Synthesis and evaluation of highly selective quinazoline-2,4-dione ligands for sphingosine-1-phosphate receptor 2

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Supplementary data

Experimental

Chemistry

All the commercially available materials and solvents were obtained from Sigma-Aldrich and Fisher Scientific without further purification. Reactions were monitored by thin-layer chromatography (TLC) using fluorescent silica gel plates (60 F_{254} from EMD Chemicals Inc.) and visualized under ultraviolet light (wavelength 254). Chromatographic purifications were performed by flash column chromatography using 230–400 mesh silica gel purchased from Silicycle. Yields refer to isolate yield and melting points were measured by MEL-TEMP 3.0 melting point apparatus without correction. ^{1}H NMR and ^{13}C NMR spectra were recorded on Varian 400 MHz instrument, are reported in ppm using the solvent residual peak as an internal standard. High-resolution positive ion mass (HRMS) analyses were conducted on a Bruker MaXis 4G Q-TOF mass spectrometer with electrospray ionization source.

General method for the syntheses of 2a-k

A mixture of 2-(1-(2-((5-chloro-2,4-dimethoxyphenyl)amino)-2-oxoethyl)-2,4-dioxo-1,4-dihydroquinazolin-3(2H)-yl)-acetic acid (**1**) (1.0 eq),[27] HATU (1.5 eq), DIPEA (2.5 eq), and dimethyl sulfoxide (15 mL/mmol) was stirred for 5 min before adding the amines (1.1 eq). The reaction mixture was stirred at RT overnight and monitored by TLC. Upon the reaction was completed, the mixture was treated with water and the precipitate was filtered. The solid product was further washed with water and cold ethanol, then dried under vacuum.

***N*-(5-chloro-2,4-dimethoxyphenyl)-2-(3-(2-((2-hydroxyethyl)-amino)-2-oxoethyl)-2,4-dioxo-3,4-dihydroquinazolin-1(2*H*)-yl)acetamide (2a)**. Following the general method, compound **2a** was obtained from compound **1** and ethanolamine as white solid. Yield: 77%, mp: 284-286 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.72 (s, 1H), 8.22 – 8.14 (m, 1H), 8.08 (d, *J* = 7.8 Hz, 1H), 7.91 (s, 1H), 7.78 (t, *J* = 7.8 Hz, 1H), 7.42 – 7.30 (m, 2H), 6.87 (s, 1H), 5.06 (s, 2H), 4.71 (t, *J* = 5.3 Hz, 1H), 4.58 (s, 2H), 3.92 (s, 3H), 3.88 (s, 3H), 3.46 – 3.37 (m, 2H), 3.21 – 3.10 (m, 2H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 166.83, 166.01, 161.33, 152.00, 150.91, 150.28, 140.65, 135.89, 128.33, 123.46, 123.26, 120.65, 115.10, 115.05, 111.40, 98.42, 60.19, 56.81, 46.69, 46.18, 43.89, 42.03. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{22}H_{24}ClN_4O_7$ 491.1328, found 491.1330.

***N*-(5-chloro-2,4-dimethoxyphenyl)-2-(3-(2-((2-(2-hydroxy-ethoxy)ethyl)amino)-2-oxoethyl)-2,4-dioxo-3,4-dihydro-quinazolin-1(2*H*)-yl)acetamide (2b)**. Following the general method, compound **2b** was obtained from compound **1** and 2-(2-aminoethoxy)ethanol as white solid. Yield: 55%, mp: 260-261 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.68 (s, 1H), 8.18 (t, *J* = 5.4 Hz, 1H), 8.04 (d, *J* = 6.7 Hz, 1H), 7.87 (s, 1H), 7.75 (t, *J* = 7.9 Hz, 1H), 7.37 – 7.27 (m, 2H), 6.84 (s, 1H), 5.02 (s, 2H), 4.56 – 4.51 (m, 3H), 3.89 (s, 3H), 3.84 (s, 3H), 3.51 – 3.44 (m, 2H), 3.43 – 3.36 (m, 3H), 3.25 – 3.16 (m, 2H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 166.83, 166.00, 161.32, 151.98, 150.89, 150.26, 140.64, 135.90, 128.32, 123.47, 123.22, 120.63, 115.11, 115.03, 111.38, 98.40, 72.60, 69.39, 60.60, 56.82, 56.77, 46.68, 43.85, 39.24. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{24}H_{28}ClN_4O_8$ 535.1599, found 535.1597.

***N*-(5-chloro-2,4-dimethoxyphenyl)-2-(3-(2-((2-(2-(2-hydroxy-ethoxy)ethoxy)ethyl)amino)-2-oxoethyl)-2,4-dioxo-3,4-dihydroquinazolin-1(2*H*)-yl)acetamide (2c)**. Following the general method, compound **2c** was obtained from compound **1** and 2-[2-(2-aminoethoxy)ethoxy]ethanol as white solid. Yield: 34%, mp: 200-201 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.67 (s, 1H), 8.19 (t, *J* = 5.5 Hz, 1H), 8.04 (d, *J* = 7.8 Hz, 1H), 7.87 (s, 1H), 7.75 (t, *J* = 7.2 Hz, 1H), 7.39 – 7.26 (m, 2H), 6.84 (s, 1H), 5.02 (s, 2H), 4.58 – 4.48 (m, 3H), 3.89 (s, 3H), 3.84 (s, 3H), 3.52 – 3.49 (m, 3H), 3.48 – 3.43 (m, 2H), 3.42 – 3.35 (m, 4H), 3.24 – 3.16 (m, 2H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 166.85, 165.99, 161.31, 151.97, 150.88, 150.26, 140.63, 135.90, 128.32, 123.46, 123.22, 120.62, 115.11, 115.03, 111.36, 98.39, 72.77, 70.11, 70.08, 69.44, 60.63, 56.82, 56.77, 46.67, 43.85, 39.19. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{26}H_{32}ClN_4O_9$ 579.1852, found 579.1853.

***N*-(5-chloro-2,4-dimethoxyphenyl)-2-(3-(2-(methylamino)-2-oxoethyl)-2,4-dioxo-3,4-dihydroquinazolin-1(2*H*)-yl)acet-amide (2d)**. Following the general method, compound **2d** was obtained from compound **1** and methylamine as white solid. Yield: 56%, mp: 307-309 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.72 (s, 1H), 8.11 – 8.03 (m, 2H), 7.91 (s, 1H), 7.78 (t, *J* = 7.6 Hz, 1H), 7.41 – 7.30 (m, 2H), 6.87 (s, 1H), 5.06 (s, 2H), 4.54 (s, 2H), 3.92 (s, 3H), 3.88 (s, 3H), 2.60 (d, *J* = 4.5 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 167.18, 166.02, 161.37, 152.00, 150.91, 150.29, 140.67, 135.89, 128.32, 123.46, 123.26, 120.62, 115.12, 111.38, 98.40, 56.83, 56.78, 46.72, 43.98, 25.94. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{21}H_{22}ClN_4O_6$ 461.1222, found 461.1225.

2-(1-(2-((5-chloro-2,4-dimethoxyphenyl)amino)-2-oxoethyl)-2,4-dioxo-1,4-dihydroquinazolin-3(2*H*)-yl)-*N*,*N*-dimethylacet-amide (2e). Following the general method, compound **2e** was obtained from compound **1** and dimethylamine as white solid. Yield: 46%, mp: 253-255 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.74 (s, 1H), 8.07 (d, *J* = 7.4 Hz, 1H), 7.93 (s, 1H), 7.78 (t, *J* = 7.7 Hz, 1H), 7.43 – 7.29 (m, 2H), 6.87 (s, 1H), 5.07 (s, 2H), 4.81 (s, 2H), 3.93 (s, 3H), 3.88 (s, 3H), 3.09 (s, 3H), 2.85 (s, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 166.08, 165.95, 161.26, 151.94, 150.85, 150.18, 140.62,

135.95, 128.32, 123.51, 123.10, 120.72, 115.13, 114.91, 111.41, 98.42, 56.86, 56.77, 46.60, 42.99, 36.22, 35.53. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{22}H_{24}ClN_4O_6$ 475.1379, found 475.1378.

***N*-(5-chloro-2,4-dimethoxyphenyl)-2-(2,4-dioxo-3-(2-oxo-2-((2-(pyridin-3-yl)ethyl)amino)ethyl)-3,4-dihydro-quinazolin-1(2*H*)-yl)acetamide (2f)**. Following the general method, compound **2f** was obtained from compound **1** and 2-(pyridin-3-yl)ethan-1-amine as white solid. Yield: 55%, mp: 248-249 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.73 (s, 1H), 8.49 – 8.38 (m, 2H), 8.28 (s, 1H), 8.09 (d, *J* = 7.5 Hz, 1H), 7.92 (s, 1H), 7.78 (d, *J* = 7.3 Hz, 1H), 7.64 (d, *J* = 7.1 Hz, 1H), 7.44 – 7.28 (m, 3H), 6.88 (s, 1H), 5.07 (s, 2H), 4.55 (s, 2H), 3.93 (s, 3H), 3.88 (s, 3H), 3.33 – 3.27 (m, 2H), 2.79 – 2.69 (m, 2H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 166.84, 166.02, 161.35, 152.01, 150.91, 150.30, 147.85, 140.66, 136.72, 135.89, 135.28, 128.34, 123.84, 123.47, 123.28, 123.26, 120.65, 115.10, 111.41, 98.43, 56.86, 56.77, 46.71, 43.96, 40.37, 32.49. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{27}H_{27}ClN_5O_6$ 552.1644, found 552.1647.

***N*-(5-chloro-2,4-dimethoxyphenyl)-2-(3-(2-((2-methoxy-phenyl)amino)-2-oxoethyl)-2,4-dioxo-3,4-dihydroquinazolin-1(2*H*)-yl)acetamide (2g)**. Following the general method, compound **2g** was obtained from compound **1** and *o*-anisidine as white solid. Yield: 52%, mp: 274-276 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.74 (s, 1H), 9.62 (s, 1H), 8.09 (d, *J* = 7.7 Hz, 1H), 7.98 – 7.88 (m, 2H), 7.84 – 7.75 (m, 1H), 7.45 – 7.29 (m, 2H), 7.10 – 7.01 (m, 2H), 6.92 – 6.82 (m, 2H), 5.08 (s, 2H), 4.88 (s, 2H), 3.92 (s, 3H), 3.87 (s, 6H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 165.98, 165.78, 161.36, 151.98, 150.93, 150.25, 149.71, 140.65, 136.02, 128.37, 127.44, 124.80, 123.57, 123.18, 121.84, 120.68 (2C), 115.18, 114.92, 111.64, 111.41, 98.43, 56.87, 56.77, 56.12, 46.68, 44.62. HRMS (ESI) m/z $[M+H]^+$ Calcd. for $C_{27}H_{26}ClN_4O_7$ 553.1485, found 553.1490.

***N*-(5-chloro-2,4-dimethoxyphenyl)-2-(3-(2-((3-methoxyphenyl)amino)-2-oxoethyl)-2,4-dioxo-3,4-dihydro-quinazolin-1(2*H*)-yl)acetamide (2h)**. Following the general method, compound **2h** was obtained from compound **1** and *m*-anisidine as white solid. Yield: 54%, mp: 257-258 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 10.32 (s, 1H), 9.74 (s, 1H), 8.10 (d, *J* = 7.1 Hz, 1H), 7.93 (s, 1H), 7.80 (t, *J* = 7.3 Hz, 1H), 7.41 (d, *J* = 8.7 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.30 (s, 1H), 7.22 (t, *J* = 8.2 Hz, 1H), 7.09 (d, *J* = 8.1 Hz, 1H), 6.87 (s, 1H), 6.64 (d, *J* = 7.8 Hz, 1H), 5.09 (s, 2H), 4.79 (s, 2H), 3.92 (s, 3H), 3.88 (s, 3H), 3.72 (s, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 165.96, 165.64, 161.36, 159.97, 151.98, 150.92, 150.24, 140.65, 140.35, 136.05, 130.04, 128.37, 123.60, 123.20, 120.67, 115.21, 114.92, 111.65, 111.41, 109.44, 105.08, 98.42, 56.86, 56.76, 55.35, 46.70, 44.54. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{27}H_{26}ClN_4O_7$ 553.1485, found 553.1491.

***N*-(5-chloro-2,4-dimethoxyphenyl)-2-(3-(2-((4-methoxy-phenyl)amino)-2-oxoethyl)-2,4-dioxo-3,4-dihydroquinazolin-1(2*H*)-yl)acetamide (2i)**. Following the general method, compound **2i** was obtained from compound **1** and *p*-anisidine as white solid. Yield: 16%, mp: 284-286 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 10.11 (s, 1H), 9.69 (s, 1H), 8.05 (d, *J* = 7.8 Hz, 1H), 7.88 (s, 1H), 7.76 (t, *J* = 7.8 Hz, 1H), 7.43 (d, *J* = 8.7 Hz, 2H), 7.38 – 7.28 (m, 2H), 6.88 – 6.81 (m, 3H), 5.04 (s, 2H), 4.71 (s, 2H), 3.88 (s, 3H), 3.84 (s, 3H), 3.68 (s, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 165.95, 165.05, 161.36, 155.66, 151.96, 150.92, 150.22, 140.64, 136.01, 132.30, 128.35, 123.56, 123.17, 120.96, 120.65, 115.18, 114.94, 114.32, 111.37, 98.39, 56.82, 56.77, 55.55, 46.68, 44.39. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{27}H_{26}ClN_4O_7$ 553.1485, found 553.1490.

***N*-(5-chloro-2,4-dimethoxyphenyl)-2-(3-(2-((2-hydroxyphenyl)amino)-2-oxoethyl)-2,4-dioxo-3,4-dihydroquinazolin-1(2H)-yl)acetamide (2j).** Following the general method, compound **2j** was obtained from compound **1** and 3-aminophenol as white solid. Yield: 62%, mp: 288-290 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 10.17 (s, 1H), 9.74 (s, 1H), 9.39 (s, 1H), 8.10 (d, *J* = 7.8 Hz, 1H), 7.93 (s, 1H), 7.80 (t, *J* = 7.6 Hz, 1H), 7.40 (d, *J* = 8.5 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.14 – 7.03 (m, 2H), 6.95 (d, *J* = 8.5 Hz, 1H), 6.87 (s, 1H), 6.46 (d, *J* = 8.0 Hz, 1H), 5.09 (s, 2H), 4.76 (s, 2H), 3.92 (s, 3H), 3.88 (s, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 165.96, 165.39, 161.36, 158.07, 151.98, 150.92, 150.25, 140.65, 140.17, 136.02, 129.88, 128.37, 123.58, 123.17, 120.68, 115.20, 114.94, 111.41, 110.95, 110.21, 106.66, 98.43, 56.86, 56.77, 46.69, 44.53. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{26}H_{24}ClN_4O_7$ 539.1328, found 539.1334.

***N*-(5-chloro-2,4-dimethoxyphenyl)-2-(3-(2-((4-hydroxy-phenyl)amino)-2-oxoethyl)-2,4-dioxo-3,4-dihydroquinazolin-1(2*H*)-yl)acetamide (2k)**. Following the general method, compound **2k** was obtained from compound **1** and 4-aminophenol as white solid. Yield: 24%, mp: 319-321 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.98 (s, 1H), 9.70 (s, 1H), 9.16 (s, 1H), 8.06 (d, *J* = 7.3 Hz, 1H), 7.88 (s, 1H), 7.76 (t, *J* = 7.4 Hz, 1H), 7.39 – 7.32 (m, 1H), 7.30 (d, *J* = 8.5 Hz, 2H), 6.84 (s, 1H), 6.65 (d, *J* = 8.8 Hz, 2H), 5.04 (s, 2H), 4.70 (s, 2H), 3.89 (s, 3H), 3.84 (s, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 165.96, 164.82, 161.36, 153.78, 151.95, 150.91, 150.22, 140.64, 135.99, 130.80, 128.34, 123.55, 123.17, 121.19, 120.63, 115.53, 115.18, 114.95, 111.35, 98.38, 56.81, 56.77, 46.67, 44.35. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{26}H_{24}ClN_4O_7$ 539.1328, found 539.1331.

2-(2,4-Dioxo-1,4-dihydroquinazolin-3(2H)-yl)-*N*-(2-methoxyphenyl)acetamide (4)

A mixture of 2-(2,4-dioxo-1,4-dihydroquinazolin-3(2*H*)-yl)acetic acid (**3**)[30] (1.10 g, 5.0 mmol), *o*-anisidine (0.68 g, 5.5 mmol), HATU (2.85 g, 7.5 mmol), DIPEA (1.61 g, 12.5 mmol), and dichloromethane (40 mL) was stirred at room temperature. The reaction was stirred at room temperature overnight until the reaction was completed as determined by TLC. Then, the mixture was concentrated under vacuum. To the residue was added 1N HCl and the mixture was

stirred for 30 min at room temperature. The solid was filtered and dried as white solid. (1.4 g, 85%). ^{1}H NMR (400 MHz, DMSO-*d6*) δ 11.54 (s, 1H), 9.59 (s, 1H), 7.93 (dd, *J* = 12.9, 7.9 Hz, 2H), 7.74 – 7.67 (m, 1H), 7.24 (t, *J* = 7.9 Hz, 2H), 7.07 (d, *J* = 3.1 Hz, 2H), 6.93 – 6.86 (m, 1H), 4.80 (s, 2H), 3.87 (s, 3H).

General method for the syntheses of 5a-h

To a round-bottomed flask equipped with a magnetic stir bar were added **4** (1.0 eq), bromides (1.1 eq), K_2CO_3 (2.0 eq), and DMF (6.0 mL/mmol). The reaction was stirred at room temperature overnight until the reaction was completed as determined by TLC. Then, the reaction mixture was treated with water, the precipitate was filtered and washed with cold ethanol. The collected solid was dried under air.

***N*-(5-chloro-2-methoxyphenyl)-2-(3-(2-((2-methoxyphenyl)amino)-2-oxoethyl)-2,4-dioxo-3,4-dihydro-quinazolin-1(2*H*)-yl)acetamide (5a)**. Following the general method, compound **5a** was obtained from compound **4** and 2-bromo-*N*-(5-chloro-2-methoxyphenyl)acetamide as white solid. Yield: 76%, mp: 218-219 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.88 (s, 1H), 9.60 (s, 1H), 8.05-8.10 (m, 2H), 7.90 (d, *J* = 7.4 Hz, 1H), 7.76 (t, *J* = 7.9 Hz, 1H), 7.39 (d, *J* = 8.4 Hz, 1H), 7.32 (t, *J* = 7.6 Hz, 1H), 7.21 – 6.98 (m, 4H), 6.86 (s, 1H), 5.12 (s, 2H), 4.85 (s, 2H), 3.86 (d, *J* = 7.6 Hz, 6H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 166.50, 165.76, 161.34, 150.92, 149.70, 148.36, 140.64, 136.05, 128.66, 128.40, 127.43, 124.79, 124.30, 124.09, 123.59, 121.84, 120.79, 120.67, 115.17, 114.89, 113.02, 111.62, 56.58, 56.13, 46.86, 44.62. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{26}H_{24}ClN_4O_6$ 523.1379, found 523.1381.

2-(1-(2-(4-Fluorophenyl)-2-oxoethyl)-2,4-dioxo-1,4-dihydro-quinazolin-3(2*H*)-yl)-*N*-(2-methoxyphenyl)acetamide (5b)

Following the general method, compound **5b** was obtained from compound **4** and 2-bromo-1-(4-fluorophenyl)ethan-1-one as white solid. Yield: 37%, mp: 224-226 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.62 (s, 1H), 8.29 – 8.18 (m, 2H), 8.12 (d, *J* = 8.1 Hz, 1H), 7.93 (d, *J* = 7.2 Hz, 1H), 7.73 (t, *J* = 7.7 Hz, 1H), 7.51 – 7.31 (m, 4H), 7.06 (s, 2H), 6.88 (s, 1H), 5.81 (s, 2H), 4.87 (s, 2H), 3.86 (s, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 192.06, 166.01 (d, *J* = 166.0 Hz), 165.73, 161.35, 150.84, 149.67, 140.57, 136.04, 131.85 (d, *J* = 10.1 Hz, 2C), 131.54 (d, *J* = 3.0 Hz), 128.46, 127.42, 124.77, 123.62, 121.80, 120.66, 116.46 (d, *J* = 22.2 Hz, 2C), 115.31, 114.88, 111.61, 56.12, 50.52, 44.60. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{25}H_{21}FN_3O_5$ 462.1460, found 462.1460.

***N*-(2-Methoxyphenyl)-2-(1-(2-(2-methoxyphenyl)-2-oxoethyl)-2,4-dioxo-1,4-dihydroquinazolin-3(2*H*)-yl)acetamide (5c)**

Following the general method, compound **5c** was obtained from compound **4** and 2-bromo-1-(2-methoxyphenyl)ethan-1-one as white solid. Yield: 59%, mp: 252-254 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.61 (s, 1H), 8.11 (d, *J* = 7.6 Hz, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.80 – 7.65 (m, 3H), 7.37 – 7.24 (m, 3H), 7.11 (t, *J* = 7.4 Hz, 1H), 7.06 (s, 2H), 6.88 (s, 1H), 5.59 (s, 2H), 4.87 (s, 2H), 4.02 (s, 3H), 3.87 (s, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 193.44, 165.75, 161.37, 160.08, 150.86, 149.66, 140.50, 136.03, 135.87, 130.58, 128.39, 127.43, 124.77, 124.65, 123.51, 121.80, 121.20, 120.66, 115.31, 114.81, 113.26, 111.60, 56.51, 56.11, 54.29, 44.57. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{26}H_{24}N_3O_6$ 474.1660, found 474.1661.

***N*-(2,6-dichloropyridin-4-yl)-2-(3-(2-((2-methoxyphenyl)-amino)-2-oxoethyl)-2,4-dioxo-3,4-dihydroquinazolin-1(2*H*)-yl)acetamide (5d)**. Following the general method, compound **5d** was obtained from compound **4** and 2-bromo-*N*-(2,6-dichloropyridin-4-yl)acetamide as white solid. Yield: 82%, mp: 298-300 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 11.25 (s, 1H), 9.62 (s, 1H), 8.11 (d, *J* = 7.8 Hz, 1H), 7.92 (d, *J* = 7.8 Hz, 1H), 7.79 (t, *J* = 7.9 Hz, 1H), 7.63 (s, 2H), 7.48 (d, *J* = 8.5 Hz, 1H), 7.36 (t, *J* = 7.5 Hz, 1H), 7.06 (s, 2H), 6.93 – 6.84 (m, 1H), 5.07 (s, 2H), 4.87 (s, 2H), 3.87 (s, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 167.77, 165.66, 161.27, 150.89, 150.28, 150.09, 149.66, 140.50, 136.06, 128.43, 127.38, 124.79, 123.74, 121.80, 120.65, 115.28, 114.86, 112.35, 111.60, 56.11, 47.16, 44.59. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{24}H_{20}Cl_2N_5O_5$ 528.0836, found 528.0838.

2-(1-(4-Fluorobenzyl)-2,4-dioxo-1,4-dihydroquinazolin-3(2*H*)-yl)-*N*-(2-methoxyphenyl)acetamide (5e). Following the general method, compound **5e** was obtained from compound **4** and 4-fluorobenzyl bromide as white solid. Yield: 51%, mp: 203-204 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.66 (s, 1H), 8.09 (d, *J* = 7.8 Hz, 1H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.71 (t, *J* = 7.8 Hz, 1H), 7.40 – 7.27 (m, 4H), 7.17 (t, *J* = 8.8 Hz, 2H), 7.07 (s, 2H), 6.93 – 6.86 (m, 1H), 5.39 (s, 2H), 4.91 (s, 2H), 3.87 (s, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 165.93, 161.79 (d, *J* = 244.4 Hz, 1C), 161.36, 160.58, 151.20, 149.82, 139.87, 135.93, 132.76, 129.03 (d, *J* = 8.1 Hz, 2C), 128.57, 127.37, 124.87, 123.60, 122.08, 120.66, 115.93 (d, *J* = 21.2 Hz, 2C), 115.44 (d, *J* = 4.0 Hz, 1C), 111.65, 56.12, 45.98, 44.73. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{24}H_{21}FN_3O_4$ 434.1511, found 434.1510.

***N*-(2-methoxyphenyl)-2-(1-(2-(4-methoxyphenyl)-2-oxoethyl)-2,4-dioxo-1,4-dihydroquinazolin-3(2*H*)-yl)acetamide (5f).**

Following the general method, compound **5f** was obtained from compound **4** and 2-bromo-4'-methoxyacetophenone as white solid. Yield: 76%, mp: 248-249 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.61 (s, 1H), 8.11 (d, *J* = 8.6 Hz, 3H), 7.93 (d,

J = 8.0 Hz, 1H), 7.73 (t, *J* = 7.9 Hz, 1H), 7.37 – 7.30 (m, 2H), 7.13 (d, *J* = 8.7 Hz, 2H), 7.06 (s, 2H), 6.92 – 6.84 (m, 1H), 5.75 (s, 2H), 4.87 (s, 2H), 3.87 (d, *J* = 9.5 Hz, 6H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 191.53, 165.74, 164.30, 161.37, 150.86, 149.67, 140.65, 136.01, 131.07, 128.43, 127.69, 127.43, 124.77, 123.54, 121.80, 120.66, 115.31, 114.86, 114.59, 111.61, 56.12 (2C), 50.19, 44.59. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{26}H_{24}N_3O_6$ 474.160, found 474.1660.

2-(1-(2-(3-Chloro-4-methoxyphenyl)-2-oxoethyl)-2,4-dioxo-1,4-dihydroquinazolin-3(2*H*)-yl)-*N*-(2-methoxyphenyl)-acetamide (5g). Following the general method, compound **5g** was obtained from compound **4** and 2-bromo-1-(3-chloro-4-methoxyphenyl)ethan-1-one as white solid. Yield: 39%, mp: 257-259 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.62 (s, 1H), 8.20 (s, 1H), 8.16 – 8.07 (m, 2H), 7.94 (d, *J* = 7.9 Hz, 1H), 7.73 (t, *J* = 7.8 Hz, 1H), 7.42 – 7.30 (m, 3H), 7.13 – 7.04 (m, 2H), 6.95 – 6.85 (m, 1H), 5.78 (s, 2H), 4.88 (s, 2H), 3.99 (s, 3H), 3.86 (s, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 191.16, 165.73, 161.35, 159.40, 150.83, 149.68, 140.58, 136.03, 130.46, 129.84, 128.45, 128.26, 127.43, 124.78, 123.60, 122.02, 121.81, 120.67, 115.30, 114.88, 113.12, 111.62, 57.23, 56.16, 50.32, 44.60. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{26}H_{23}ClN_3O_6$ 508.1270, found 508.1274.

2-(1-(2-(3-chloro-4-ethoxyphenyl)-2-oxoethyl)-2,4-dioxo-1,4-dihydroquinazolin-3(2*H*)-yl)-*N*-(2-methoxyphenyl)acetamide (5h). Following the general method, compound **5h** was obtained from compound **4** and 2-bromo-1-(3-chloro-4-ethoxyphenyl)ethan-1-one as white solid. Yield: 15%, mp: 227-228 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.58 (s, 1H), 8.16 (s, 1H), 8.07 (t, *J* = 7.9 Hz, 2H), 7.89 (d, *J* = 7.7 Hz, 1H), 7.73 – 7.66 (m, 1H), 7.37 – 7.27 (m, 3H), 7.02 (s, 2H), 6.89 – 6.82 (m, 1H), 5.74 (s, 2H), 4.83 (s, 2H), 4.31 – 4.20 (m, 2H), 3.83 (s, 3H), 1.37 (t, *J* = 6.7 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 191.12, 165.70, 161.33, 158.71, 150.81, 149.65, 140.57, 136.02, 130.51, 129.79, 128.43, 128.06, 127.41, 124.76, 123.58, 122.09, 121.79, 120.65, 115.30, 114.85, 113.74, 111.60, 65.44, 56.11, 50.30, 44.56, 14.79. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{27}H_{25}ClN_3O_6$ 522.1426, found 522.1428.

General method for the syntheses of 7a-e

To a round-bottomed flask equipped with a magnetic stir bar were added isatoic anhydride (1.0 eq), amines (1.0 eq), Et_3N (5.0 eq), and ethyl acetate (3.0 mL/mmol). The reaction mixture was stirred at 80 °C overnight until the reaction was completed as determined by TLC. After cooling to room temperature, the mixture was washed with 1 N NaOH (aqueous), saturated brine, and dried over anhydrous $MgSO_4$. After filtering and concentration, the crude product was obtained which was used directly for the next step.

To a round-bottomed flask equipped with a magnetic stir bar were added crude intermediates (1.0 eq), triphosgene (0.5 eq), and dichloromethane (5.0 mL/mmol). After 5 min, DIPEA (2.0 eq) was added dropwise and the mixture was stirred at room temperature for 3 h until the reaction was completed as determined by TLC. After removal of the solvent under vacuum, to the residue was added 1 N HCl and the mixture was stirred for 30 min at room temperature. The formed solid was filtered and washed with ethyl ether. After drying, the pure product was collected as white solid.

3-Benzylquinazoline-2,4(1*H*,3*H*)-dione (7a). Following the general method, compound **7a** was obtained from isatoic anhydride and benzylamine. Yield: 93%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.56 (s, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.67 (t, *J* = 7.6 Hz, 1H), 7.31 (d, *J* = 3.9 Hz, 3H), 7.21 (t, *J* = 8.1 Hz, 2H), 5.09 (s, 2H).

3-(2-Fluoroethyl)quinazoline-2,4(1*H*,3*H*)-dione (7b). Following the general method, compound **7b** was obtained from isatoic anhydride and 2-fluoroethylamine hydrochloride. Yield: 37%. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 10.79 (s, 1H), 8.47 (d, *J* = 8.0 Hz, 1H), 8.12 (t, *J* = 7.6 Hz, 1H), 7.78 – 7.64 (m, 2H), 5.17 (t, *J* = 5.5 Hz, 1H), 5.05 (t, *J* = 5.5 Hz, 1H), 4.82 (t, *J* = 5.5 Hz, 1H), 4.76 (t, *J* = 5.5 Hz, 1H).

3-Methylquinazoline-2,4(1*H*,3*H*)-dione (7c). Following the general method, compound **7c** was obtained from isatoic anhydride and methylamine hydrochloride. Yield: 73%. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 11.44 (s, 1H), 7.91 (d, *J* = 7.9 Hz, 1H), 7.64 (t, *J* = 7.7 Hz, 1H), 7.24 – 7.11 (m, 2H), 3.25 (s, 3H).

3-Ethylquinazoline-2,4(1*H*,3*H*)-dione (7d). Following the general method, compound **7d** was obtained from isatoic anhydride and ethylamine. Yield: 65%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.23 (s, 1H), 8.14 (d, *J* = 7.9 Hz, 1H), 7.61 (t, *J* = 7.7 Hz, 1H), 7.23 (t, *J* = 7.6 Hz, 1H), 7.13 (d, *J* = 8.1 Hz, 1H), 4.17 (q, *J* = 7.1 Hz, 2H), 1.32 (t, *J* = 7.1 Hz, 3H).

***N*-cyclopentyl-4-(2,4-dioxo-1,4-dihydroquinazolin-3(2*H*)-yl)-butanamide (7e)**. Following the general method, compound **7e** was obtained from isatoic anhydride and 4-amino-*N*-cyclopentylbutanamide. Yield: 86%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.71 (s, 1H), 8.12 (d, *J* = 7.8 Hz, 1H), 7.61 (t, *J* = 7.7 Hz, 1H), 7.23 (t, *J* = 7.6 Hz, 1H), 7.13 (d, *J* = 8.2 Hz, 1H), 6.19 (d, *J* = 7.0 Hz, 1H), 4.25 – 4.10 (m, 3H), 2.26 (t, *J* = 7.0 Hz, 2H), 2.08 (p, *J* = 6.7 Hz, 2H), 2.01 – 1.90 (m, 2H), 1.74 – 1.65 (m, 2H), 1.63 – 1.53 (m, 2H), 1.48 – 1.35 (m, 2H).

General method for the syntheses of 8a-e or 9a-e

To a round-bottomed flask equipped with a magnetic stir bar were added **7a-e** (1.0 eq), 2-bromo-1-(3-chloro-4-ethoxyphenyl)ethan-1-one or 2-bromo-*N*-(5-chloro-2,4-dimethoxyphenyl)acetamide (1.2 eq), K_2CO_3 (2.0 eq), and DMF

(6.0 mL/mmol). The reaction was stirred at room temperature overnight until the reaction was completed as determined by TLC. Then, the reaction mixture was treated with water and the precipitate was filtered. The collected solid was washed with water and cold acetone as the white solid product.

3-Benzyl-1-(2-(3-chloro-4-ethoxyphenyl)-2-oxoethyl)-quinazoline-2,4(1*H*,3*H*)-dione (8a). Following the general method, compound **8a** was obtained from **7a** and 2-bromo-1-(3-chloro-4-ethoxyphenyl)ethan-1-one. Yield: 58%, mp: 196-197 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 7.9 Hz, 1H), 8.07 (d, *J* = 2.1 Hz, 1H), 7.93 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.56 (t, *J* = 7.8 Hz, 1H), 7.51 (d, *J* = 7.1 Hz, 2H), 7.31 (t, *J* = 7.3 Hz, 2H), 7.26 – 7.21 (m, 2H), 6.99 (d, *J* = 8.7 Hz, 1H), 6.82 (d, *J* = 8.5 Hz, 1H), 5.53 (s, 2H), 5.29 (s, 2H), 4.22 (q, *J* = 6.9 Hz, 2H), 1.53 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 191.23, 161.48, 158.72, 150.96, 140.57, 137.44, 135.98, 130.52, 129.81, 128.79, 128.50, 128.03, 127.91, 127.63, 123.54, 122.11, 115.22, 114.96, 113.71, 65.44, 50.37, 44.70, 14.79. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{25}H_{22}ClN_2O_4$ 449.1263, found 449.1264.

1-(2-(3-Chloro-4-ethoxyphenyl)-2-oxoethyl)-3-(2-fluoroethyl)-quinazoline-2,4(1*H*,3*H*)-dione (8b). Following the general method, compound **8b** was obtained from **7b** and 2-bromo-1-(3-chloro-4-ethoxyphenyl)ethan-1-one. Yield: 38%, mp: 197-199 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.19 (s, 1H), 8.10 (t, *J* = 6.9 Hz, 2H), 7.71 (t, *J* = 7.6 Hz, 1H), 7.40 – 7.29 (m, 3H), 5.77 (s, 2H), 4.75 – 4.66 (m, 1H), 4.64 – 4.56 (m, 1H), 4.39 – 4.21 (m, 4H), 1.41 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 191.18, 161.54, 158.73, 150.85, 140.54, 135.95, 130.52, 129.80, 128.43, 128.04, 123.53, 122.12, 115.21, 114.92, 113.73, 81.10 (d, *J* = 166.7 Hz), 65.45, 50.29, 41.69 (d, *J* = 22.2 Hz), 14.79. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{20}H_{19}ClFN_2O_4$ 405.1012, found 405.1012.

1-(2-(3-Chloro-4-ethoxyphenyl)-2-oxoethyl)-3-methylquinazoline-2,4(1*H*,3*H*)-dione (8c). Following the general method, compound **8c** was obtained from **7c** and 2-bromo-1-(3-chloro-4-ethoxyphenyl)ethan-1-one. Yield: 53%, mp: 182-184 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 7.9 Hz, 1H), 8.09 (d, *J* = 2.0 Hz, 1H), 7.96 (dd, *J* = 8.6, 2.0 Hz, 1H), 7.56 (t, *J* = 7.9 Hz, 1H), 7.26 – 7.22 (m, 1H), 7.02 (d, *J* = 8.6 Hz, 1H), 6.82 (d, *J* = 8.4 Hz, 1H), 5.55 (s, 2H), 4.23 (q, *J* = 7.0 Hz, 2H), 3.51 (s, 3H), 1.54 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 191.28, 161.64, 158.71, 151.05, 140.41, 135.67, 130.49, 129.77, 128.28, 128.08, 123.34, 122.11, 115.05, 114.96, 113.73, 65.45, 50.23, 28.56, 14.79. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{19}H_{18}ClN_2O_4$ 373.0950, found 373.0949.

1-(2-(3-Chloro-4-ethoxyphenyl)-2-oxoethyl)-3-ethyl-quinazoline-2,4(1*H*,3*H*)-dione (8d). Following the general method, compound **8d** was obtained from **7d** and 2-bromo-1-(3-chloro-4-ethoxyphenyl)ethan-1-one. Yield: 23%, mp: 180-182 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 7.8 Hz, 1H), 8.09 (d, *J* = 2.1 Hz, 1H), 7.96 (d, *J* = 8.6 Hz, 1H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.26 – 7.20 (m, 1H), 7.02 (d, *J* = 8.6 Hz, 1H), 6.82 (d, *J* = 8.4 Hz, 1H), 5.54 (s, 2H), 4.26 – 4.14 (m, 4H), 1.53 (t, *J* = 6.1 Hz, 3H), 1.31 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 191.30, 161.18, 158.71, 150.61, 140.50, 135.72, 130.50, 129.79, 128.31, 128.06, 123.36, 122.10, 115.09, 115.08, 113.73, 65.44, 50.19, 36.76, 14.80, 13.29. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{20}H_{20}ClN_2O_4$ 387.1106, found 387.1108.

4-(1-(2-(3-Chloro-4-ethoxyphenyl)-2-oxoethyl)-2,4-dioxo-1,4-dihydroquinazolin-3(2*H*)-yl)-*N*-cyclopentylbutanamide (8e).

Following the general method, compound **8e** was obtained from **7e** and 2-bromo-1-(3-chloro-4-ethoxyphenyl)ethan-1-one. Yield: 70%, mp: 250-251 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 7.6 Hz, 1H), 8.09 (s, 1H), 7.99 – 7.92 (m, 1H), 7.77 (d, *J* = 11.3 Hz, 1H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.03 (d, *J* = 8.7 Hz, 1H), 6.84 (d, *J* = 8.5 Hz, 1H), 6.20 (s, 1H), 5.53 (s, 2H), 4.26 – 4.15 (m, 5H), 2.24 – 2.19 (m, 2H), 2.11 – 2.04 (m, 2H), 1.98 – 1.90 (m, 2H), 1.71 – 1.62 (m, 2H), 1.55 – 1.50 (m, 3H), 1.44 – 1.36 (m, 2H), 1.29 – 1.23 (m, 2H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 191.29, 171.06, 161.40, 158.69, 150.78, 140.52, 135.72, 130.49, 129.78, 128.38, 128.06, 123.33, 122.09, 115.05, 113.72, 109.99, 65.43, 50.49, 50.20, 41.27, 33.36, 32.66, 24.18, 23.80, 14.78. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{27}H_{31}ClN_3O_5$ 512.1947, found 512.1946.

2-(3-Benzyl-2,4-dioxo-3,4-dihydroquinazolin-1(2*H*)-yl)-*N*-(5-chloro-2,4-dimethoxyphenyl)acetamide (9a).

Following the general method, compound **9a** was obtained from **7a** and 2-bromo-*N*-(5-chloro-2,4-dimethoxyphenyl)-acetamide. Yield: 52%, mp: 234-237 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.76 (s, 1H), 8.10 (d, *J* = 7.5 Hz, 1H), 7.88 (s, 1H), 7.78 (t, *J* = 7.7 Hz, 1H), 7.41 – 7.22 (m, 7H), 6.87 (s, 1H), 5.17 (s, 2H), 5.07 (s, 2H), 3.92 (s, 3H), 3.87 (s, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 166.06, 161.50, 152.00, 151.07, 150.31, 140.65, 137.46, 135.94, 128.77, 128.40, 127.93, 127.60, 123.47, 123.31, 120.59, 115.06, 115.01, 111.35, 98.37, 56.81, 56.75, 46.72, 44.73. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{25}H_{23}ClN_3O_5$ 480.1321, found 480.1324.

***N*-(5-Chloro-2,4-dimethoxyphenyl)-2-(3-(2-fluoroethyl)-2,4-dioxo-3,4-dihydroquinazolin-1(2*H*)-yl)acetamide (9b)**.

Following the general method, compound **9b** was obtained from **7b** and 2-bromo-*N*-(5-chloro-2,4-dimethoxyphenyl)-acetamide. Yield: 50%, mp: 268-270 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.74 (s, 1H), 8.09 (d, *J* = 7.9 Hz, 1H), 7.89 (s, 1H), 7.78 (t, *J* = 7.9 Hz, 1H), 7.42 – 7.28 (m, 2H), 6.87 (s, 1H), 5.06 (s, 2H), 4.72 (t, *J* = 4.9 Hz, 1H), 4.60 (t, *J* = 4.9 Hz, 1H), 4.35 (t, *J* = 4.8 Hz, 1H), 4.29 (t, *J* = 4.7 Hz, 1H), 3.90 (d, *J* = 17.3 Hz, 6H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 166.05, 161.58, 152.03, 150.96, 150.35, 140.61, 135.92, 128.35, 123.48, 123.36, 120.57, 115.07, 114.99, 111.37, 98.38, 81.12 (d, *J* =

167.7 Hz, 1C), 56.82, 56.76, 46.69, 41.68 (d, *J* = 22.2 Hz, 1C). HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{20}H_{20}ClFN_3O_5$ 436.1070, found 436.1073.

***N*-(5-Chloro-2,4-dimethoxyphenyl)-2-(3-methyl-2,4-dioxo-3,4-dihydroquinazolin-1(2*H*)-yl)acetamide (9c)**.

Following the general method, compound **9c** was obtained from **7c** and 2-bromo-*N*-(5-chloro-2,4-dimethoxyphenyl)acetamide. Yield: 74%, mp: 314-315 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.72 (s, 1H), 8.08 (d, *J* = 7.8 Hz, 1H), 7.87 (s, 1H), 7.75 (t, *J* = 7.9 Hz, 1H), 7.40 – 7.27 (m, 2H), 6.87 (s, 1H), 5.05 (s, 2H), 3.90 (d, *J* = 16.5 Hz, 6H), 3.34 (s, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 166.16, 161.71, 152.05, 151.18, 150.42, 140.49, 135.66, 128.21, 123.44, 123.31, 120.57, 115.05, 114.93, 111.36, 98.41, 56.83, 56.78, 46.65, 28.59. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{19}H_{19}ClN_3O_5$ 404.1008, found 404.1009.

***N*-(5-Chloro-2,4-dimethoxyphenyl)-2-(3-ethyl-2,4-dioxo-3,4-dihydroquinazolin-1(2*H*)-yl)acetamide (9d)**.

Following the general method, compound **9d** was obtained from **7d** and 2-bromo-*N*-(5-chloro-2,4-dimethoxyphenyl)-acetamide. Yield: 26%, mp: 263-264 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.69 (s, 1H), 8.04 (d, *J* = 7.8 Hz, 1H), 7.85 (s, 1H), 7.71 (t, *J* = 7.7 Hz, 1H), 7.35 – 7.24 (m, 2H), 6.82 (s, 1H), 4.99 (s, 2H), 3.97 (q, *J* = 7.0 Hz, 2H), 3.85 (d, *J* = 16.2 Hz, 6H), 1.14 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 166.14, 161.22, 151.98, 150.72, 150.34, 140.57, 135.67, 128.22, 123.33, 123.29, 120.63, 115.14, 114.93, 111.34, 98.38, 56.81, 56.76, 46.57, 36.76, 13.28. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{20}H_{21}ClN_3O_5$ 418.1164, found 418.1167.

