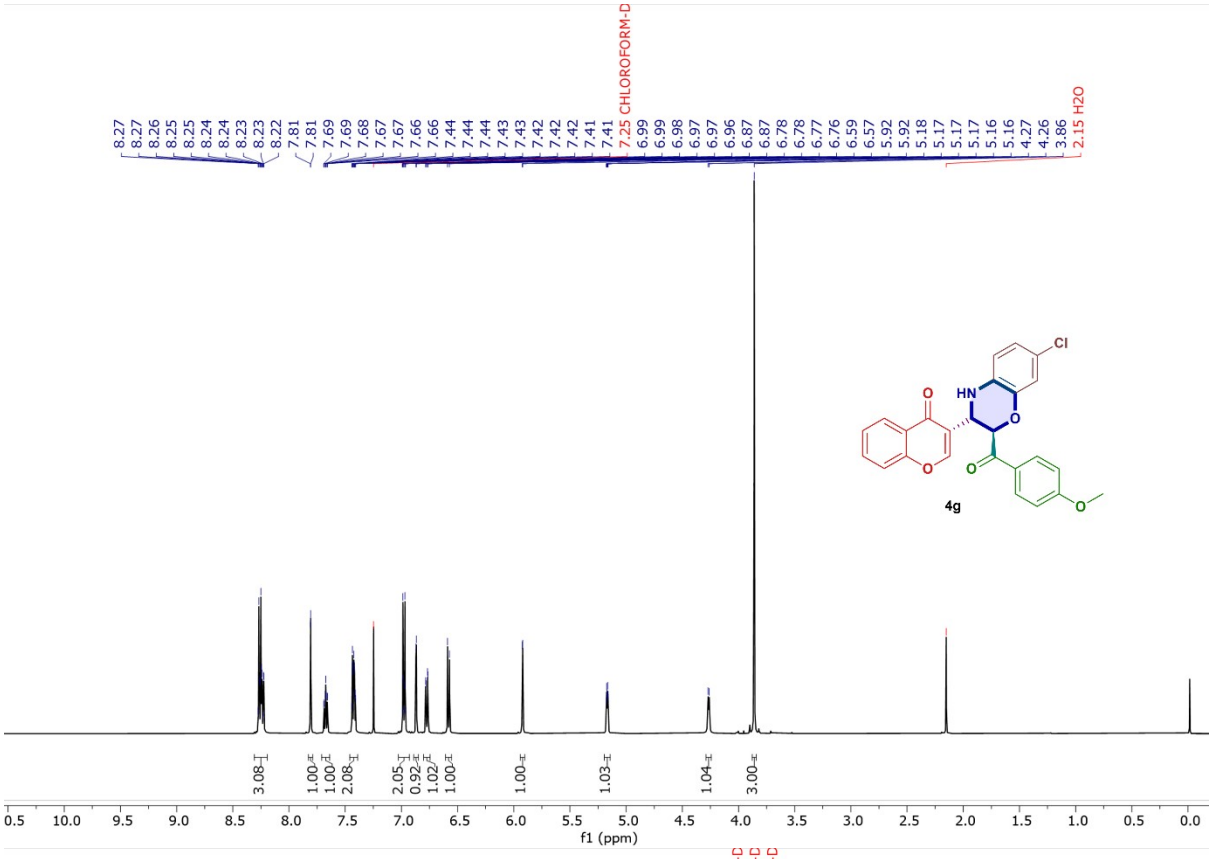
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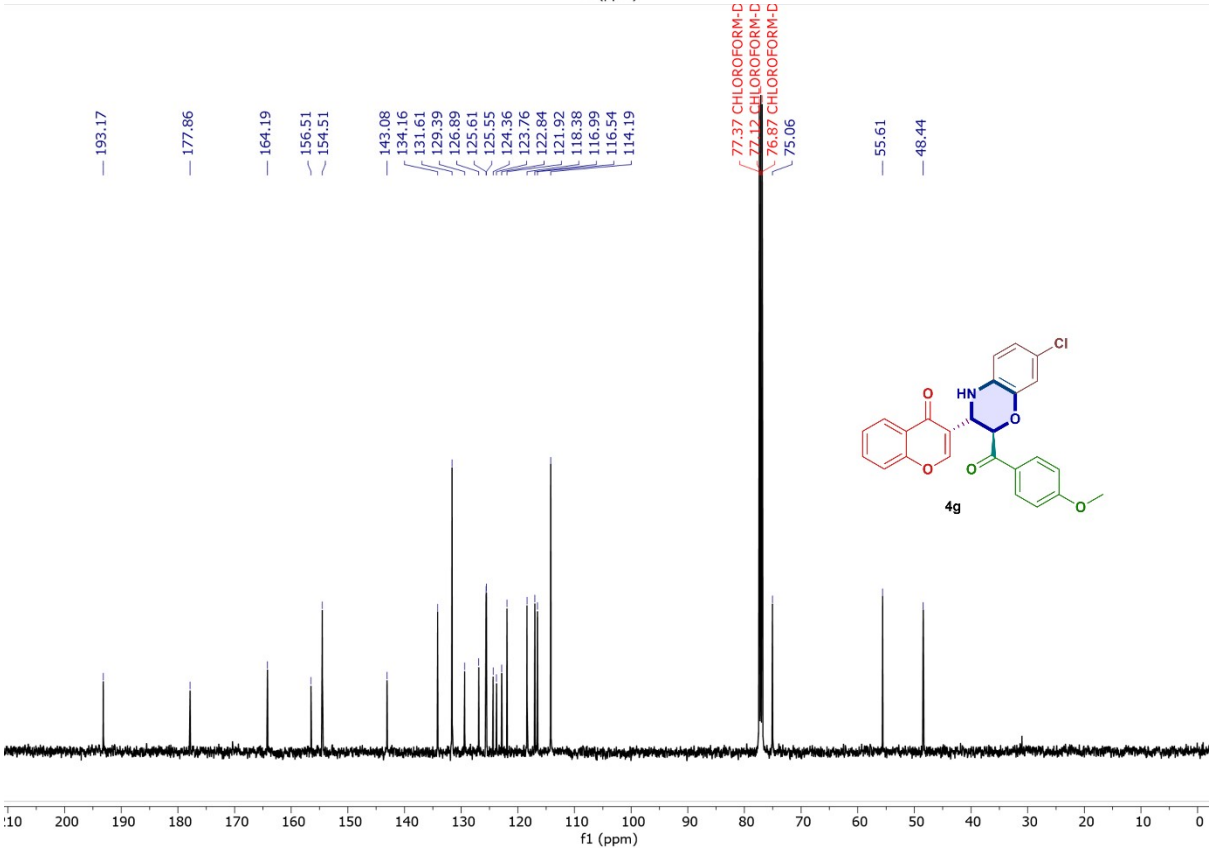
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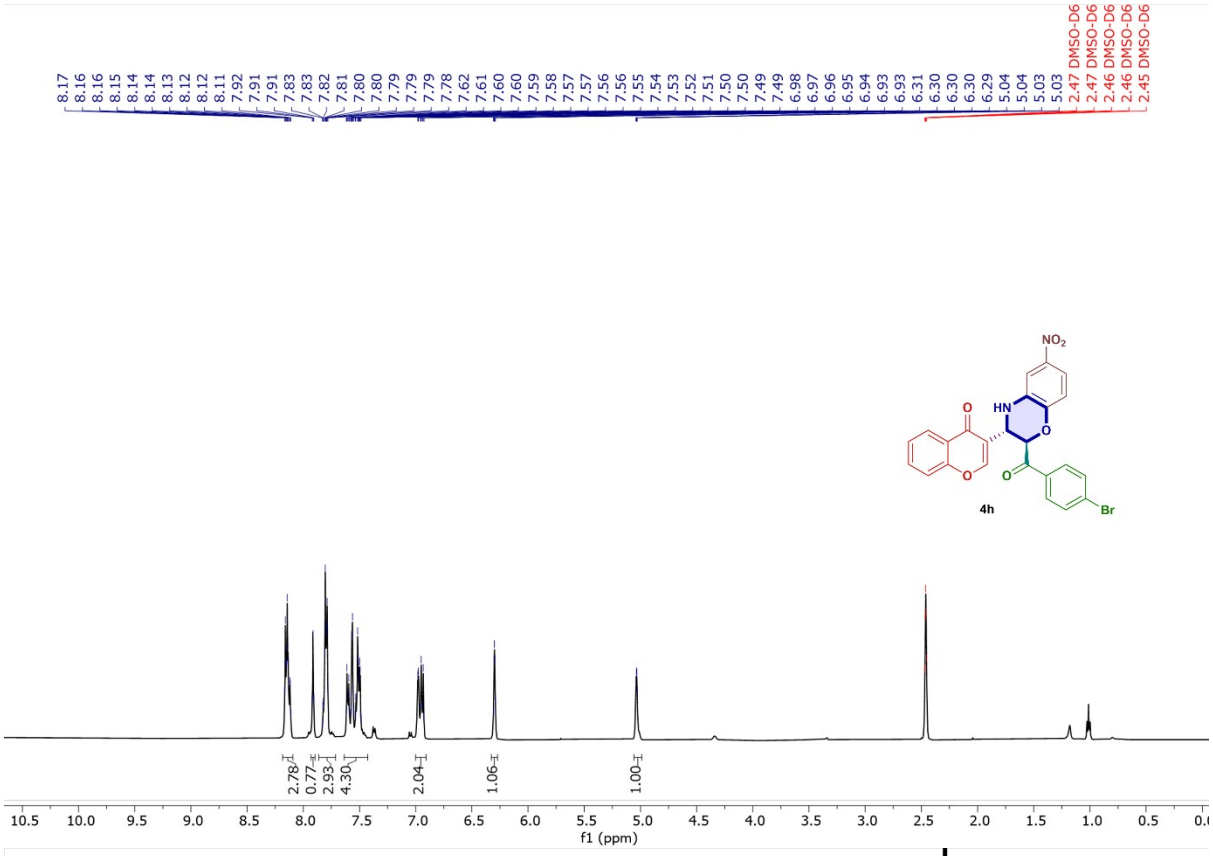
4g
f1 (ppm)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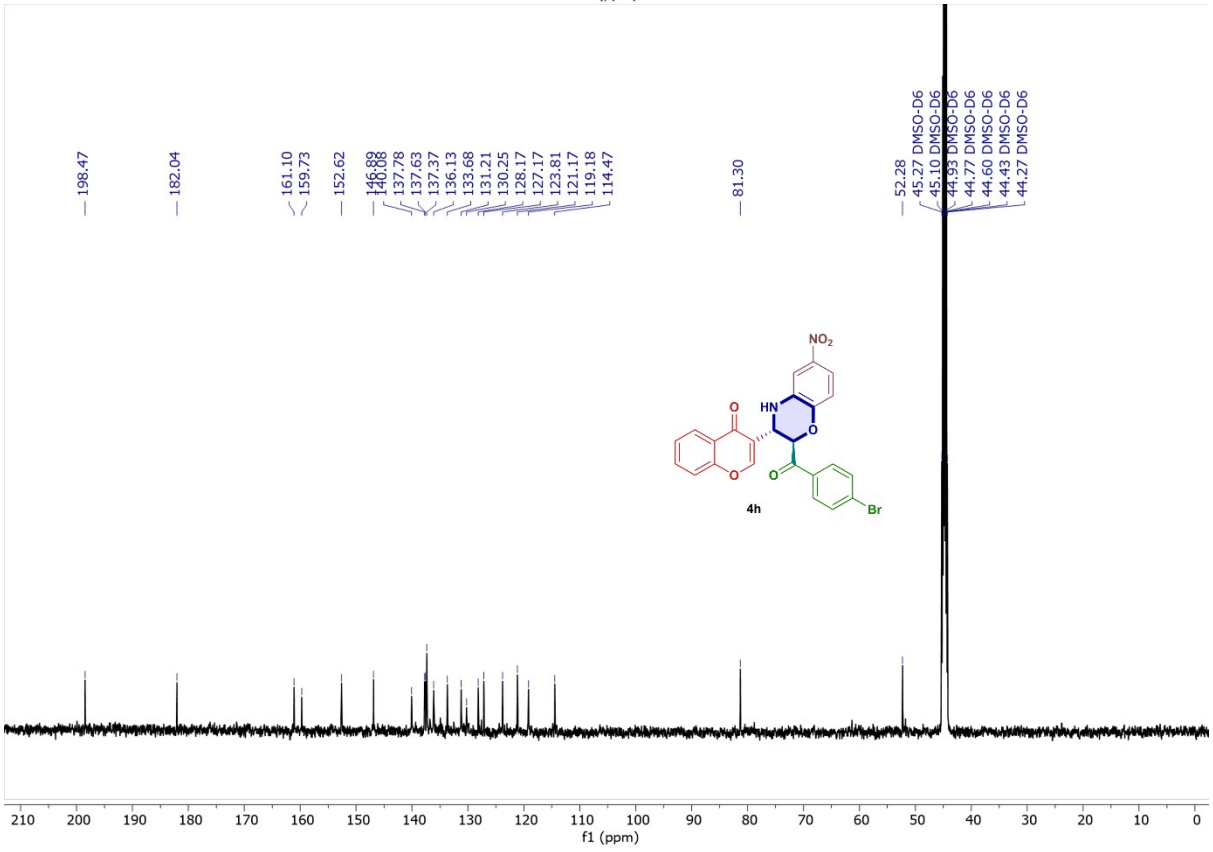
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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140.08
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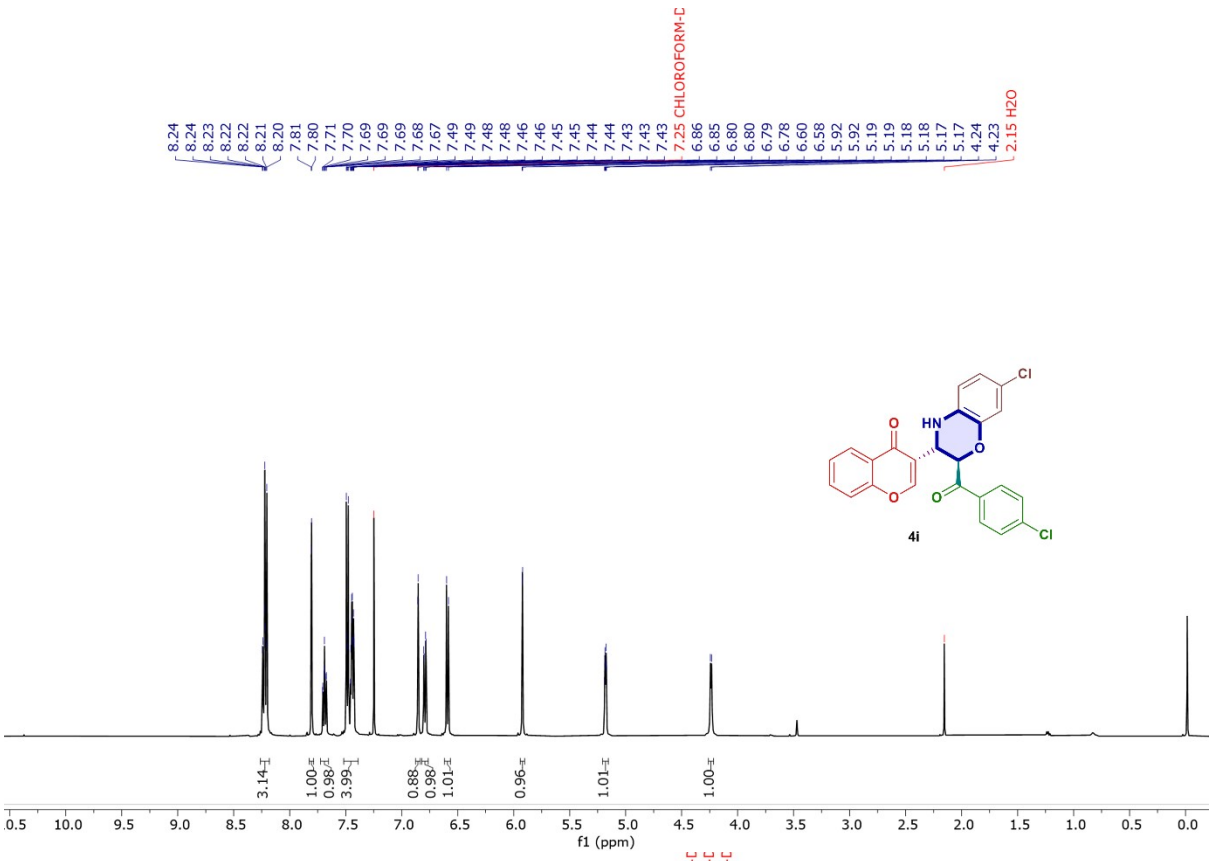
137.63
137.37
136.13
133.68
131.21
130.25
128.17
127.17
123.81
121.17
119.18
114.47
81.30
52.28
45.27 DMSO-D6
45.10 DMSO-D6
44.93 DMSO-D6
44.77 DMSO-D6
44.60 DMSO-D6
44.43 DMSO-D6
44.27 DMSO-D6
NO2
HN
O
O
O
O
Br
4h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.71
7.70
7.69
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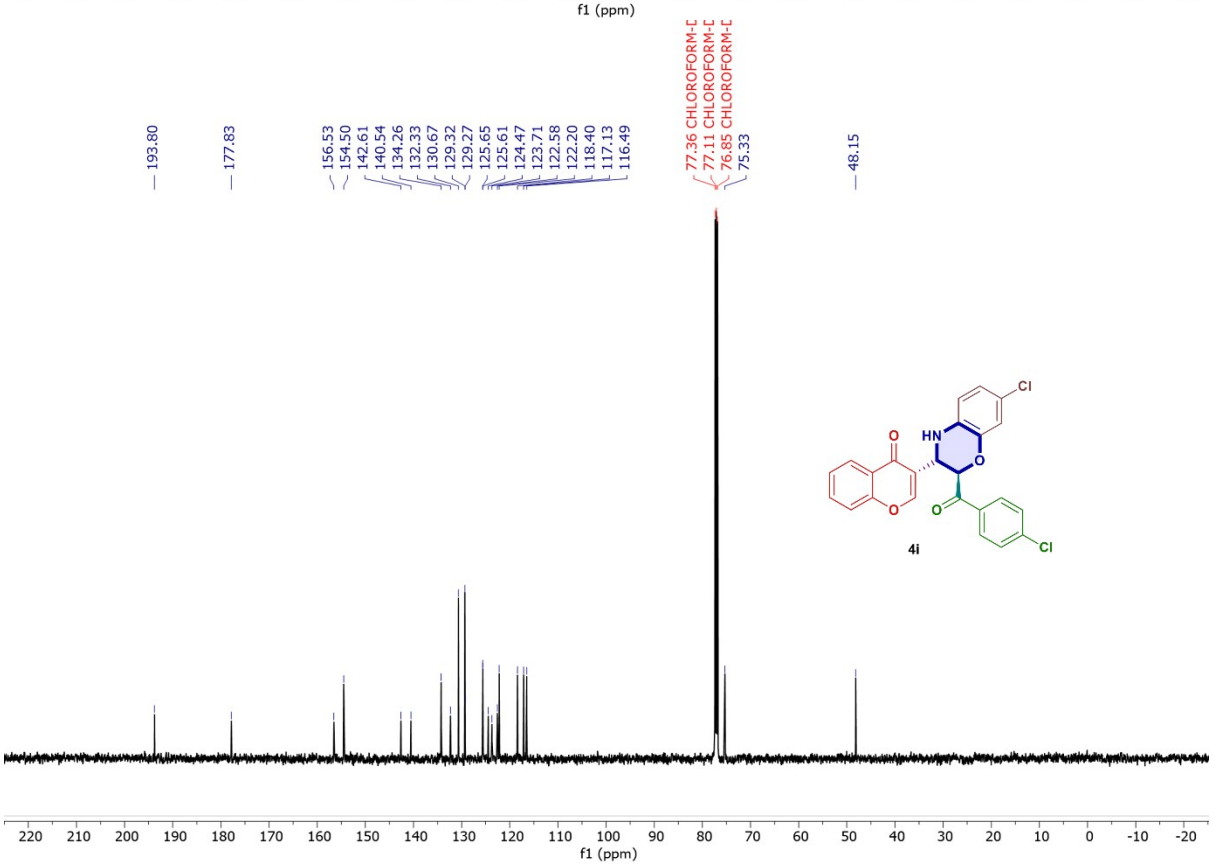
7.69
7.68
7.67
7.49
7.49
7.48
7.48
7.46
7.46
7.45
7.45
7.44
7.44
7.43
7.43
7.43
7.25 CHLOROFORM-D
6.86
6.85
6.80
6.80
6.79
6.78
6.60
6.58
5.92
5.92
5.19
5.19
5.18
5.18
5.17
5.17
4.24
4.23
2.15 H2O
Cl
HN
O
O
O
O
Cl
4i
3.14
1.00
0.98
3.99
0.88
0.98
1.01
0.96
1.01
1.00
f1 (ppm)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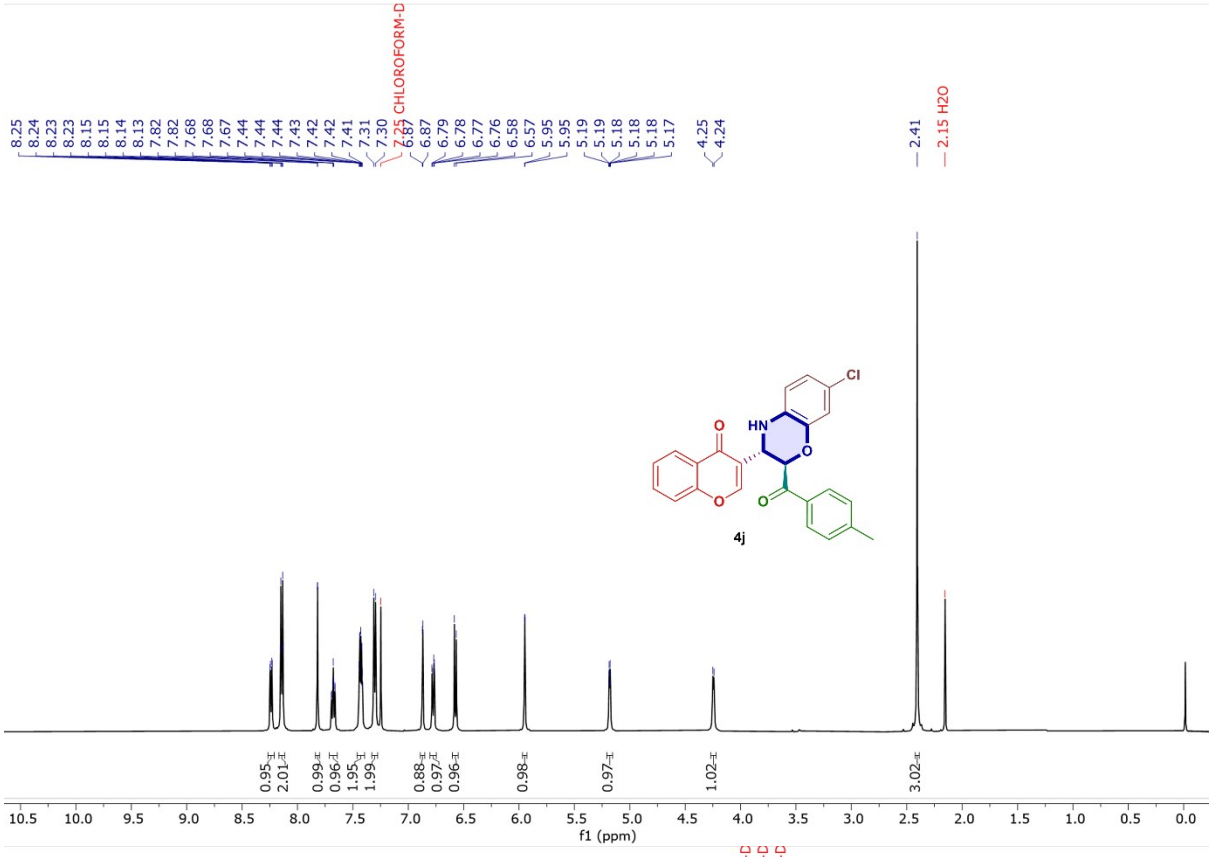
129.27
125.65
125.61
124.47
123.71
122.58
122.20
118.40
117.13
116.49
77.36 CHLOROFORM-D
77.11 CHLOROFORM-D
76.85 CHLOROFORM-D
75.33
48.15
Cl
HN
O
O
O
O
Cl
4i
f1 (ppm)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8.13
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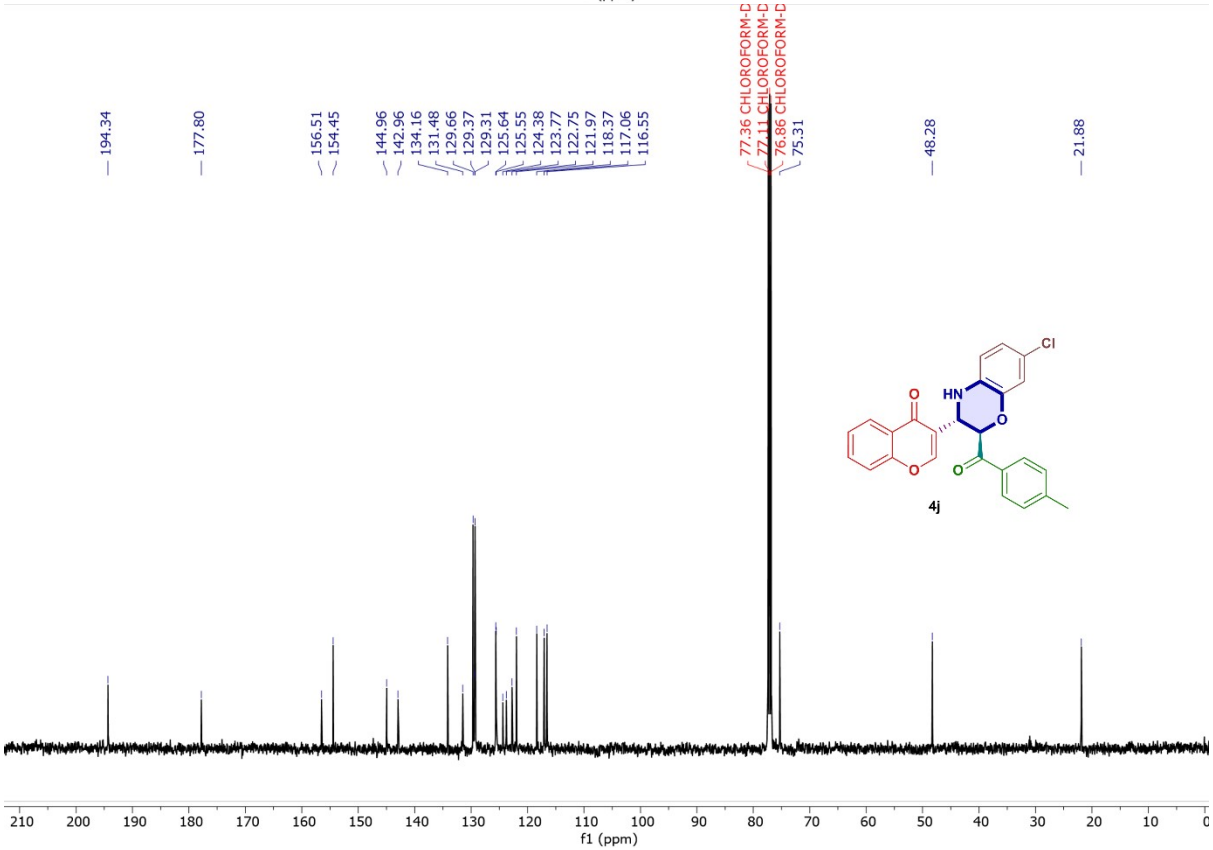
7.82
7.68
7.68
7.67
7.44
7.44
7.44
7.43
7.42
7.42
7.41
7.31
7.30
7.25 CHLOROFORM-D
6.87
6.87
6.79
6.78
6.77
6.76
6.58
6.57
5.95
5.95
5.19
5.19
5.18
5.18
5.18
5.17
4.25
4.24
2.41
2.15 H2O
Cl
HN
O
O
O
4j
0.95
2.01
0.99
0.96
1.95
1.99
0.88
0.97
0.96
0.98
0.97
1.02
3.02
f1 (ppm)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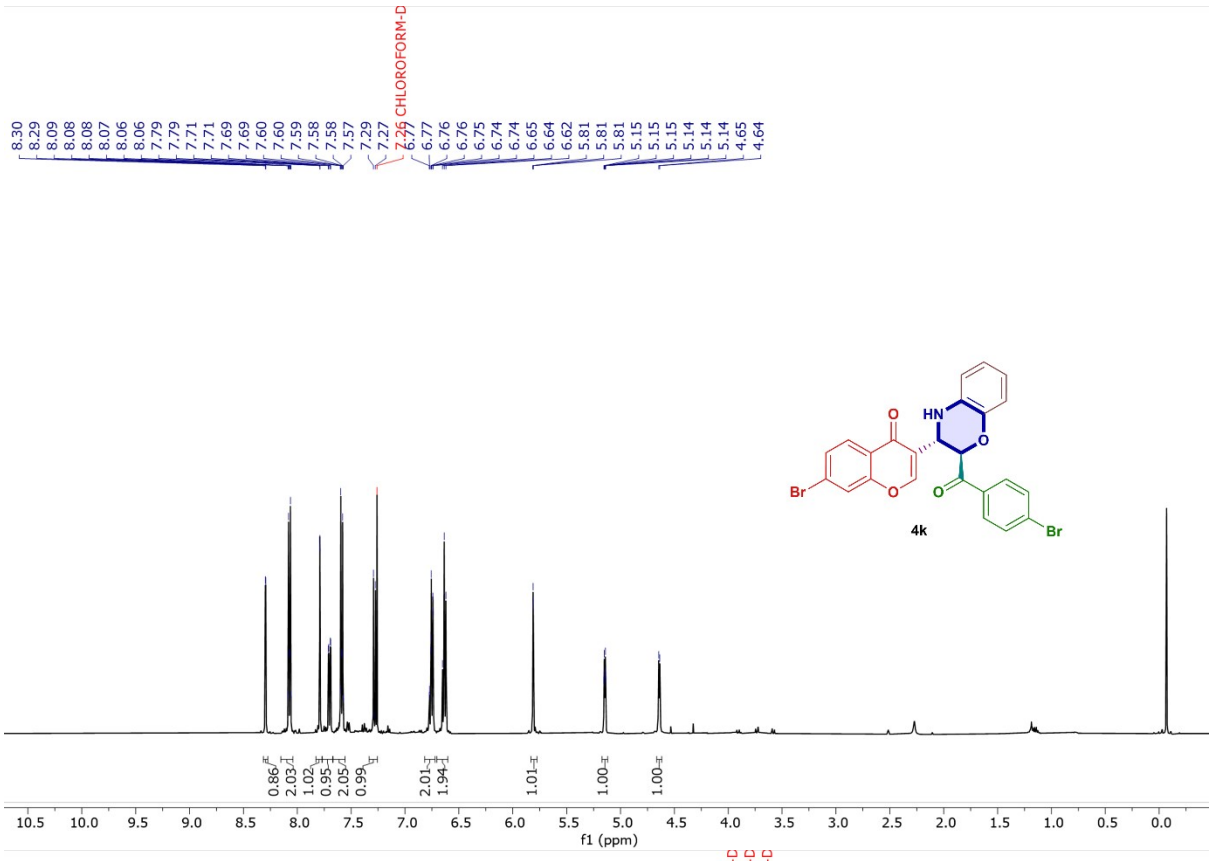
129.31
125.64
125.55
124.38
123.77
122.75
121.97
118.37
117.06
116.55
77.36 CHLOROFORM-D
77.11 CHLOROFORM-D
76.86 CHLOROFORM-D
75.31
48.28
21.88
Cl
HN
O
O
O
4j
f1 (ppm)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8.07
8.06
8.06
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7.79
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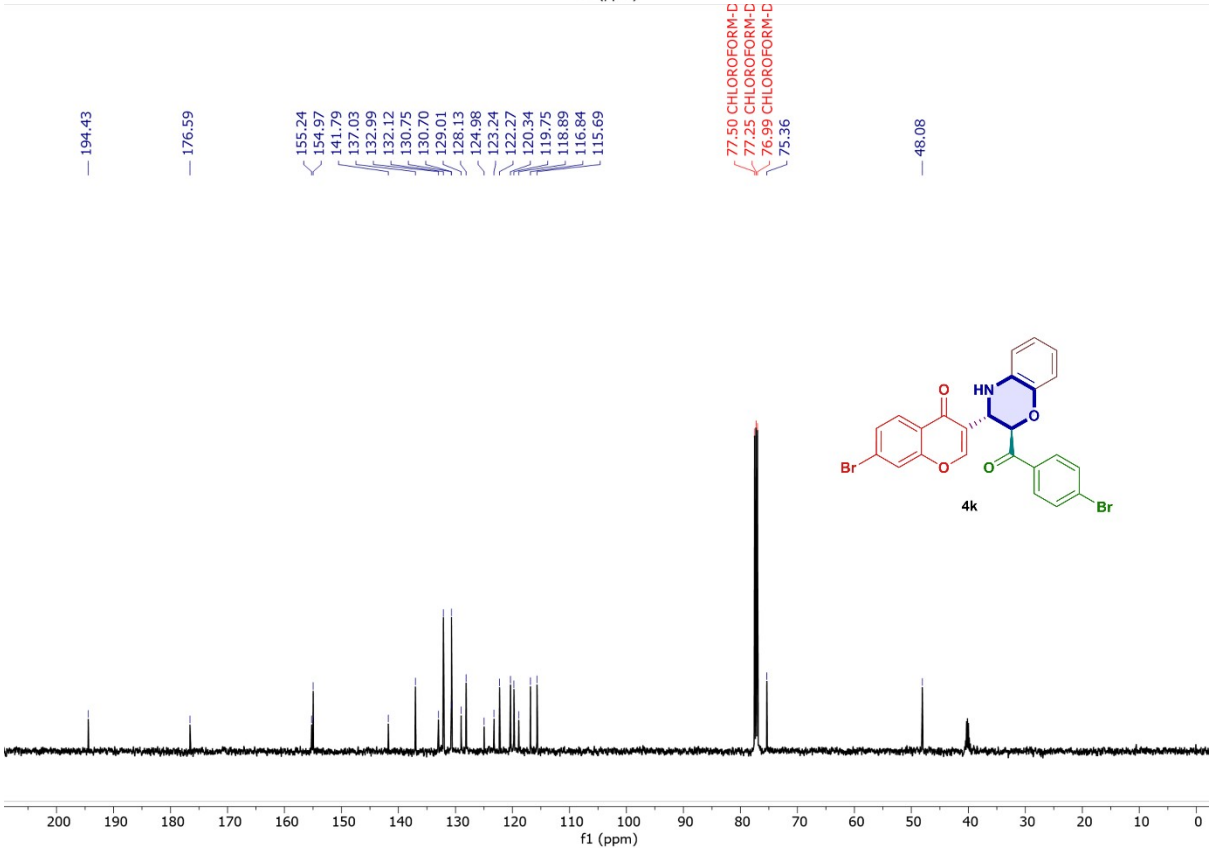
7.71
7.69
7.69
7.60
7.60
7.59
7.58
7.58
7.57
7.29
7.27
7.26 CHLOROFORM-D
6.77
6.76
6.76
6.75
6.74
6.74
6.65
6.64
6.62
5.81
5.81
5.81
5.15
5.15
5.15
5.14
5.14
5.14
4.65
4.64
O
HN
O
Br
O
O
Br
4k
0.86
2.03
1.02
0.95
2.05
0.99
2.01
1.94
1.01
1.00
1.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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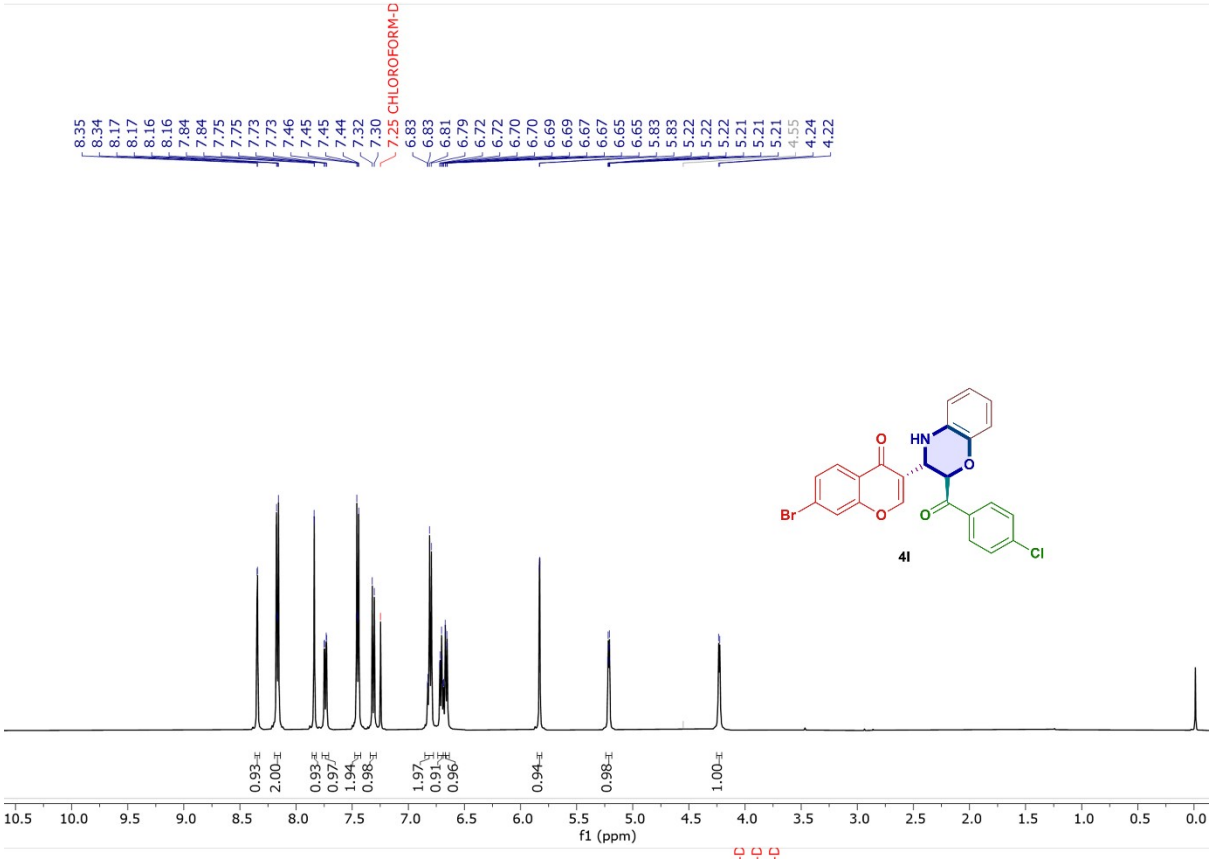
130.70
129.01
128.13
124.98
123.24
122.27
120.34
119.75
118.89
116.84
115.69
77.50 CHLOROFORM-D
77.25 CHLOROFORM-D
76.99 CHLOROFORM-D
75.36
48.08
O
HN
O
Br
O
O
Br
4k
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.16
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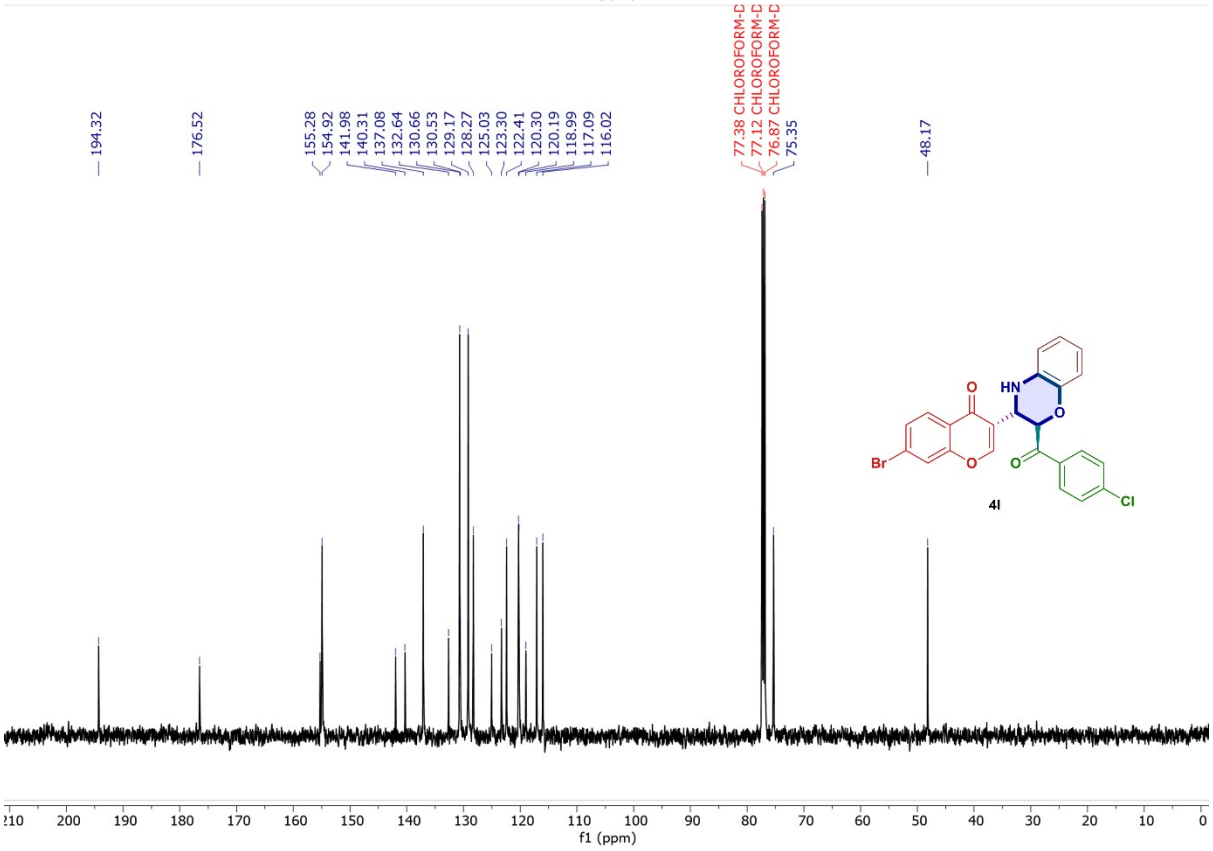
7.84
7.75
7.75
7.73
7.73
7.46
7.45
7.45
7.44
7.32
7.30
7.25 CHLOROFORM-D
6.83
6.83
6.81
6.79
6.72
6.72
6.70
6.70
6.69
6.69
6.67
6.67
6.65
6.65
5.83
5.83
5.22
5.22
5.22
5.21
5.21
5.21
4.55
4.24
4.22
0.93
2.00
0.93
0.97
1.94
0.98
1.97
0.91
0.96
0.94
0.98
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
HN
O
O
Br
O
Cl
4l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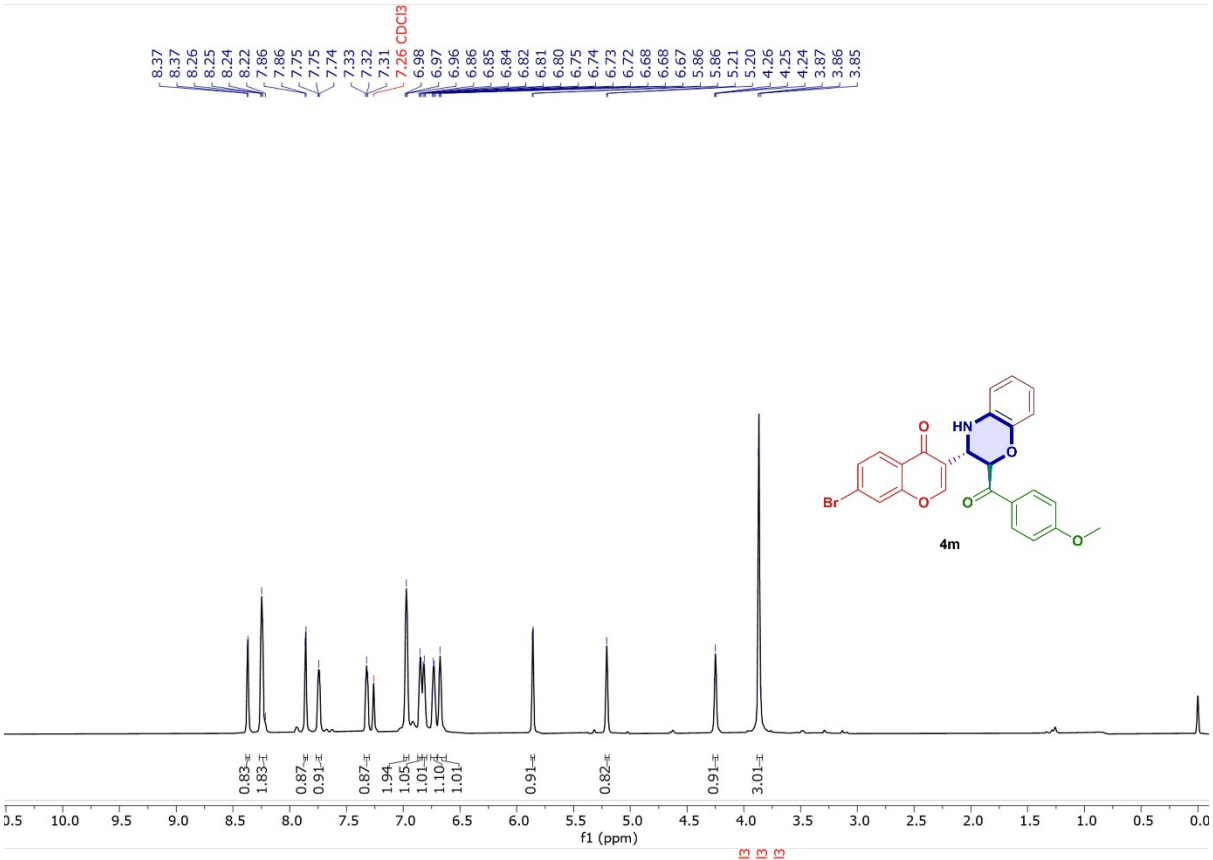
140.31
137.08
132.64
130.66
130.53
129.17
128.27
125.03
123.30
122.41
120.30
120.19
118.99
117.09
116.02
77.38 CHLOROFORM-D
77.12 CHLOROFORM-D
76.87 CHLOROFORM-D
75.35
48.17
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
HN
O
O
Br
O
Cl
4l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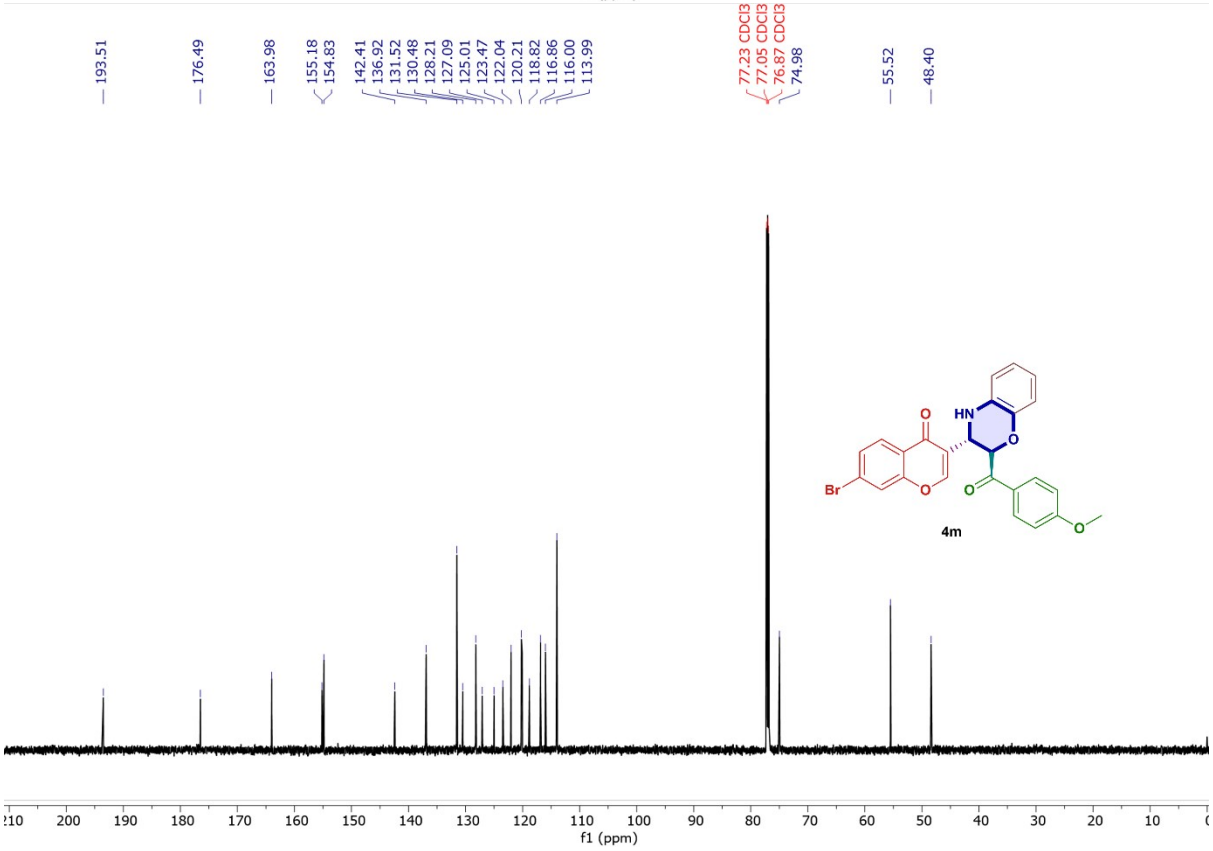
8.22
7.86
7.86
7.75
7.75
7.74
7.33
7.32
7.31
7.26 CDCl3
6.98
6.97
6.96
6.86
6.85
6.84
6.82
6.81
6.80
6.75
6.74
6.73
6.72
6.68
6.68
6.67
5.86
5.86
5.21
5.20
4.26
4.25
4.24
3.87
3.86
3.85
0.83
1.83
0.87
0.91
0.87
1.94
1.05
1.01
1.10
1.01
0.91
0.82
0.91
3.01
f1 (ppm)
4m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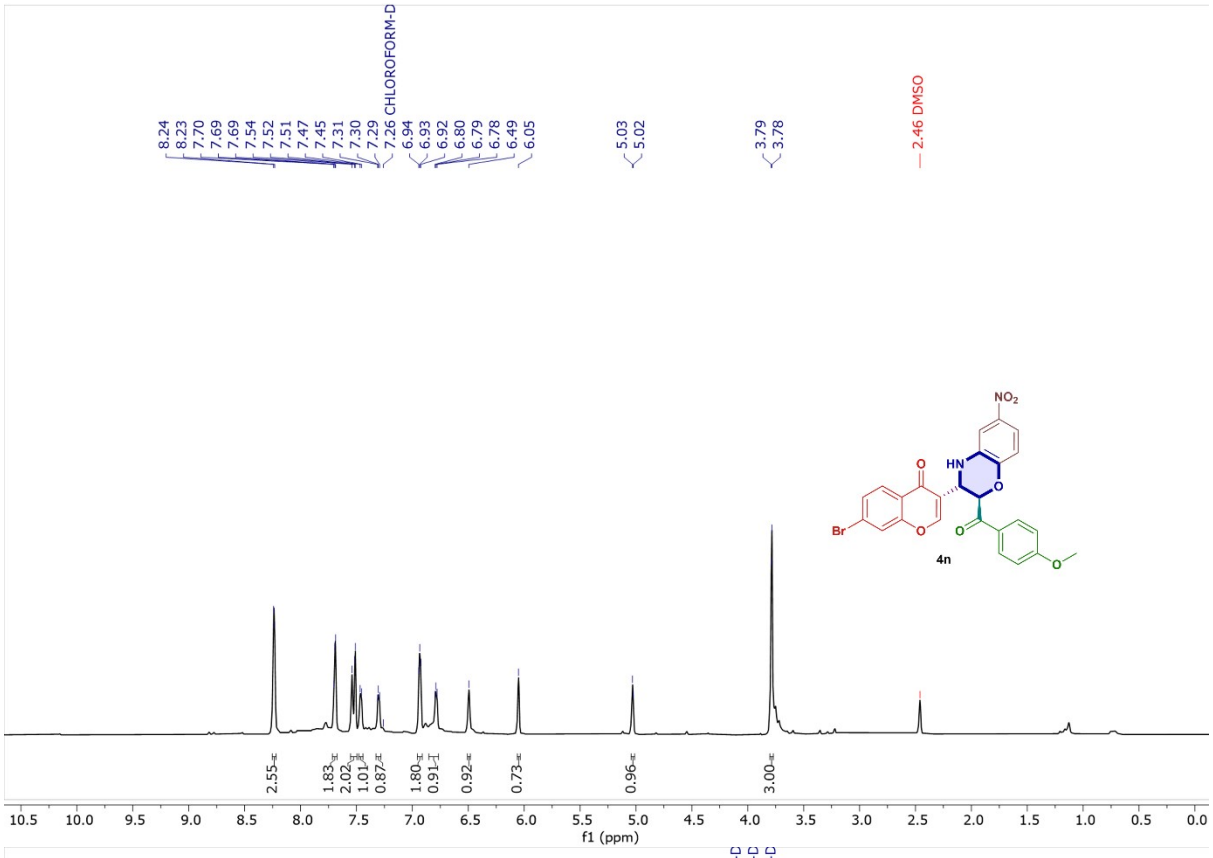
154.83
142.41
136.92
131.52
130.48
128.21
127.09
125.01
123.47
122.04
120.21
118.82
116.86
116.00
113.99
77.23 CDCl3
77.05 CDCl3
76.87 CDCl3
74.98
55.52
48.40
f1 (ppm)
4m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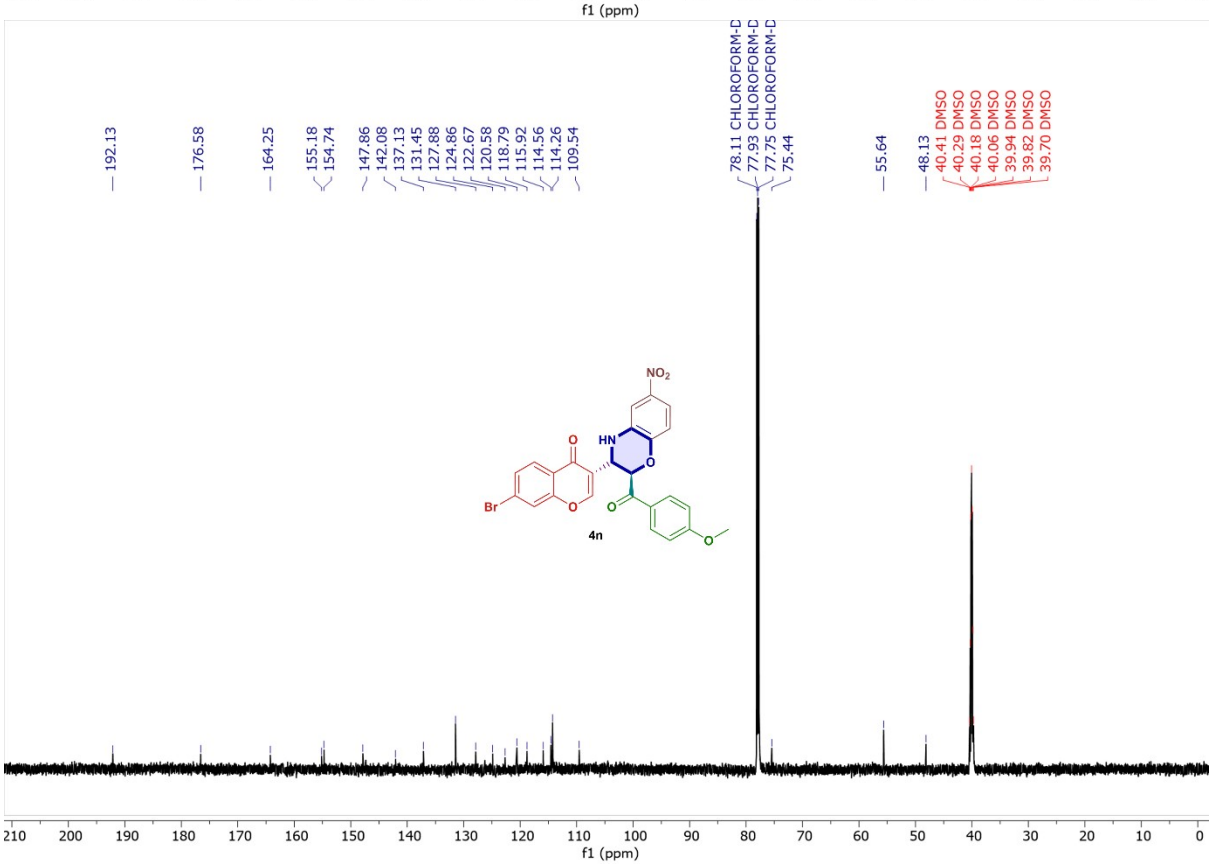
7.69
7.69
7.54
7.52
7.51
7.47
7.45
7.31
7.30
7.29
7.26 CHLOROFORM-D
6.94
6.93
6.92
6.80
6.79
6.78
6.49
6.05
5.03
5.02
3.79
3.78
2.46 DMSO
NO2
HN
O
Br
4n
2.55
1.83
2.02
1.01
0.87
1.80
0.91
0.92
0.73
0.96
3.00
f1 (ppm)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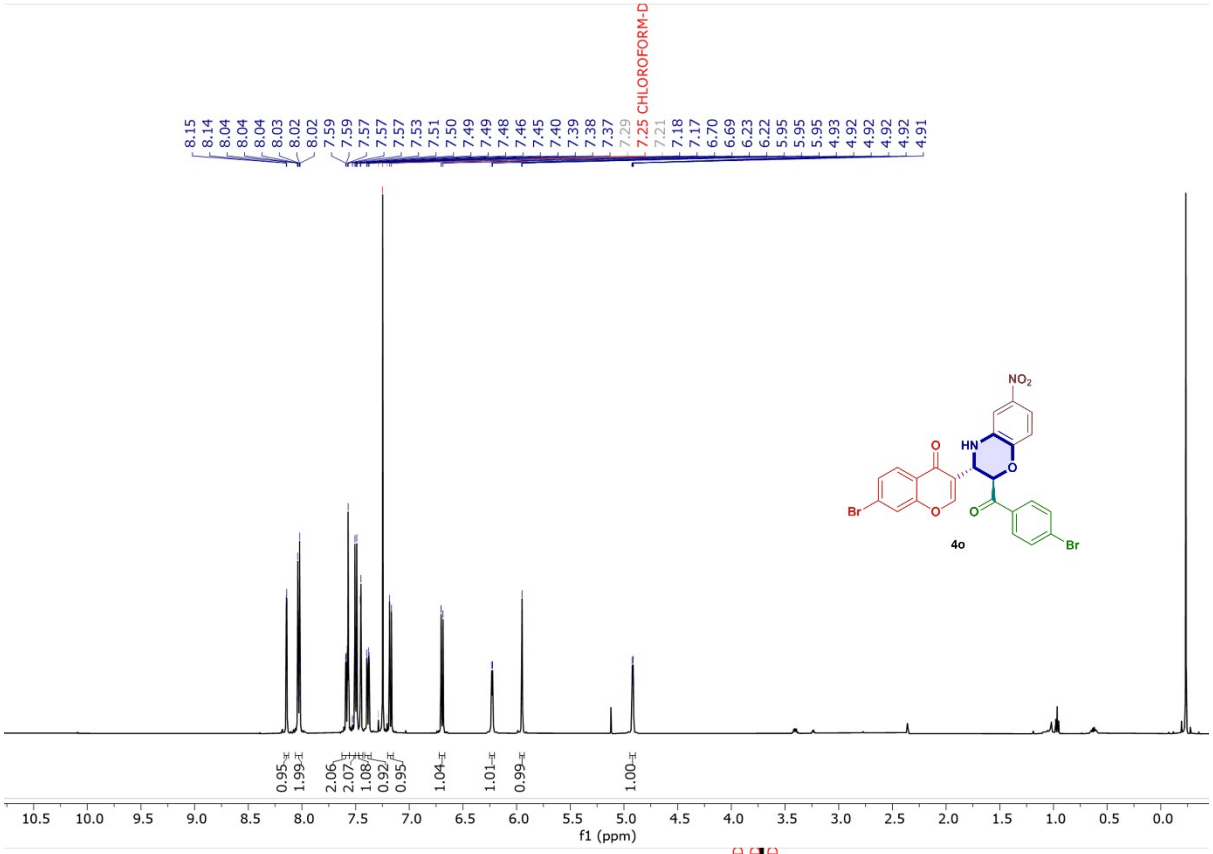
142.08
137.13
131.45
127.88
124.86
122.67
120.58
118.79
115.92
114.56
114.26
109.54
78.11 CHLOROFORM-D
77.93 CHLOROFORM-D
77.75 CHLOROFORM-D
75.44
55.64
48.13
40.41 DMSO
40.29 DMSO
40.18 DMSO
40.06 DMSO
39.94 DMSO
39.82 DMSO
39.70 DMSO
NO2
HN
O
Br
4n
f1 (ppm)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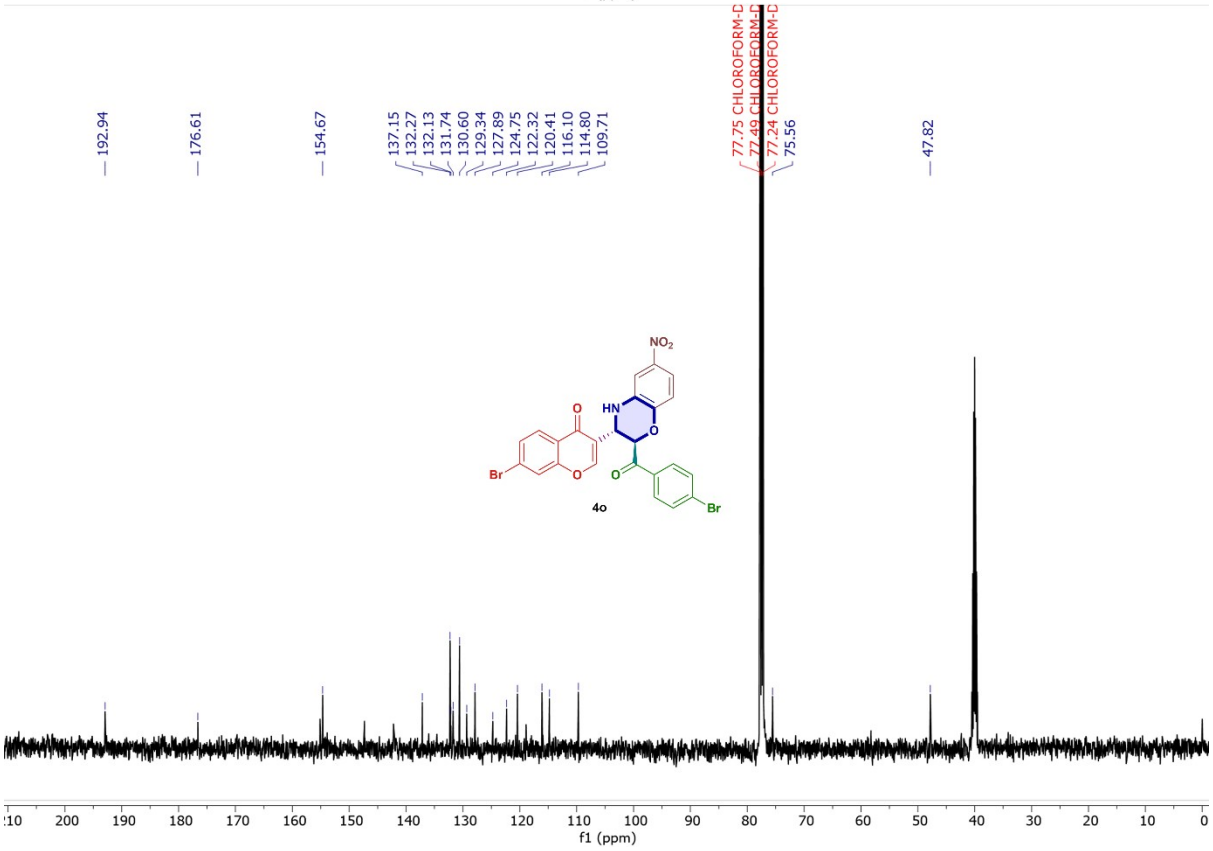
7.53
7.51
7.50
7.49
7.49
7.48
7.46
7.45
7.40
7.39
7.38
7.37
7.29
7.25 CHLOROFORM-D
7.21
7.18
7.17
6.70
6.69
6.23
6.22
5.95
5.95
5.95
4.93
4.92
4.92
4.92
4.92
4.91
0.95
1.99
2.06
2.07
1.08
0.92
0.95
1.04
1.01
0.99
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
NO2
HN
O
O
Br
O
Br
4o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130.60
129.34
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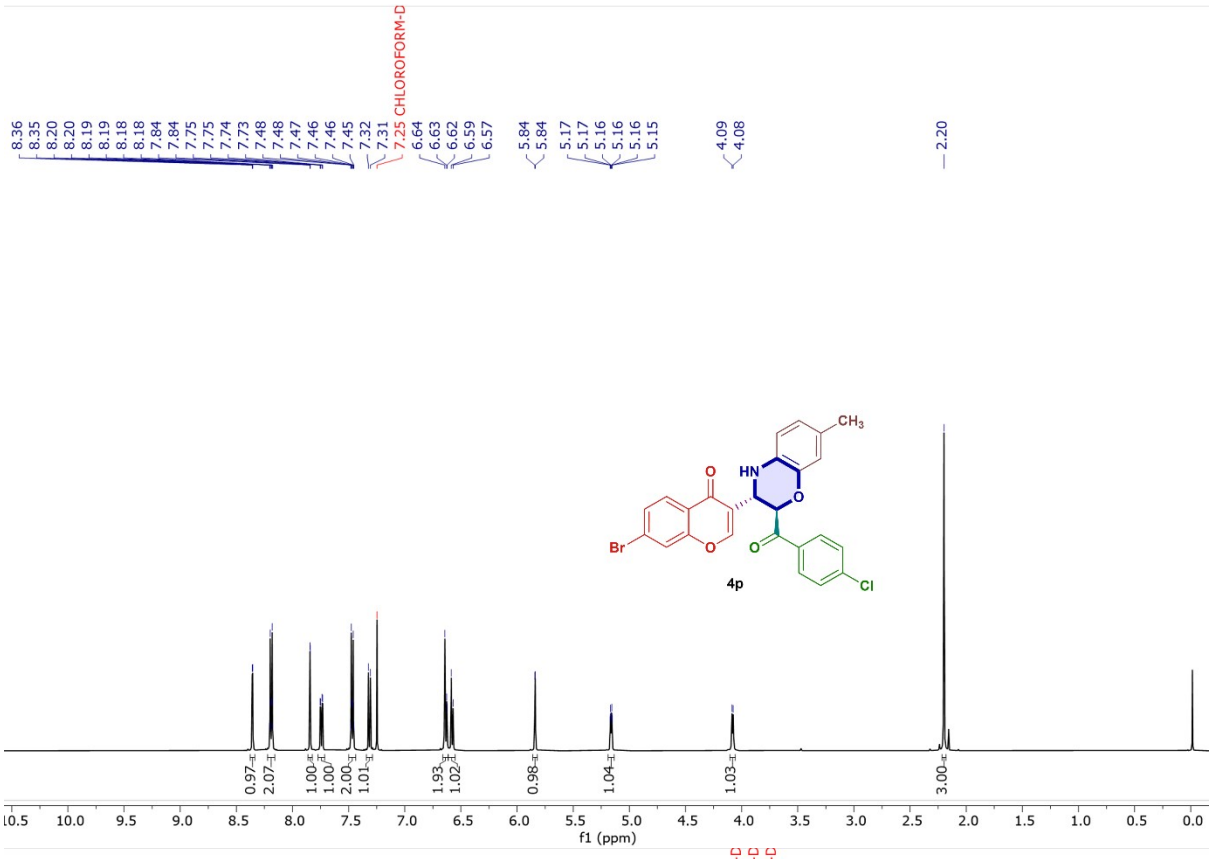
124.75
122.32
120.41
116.10
114.80
109.71
77.75 CHLOROFORM-D
77.49 CHLOROFORM-D
77.24 CHLOROFORM-D
75.56
47.82
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
