Supplementary Information

Visible-light photoredox-catalyzed four component reaction for the construction of sulfone-containing quinoxalin-2(1H)-ones

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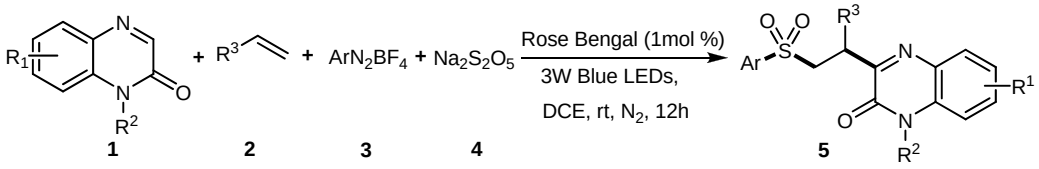
1. General information

All commercially available reagent grade chemicals were purchased from Adamas, Strem, MERYER, Alfa Aesarand Energy Chemical Company and used as received without further purification unless otherwise stated. ^{1}H NMR and ^{13}C NMR were recorded in $CDCl_3$ on a BrukerAvance III 500MHz or 400 MHz spectrometer with TMS as internal standard at room temperature, the chemical shifts (δ) were expressed in ppm and J values were given in Hz. The following abbreviations are used to indicate the multiplicity: singlet (s), doublet (d), triplet (t), quartet (q), doublet of doublets (dd), doublet of triplets (dt), and multiplet (m). All first order splitting patterns were assigned on the basis of the appearance of the multiplet. Splitting patterns that could not be easily interpreted were designated as multiplet (m). High-resolution mass spectra (HRMS) were obtained on an LTQ Orbitrap XL mass spectrometry equipped with an ESI source. Column chromatography was performed on silica gel (200-300 mesh).

2. General procedure for visible-light photoredox-catalyzed four component reaction leading to sulfone-containing quinoxalin-2(1H)-ones.

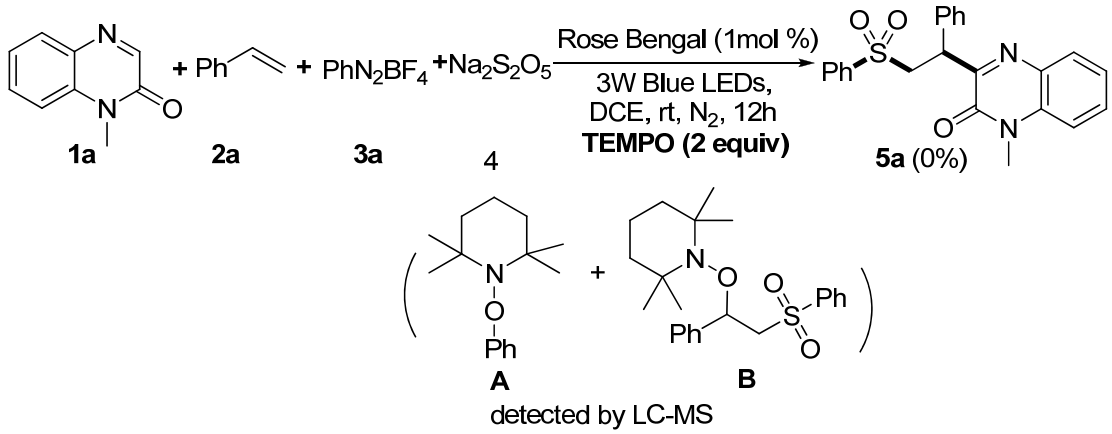


1 2 3 4 5

A mixture of quinoxalin-2(1H)-ones **1** (0.1mmol), aryldiazoniumtetrafluoroborate **3** (0.2mmol), $Na_2S_2O_5$ **4** (0.3mmol), and Rose Bengal (1 mol%), and DCE(2 mL) in a tube (20 mL). Then, the tube was filled with N_2. Alkene **2** (0.2 mmol) and DCE (2 mL) was added in tube under nitrogen atmosphere. The reaction mixture was stirred and irradiated by 3 W blue LEDs at room temperature for 12h. After completion of the reaction, the reaction mixture was concentrated in vacuum. The residue was purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate as eluent to give the desired product **5**.