4-(1-(2-((5-Chloro-2,4-dimethoxyphenyl)amino)-2-oxoethyl)-2,4-dioxo-1,4-dihydroquinazolin-3(2*H*)-yl)-*N*-cyclo-pentyl-butanamide (9e). Following the general method, compound **9e** was obtained from **7e** and 2-bromo-*N*-(5-chloro-2,4-dimethoxy-phenyl)acetamide. Yield: 52%, mp: 260-262 °C. ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.73 (s, 1H), 8.08 (d, *J* = 7.5 Hz, 1H), 7.86 (s, 1H), 7.80 – 7.70 (m, 2H), 7.40 – 7.27 (m, 2H), 6.87 (s, 1H), 5.04 (s, 2H), 4.02 – 3.83 (m, 9H), 2.08 (t, *J* = 7.5 Hz, 2H), 1.87 – 1.78 (m, 2H), 1.77 – 1.66 (m, 2H), 1.64 – 1.54 (m, 2H), 1.50 – 1.41 (m, 2H), 1.35 – 1.25 (m, 2H). ^{13}C NMR (101 MHz, DMSO-*d6*) δ 171.16, 166.16, 161.47, 152.07, 150.92, 150.44, 140.58, 135.69, 128.32, 123.47, 123.29, 120.56, 115.16, 114.90, 111.37, 98.39, 56.83, 56.76, 50.52, 46.65, 41.32, 33.40, 32.67, 24.11, 23.82. HRMS (ESI) m/z $[M+H]^+$ Calcd for $C_{27}H_{32}ClN_4O_6$ 543.2005, found 543.2004.

2-(2,4-Dioxo-1,4-dihydroquinazolin-3(2*H*)-yl)-*N*-(2-hydroxyethyl)-acetamide (10)

A mixture of 2-(2,4-dioxo-1,4-dihydroquinazolin-3(2*H*)-yl)acetic acid (**3**) (0.44 g, 2.0 mmol), ethanolamine (0.15 g, 2.4 mmol), HATU (1.14 g, 3.0 mmol), DIPEA (0.65 g, 5.0 mmol), and dichloromethane (15 mL) was stirred at room temperature. The reaction was stirred at room temperature overnight until the reaction was completed as determined by TLC. Then, the mixture was concentrated under vacuum. To the residue was added 1N HCl and the mixture was stirred for 30 min at room temperature. The solid was filtered and dried as white solid. (0.24 g, 46%). ^{1}H NMR (400 MHz, DMSO-*d6*) δ 11.41 (s, 1H), 8.13 (s, 1H), 7.92 (d, *J* = 7.3 Hz, 1H), 7.67 (t, *J* = 7.4 Hz, 1H), 7.21 (t, *J* = 8.2 Hz, 2H), 4.69 (s, 1H), 4.48 (s, 2H), 3.39 (s, 2H), 3.13 (s, 2H).

***tert*-Butyl 2-(3-(2-((2-hydroxyethyl)amino)-2-oxoethyl)-2,4-dioxo-3,4-dihydroquinazolin-1(2*H*)-yl)acetate (11)**

To a round-bottomed flask equipped with a magnetic stir bar were added **10** (0.60 g, 2.3 mmol), *tert*-butyl bromoacetate (0.47 g, 2.4 mmol), K_2CO_3 (138 mg, 2.0 eq), and DMF (10 mL). The reaction was stirred at room temperature overnight until the reaction was completed as determined by TLC. Then, the reaction mixture was diluted with ethyl acetate and washed with water and saturated brine. After drying over $MgSO_4$, the mixture was filtered and the filtrate was concentrated under vacuum. The residue was purified by flash chromatography with eluent of ethyl acetate (0.5 g, 58%).

2-(3-(2-((2-Hydroxyethyl)amino)-2-oxoethyl)-2,4-dioxo-3,4-dihydroquinazolin-1(2*H*)-yl)acetic acid (12)

To a round-bottomed flask equipped with a magnetic stir bar were added **11** (0.50 g, 1.3 mmol), trifluoroacetic acid (5 mL), and dichloromethane (5 mL). The reaction was stirred at room temperature for 3 h until the reaction was completed as determined by TLC. Then, the reaction mixture was concentrated under vacuum to give white solid product (0.4 g, 96%). ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.41 (t, *J* = 5.3 Hz, 1H), 8.07 (d, *J* = 7.8 Hz, 1H), 7.78 (t, *J* = 7.8 Hz, 1H), 7.43 – 7.28 (m, 2H), 4.88 (s, 2H), 4.55 (s, 2H), 4.39 (t, *J* = 5.3 Hz, 2H), 3.49 – 3.38 (m, 3H).

***N*-(5-Chloro-4-hydroxy-2-methoxyphenyl)-2-(3-(2-((2-hydroxyethyl)amino)-2-oxoethyl)-2,4-dioxo-3,4-dihydro-quinazolin-1(2*H*)-yl)acetamide (13)**

A mixture of **12** (96 mg, 0.30 mmol), 4-amino-2-chloro-5-methoxyphenol (57 mg, 0.33 mmol), HATU (171 mg, 0.45 mmol), DIPEA (97 mg, 0.75 mmol), and dimethyl sulfoxide (3 mL) was stirred at room temperature. The reaction was stirred at room temperature for overnight until the reaction was completed as determined by TLC. Then, the mixture was diluted with water and the precipitate was filtered and dried as white solid. (50 mg, 35%). ^{1}H NMR (400 MHz, DMSO-

d6) δ 10.04 (s, 1H), 9.61 (s, 1H), 8.16 (s, 1H), 8.07 (d, *J* = 8.0 Hz, 1H), 7.83 – 7.72 (m, 2H), 7.34 (dd, *J* = 16.4, 8.4 Hz, 2H), 6.66 (s, 1H), 5.03 (s, 2H), 4.69 (s, 1H), 4.57 (s, 2H), 3.80 (s, 3H), 3.40 (dd, *J* = 11.0, 5.4 Hz, 2H), 3.14 (dd, *J* = 11.5, 5.8 Hz, 2H).

Radiochemistry

[^{11}C]CO_2 was produced via a ^{14}N(p,α)^{11}C reaction with a 40 μA beam of 16 MeV protons on a target of 0.5% O_2 in N_2 for 25 min with a JSW BC-16/8 cyclotron, and shunted to a GE PETtrace MeI Microlab to convert [^{11}C]CH_3I.

Radiosynthesis of [^{11}C]2a

[^{11}C]CH_3I was released with helium at a flow rate of 20 mL/min to a reaction vessel containing ~1.0 mg of precursor **13**, 2 μL of 5 M NaOH, and 300 μL of DMSO at room temperature. Once the radioactivity reached the maximum, the reaction mixture was heated at 90 °C for 5 min. After quenching with 1.5 mL of HPLC mobile phase (30% acetonitrile in 0.1 M ammonium formate buffer, pH = 4.5). The reactive mixture was loaded onto a semi-preparative C-18 column (Agilent SB-C18,250 x 9.6 mm, 5 μm), then eluted from the column using above mentioned HPLC mobile phase at a flow rate of 4.0 mL/min. The radioactive product fraction was collected to 50 mL of Milli-Q water, followed by trapping on a C18 Sep-Pak Plus cartridge. The C18 cartridge was further washed with 20 mL of Milli-Q water to remove the solvent residue. Then, the radioactive product was eluted out from the C18 cartridge with 0.6 mL of ethanol and 5.4 mL of 0.9% saline. Radiochemical purity was determined by analytical HPLC on a reverse-phase analytical column (Agilent SB-C18, 250 X 4.6 mm, 5 μm) with a mobile phase of 55% 0.1 M ammonium formate (pH 4.5) in acetonitrile and flow rate of 1.0 mL/min (Figure S1).

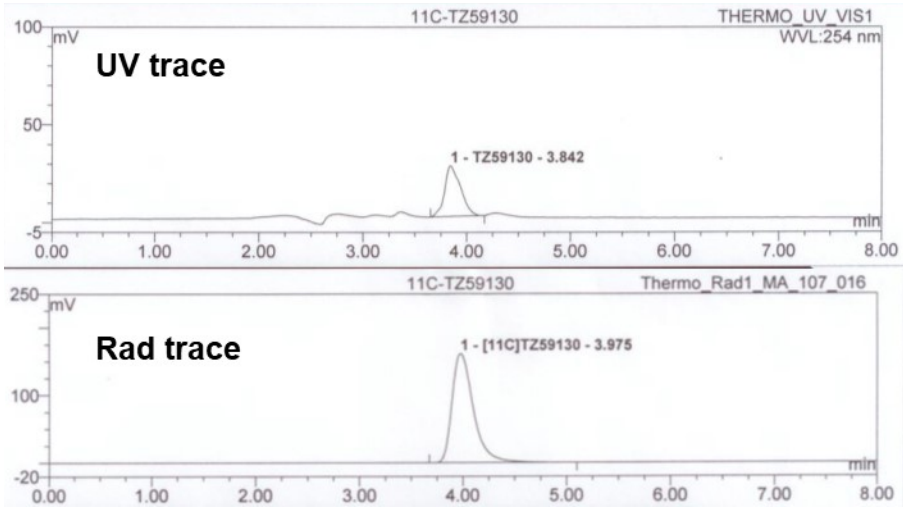


Figure S1. The analytical HPLC trace of [^{11}C]2a

Radiosynthesis of [^{11}C]2i

[^{11}C]CH_3I was released with helium at a flow rate of 20 mL/min to a reaction vessel containing ~1.0 mg of precursor **2k**, 2 μL of 5 M NaOH, and 300 μL of DMSO at room temperature. Once the radioactivity reaches the maximum, the reaction mixture was heated at 90 °C for 5 min. After quenching with 1.5 mL of HPLC mobile phase (45% acetonitrile in 0.1 M ammonium formate buffer, pH = 4.5). The reactive mixture was loaded onto a semi-preparative C-18 column (Agilent SB-C18,250 x 9.6 mm, 5 μm), then eluted from the column using above mentioned HPLC mobile phase at a flow rate of 4.0 mL/min. The radioactive product fraction was collected to 50 mL of Milli-Q water, followed by trapping on a C18 Sep-Pak Plus cartridge. The C18 cartridge was further washed with 20 mL of Milli-Q water to remove the solvent residue. Then, the radioactive product was eluted out from the C18 cartridge with 0.6 mL of ethanol and 5.4 mL of 5% Kolliphor® HS 15 solution. Radiochemical purity was determined by analytical HPLC on a reverse-phase analytical column (Agilent SB-C18, 250 X 4.6 mm, 5 μm) with a mobile phase of 25% 0.1 M ammonium formate (pH 4.5) in acetonitrile and flow rate of 1.0 mL/min (Figure S2).

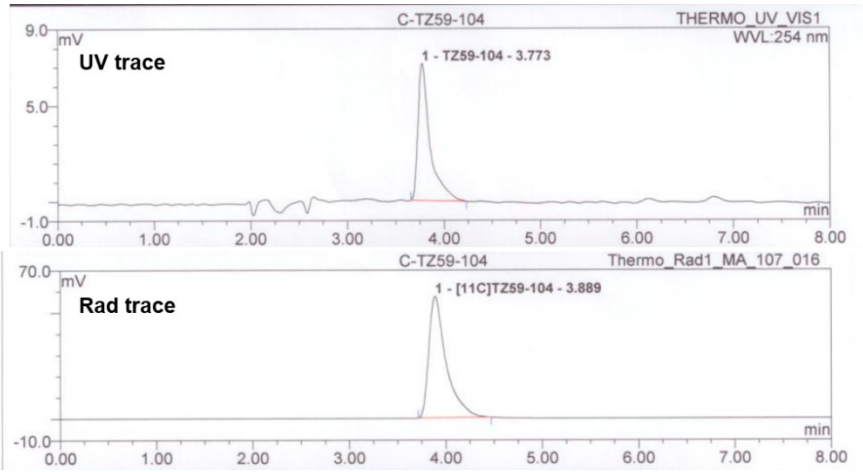


Figure S2. The analytical HPLC trace of [^{11}C]2i

***In vitro* binding assay**

The binding potency of newly synthesized compounds to S1PR2 was determined by a [^{32}P]S1P competitive binding assay according to our previously reported protocol[24]. Briefly, increasing concentrations of compounds (0.01, 0.1, 1.0, 10, 100, and 1000 nM) were incubated with ChemiSCREEN™ human recombinant S1PR2 lysophospholipid receptor membrane (Millipore, Billerica, MA) (~1 μg/well) and [^{32}P]S1P (0.1 nM) in a 96-well poly-L-lysine microplate for 60 min. The reaction was terminated by collecting the membranes onto 96-well glass fiber filtration plates (Millipore, Billerica, MA). After washing with cold assay buffer (50 mM HEPES Na, pH 7.5, 5 mM $MgCl_2$, 1 mM $CaCl_2$, and 0.5% fatty acid-free bovine serum albumin), the filter-bound radioactivity was measured by a Beckman LS 3801 scintillation counter using Cherenkov counting. The binding affinity of compounds toward the other four S1PRs was similarly determined using the above procedure. Human recombinant S1PR1, 2, 3, and 5 lysophospholipid receptor membranes were purchased from Millipore (Millipore, Billerica, MA) and human recombinant S1PR4 lysophospholipid receptor membrane was purchased from Muiltispan (Multispan, Hayward, CA). IC_{50} values were calculated using GraphPad Prism (GraphPadSoftware, Inc., San Diego, CA).

Tissue distribution studies of [^{11}C]2a and [^{11}C]2i in rodents

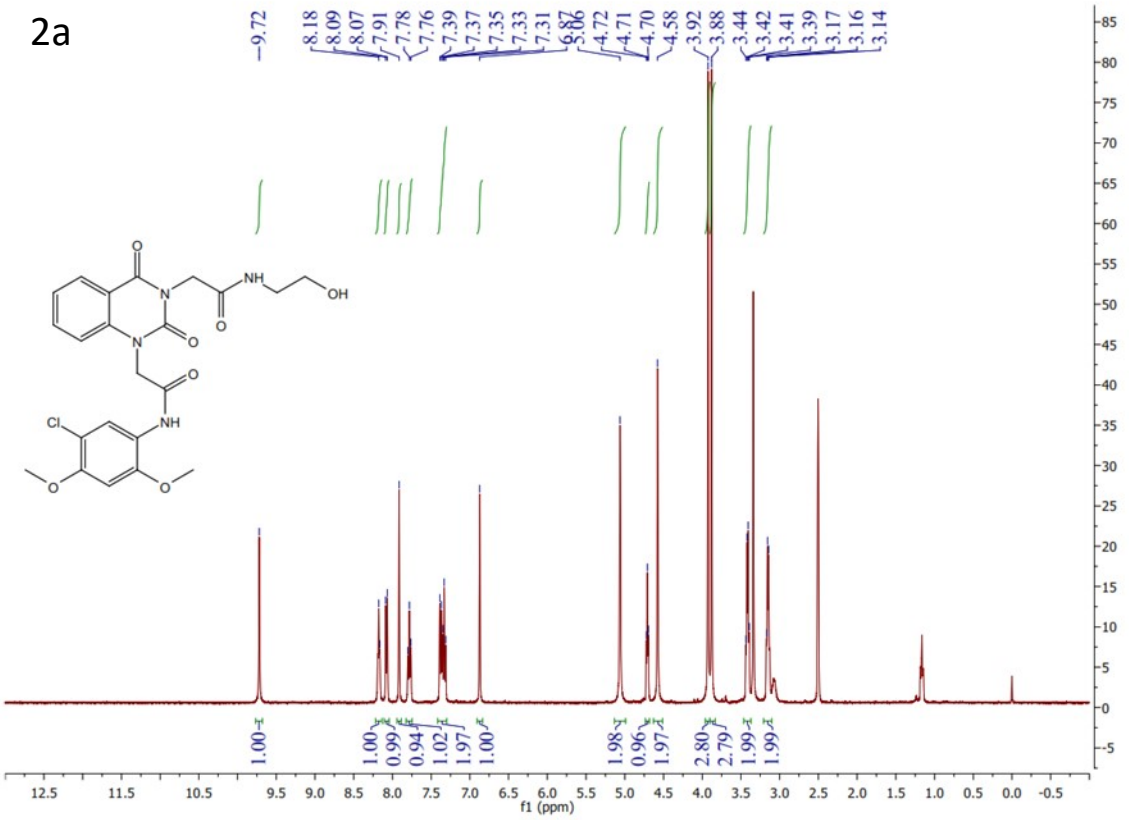
***Ex-vivo* tissue distribution of [^{11}C]2a**

A solution of [^{11}C]**2a** (~3.7 MBq/100 μL) in 10% ethanol in 0.9% saline was injected via the tail vein into adult male Sprague Dawley (SD) rats (n = 12, 8 weeks, 200-250 g, Charles River) under 2-3% isoflurane/oxygen anesthesia. The rats were euthanized under anesthesia at 5, 30, and 60 min post-injection (n = 4 for each group). Organs of blood, heart, lung, muscle, pancreas, spleen, kidney, liver, thymus, and brain were dissected and collected for counting. All the samples were counted with a dilution of the injectate on an automated well counter (Beckman Gamma 8000 well counter). Tissues were weighed and the uptake was reported as background and decay-corrected percent injected dose per gram (% ID/gram).

***Ex-vivo* tissue distribution of [^{11}C]2i in SJL mice**

The *ex-vivo* biodistribution study of [^{11}C]**2i** in normal female SJL mice (8 weeks, 16-22 g) was performed using a similar experimental procedure as the study of [^{11}C]**2a**.

2a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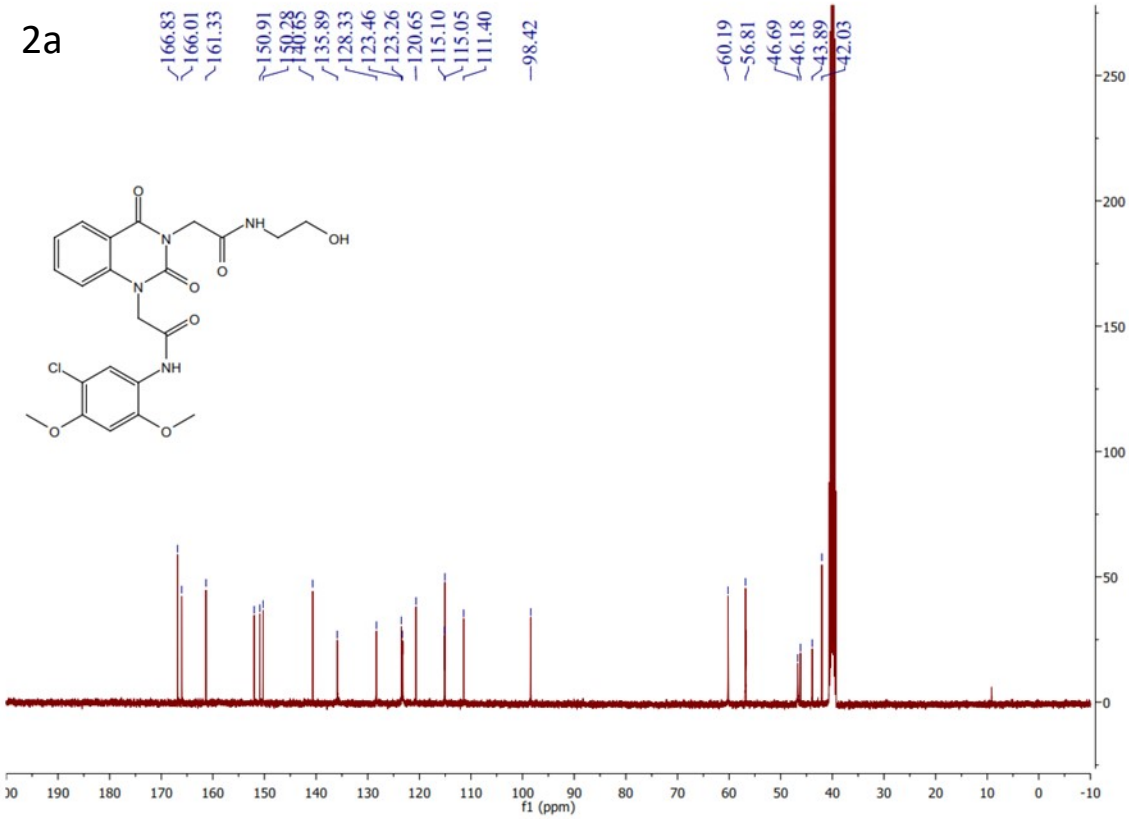
2a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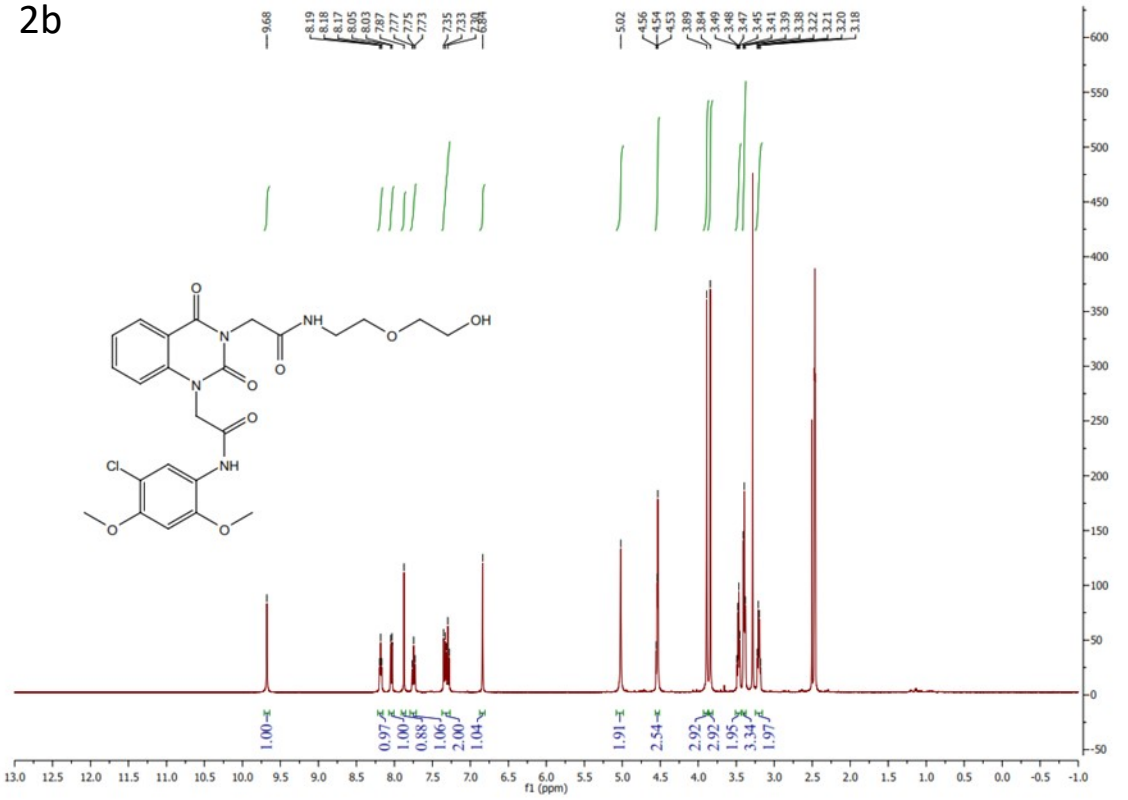
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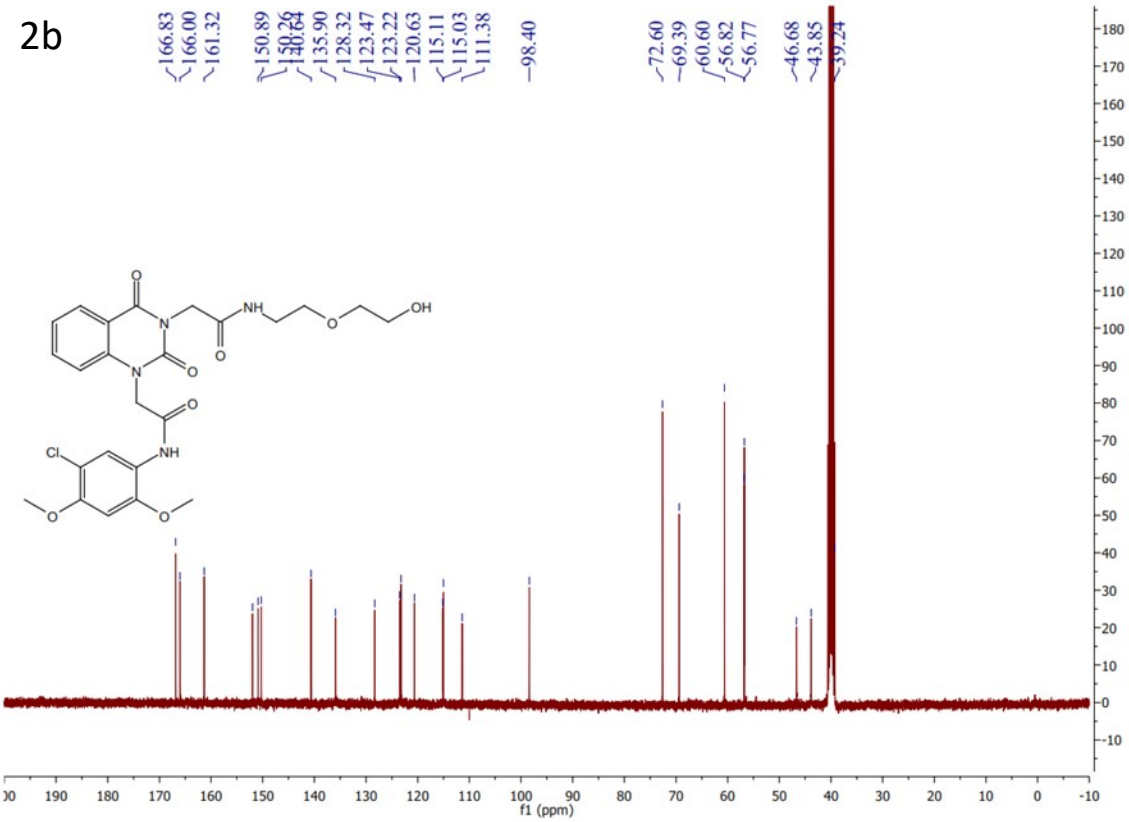
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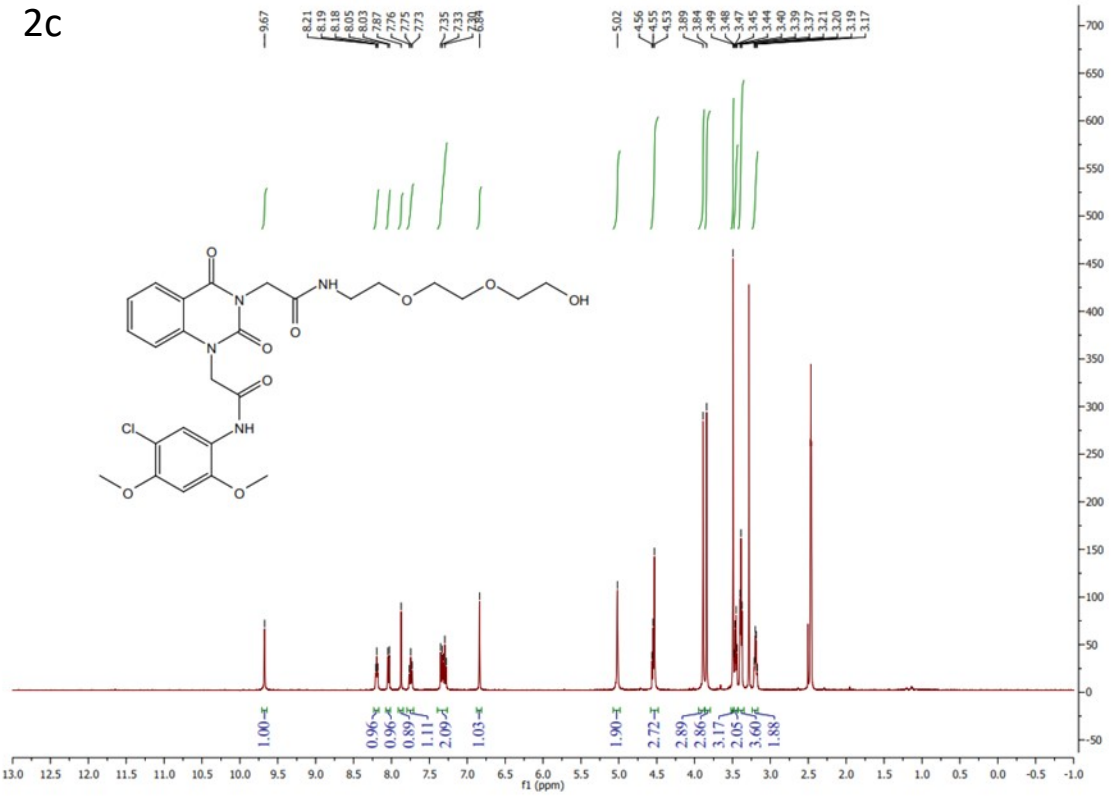
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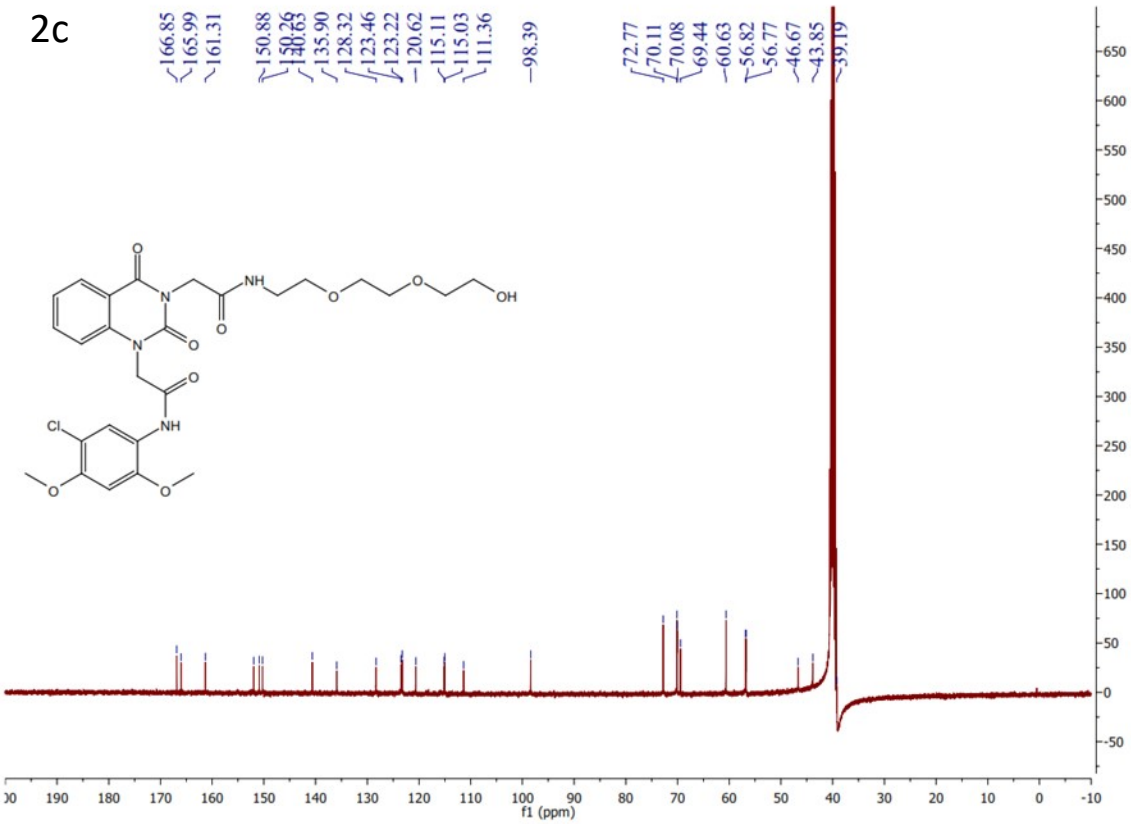
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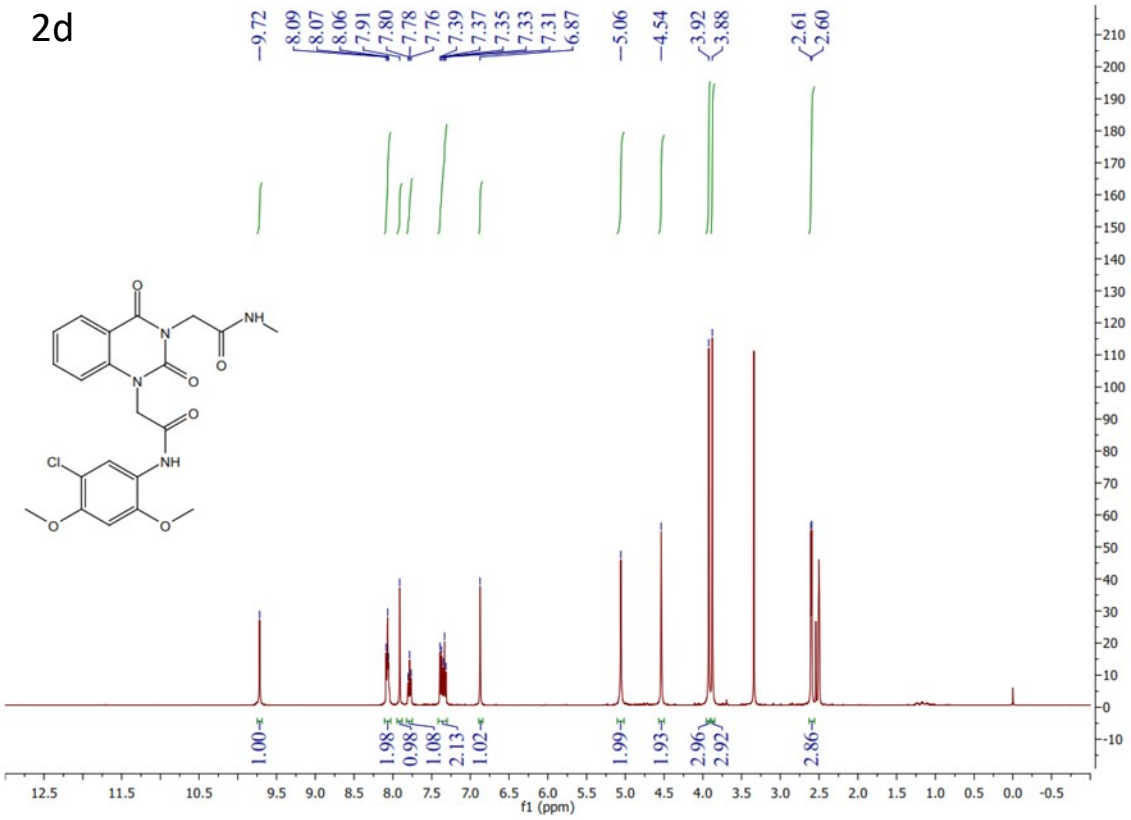
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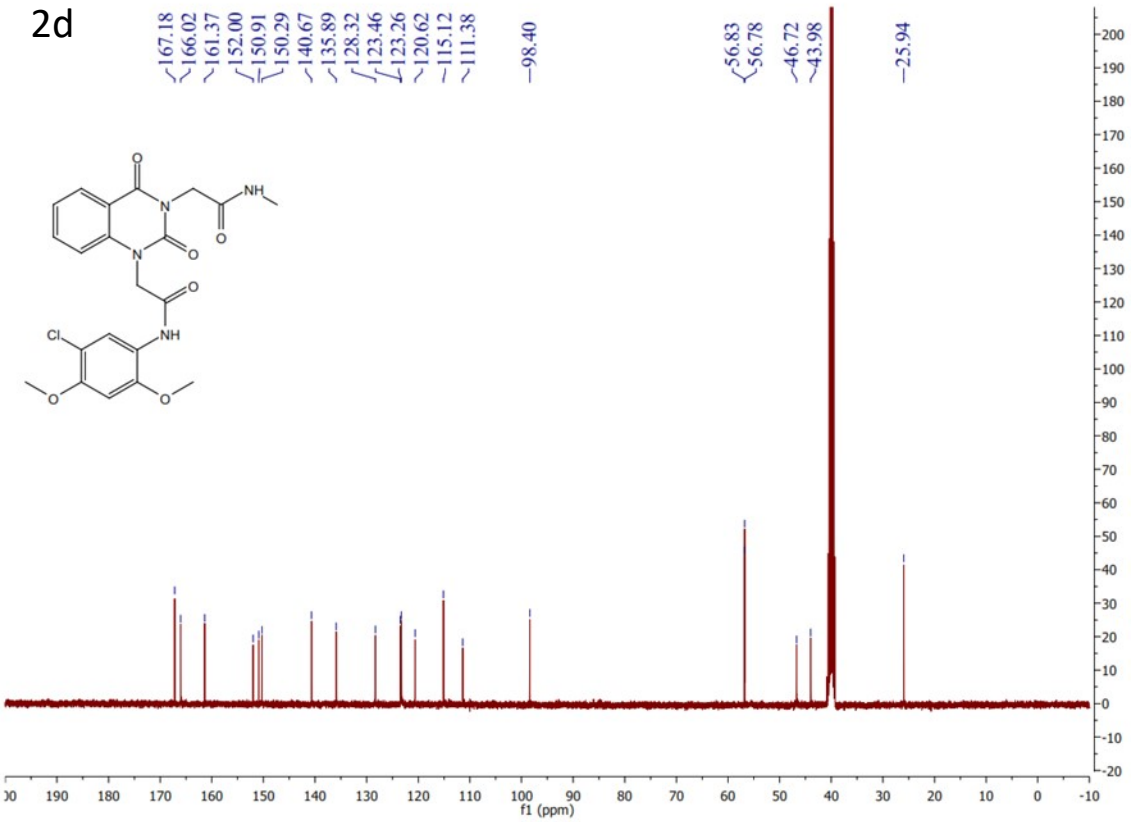
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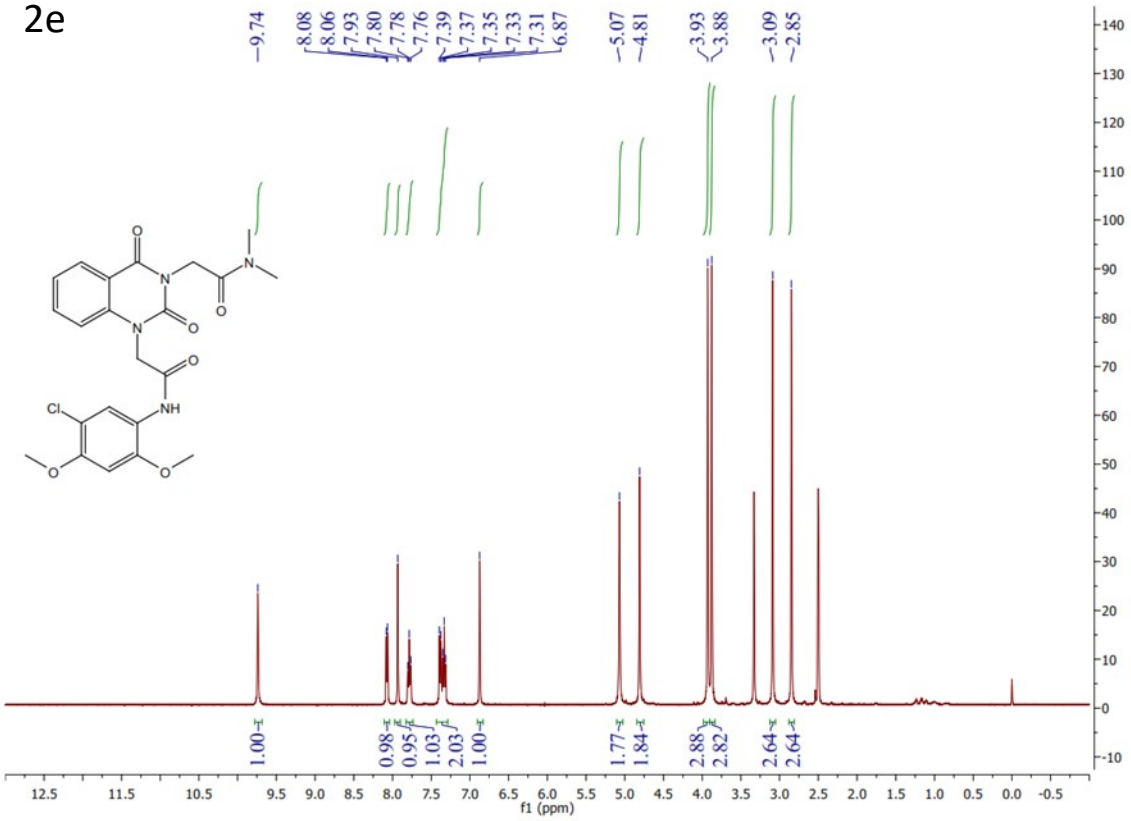
2e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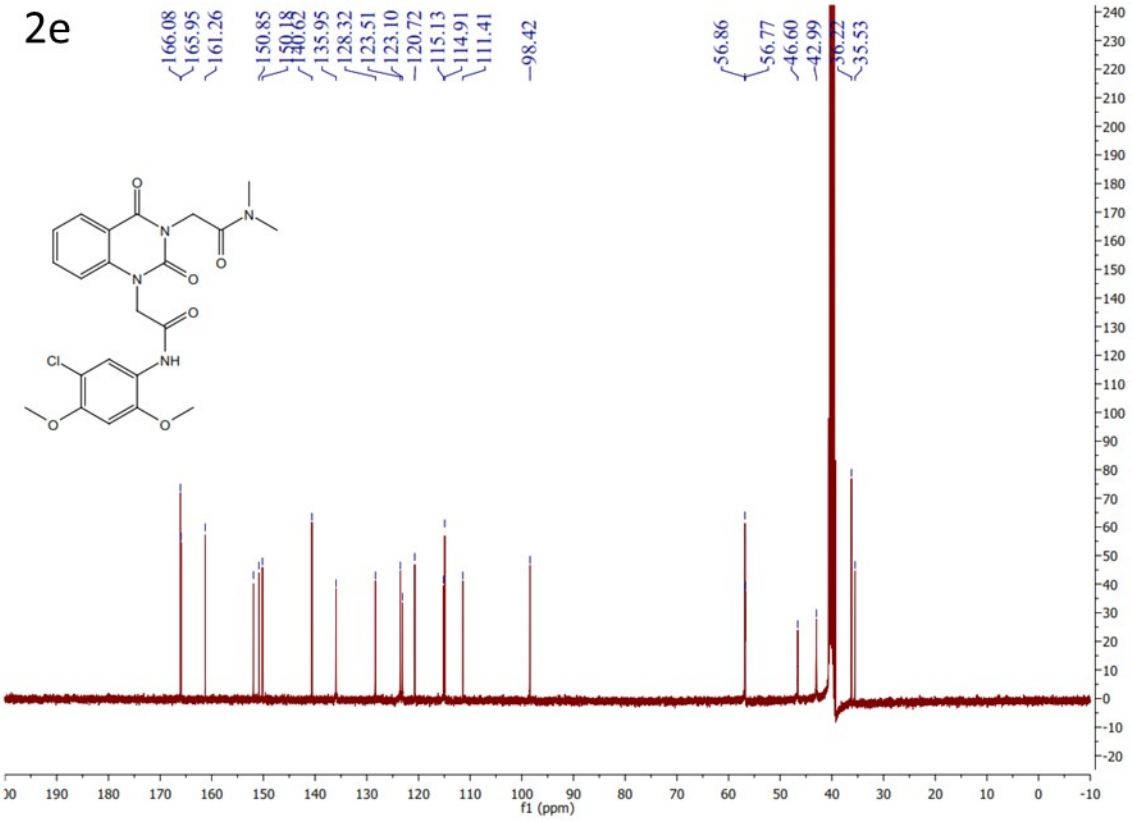
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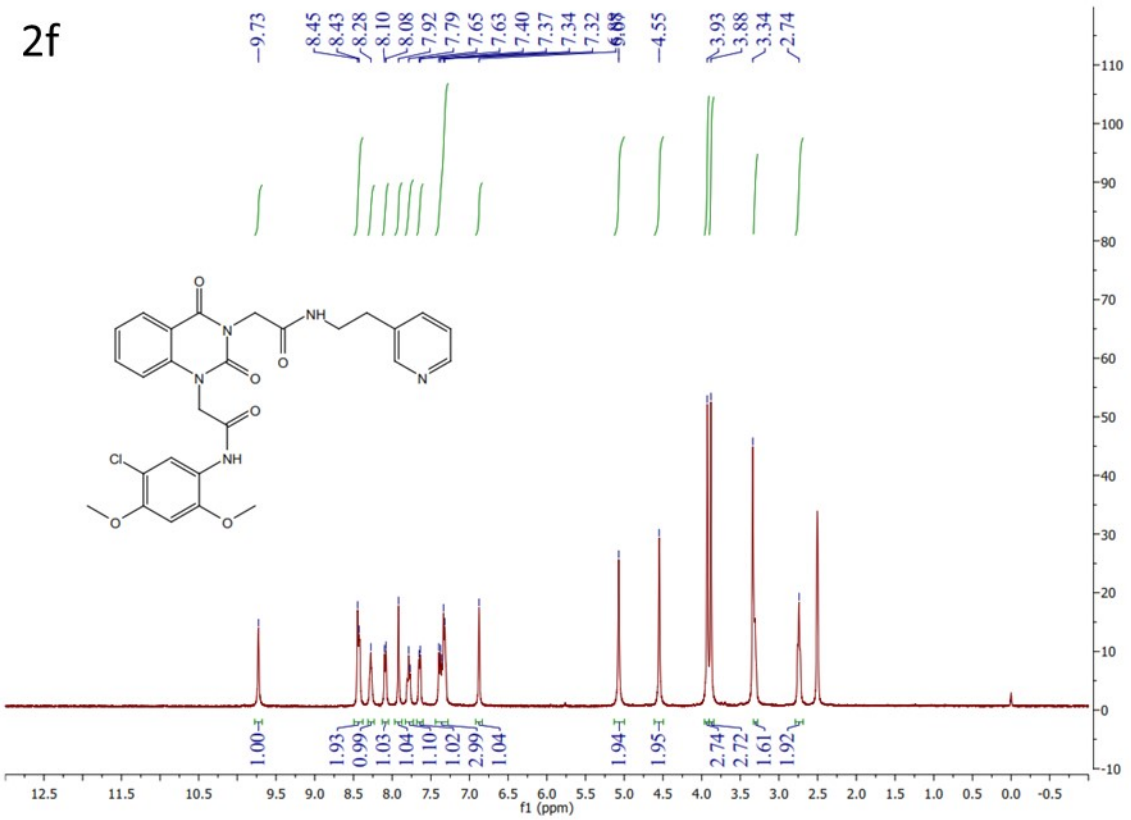
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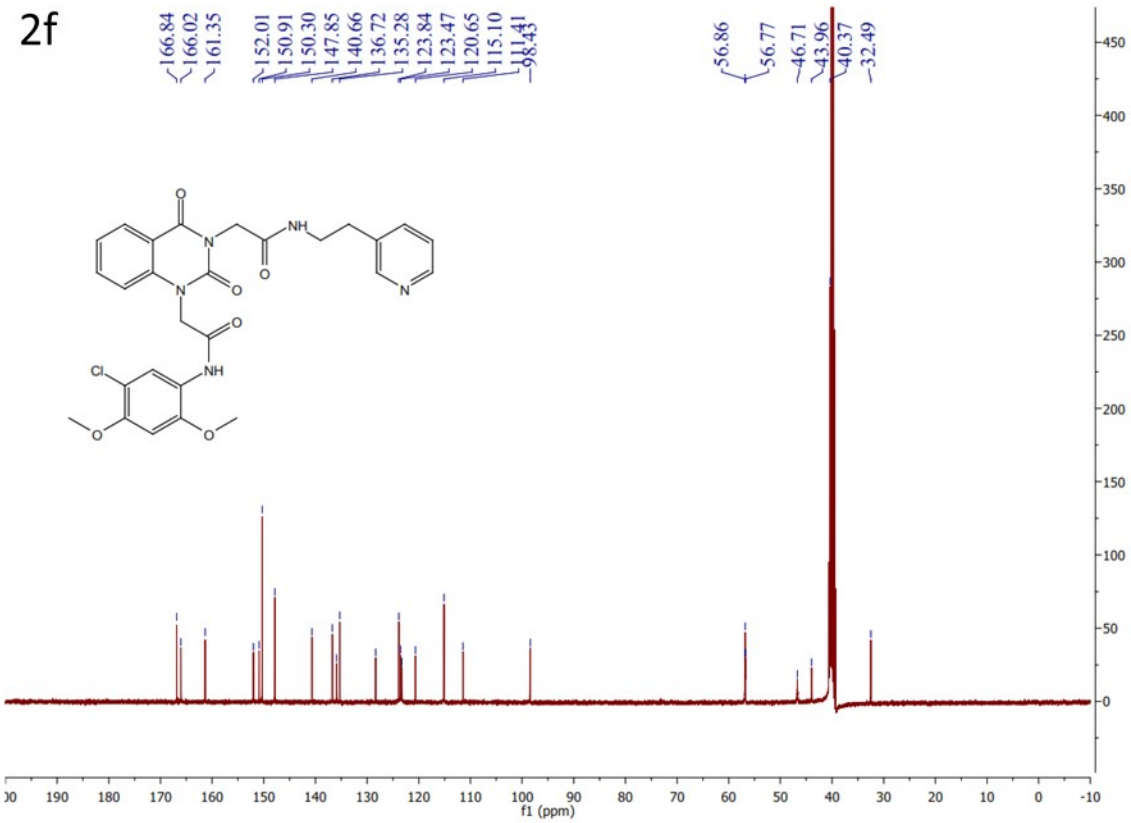
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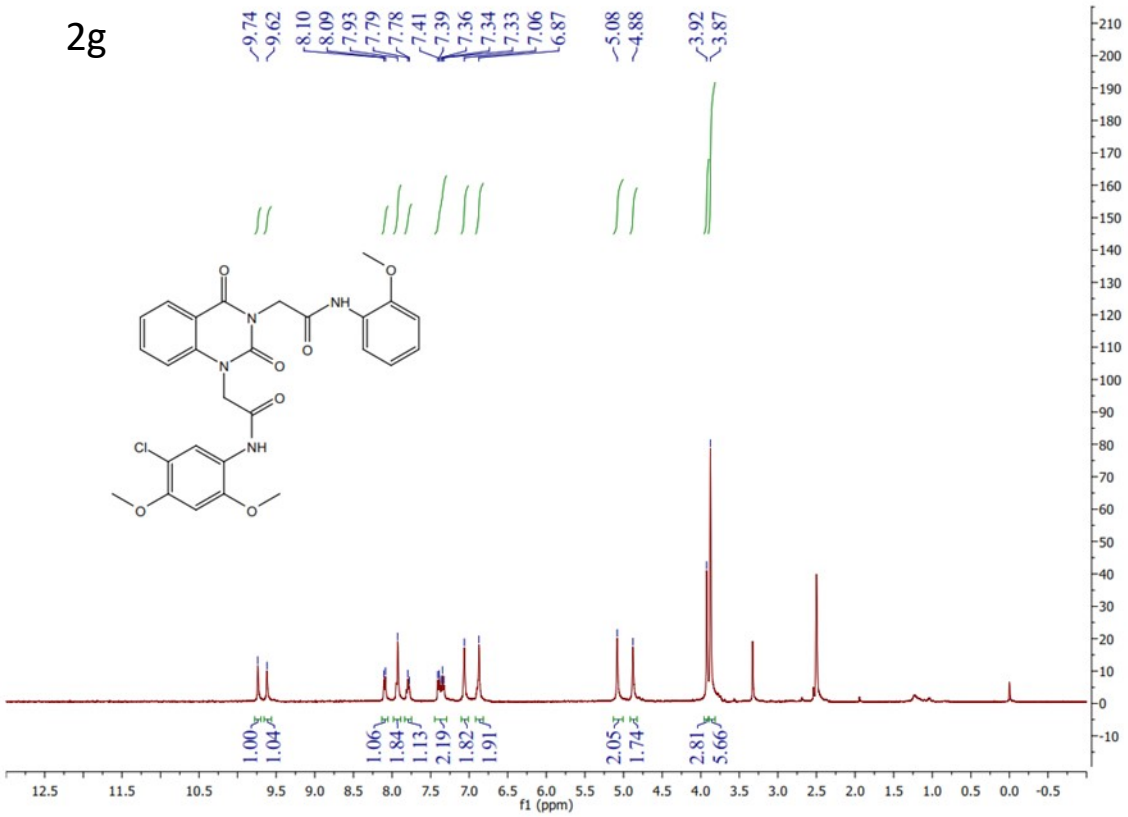
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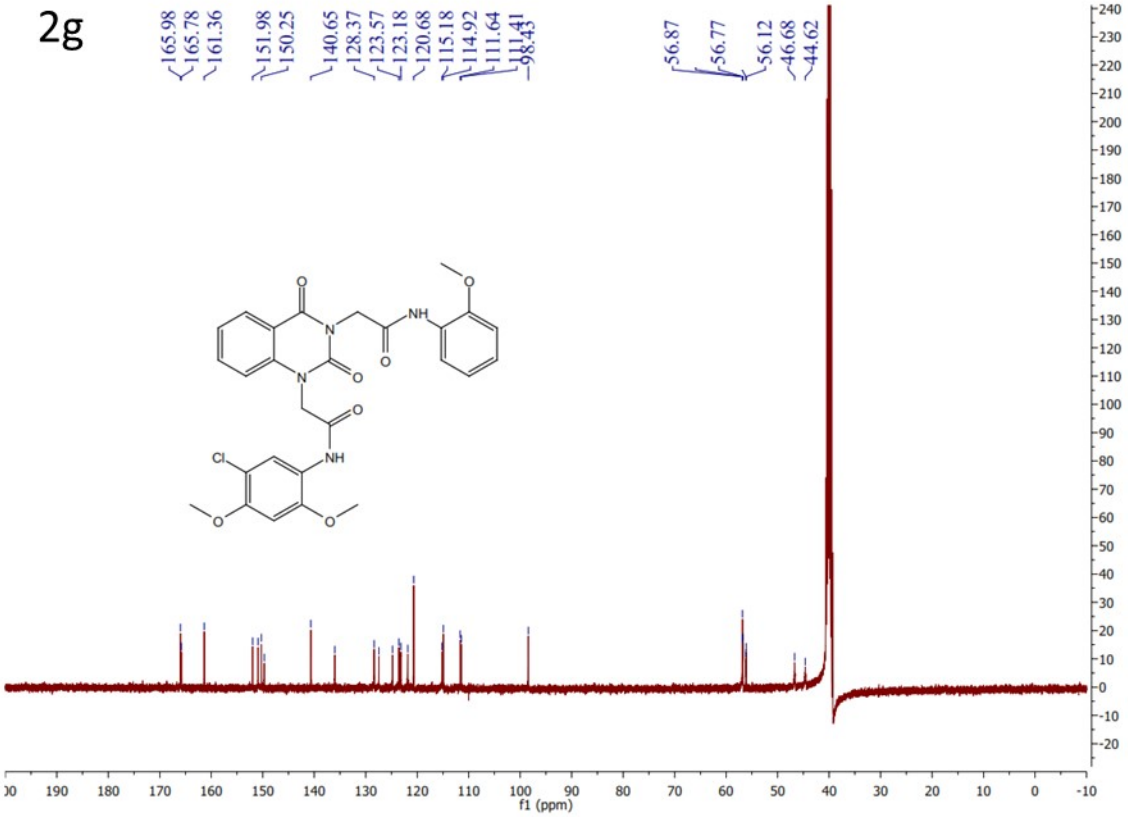
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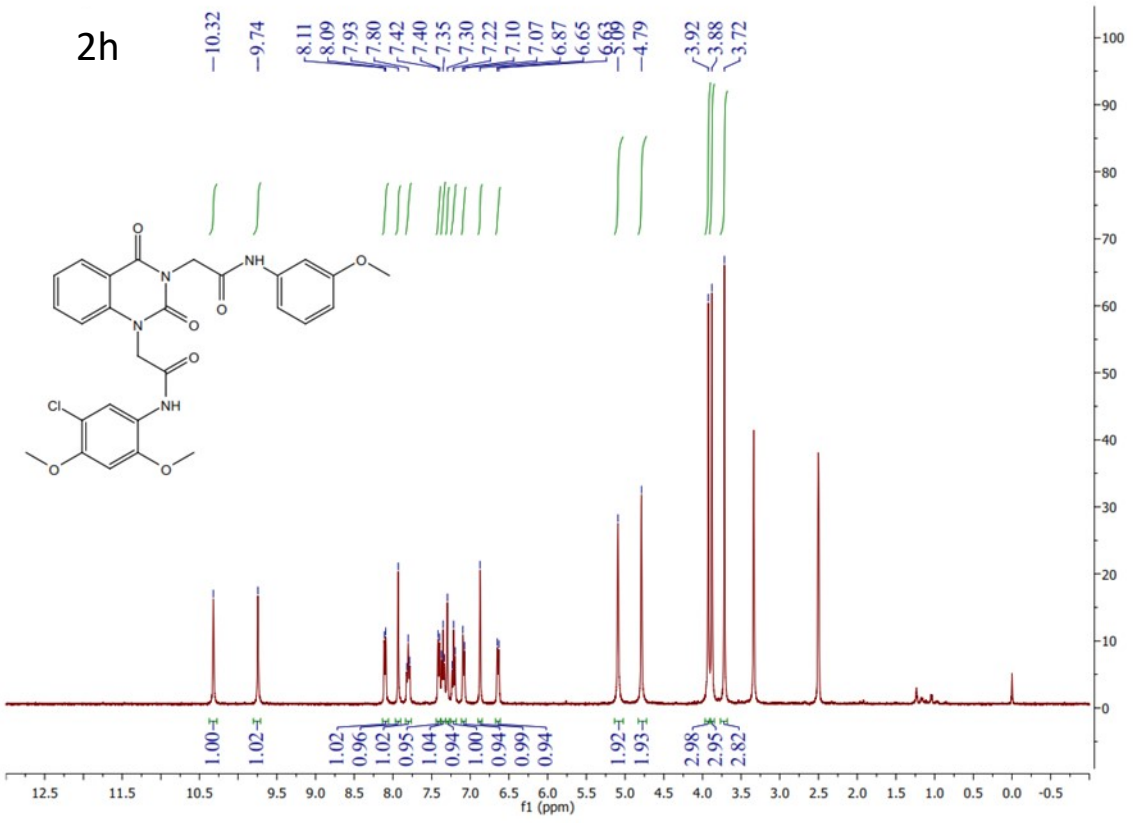
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1.04
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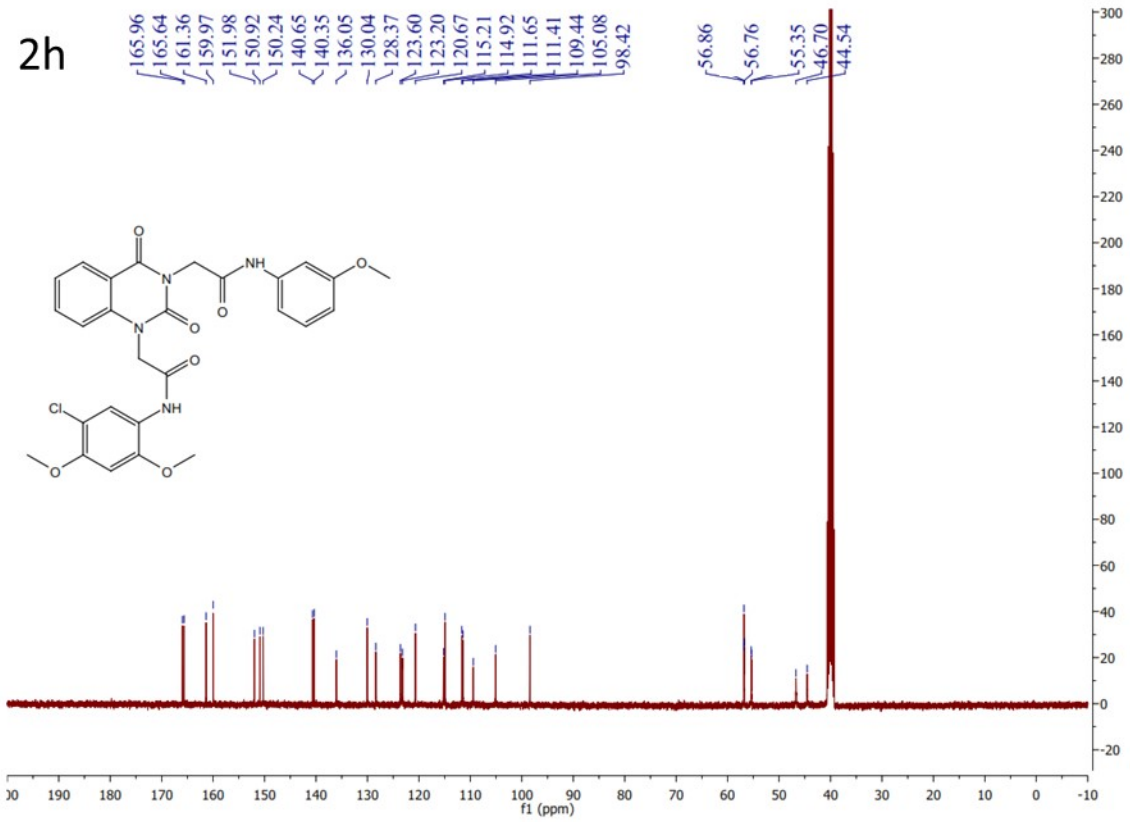
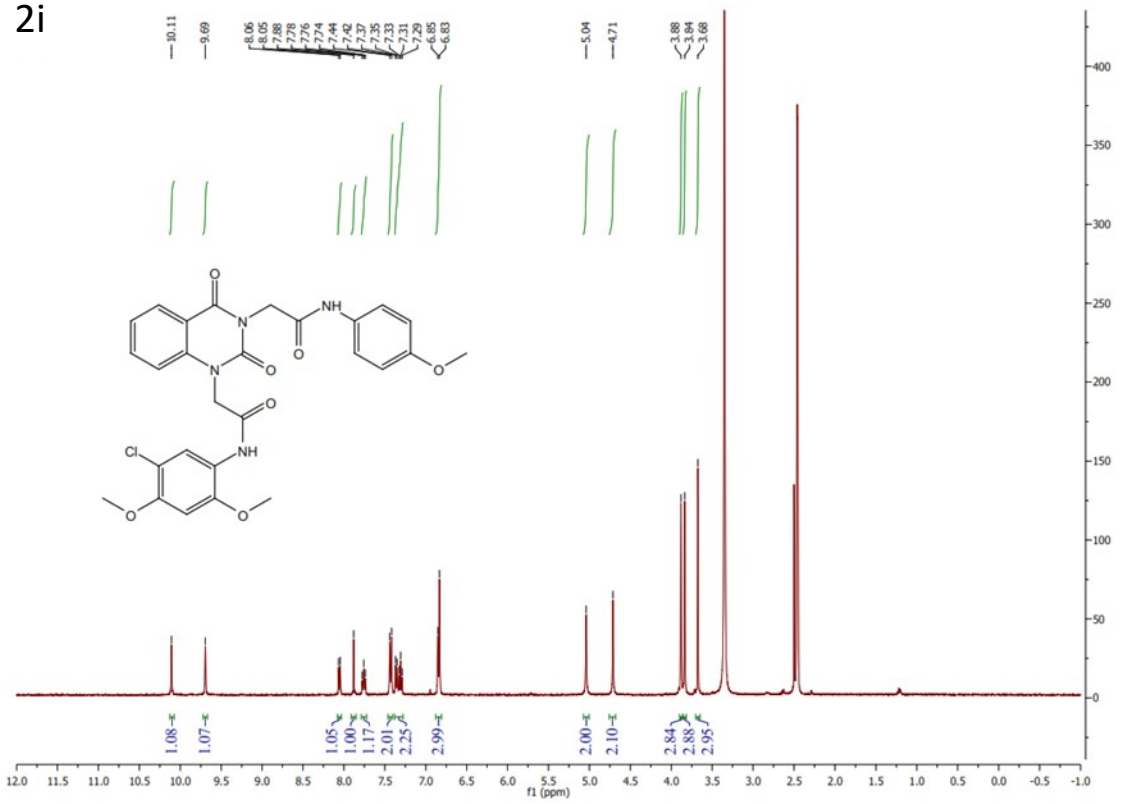
0.94
0.99
0.94
1.92
1.93
2.98
2.95
2.82
f1 (ppm)