NO2
HN
O
O
Br
O
Br
4o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8.18
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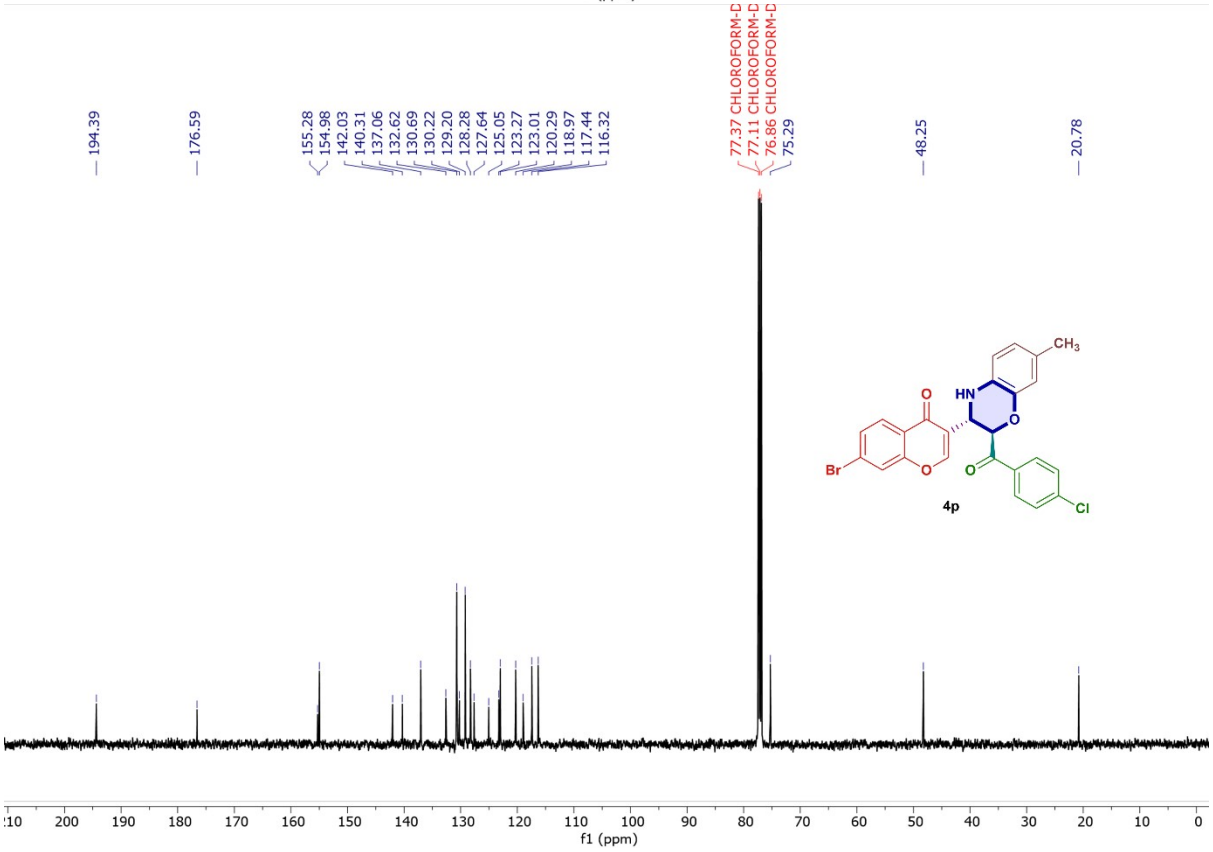
7.84
7.75
7.75
7.74
7.73
7.48
7.48
7.47
7.46
7.46
7.45
7.32
7.31
7.25 CHLOROFORM-D
6.64
6.63
6.62
6.59
6.57
5.84
5.84
5.17
5.17
5.16
5.16
5.16
5.15
4.09
4.08
2.20
CH3
HN
O
O
Br
O
O
Cl
4p
0.97
2.07
1.00
1.00
2.00
1.01
1.93
1.02
0.98
1.04
1.03
3.00
f1 (ppm)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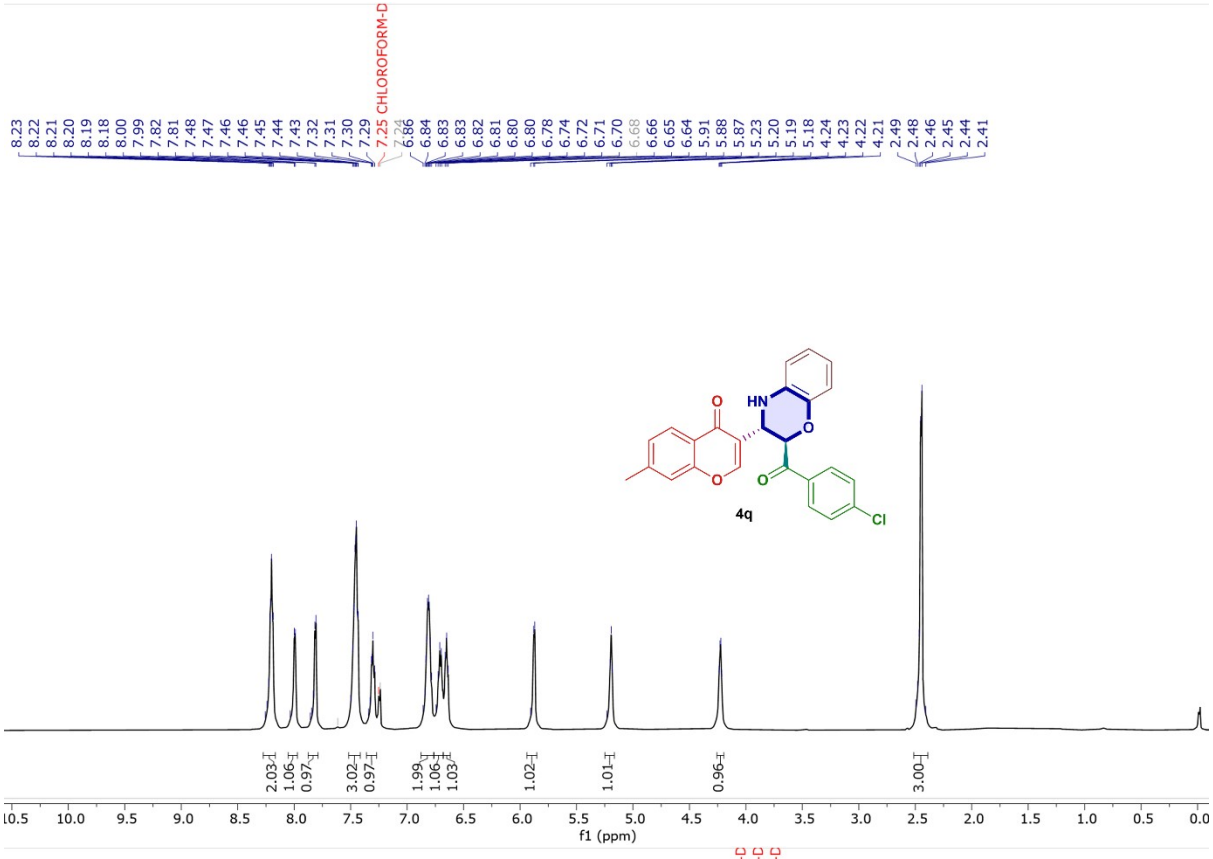
130.69
130.22
129.20
128.28
127.64
125.05
123.27
123.01
120.29
118.97
117.44
116.32
77.37 CHLOROFORM-D
77.11 CHLOROFORM-D
76.86 CHLOROFORM-D
75.29
48.25
20.78
CH3
HN
O
O
Br
O
O
Cl
4p
f1 (ppm)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7.82
7.81
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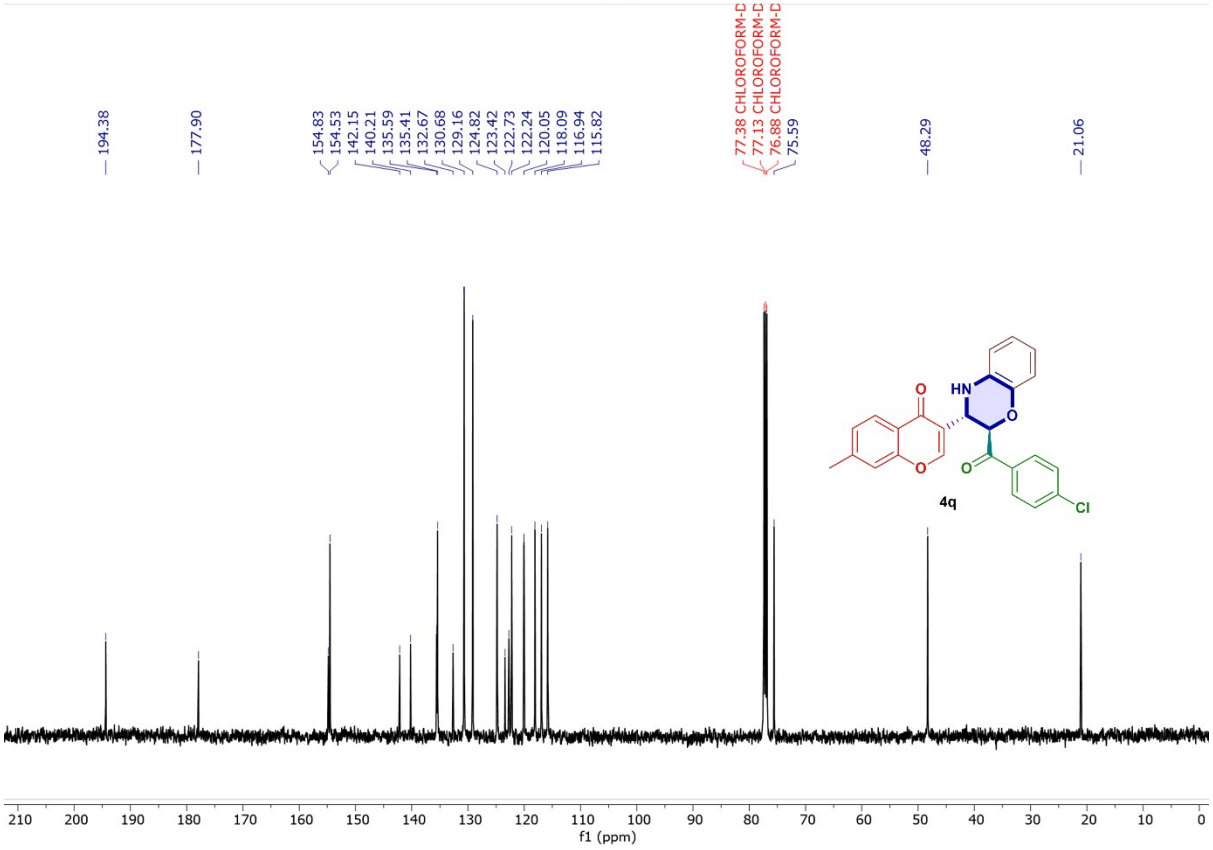
7.46
7.46
7.45
7.44
7.43
7.32
7.31
7.30
7.29
7.25 CHLOROFORM-D
7.24
6.86
6.84
6.83
6.82
6.81
6.80
6.80
6.78
6.74
6.72
6.71
6.70
6.68
6.66
6.65
6.64
5.91
5.88
5.87
5.23
5.20
5.19
5.18
4.24
4.23
4.22
4.21
2.49
2.48
2.46
2.45
2.44
2.41
O
HN
O
O
O
Cl
4q
2.03
1.06
0.97
3.02
0.97
1.99
1.06
1.03
1.02
1.01
0.96
3.00
f1 (ppm)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135.59
135.41
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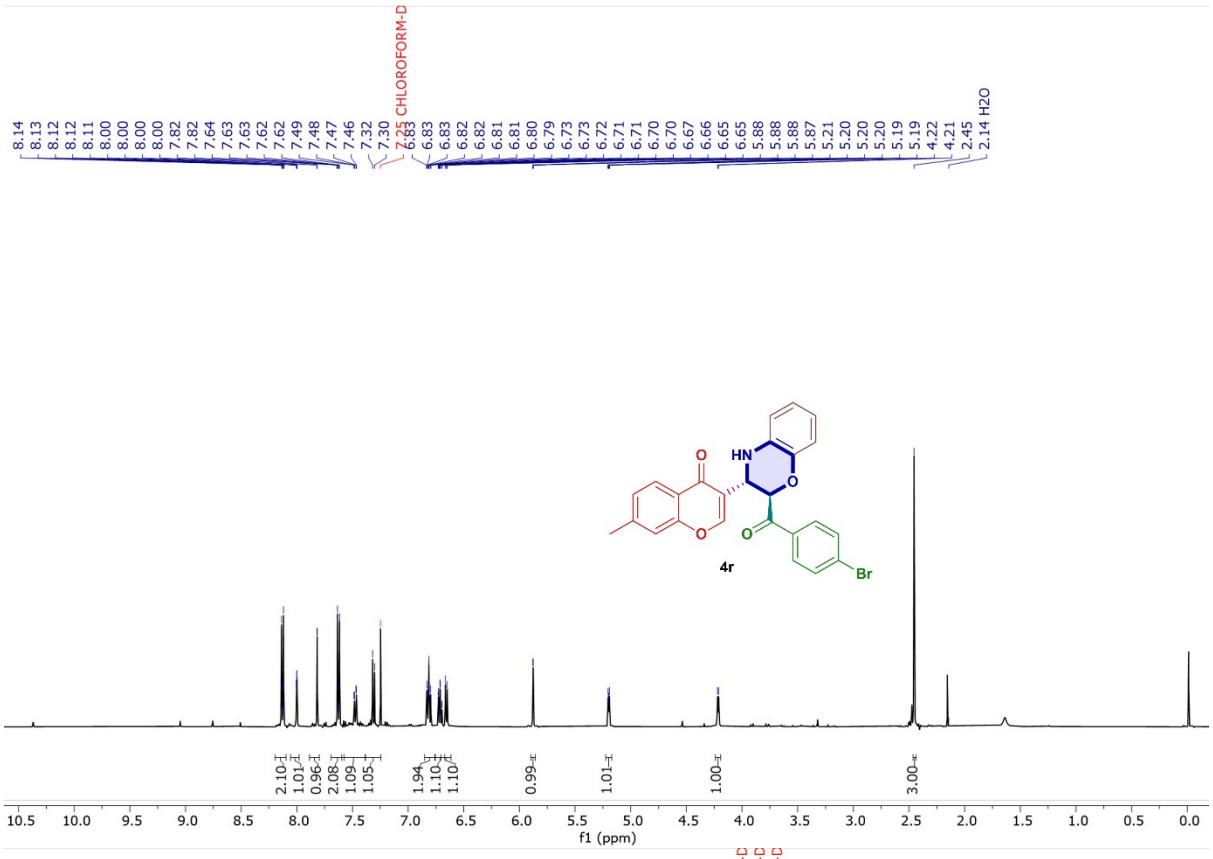
130.68
129.16
124.82
123.42
122.73
122.24
120.05
118.09
116.94
115.82
77.38 CHLOROFORM-D
77.13 CHLOROFORM-D
76.88 CHLOROFORM-D
75.59
48.29
21.06
O
HN
O
O
O
Cl
4q
f1 (ppm)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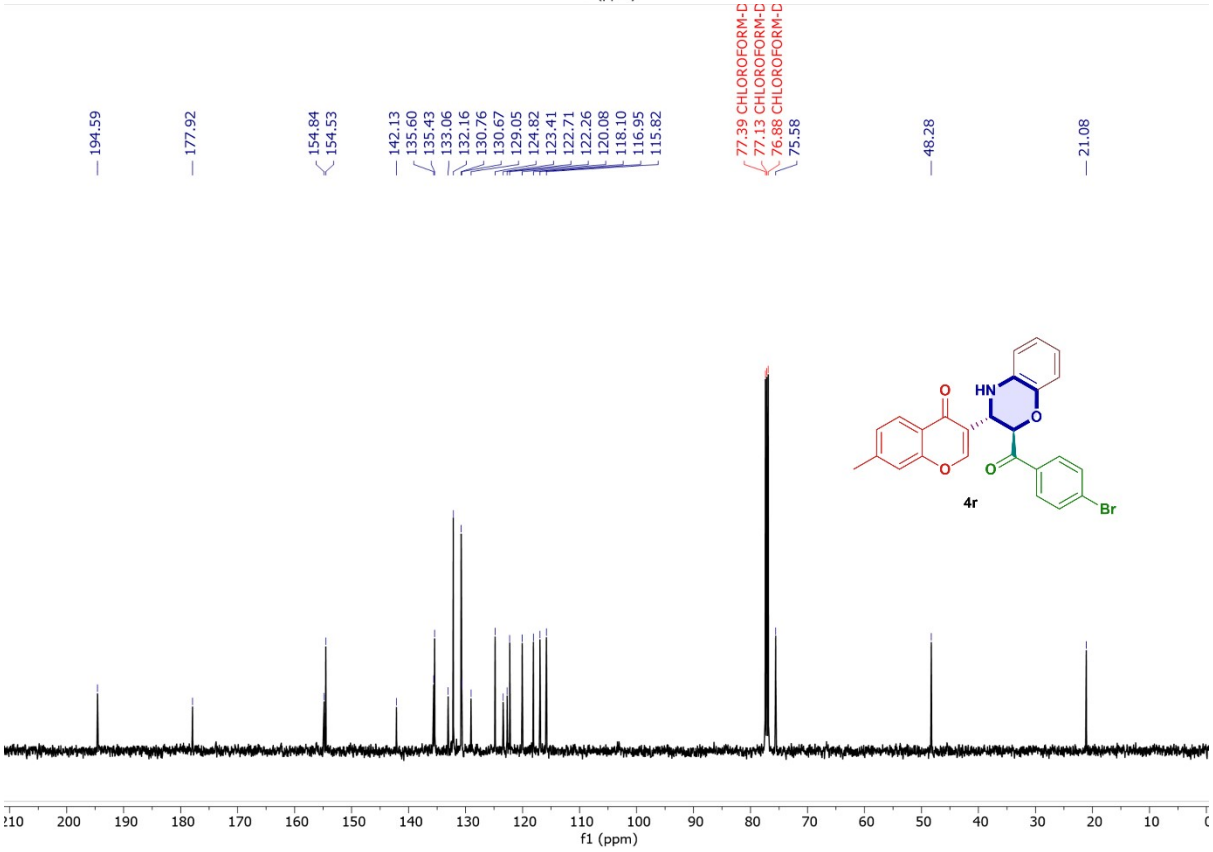
7.82
7.64
7.63
7.63
7.62
7.62
7.49
7.48
7.47
7.46
7.32
7.30
7.25 CHLOROFORM-D
6.83
6.83
6.82
6.82
6.81
6.80
6.79
6.73
6.73
6.72
6.71
6.71
6.70
6.70
6.67
6.66
6.65
5.88
5.88
5.88
5.87
5.21
5.20
5.20
5.19
5.19
4.22
4.21
2.45
2.14 H2O
O
HN
O
O
O
Br
4r
2.10
1.01
0.96
2.08
1.09
1.05
1.94
1.10
1.10
0.99
1.01
1.00
3.00
f1 (ppm)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154.53
142.13
135.60
135.43
133.06
132.16
130.76
130.67
129.05
124.82
123.41
122.71
122.26
120.08
118.10
116.95
115.82
77.39 CHLOROFORM-D
77.13 CHLOROFORM-D
76.88 CHLOROFORM-D
75.58
48.28
21.08
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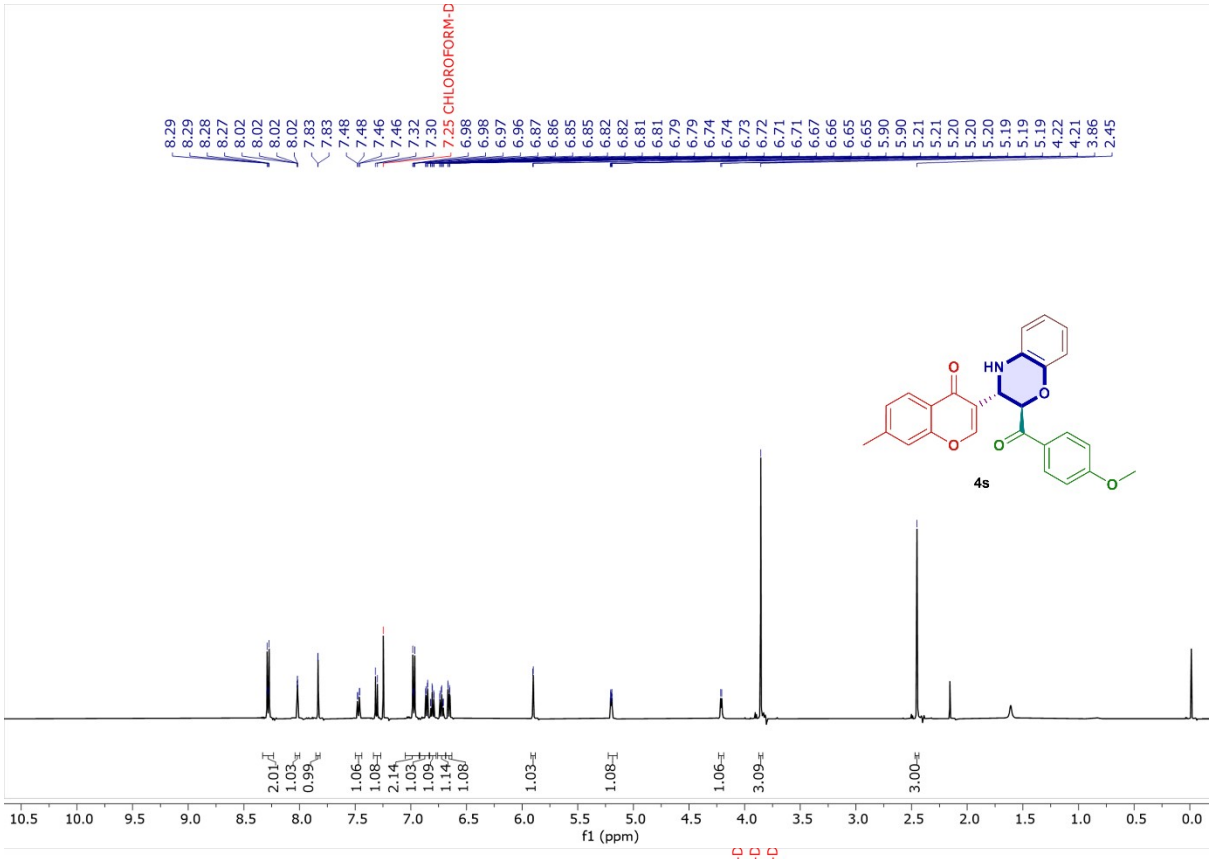
HN
O
O
O
Br
4r
f1 (ppm)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7.46
7.46
7.32
7.30
7.25 CHLOROFORM-D
6.98
6.98
6.97
6.96
6.87
6.86
6.85
6.85
6.82
6.82
6.81
6.81
6.79
6.79
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6.74
6.73
6.72
6.71
6.71
6.67
6.66
6.65
6.65
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5.90
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5.20
5.20
5.20
5.19
5.19
5.19
4.22
4.21
3.86
2.45
HN
O
O
O
O
4s
2.01
1.03
0.99
1.06
1.08
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1.14
1.08
1.03
1.08
1.06
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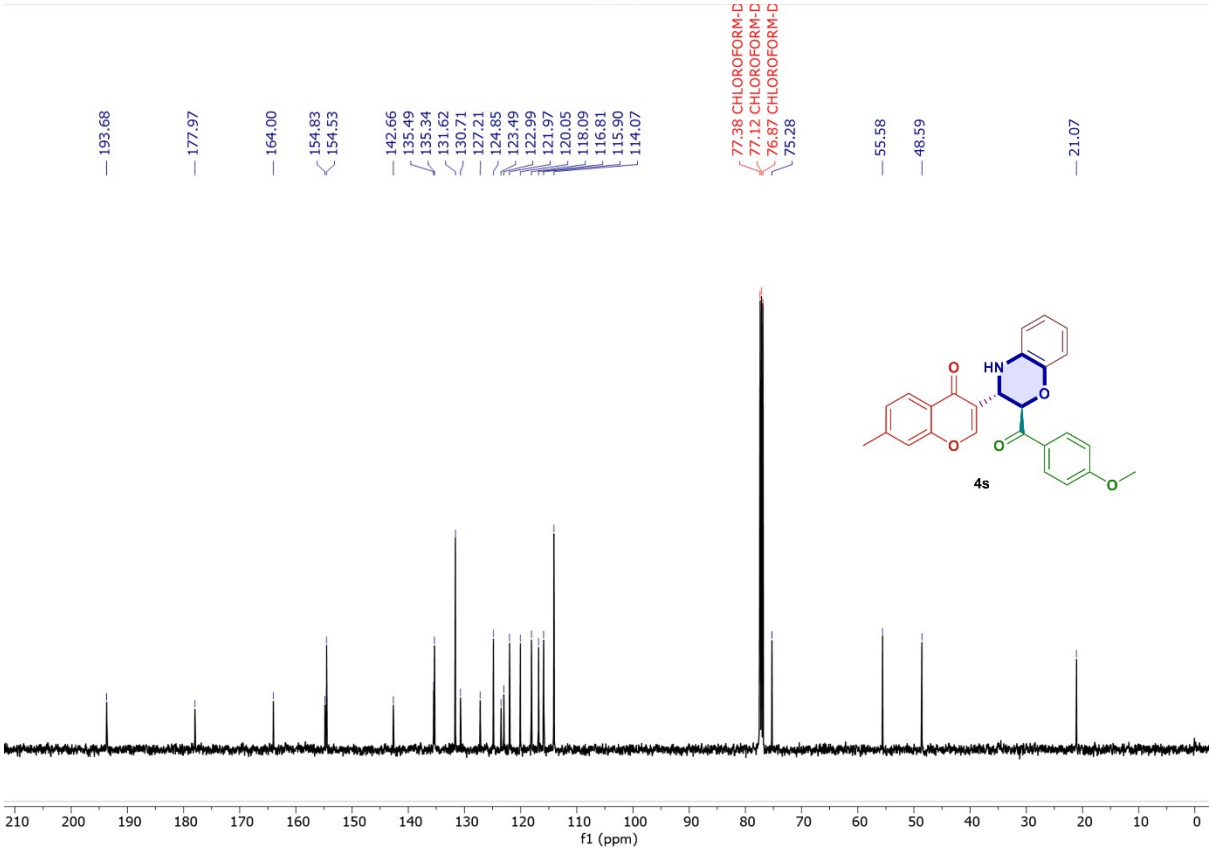
3.00
f1 (ppm)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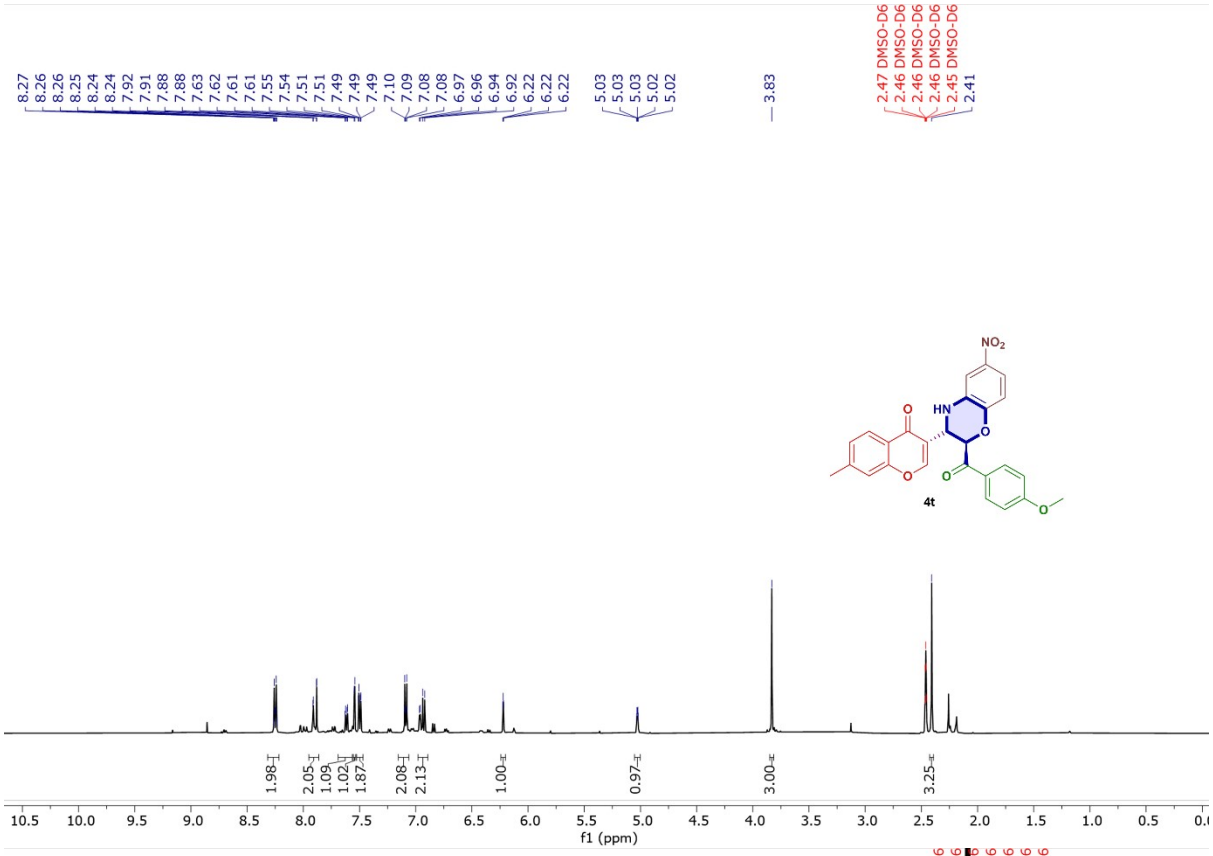
135.34
131.62
130.71
127.21
124.85
123.49
122.99
121.97
120.05
118.09
116.81
115.90
114.07
77.38 CHLOROFORM-D
77.12 CHLOROFORM-D
76.87 CHLOROFORM-D
75.28
55.58
48.59
21.07
HN
O
O
O
O
4s
f1 (ppm)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7.61
7.55
7.54
7.51
7.51
7.49
7.49
7.49
7.10
7.09
7.08
7.08
6.97
6.96
6.94
6.92
6.22
6.22
6.22
5.03
5.03
5.03
5.02
5.02
3.83
2.47 DMSO-D6
2.46 DMSO-D6
2.46 DMSO-D6
2.46 DMSO-D6
2.45 DMSO-D6
2.41
NO2
HN
O
O
O
O
O
4t
1.98
2.05
1.09
1.02
1.87
2.08
2.13
1.00
0.97
3.00
3.25
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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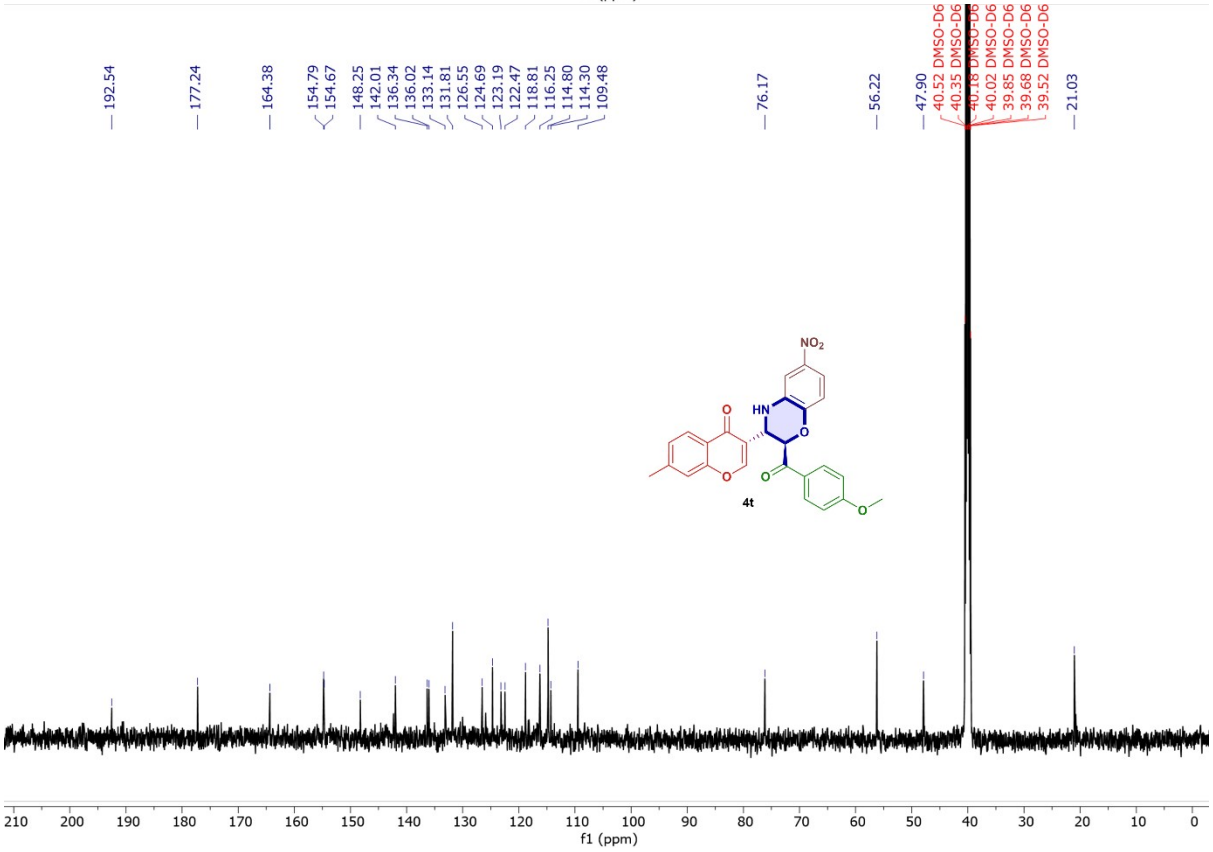
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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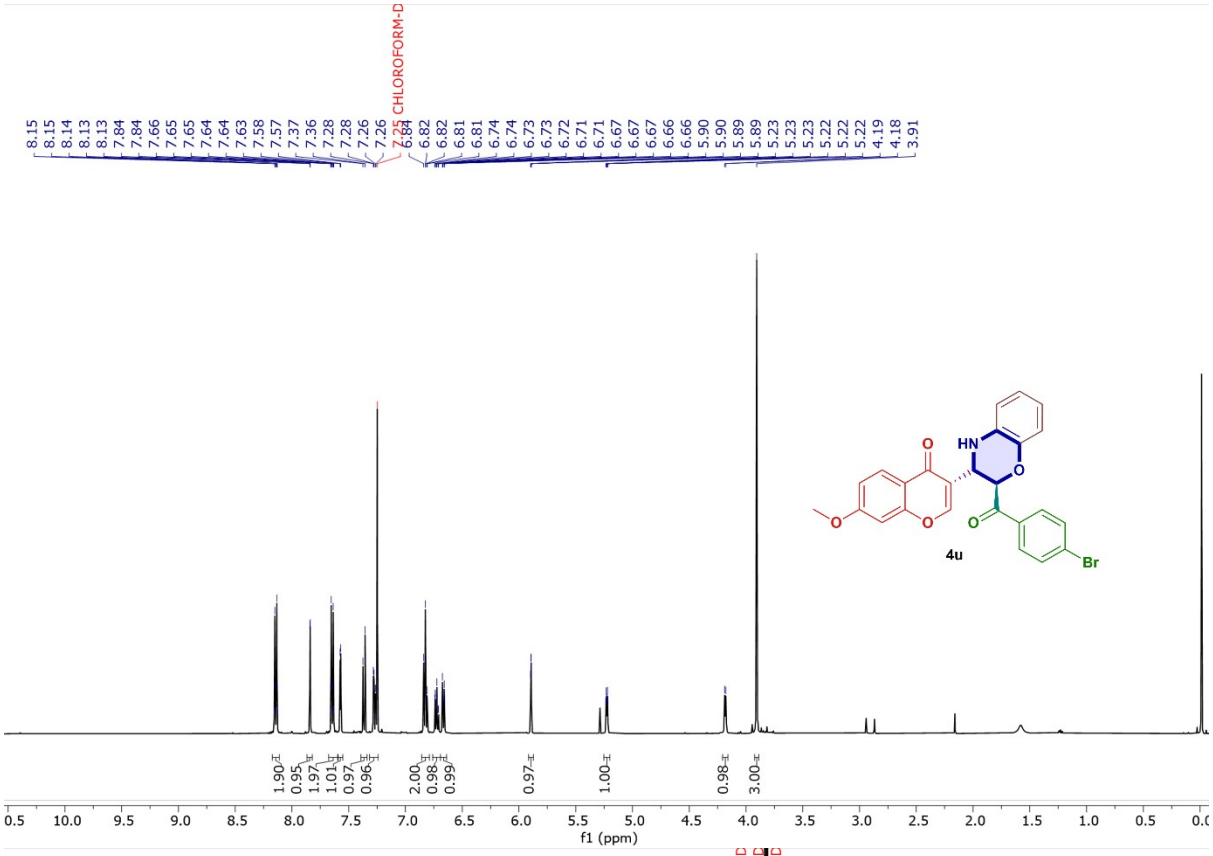
131.81
126.55
124.69
123.19
122.47
118.81
116.25
114.80
114.30
109.48
76.17
56.22
47.90
40.52 DMSO-D6
40.35 DMSO-D6
40.18 DMSO-D6
40.02 DMSO-D6
39.85 DMSO-D6
39.68 DMSO-D6
39.52 DMSO-D6
21.03
NO2
HN
O
O
O
O
O
4t
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.65
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7.63
7.58
7.57
7.37
7.36
7.28
7.28
7.26
7.26
7.25 CHLOROFORM-D
6.84
6.82
6.82
6.81
6.81
6.74
6.74
6.73
6.73
6.72
6.71
6.71
6.67
6.67
6.67
6.66
6.66
5.90
5.90
5.89
5.89
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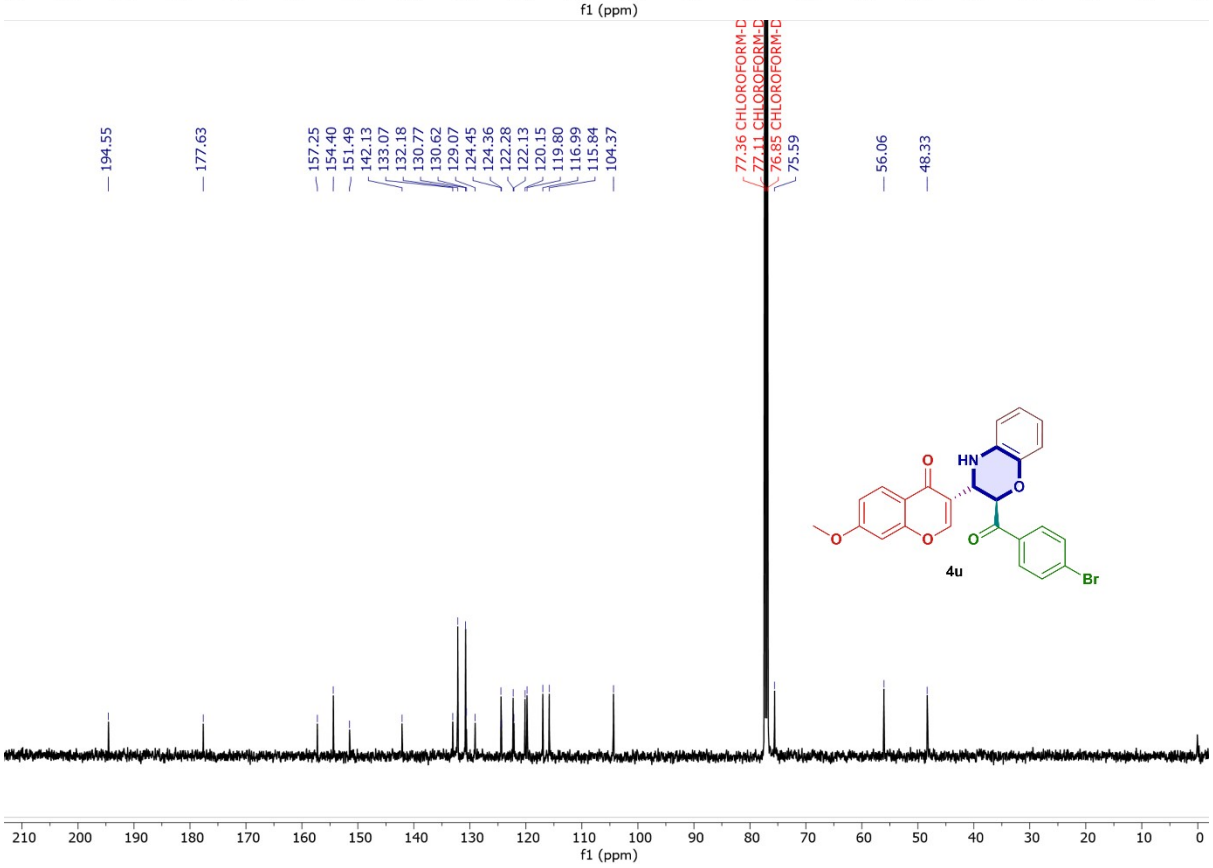
5.23
5.22
5.22
5.22
4.19
4.18
3.91
1.90
0.95
1.97
1.01
0.97
0.96
2.00
0.98
0.99
0.97
1.00
0.98
3.00
f1 (ppm)
4u
Br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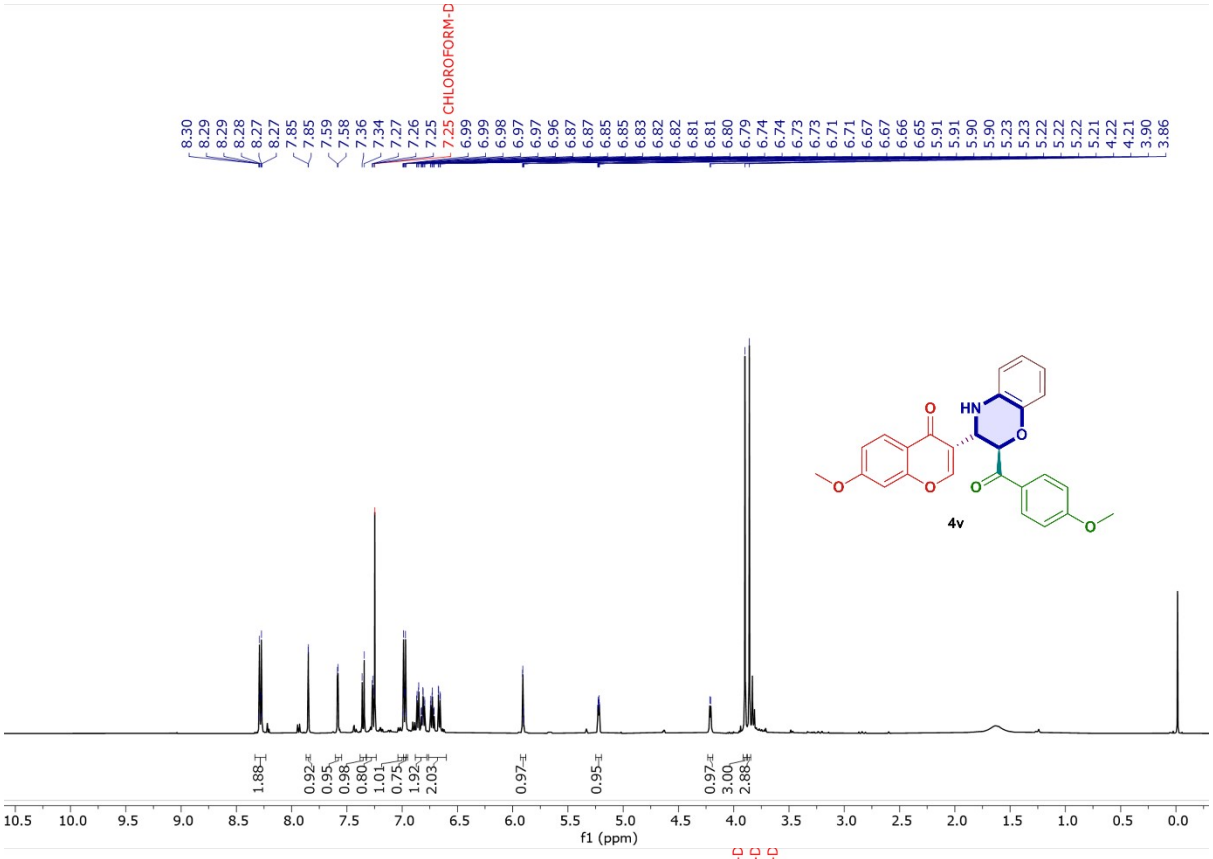
133.07
132.18
130.77
130.62
129.07
124.45
124.36
122.28
122.13
120.15
119.80
116.99
115.84
104.37
77.36 CHLOROFORM-D
77.11 CHLOROFORM-D
76.85 CHLOROFORM-D
75.59
56.06
48.33
f1 (ppm)
4u
Br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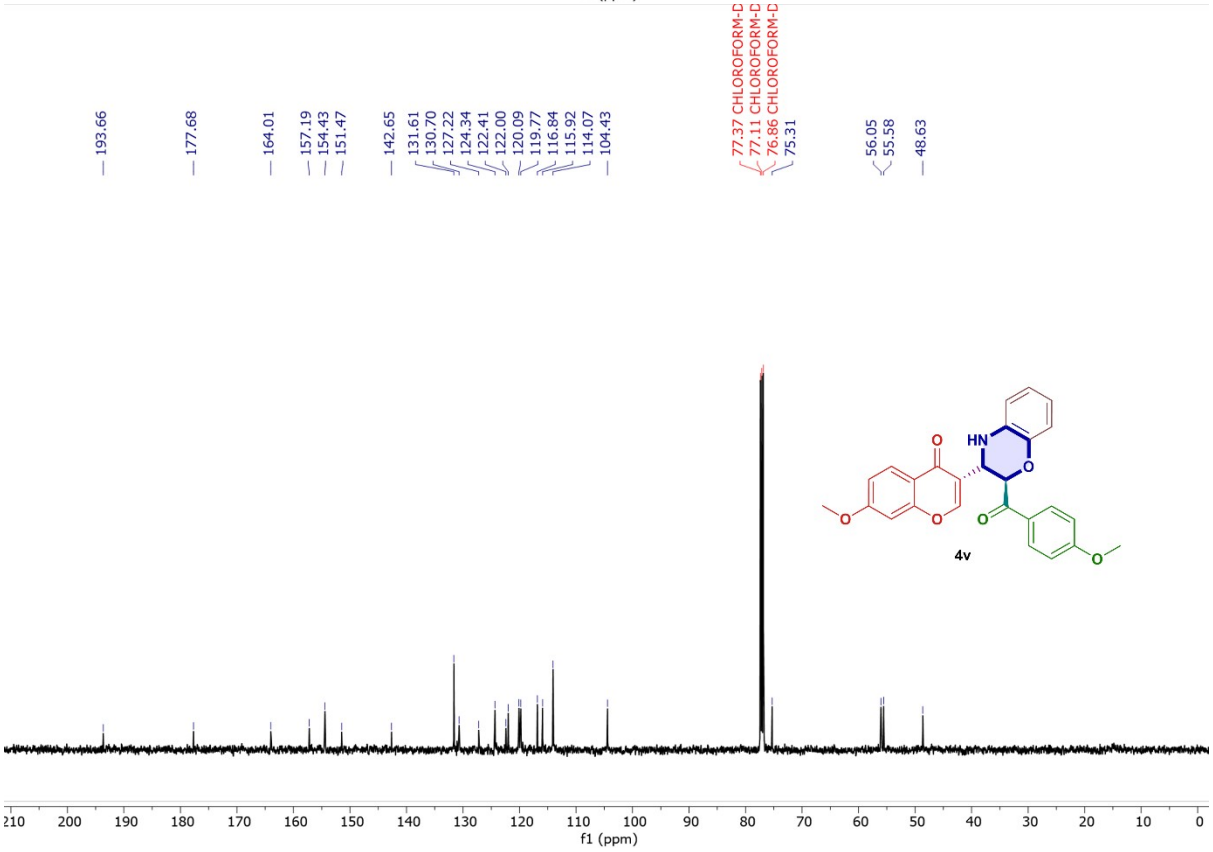
8.27
7.85
7.85
7.59
7.58
7.36
7.34
7.27
7.26
7.25
7.25 CHLOROFORM-D
6.99
6.99
6.98
6.97
6.97
6.96
6.87
6.87
6.85
6.85
6.83
6.82
6.82
6.81
6.81
6.80
6.79
6.74
6.74
6.73
6.73
6.71
6.67
6.67
6.66
6.65
5.91
5.91
5.90
5.90
5.23
5.23
5.22
5.22
5.22
5.21
4.22
4.21
3.90
3.86
HN
O
O
O
O
O
4v
1.88
0.92
0.95
0.98
0.80
1.01
0.75
1.92
2.03
0.97
0.95
0.97
3.00
2.88
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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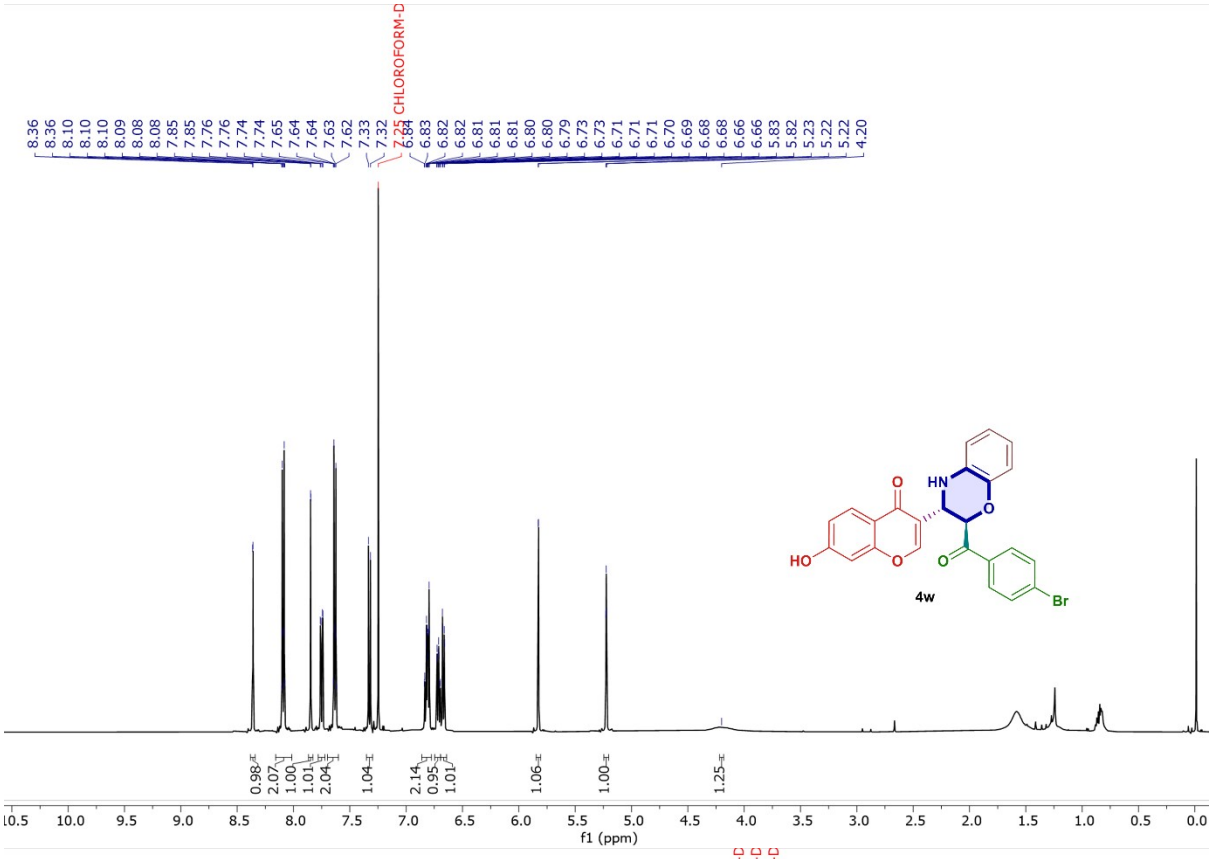
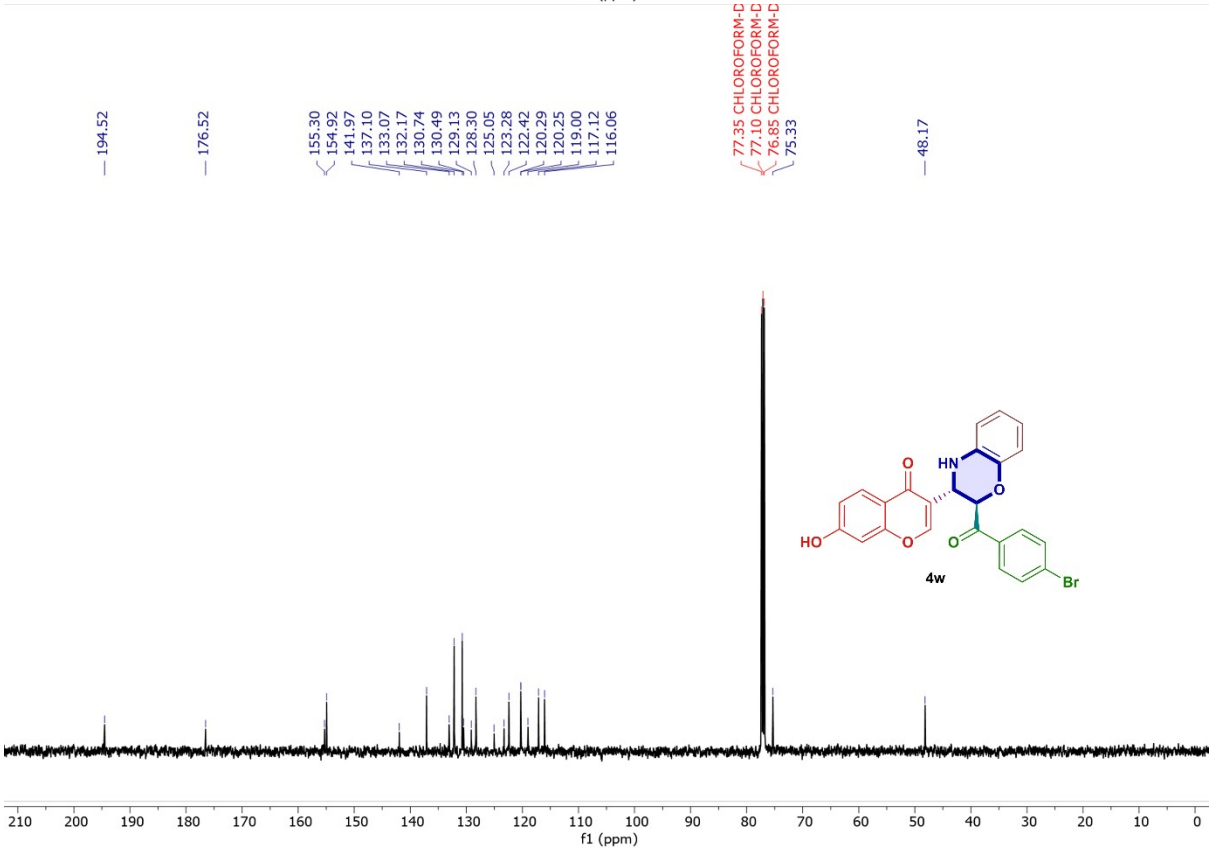
151.47
142.65
131.61
130.70
127.22
124.34
122.41
122.00
120.09
119.77
116.84
115.92
114.07
104.43
77.37 CHLOROFORM-D
77.11 CHLOROFORM-D
76.86 CHLOROFORM-D
75.31
56.05
55.58
48.63
HN
O
O
O
O
O
4v
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