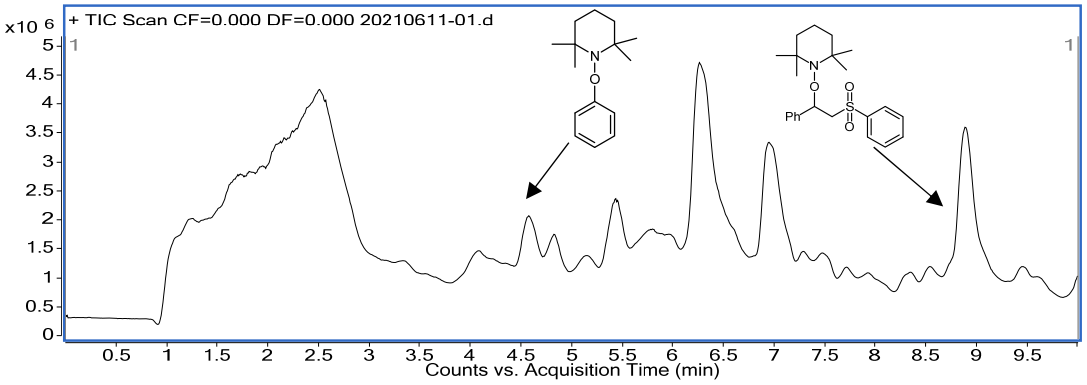
3. Preliminary mechanistic studies

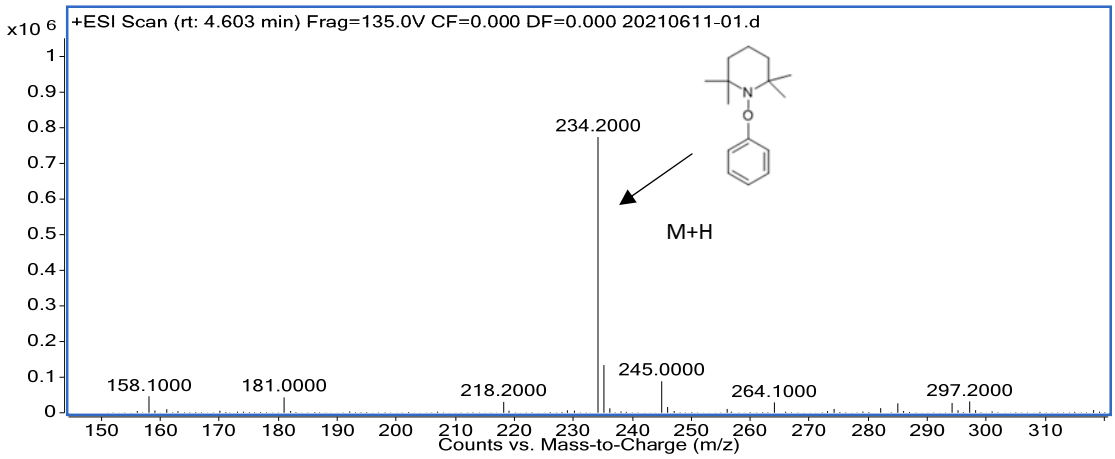
3.1 The addition of TEMPO in the model reaction system.

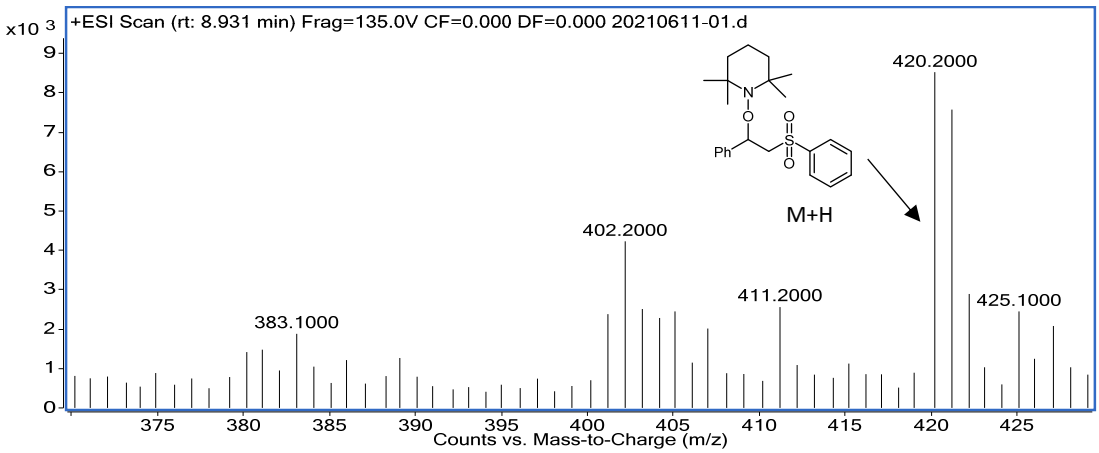


A mixture of 1-methylquinoxalin-2(1H)-one (**1a**), phenyldiazoniumtetrafluoroborate (**3a**), $Na_2S_2O_5$ (**4**), Rose Bengal (1 mol%), and TEMPO (0.2 mmol) in a 20mL tube. Then, the tube was filled with N_2. Styrene **2a** (0.2 mmol) and DCE (2 mL) were added in tube under nitrogen atmosphere. The reaction mixture was stirred and irradiated by 3 W blue LEDs at room temperature for

12h. After completion of the reaction, the reaction mixture was concentrated in vacuum. None of the desired product **5a** was detected and TEMPO trapped complexes **A** and **B** were detected by LC-MS. The above result indicated that a radical process should be involved in this reaction.