2h
165.96
165.64
161.36
159.97
151.98
150.92
150.24
140.65
140.35
136.05
130.04
128.37
123.60
123.20
120.67
115.21
114.92
111.65
111.41
109.44
105.08
98.42
56.86
56.76
55.35
46.70
44.54
f1 (ppm)

2i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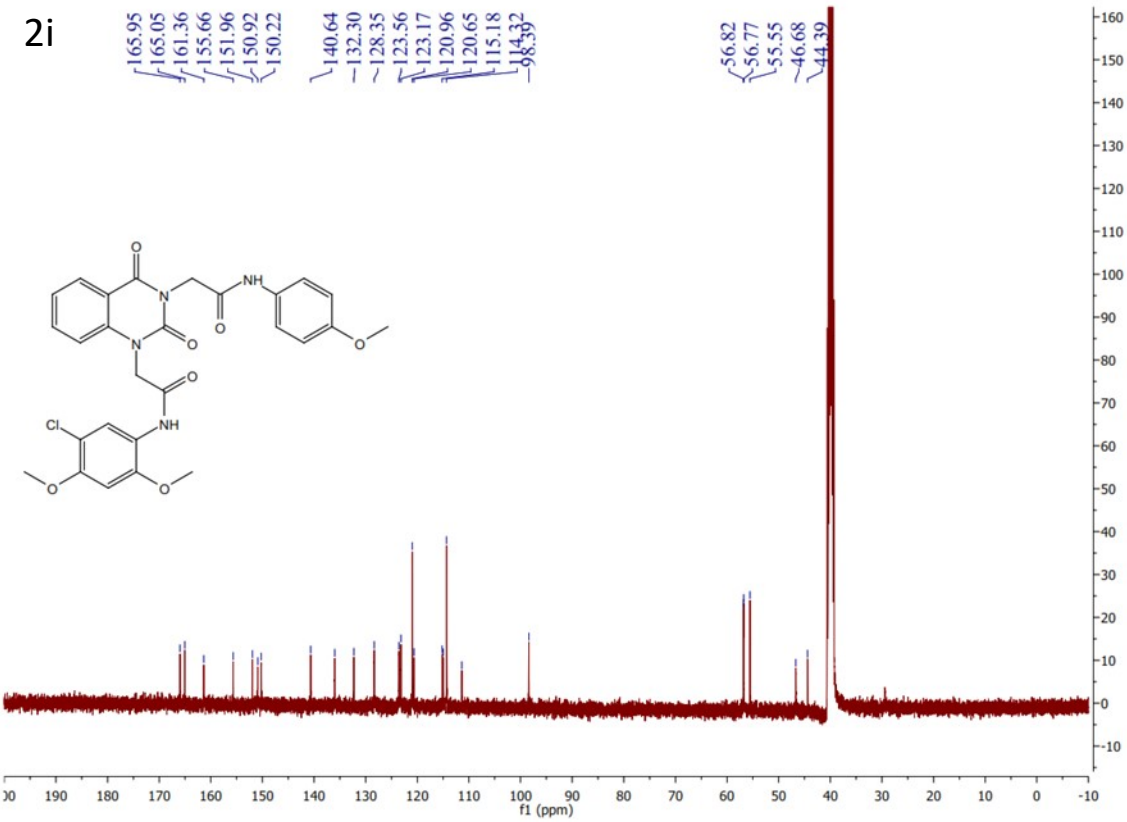
8.05
7.88
7.78
7.76
7.74
7.44
7.42
7.37
7.35
7.33
7.31
7.29
6.85
6.83
5.04
4.71
3.88
3.84
3.68
1.08
1.07
1.05
1.00
1.17
2.01
2.25
2.99
2.00
2.10
2.84
2.88
2.95
f1 (ppm)

2i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165.05
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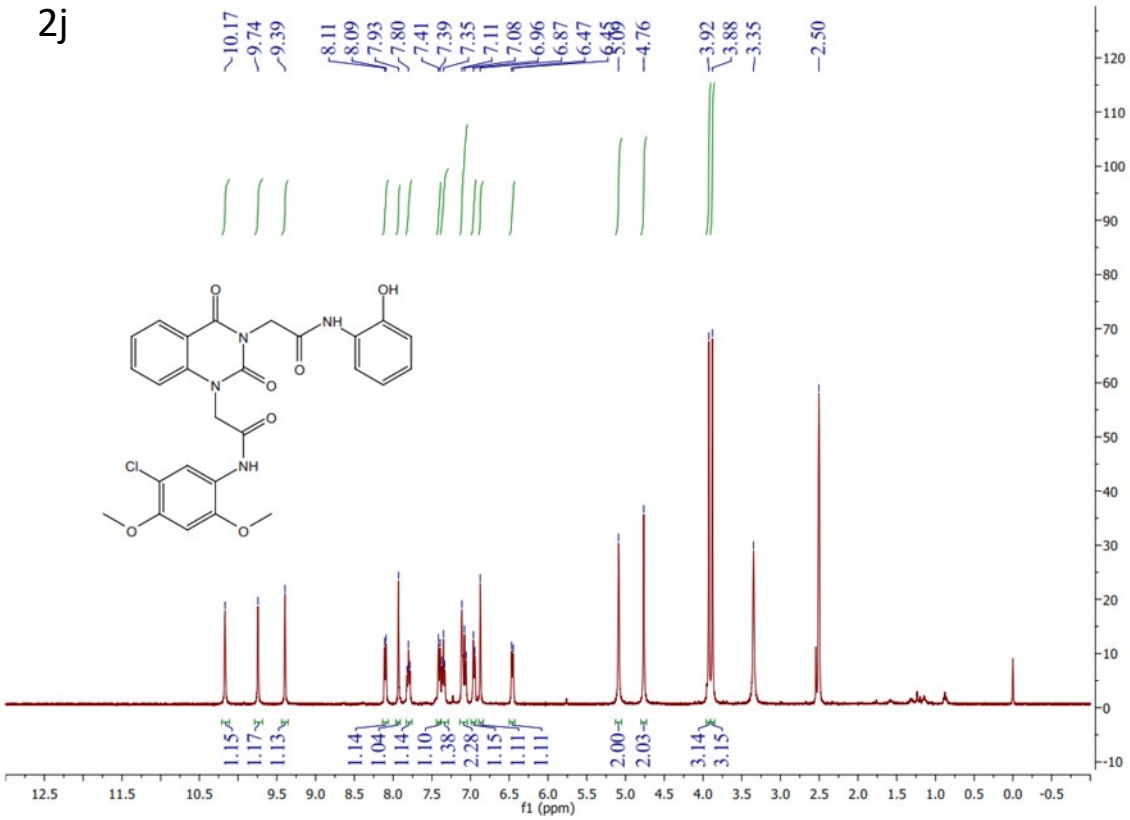
155.66
151.96
150.92
150.22
140.64
132.30
128.35
123.56
123.17
120.96
120.65
115.18
114.32
98.39
56.82
56.77
55.55
46.68
44.39
f1 (ppm)

2j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9.74
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7.93
7.80
7.41
7.39
7.35
7.11
7.08
6.96
6.87
6.47
6.45
5.00
4.76
3.92
3.88
3.35
2.50
1.15
1.17
1.13
1.14
1.04
1.14
1.10
1.38
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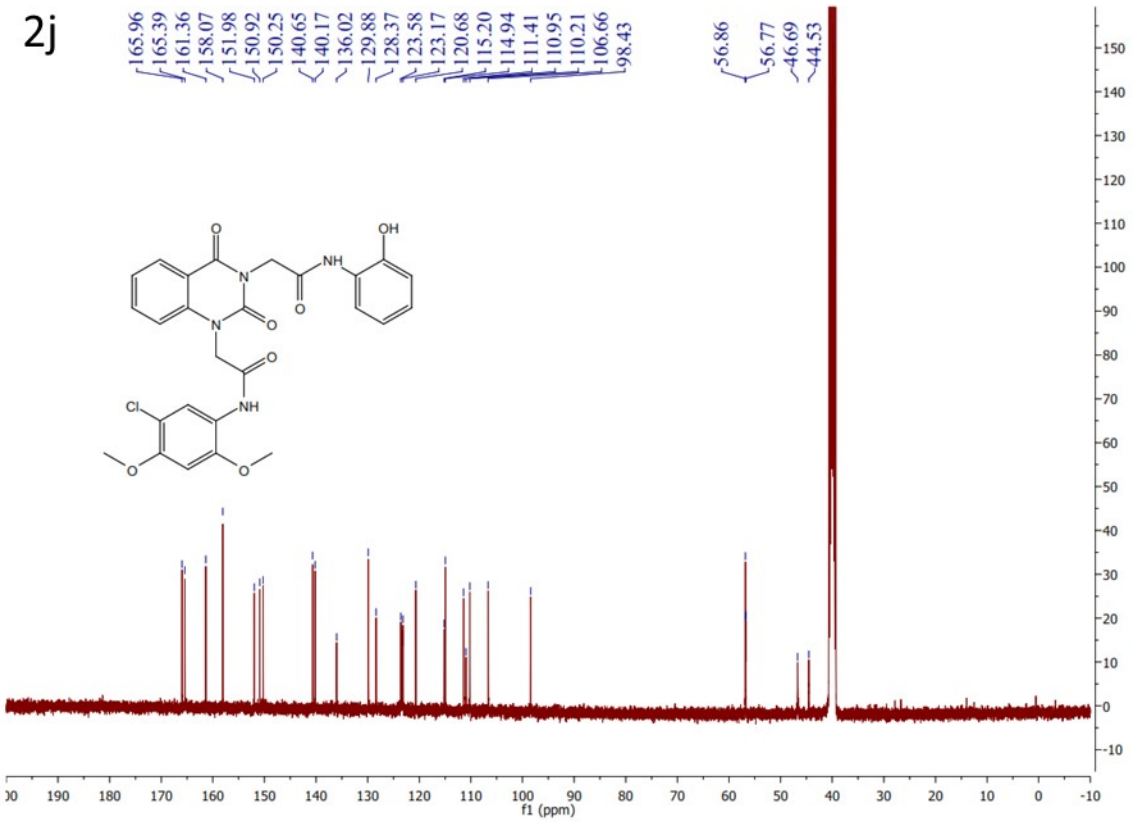
1.15
1.11
1.11
2.00
2.03
3.14
3.15
f1 (ppm)

2j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165.39
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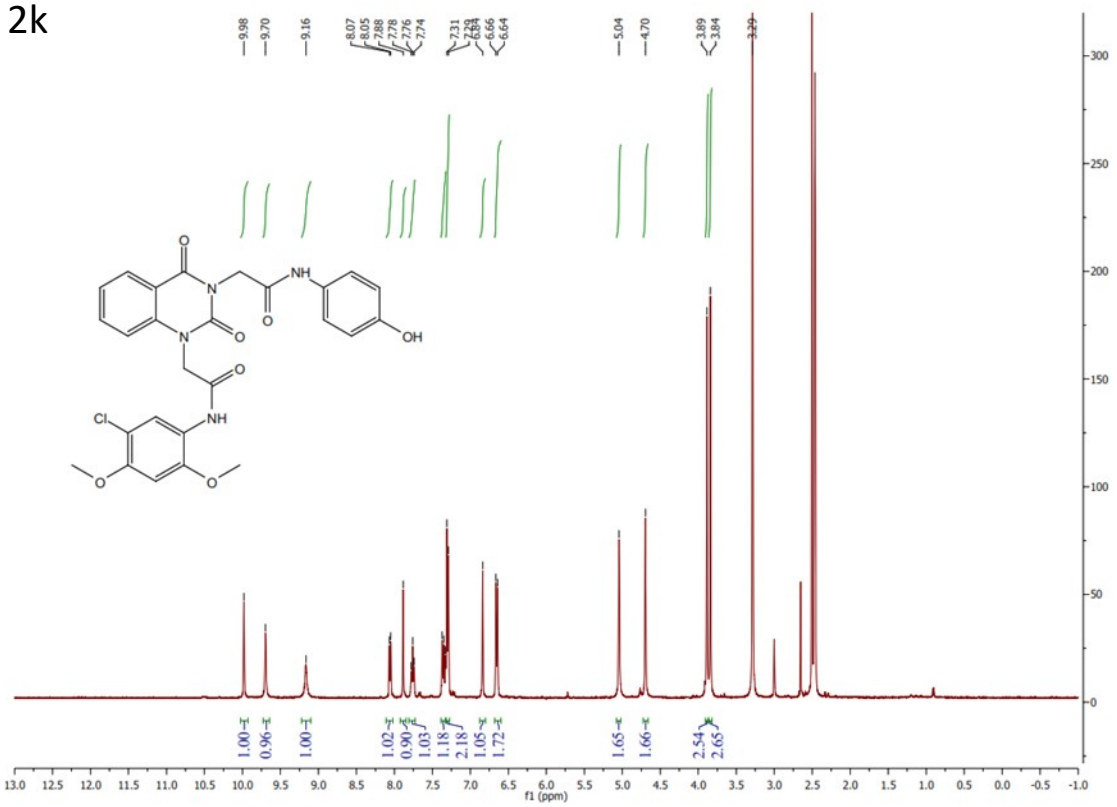
158.07
151.98
150.92
150.25
140.65
140.17
136.02
129.88
128.37
123.58
123.17
120.68
115.20
114.94
111.41
110.95
110.21
106.66
98.43
56.86
56.77
46.69
44.53
f1 (ppm)

2k


9.98
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9.16
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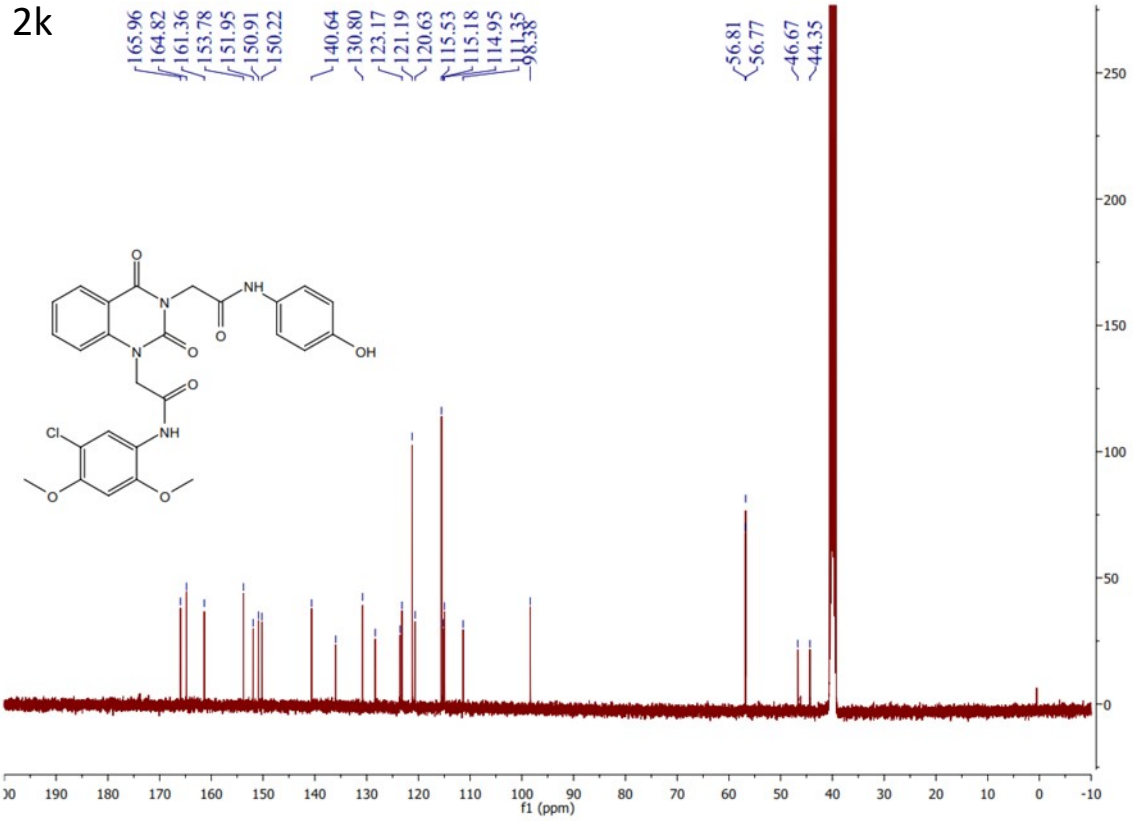
8.05
7.88
7.78
7.76
7.74
7.31
7.29
6.84
6.66
6.64
5.04
4.70
3.89
3.84
3.29
1.00
0.96
1.00
1.02
0.90
1.03
1.18
2.18
1.05
1.72
1.65
1.66
2.54
2.65
f1 (ppm)

2k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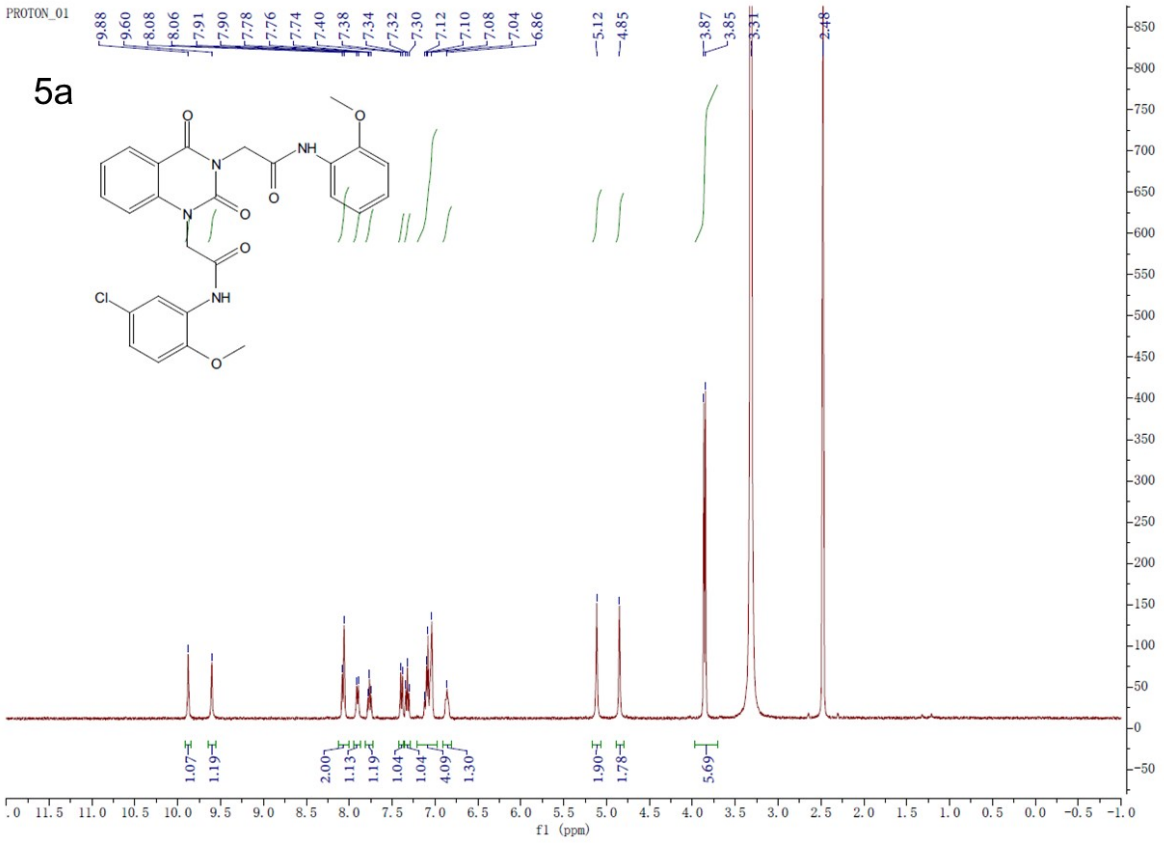
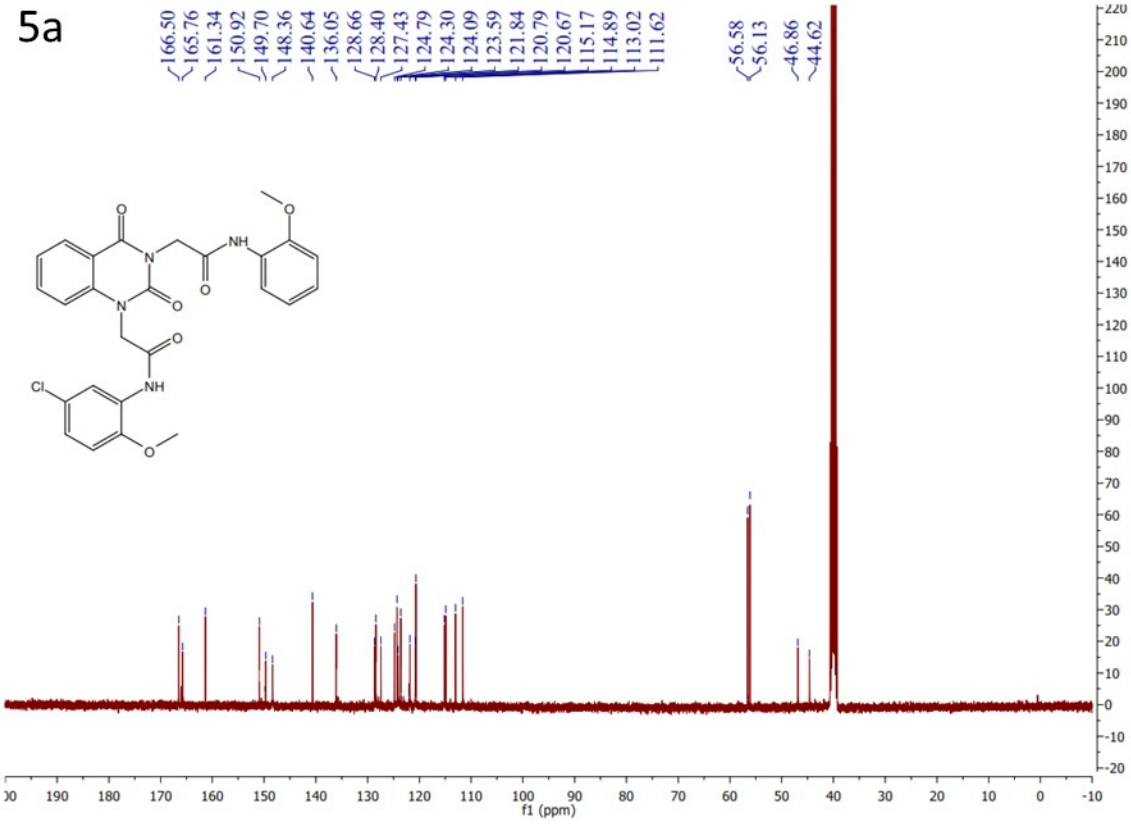
161.36
153.78
151.95
150.91
150.22
140.64
130.80
123.17
121.19
120.63
115.53
115.18
114.95
111.35
98.38
56.81
56.77
46.67
44.35
f1 (ppm)