CHLOROFORM-D
8.36
8.36
8.10
8.10
8.10
8.09
8.08
8.08
8.08
7.85
7.85
7.76
7.76
7.76
7.74
7.74
7.65
7.64
7.64
7.63
7.62
7.33
7.32
7.25
6.84
6.83
6.82
6.82
6.81
6.81
6.81
6.80
6.80
6.79
6.73
6.73
6.71
6.71
6.71
6.70
6.69
6.68
6.68
6.66
6.66
5.83
5.82
5.23
5.22
5.22
4.20
0.98
2.07
1.00
1.01
2.04
1.04
2.14
0.95
1.01
1.06
1.00
1.25
f1 (ppm)
HO
O
HN
O
O
O
Br
4w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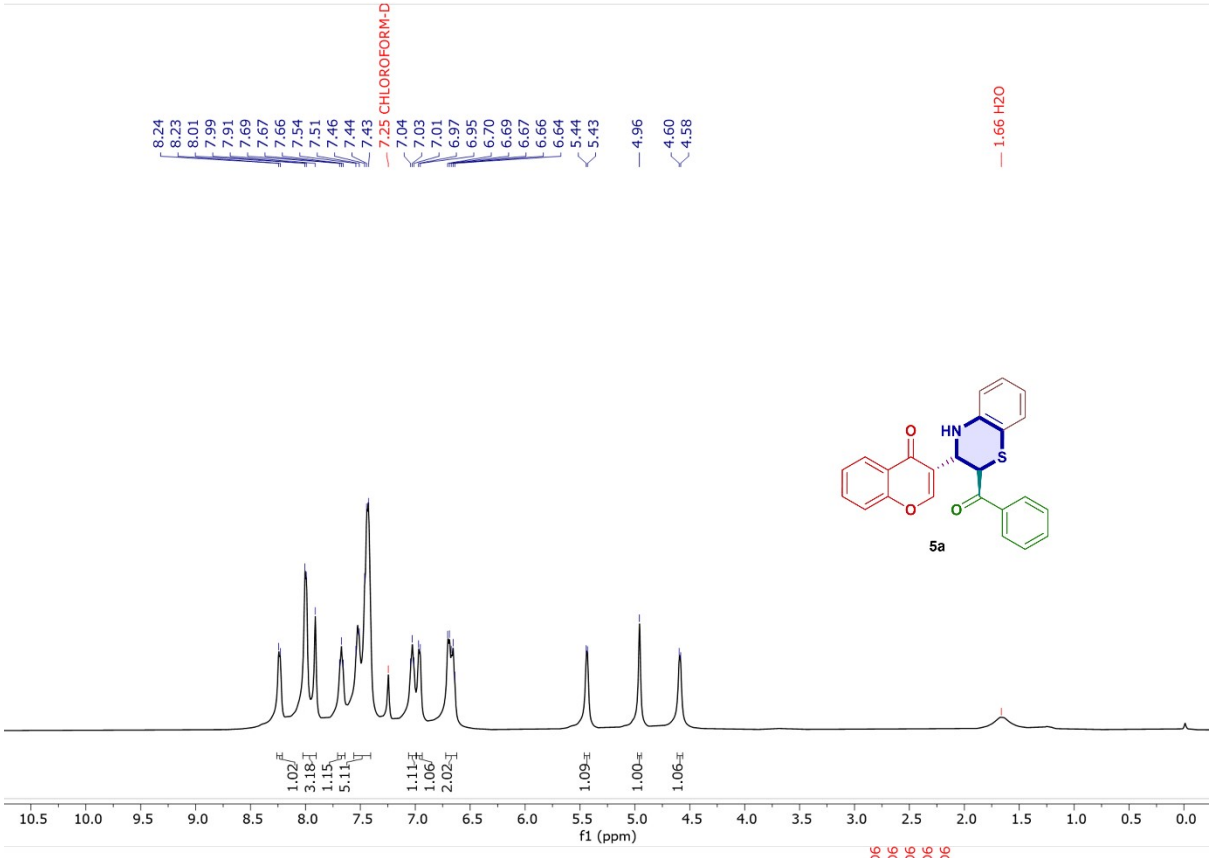
137.10
133.07
132.17
130.74
130.49
129.13
128.30
125.05
123.28
122.42
120.29
120.25
119.00
117.12
116.06
77.35 CHLOROFORM-D
77.10 CHLOROFORM-D
76.85 CHLOROFORM-D
75.33
48.17
f1 (ppm)
HO
O
HN
O
O
O
Br
4w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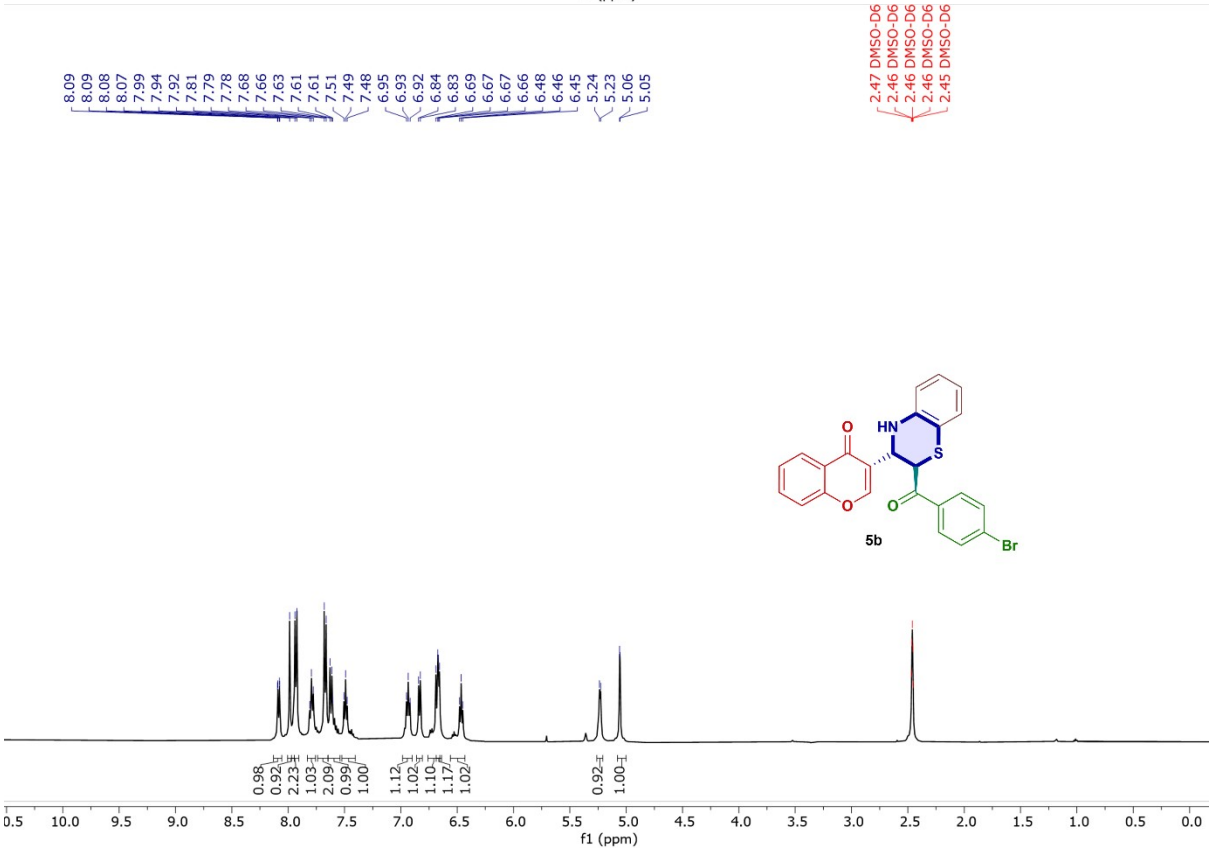
8.23
8.01
7.99
7.91
7.69
7.67
7.66
7.54
7.51
7.46
7.44
7.43
7.25 CHLOROFORM-D
7.04
7.03
7.01
6.97
6.95
6.70
6.69
6.67
6.66
6.64
5.44
5.43
4.96
4.60
4.58
1.66 H2O
HN
S
O
O
O
5a
1.02
3.18
1.15
5.11
1.11
1.06
2.02
1.09
1.00
1.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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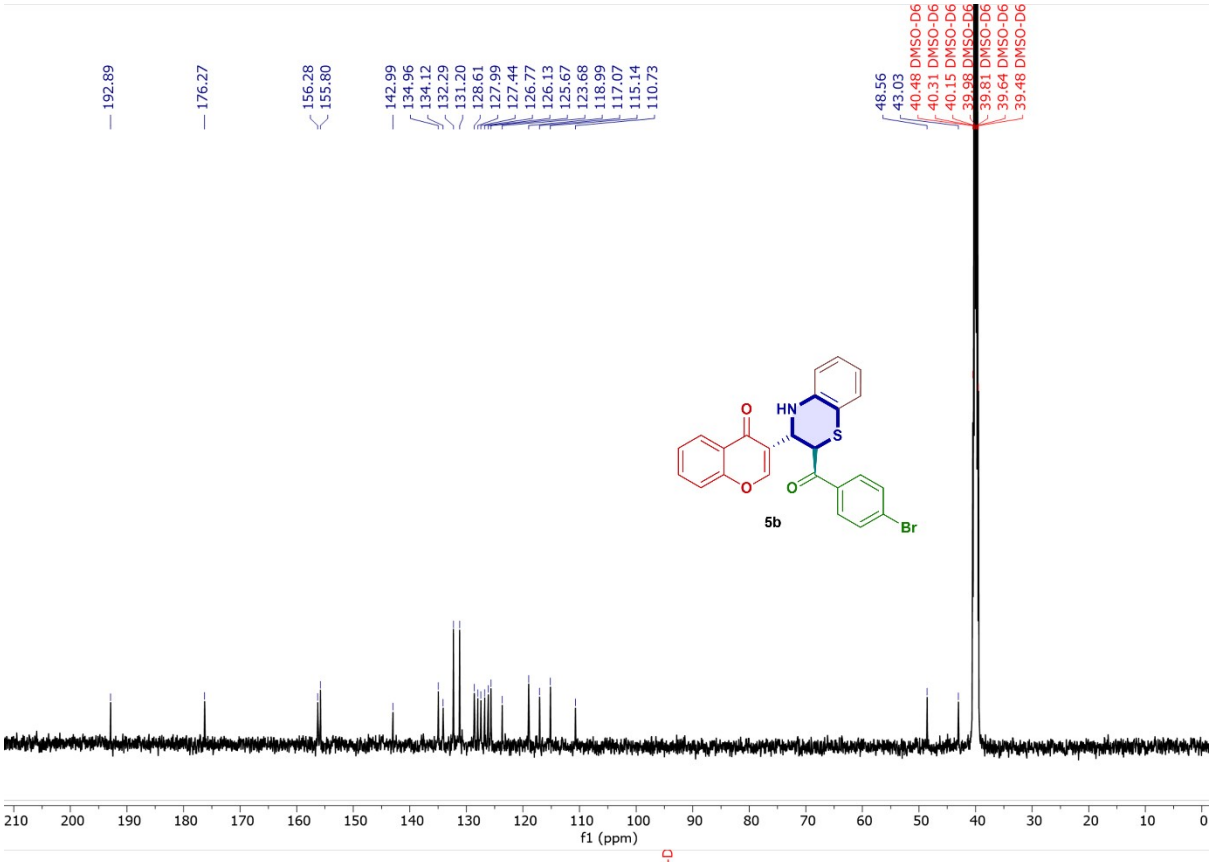
8.08
8.07
7.99
7.94
7.92
7.81
7.79
7.78
7.68
7.66
7.63
7.61
7.61
7.51
7.49
7.48
6.95
6.93
6.92
6.84
6.83
6.69
6.67
6.67
6.66
6.48
6.46
6.45
5.24
5.23
5.06
5.05
2.47 DMSO-D6
2.46 DMSO-D6
2.46 DMSO-D6
2.46 DMSO-D6
2.45 DMSO-D6
HN
S
O
O
O
Br
5b
0.98
0.92
2.23
1.03
2.09
0.99
1.00
1.12
1.02
1.10
1.17
1.02
0.92
1.00
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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134.12
132.29
131.20
128.61
127.99
127.44
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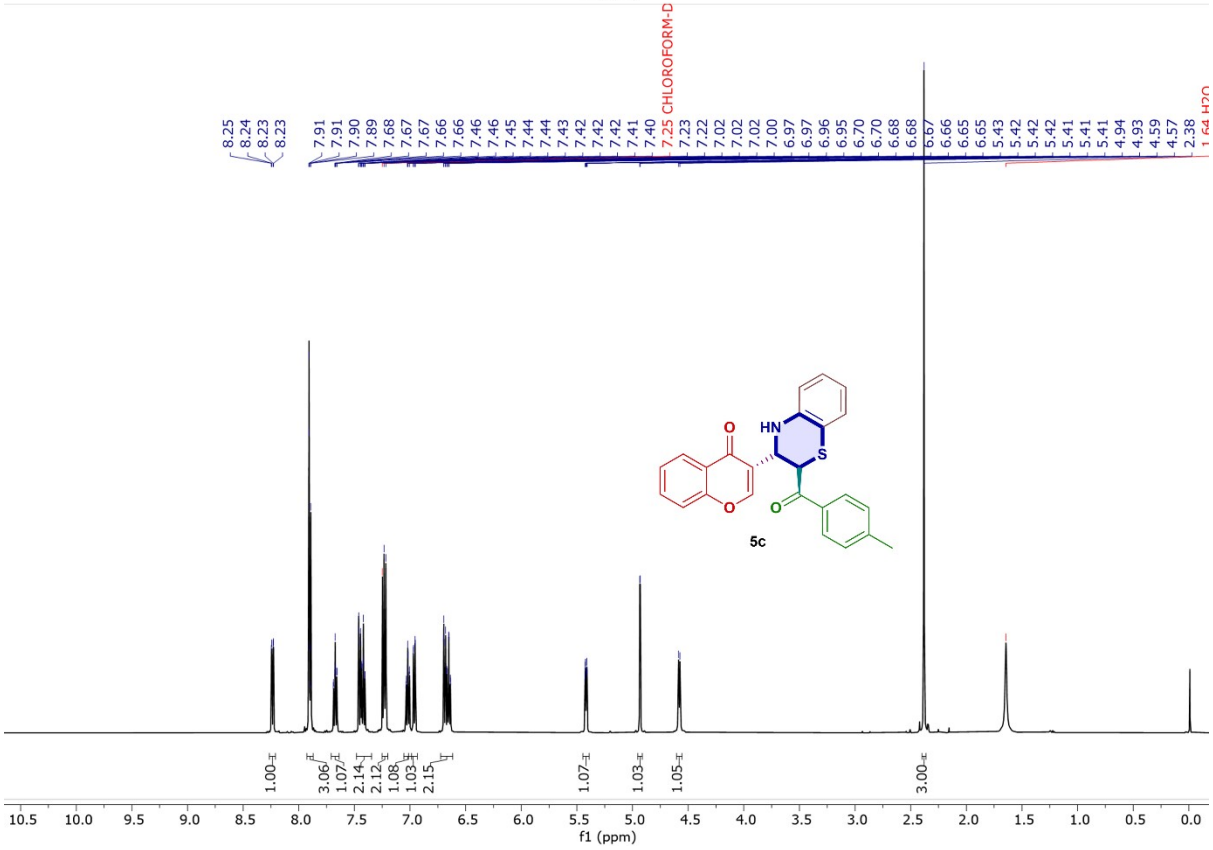
126.13
125.67
123.68
118.99
117.07
115.14
110.73
48.56
43.03
40.48 DMSO-D6
40.31 DMSO-D6
40.15 DMSO-D6
39.98 DMSO-D6
39.81 DMSO-D6
39.64 DMSO-D6
39.48 DMSO-D6
O
HN
S
O
O
Br
5b
f1 (ppm)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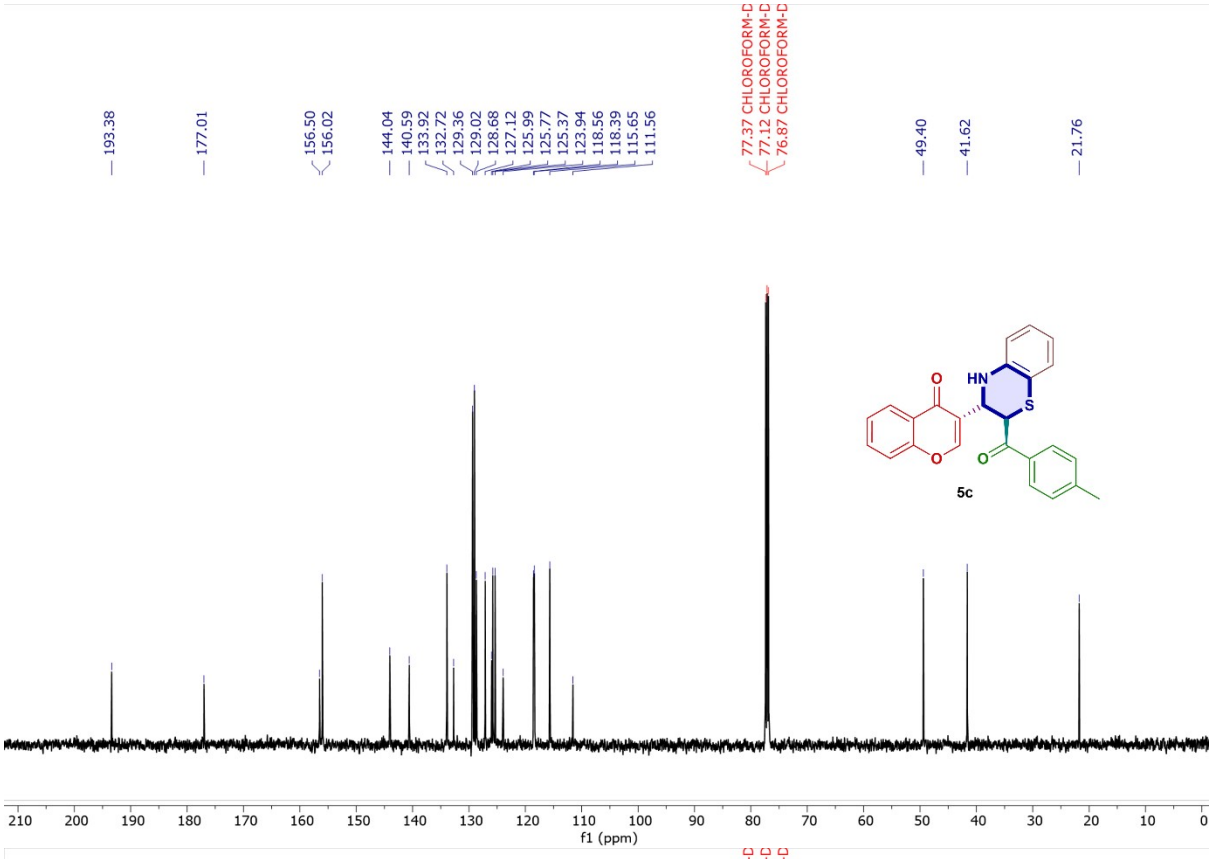
7.91
7.90
7.89
7.68
7.67
7.67
7.66
7.66
7.46
7.46
7.45
7.44
7.44
7.43
7.42
7.42
7.42
7.41
7.40
7.25 CHLOROFORM-D
7.23
7.22
7.02
7.02
7.02
7.00
6.97
6.97
6.96
6.95
6.70
6.70
6.68
6.68
6.67
6.66
6.65
6.65
5.43
5.42
5.42
5.42
5.41
5.41
5.41
4.94
4.93
4.59
4.57
2.38
1.64 H2O
1.00
3.06
1.07
2.14
2.12
1.08
1.03
2.15
1.07
1.03
1.05
3.00
O
HN
S
O
O
5c
f1 (ppm)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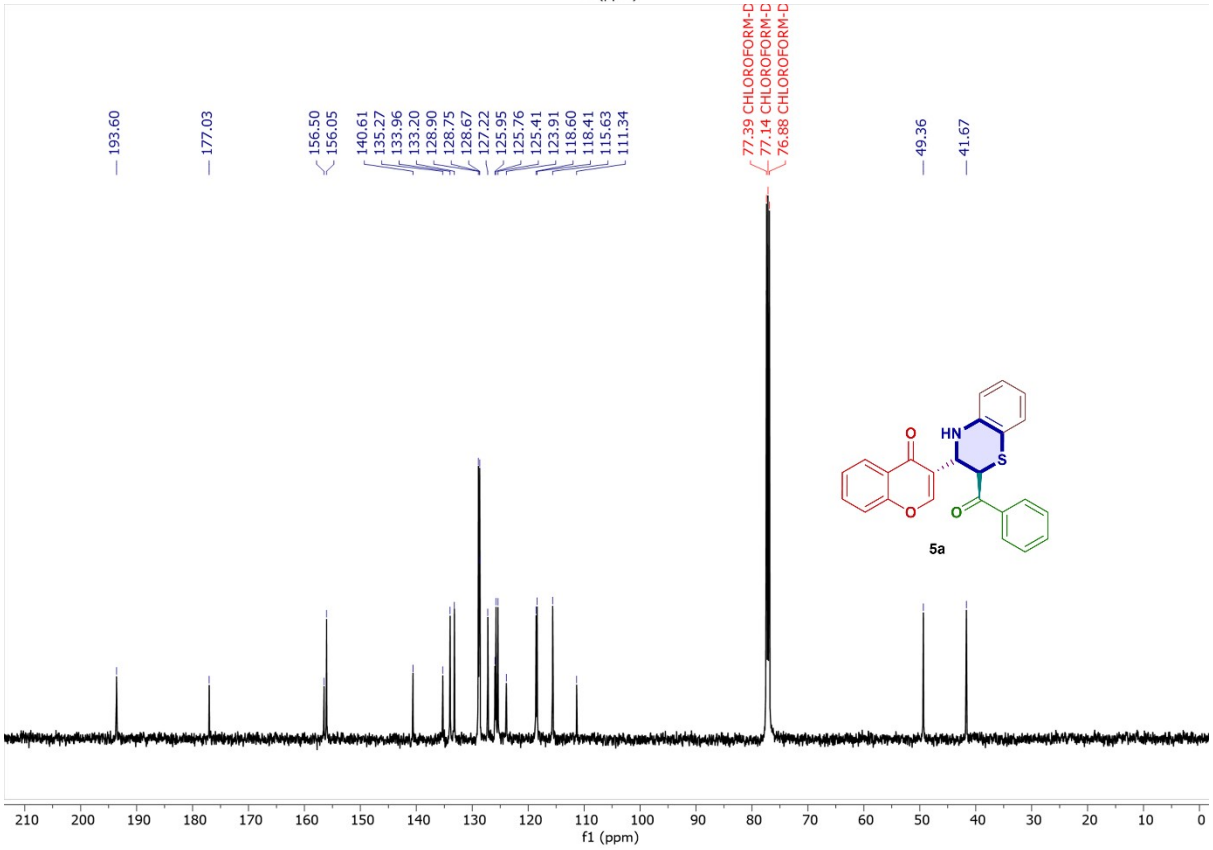
133.92
132.72
129.36
129.02
128.68
127.12
125.99
125.77
125.37
123.94
118.56
118.39
115.65
111.56
77.37 CHLOROFORM-D
77.12 CHLOROFORM-D
76.87 CHLOROFORM-D
49.40
41.62
21.76
HN
S
O
O
O
5c
f1 (ppm)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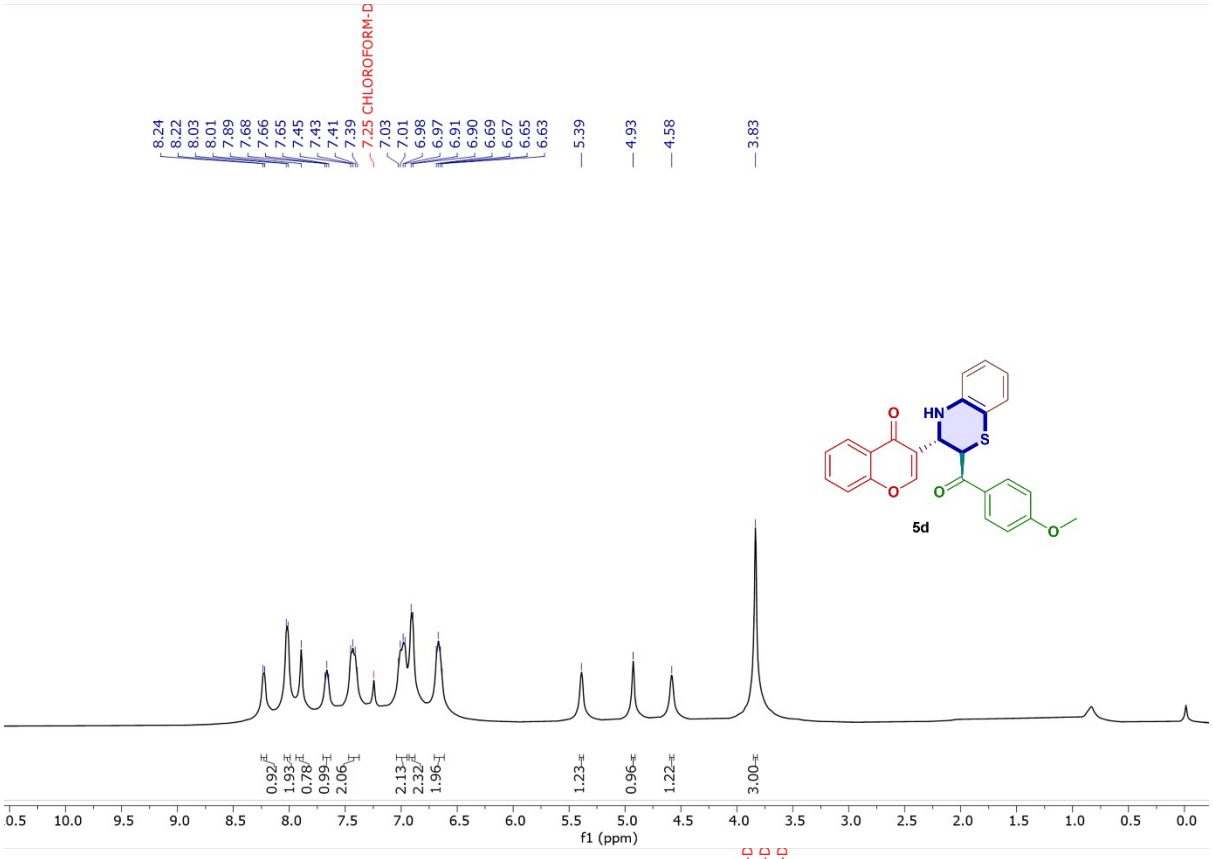
156.05
140.61
135.27
133.96
133.20
128.90
128.75
128.67
127.22
125.95
125.76
125.41
123.91
118.60
118.41
115.63
111.34
77.39 CHLOROFORM-D
77.14 CHLOROFORM-D
76.88 CHLOROFORM-D
49.36
41.67
HN
S
O
O
O
5a
f1 (ppm)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8.22
8.03
8.01
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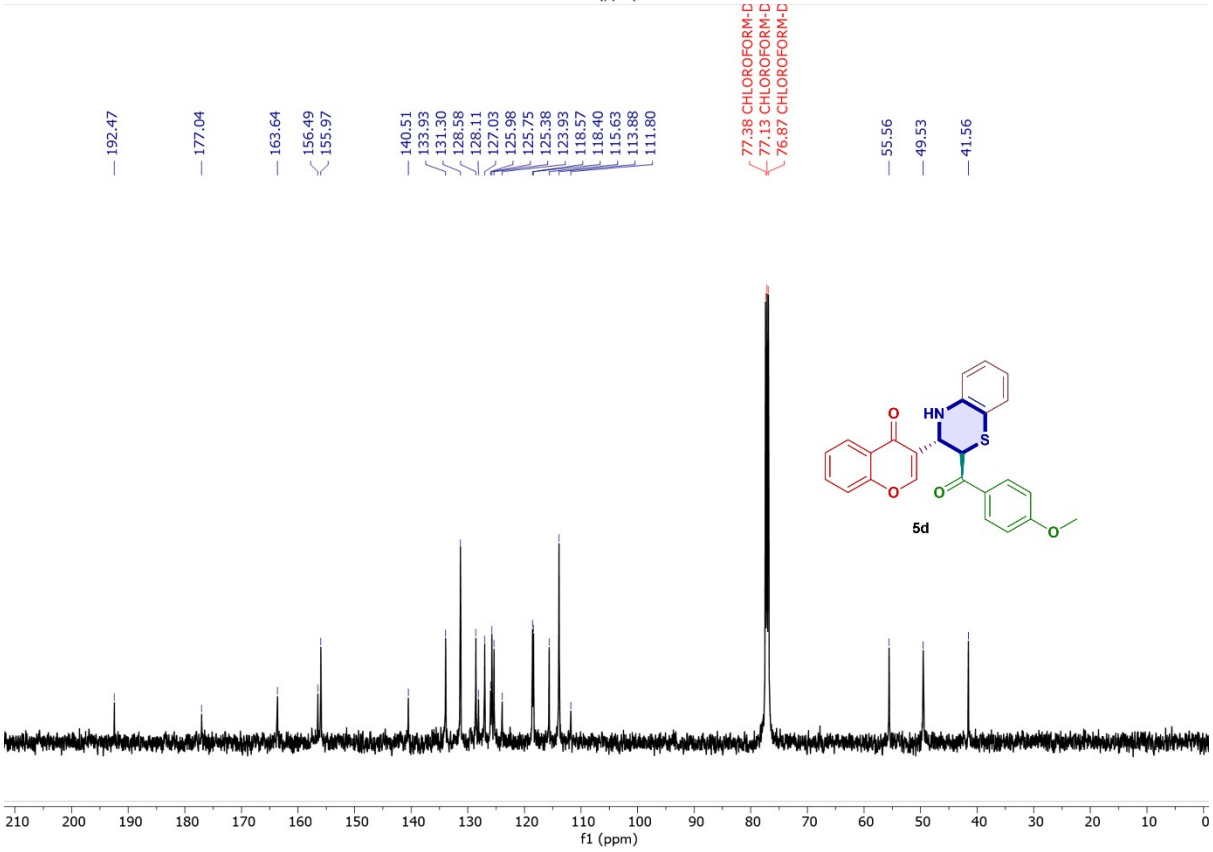
7.68
7.66
7.65
7.45
7.43
7.41
7.39
7.25 CHLOROFORM-D
7.03
7.01
6.98
6.97
6.91
6.90
6.69
6.67
6.65
6.63
5.39
4.93
4.58
3.83
HN
S
O
O
O
O
5d
0.92
1.93
0.78
0.99
2.06
2.13
2.32
1.96
1.23
0.96
1.22
3.00
f1 (ppm)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140.51
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131.30
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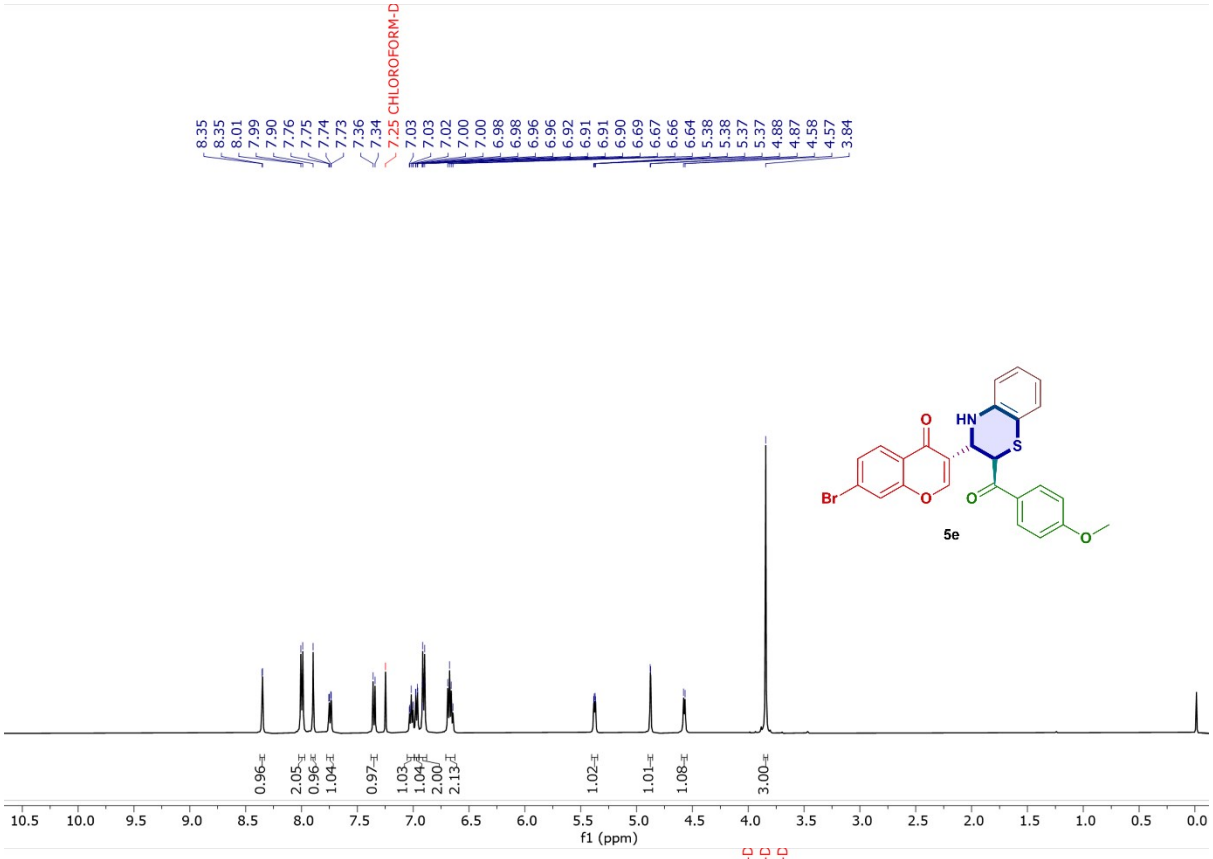
128.11
127.03
125.98
125.75
125.38
123.93
118.57
118.40
115.63
113.88
111.80
77.38 CHLOROFORM-D
77.13 CHLOROFORM-D
76.87 CHLOROFORM-D
55.56
49.53
41.56
HN
S
O
O
O
O
5d
f1 (ppm)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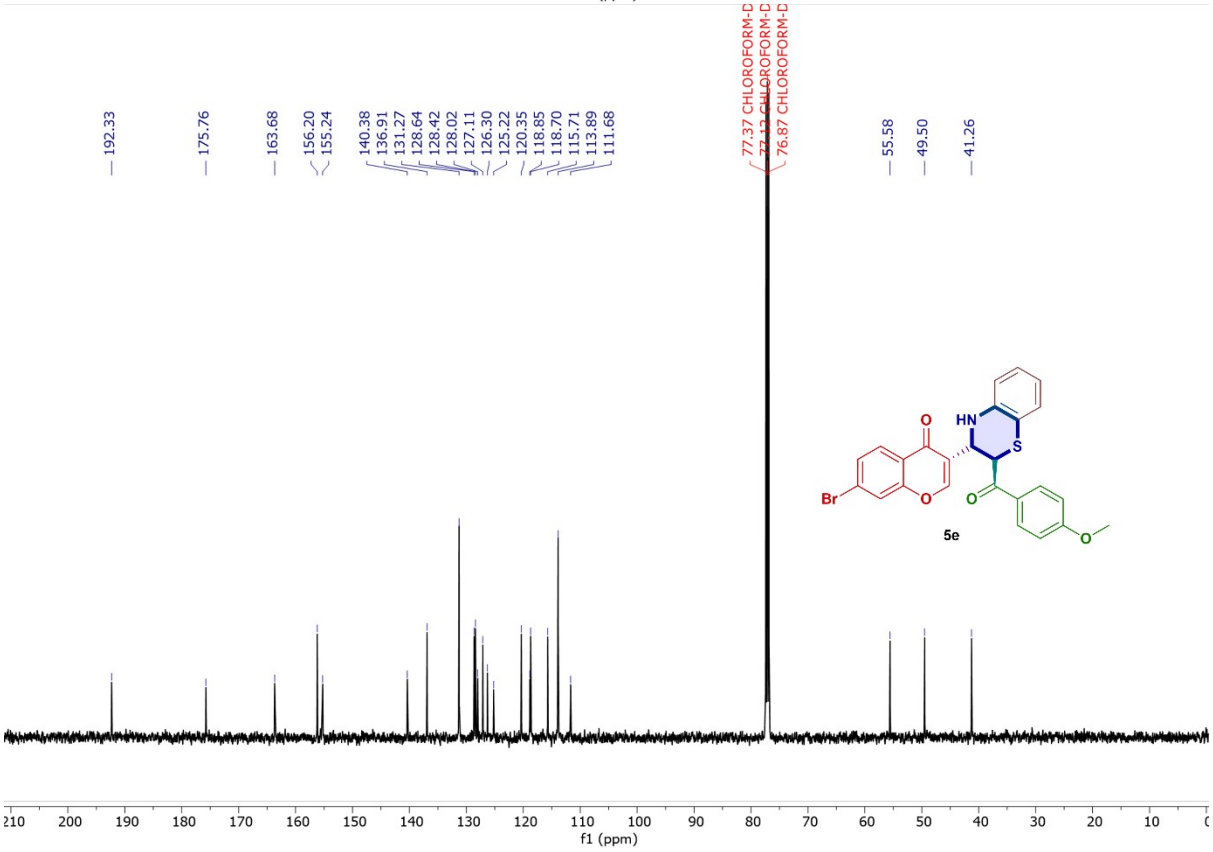
8.35
8.01
7.99
7.90
7.76
7.75
7.74
7.73
7.36
7.34
7.25 CHLOROFORM-D
7.03
7.03
7.02
7.00
7.00
6.98
6.98
6.96
6.96
6.92
6.91
6.91
6.90
6.69
6.67
6.66
6.64
5.38
5.38
5.37
5.37
4.88
4.87
4.58
4.57
3.84
0.96
2.05
0.96
1.04
0.97
1.03
1.04
2.00
2.13
1.02
1.01
1.08
3.00
f1 (ppm)
5e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175.76
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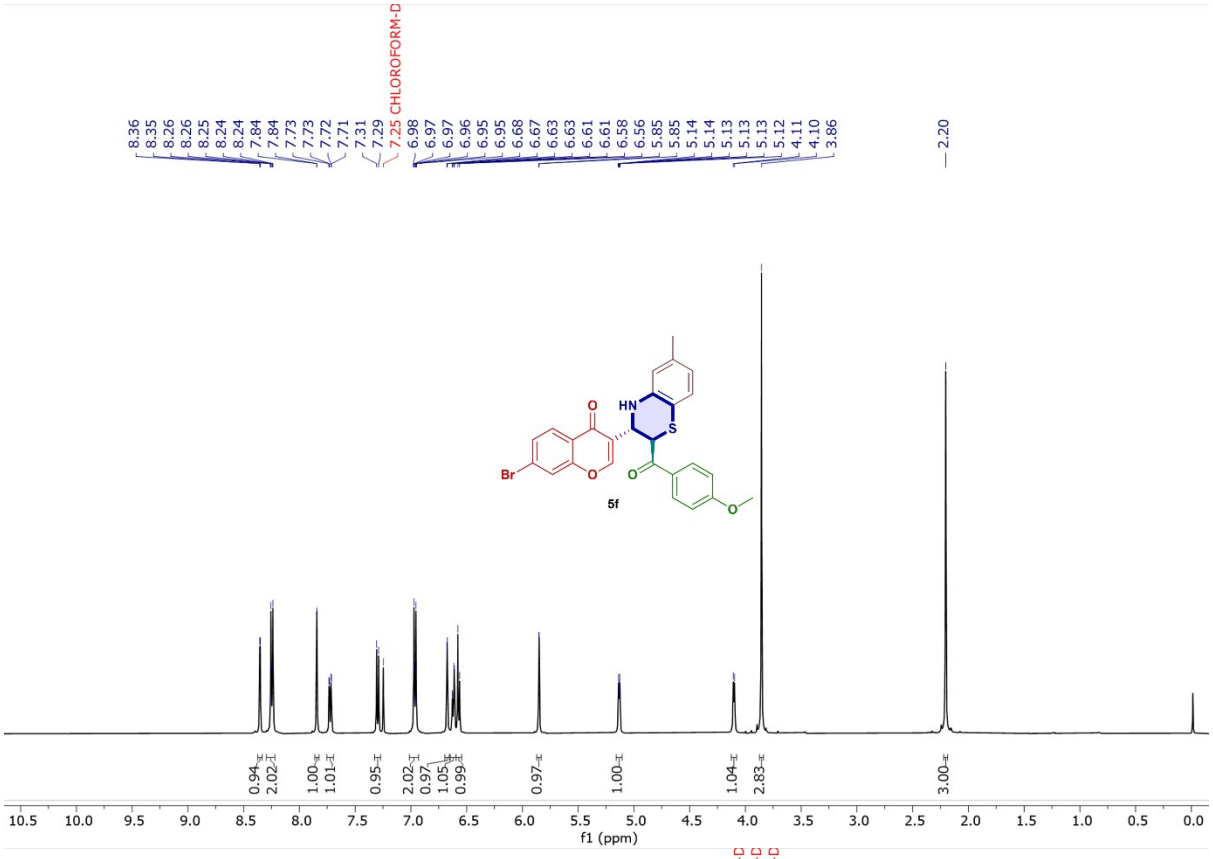
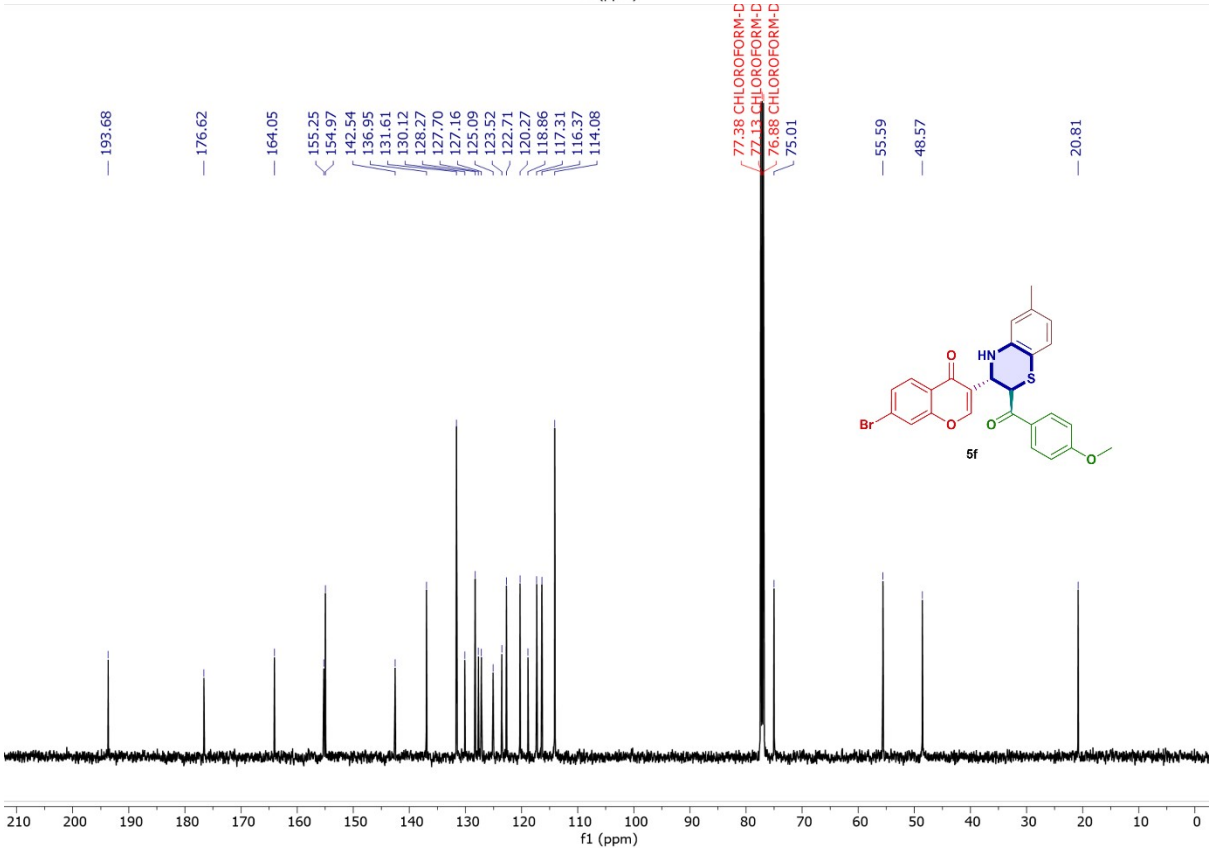
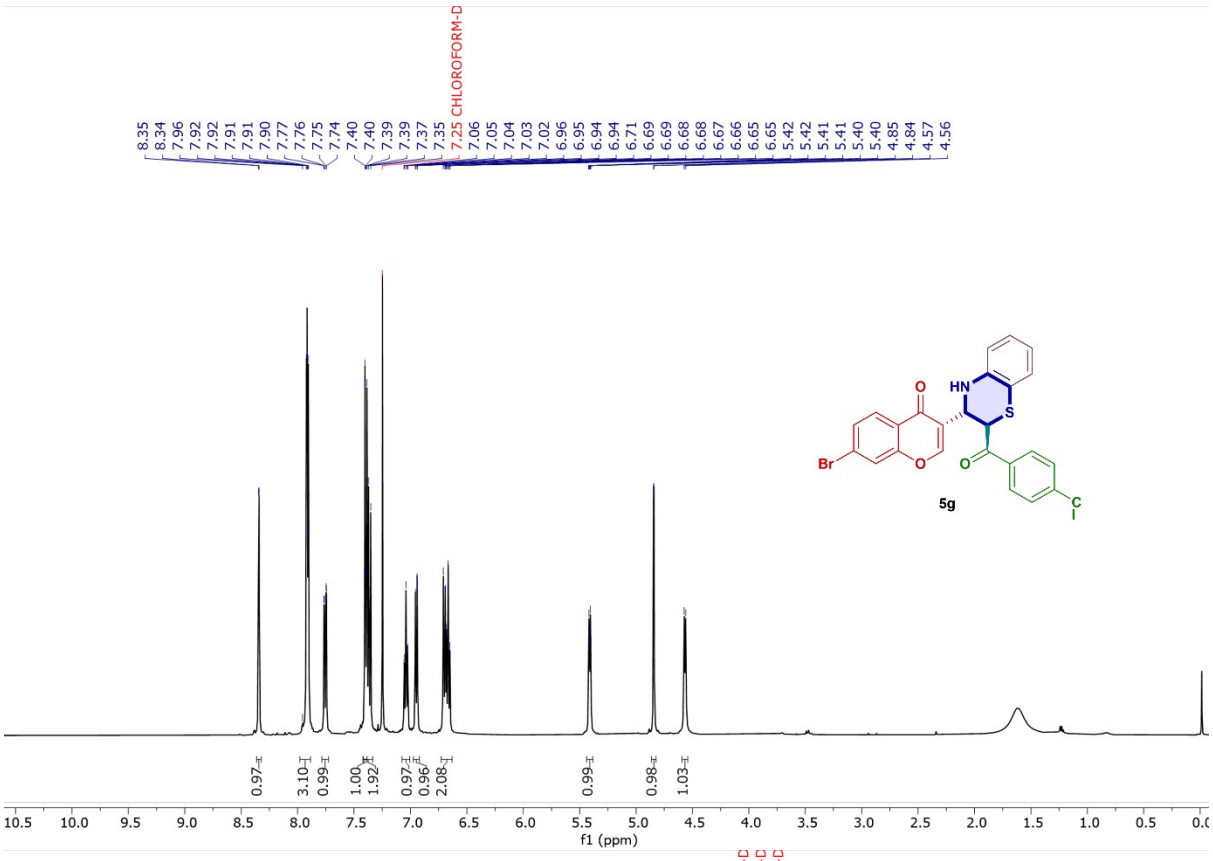
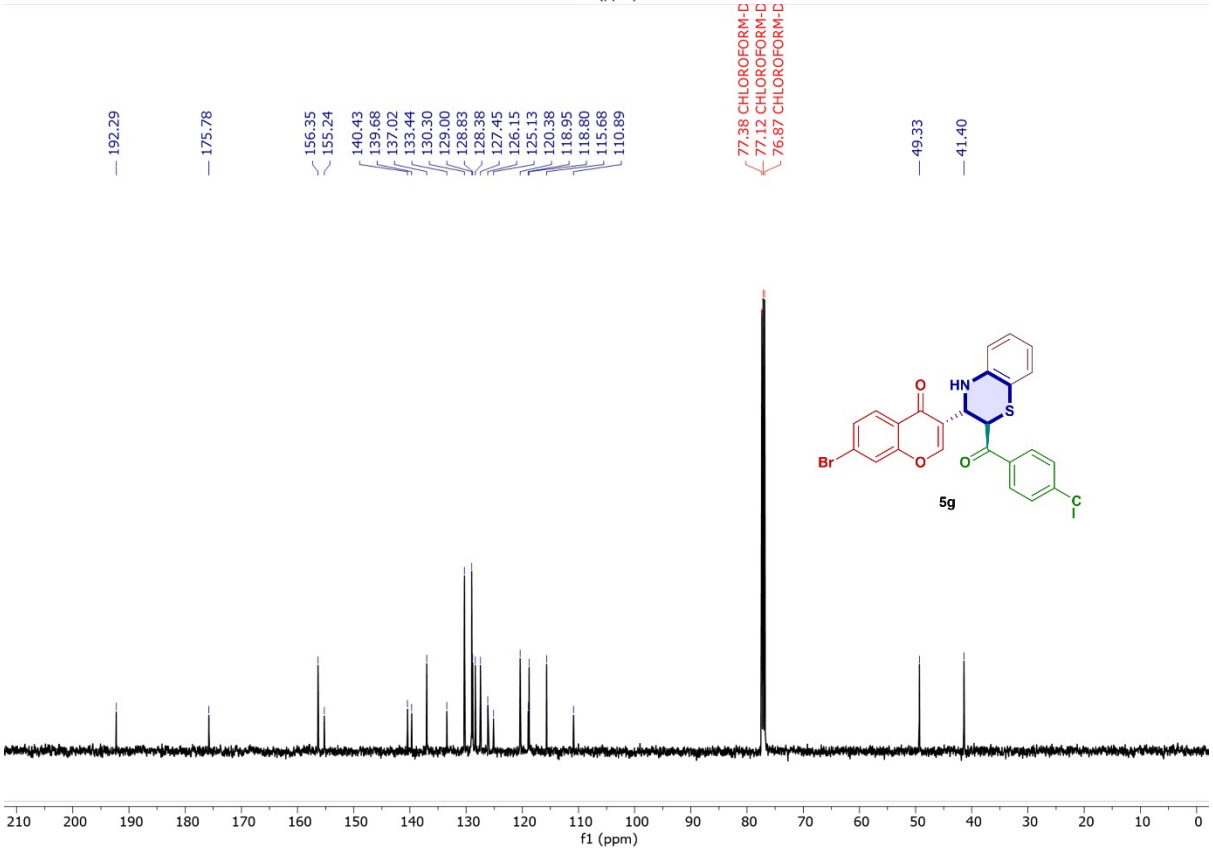
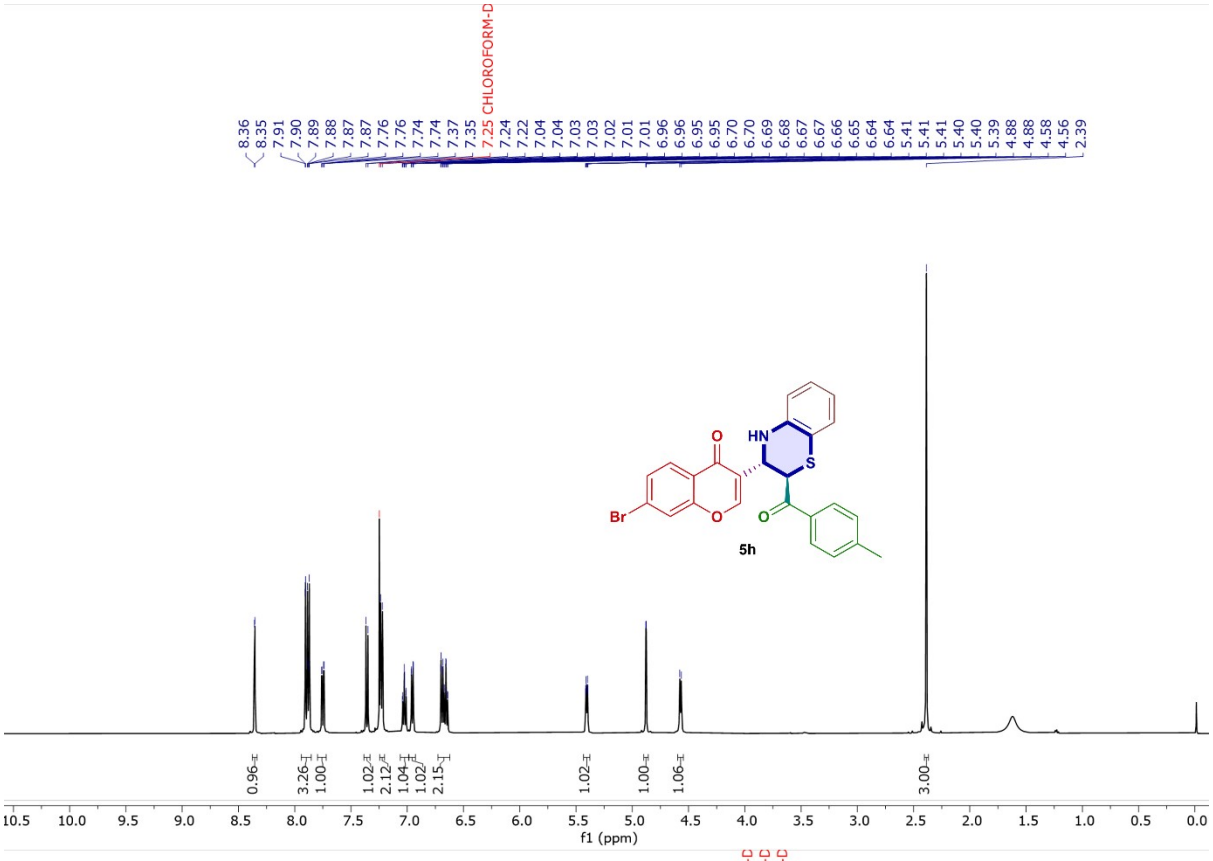
156.20
155.24
140.38
136.91
131.27
128.64
128.42
128.02
127.11
126.30
125.22
120.35
118.85
118.70
115.71
113.89
111.68
77.37 CHLOROFORM-D
77.13 CHLOROFORM-D
76.87 CHLOROFORM-D
55.58
49.50
41.26
f1 (ppm)
5e

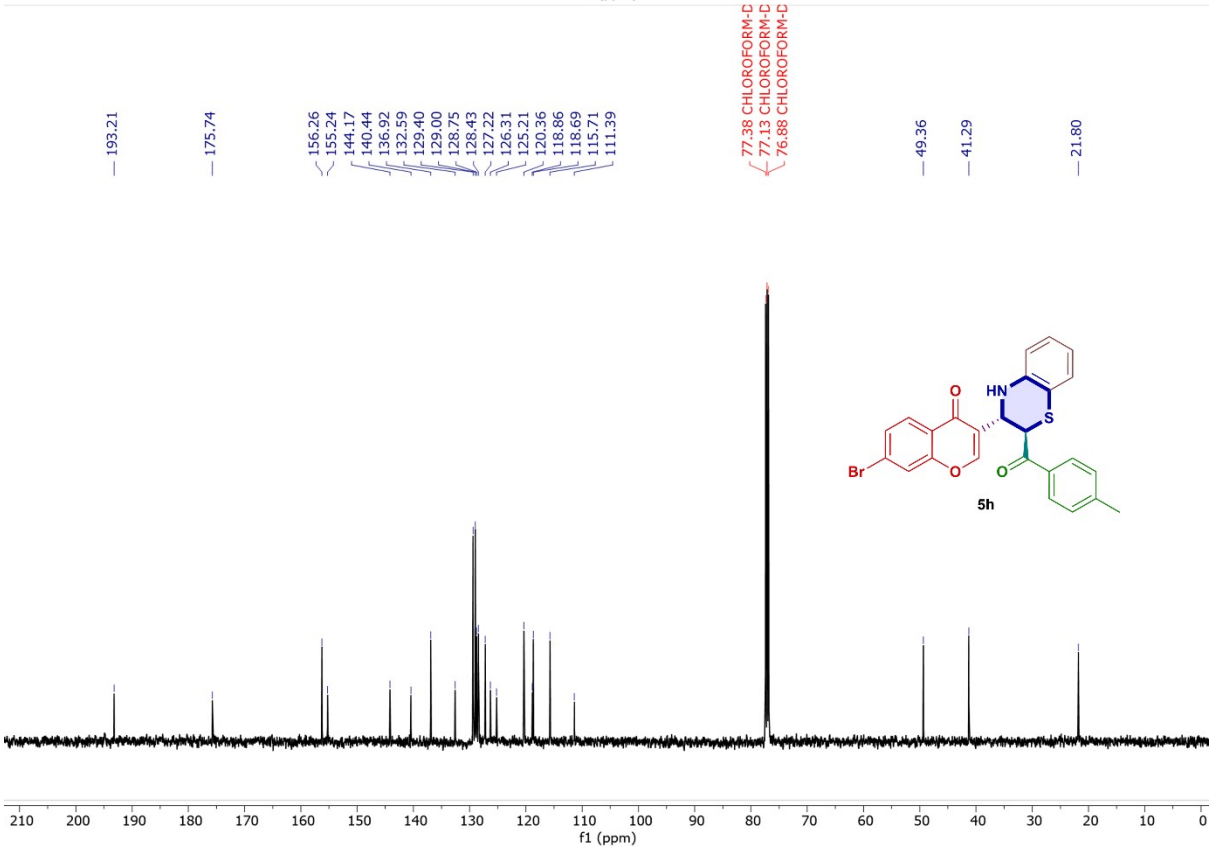

8.36
8.35
8.26
8.26
8.25
8.24
8.24
7.84
7.84
7.73
7.73
7.72
7.71
7.31
7.29
7.25 CHLOROFORM-D
6.98
6.97
6.97
6.96
6.95
6.95
6.68
6.67
6.63
6.63
6.61
6.61
6.58
6.56
5.85
5.85
5.14
5.14
5.13
5.13
5.13
5.12
4.11
4.10
3.86
2.20
0.94
2.02
1.00
1.01
0.95
2.02
0.97
1.05
0.99
0.97
1.00
1.04
2.83
3.00
f1 (ppm)

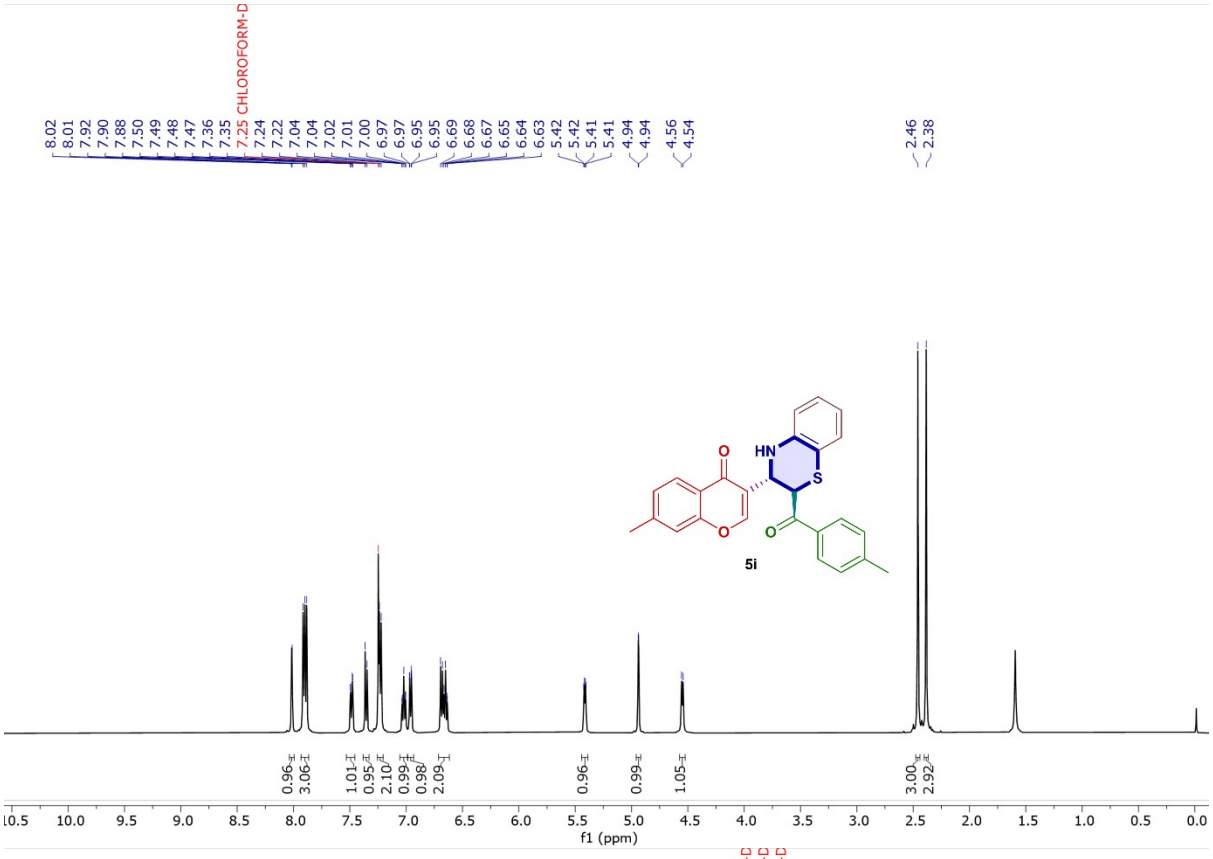

193.68
176.62
164.05
155.25
154.97
142.54
136.95
131.61
130.12
128.27
127.70
127.16
125.09
123.52
122.71
120.27
118.86
117.31
116.37
114.08
77.38 CHLOROFORM-D
77.13 CHLOROFORM-D
76.88 CHLOROFORM-D
75.01
55.59
48.57
20.81
f1 (ppm)

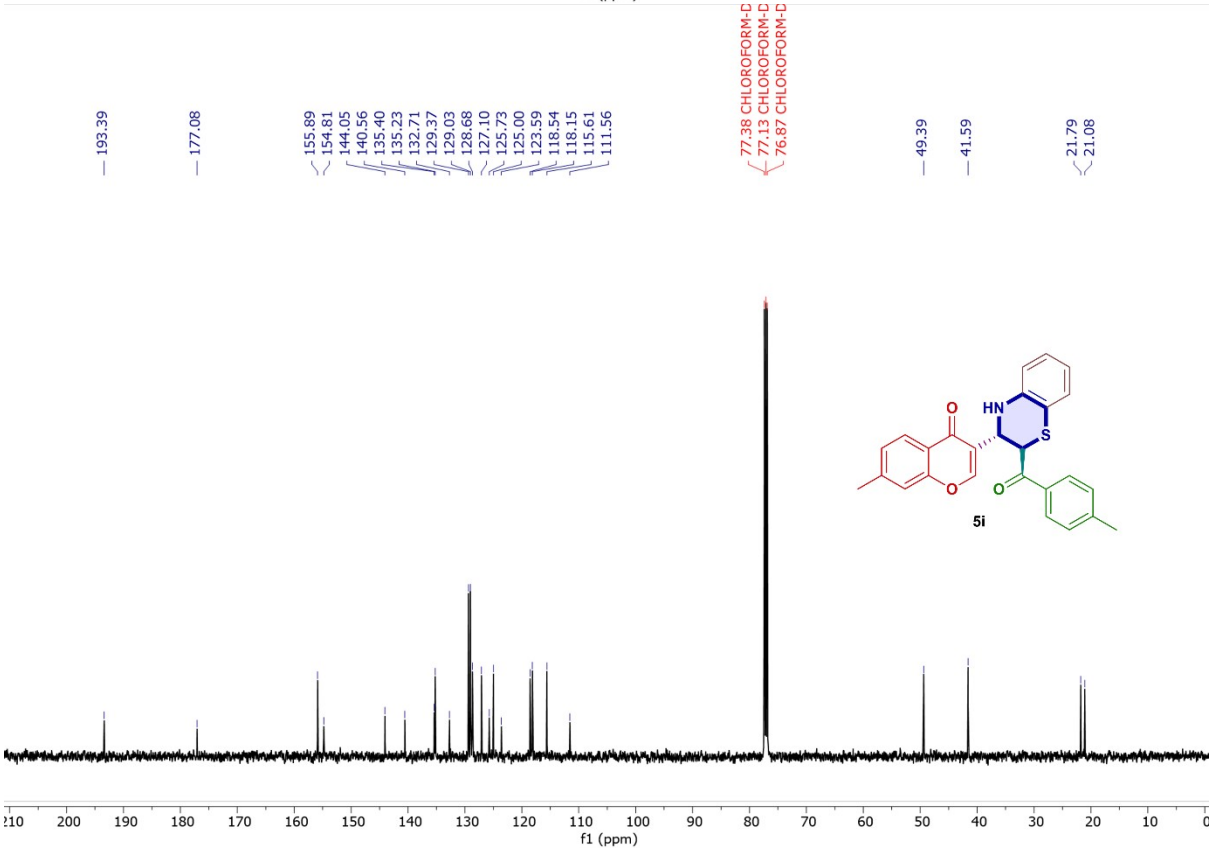

8.35
8.34
7.96
7.92
7.92
7.91
7.91
7.90
7.77
7.76
7.75
7.74
7.40
7.40
7.39
7.39
7.37
7.35
7.25 CHLOROFORM-D
7.06
7.05
7.04
7.03
7.02
6.96
6.95
6.94
6.94
6.71
6.69
6.69
6.68
6.68
6.67
6.66
6.65
6.65
5.42
5.42
5.41
5.41
5.40
5.40
4.85
4.84
4.57
4.56
0.97
3.10
0.99
1.00
1.92
0.97
0.96
2.08
0.99
0.98
1.03
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
O
HN
S
Br
O
O
5g