PROTON_01
5a
9.88
9.60
8.08
8.06
7.91
7.90
7.78
7.76
7.74
7.40
7.38
7.34
7.32
7.30
7.12
7.10
7.08
7.04
6.86
5.12
4.85
3.87
3.85
3.31
2.48
1.07
1.19
2.00
1.13
1.19
1.04
1.04
4.09
1.30
1.90
1.78
5.69
f1 (ppm)


5a
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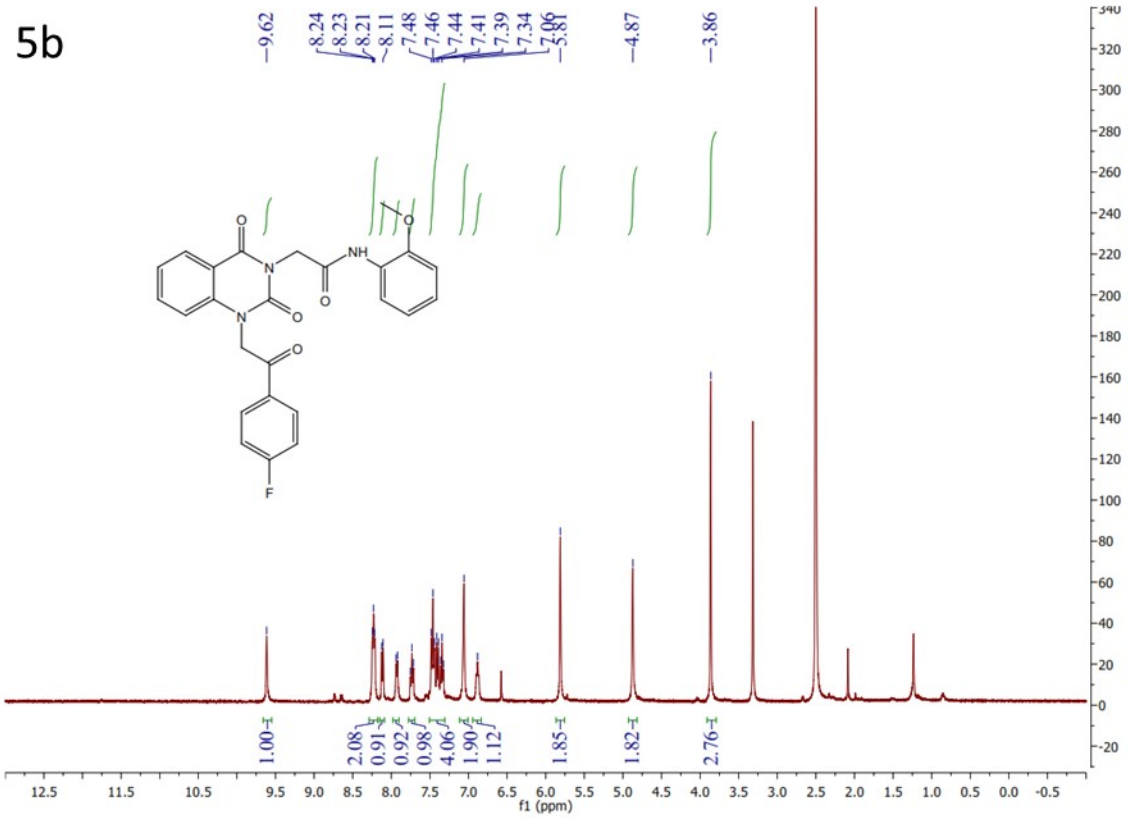
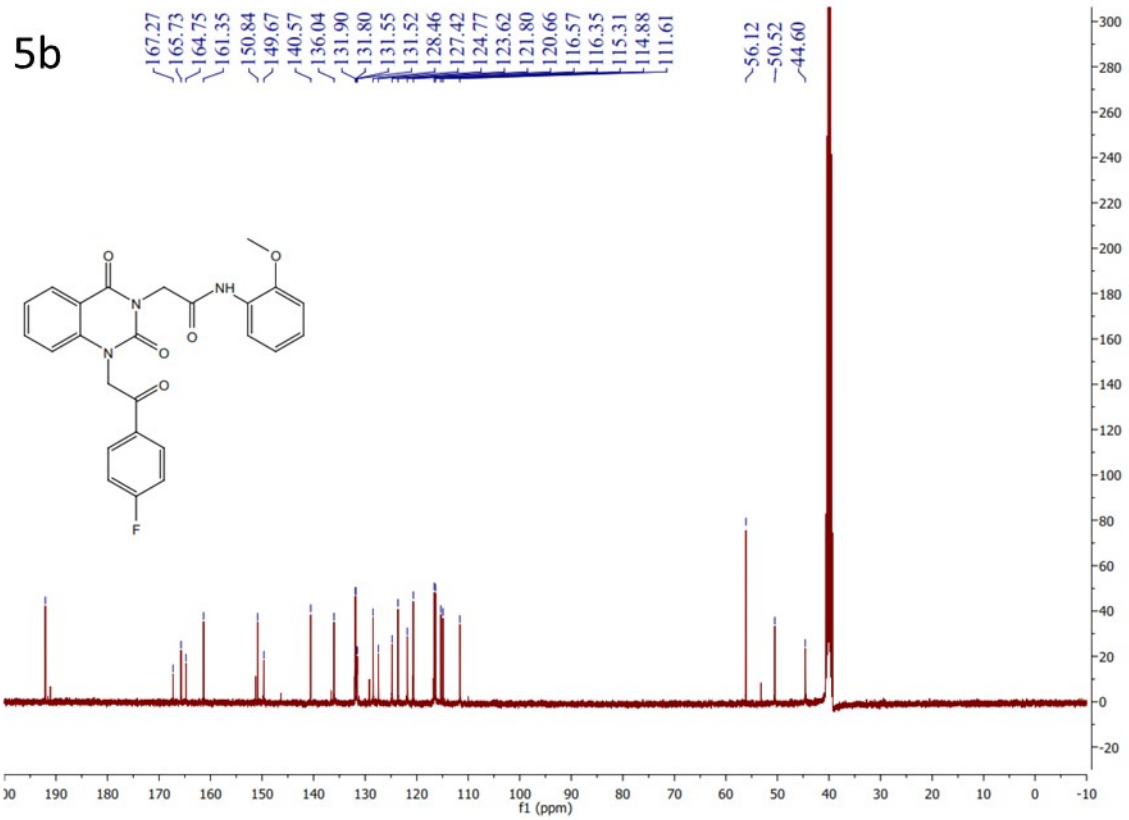
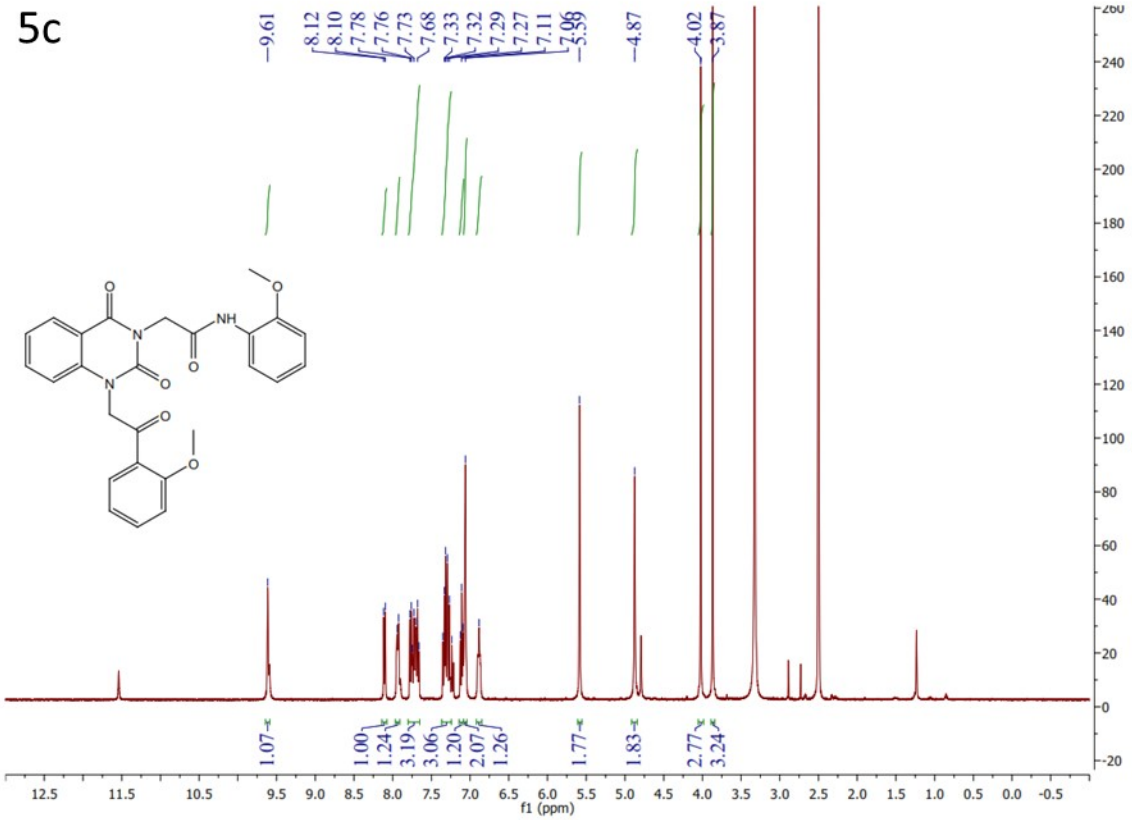
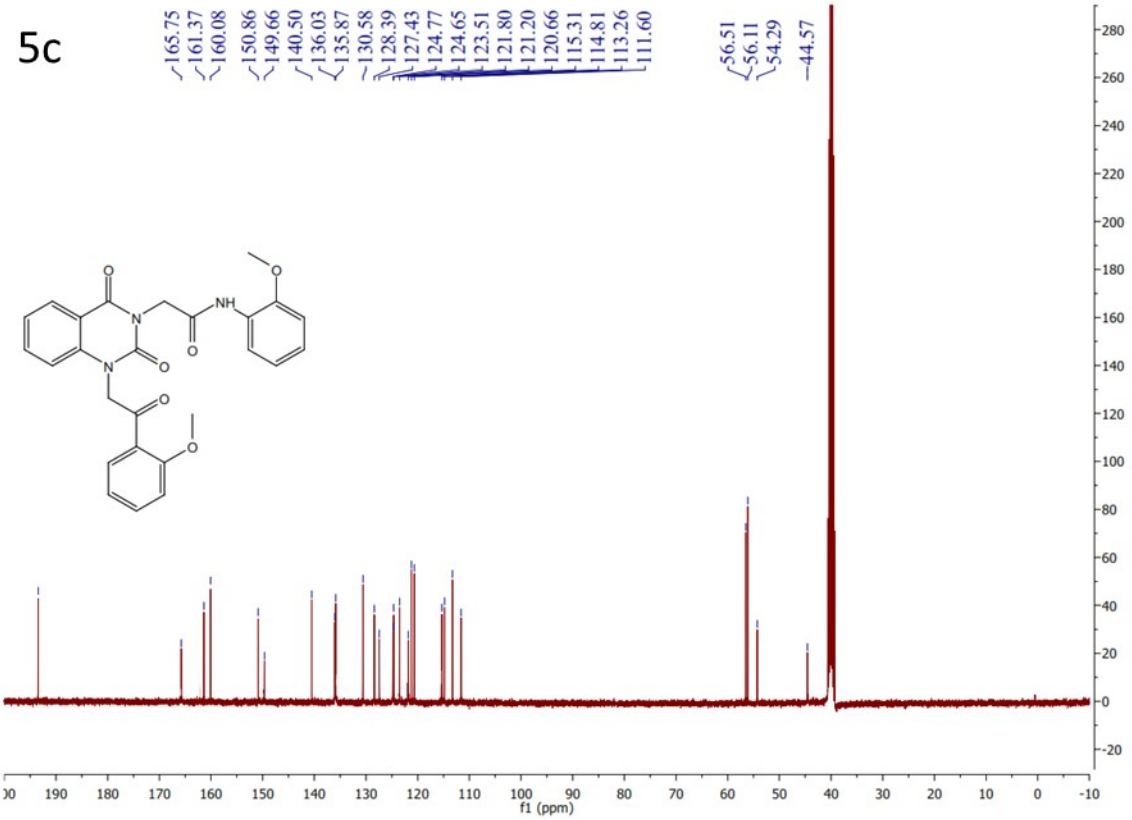
165.76
161.34
150.92
149.70
148.36
140.64
136.05
128.66
128.40
127.43
124.79
124.30
124.09
123.59
121.84
120.79
120.67
115.17
114.89
113.02
111.62
56.58
56.13
46.86
44.62
f1 (ppm)


5b
9.62
8.24
8.23
8.21
8.11
7.48
7.46
7.44
7.41
7.39
7.34
7.06
5.81
4.87
3.86
1.00
2.08
0.91
0.92
0.98
4.06
1.90
1.12
1.85
1.82
2.76
f1 (ppm)


5b
167.27
165.73
164.75
161.35
150.84
149.67
140.57
136.04
131.90
131.80
131.55
131.52
128.46
127.42
124.77
123.62
121.80
120.66
116.57
116.35
115.31
114.88
111.61
56.12
50.52
44.60
f1 (ppm)


5c
9.61
8.12
8.10
7.78
7.76
7.73
7.68
7.33
7.32
7.29
7.27
7.11
5.98
5.97
4.87
4.02
3.87
1.07
1.00
1.24
3.19
3.06
1.20
2.07
1.26
1.77
1.83
2.77
3.24
f1 (ppm)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165.75
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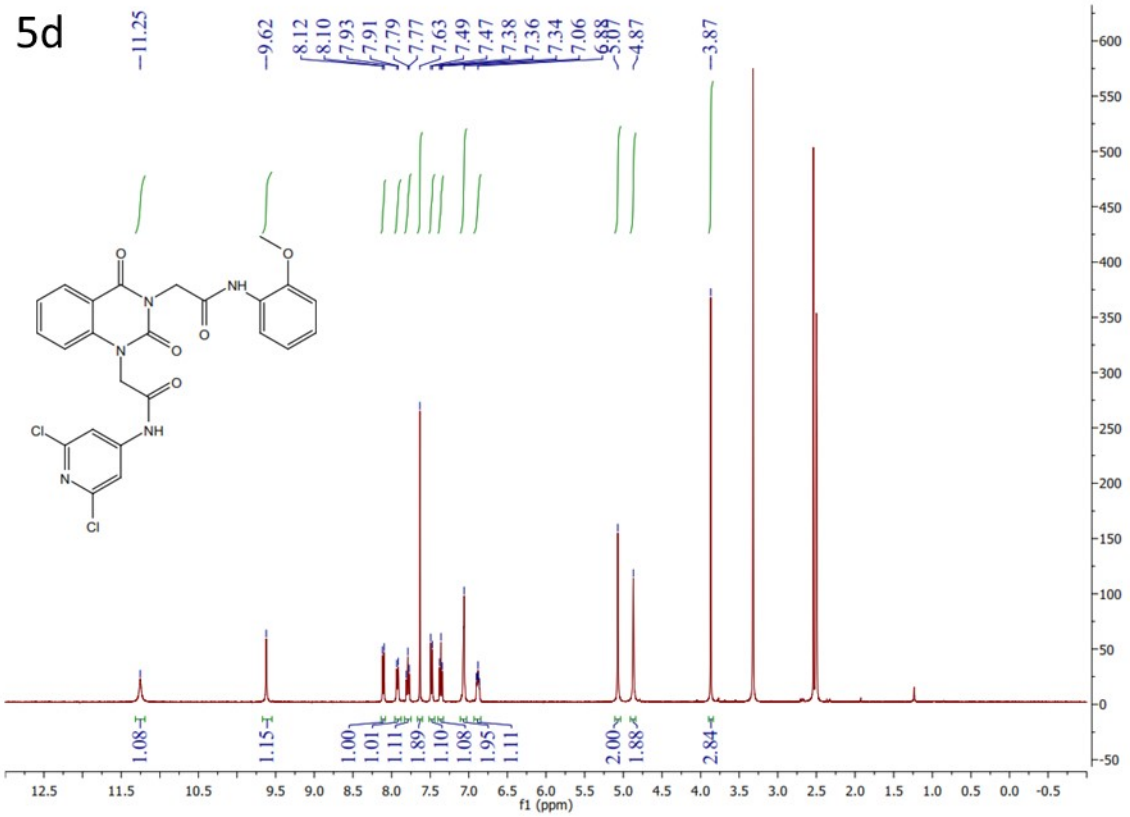
160.08
150.86
149.66
140.50
136.03
135.87
130.58
128.39
127.43
124.77
124.65
123.51
121.80
121.20
120.66
115.31
114.81
113.26
111.60
56.51
56.11
54.29
44.57
f1 (ppm)


5d
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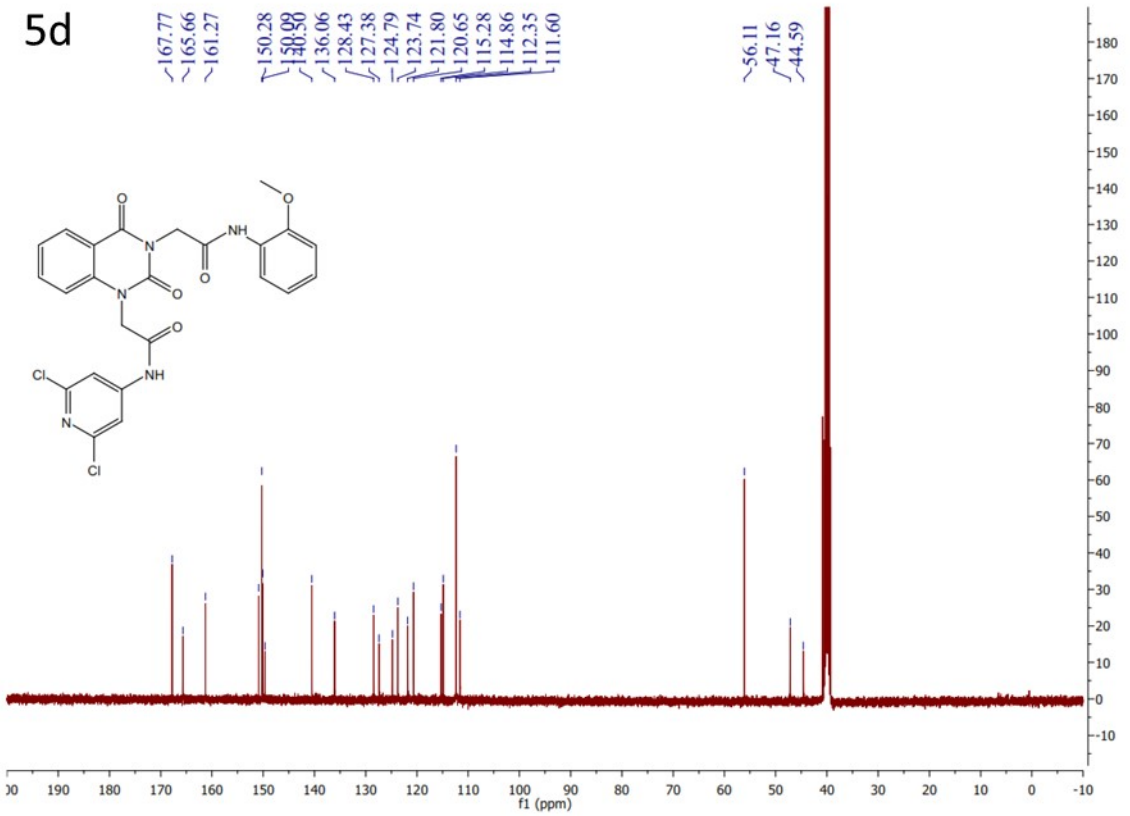
8.12
8.10
7.93
7.91
7.79
7.77
7.63
7.49
7.47
7.38
7.36
7.34
7.06
6.88
5.07
4.87
3.87
1.08
1.15
1.00
1.01
1.11
1.89
1.10
1.08
1.95
1.11
2.00
1.88
2.84
f1 (ppm)


5d
167.77
165.66
161.27
150.28
140.30
136.06
128.43
127.38
124.79
123.74
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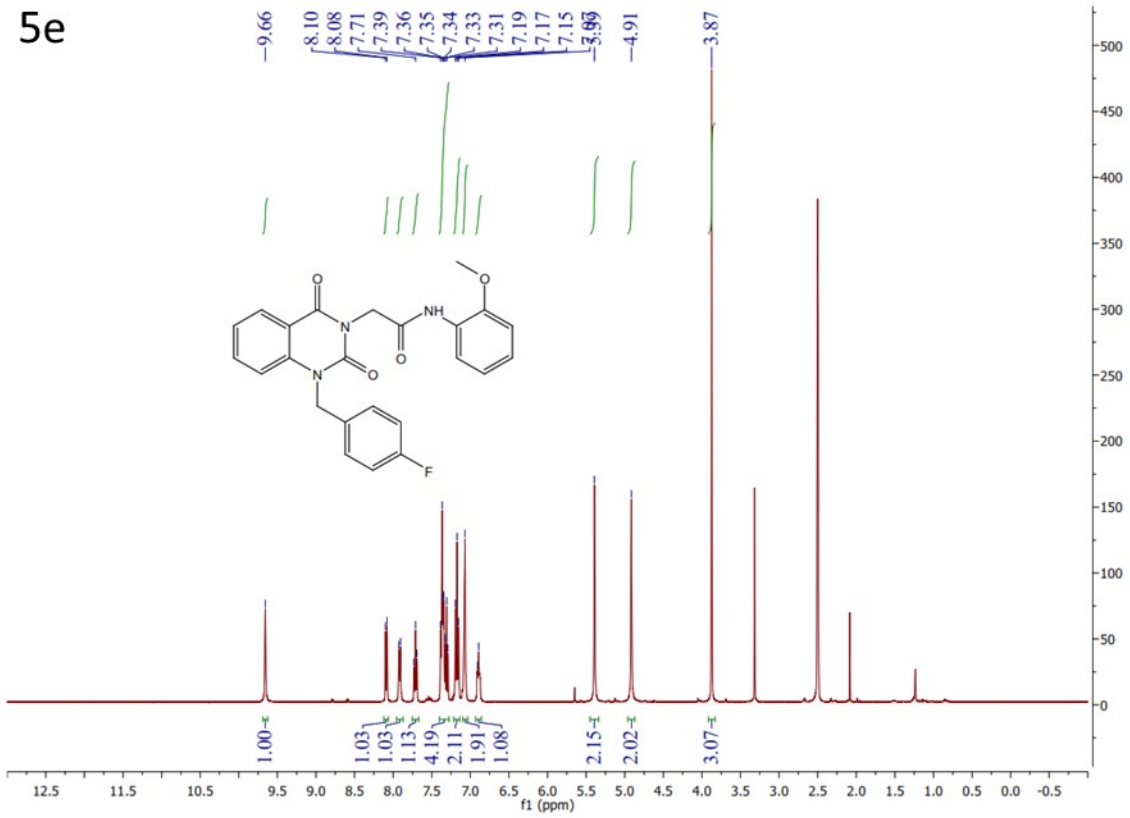
120.65
115.28
114.86
112.35
111.60
56.11
47.16
44.59
f1 (ppm)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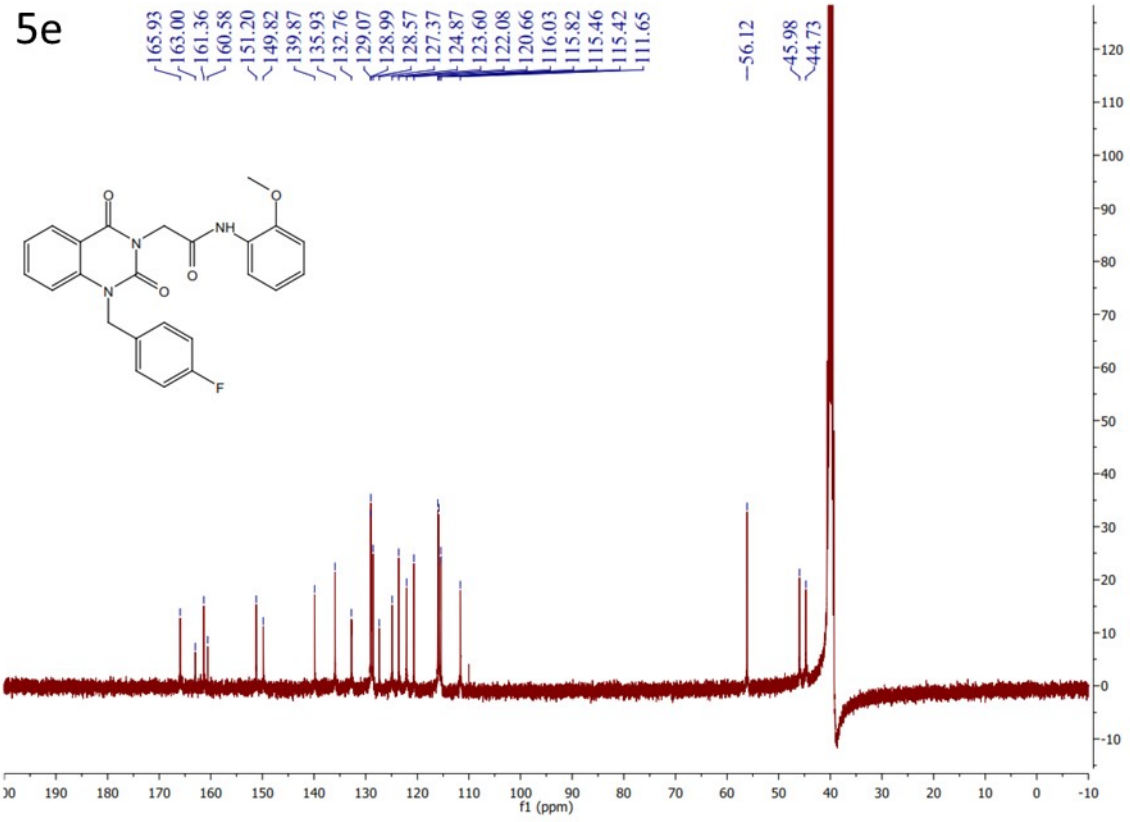
8.10
8.08
7.71
7.39
7.36
7.35
7.34
7.33
7.31
7.19
7.17
7.15
4.91
3.87
1.00
1.03
1.03
1.13
4.19
2.11
1.91
1.08
2.15
2.02
3.07
f1 (ppm)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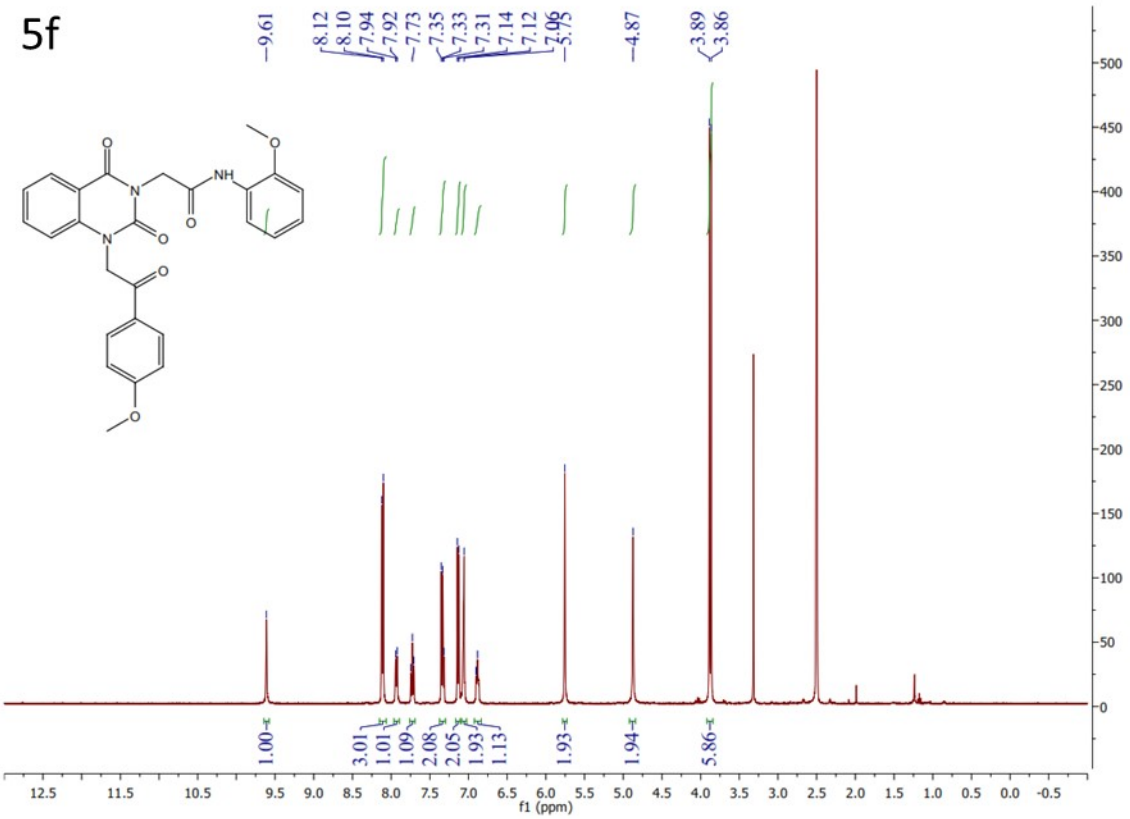
161.36
160.58
151.20
149.82
139.87
135.93
132.76
129.07
128.99
128.57
127.37
124.87
123.60
122.08
120.66
116.03
115.82
115.46
115.42
111.65
56.12
45.98
44.73
f1 (ppm)


5f
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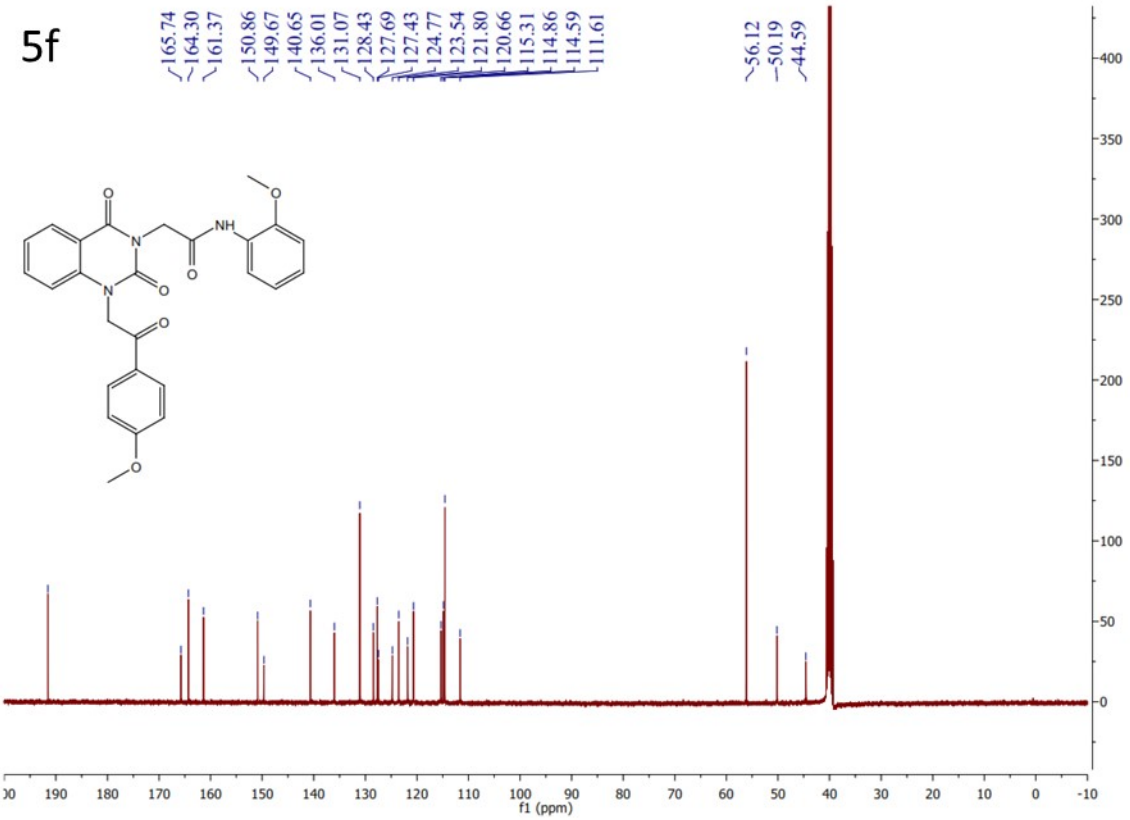
8.10
7.94
7.92
7.73
7.35
7.33
7.31
7.14
7.12
7.06
5.75
4.87
3.89
3.86
1.00
3.01
1.01
1.09
2.08
2.05
1.93
1.13
1.93
1.94
5.86
f1 (ppm)


5f
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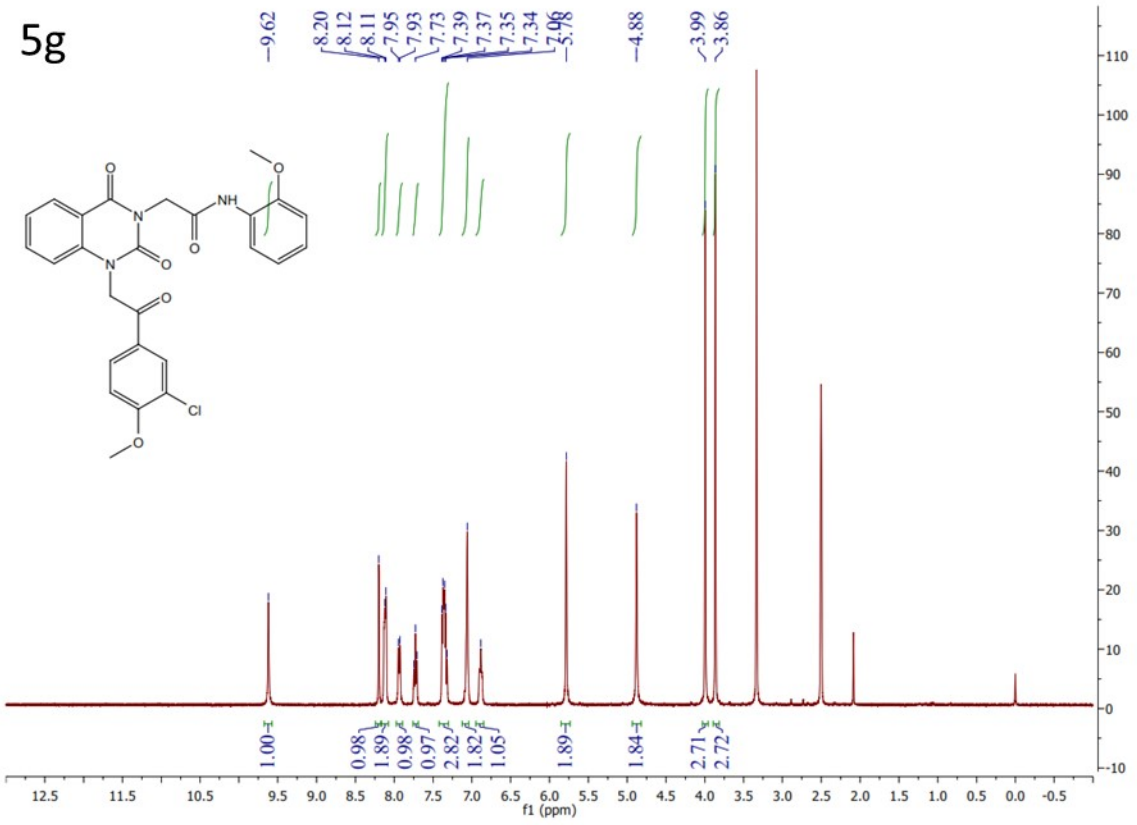
149.67
140.65
136.01
131.07
128.43
127.69
127.43
124.77
123.54
121.80
120.66
115.31
114.86
114.59
111.61
56.12
50.19
44.59
f1 (ppm)


5g
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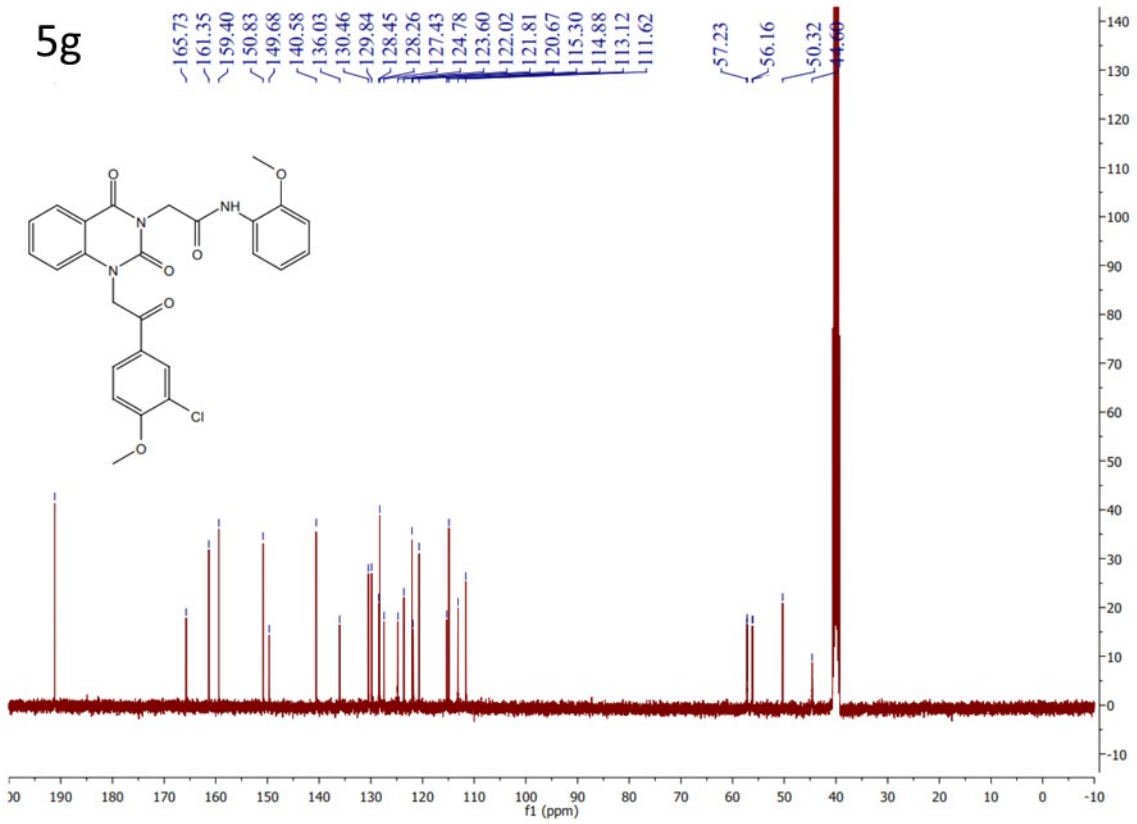
8.20
8.12
8.11
7.95
7.93
7.73
7.39
7.37
7.35
7.34
4.88
3.99
3.86
1.00
0.98
1.89
0.98
0.97
2.82
1.82
1.05
1.89
1.84
2.71
2.72
f1 (ppm)