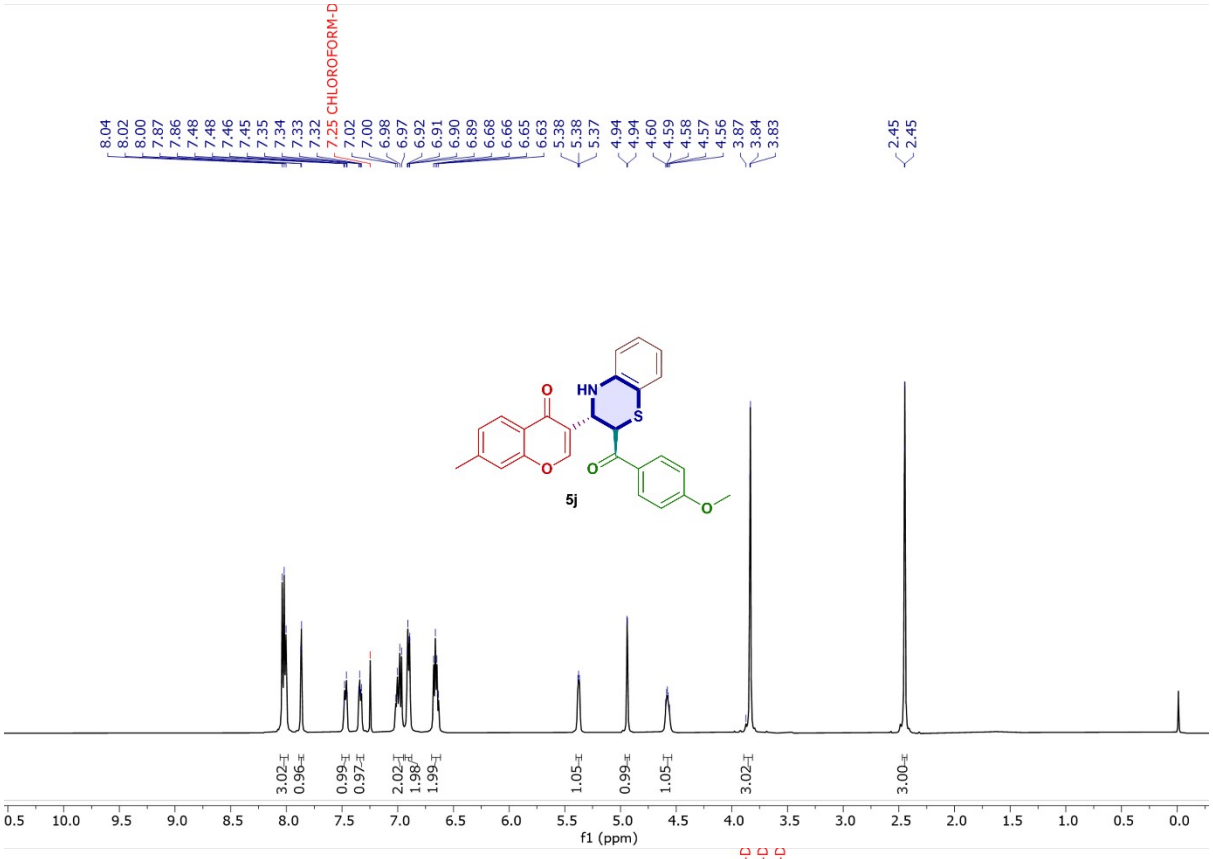

192.29
175.78
156.35
155.24
140.43
139.68
137.02
133.44
130.30
129.00
128.83
128.38
127.45
126.15
125.13
120.38
118.95
118.80
115.68
110.89
77.38 CHLOROFORM-D
77.12 CHLOROFORM-D
76.87 CHLOROFORM-D
49.33
41.40
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
O
HN
S
Br
O
O
5g

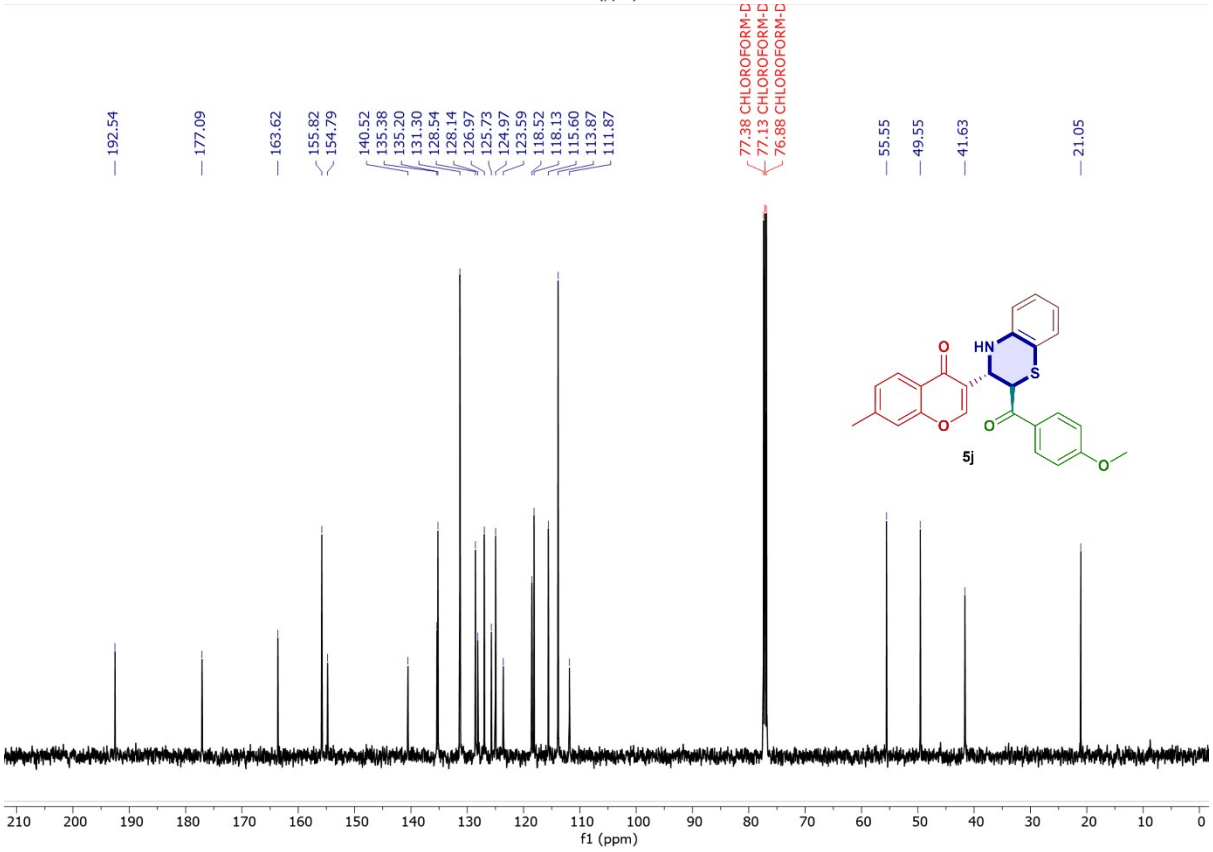

CHLOROFORM-D
8.36 8.35 7.91 7.90 7.89 7.88 7.87 7.87 7.87 7.76 7.76 7.74 7.74 7.37 7.35 7.25 7.24 7.22 7.04 7.04 7.03 7.03 7.02 7.01 7.01 6.96 6.96 6.95 6.95 6.70 6.70 6.69 6.68 6.67 6.67 6.66 6.65 6.64 6.64 5.41 5.41 5.41 5.40 5.40 5.39 4.88 4.88 4.58 4.56 2.39
HN
S
O
Br
O
O
5h
0.96 3.26 1.00 1.02 2.12 1.04 1.02 2.15 1.02 1.00 1.06 3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

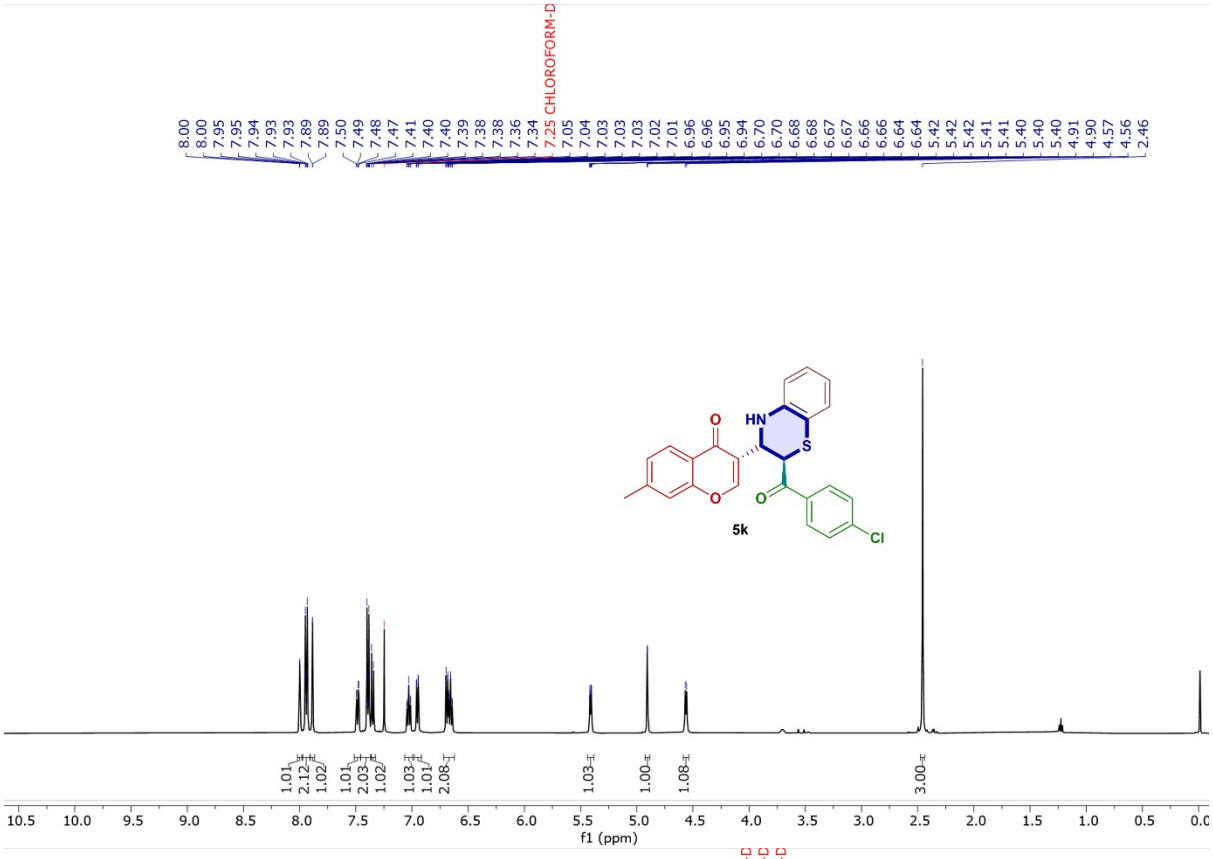

193.21
175.74
156.26 155.24 144.17 140.44 136.92 132.59 129.40 129.00 128.75 128.43 127.22 126.31 125.21 120.36 118.86 118.69 115.71 111.39
77.38 CHLOROFORM-D
77.13 CHLOROFORM-D
76.88 CHLOROFORM-D
49.36
41.29
21.80
HN
S
O
Br
O
O
5h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

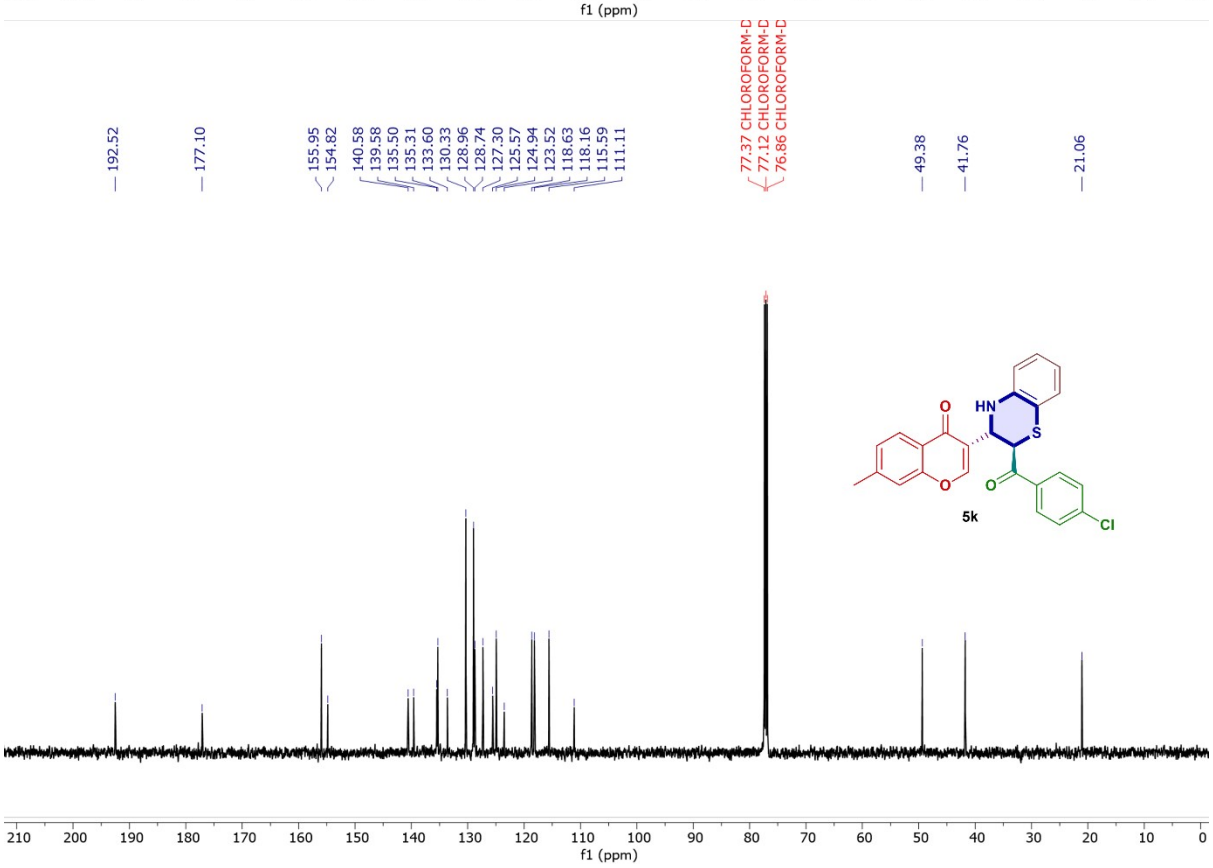

8.02
8.01
7.92
7.90
7.88
7.50
7.49
7.48
7.47
7.36
7.35
7.25 CHLOROFORM-D
7.24
7.22
7.04
7.04
7.02
7.01
7.00
6.97
6.97
6.95
6.95
6.69
6.68
6.67
6.65
6.64
6.63
5.42
5.42
5.41
5.41
4.94
4.94
4.56
4.54
2.46
2.38
HN
S
O
O
O
5i
0.96
3.06
1.01
0.95
2.10
0.99
0.98
2.09
0.96
0.99
1.05
3.00
2.92
f1 (ppm)

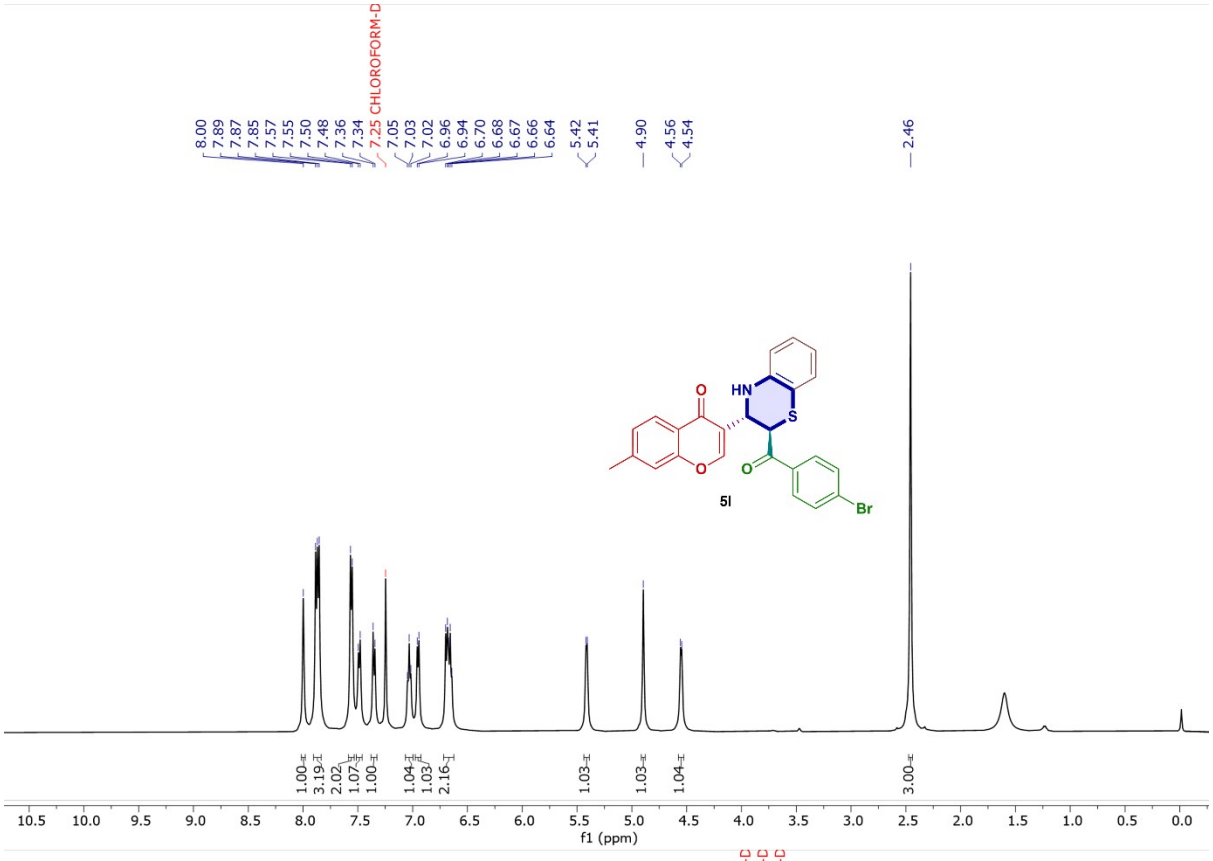

193.39
177.08
155.89
154.81
144.05
140.56
135.40
135.23
132.71
129.37
129.03
128.68
127.10
125.73
125.00
123.59
118.54
118.15
115.61
111.56
77.38 CHLOROFORM-D
77.13 CHLOROFORM-D
76.87 CHLOROFORM-D
49.39
41.59
21.79
21.08
HN
S
O
O
O
5i
f1 (ppm)

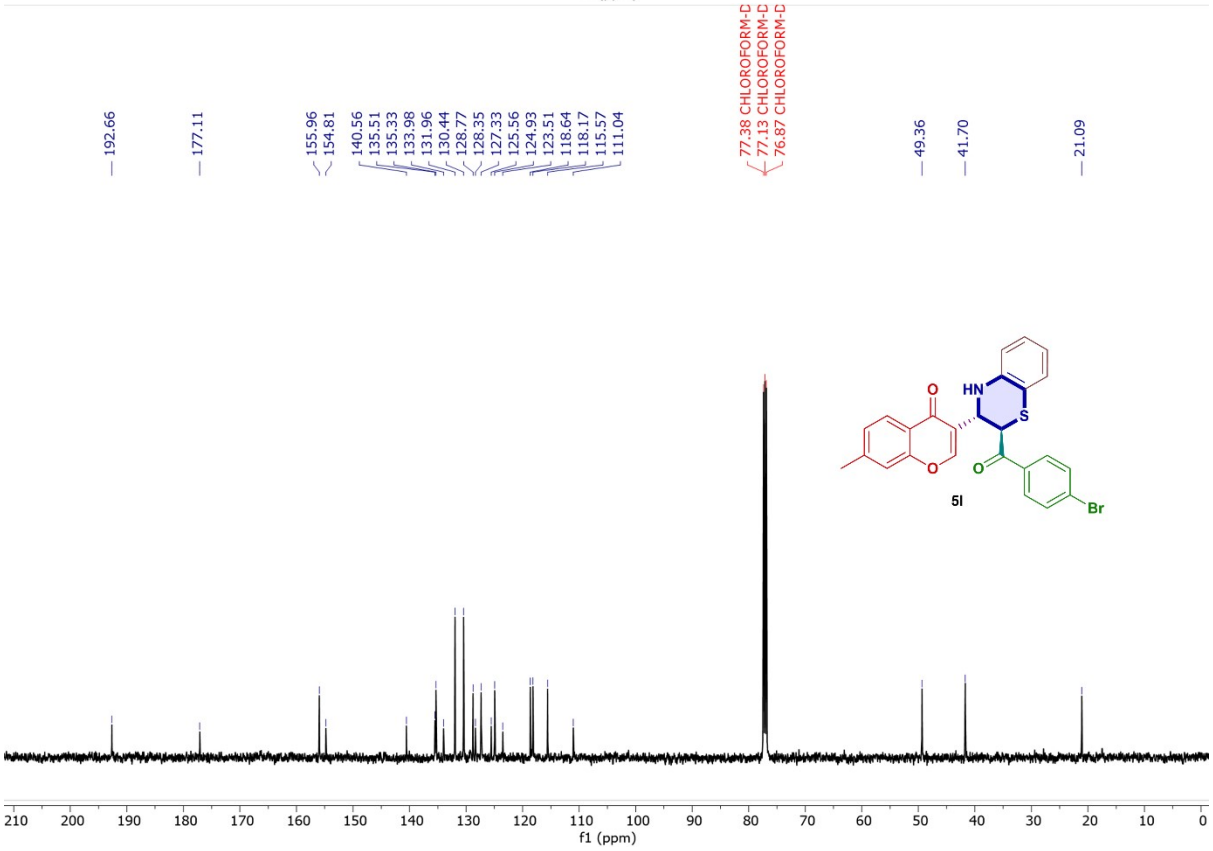

CHLOROFORM-D
8.04
8.02
8.00
7.87
7.86
7.48
7.48
7.46
7.45
7.35
7.34
7.33
7.32
7.25
7.02
7.00
6.98
6.97
6.92
6.91
6.90
6.89
6.68
6.66
6.65
6.63
5.38
5.38
5.37
4.94
4.94
4.60
4.59
4.58
4.57
4.56
3.87
3.84
3.83
2.45
2.45
HN
S
O
O
O
O
5j
3.02
0.96
0.99
0.97
2.02
1.98
1.99
1.05
0.99
1.05
3.02
3.00
f1 (ppm)

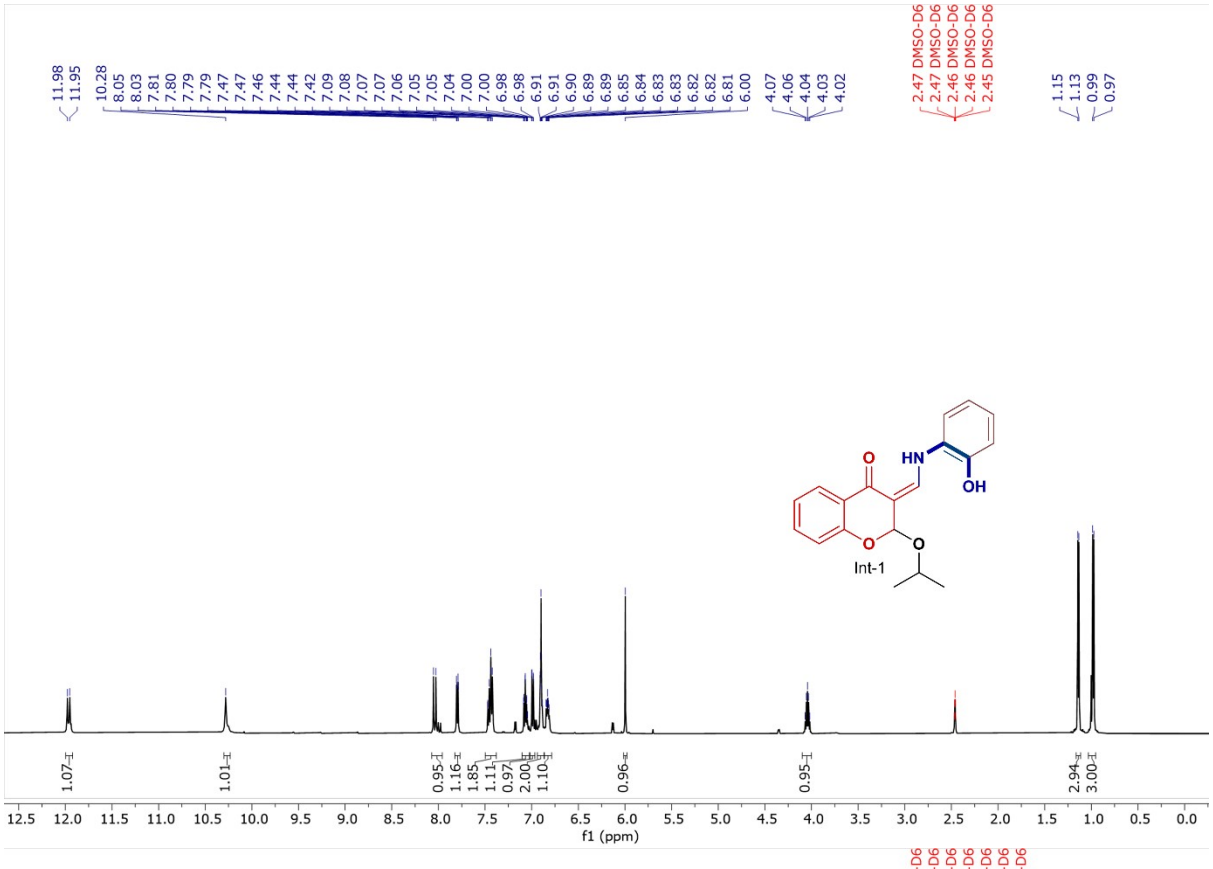

192.54
177.09
163.62
155.82
154.79
140.52
135.38
135.20
131.30
128.54
128.14
126.97
125.73
124.97
123.59
118.52
118.13
115.60
113.87
111.87
77.38 CHLOROFORM-D
77.13 CHLOROFORM-D
76.88 CHLOROFORM-D
55.55
49.55
41.63
21.05
HN
S
O
O
O
O
5j
f1 (ppm)

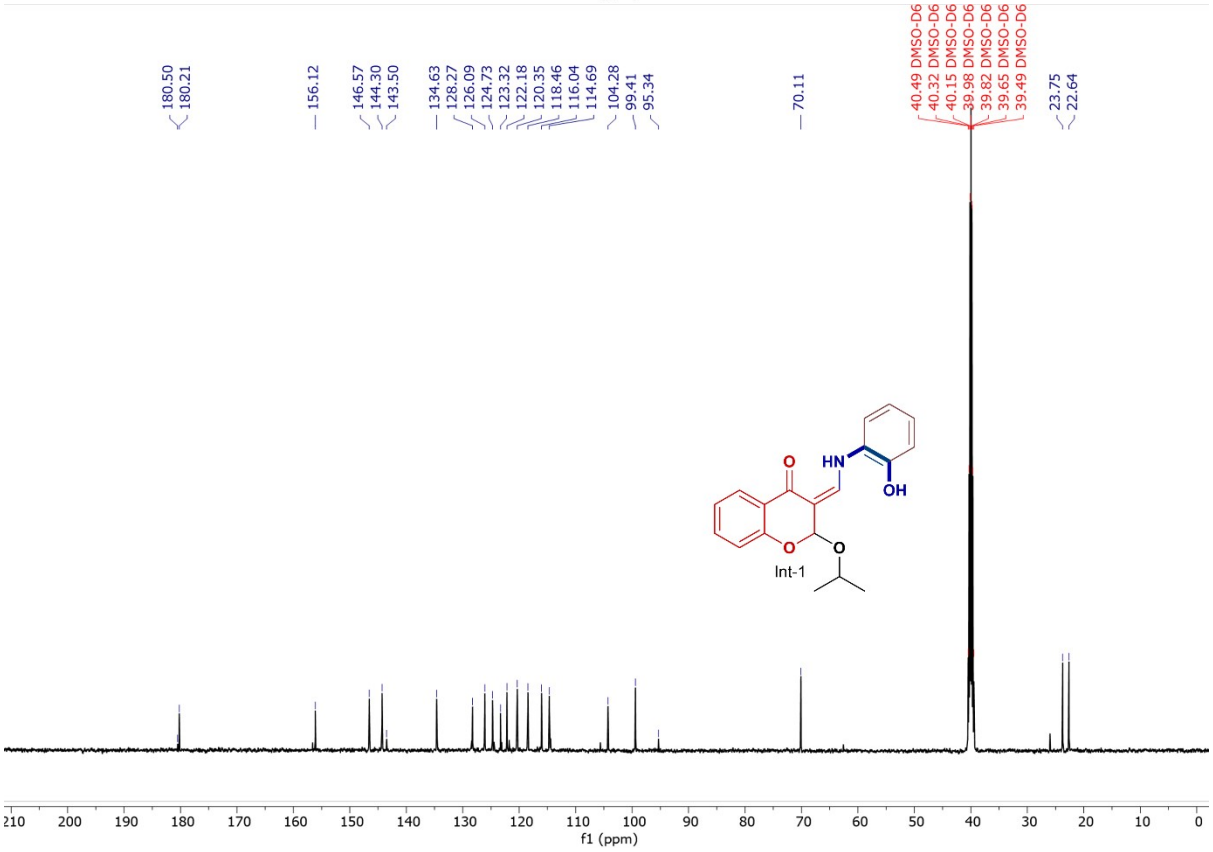

8.00
8.00
7.95
7.95
7.94
7.93
7.93
7.89
7.89
7.50
7.49
7.48
7.47
7.41
7.40
7.40
7.39
7.38
7.38
7.36
7.34
7.25 CHLOROFORM-D
7.05
7.04
7.03
7.03
7.03
7.02
7.01
6.96
6.96
6.95
6.94
6.70
6.70
6.68
6.68
6.67
6.67
6.66
6.66
6.64
6.64
5.42
5.42
5.42
5.41
5.41
5.40
5.40
5.40
4.91
4.90
4.57
4.56
2.46
O
HN
S
O
O
Cl
5k
1.01
2.12
1.02
1.01
2.03
1.02
1.03
1.01
2.08
1.03
1.00
1.08
3.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

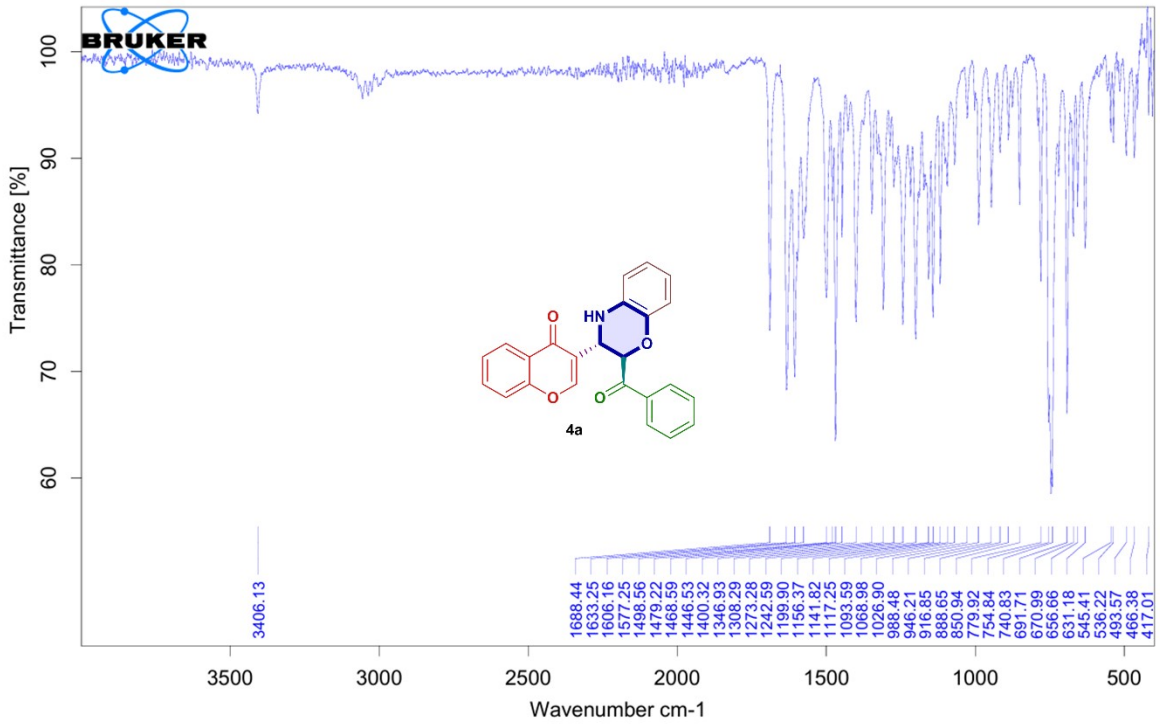

192.52
177.10
155.95
154.82
140.58
139.58
135.50
135.31
133.60
130.33
128.96
128.74
127.30
125.57
124.94
123.52
118.63
118.16
115.59
111.11
77.37 CHLOROFORM-D
77.12 CHLOROFORM-D
76.86 CHLOROFORM-D
49.38
41.76
21.06
O
HN
S
O
O
Cl
5k
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

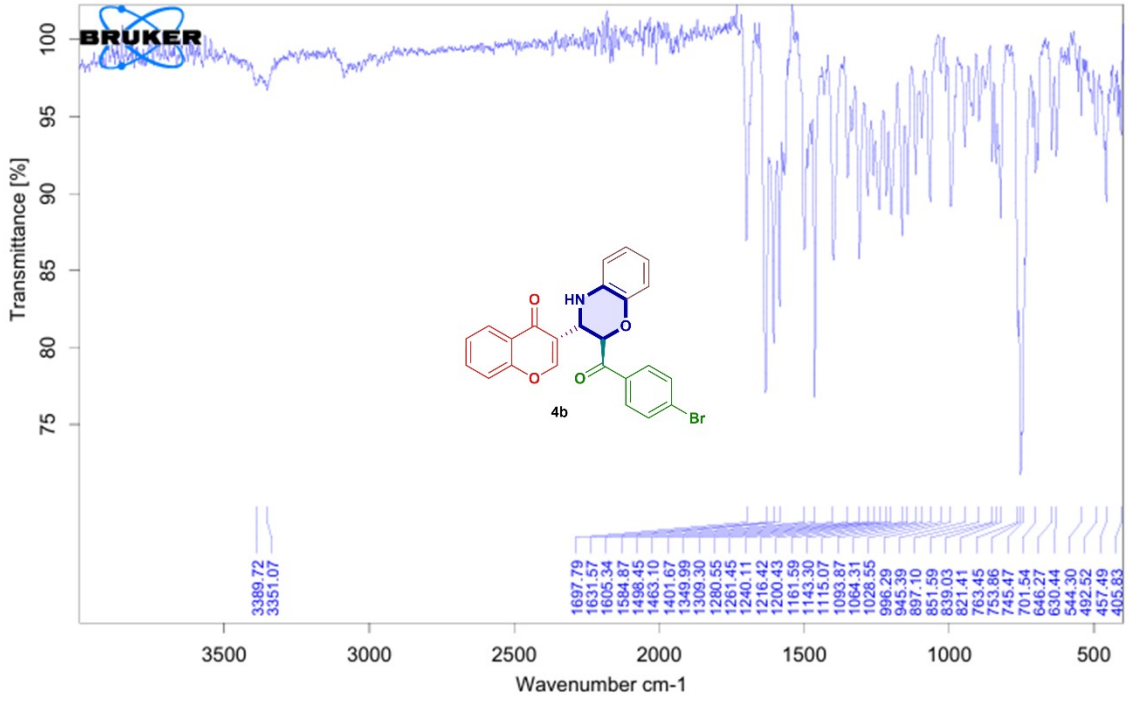

8.00
7.89
7.87
7.85
7.57
7.55
7.50
7.48
7.36
7.34
7.25 CHLOROFORM-D
7.05
7.03
7.02
6.96
6.94
6.70
6.68
6.67
6.66
6.64
5.42
5.41
4.90
4.56
4.54
2.46
1.00
3.19
2.02
1.07
1.00
1.04
1.03
2.16
1.03
1.03
1.04
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
HN
S
O
O
O
Br
5l

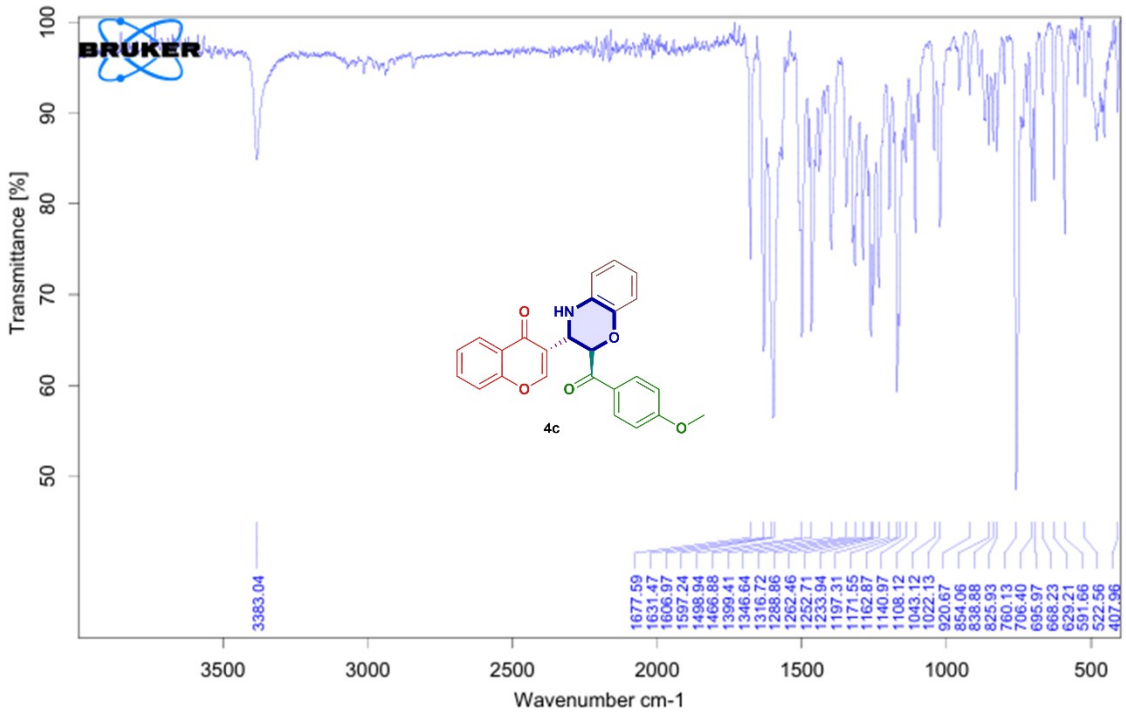

192.66
177.11
155.96
154.81
140.56
135.51
135.33
133.98
131.96
130.44
128.77
128.35
127.33
125.56
124.93
123.51
118.64
118.17
115.57
111.04
77.38 CHLOROFORM-D
77.13 CHLOROFORM-D
76.87 CHLOROFORM-D
49.36
41.70
21.09
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
HN
S
O
O
O
Br
5l

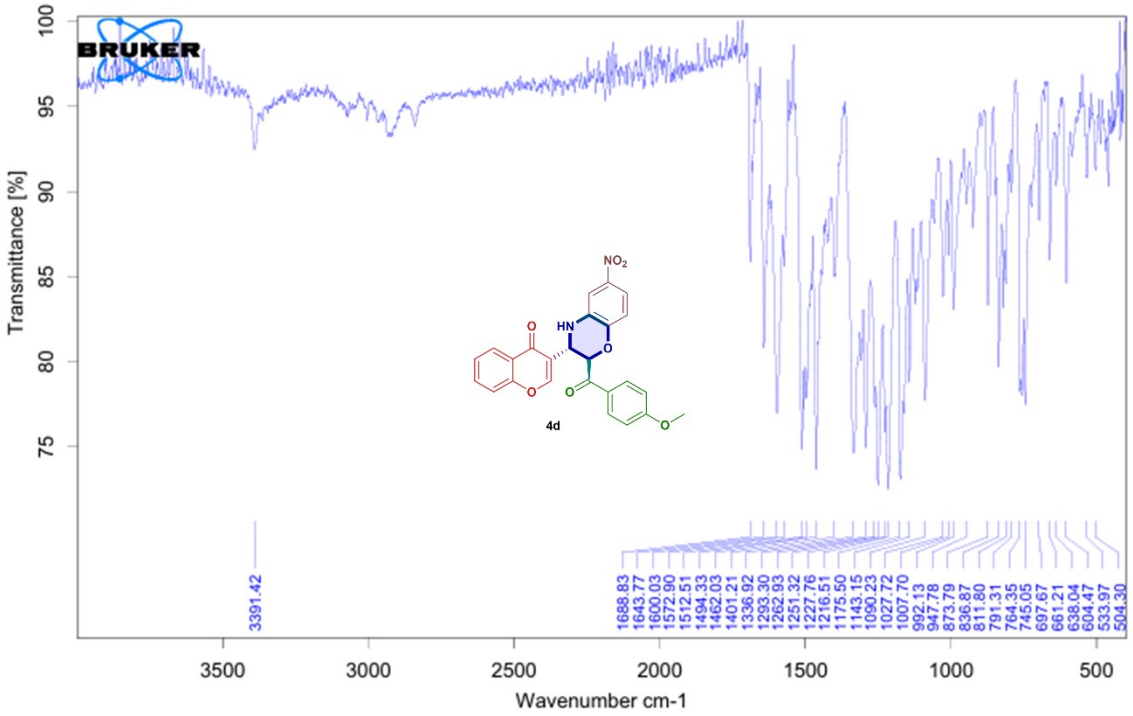

11.98
11.95
10.28
8.05
8.03
7.81
7.80
7.79
7.79
7.47
7.47
7.46
7.44
7.44
7.42
7.09
7.08
7.07
7.07
7.06
7.05
7.05
7.04
7.00
7.00
6.98
6.98
6.91
6.91
6.90
6.89
6.89
6.85
6.84
6.83
6.83
6.82
6.82
6.81
6.00
4.07
4.06
4.04
4.03
4.02
2.47 DMSO-D6
2.47 DMSO-D6
2.46 DMSO-D6
2.46 DMSO-D6
2.46 DMSO-D6
2.45 DMSO-D6
1.15
1.13
0.99
0.97
O
HN
OH
O
O
Int-1
1.07
1.01
0.95
1.16
1.85
1.11
0.97
2.00
1.10
0.96
0.95
2.94
3.00
f1 (ppm)


180.50
180.21
156.12
146.57
144.30
143.50
134.63
128.27
126.09
124.73
123.32
122.18
120.35
118.46
116.04
114.69
104.28
99.41
95.34
70.11
40.49 DMSO-D6
40.32 DMSO-D6
40.15 DMSO-D6
39.98 DMSO-D6
39.82 DMSO-D6
39.65 DMSO-D6
39.49 DMSO-D6
23.75
22.64
O
HN
OH
O
O
Int-1
f1 (ppm)


BRUKER
Transmittance [%]
100
90
80
70
60
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
4a
3406.13
1688.44
1633.25
1606.16
1577.25
1498.56
1479.22
1468.59
1446.53
1400.32
1346.93
1308.29
1273.28
1242.59
1199.90
1156.37
1141.82
1117.25
1093.59
1068.98
1026.90
988.48
946.21
916.85
888.65
850.94
779.92
754.84
740.83
691.71
670.99
656.66
631.18
545.41
536.22
493.57
466.38
417.01


BRUKER
Transmittance [%]
100
95
90
85
80
75
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
4b
Br
3389.72
3351.07
1697.79
1631.57
1605.34
1584.87
1498.45
1463.10
1401.67
1349.99
1309.30
1280.55
1261.45
1240.11
1216.42
1200.43
1161.59
1143.30
1115.07
1093.87
1064.31
1028.55
996.29
945.39
897.10
851.59
839.03
821.41
763.45
753.86
745.47
701.54
646.27
630.44
544.30
492.52
457.49
405.83


BRUKER
Transmittance [%]
100
90
80
70
60
50
3383.04
1677.59
1631.47
1606.97
1597.24
1498.94
1466.88
1399.41
1346.64
1316.72
1288.86
1262.46
1252.71
1233.94
1197.31
1171.55
1162.87
1140.97
1108.12
1043.12
1022.13
920.67
854.06
838.88
825.93
760.13
706.40
695.97
668.23
629.21
591.66
522.56
407.96
O
HN
O
O
O
4c
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1