5g
165.73
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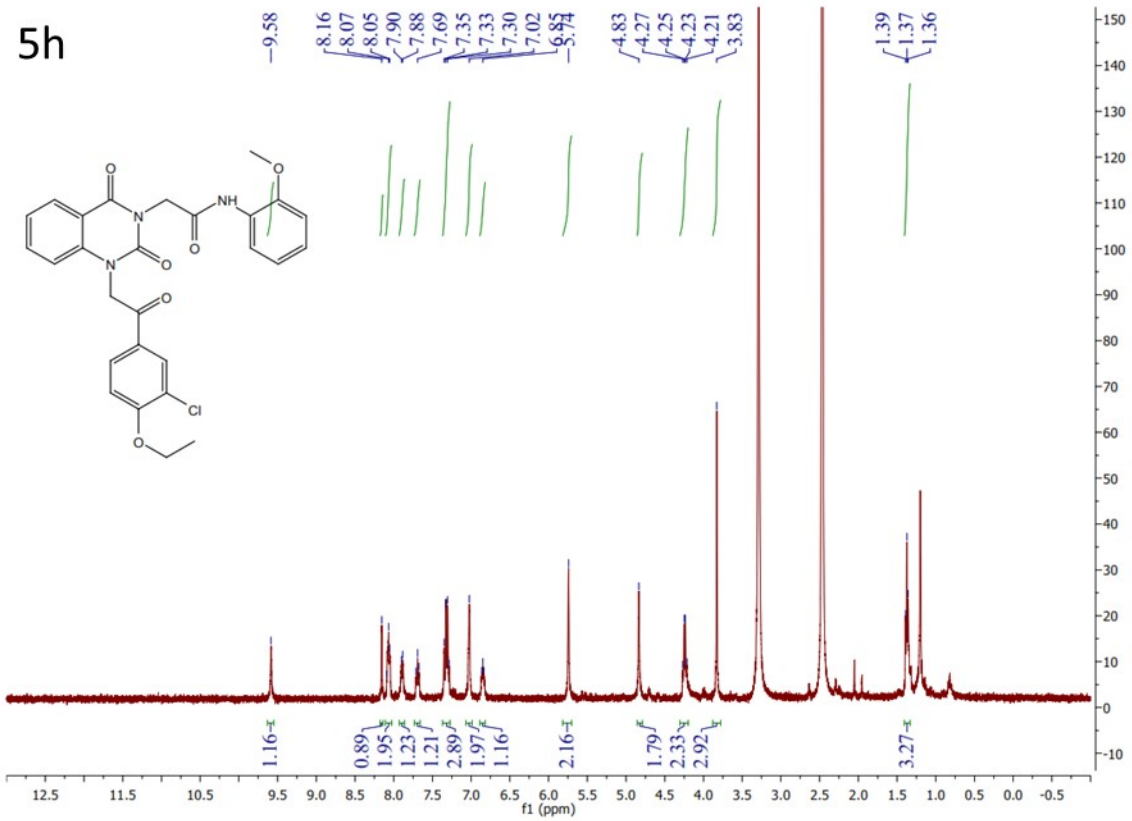
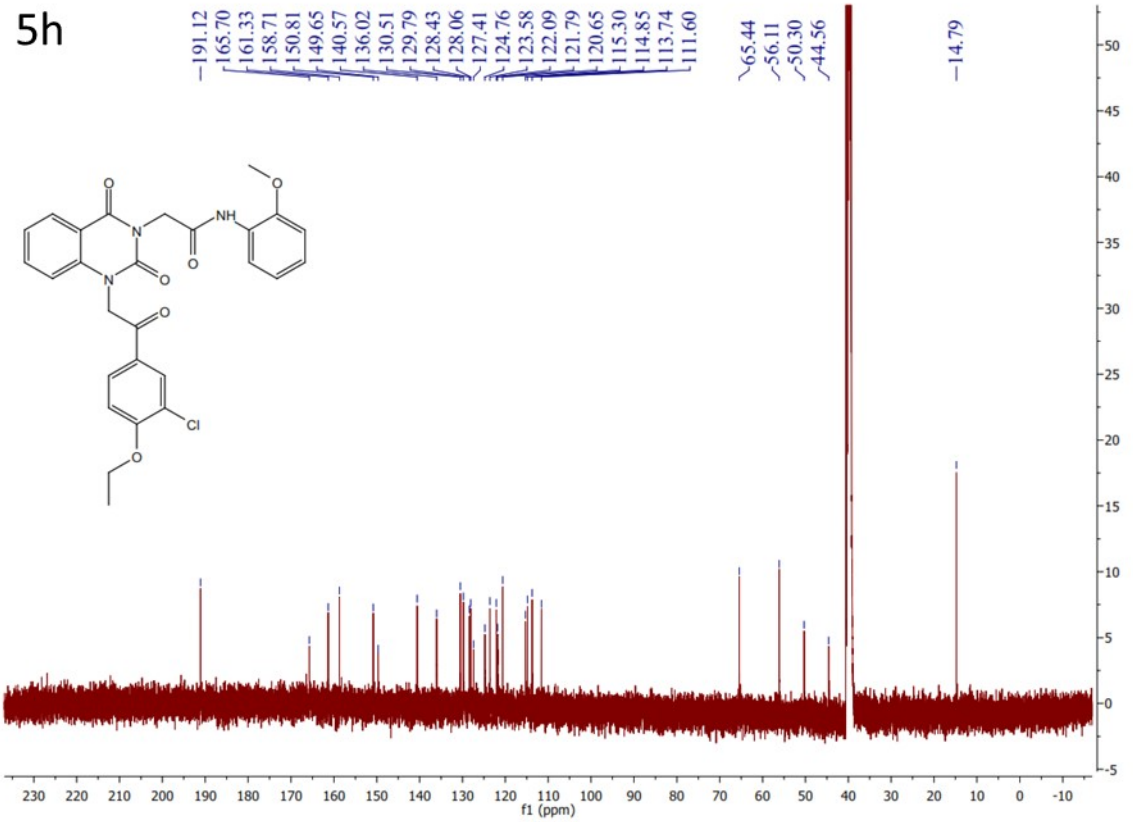
159.40
150.83
149.68
140.58
136.03
130.46
129.84
128.45
128.26
127.43
124.78
123.60
122.02
121.81
120.67
115.30
114.88
113.12
111.62
57.23
56.16
50.32
44.60
f1 (ppm)


5h
9.58
8.16
8.07
8.05
7.90
7.88
7.69
7.35
7.33
7.30
7.02
6.85
5.74
4.83
4.27
4.25
4.23
4.21
3.83
1.39
1.37
1.36
1.16
0.89
1.95
1.23
1.21
2.89
1.97
1.16
2.16
1.79
2.33
2.92
3.27
f1 (ppm)


5h
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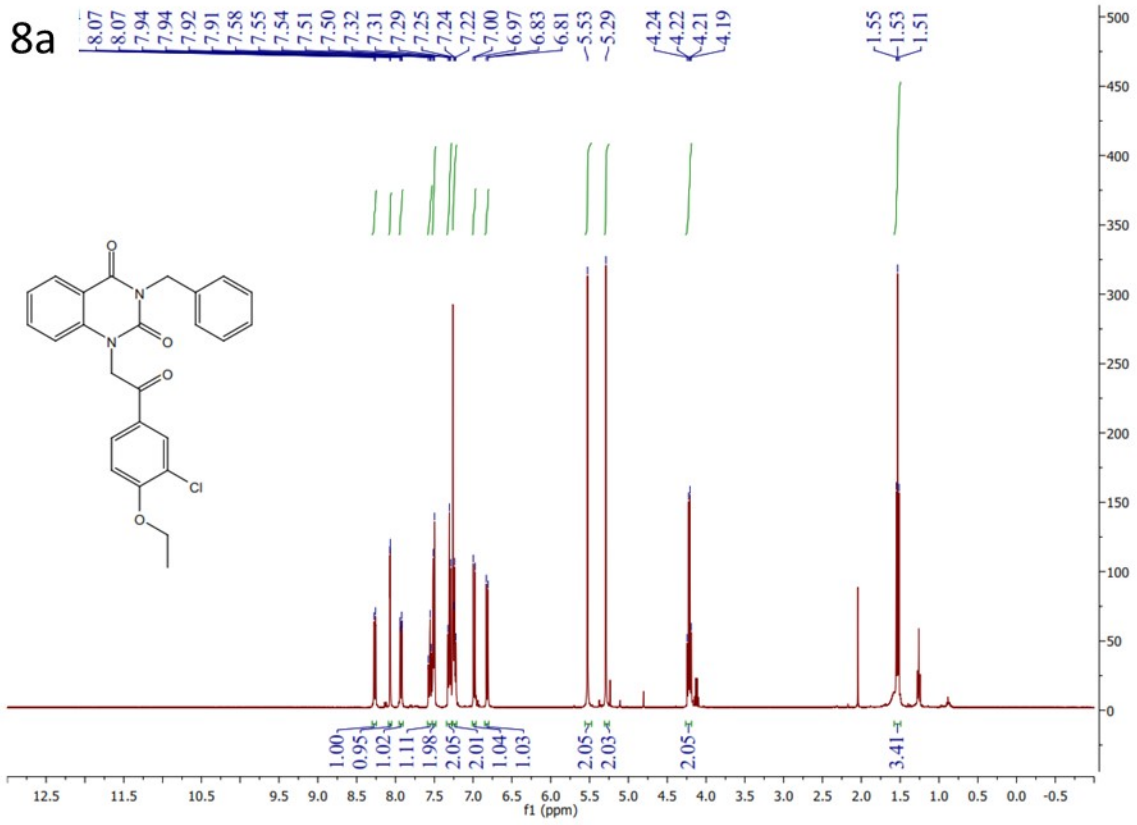
150.81
149.65
140.57
136.02
130.51
129.79
128.43
128.06
127.41
124.76
123.58
122.09
121.79
120.65
115.30
114.85
113.74
111.60
65.44
56.11
50.30
44.56
14.79
f1 (ppm)


8a
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8.07
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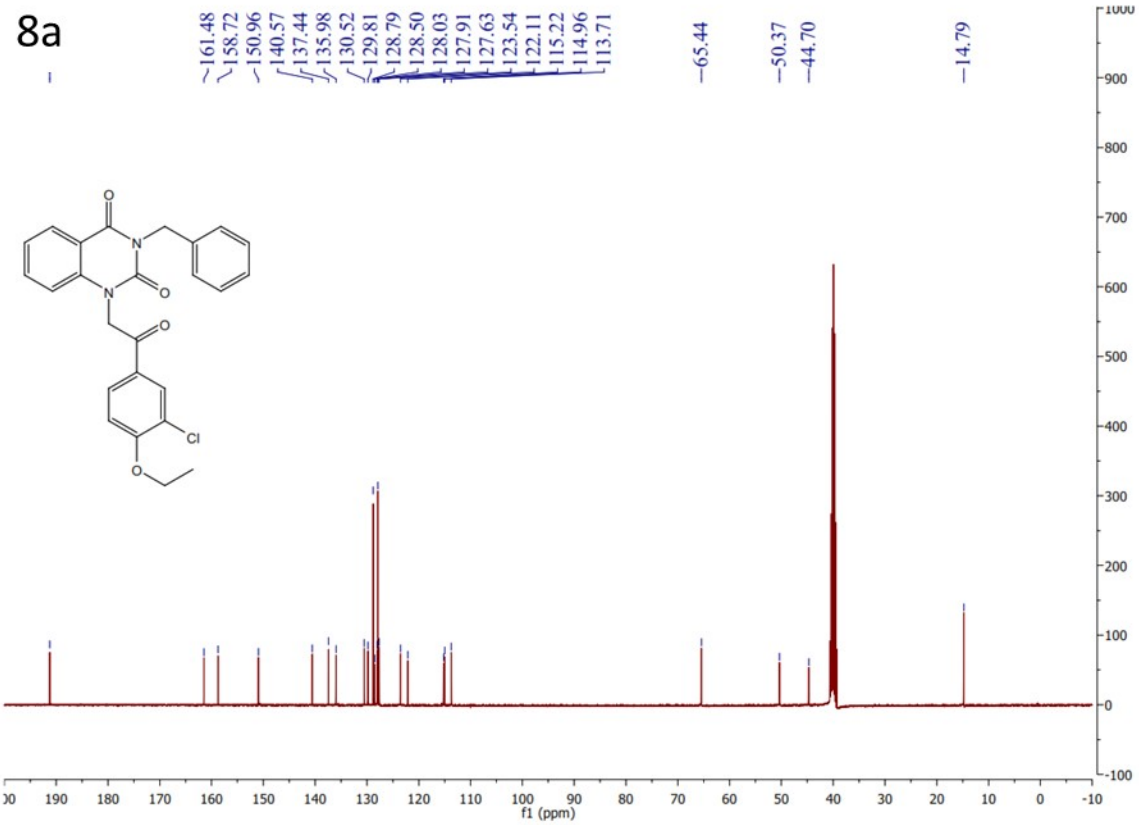
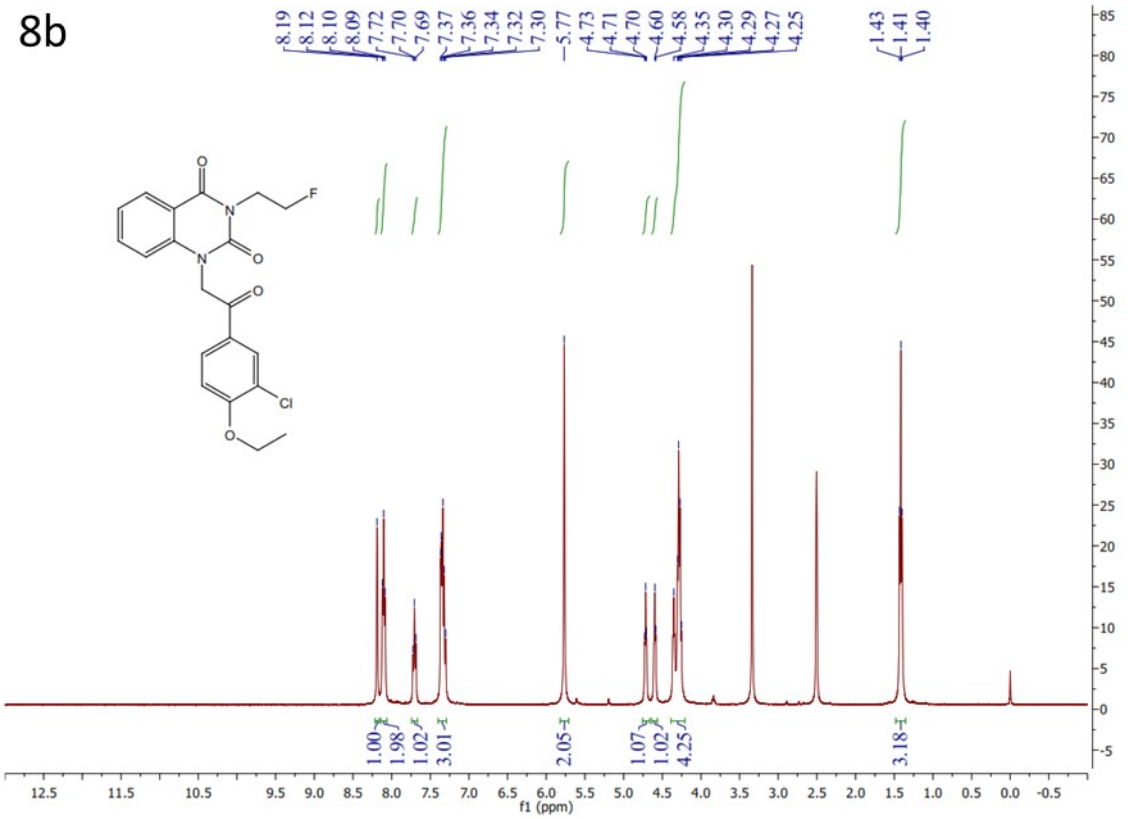
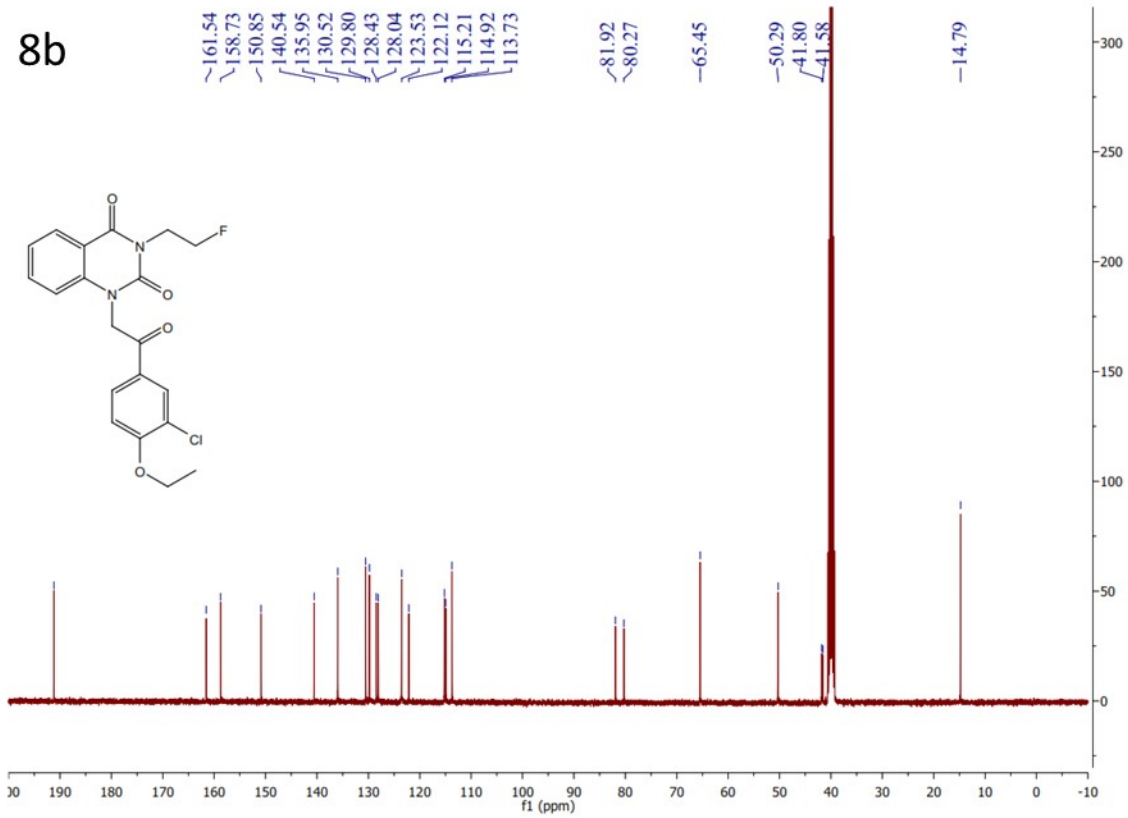
7.94
7.92
7.91
7.58
7.55
7.54
7.51
7.50
7.32
7.31
7.29
7.25
7.24
7.22
7.00
6.97
6.83
6.81
5.53
5.29
4.24
4.22
4.21
4.19
1.55
1.53
1.51
1.00
0.95
1.02
1.11
1.98
2.05
2.01
1.04
1.03
2.05
2.03
2.05
3.41
f1 (ppm)

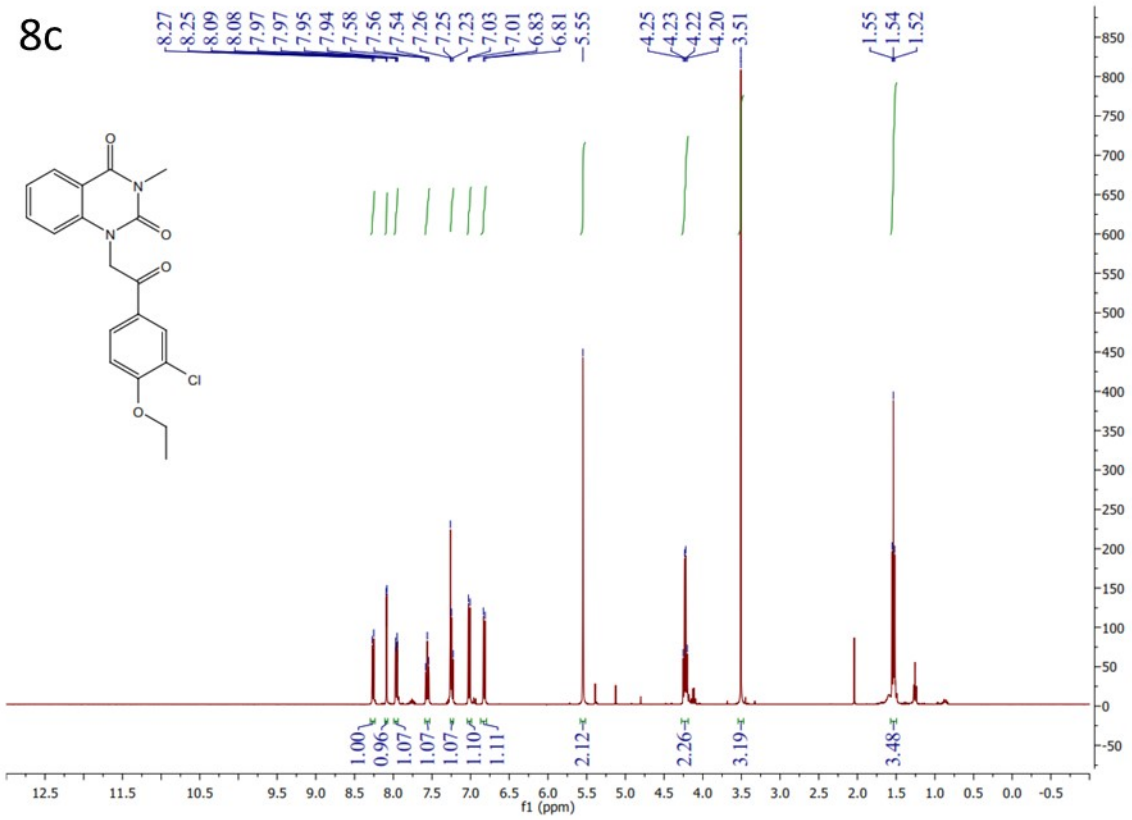

8a
161.48
158.72
150.96
140.57
137.44
135.98
130.52
129.81
128.79
128.50
128.03
127.91
127.63
123.54
122.11
115.22
114.96
113.71
65.44
50.37
44.70
14.79
f1 (ppm)

8b


8.19
8.12
8.10
8.09
7.72
7.70
7.69
7.37
7.36
7.34
7.32
7.30
5.77
4.73
4.71
4.70
4.60
4.58
4.35
4.30
4.29
4.27
4.25
1.43
1.41
1.40
1.00
1.98
1.02
3.01
2.05
1.07
1.02
4.25
3.18
f1 (ppm)

8b


161.54
158.73
150.85
140.54
135.95
130.52
129.80
128.43
128.04
123.53
122.12
115.21
114.92
113.73
81.92
80.27
65.45
50.29
41.80
41.58
14.79
f1 (ppm)


8c
8.27
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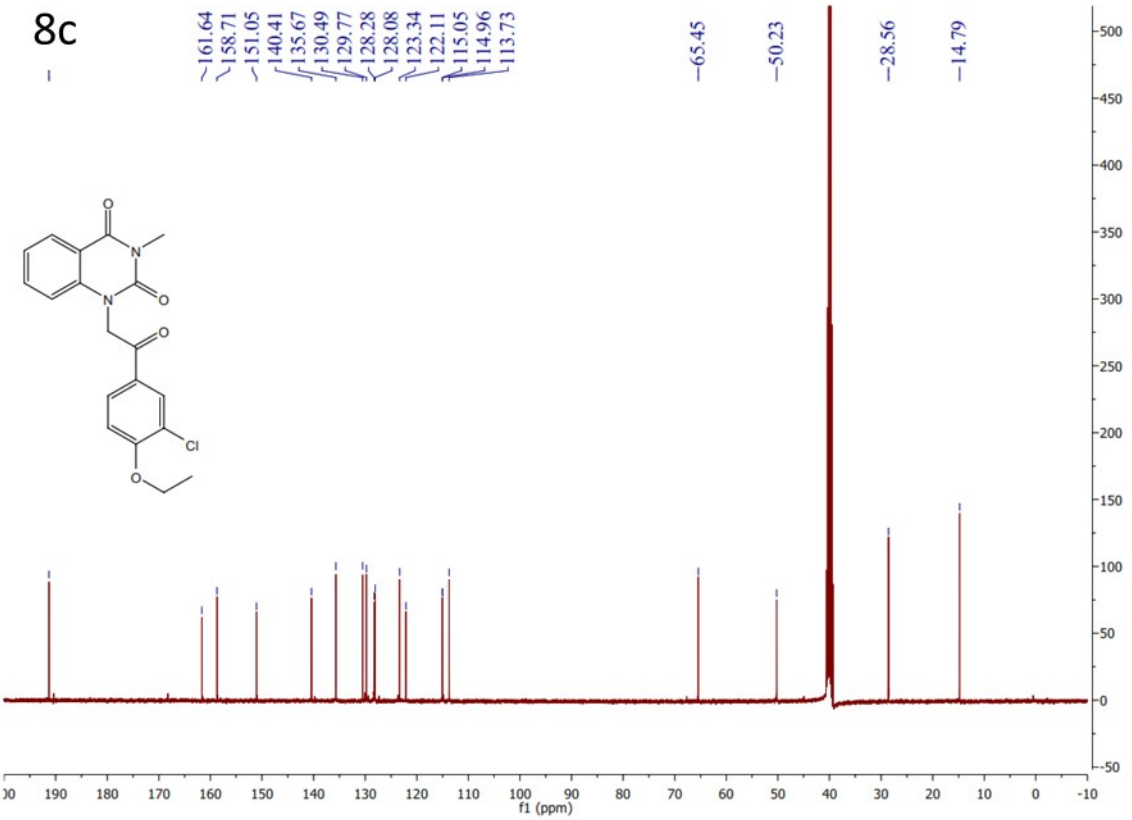
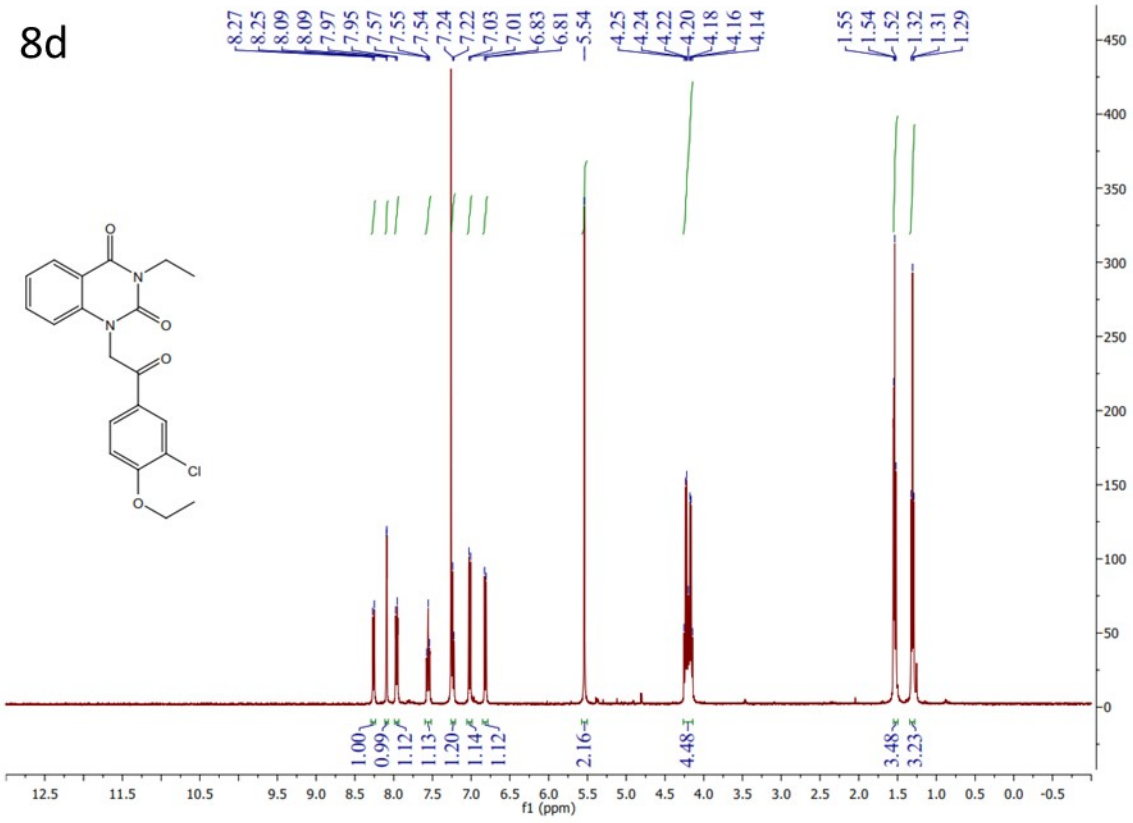
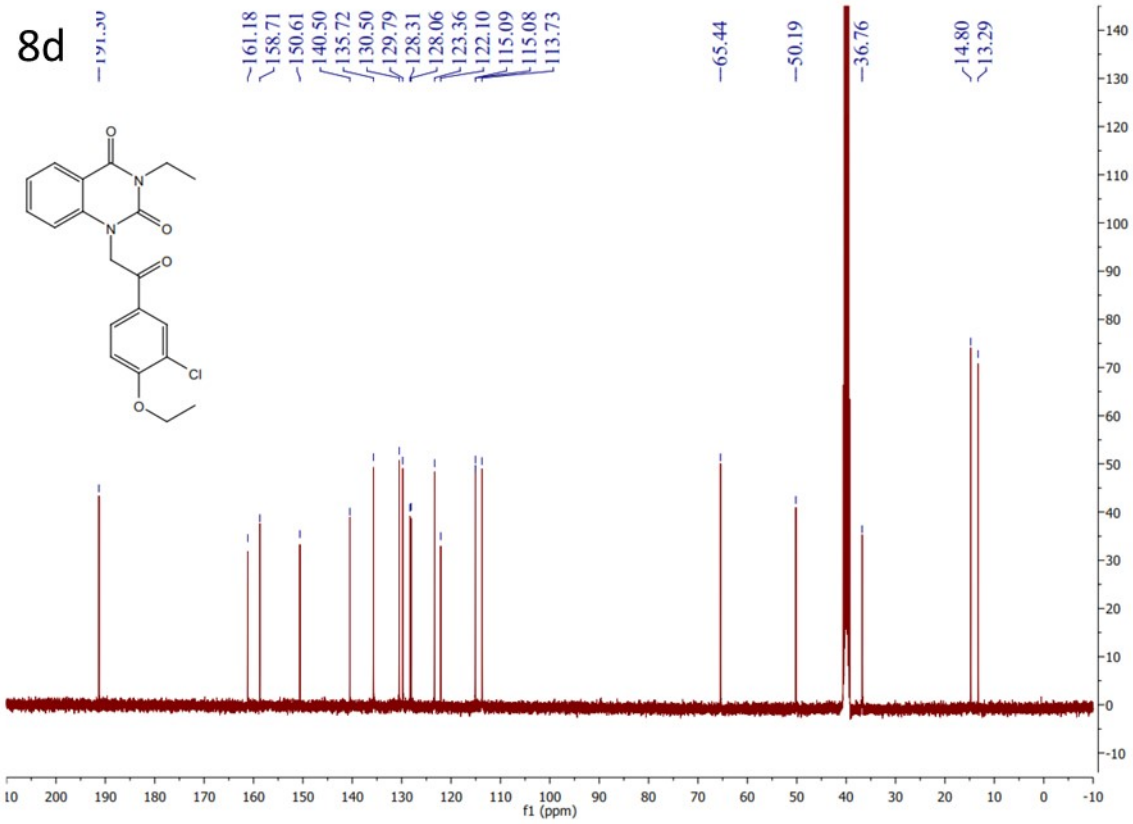
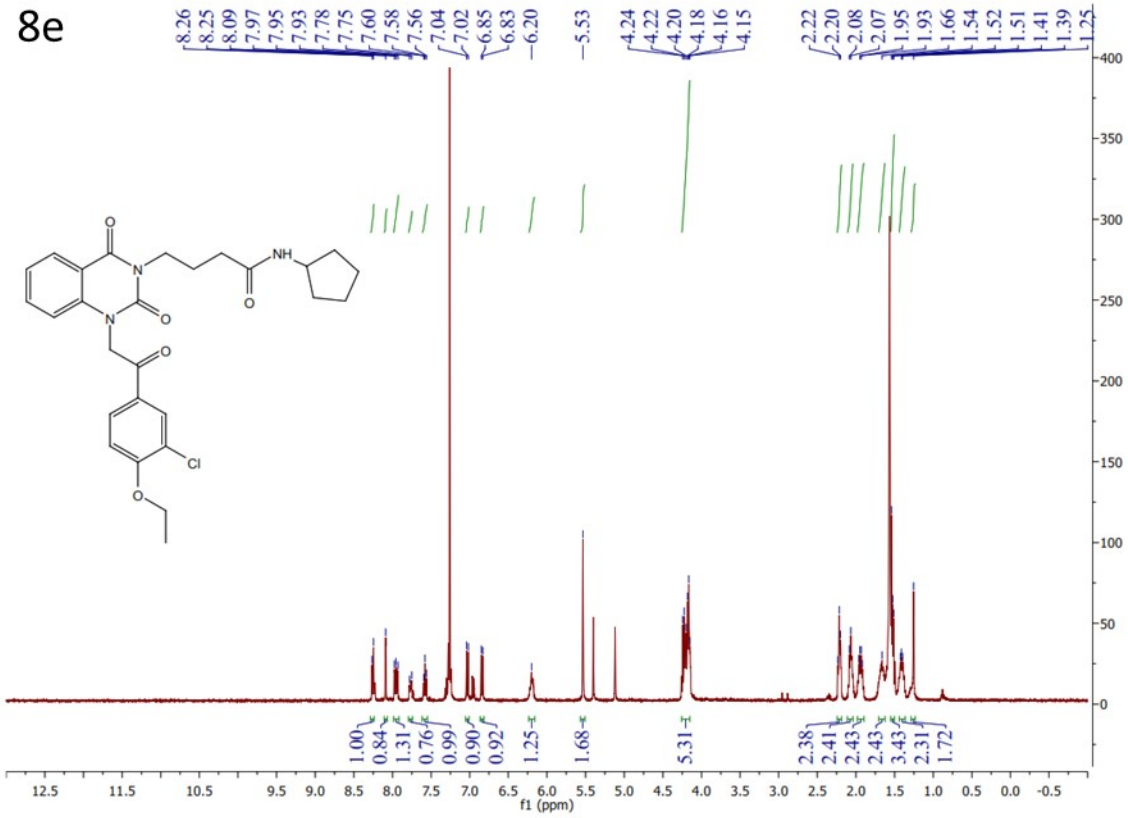
8.08
7.97
7.97
7.95
7.94
7.58
7.56
7.54
7.26
7.25
7.23
7.03
7.01
6.83
6.81
5.55
4.25
4.23
4.22
4.20
3.51
1.55
1.54
1.52
1.00
0.96
1.07
1.07
1.07
1.10
1.11
2.12
2.26
3.19
3.48
f1 (ppm)


8c
161.64
158.71
151.05
140.41
135.67
130.49
129.77
128.28
128.08
123.34
122.11
115.05
114.96
113.73
65.45
50.23
28.56
14.79
f1 (ppm)

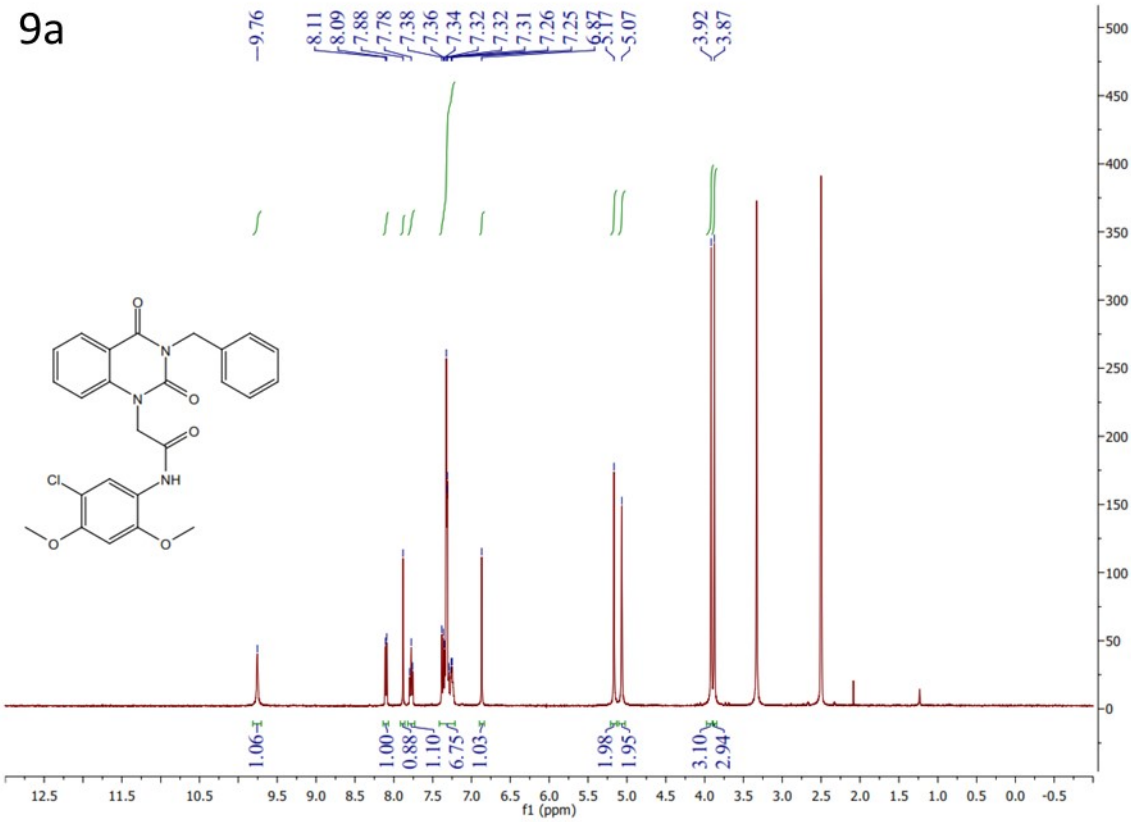

8d
8.27
8.25
8.09
8.09
7.97
7.95
7.57
7.55
7.54
7.24
7.22
7.03
7.01
6.83
6.81
5.54
4.25
4.24
4.22
4.20
4.18
4.16
4.14
1.55
1.54
1.52
1.32
1.31
1.29
1.00
0.99
1.12
1.13
1.20
1.14
1.12
2.16
4.48
3.48
3.23
f1 (ppm)


8d
161.18
158.71
150.61
140.50
135.72
130.50
129.79
128.31
128.06
123.36
122.10
115.09
115.08
113.73
65.44
50.19
36.76
14.80
13.29
f1 (ppm)

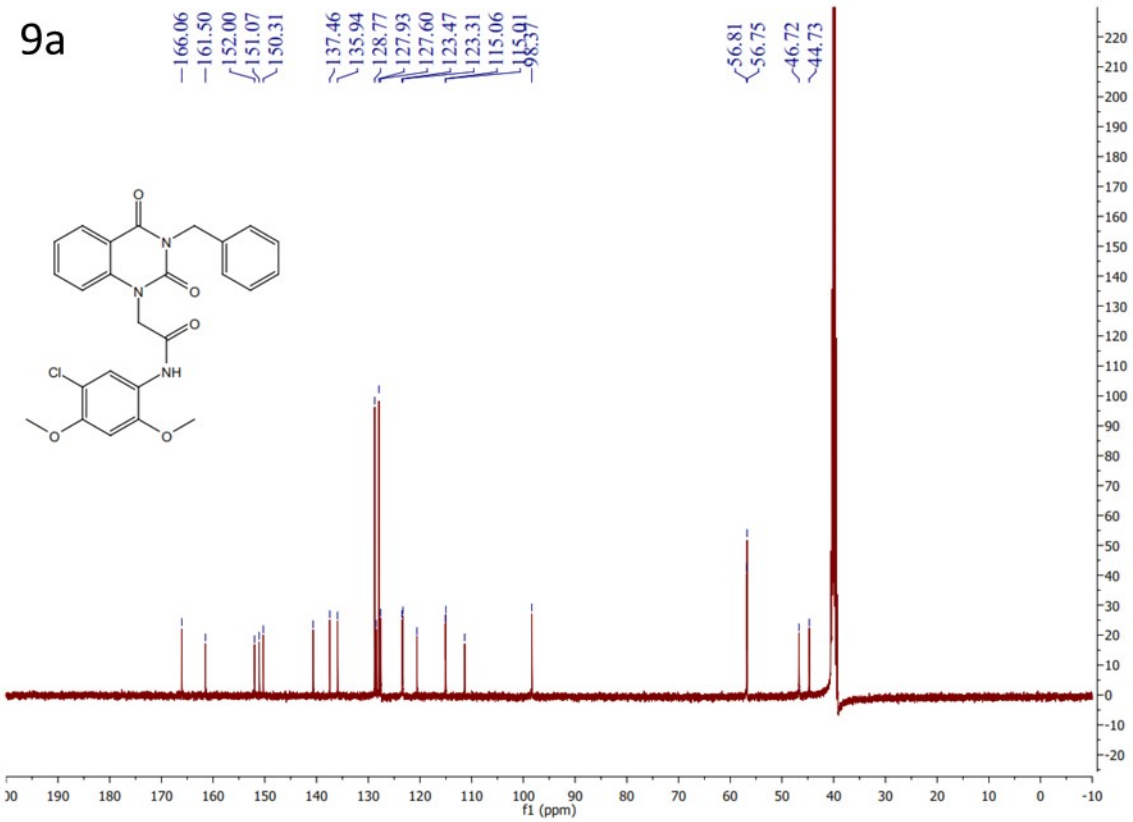
8e


8.26
8.25
8.09
7.97
7.95
7.93
7.78
7.75
7.60
7.58
7.56
7.04
7.02
6.85
6.83
6.20
5.53
4.24
4.22
4.20
4.18
4.16
4.15
2.22
2.20
2.08
2.07
1.95
1.93
1.66
1.54
1.52
1.51
1.41
1.39
1.25
1.00
0.84
1.31
0.76
0.99
0.90
0.92
1.25
1.68
5.31
2.38
2.41
2.43
2.43
3.43
2.31
1.72
f1 (ppm)

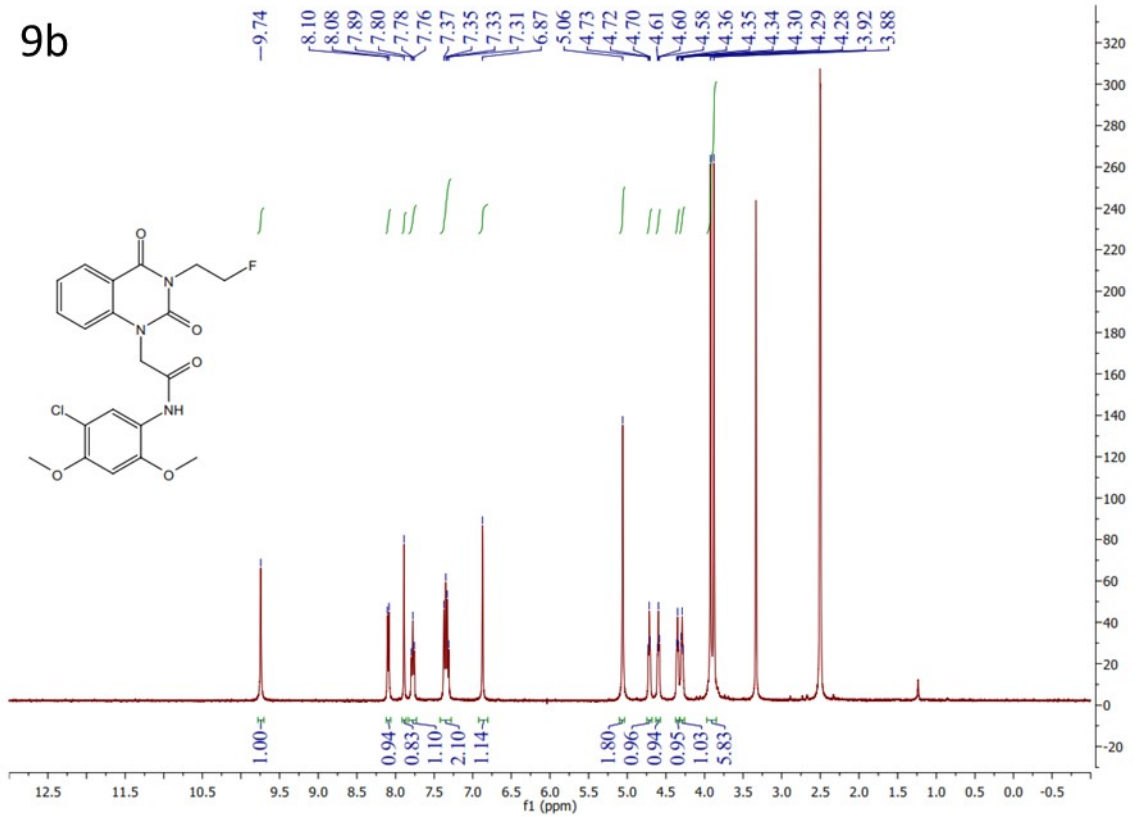
9a


9.76
8.11
8.09
7.88
7.78
7.38
7.36
7.34
7.32
7.32
7.31
7.26
7.25
6.87
5.17
5.07
3.92
3.87
1.06
1.00
0.88
1.10
6.75
1.03
1.98
1.95
3.10
2.94
f1 (ppm)

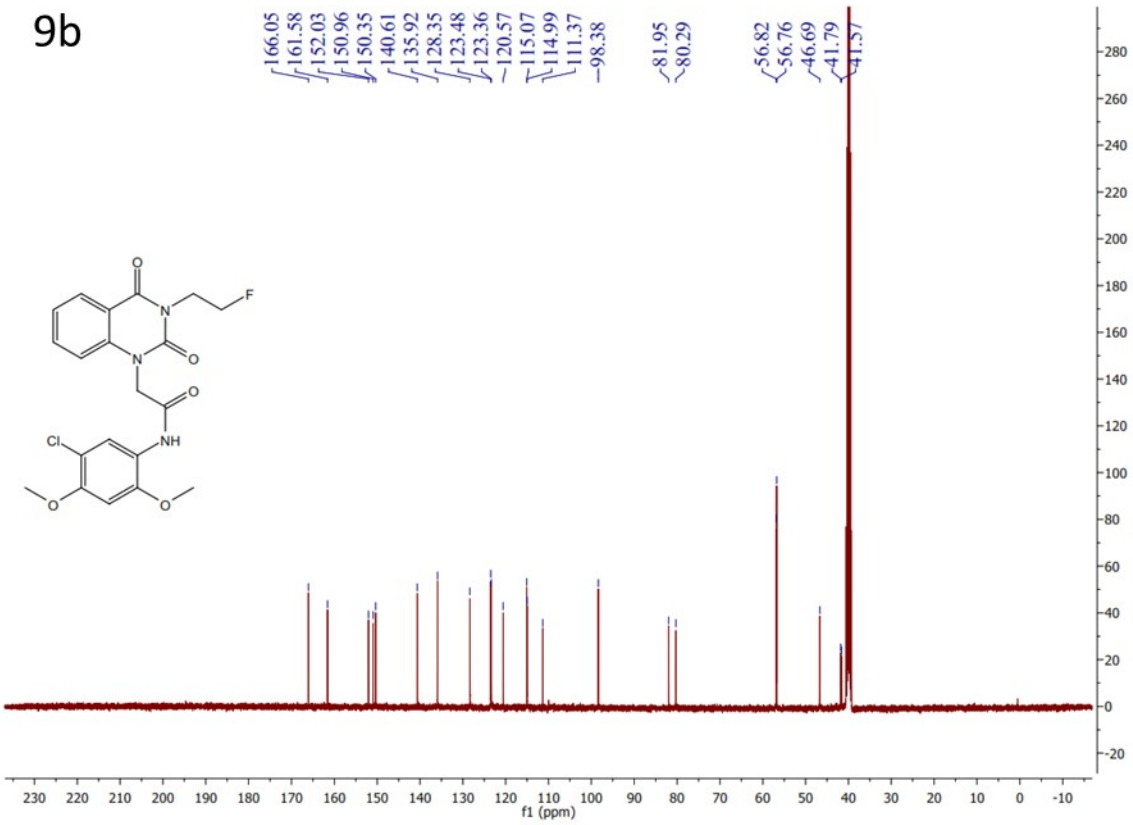
9a


166.06
161.50
152.00
151.07
150.31
137.46
135.94
128.77
127.93
127.60
123.47
123.31
115.06
115.01
98.37
56.81
56.75
46.72
44.73
f1 (ppm)

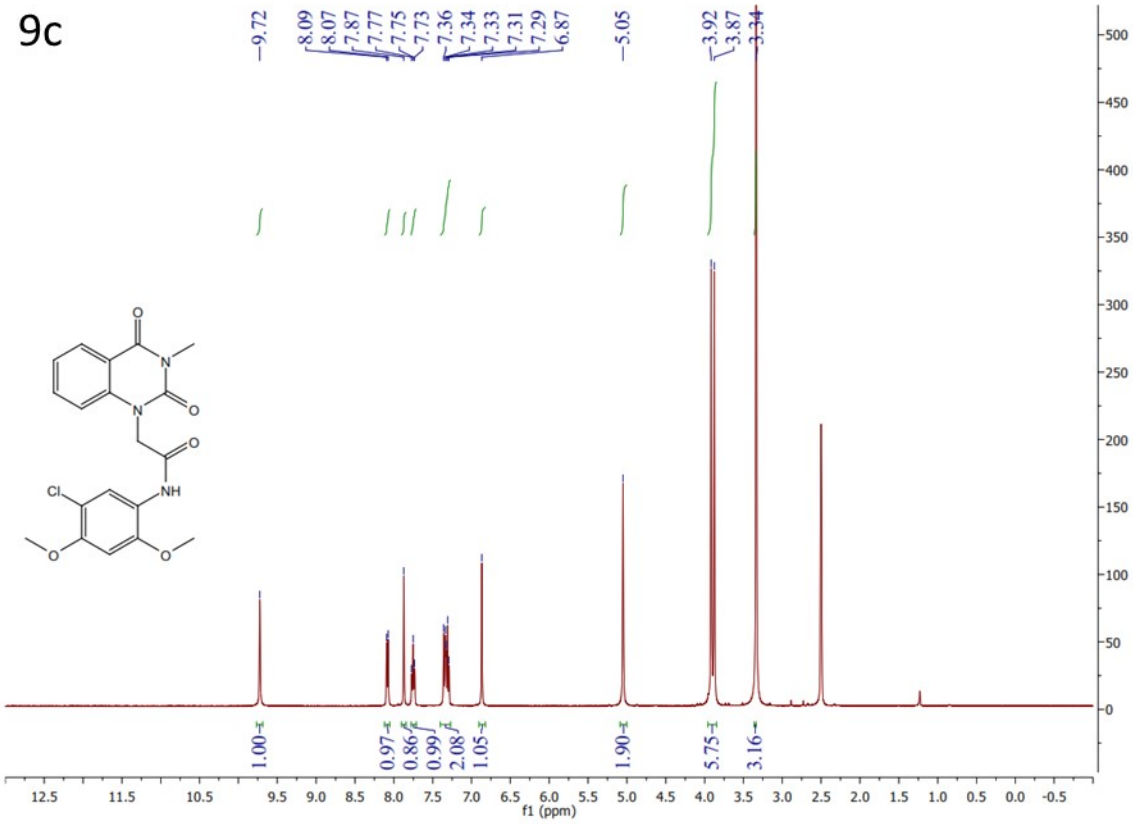
9b

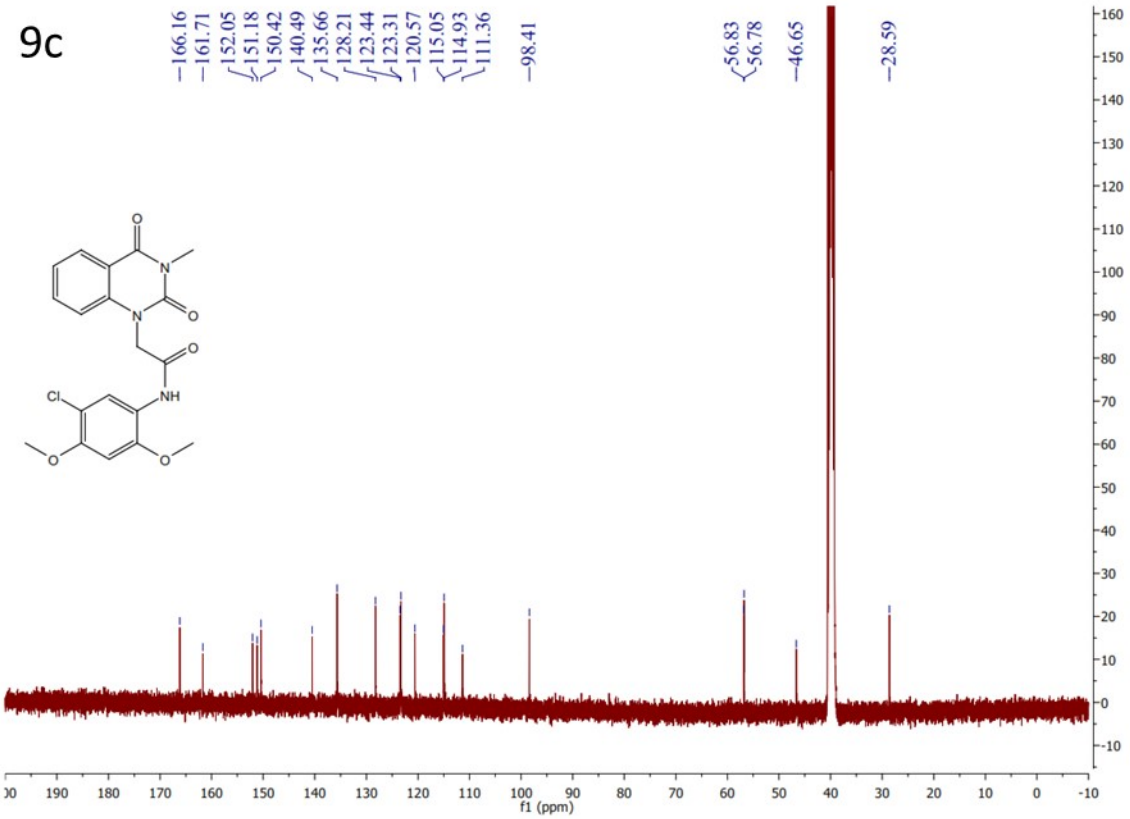

9.74
8.10
8.08
7.89
7.80
7.78
7.76
7.37
7.35
7.33
7.31
6.87
5.06
4.73
4.72
4.70
4.61
4.60
4.58
4.36
4.35
4.34
4.30
4.29
4.28
3.92
3.88
1.00
0.94
0.83
1.10
2.10
1.14
1.80
0.96
0.94
0.95
1.03
5.83
f1 (ppm)

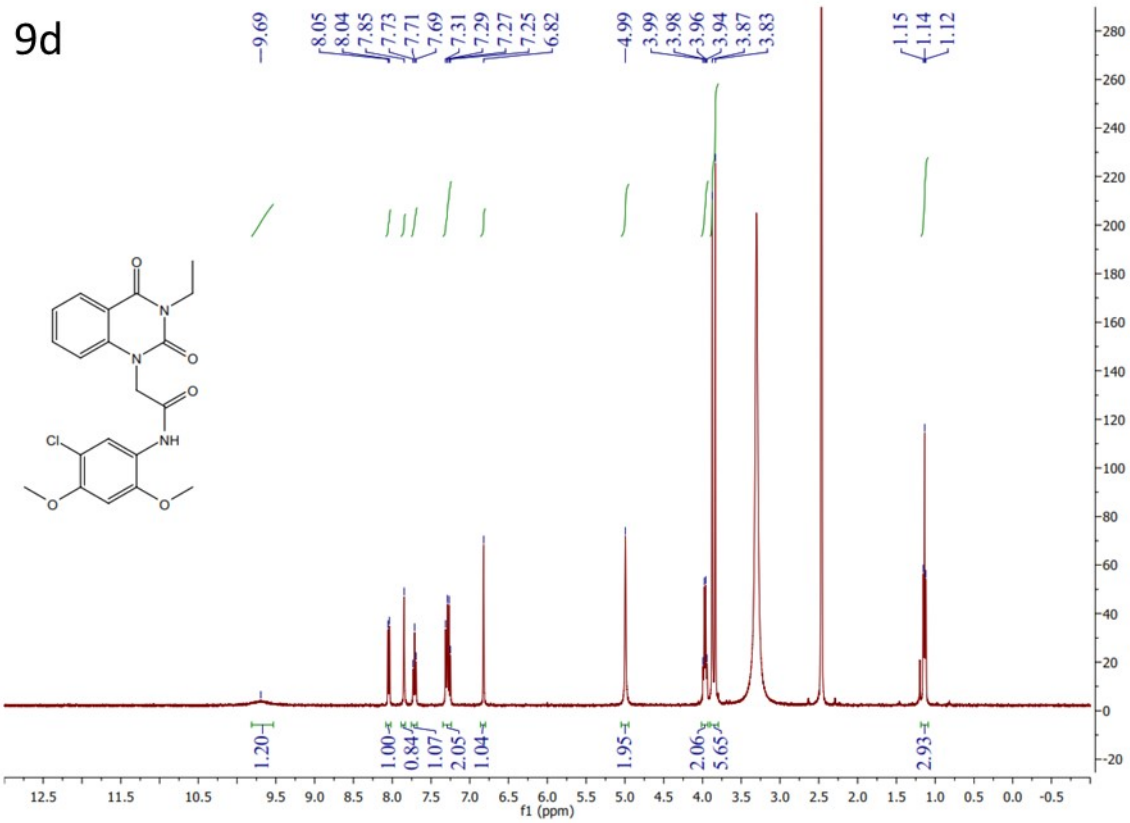
9b


166.05
161.58
152.03
150.96
150.35
140.61
135.92
128.35
123.48
123.36
120.57
115.07
114.99
111.37
98.38
81.95
80.29
56.82
56.76
46.69
41.79
41.57
f1 (ppm)

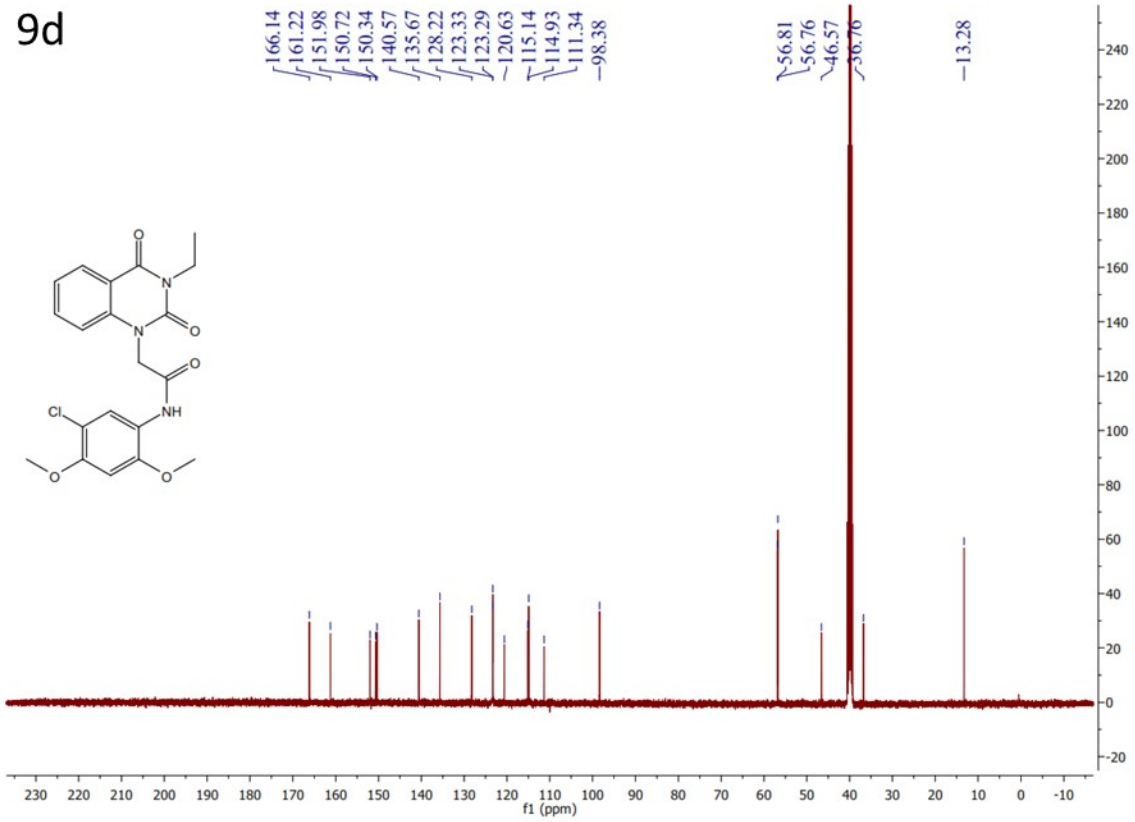
9c


9.72
8.09
8.07
7.87
7.77
7.75
7.73
7.36
7.34
7.33
7.31
7.29
6.87
5.05
3.92
3.87
3.34
1.00
0.97
0.86
0.99
2.08
1.05
1.90
5.75
3.16
f1 (ppm)

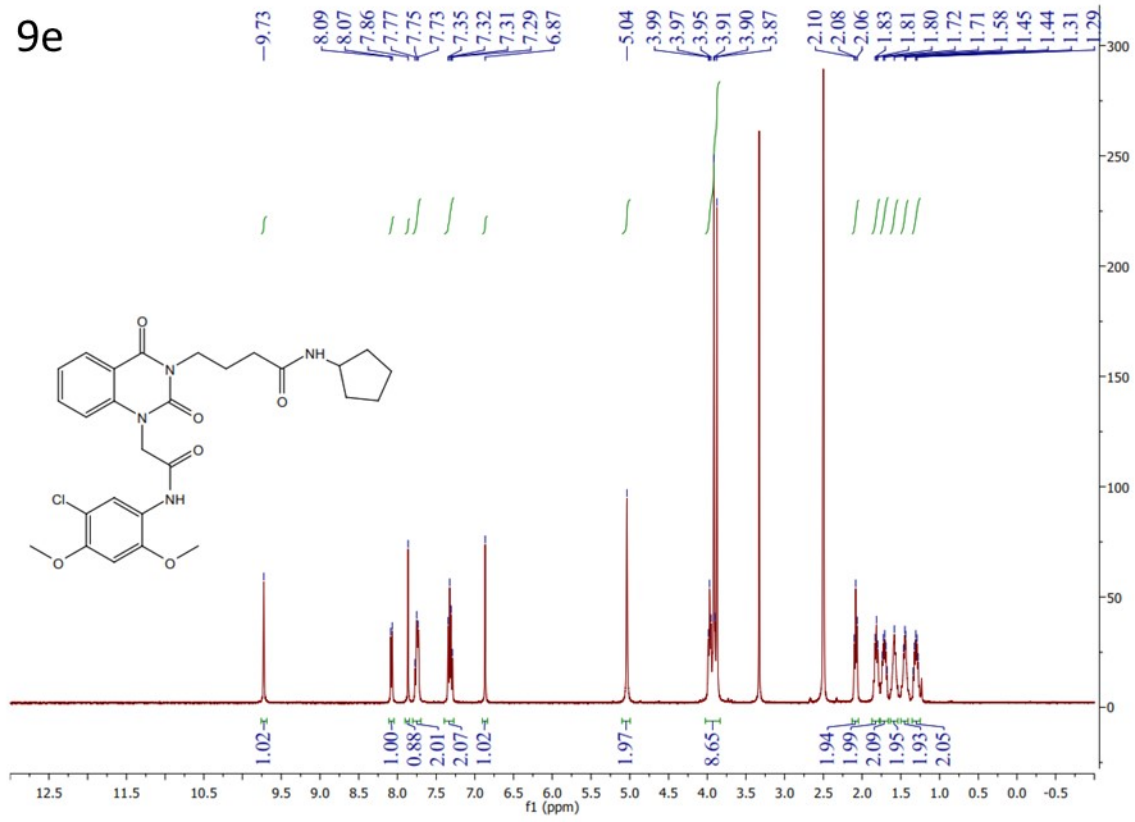

9c
166.16
161.71
152.05
151.18
150.42
140.49
135.66
128.21
123.44
123.31
120.57
115.05
114.93
111.36
98.41
56.83
56.78
46.65
28.59
f1 (ppm)

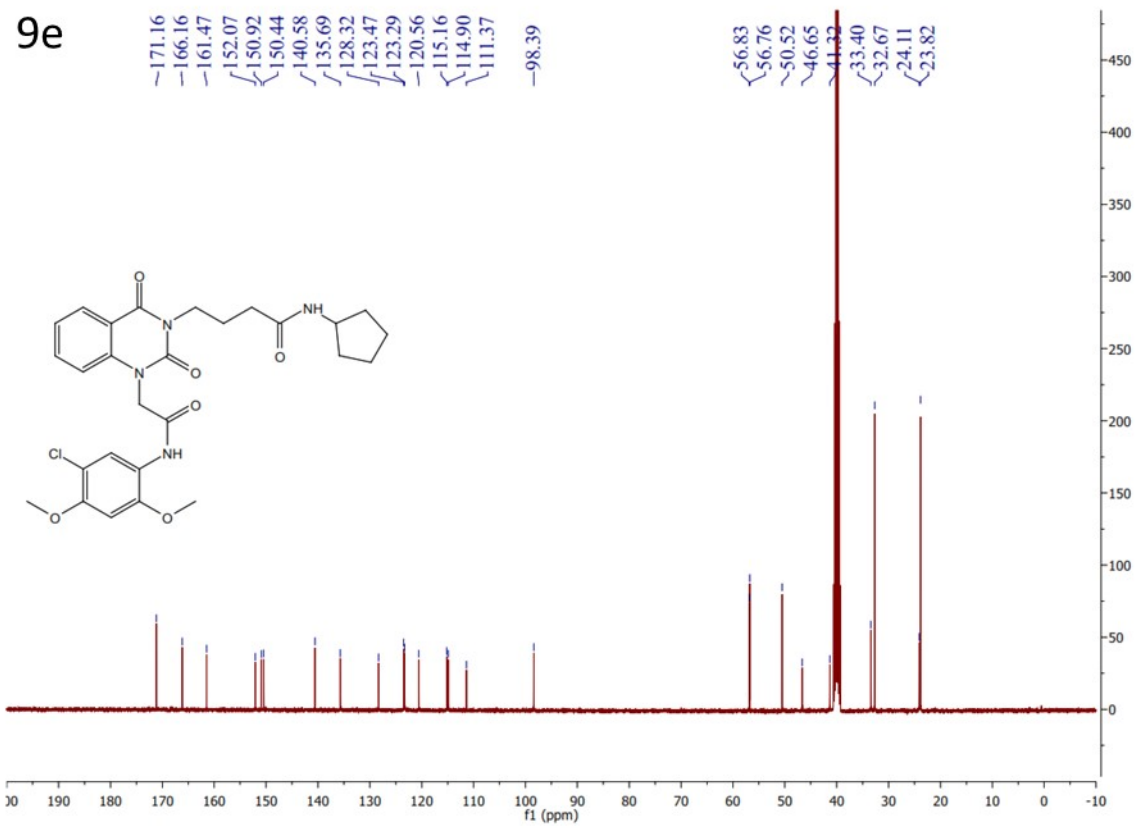

9d
9.69
8.05
8.04
7.85
7.73
7.71
7.69
7.31
7.29
7.27
7.25
6.82
4.99
3.99
3.98
3.96
3.94
3.87
3.83
1.15
1.14
1.12
1.20
1.00
0.84
1.07
2.05
1.04
1.95
2.06
5.65
2.93
f1 (ppm)

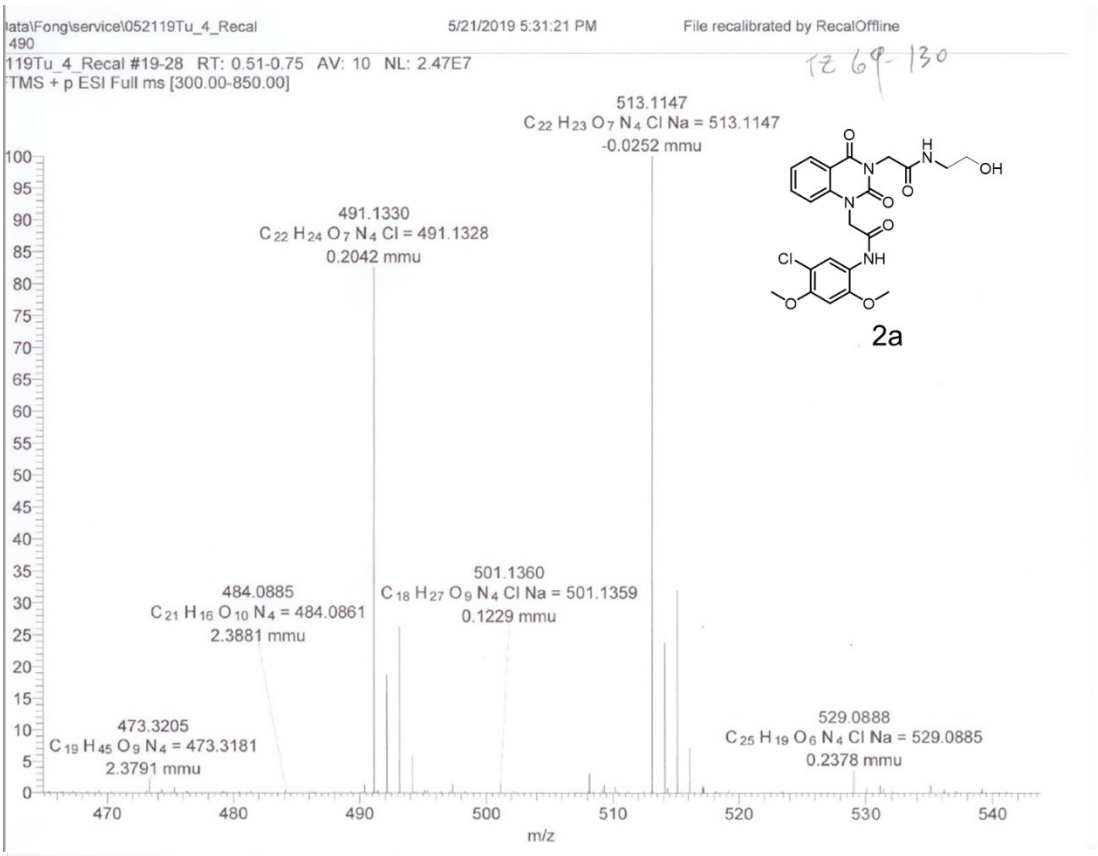
9d

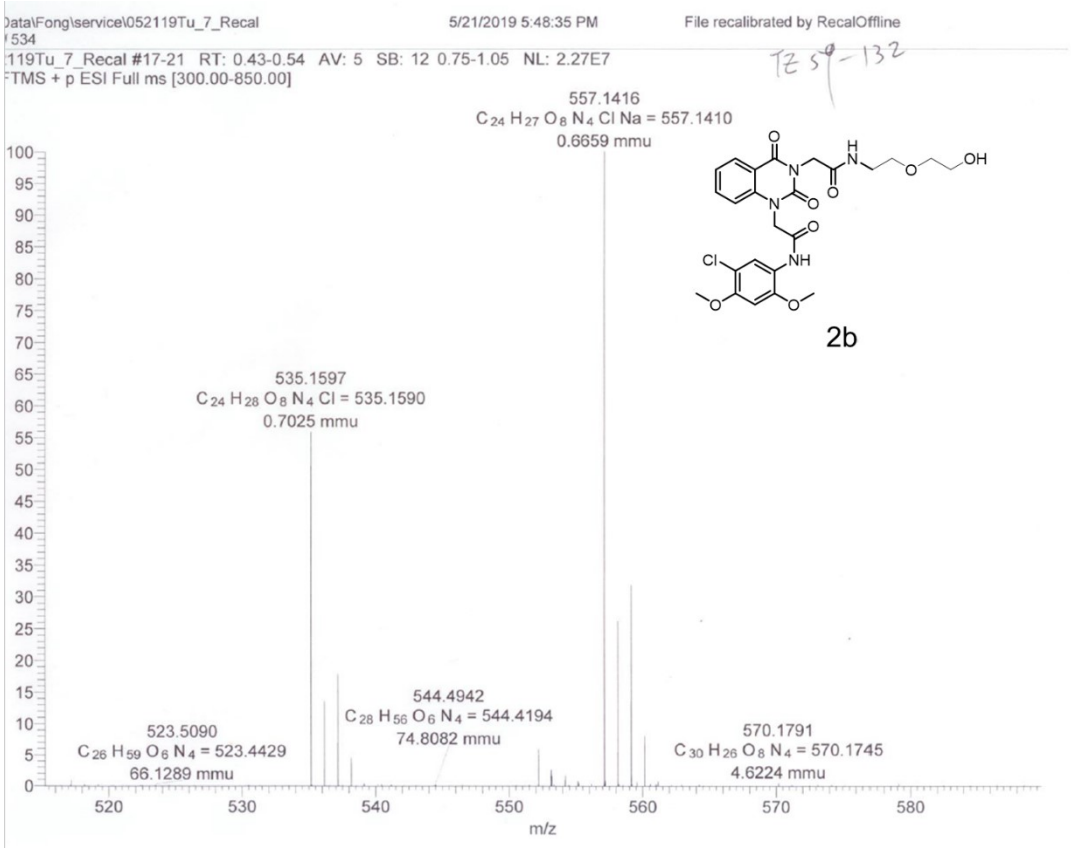

166.14
161.22
151.98
150.72
150.34
140.57
135.67
128.22
123.33
123.29
120.63
115.14
114.93
111.34
98.38
56.81
56.76
46.57
36.76
13.28
f1 (ppm)

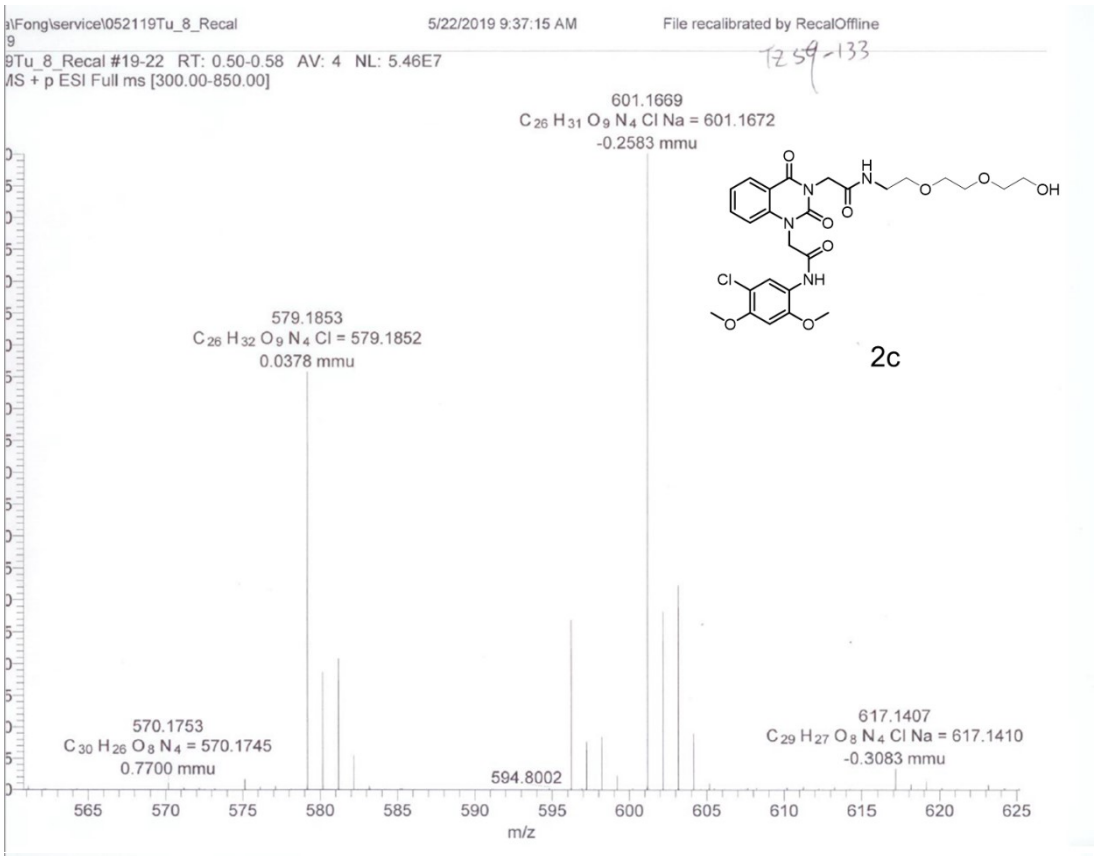
9e


9.73
8.09
8.07
7.86
7.77
7.75
7.73
7.35
7.32
7.31
7.29
6.87
5.04
3.99
3.97
3.95
3.91
3.90
3.87
2.10
2.08
2.06
1.83
1.81
1.80
1.72
1.71
1.58
1.45
1.44
1.31
1.29
1.02
1.00
0.88
2.01
2.07
1.02
1.97
8.65
1.94
1.99
2.09
1.95
1.93
2.05
f1 (ppm)

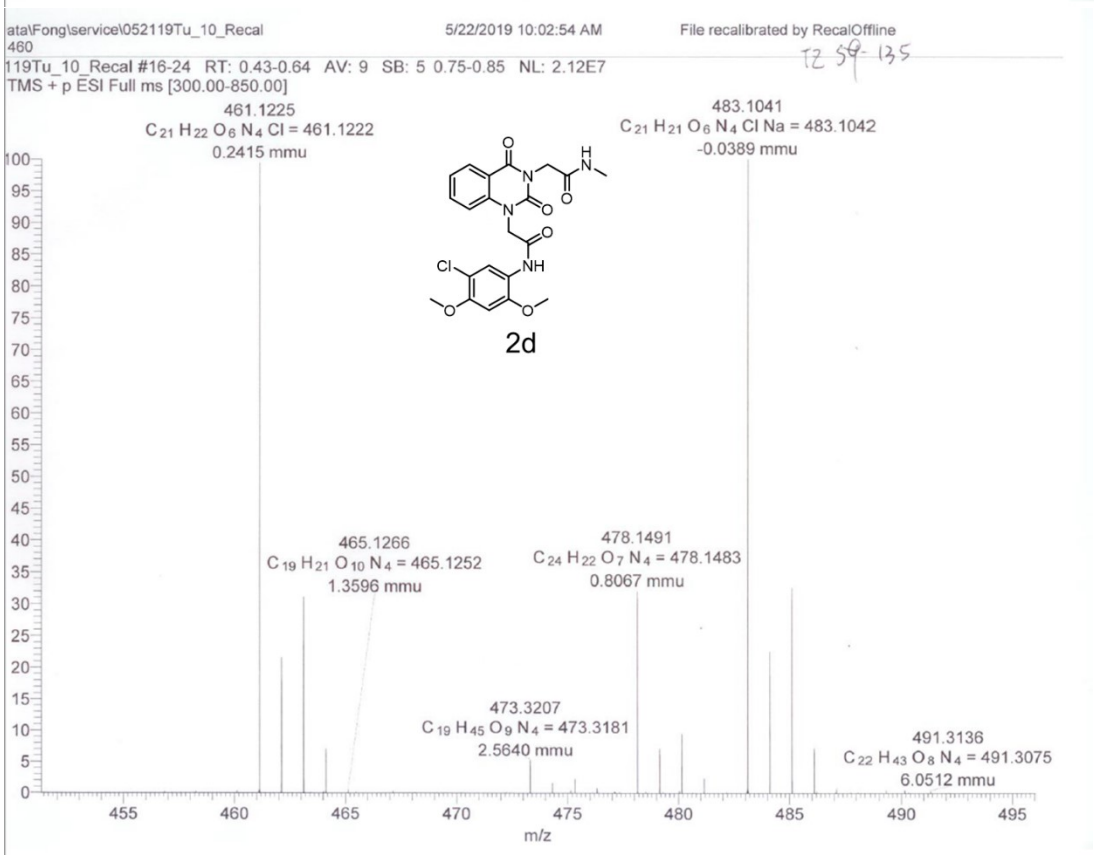

9e
171.16
166.16
161.47
152.07
150.92
150.44
140.58
135.69
128.32
123.47
123.29
120.56
115.16
114.90
111.37
98.39
56.83
56.76
50.52
46.65
41.32
33.40
32.67
24.11
23.82
O
N
O
NH
O
O
N
O
NH
Cl
O
O
450
400
350
300
250
200
150
100
50
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


lata\Fong\service\052119Tu_4_Recal
5/21/2019 5:31:21 PM
File recalibrated by RecalOffline
490
119Tu_4_Recal #19-28 RT: 0.51-0.75 AV: 10 NL: 2.47E7
TMS + p ESI Full ms [300.00-850.00]
TZ 69-130
513.1147
C22 H23 O7 N4 Cl Na = 513.1147
-0.0252 mmu
491.1330
C22 H24 O7 N4 Cl = 491.1328
0.2042 mmu
501.1360
C18 H27 O9 N4 Cl Na = 501.1359
0.1229 mmu
484.0885
C21 H16 O10 N4 = 484.0861
2.3881 mmu
473.3205
C19 H45 O9 N4 = 473.3181
2.3791 mmu
529.0888
C25 H19 O6 N4 Cl Na = 529.0885
0.2378 mmu
m/z
2a

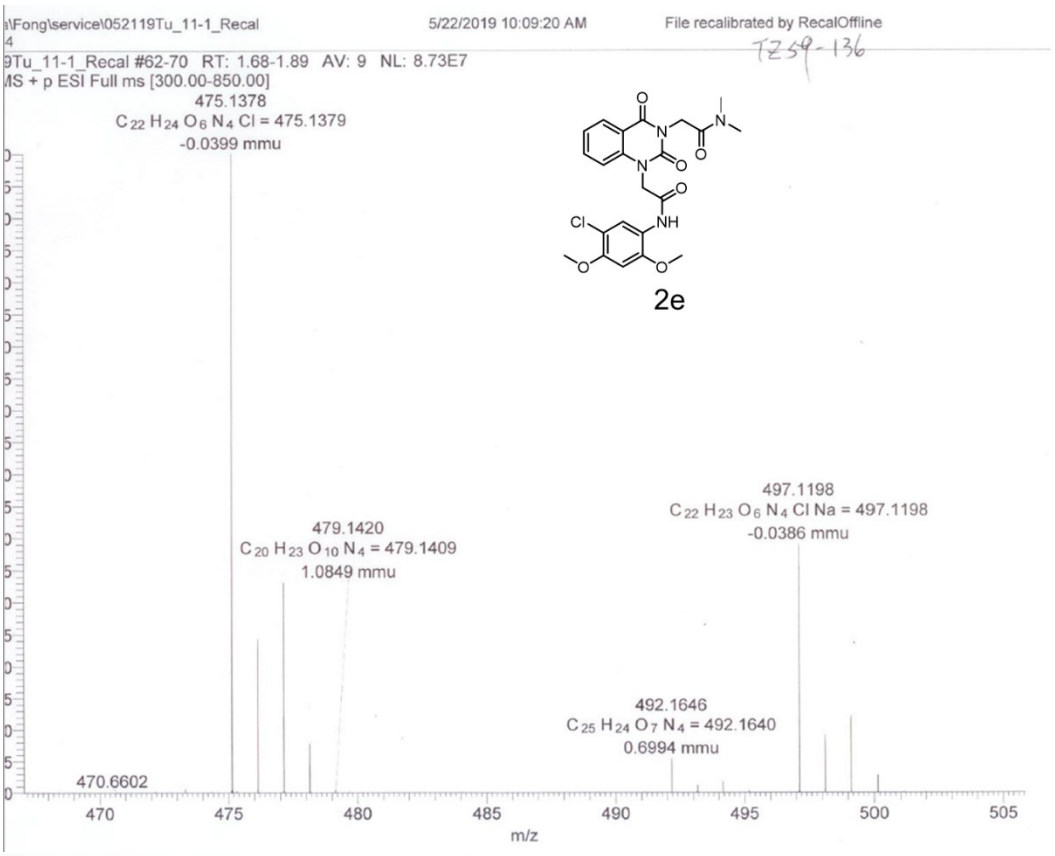

Data\Fong\service\052119Tu_7_Recal
5/21/2019 5:48:35 PM
File recalibrated by RecalOffline
534
119Tu_7_Recal #17-21 RT: 0.43-0.54 AV: 5 SB: 12 0.75-1.05 NL: 2.27E7
TMS + p ESI Full ms [300.00-850.00]
TZ 59-132
557.1416
C24 H27 O8 N4 Cl Na = 557.1410
0.6659 mmu
535.1597
C24 H28 O8 N4 Cl = 535.1590
0.7025 mmu
544.4942
C28 H56 O6 N4 = 544.4194
74.8082 mmu
523.5090
C26 H59 O6 N4 = 523.4429
66.1289 mmu
570.1791
C30 H26 O8 N4 = 570.1745
4.6224 mmu
m/z
2b

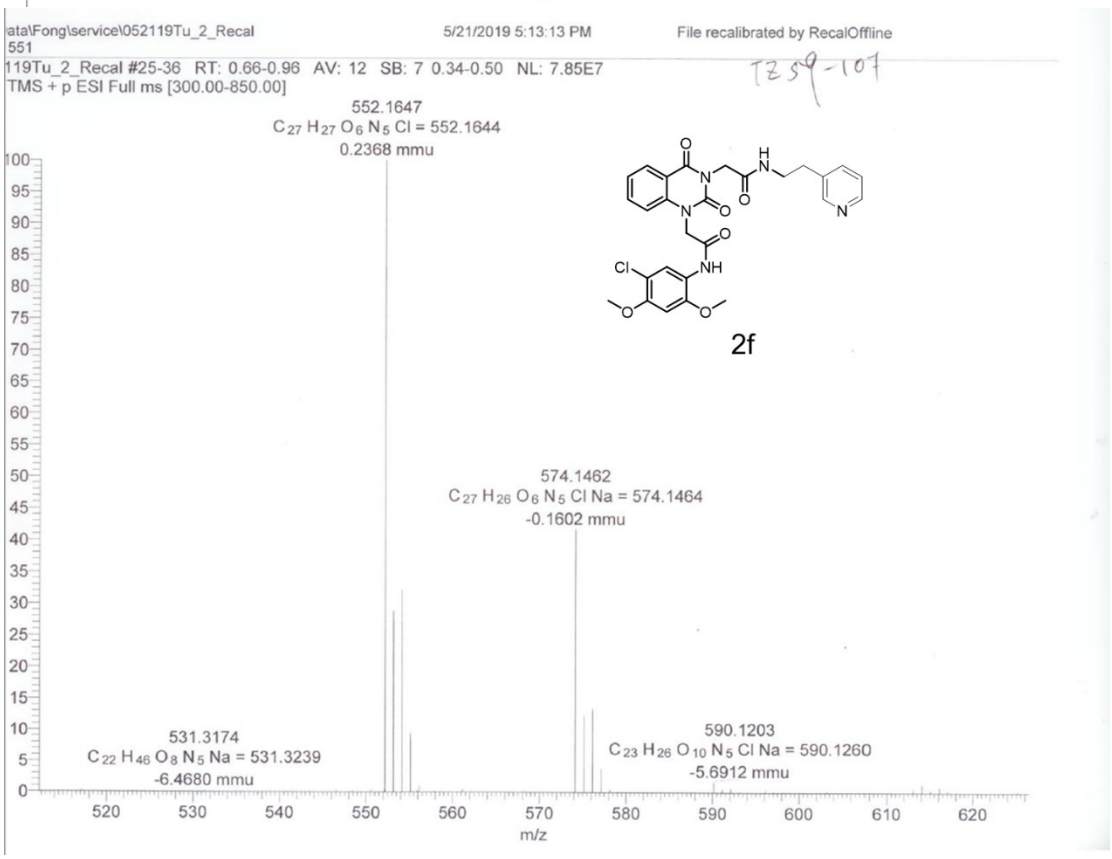

a\Fong\service\052119Tu_8_Recal
5/22/2019 9:37:15 AM
File recalibrated by RecalOffline
9Tu_8_Recal #19-22 RT: 0.50-0.58 AV: 4 NL: 5.46E7
MS + p ESI Full ms [300.00-850.00]
601.1669
C26 H31 O9 N4 Cl Na = 601.1672
-0.2583 mmu
579.1853
C26 H32 O9 N4 Cl = 579.1852
0.0378 mmu
570.1753
C30 H26 O8 N4 = 570.1745
0.7700 mmu
594.8002
617.1407
C29 H27 O8 N4 Cl Na = 617.1410
-0.3083 mmu
m/z