BRUKER
Transmittance [%]
100
95
90
85
80
75
3391.42
1688.83
1643.77
1600.03
1572.90
1512.51
1494.33
1462.03
1401.21
1336.92
1293.30
1262.93
1251.32
1227.76
1216.51
1175.50
1143.15
1090.23
1027.72
1007.70
992.13
947.78
873.79
836.87
811.80
791.31
764.35
745.05
697.67
661.21
638.04
604.47
533.97
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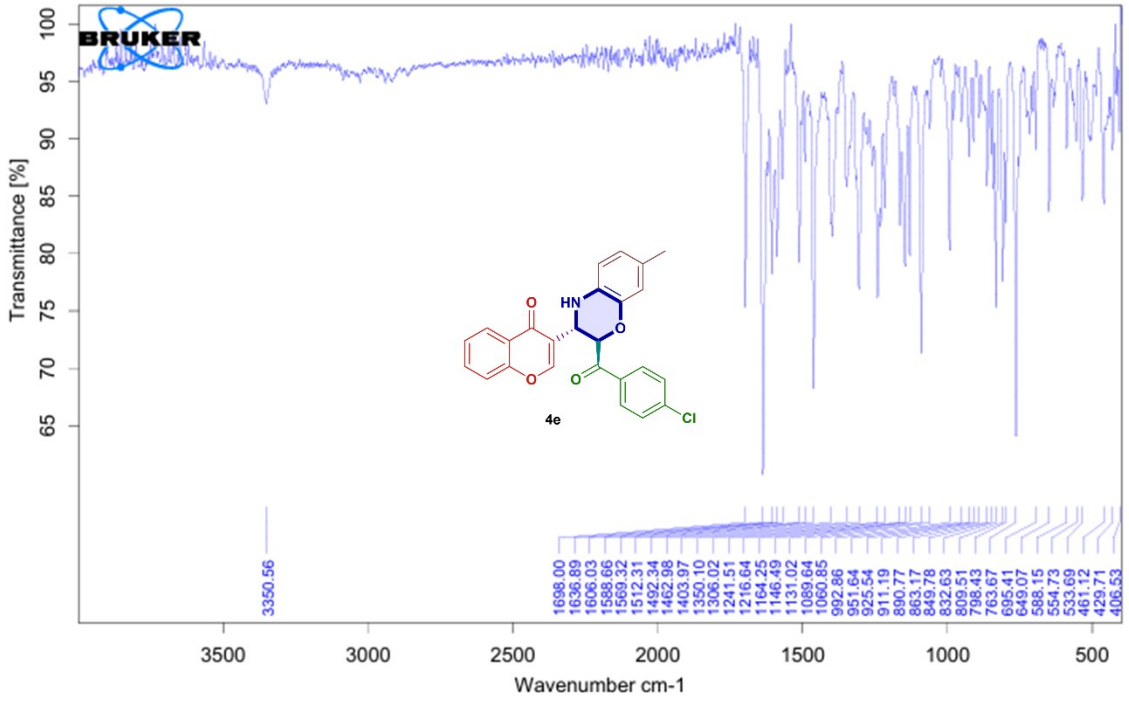
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4e
Cl
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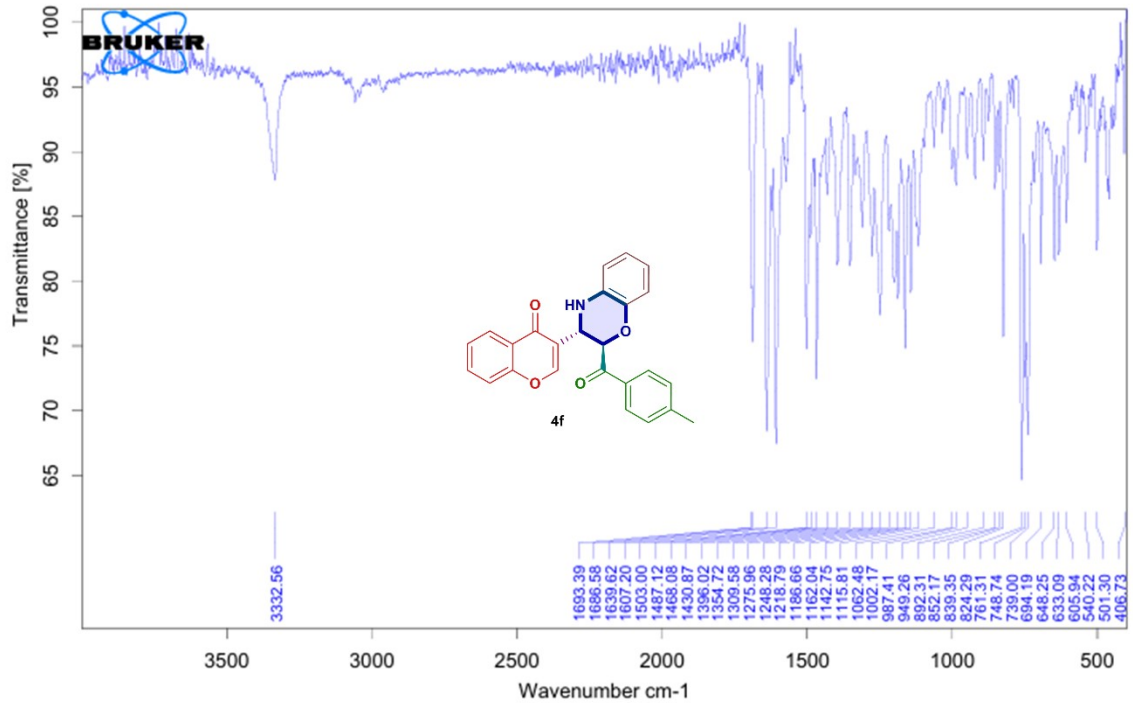
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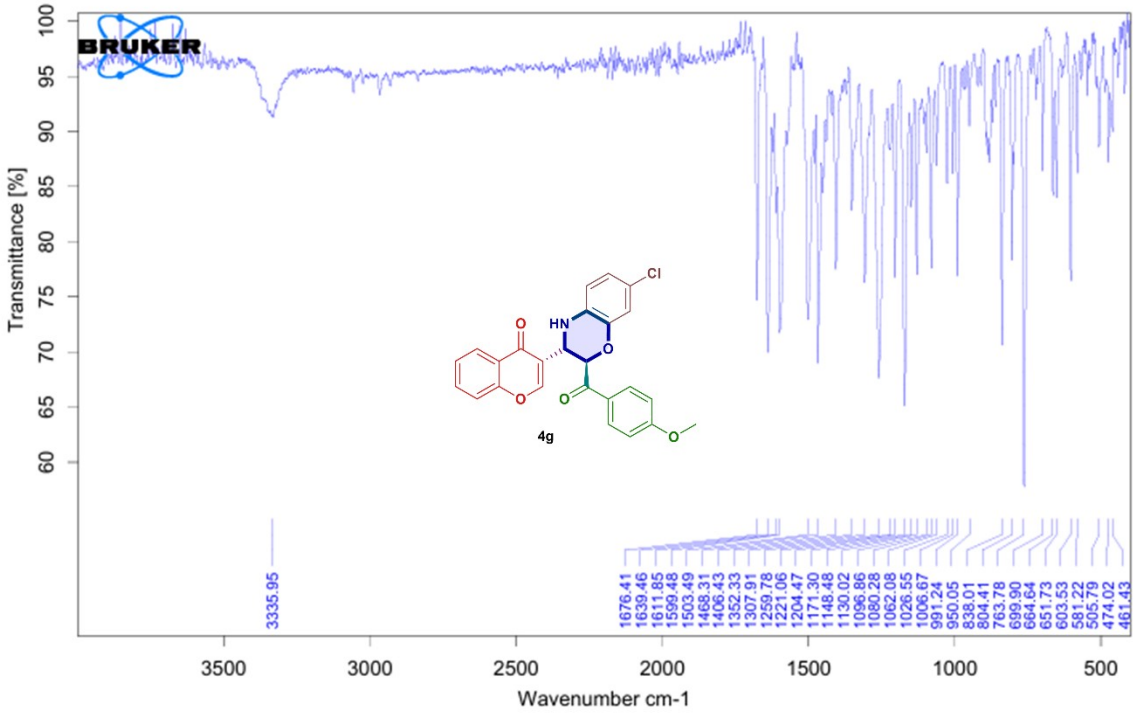
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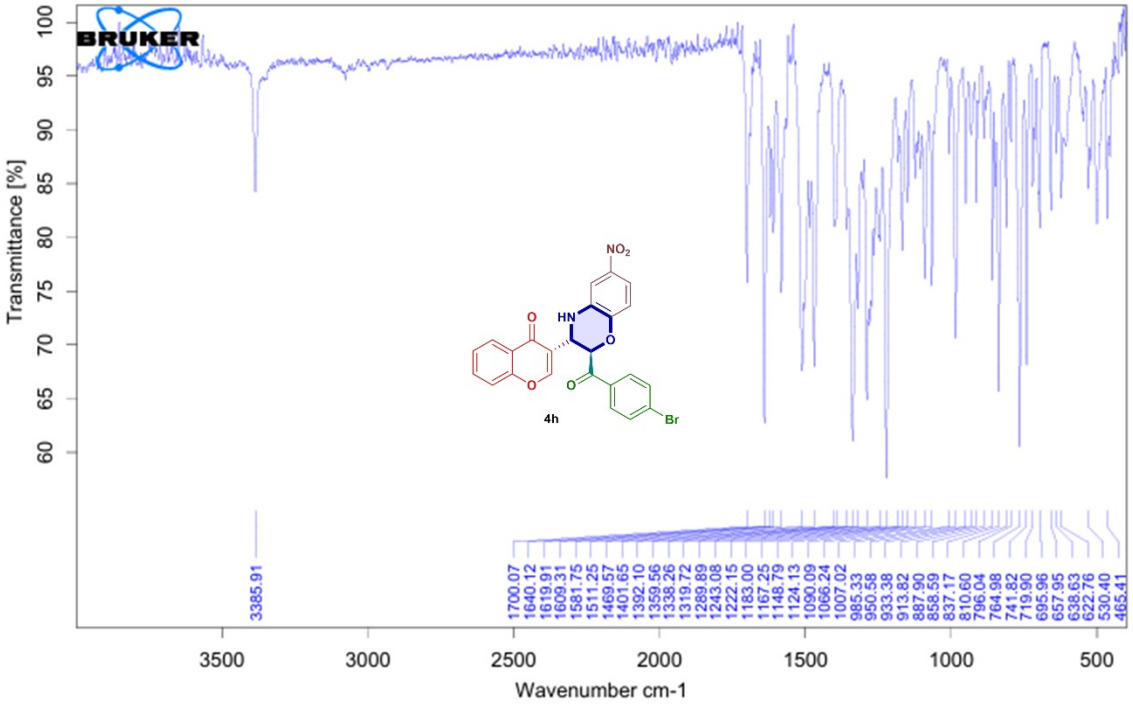
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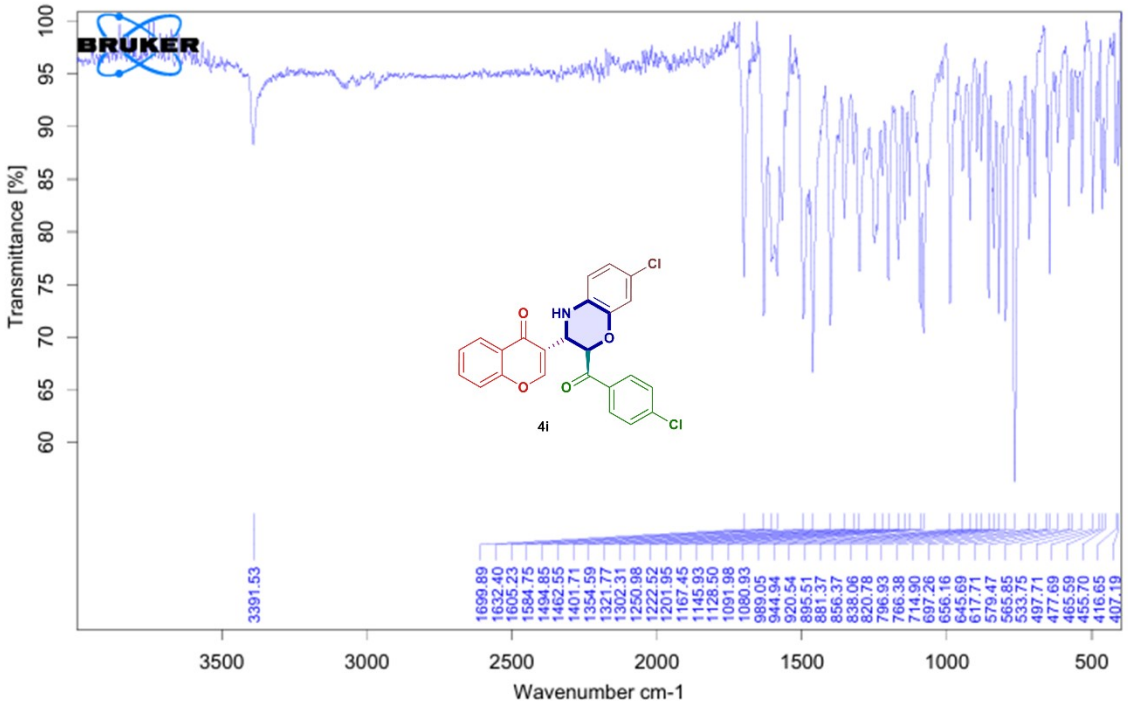
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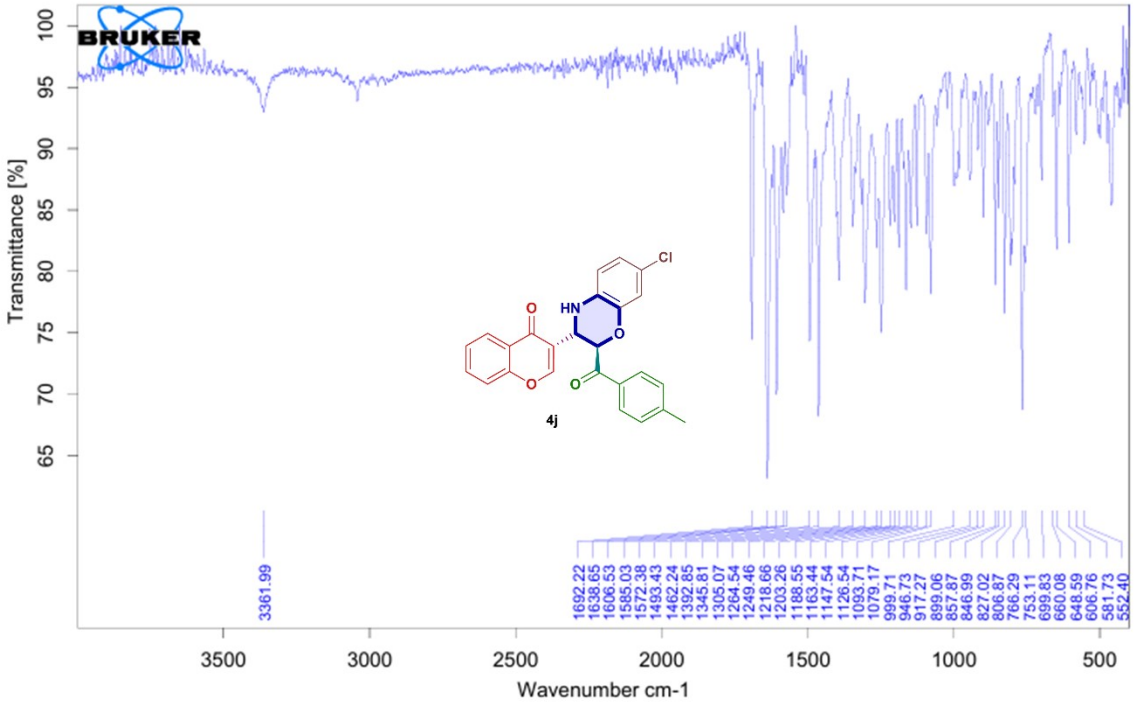
Wavenumber cm-1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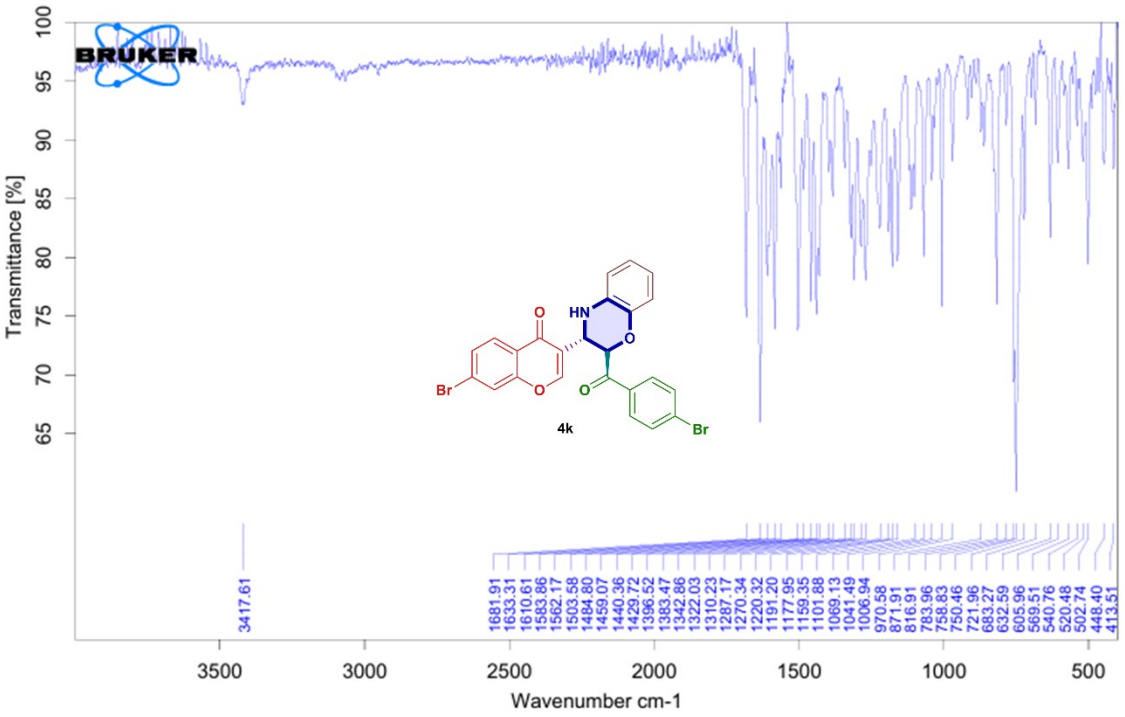
Wavenumber cm-1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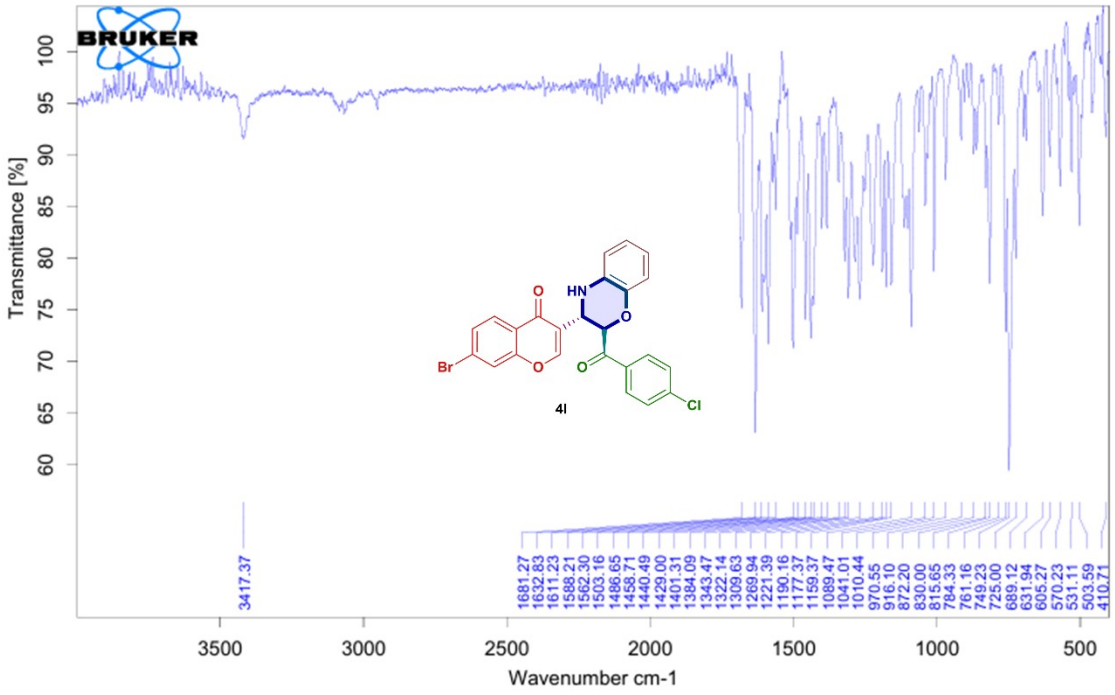
Br
4k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Transmittance [%]
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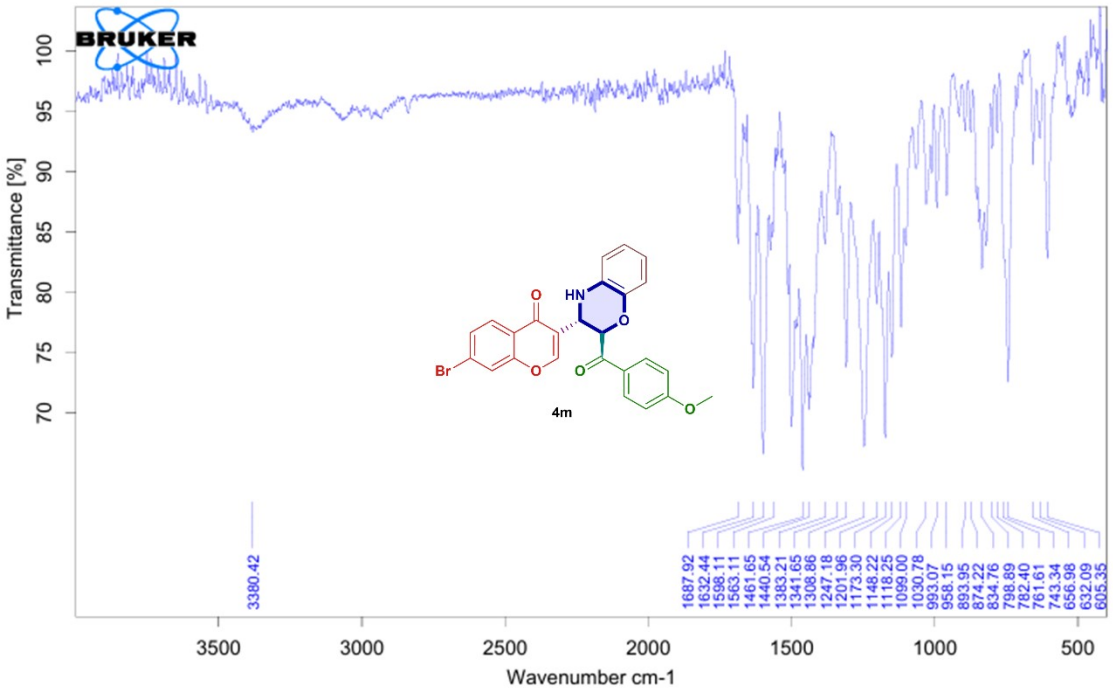
O
O
Cl
4l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Br
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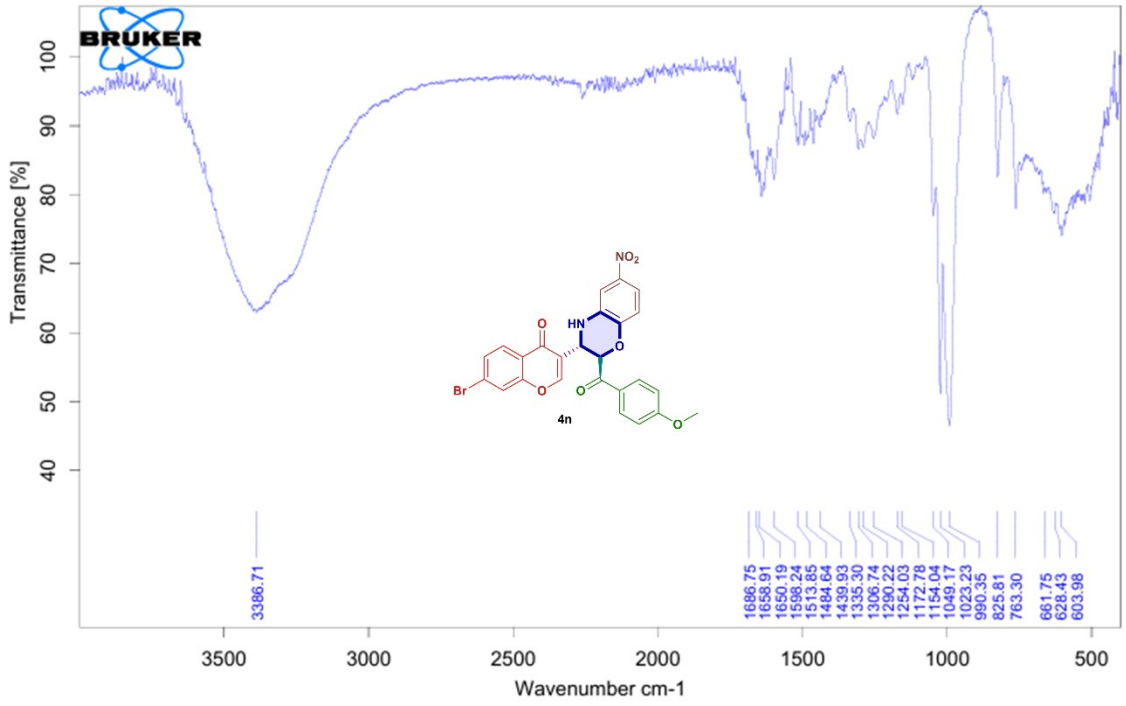
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Wavenumber cm-1
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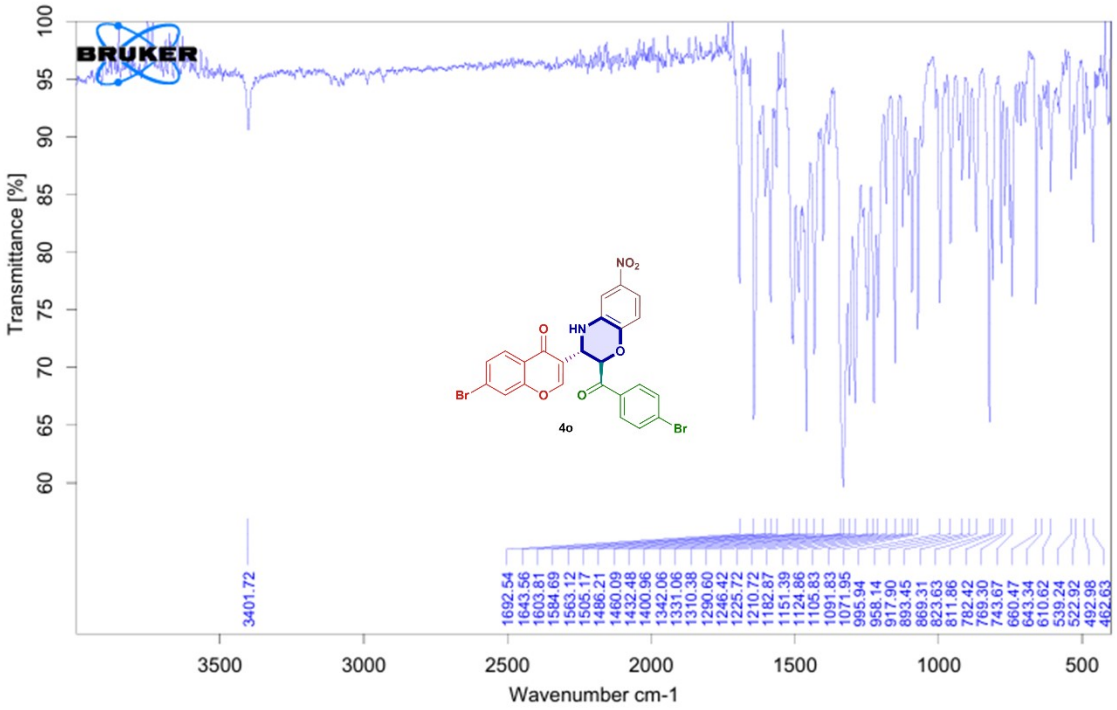
4n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4o
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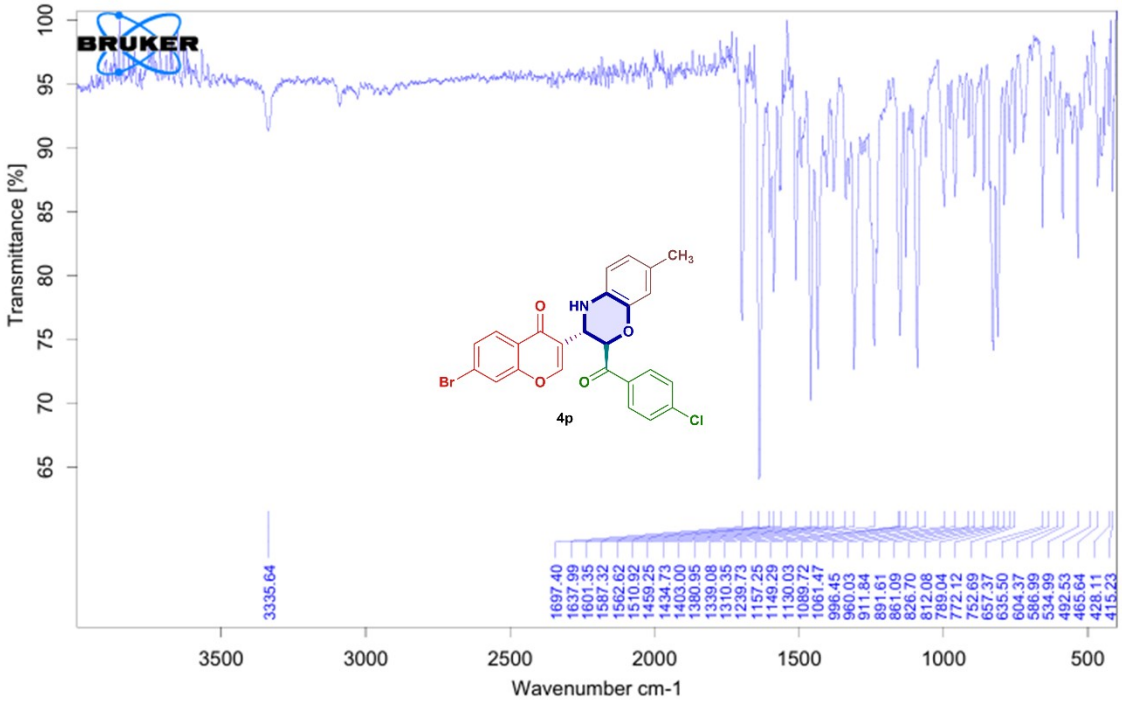
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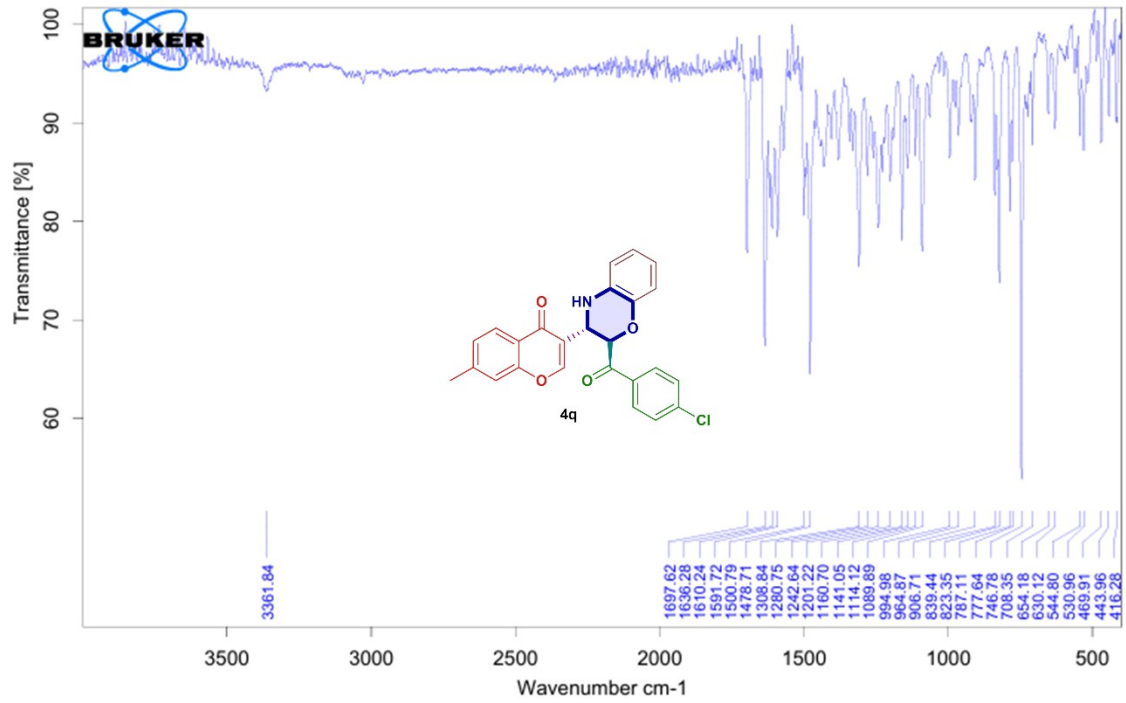
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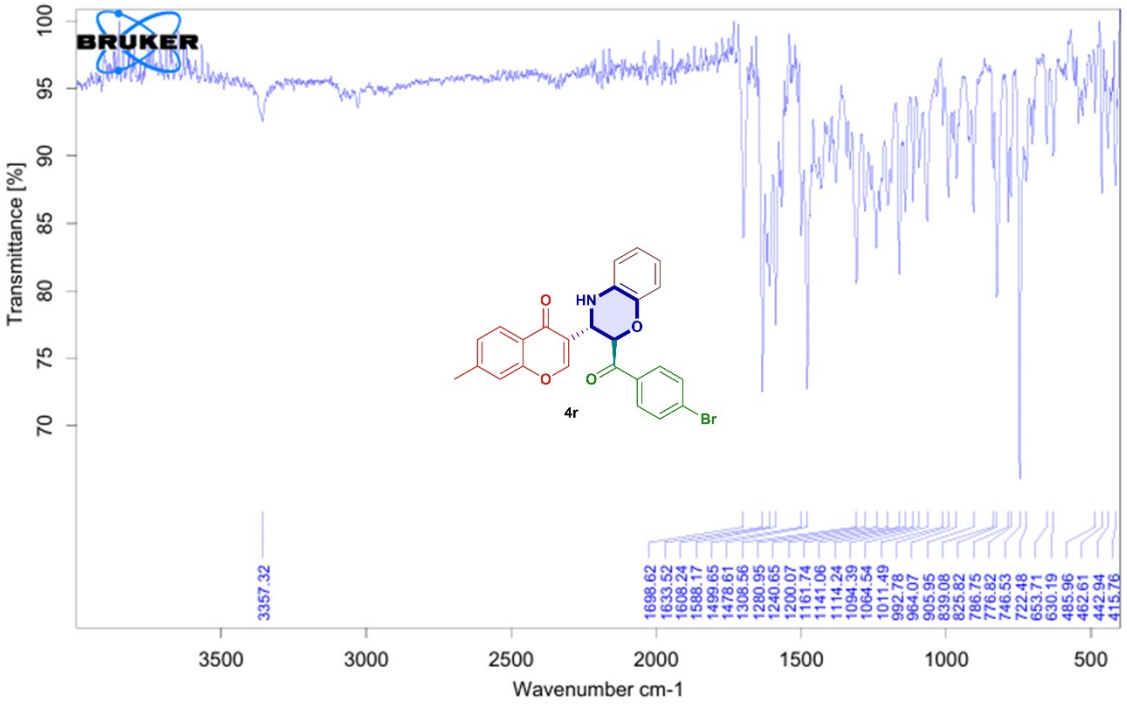
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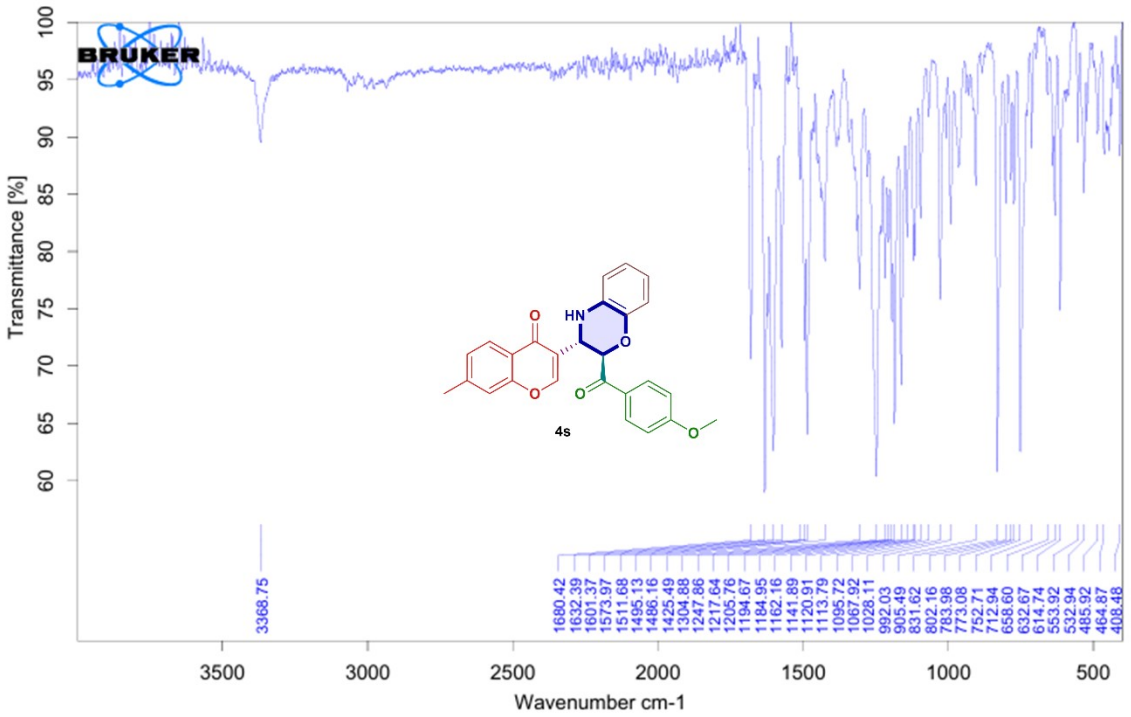
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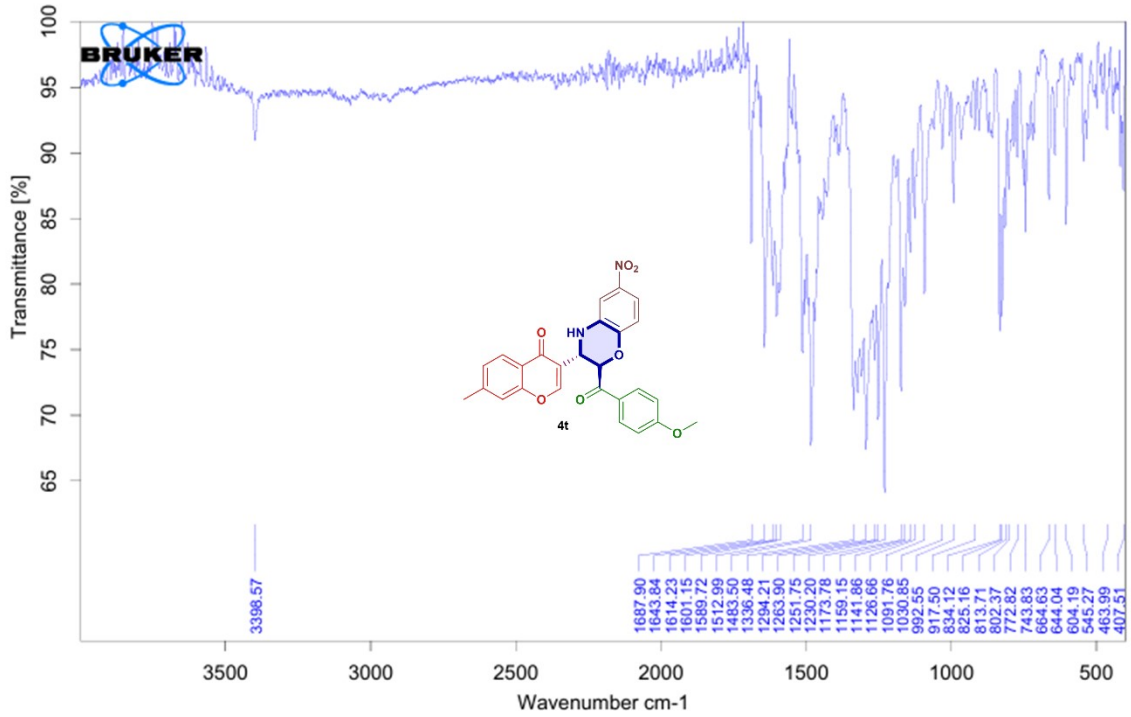
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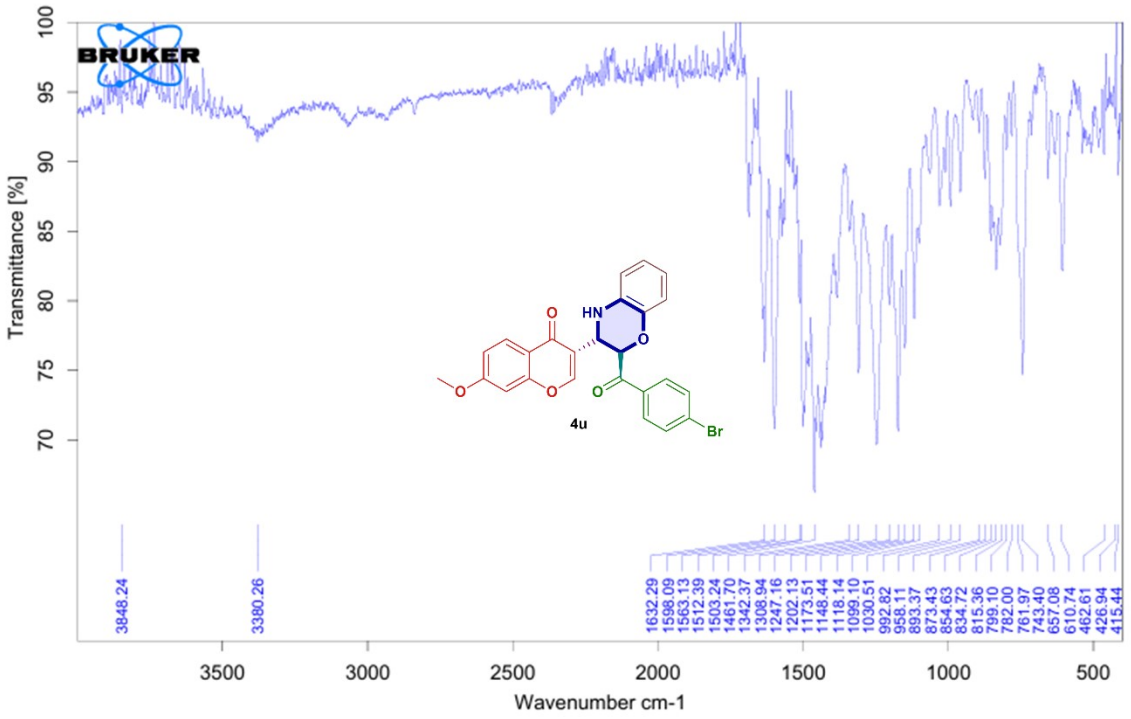
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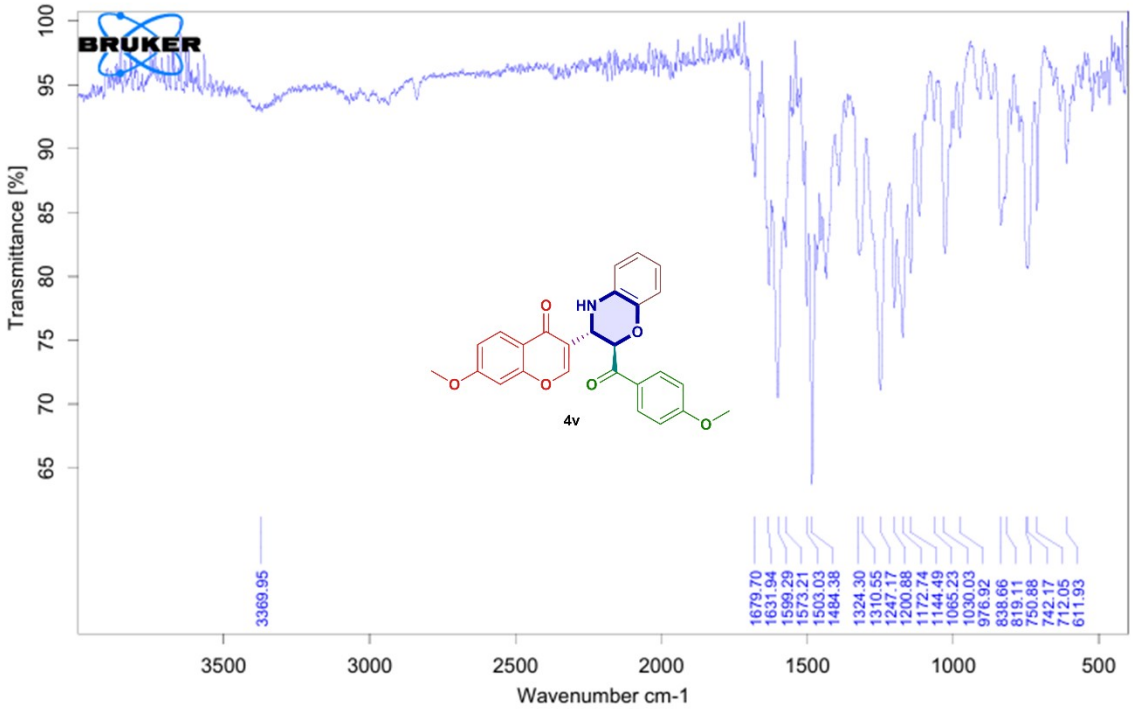
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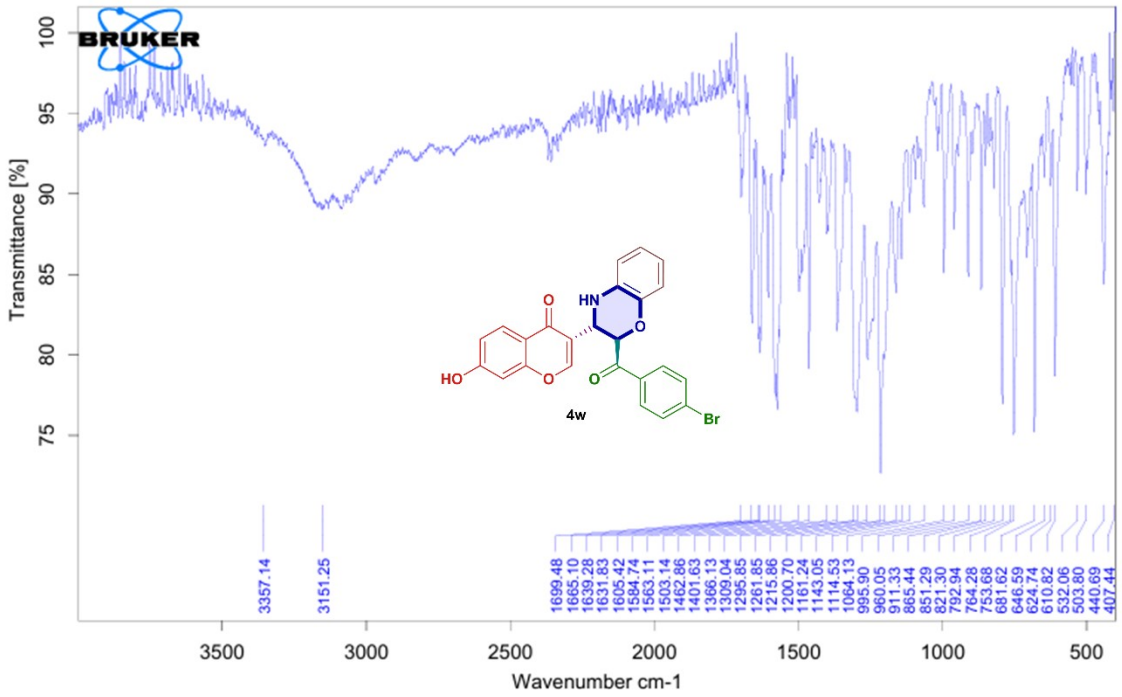
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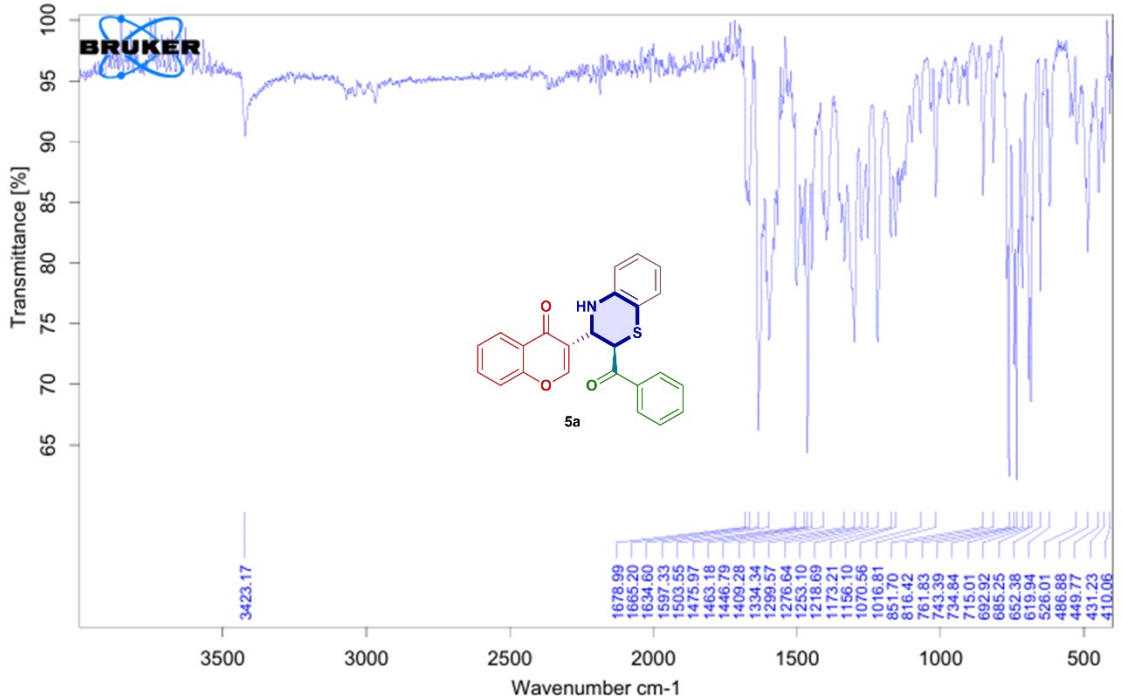
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1463.18
1446.79
1409.28
1334.34
1299.57
1276.64
1253.10
1218.69
1173.21
1156.10
1070.56
1016.81
851.70
816.42
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743.39
734.84
715.01
692.92
685.25
652.38
619.94
526.01
486.88
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HN
S
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O
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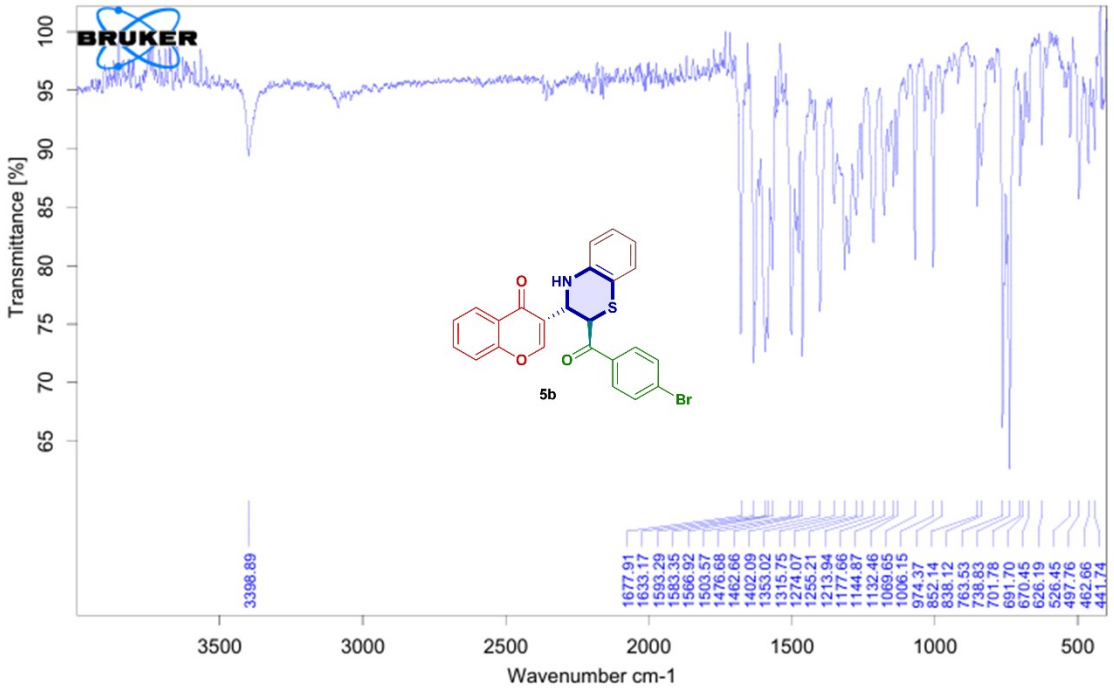
2000
1500
1000
500
Wavenumber cm-1