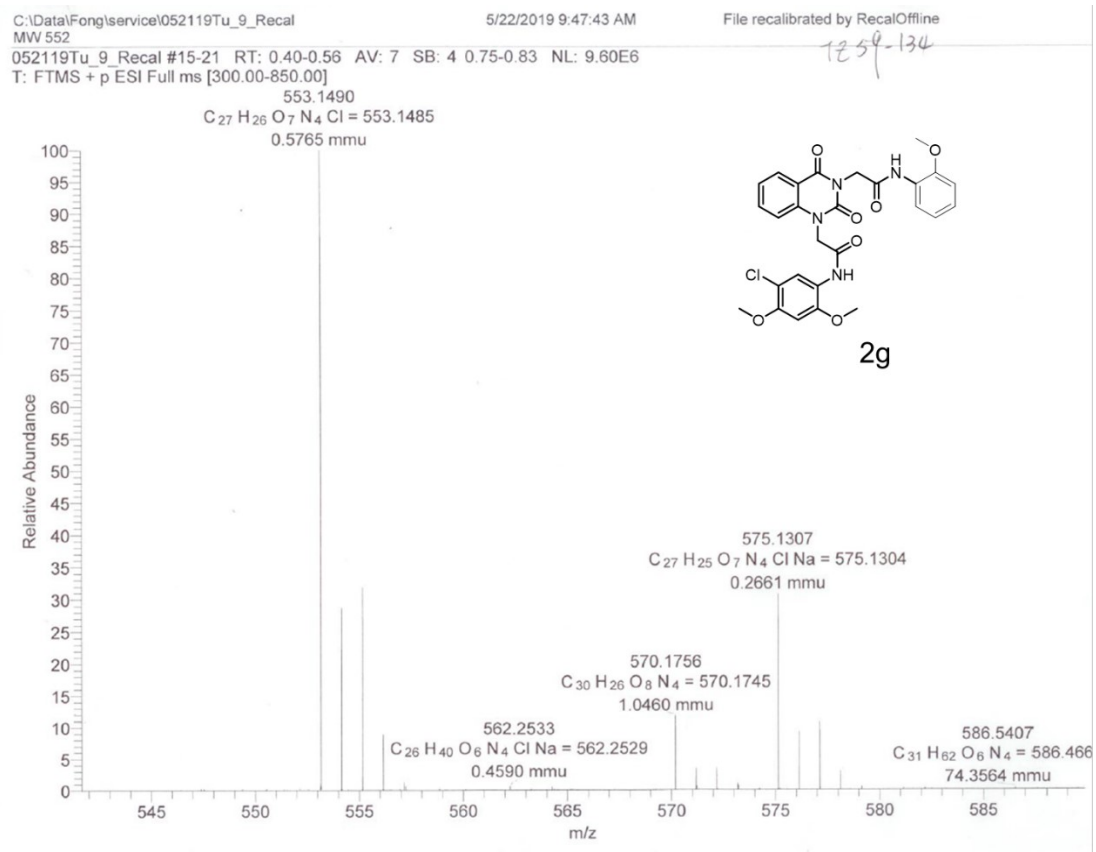
2c

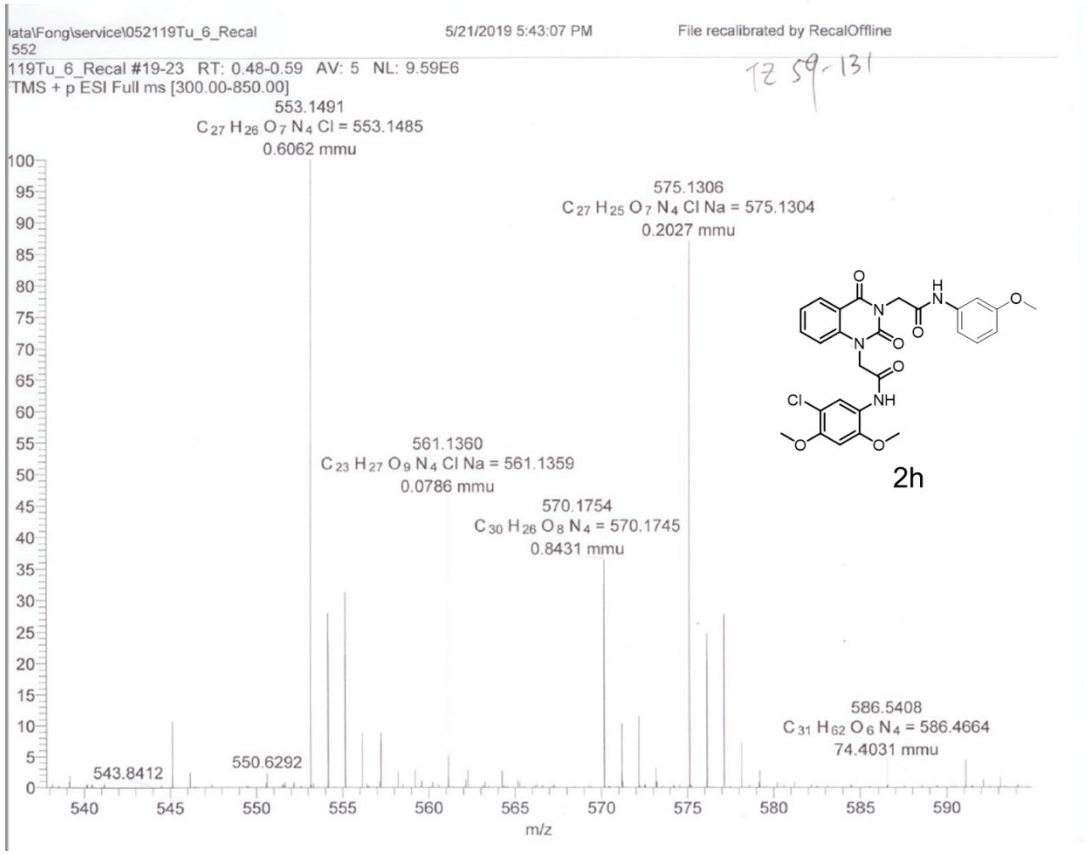

ata\Fong\service\052119Tu_10_Recal
5/22/2019 10:02:54 AM
File recalibrated by RecalOffline
119Tu_10_Recal #16-24 RT: 0.43-0.64 AV: 9 SB: 5 0.75-0.85 NL: 2.12E7
TMS + p ESI Full ms [300.00-850.00]
461.1225
C21 H22 O6 N4 Cl = 461.1222
0.2415 mmu
483.1041
C21 H21 O6 N4 Cl Na = 483.1042
-0.0389 mmu
465.1266
C19 H21 O10 N4 = 465.1252
1.3596 mmu
478.1491
C24 H22 O7 N4 = 478.1483
0.8067 mmu
473.3207
C19 H45 O9 N4 = 473.3181
2.5640 mmu
491.3136
C22 H43 O8 N4 = 491.3075
6.0512 mmu
m/z

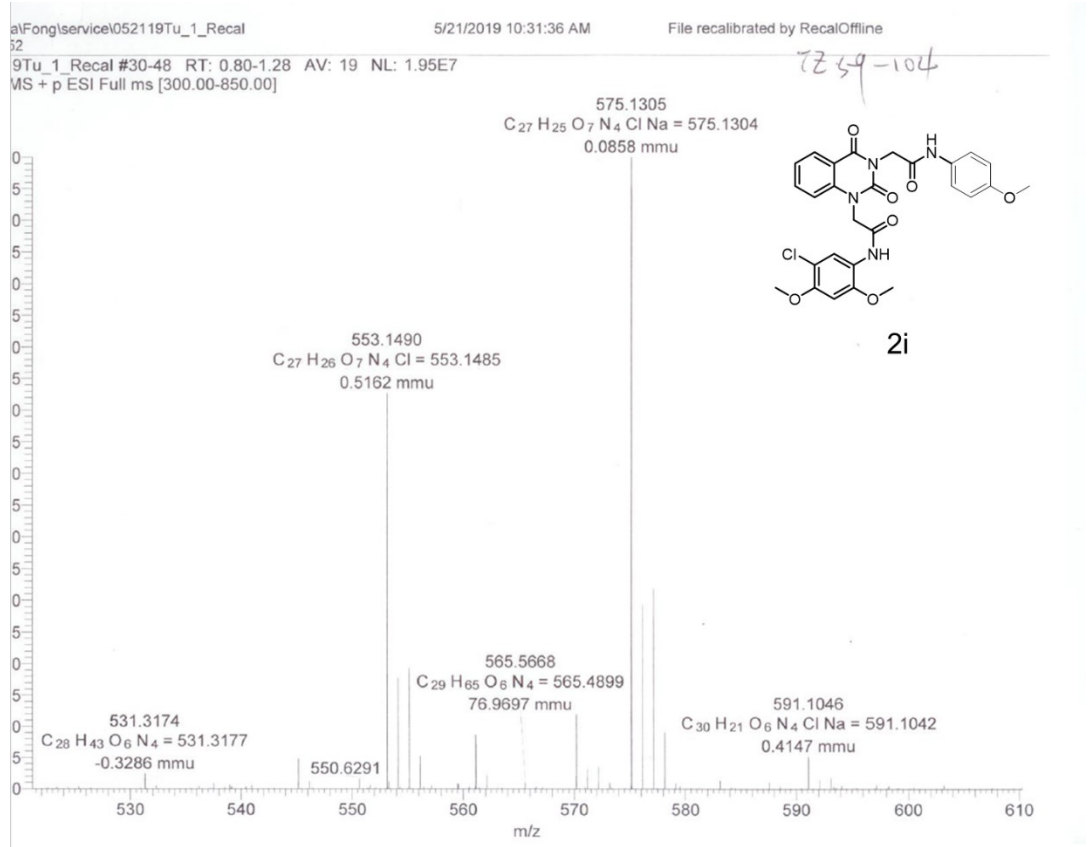
2d

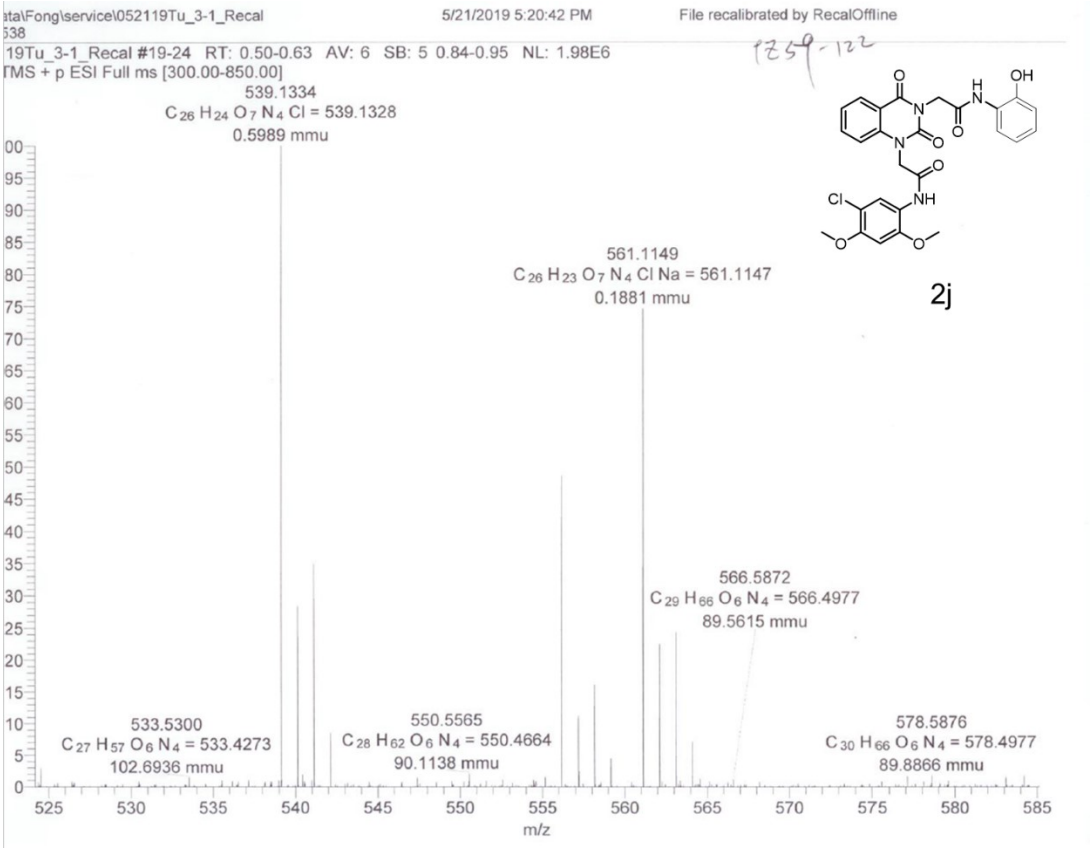

\Fong\service\052119Tu_11-1_Recal
5/22/2019 10:09:20 AM
File recalibrated by RecalOffline
TZ59-136
9Tu_11-1_Recal #62-70 RT: 1.68-1.89 AV: 9 NL: 8.73E7
MS + p ESI Full ms [300.00-850.00]
475.1378
C22 H24 O6 N4 Cl = 475.1379
-0.0399 mmu
2e
497.1198
C22 H23 O6 N4 Cl Na = 497.1198
-0.0386 mmu
479.1420
C20 H23 O10 N4 = 479.1409
1.0849 mmu
492.1646
C25 H24 O7 N4 = 492.1640
0.6994 mmu
470.6602
m/z

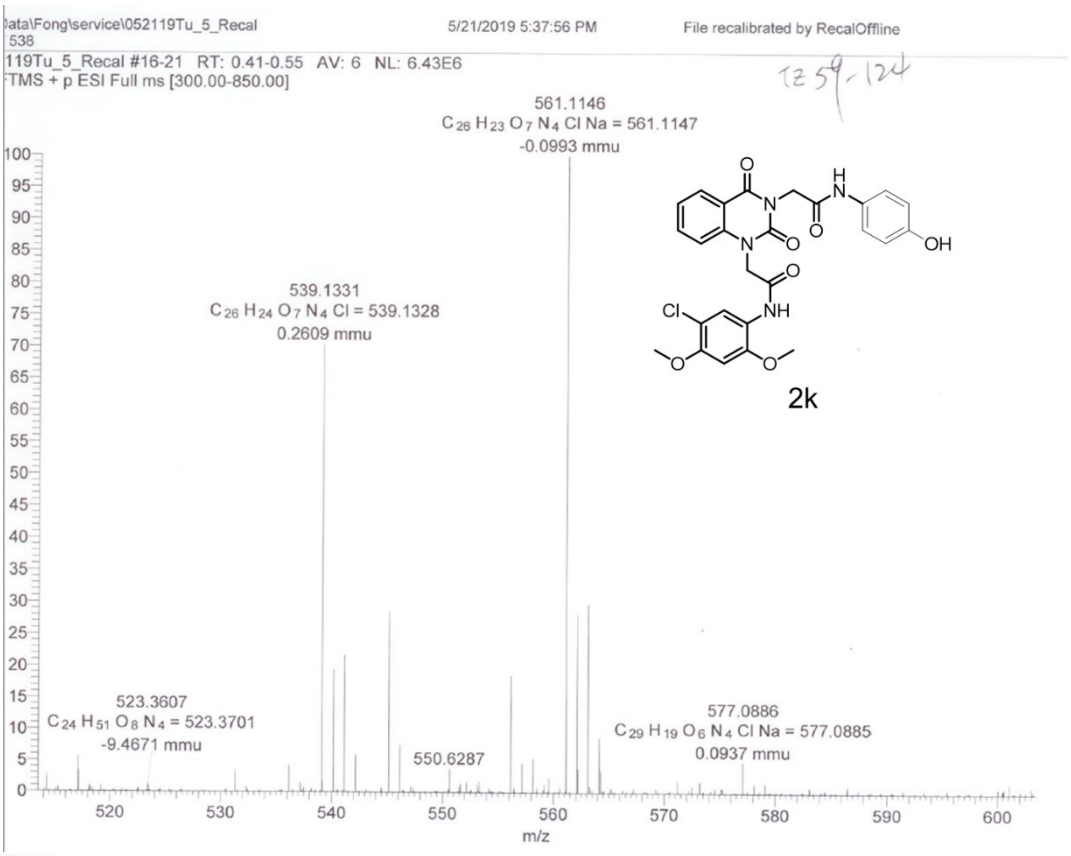

ata\Fong\service\052119Tu_2_Recal
5/21/2019 5:13:13 PM
File recalibrated by RecalOffline
551
119Tu_2_Recal #25-36 RT: 0.66-0.96 AV: 12 SB: 7 0.34-0.50 NL: 7.85E7
TMS + p ESI Full ms [300.00-850.00]
TZ59-107
552.1647
C27 H27 O6 N5 Cl = 552.1644
0.2368 mmu
2f
574.1462
C27 H26 O6 N5 Cl Na = 574.1464
-0.1602 mmu
531.3174
C22 H46 O8 N5 Na = 531.3239
-6.4680 mmu
590.1203
C23 H26 O10 N5 Cl Na = 590.1260
-5.6912 mmu
m/z

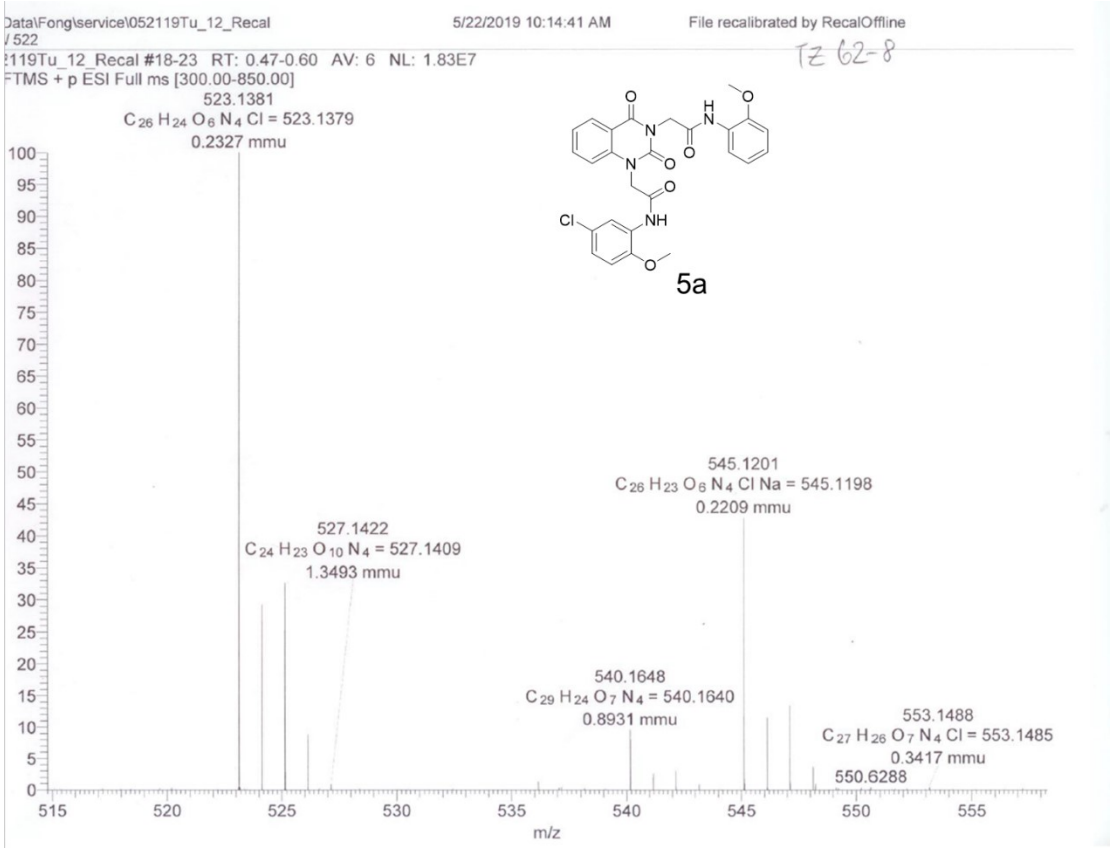

C:\Data\Fong\service\052119Tu_9_Recal
5/22/2019 9:47:43 AM
File recalibrated by RecalOffline
MW 552
052119Tu_9_Recal #15-21 RT: 0.40-0.56 AV: 7 SB: 4 0.75-0.83 NL: 9.60E6
T: FTMS + p ESI Full ms [300.00-850.00]
553.1490
C27 H26 O7 N4 Cl = 553.1485
0.5765 mmu
575.1307
C27 H25 O7 N4 Cl Na = 575.1304
0.2661 mmu
570.1756
C30 H26 O8 N4 = 570.1745
1.0460 mmu
562.2533
C26 H40 O6 N4 Cl Na = 562.2529
0.4590 mmu
586.5407
C31 H62 O6 N4 = 586.466
74.3564 mmu
Relative Abundance
m/z
2g

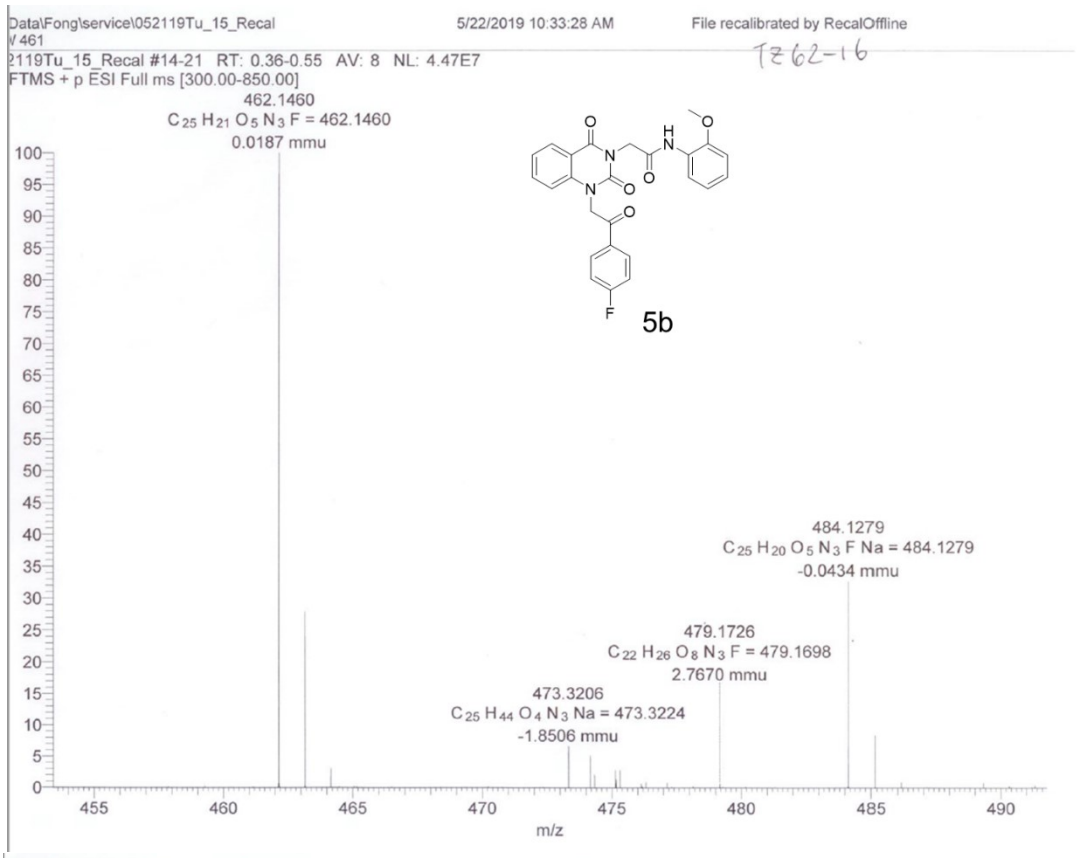

ata\Fong\service\052119Tu_6_Recal
5/21/2019 5:43:07 PM
File recalibrated by RecalOffline
552
119Tu_6_Recal #19-23 RT: 0.48-0.59 AV: 5 NL: 9.59E6
TMS + p ESI Full ms [300.00-850.00]
553.1491
C27 H26 O7 N4 Cl = 553.1485
0.6062 mmu
575.1306
C27 H25 O7 N4 Cl Na = 575.1304
0.2027 mmu
561.1360
C23 H27 O9 N4 Cl Na = 561.1359
0.0786 mmu
570.1754
C30 H26 O8 N4 = 570.1745
0.8431 mmu
586.5408
C31 H62 O6 N4 = 586.4664
74.4031 mmu
543.8412
550.6292
m/z
2h

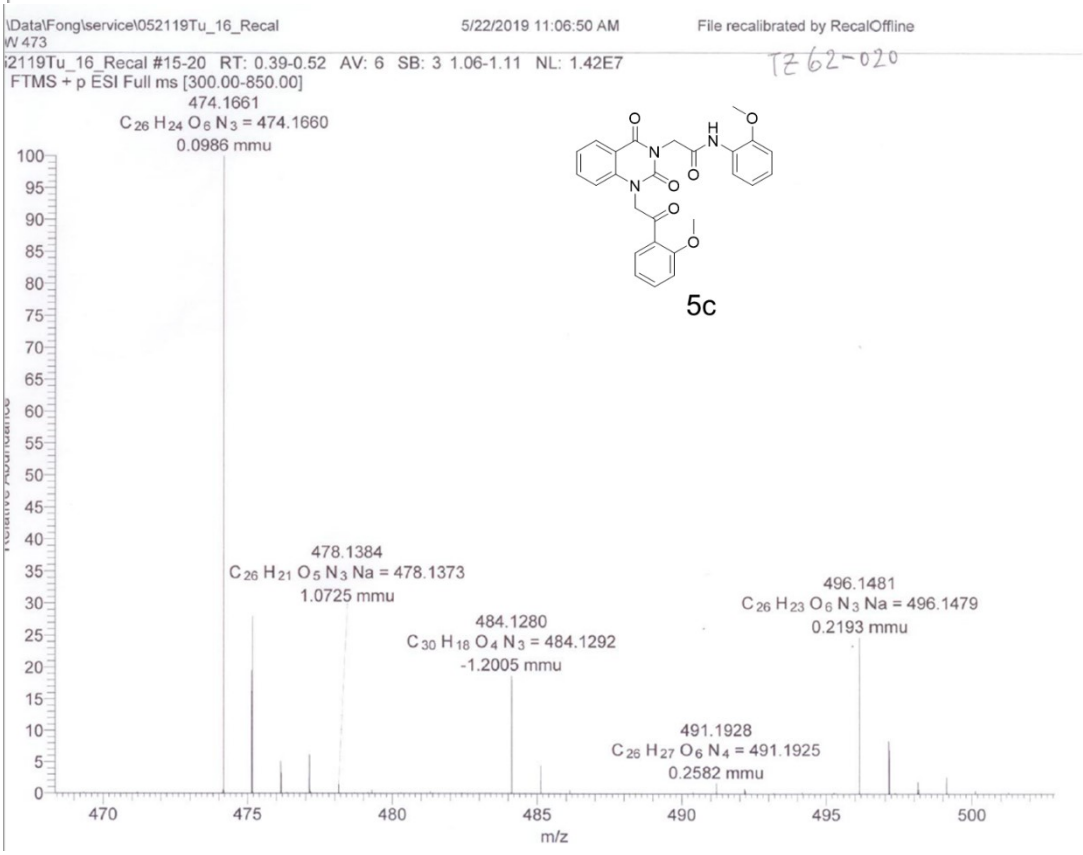

a\Fong\service\052119Tu_1_Recal
5/21/2019 10:31:36 AM
File recalibrated by RecalOffline
9Tu_1_Recal #30-48 RT: 0.80-1.28 AV: 19 NL: 1.95E7
MS + p ESI Full ms [300.00-850.00]
TZ59-104
575.1305
C27 H25 O7 N4 Cl Na = 575.1304
0.0858 mmu
2i
553.1490
C27 H26 O7 N4 Cl = 553.1485
0.5162 mmu
565.5668
C29 H65 O6 N4 = 565.4899
76.9697 mmu
591.1046
C30 H21 O6 N4 Cl Na = 591.1042
0.4147 mmu
531.3174
C28 H43 O6 N4 = 531.3177
-0.3286 mmu
550.6291
m/z

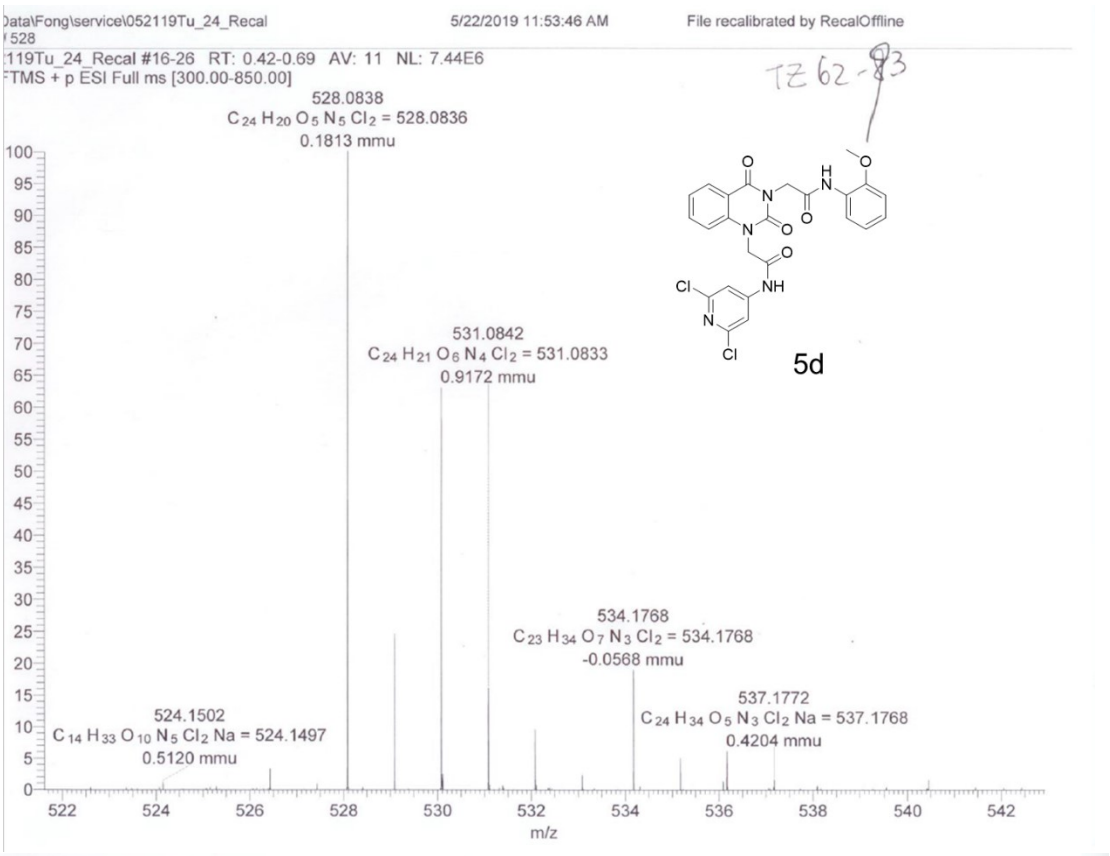

ata\Fong\service\052119Tu_3-1_Recal
5/21/2019 5:20:42 PM
File recalibrated by RecalOffline
19Tu_3-1_Recal #19-24 RT: 0.50-0.63 AV: 6 SB: 5 0.84-0.95 NL: 1.98E6
TMS + p ESI Full ms [300.00-850.00]
TZ59-122
539.1334
C26 H24 O7 N4 Cl = 539.1328
0.5989 mmu
2j
561.1149
C26 H23 O7 N4 Cl Na = 561.1147
0.1881 mmu
566.5872
C29 H66 O6 N4 = 566.4977
89.5615 mmu
533.5300
C27 H57 O6 N4 = 533.4273
102.6936 mmu
550.5565
C28 H62 O6 N4 = 550.4664
90.1138 mmu
578.5876
C30 H66 O6 N4 = 578.4977
89.8866 mmu
m/z

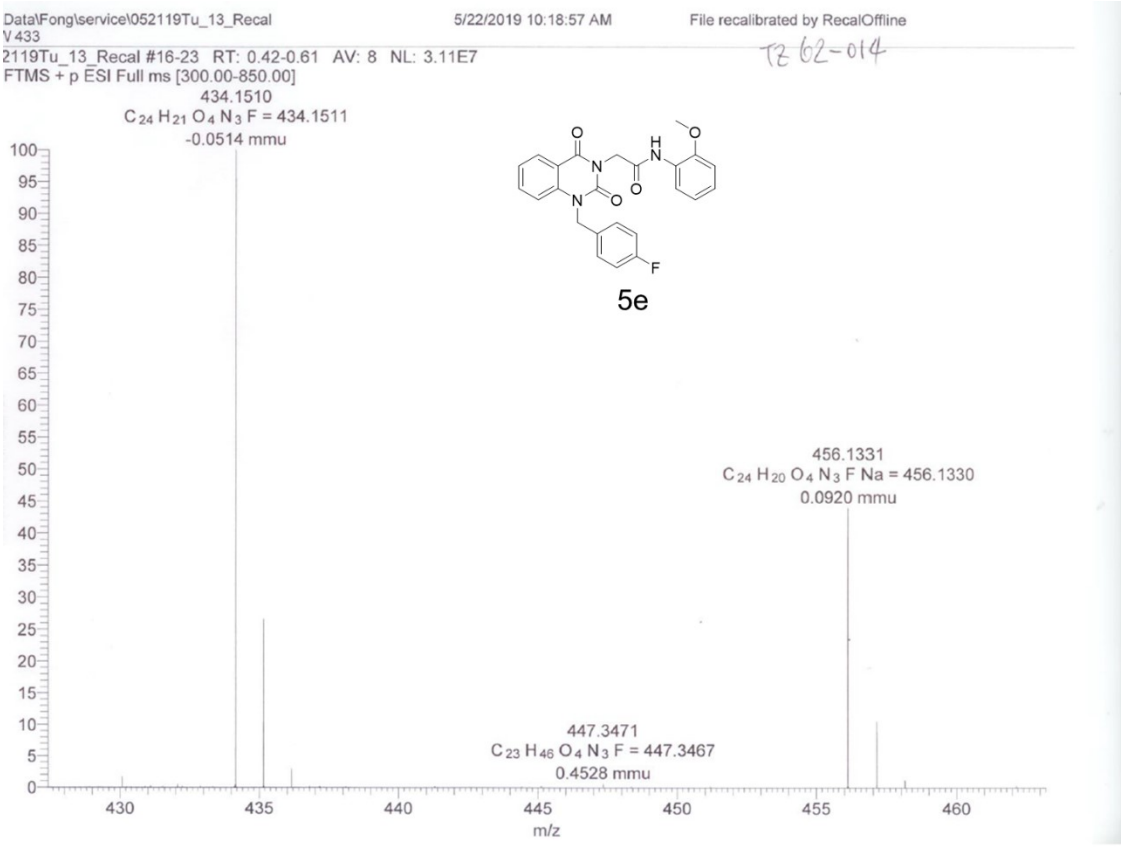

Data\Fong\service\052119Tu_5_Recal
538
119Tu_5_Recal #16-21 RT: 0.41-0.55 AV: 6 NL: 6.43E6
TMS + p ESI Full ms [300.00-850.00]
5/21/2019 5:37:56 PM
File recalibrated by RecalOffline
TZ 59-124
561.1146
C26 H23 O7 N4 Cl Na = 561.1147
-0.0993 mmu
539.1331
C26 H24 O7 N4 Cl = 539.1328
0.2609 mmu
523.3607
C24 H51 O8 N4 = 523.3701
-9.4671 mmu
550.6287
577.0886
C29 H19 O6 N4 Cl Na = 577.0885
0.0937 mmu
m/z
2k

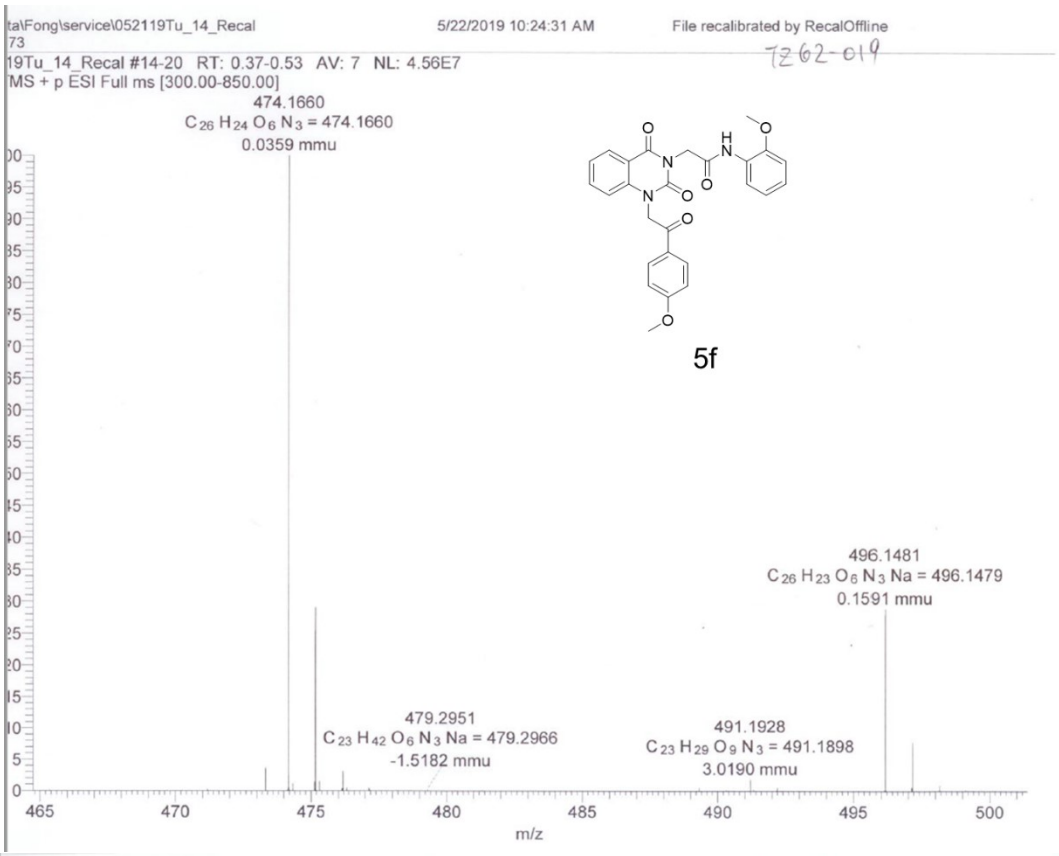

Data\Fong\service\052119Tu_12_Recal
522
119Tu_12_Recal #18-23 RT: 0.47-0.60 AV: 6 NL: 1.83E7
TMS + p ESI Full ms [300.00-850.00]
5/22/2019 10:14:41 AM
File recalibrated by RecalOffline
TZ 62-8
523.1381
C26 H24 O6 N4 Cl = 523.1379
0.2327 mmu
545.1201
C26 H23 O6 N4 Cl Na = 545.1198
0.2209 mmu
527.1422
C24 H23 O10 N4 = 527.1409
1.3493 mmu
540.1648
C29 H24 O7 N4 = 540.1640
0.8931 mmu
553.1488
C27 H26 O7 N4 Cl = 553.1485
0.3417 mmu
550.6288
m/z
5a


Data\Fong\service\052119Tu_15_Recal
5/22/2019 10:33:28 AM
File recalibrated by RecalOffline
TZ62-16
2119Tu_15_Recal #14-21 RT: 0.36-0.55 AV: 8 NL: 4.47E7
FTMS + p ESI Full ms [300.00-850.00]
462.1460
C25 H21 O5 N3 F = 462.1460
0.0187 mmu
484.1279
C25 H20 O5 N3 F Na = 484.1279
-0.0434 mmu
479.1726
C22 H26 O8 N3 F = 479.1698
2.7670 mmu
473.3206
C25 H44 O4 N3 Na = 473.3224
-1.8506 mmu
5b
m/z

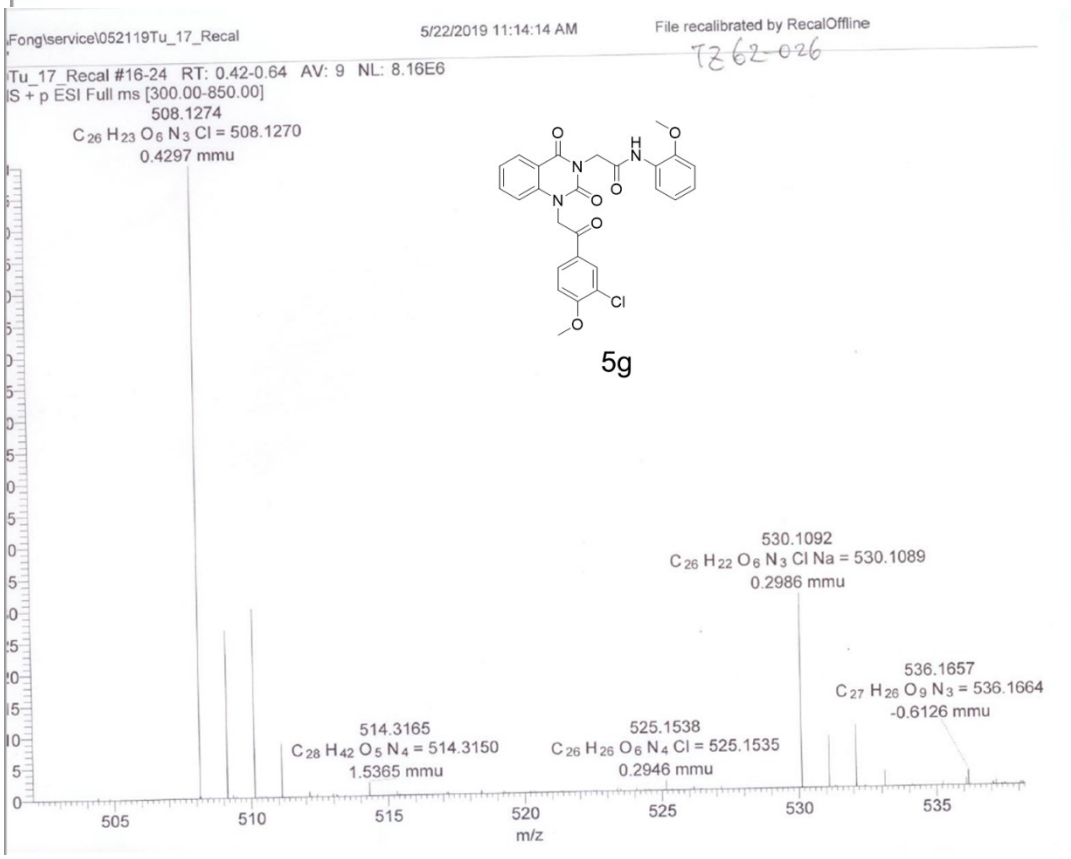

\Data\Fong\service\052119Tu_16_Recal
5/22/2019 11:06:50 AM
File recalibrated by RecalOffline
TZ62-020
2119Tu_16_Recal #15-20 RT: 0.39-0.52 AV: 6 SB: 3 1.06-1.11 NL: 1.42E7
FTMS + p ESI Full ms [300.00-850.00]
474.1661
C26 H24 O6 N3 = 474.1660
0.0986 mmu
478.1384
C26 H21 O5 N3 Na = 478.1373
1.0725 mmu
484.1280
C30 H18 O4 N3 = 484.1292
-1.2005 mmu
496.1481
C26 H23 O6 N3 Na = 496.1479
0.2193 mmu
491.1928
C26 H27 O6 N4 = 491.1925
0.2582 mmu
5c
m/z