BRUKER
Transmittance [%]
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80
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O
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1566.92
1503.57
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1462.66
1402.09
1353.02
1315.75
1274.07
1255.21
1213.94
1177.66
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1132.46
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1006.15
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852.14
838.12
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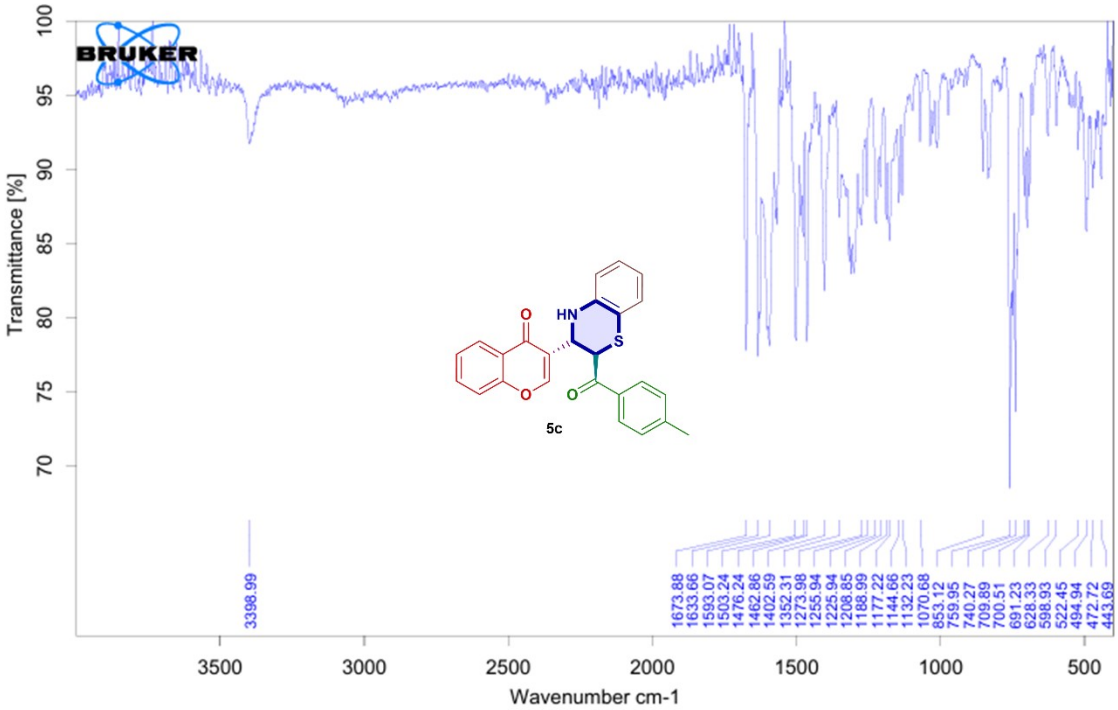
Wavenumber cm-1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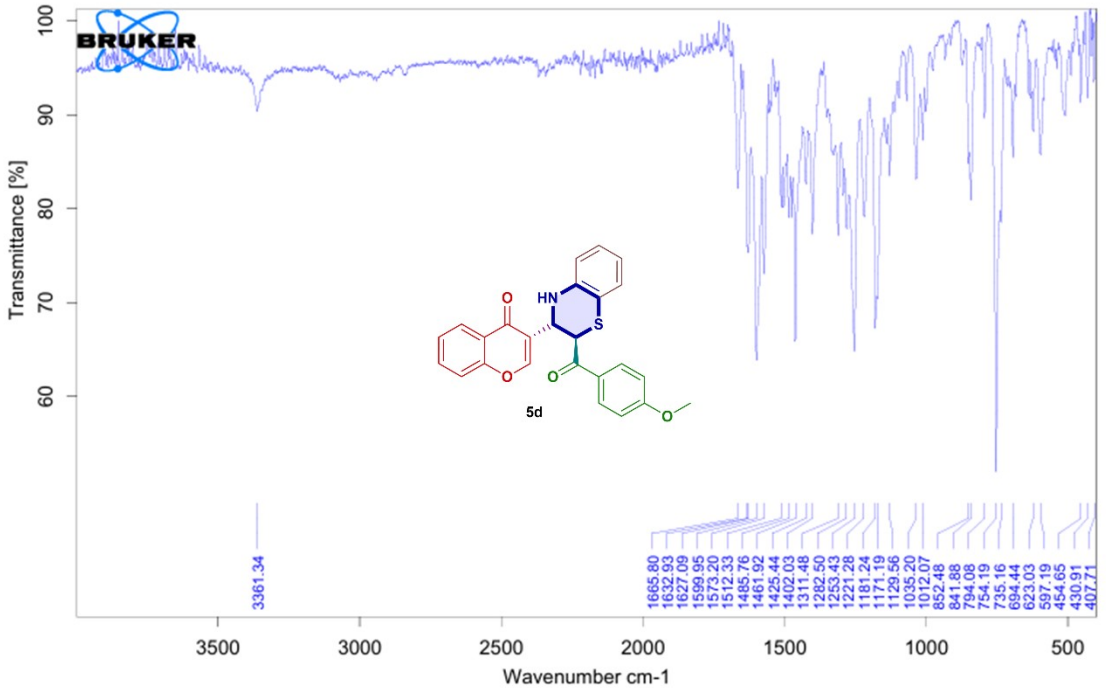
Wavenumber cm-1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1253.43
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1171.19
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1035.20
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852.48
841.88
794.08
754.19
735.16
694.44
623.03
597.19
454.65
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O
O
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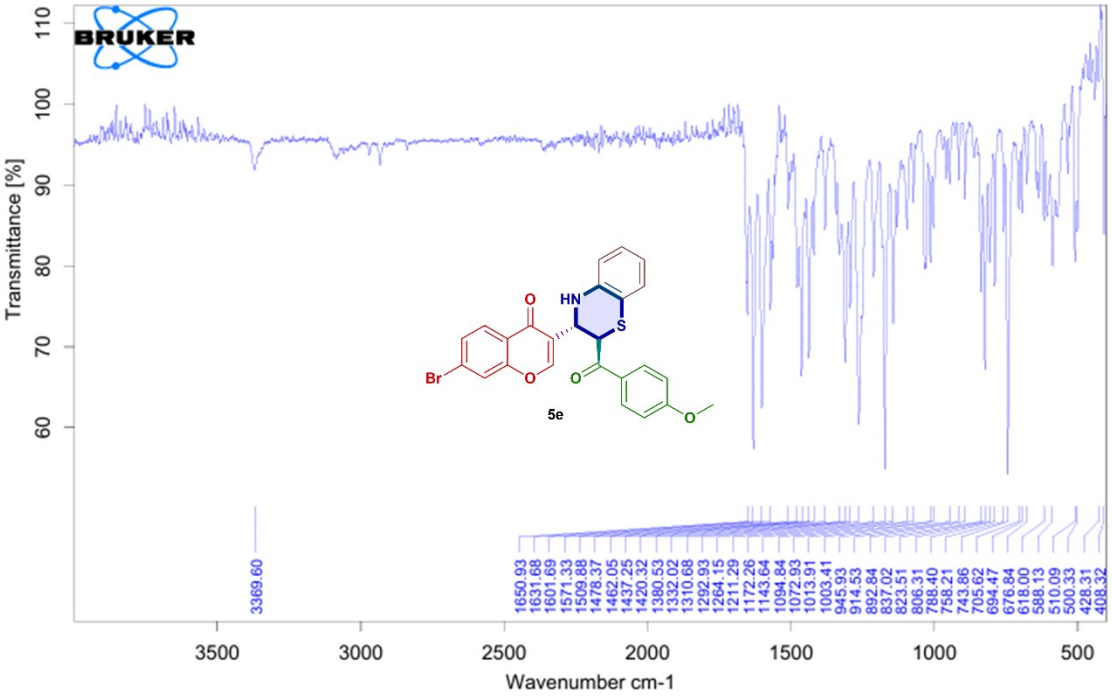
2000
1500
1000
500
Wavenumber cm-1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618.00
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O
Br
O
5e
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2000
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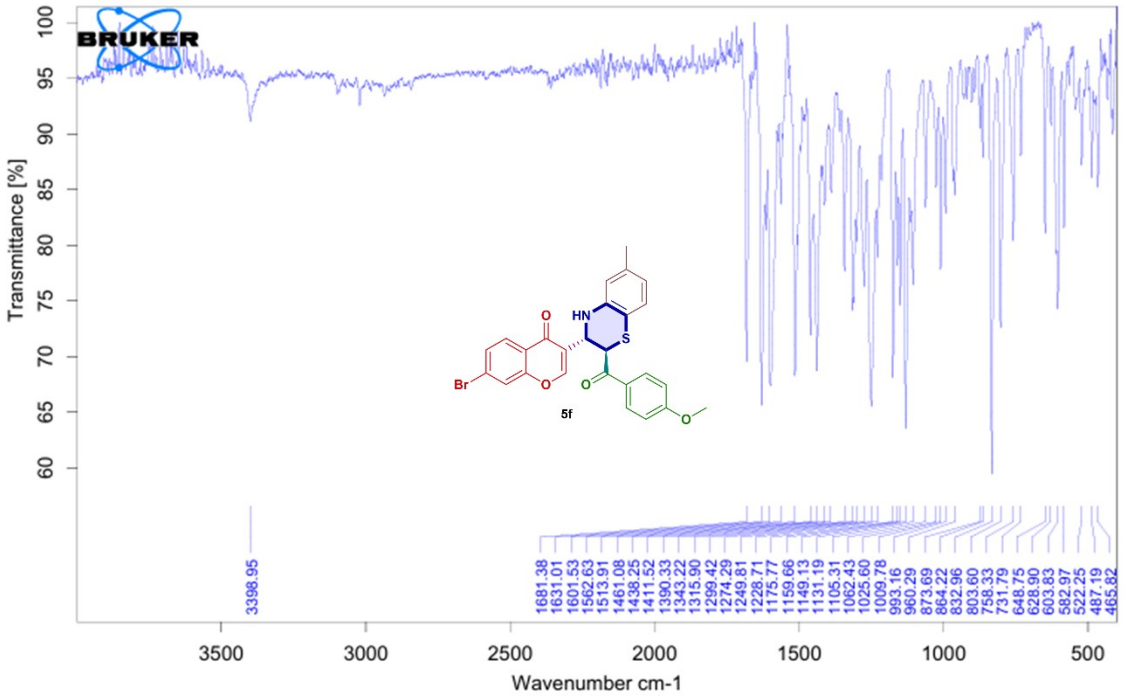
500
Wavenumber cm-1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2500
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HN
S
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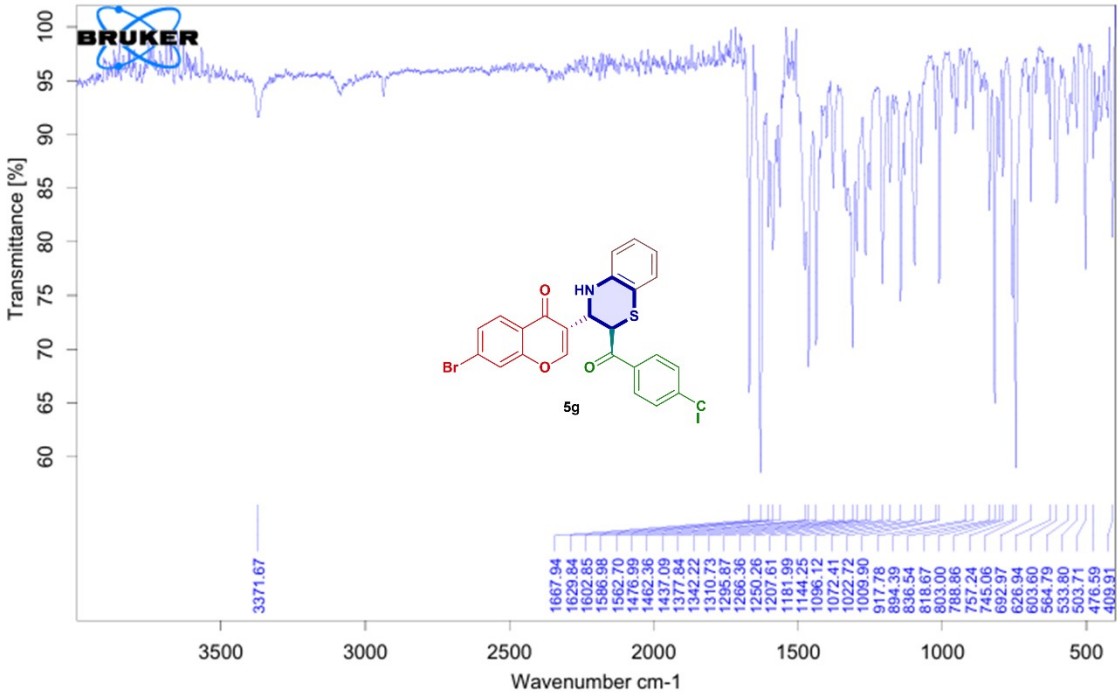
O
Br
O
5f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Transmittance [%]
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1500
1000
500
Wavenumber cm-1
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1586.98
1562.70
1476.99
1462.36
1437.09
1377.84
1342.22
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1207.61
1181.99
1144.25
1096.12
1072.41
1022.72
1009.90
917.78
894.39
836.54
818.67
803.00
788.86
757.24
745.06
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476.59
409.91
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S
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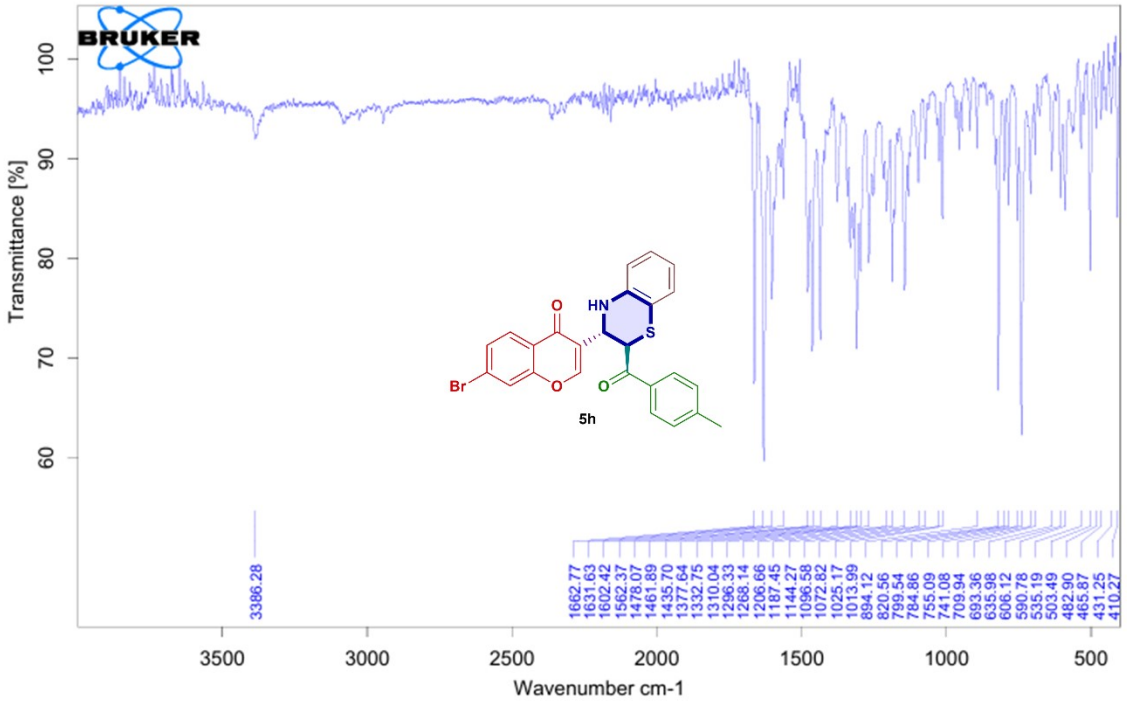
O
Br
O
Cl
5g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1310.04
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1268.14
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1025.17
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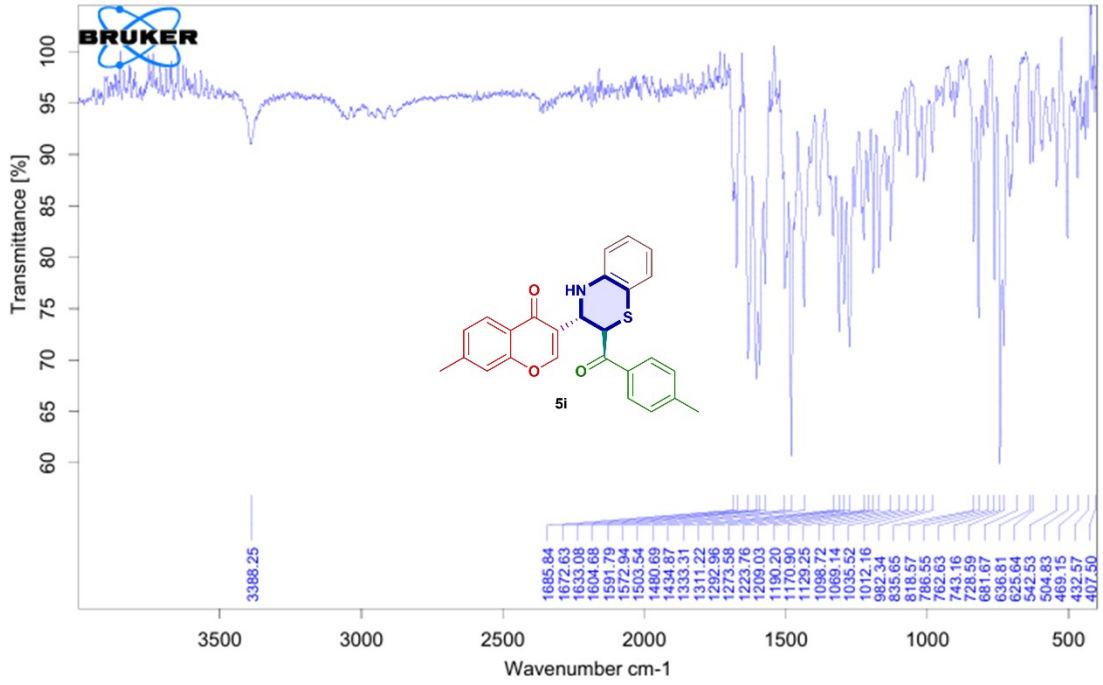
2500
2000
1500
1000
500
Wavenumber cm-1


BRUKER
Transmittance [%]
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1273.58
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1098.72
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786.55
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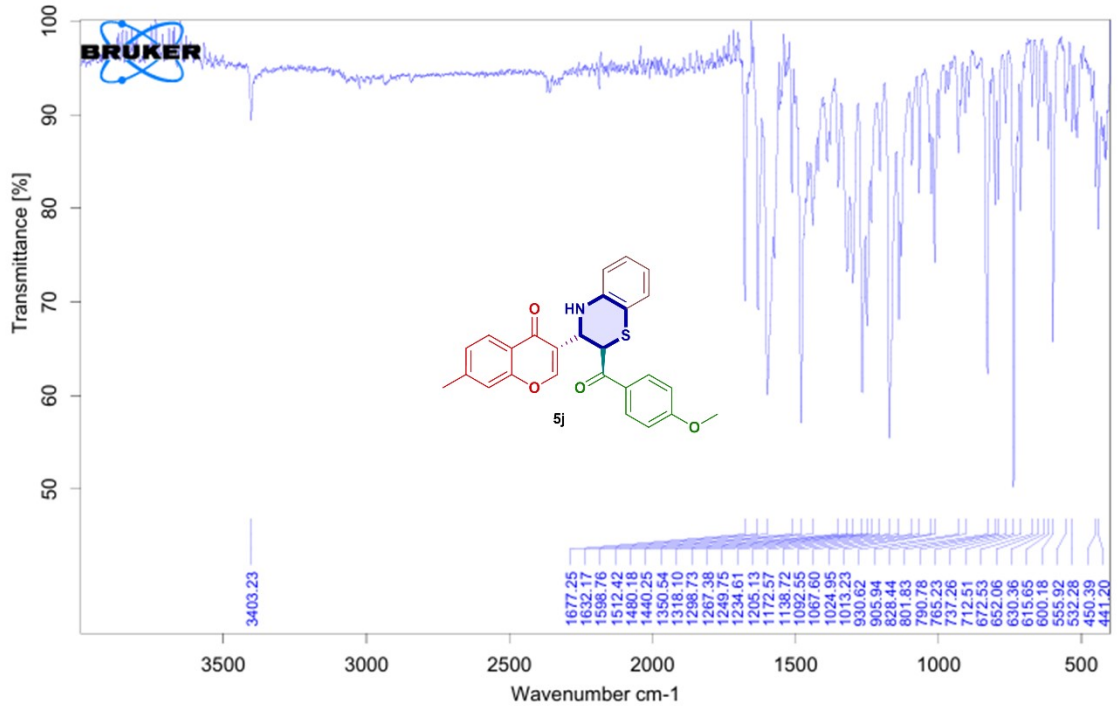
Wavenumber cm-1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Transmittance [%]
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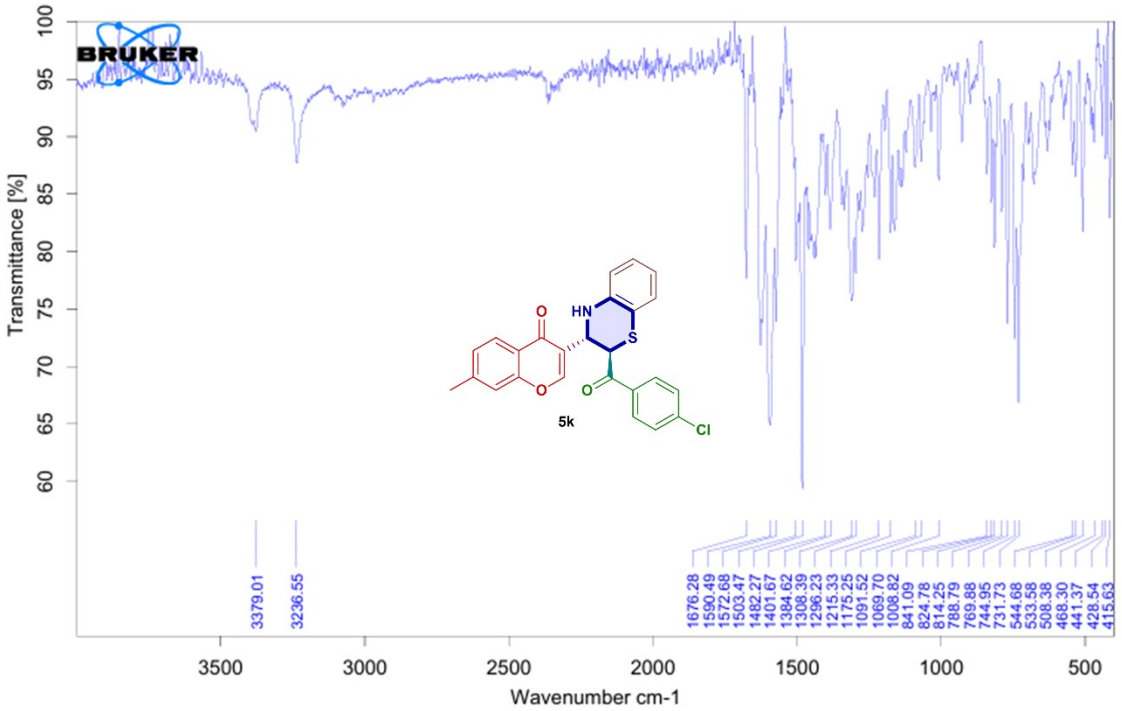
Wavenumber cm-1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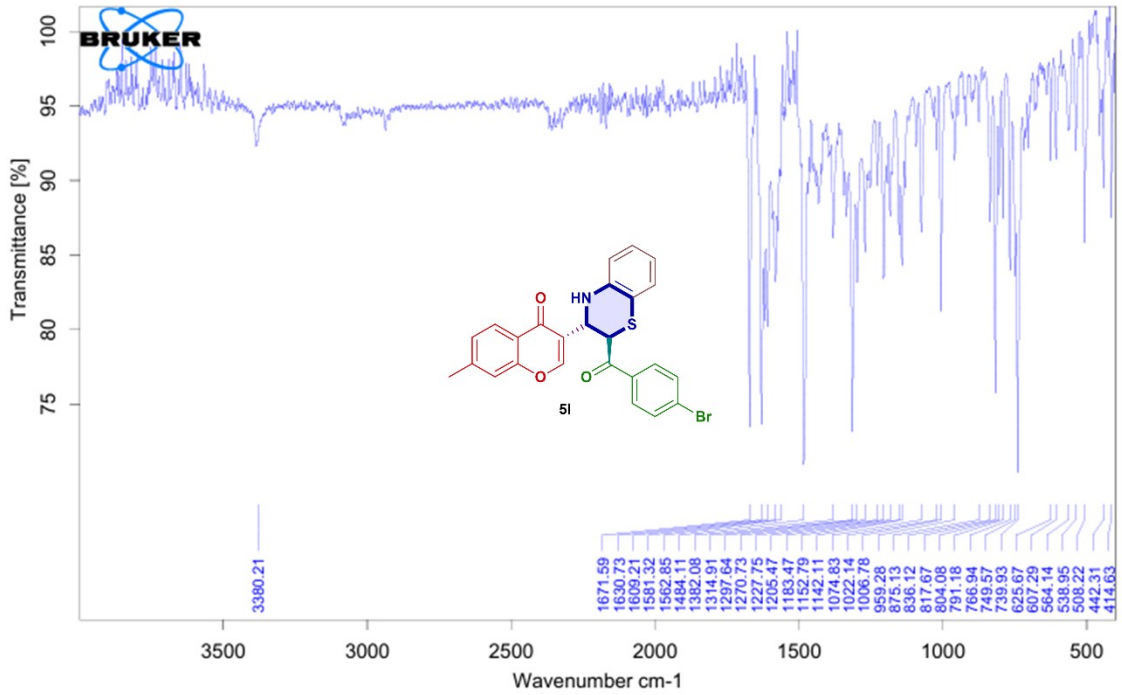
BRUKER
Transmittance [%]
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1152.79
1142.11
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804.08
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766.94
749.57
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625.67
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564.14
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508.22
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Br
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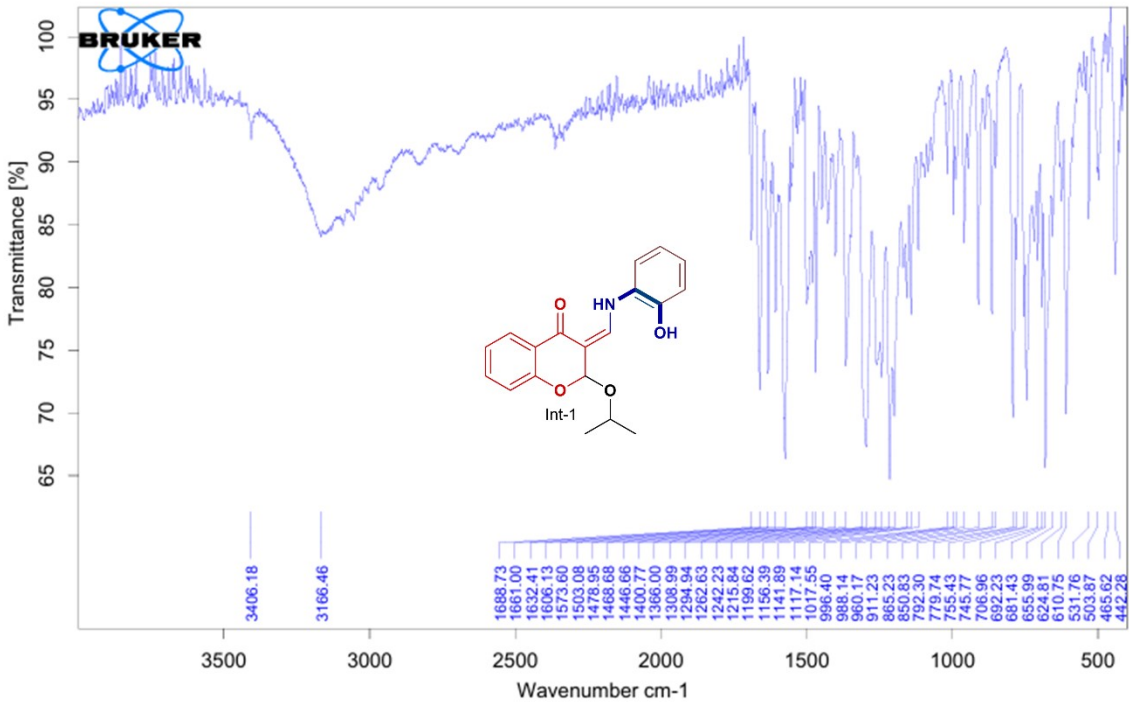
Wavenumber cm-1


BRUKER
Transmittance [%]
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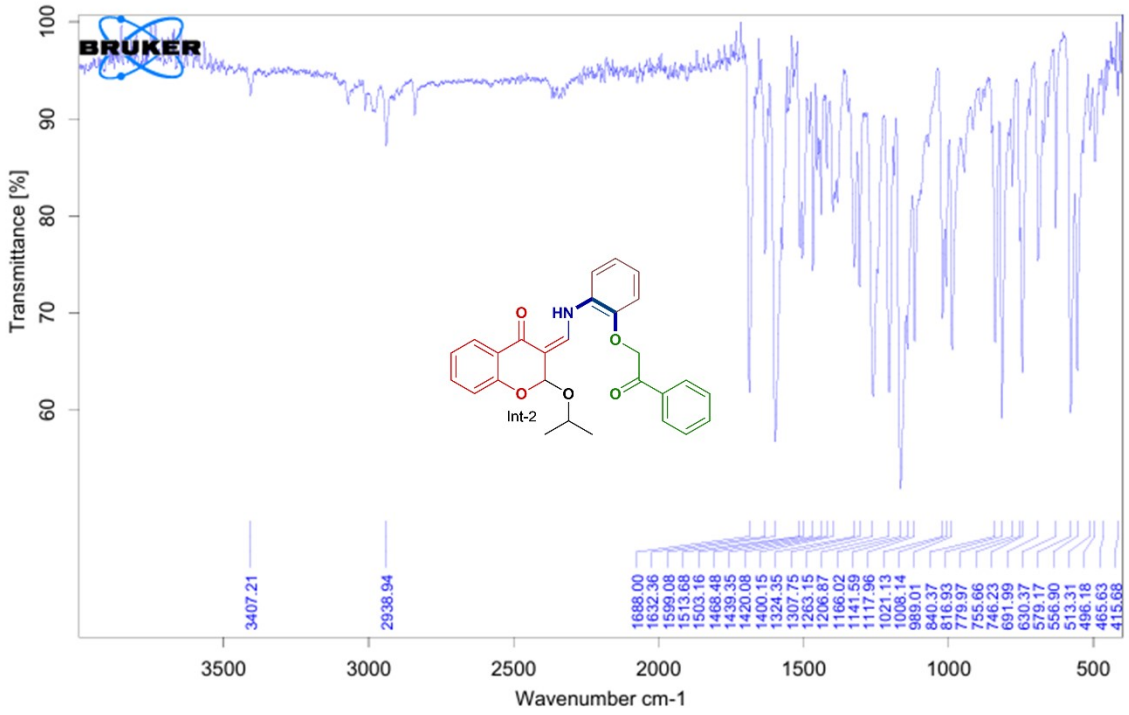
Wavenumber cm-1

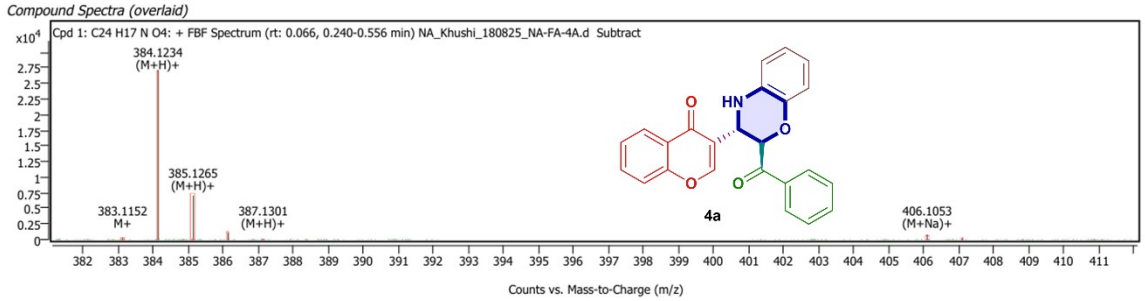


Compound Details

Cpd. 1: C24 H17 N O4

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C24 H17 N O4	383.1160	99.61	FBF	0.71315738593882	Positive

Compound Spectra (overlaid)

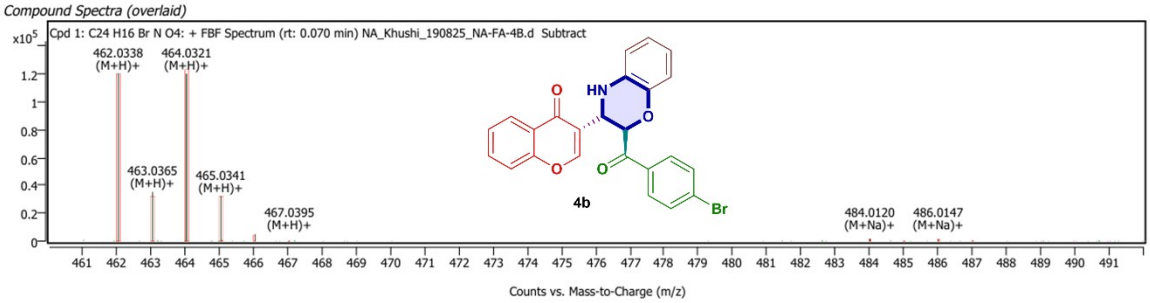


Compound Details

Cpd. 1: C24 H16 Br N O4

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C24 H16 Br N O4	461.0263	99.25	FBF	0.101133810556293	Positive

Compound Spectra (overlaid)

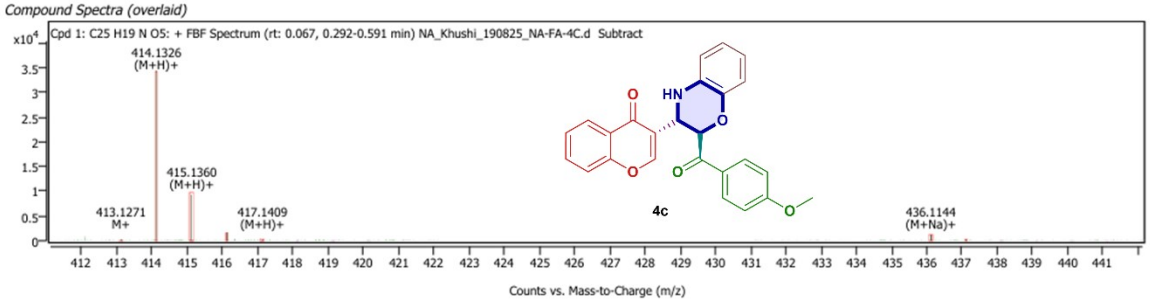


Compound Details

Cpd. 1: C25 H19 N O5

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C25 H19 N O5	413.1254	97.48	FBF	-2.35318308192693	Positive

Compound Spectra (overlaid)

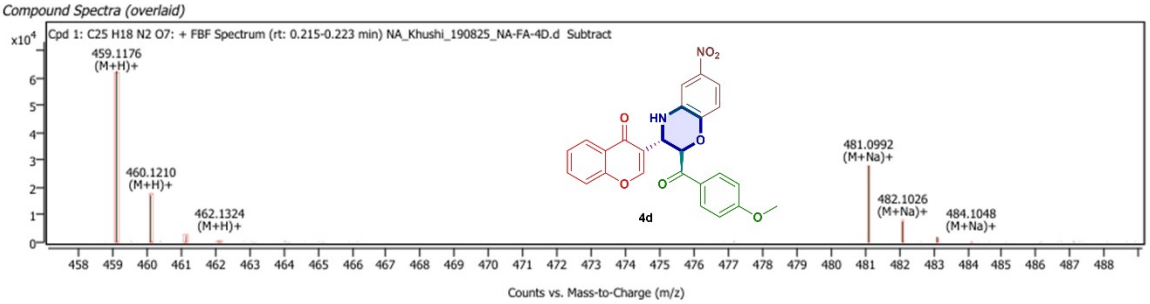


Compound Details

Cpd. 1: C25 H18 N2 O7

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C25 H18 N2 O7	458.1103	97.03	FBF	-2.46020031012398	Positive

Compound Spectra (overlaid)

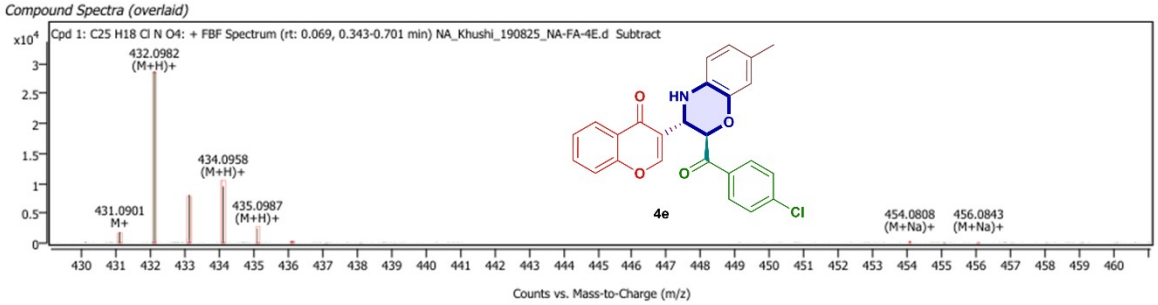


Compound Details

Cpd. 1: C25 H18 Cl N O4

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C25 H18 Cl N O4	431.0907	91.73	FBF	-3.95027194617228	Positive

Compound Spectra (overlaid)

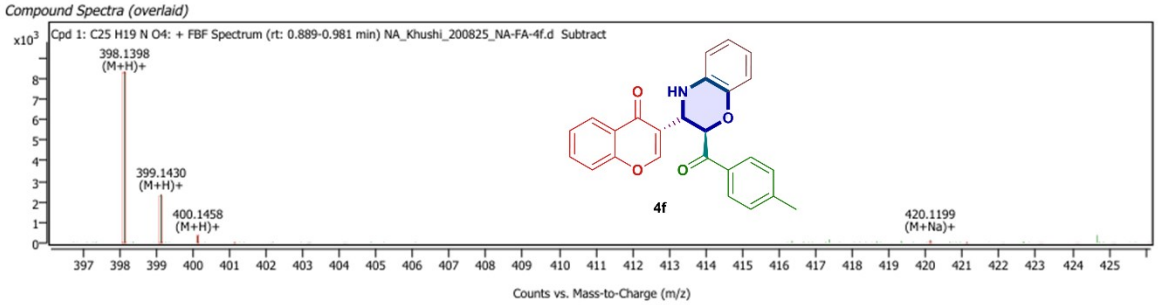


Compound Details

Cpd. 1: C25 H19 N O4

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C25 H19 N O4	397.1325	96.81	FBF	2.67355003144451	Positive

Compound Spectra (overlaid)

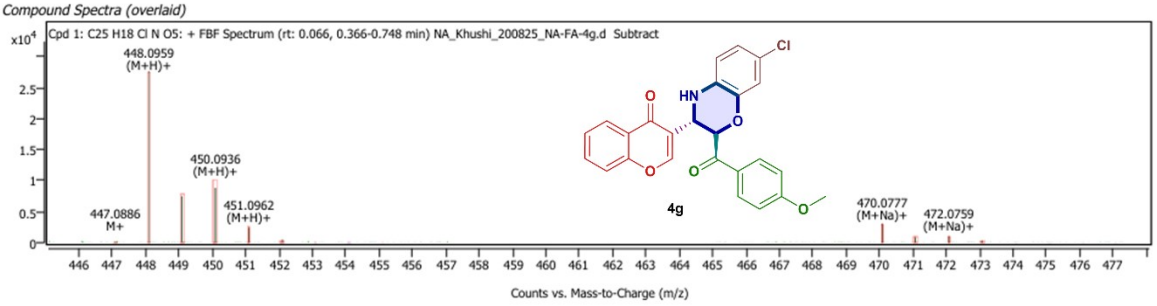


Compound Details

Cpd. 1: C25 H18 Cl N O5

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C25 H18 Cl N O5	447.0885	95.43	FBF	2.47936351610189	Positive

Compound Spectra (overlaid)

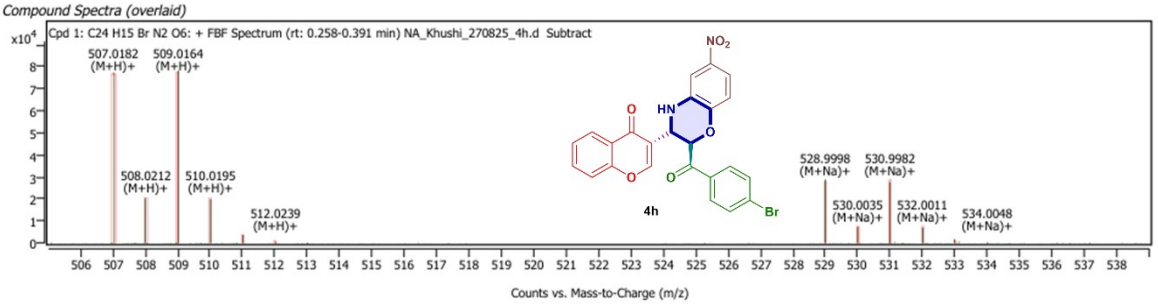


Compound Details

Cpd. 1: C24 H15 Br N2 O6

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C24 H15 Br N2 O6	506.0108	99.11	FBF	-1.1256816492227	Positive

Compound Spectra (overlaid)

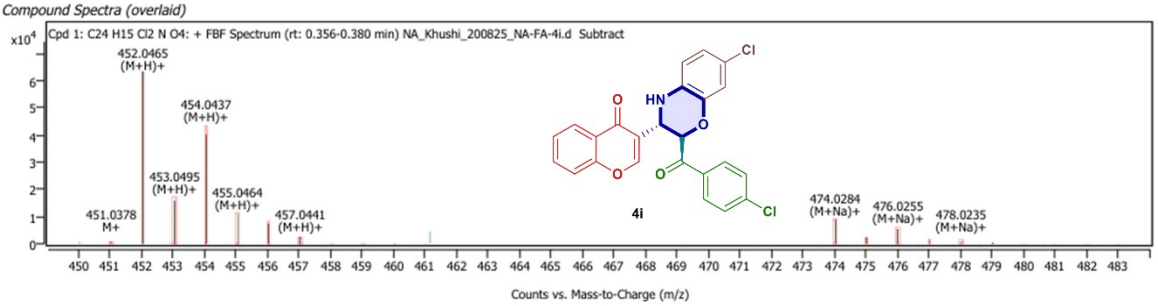


Compound Details

Cpd. 1: C24 H15 Cl2 N O4

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C24 H15 Cl2 N O4	451.0389	96.18	FBF	2.48373939518265	Positive

Compound Spectra (overlaid)

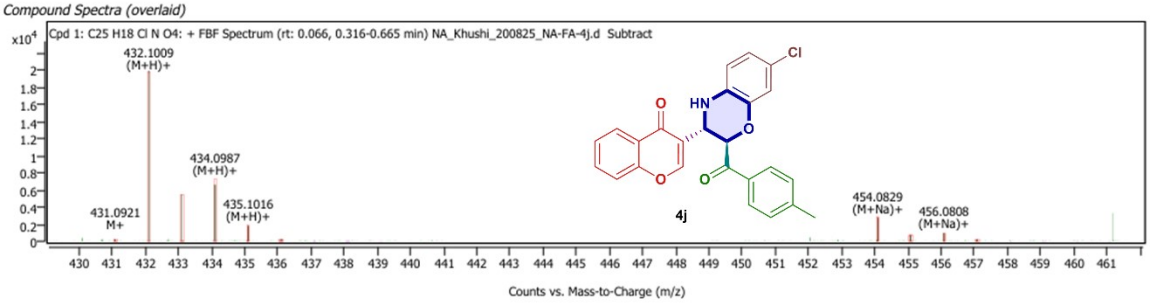


Compound Details

Cpd. 1: C25 H18 Cl N O4

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C25 H18 Cl N O4	431.0935	96.40	FBF	2.52486364146582	Positive