Data\Fong\service\052119Tu_24_Recal
5/22/2019 11:53:46 AM
File recalibrated by RecalOffline
119Tu_24_Recal #16-26 RT: 0.42-0.69 AV: 11 NL: 7.44E6
FTMS + p ESI Full ms [300.00-850.00]
528.0838
C24 H20 O5 N5 Cl2 = 528.0836
0.1813 mmu
531.0842
C24 H21 O6 N4 Cl2 = 531.0833
0.9172 mmu
534.1768
C23 H34 O7 N3 Cl2 = 534.1768
-0.0568 mmu
537.1772
C24 H34 O5 N3 Cl2 Na = 537.1768
0.4204 mmu
524.1502
C14 H33 O10 N5 Cl2 Na = 524.1497
0.5120 mmu
m/z
TZ 62-83
5d

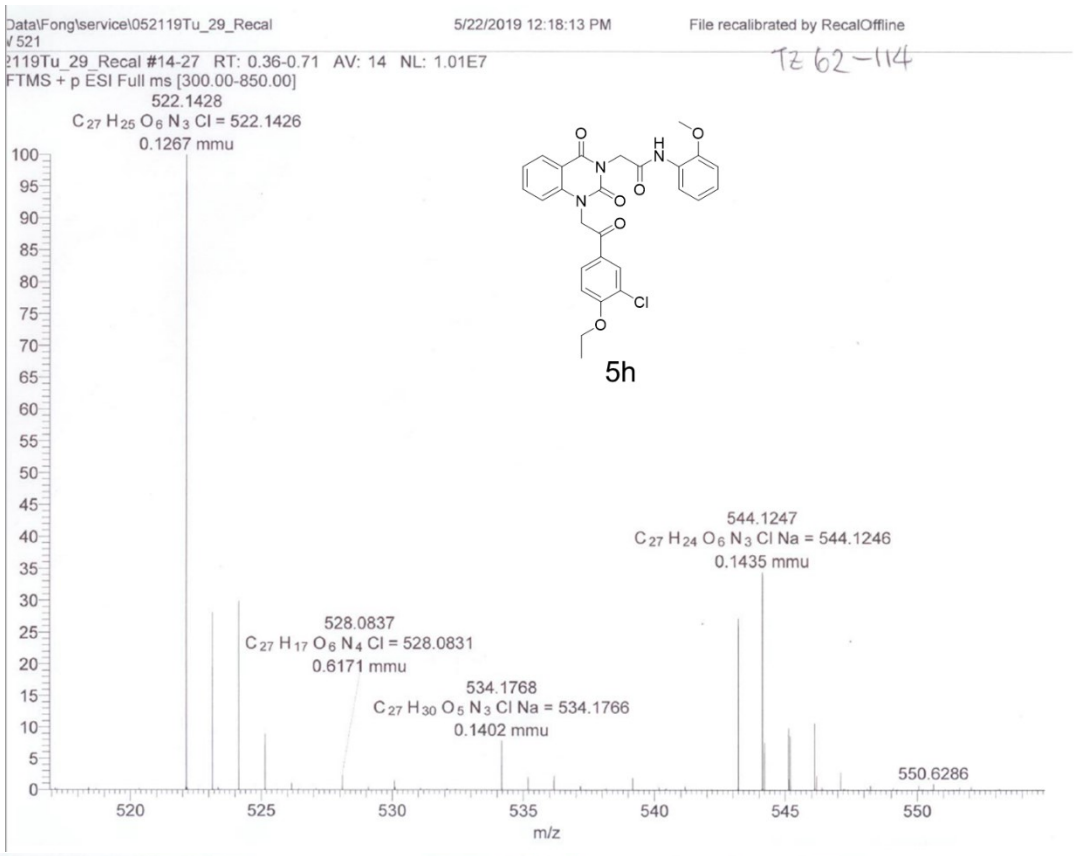

Data\Fong\service\052119Tu_13_Recal
5/22/2019 10:18:57 AM
File recalibrated by RecalOffline
2119Tu_13_Recal #16-23 RT: 0.42-0.61 AV: 8 NL: 3.11E7
FTMS + p ESI Full ms [300.00-850.00]
434.1510
C24 H21 O4 N3 F = 434.1511
-0.0514 mmu
456.1331
C24 H20 O4 N3 F Na = 456.1330
0.0920 mmu
447.3471
C23 H46 O4 N3 F = 447.3467
0.4528 mmu
m/z
TZ 62-014
5e

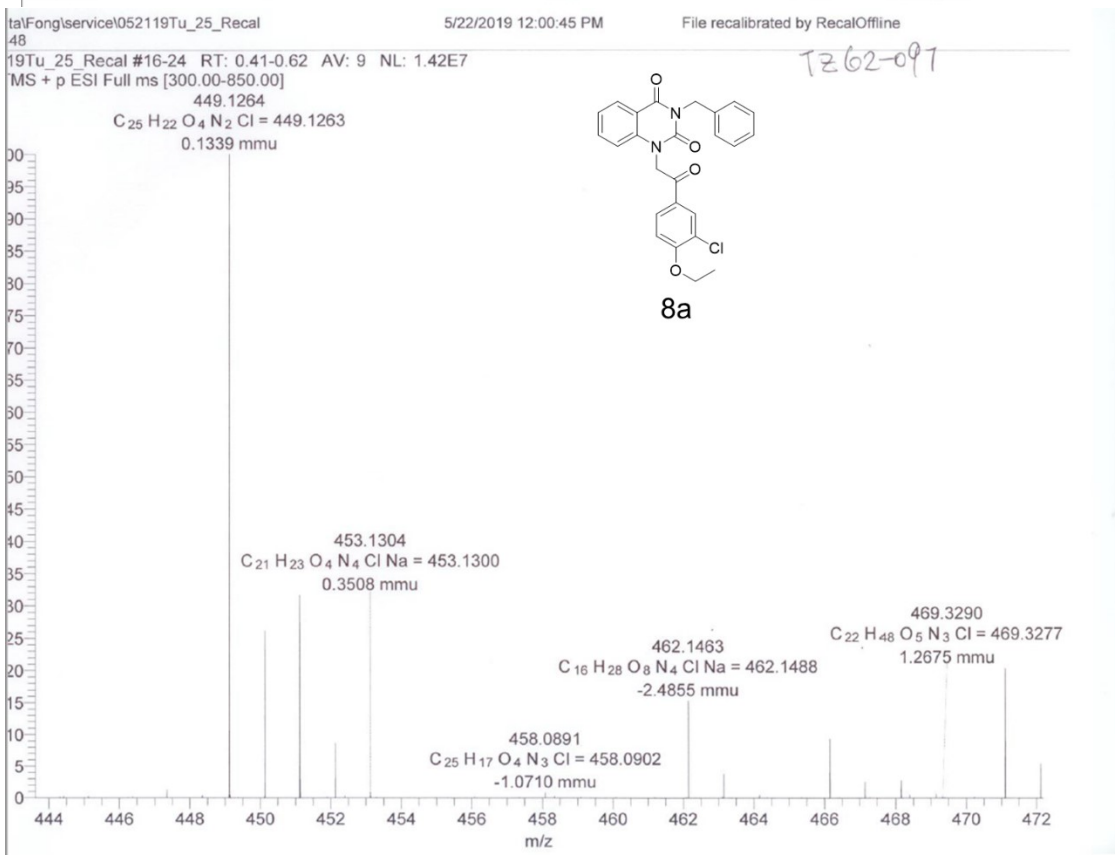

ta\Fong\service\052119Tu_14_Recal
5/22/2019 10:24:31 AM
File recalibrated by RecalOffline
TZ62-019
19Tu_14_Recal #14-20 RT: 0.37-0.53 AV: 7 NL: 4.56E7
MS + p ESI Full ms [300.00-850.00]
474.1660
C26 H24 O6 N3 = 474.1660
0.0359 mmu
496.1481
C26 H23 O6 N3 Na = 496.1479
0.1591 mmu
479.2951
C23 H42 O6 N3 Na = 479.2966
-1.5182 mmu
491.1928
C23 H29 O9 N3 = 491.1898
3.0190 mmu
m/z

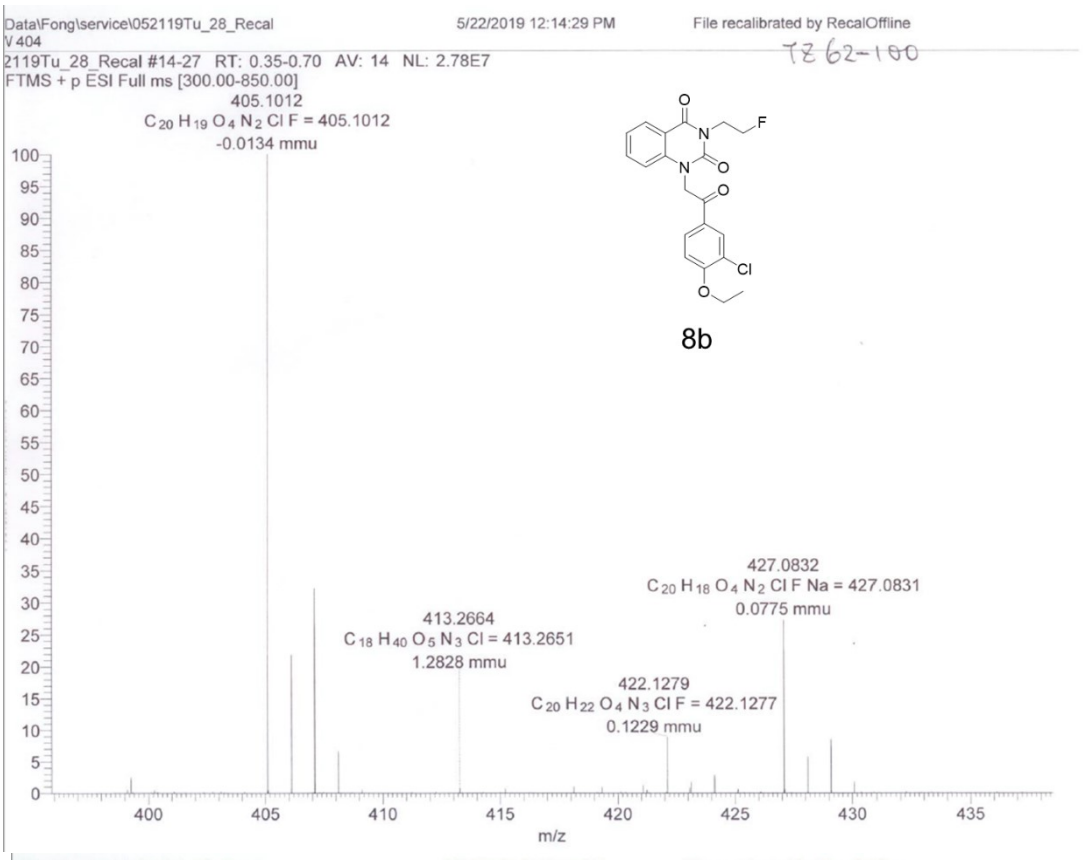
5f

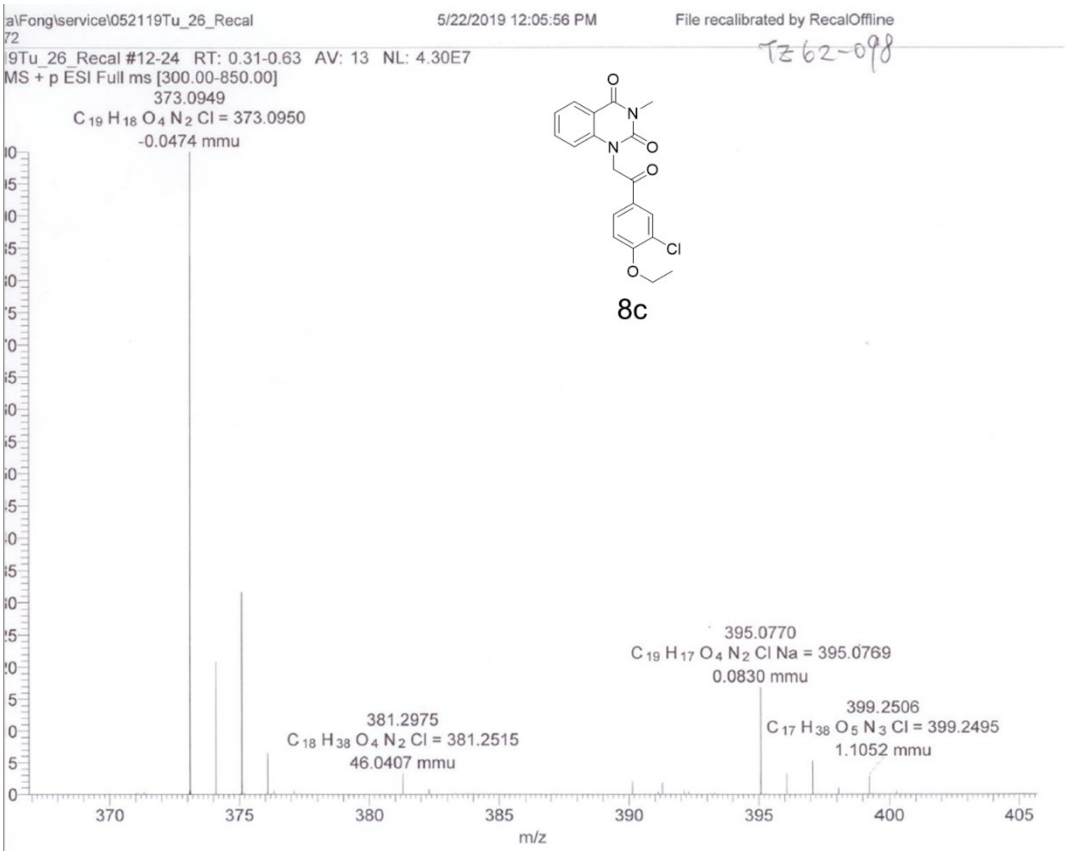

Fong\service\052119Tu_17_Recal
5/22/2019 11:14:14 AM
File recalibrated by RecalOffline
TZ62-026
Tu_17_Recal #16-24 RT: 0.42-0.64 AV: 9 NL: 8.16E6
S + p ESI Full ms [300.00-850.00]
508.1274
C26 H23 O6 N3 Cl = 508.1270
0.4297 mmu
530.1092
C26 H22 O6 N3 Cl Na = 530.1089
0.2986 mmu
536.1657
C27 H26 O9 N3 = 536.1664
-0.6126 mmu
514.3165
C28 H42 O5 N4 = 514.3150
1.5365 mmu
525.1538
C26 H26 O6 N4 Cl = 525.1535
0.2946 mmu
m/z

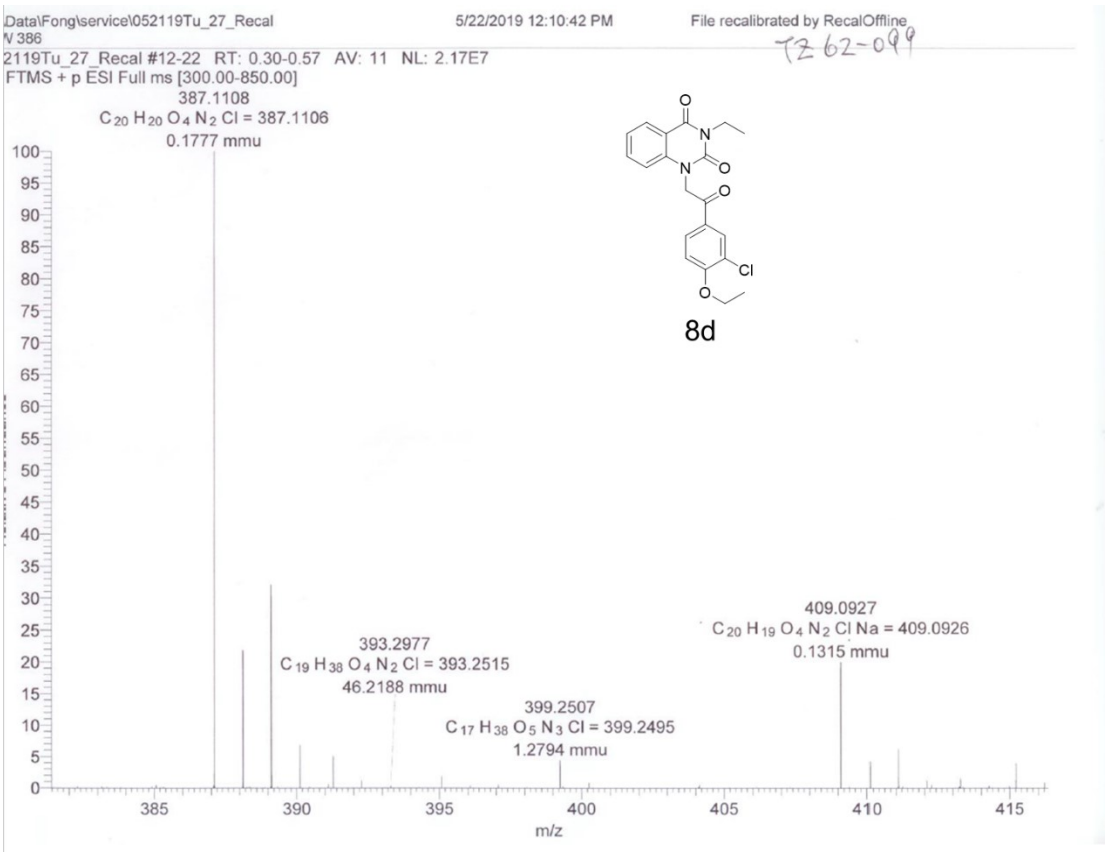
5g

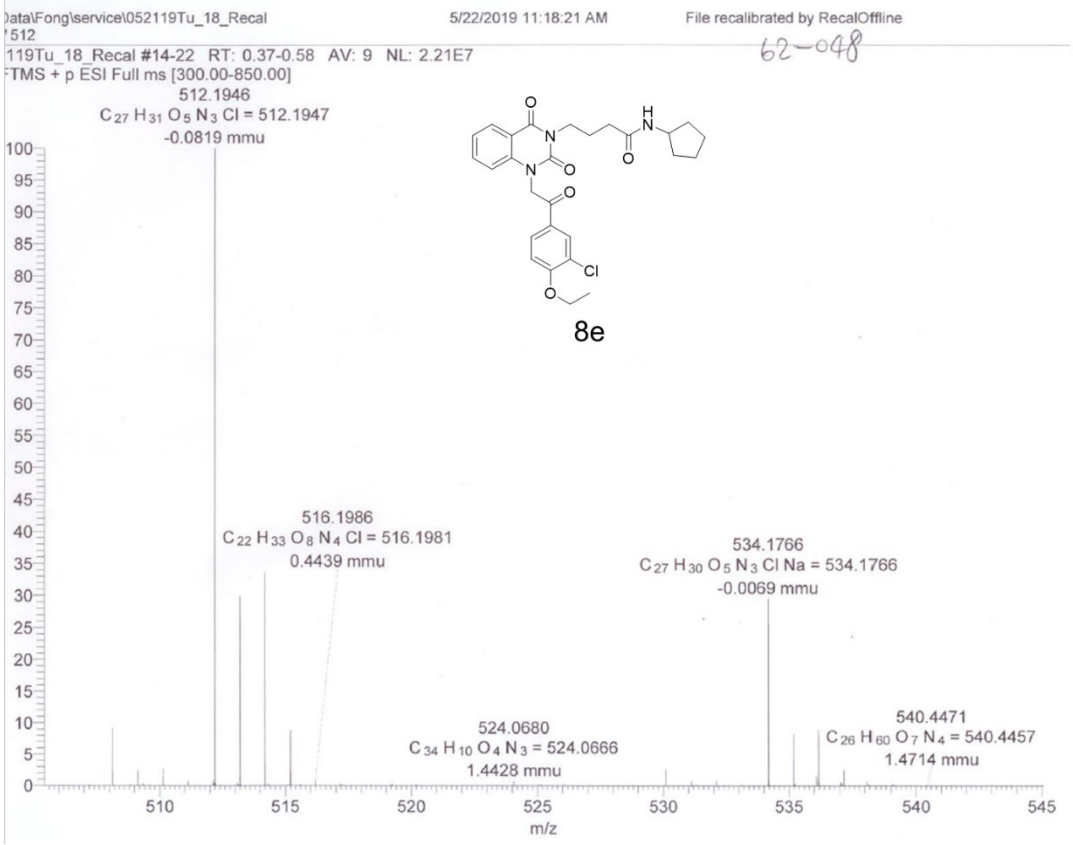

Data\Fong\service\052119Tu_29_Recal
5/22/2019 12:18:13 PM
File recalibrated by RecalOffline
TZ 62-114
2119Tu_29_Recal #14-27 RT: 0.36-0.71 AV: 14 NL: 1.01E7
FTMS + p ESI Full ms [300.00-850.00]
522.1428
C27 H25 O6 N3 Cl = 522.1426
0.1267 mmu
5h
544.1247
C27 H24 O6 N3 Cl Na = 544.1246
0.1435 mmu
528.0837
C27 H17 O6 N4 Cl = 528.0831
0.6171 mmu
534.1768
C27 H30 O5 N3 Cl Na = 534.1766
0.1402 mmu
550.6286
m/z

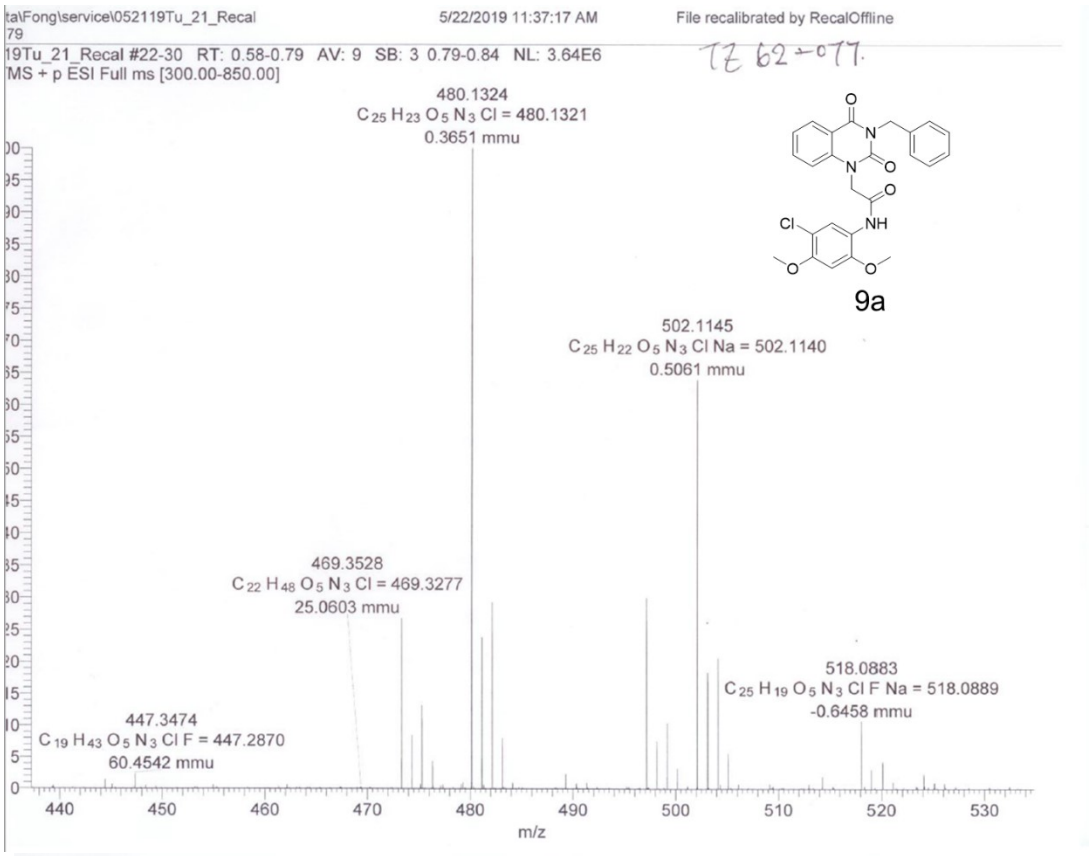

ta\Fong\service\052119Tu_25_Recal
5/22/2019 12:00:45 PM
File recalibrated by RecalOffline
48
19Tu_25_Recal #16-24 RT: 0.41-0.62 AV: 9 NL: 1.42E7
TMS + p ESI Full ms [300.00-850.00]
TZ62-097
449.1264
C25 H22 O4 N2 Cl = 449.1263
0.1339 mmu
8a
453.1304
C21 H23 O4 N4 Cl Na = 453.1300
0.3508 mmu
462.1463
C16 H28 O8 N4 Cl Na = 462.1488
-2.4855 mmu
469.3290
C22 H48 O5 N3 Cl = 469.3277
1.2675 mmu
458.0891
C25 H17 O4 N3 Cl = 458.0902
-1.0710 mmu
m/z

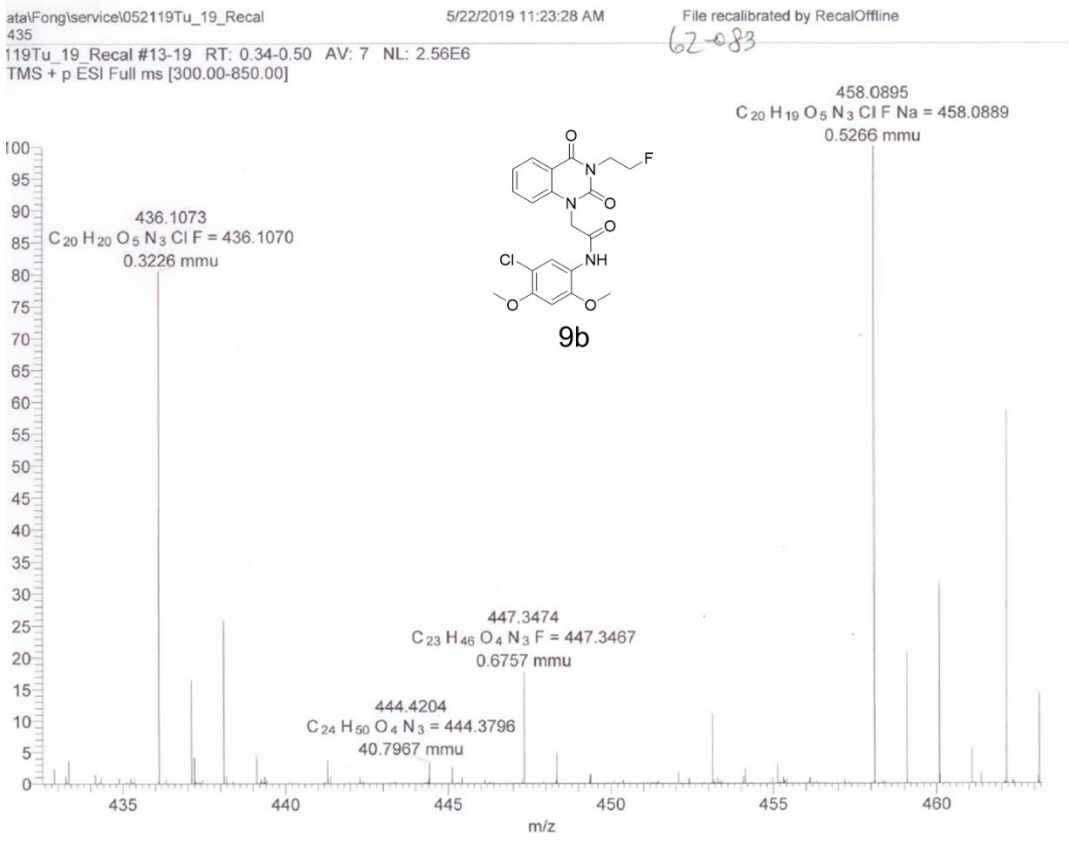

Data\Fong\service\052119Tu_28_Recal
5/22/2019 12:14:29 PM
File recalibrated by RecalOffline
V 404
2119Tu_28_Recal #14-27 RT: 0.35-0.70 AV: 14 NL: 2.78E7
FTMS + p ESI Full ms [300.00-850.00]
405.1012
C20 H19 O4 N2 Cl F = 405.1012
-0.0134 mmu
TZ 62-100
8b
427.0832
C20 H18 O4 N2 Cl F Na = 427.0831
0.0775 mmu
413.2664
C18 H40 O5 N3 Cl = 413.2651
1.2828 mmu
422.1279
C20 H22 O4 N3 Cl F = 422.1277
0.1229 mmu
m/z

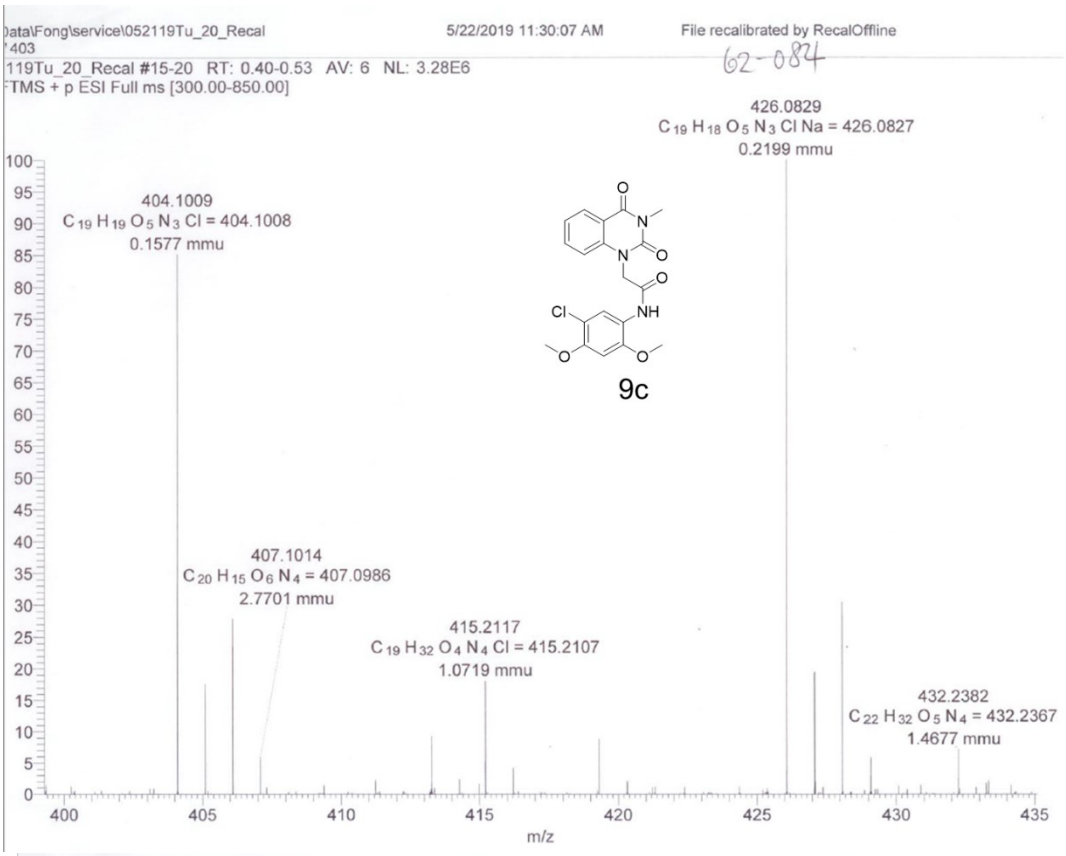

a\Fong\service\052119Tu_26_Recal
5/22/2019 12:05:56 PM
File recalibrated by RecalOffline
72
9Tu_26_Recal #12-24 RT: 0.31-0.63 AV: 13 NL: 4.30E7
MS + p ESI Full ms [300.00-850.00]
373.0949
C19 H18 O4 N2 Cl = 373.0950
-0.0474 mmu
TZ 62-098
8c
395.0770
C19 H17 O4 N2 Cl Na = 395.0769
0.0830 mmu
399.2506
C17 H38 O5 N3 Cl = 399.2495
1.1052 mmu
381.2975
C18 H38 O4 N2 Cl = 381.2515
46.0407 mmu
m/z

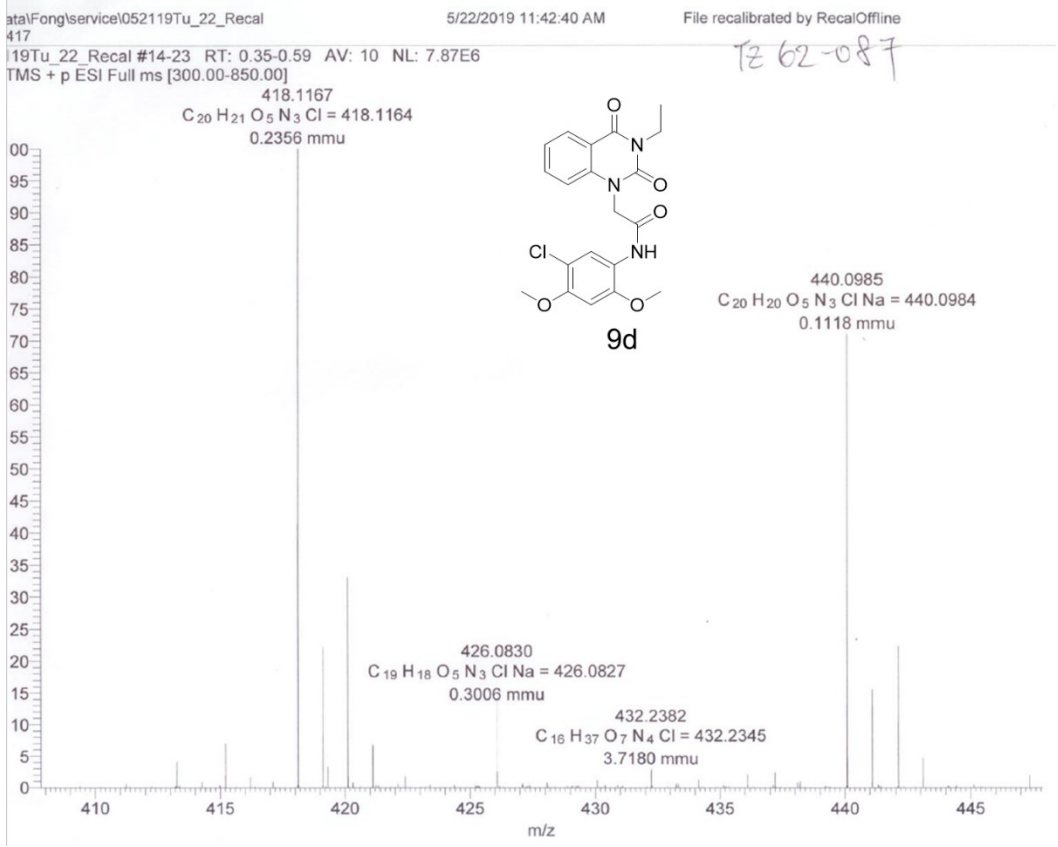

Data\Fong\service\052119Tu_27_Recal
5/22/2019 12:10:42 PM
File recalibrated by RecalOffline
TZ 62-099
2119Tu_27_Recal #12-22 RT: 0.30-0.57 AV: 11 NL: 2.17E7
FTMS + p ESI Full ms [300.00-850.00]
387.1108
C20 H20 O4 N2 Cl = 387.1106
0.1777 mmu
393.2977
C19 H38 O4 N2 Cl = 393.2515
46.2188 mmu
399.2507
C17 H38 O5 N3 Cl = 399.2495
1.2794 mmu
409.0927
C20 H19 O4 N2 Cl Na = 409.0926
0.1315 mmu
m/z
8d

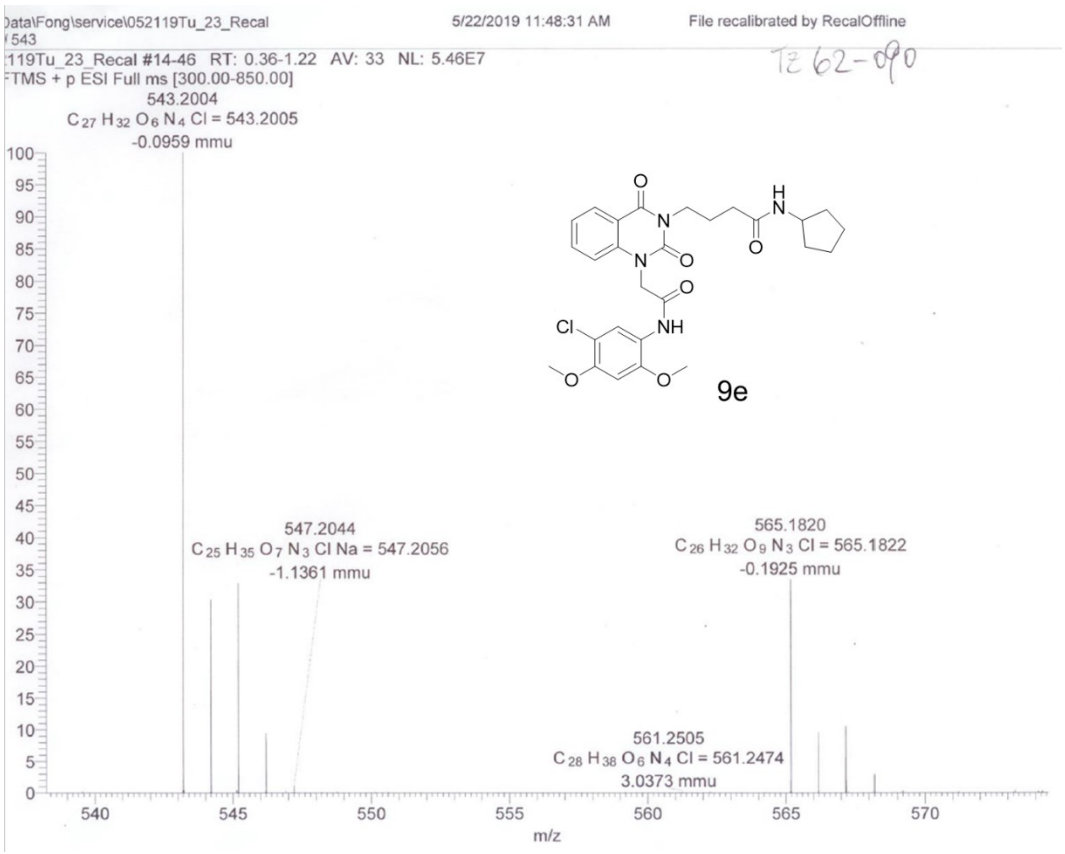

Data\Fong\service\052119Tu_18_Recal
5/22/2019 11:18:21 AM
File recalibrated by RecalOffline
62-048
119Tu_18_Recal #14-22 RT: 0.37-0.58 AV: 9 NL: 2.21E7
TMS + p ESI Full ms [300.00-850.00]
512.1946
C27 H31 O5 N3 Cl = 512.1947
-0.0819 mmu
516.1986
C22 H33 O8 N4 Cl = 516.1981
0.4439 mmu
524.0680
C34 H10 O4 N3 = 524.0666
1.4428 mmu
534.1766
C27 H30 O5 N3 Cl Na = 534.1766
-0.0069 mmu
540.4471
C26 H60 O7 N4 = 540.4457
1.4714 mmu
m/z
8e


ta\Fong\service\052119Tu_21_Recal
79
5/22/2019 11:37:17 AM
File recalibrated by RecalOffline
19Tu_21_Recal #22-30 RT: 0.58-0.79 AV: 9 SB: 3 0.79-0.84 NL: 3.64E6
MS + p ESI Full ms [300.00-850.00]
TZ 62-077.
480.1324
C25 H23 O5 N3 Cl = 480.1321
0.3651 mmu
9a
502.1145
C25 H22 O5 N3 Cl Na = 502.1140
0.5061 mmu
469.3528
C22 H48 O5 N3 Cl = 469.3277
25.0603 mmu
518.0883
C25 H19 O5 N3 Cl F Na = 518.0889
-0.6458 mmu
447.3474
C19 H43 O5 N3 Cl F = 447.2870
60.4542 mmu
m/z


ata\Fong\service\052119Tu_19_Recal
435
5/22/2019 11:23:28 AM
File recalibrated by RecalOffline
62-083
119Tu_19_Recal #13-19 RT: 0.34-0.50 AV: 7 NL: 2.56E6
TMS + p ESI Full ms [300.00-850.00]
458.0895
C20 H19 O5 N3 Cl F Na = 458.0889
0.5266 mmu
9b
436.1073
C20 H20 O5 N3 Cl F = 436.1070
0.3226 mmu
447.3474
C23 H46 O4 N3 F = 447.3467
0.6757 mmu
444.4204
C24 H50 O4 N3 = 444.3796
40.7967 mmu
m/z


)ata\Fong\service\052119Tu_20_Recal
5/22/2019 11:30:07 AM
File recalibrated by RecalOffline
62-084
119Tu_20_Recal #15-20 RT: 0.40-0.53 AV: 6 NL: 3.28E6
TMS + p ESI Full ms [300.00-850.00]
426.0829
C19 H18 O5 N3 Cl Na = 426.0827
0.2199 mmu
404.1009
C19 H19 O5 N3 Cl = 404.1008
0.1577 mmu
9c
407.1014
C20 H15 O6 N4 = 407.0986
2.7701 mmu
415.2117
C19 H32 O4 N4 Cl = 415.2107
1.0719 mmu
432.2382
C22 H32 O5 N4 = 432.2367
1.4677 mmu
m/z


ata\Fong\service\052119Tu_22_Recal
5/22/2019 11:42:40 AM
File recalibrated by RecalOffline
TZ 62-087
19Tu_22_Recal #14-23 RT: 0.35-0.59 AV: 10 NL: 7.87E6
TMS + p ESI Full ms [300.00-850.00]
418.1167
C20 H21 O5 N3 Cl = 418.1164
0.2356 mmu
9d
440.0985
C20 H20 O5 N3 Cl Na = 440.0984
0.1118 mmu
426.0830
C19 H18 O5 N3 Cl Na = 426.0827
0.3006 mmu
432.2382
C16 H37 O7 N4 Cl = 432.2345
3.7180 mmu
m/z


Data\Fong\service\052119Tu_23_Recal
5/22/2019 11:48:31 AM
File recalibrated by RecalOffline
543
119Tu_23_Recal #14-46 RT: 0.36-1.22 AV: 33 NL: 5.46E7
FTMS + p ESI Full ms [300.00-850.00]
543.2004
C27 H32 O6 N4 Cl = 543.2005
-0.0959 mmu
TZ 62-090
9e
547.2044
C25 H35 O7 N3 Cl Na = 547.2056
-1.1361 mmu
565.1820
C26 H32 O9 N3 Cl = 565.1822
-0.1925 mmu
561.2505
C28 H38 O6 N4 Cl = 561.2474
3.0373 mmu
m/z