Compound Spectra (overlaid)

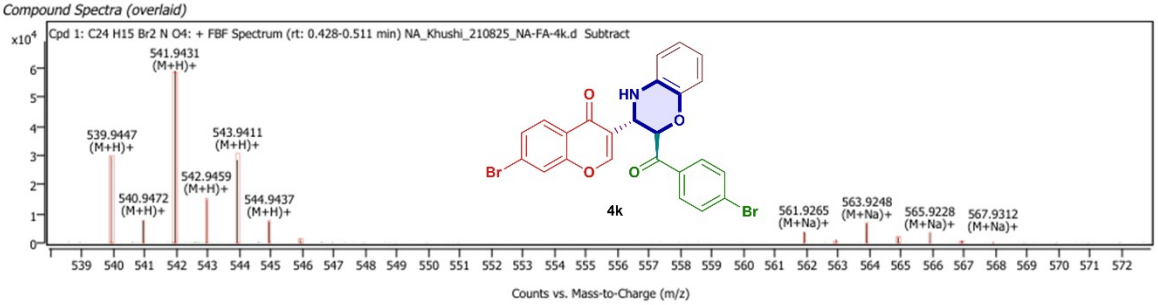


Compound Details

Cpd. 1: C24 H15 Br2 N O4

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C24 H15 Br2 N O4	538.9374	98.12	FBF	1.17563972342711	Positive

Compound Spectra (overlaid)

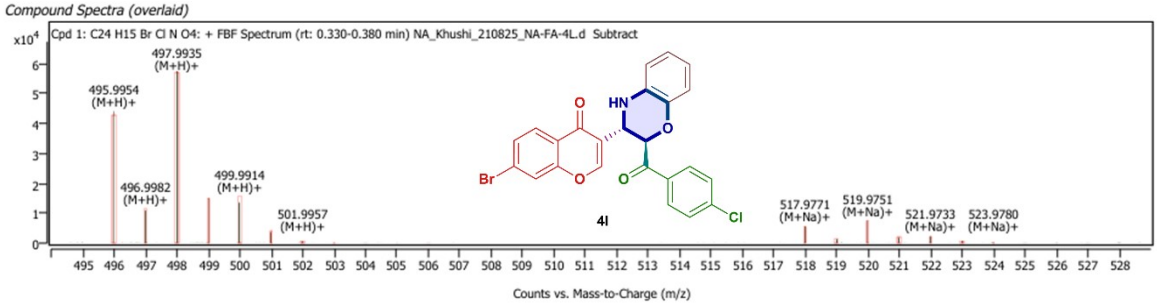


Compound Details

Cpd. 1: C24 H15 Br Cl N O4

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C24 H15 Br Cl N O4	494.9880	98.23	FBF	1.48054769240496	Positive

Compound Spectra (overlaid)

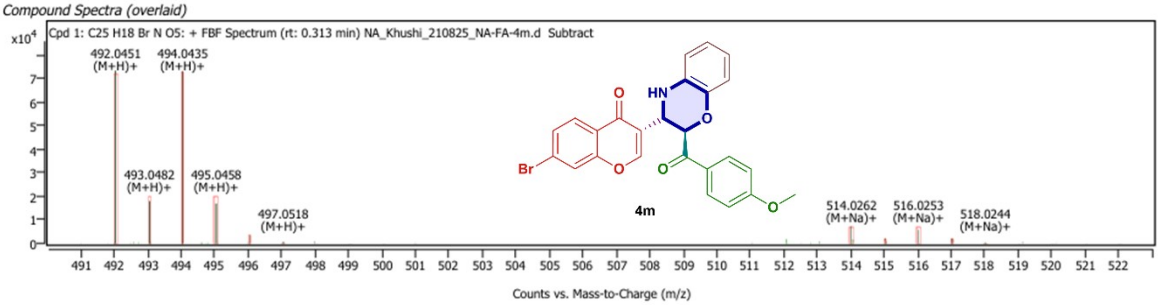


Compound Details

Cpd. 1: C25 H18 Br N O5

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C25 H18 Br N O5	491.0376	95.88	FBF	1.63767485593487	Positive

Compound Spectra (overlaid)

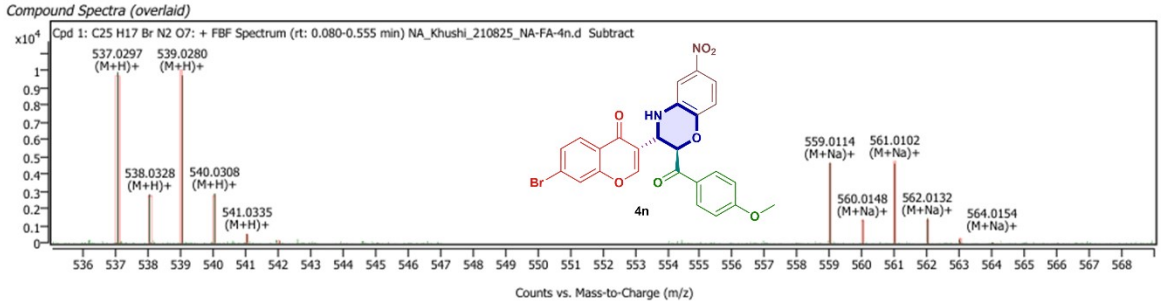


Compound Details

Cpd. 1: C25 H17 Br N2 O7

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C25 H17 Br N2 O7	536.0224	99.27	FBF	0.87648218926999	Positive

Compound Spectra (overlaid)

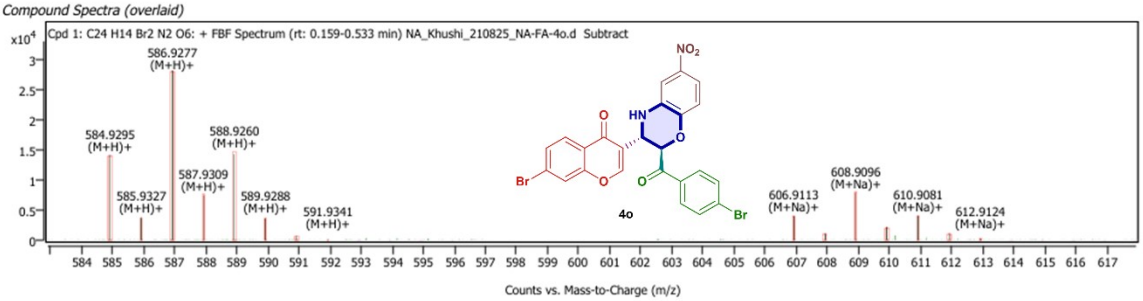


Compound Details

Cpd. 1: C24 H14 Br2 N2 O6

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C24 H14 Br2 N2 O6	583.9222	99.67	FBF	0.614969299916012	Positive

Compound Spectra (overlaid)

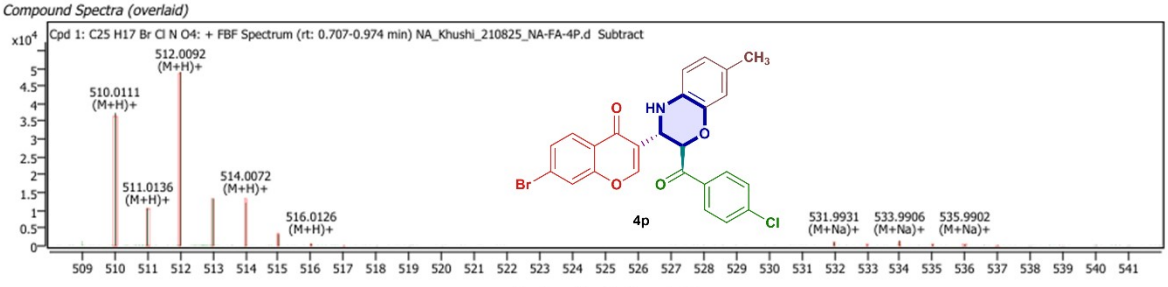


Compound Details

Cpd. 1: C25 H17 Br Cl N O4

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C25 H17 Br Cl N O4	509.0037	97.32	FBF	1.54653144805661	Positive

Compound Spectra (overlaid)

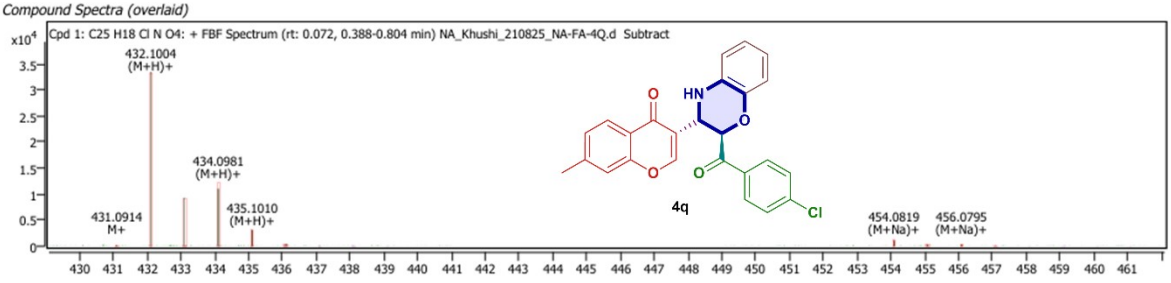


Compound Details

Cpd. 1: C25 H18 Cl N O4

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C25 H18 Cl N O4	431.0930	97.63	FBF	1.345286968	Positive

Compound Spectra (overlaid)

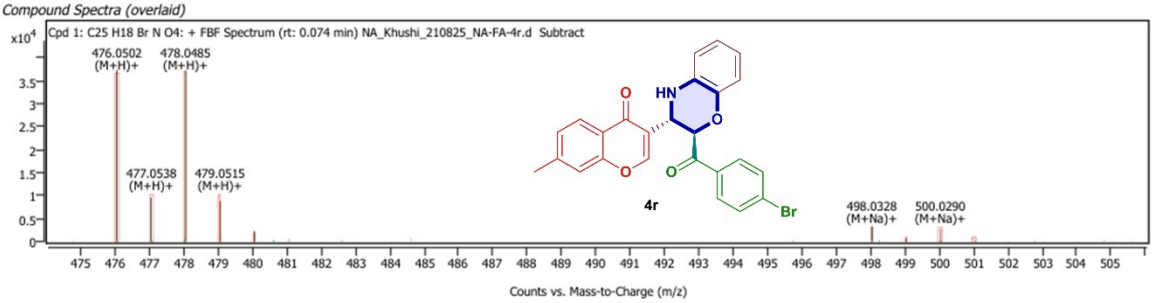


Compound Details

Cpd. 1: C25 H18 Br N O4

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C25 H18 Br N O4	475.0429	95.88	FBF	2.14594375717866	Positive

Compound Spectra (overlaid)

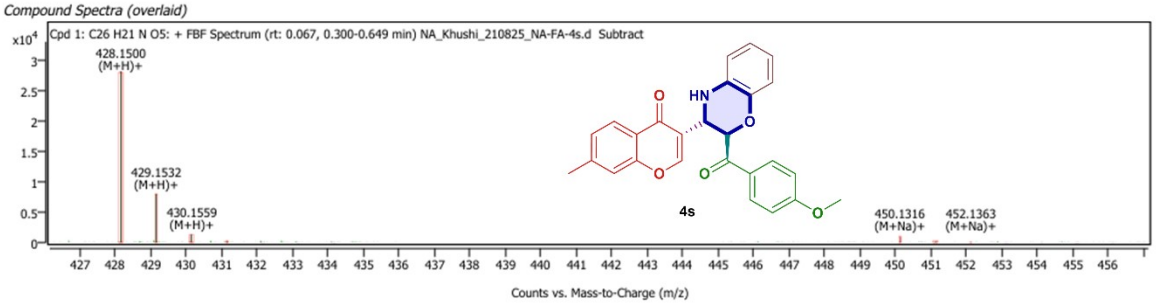


Compound Details

Cpd. 1: C26 H21 N O5

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C26 H21 N O5	427.1427	98.66	FBF	1.64885942026727	Positive

Compound Spectra (overlaid)

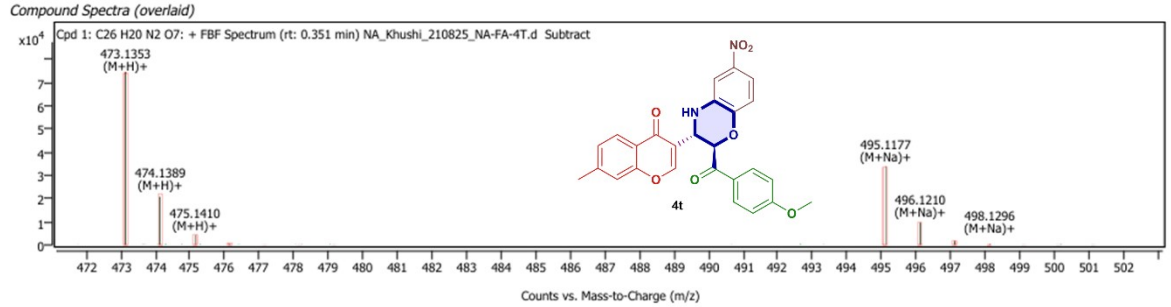


Compound Details

Cpd. 1: C26 H20 N2 O7

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C26 H20 N2 O7	472.1282	97.15	FBF	2.46837277857487	Positive

Compound Spectra (overlaid)

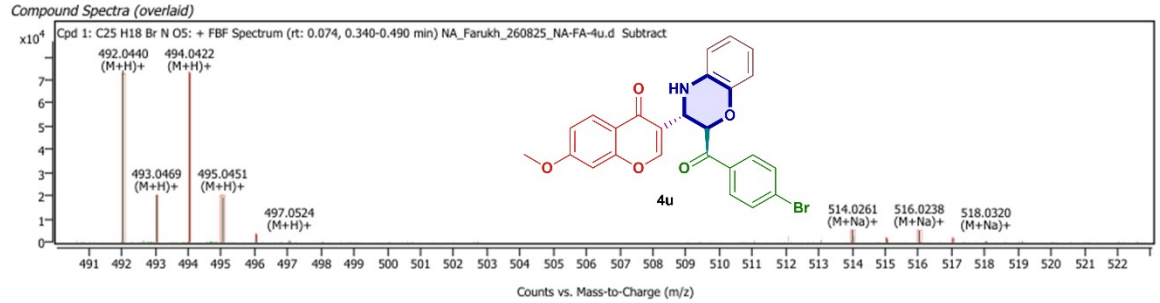


Compound Details

Cpd. 1: C25 H18 Br N O5

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C25 H18 Br N O5	491.0366	99.27	FBF	-0.438562380199797	Positive

Compound Spectra (overlaid)

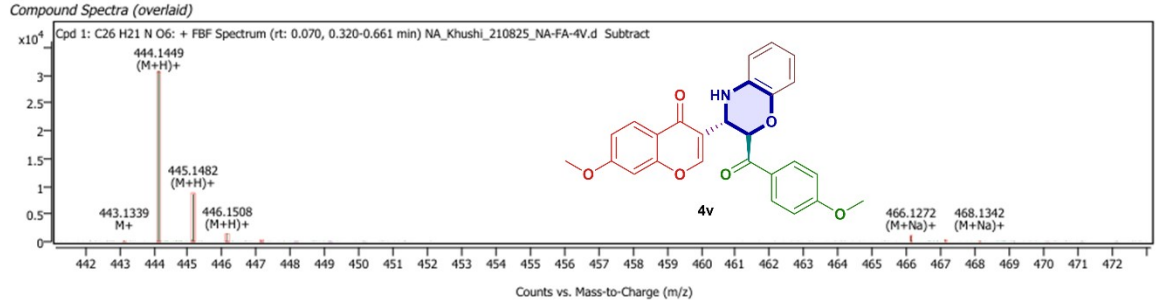


Compound Details

Cpd. 1: C26 H21 N O6

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C26 H21 N O6	443.1376	98.48	FBF	1.65657813178911	Positive

Compound Spectra (overlaid)

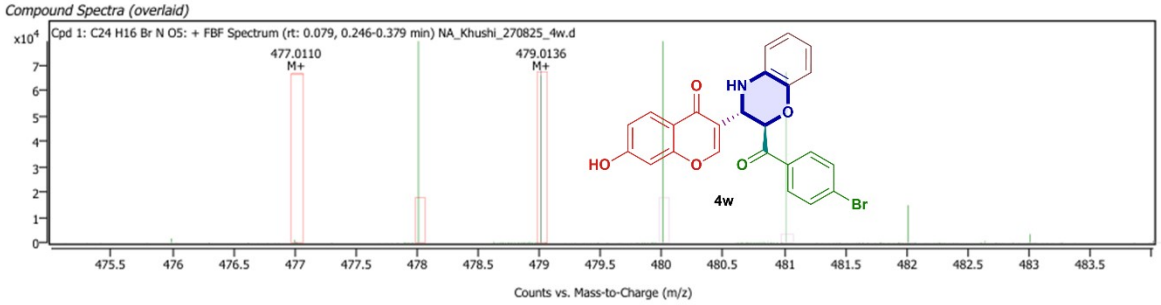


Compound Details

Cpd. 1: C24 H16 Br N O5

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C24 H16 Br N O5	477.0158	19.50	FBF	-11.2914555641035	Positive

Compound Spectra (overlaid)

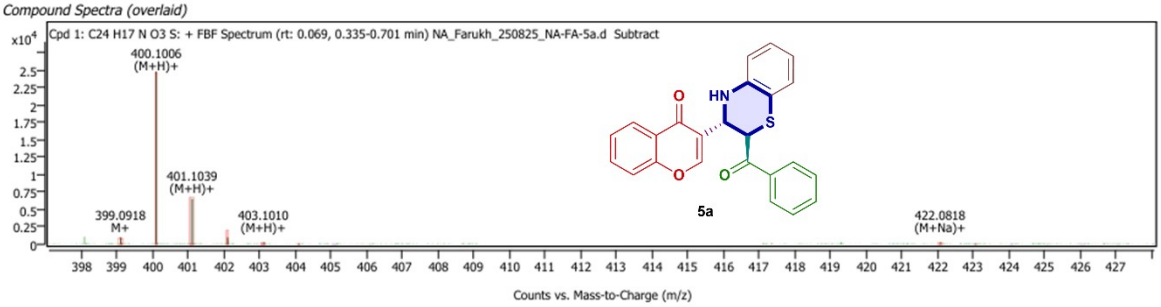


Compound Details

Cpd. 1: C24 H17 N O3 S

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C24 H17 N O3 S	399.0933	94.39	FBF	0.867901099842326	Positive

Compound Spectra (overlaid)

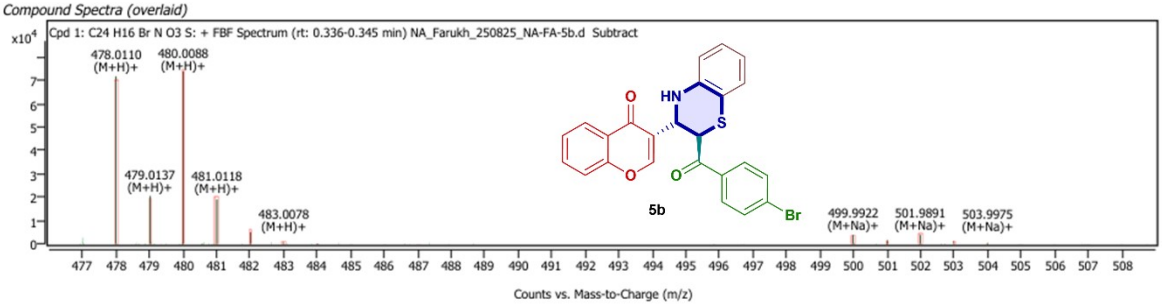


Compound Details

Cpd. 1: C24 H16 Br N O3 S

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C24 H16 Br N O3 S	477.0034	98.78	FBF	-0.0358432461455847	Positive

Compound Spectra (overlaid)

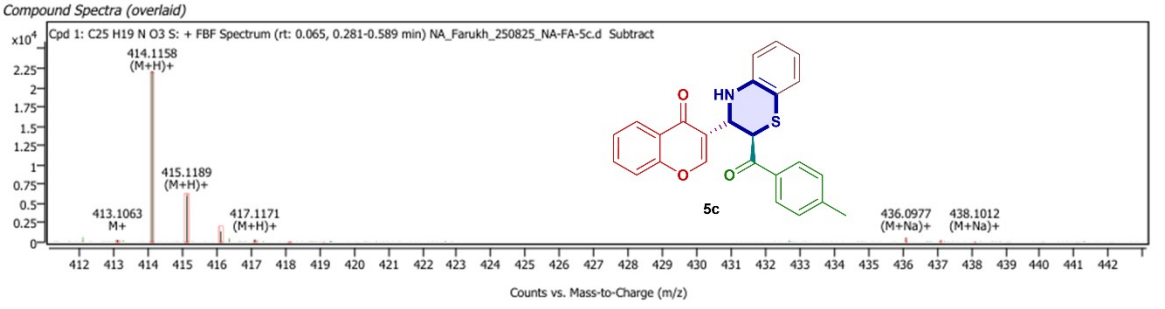


Compound Details

Cpd. 1: C25 H19 N O3 S

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C25 H19 N O3 S	413.1085	98.22	FBF	-0.121491608889175	Positive

Compound Spectra (overlaid)

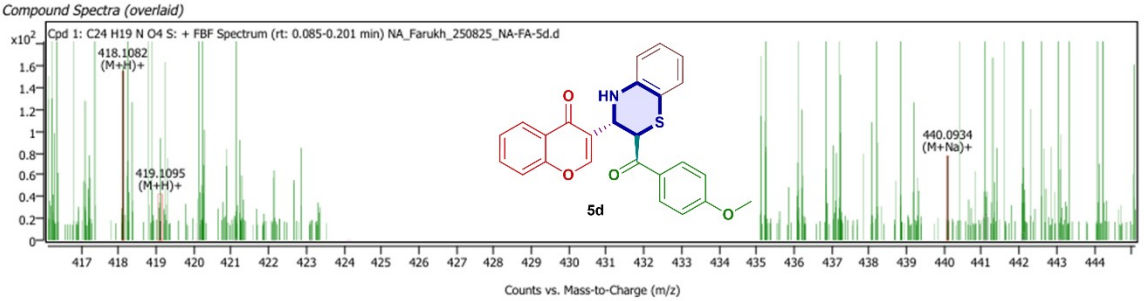


Compound Details

Cpd. 1: C24 H19 N O4 S

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C24 H19 N O4 S	417.1018	46.53	FBF	-4.12601541457517	Positive

Compound Spectra (overlaid)

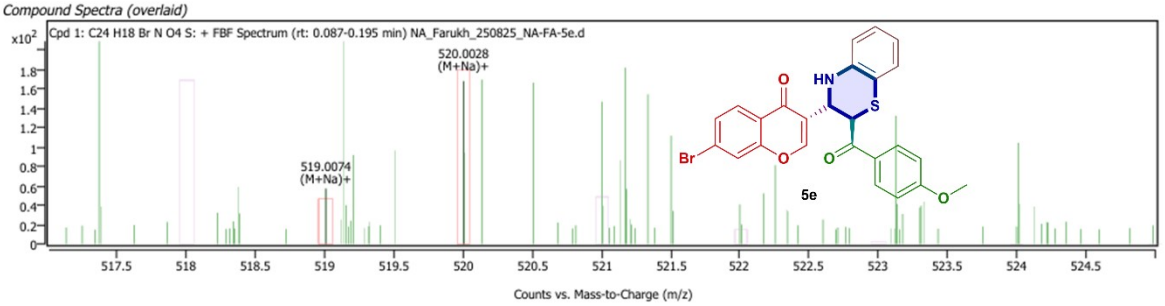


Compound Details

Cpd. 1: C24 H18 Br N O4 S

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C24 H18 Br N O4 S	495.0153	46.91	FBF	2.59761187760021	Positive

Compound Spectra (overlaid)

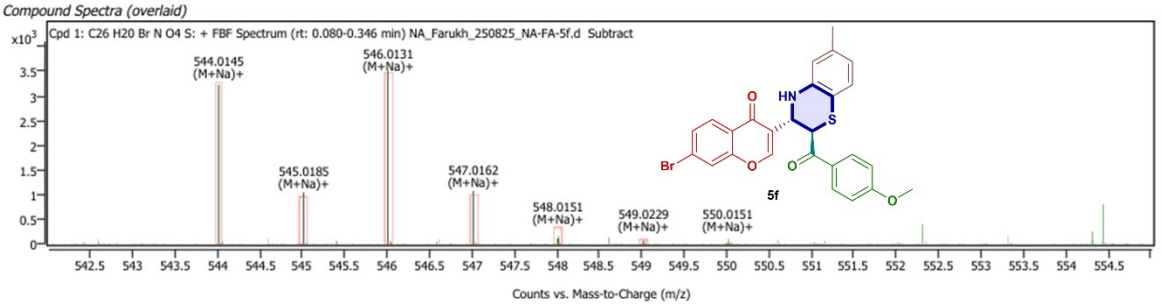


Compound Details

Cpd. 1: C26 H20 Br N O4 S

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C26 H20 Br N O4 S	521.0256	73.93	FBF	-7.71356243789015	Positive

Compound Spectra (overlaid)

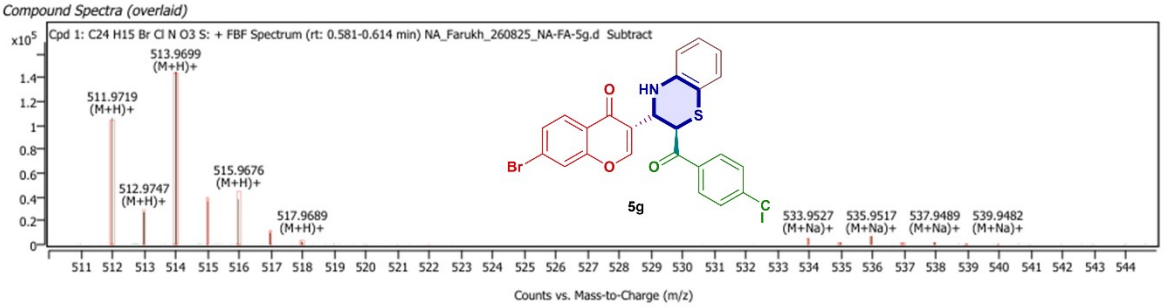


Compound Details

Cpd. 1: C24 H15 Br Cl N O3 S

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C24 H15 Br Cl N O3 S	510.9645	97.80	FBF	0.162886135924849	Positive

Compound Spectra (overlaid)

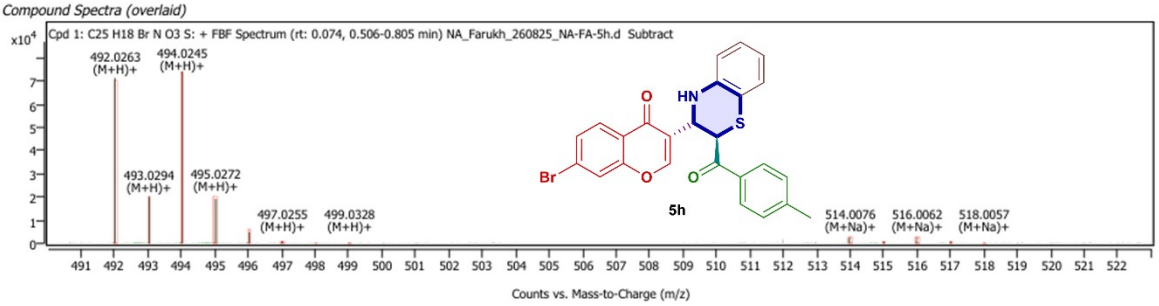


Compound Details

Cpd. 1: C25 H18 Br N O3 S

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C25 H18 Br N O3 S	491.0189	98.79	FBF	-0.261817294487753	Positive

Compound Spectra (overlaid)

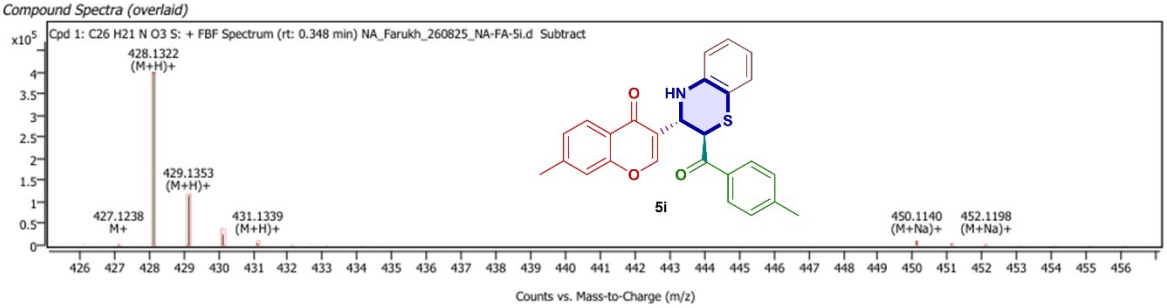


Compound Details

Cpd. 1: C26 H21 N O3 S

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C26 H21 N O3 S	427.1249	96.52	FBF	1.58912054041195	Positive

Compound Spectra (overlaid)

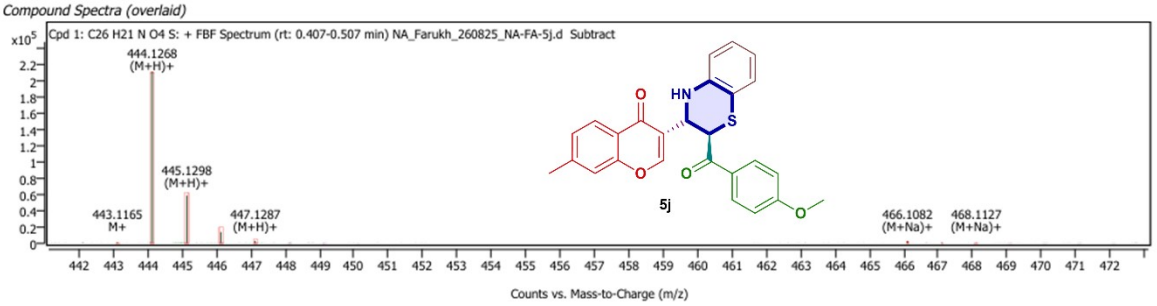


Compound Details

Cpd. 1: C26 H21 N O4 S

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C26 H21 N O4 S	443.1195	97.47	FBF	0.787567779243898	Positive

Compound Spectra (overlaid)

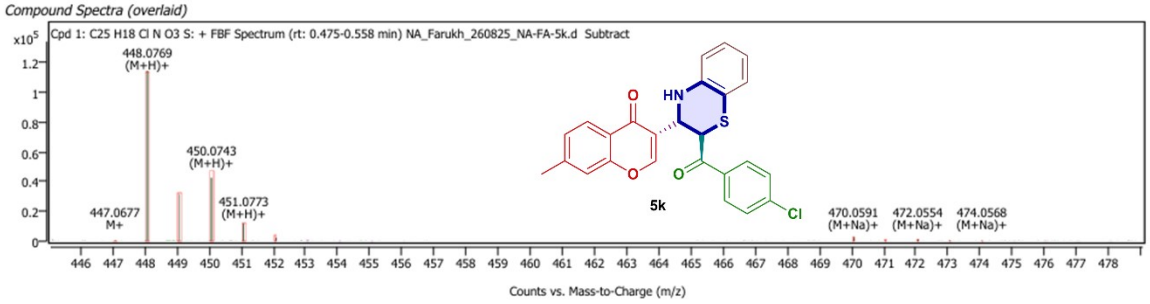


Compound Details

Cpd. 1: C25 H18 Cl N O3 S

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C25 H18 Cl N O3 S	447.0695	98.87	FBF	-0.163038303836211	Positive

Compound Spectra (overlaid)

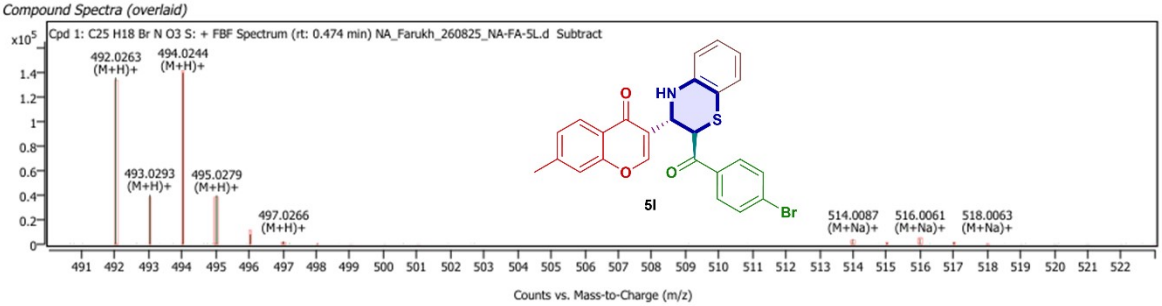


Compound Details

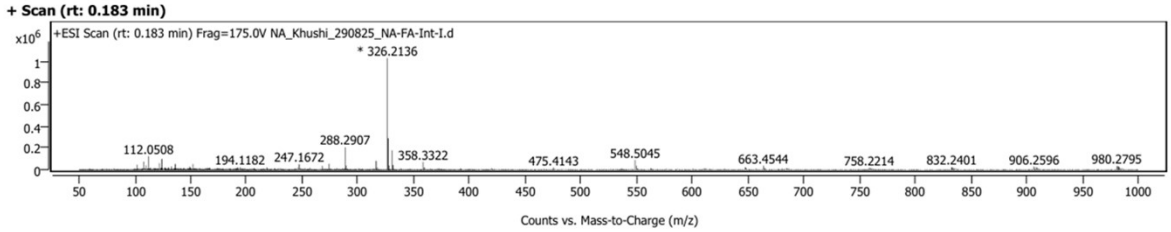
Cpd. 1: C25 H18 Br N O3 S

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C25 H18 Br N O3 S	491.0190	98.75	FBF	-0.0940643091961051	Positive

Compound Spectra (overlaid)



+ Scan (rt: 0.183 min)

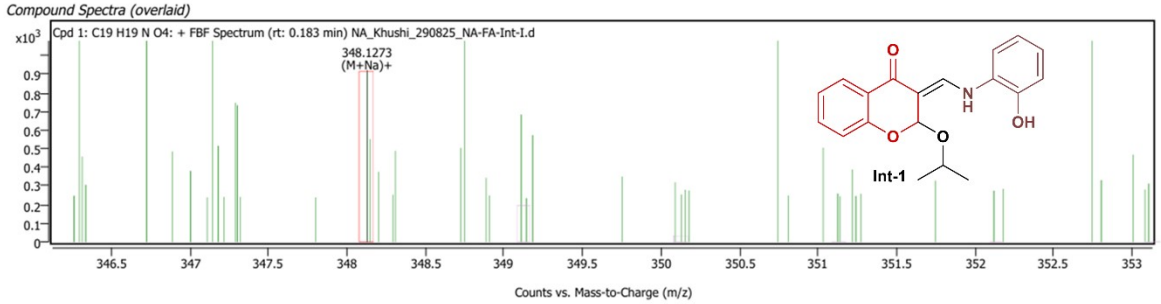


Compound Details

Cpd. 1: C19 H19 N O4

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C19 H19 N O4	325.1381	2.71	FBF	20.5697068166394	Positive

Compound Spectra (overlaid)

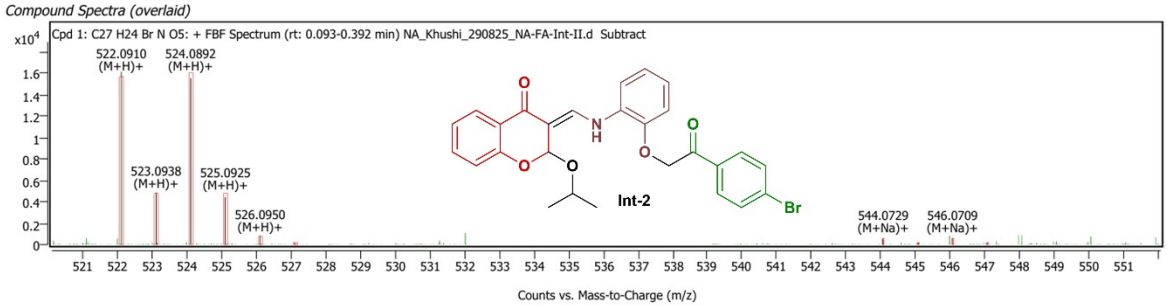


Compound Details

Cpd. 1: C27 H24 Br N O5

Formula	Mass	Score	Algorithm	Diff (Tgt, ppm)	Polarity
C27 H24 Br N O5	521.0836	98.57	FBF	-0.347761206503183	Positive

Compound Spectra (overlaid)



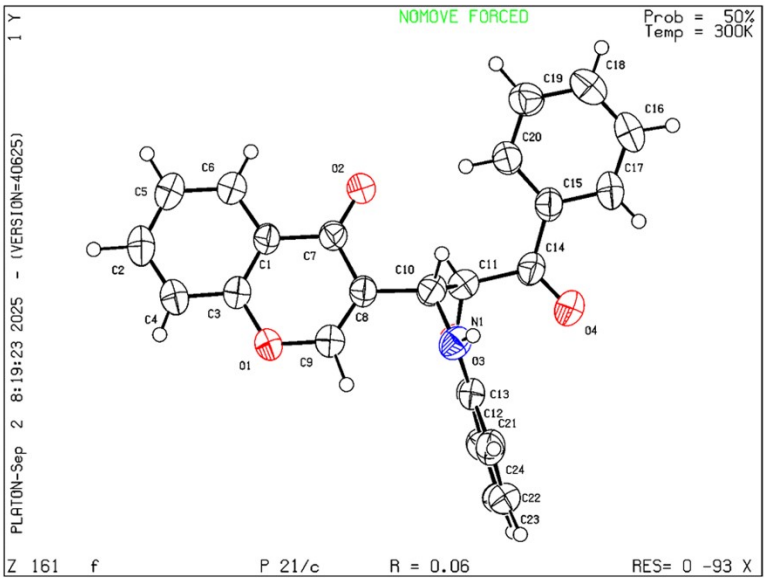


Figure S1. Single crystal-XRD image of **4a**

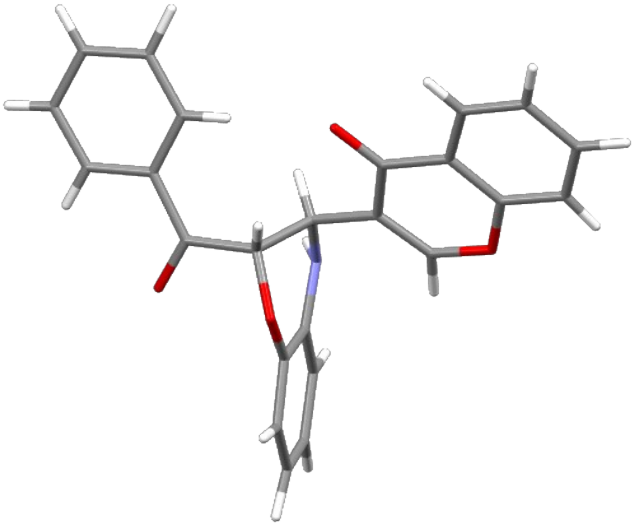


Figure S2. Single crystal-XRD image of **4a** using Mercury software

Table S1. Single crystal-XRD data of **4a**

Molecule code	**4a**
CCDC number	2484494
Empirical formula	$C_{24}H_{17}NO_4$
Formula weight (g/mol.)	383.38
Temperature (K)	300
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	P 21/c
Unit cell dimensions	A = 20.836(4) Å
	B = 7.1335(13) Å
	C = 21.837(5) Å
	α = 90°, β = 146.592(5)°, ϒ = 90°
Volume ($Å^3$)	1787.1(6)
Density(calculated) (g/cm^3)	1.425
Absorption coefficient (mm^{-1})	0.098
F(000)	800.0
Crystal size (mm^3)	0.0206 x 0.0089 x 0.0219
Theta maximum for data collection	19.6732°
Index ranges	-24 ≤ h ≤ 24, -8 ≤ k ≤ 8, -26 ≤ l ≤ 26
Reflections collected	3218
Independent reflections	3218 [R(int) = 0.1864]
Coverage of independent reflections	99.7%
Absorption correction	Multi-scan
Max. and min. Transmission	0.910 and 0.990
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3218 / 0 / 307
Goodness-of-fit on F^2	1.095
Final r indices [i>2sigma(i)]	0.043
R indices (all data)	0.0824
Largest diff. Peak and hole ($e.Å^{-3}$)	0.219 and -0.190

- Google Drive link for the CIF file of the above table: https://drive.google.com/drive/folders/1t-gmXgo8gv0lBObNm6fOiGdD3iiw5232?usp=sharing

f.cif

.cif file:

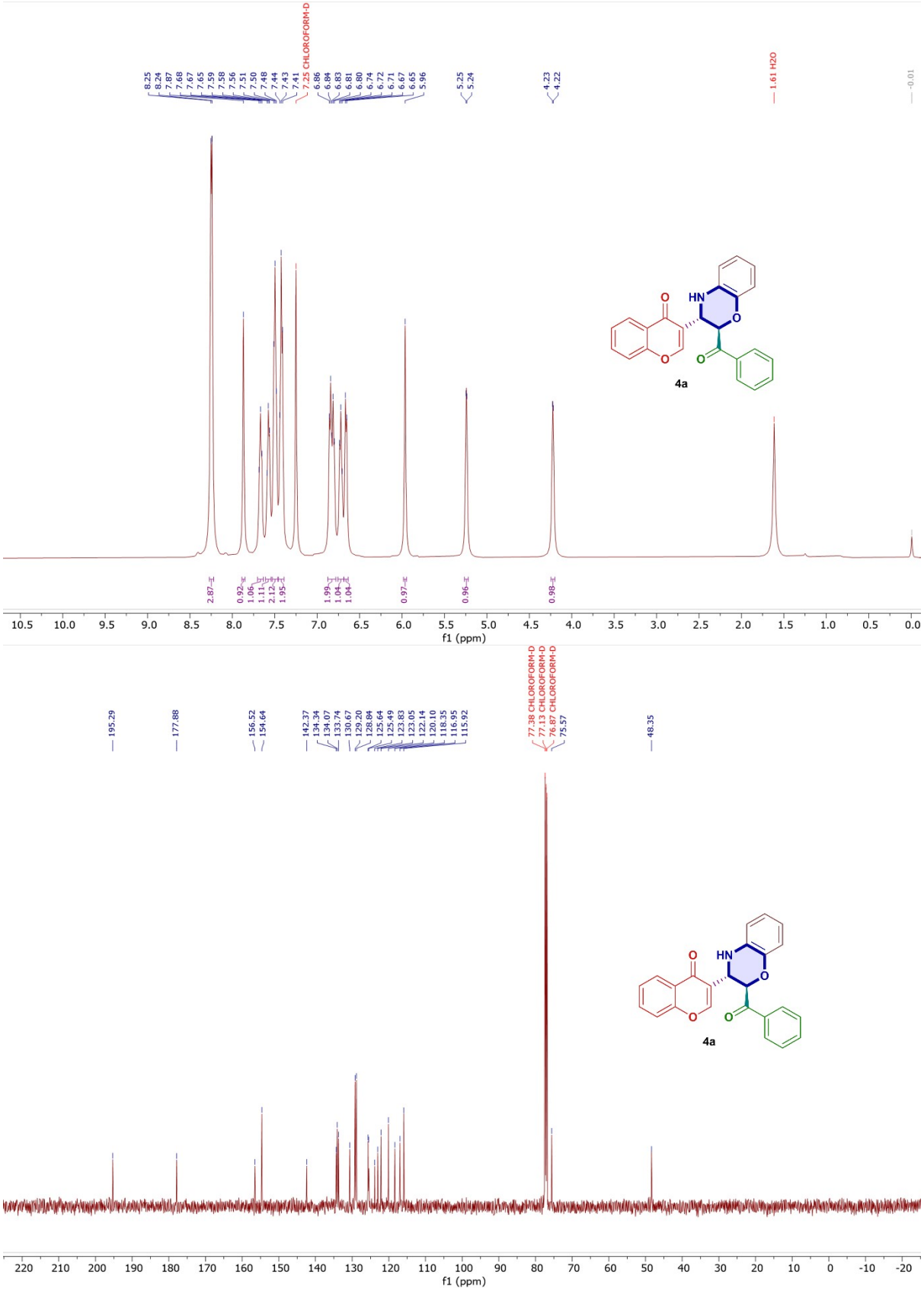


Figure S3. Crude ^{1}H and ^{13}C-NMR of **4a**

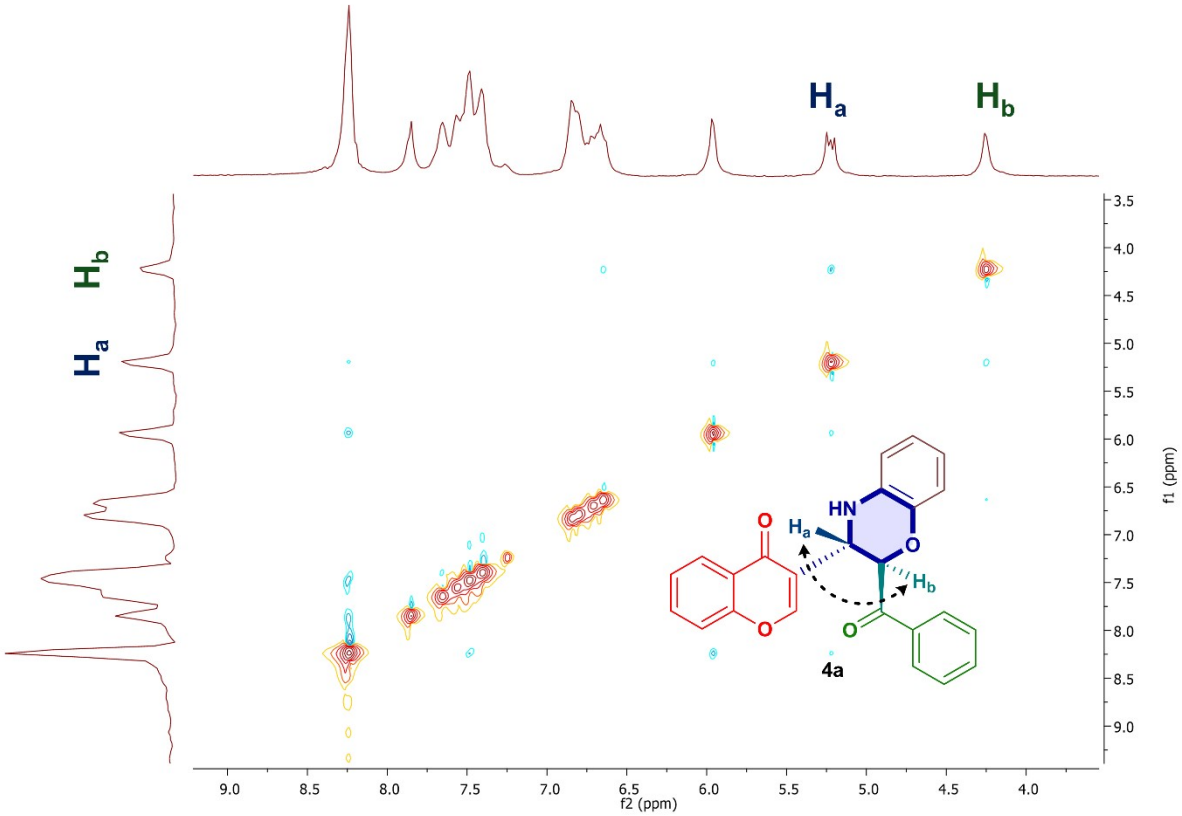


Figure S4.**1H-1H NOESY** experiment of **4a**