2. On/off experiments.

A mixture of1-methylquinoxalin-2(1H)-one (**1a**),

phenyldiazoniumtetrafluoroborate (**3a**), $Na_2S_2O_5$ (**4**), and Rose Bengal (1 mol%) in a 20mL tube. Then, the tube was filled with N_2. Styrene **2a** and DCE (2 mL) were added in tube under nitrogen atmosphere. The reaction mixture was stirred and irradiated by 3 W blue LEDs at room temperature under nitrogen atmosphere for 3h, the corresponding product was isolated in 36% yield. The reaction mixture was stirred and irradiated by 3 W blue LEDs at room temperature under nitrogen atmosphere for 3h, then the reaction mixture was continuously stirred in the dark for 3h, the desired product was obtained in 36.1% yield. Furthermore, when the reaction mixture was stirred and irradiated by 3 W blue LEDs at room temperature under nitrogen atmosphere for 6h, the desired product was isolated in 57% yield. Moreover, the reaction mixture was stirred and irradiated by 3 W blue LEDs at room temperature under nitrogen atmosphere for 6h, then the reaction mixture was continuously stirred in the dark for 3h, the desired product was obtained in 57% yield. The above results indicated that the continuous visible light irradiation is essential for promoting this transformation (Fig. S1).

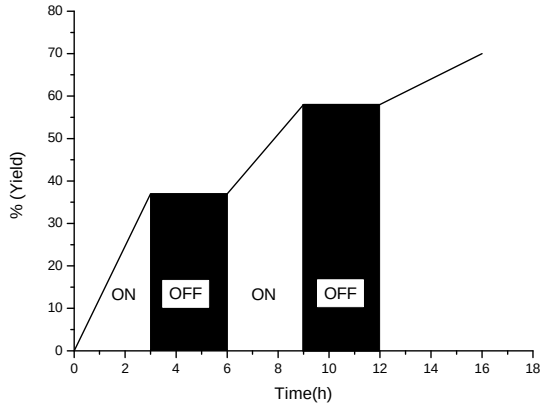
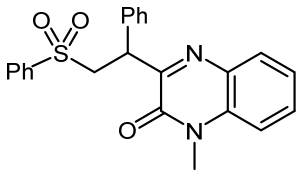
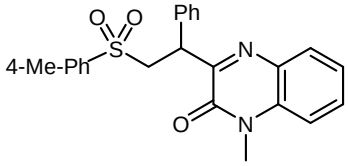


Fig. S1 On/off experiments

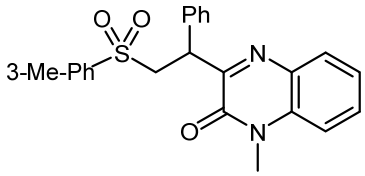
4. Characterization data of products



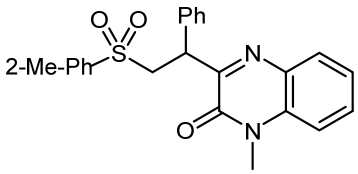
1,6-dimethyl-3-(1-phenyl-2-(phenylsulfonyl)ethyl)-5-vinylpyrazin-2(1H)-one (5a), ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.82 (d, J = 8.0 Hz, 2H), 7.77 (d, J = 8.0 Hz, 1H), 7.53 - 7.49(m, 1H), 7.38 - 7.30(m, 6H), 7.21 (t, J = 7.9 Hz, 3H), 7.17 - 7.14 (m, 1H), 5.28 (dd,J_1 = 3.4 Hz, J_2 = 10.0 Hz, 1H), 4.79 (dd,J_1 = 10.0 Hz, J_2 = 14.4 Hz, 1H), 3.64 (dd,J_1 = 3.4 Hz, J_2 = 14.4 Hz, 1H), 3.57 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.4, 153.9, 139.4, 138.4, 133.1, 133.0, 132.1, 130.3, 130.1, 128.8, 128.8, 128.3, 127.6, 123.6, 113.5, 59.3, 42.1, 29.1; ESI HRMS: calculated for $C_{23}H_{21}N_2O_3S$ $[M+H]^+$ 405.1273, found 405.1261.



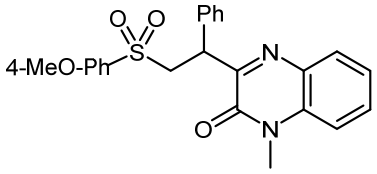
1-methyl-3-(1-phenyl-2-tosylethyl)quinoxalin-2(1H)-one (5b), ^{1}H NMR(500 MHz, $CDCl_3$): δ 7.74 (d, J = 8.0 Hz, 1H), 7.68 (d, J = 8.0 Hz, 2H), 7.47 (t, J = 7.8 Hz, 1H), 7.34 - 7.30(m, 3H), 7.23 - 7.15 (m, 4H), 7.05 (d, J = 8.2 Hz, 2H), 5.26 (dd,J_1 = 3.0 Hz, J_2 = 10.2 Hz, 1H), 4.78 (dd,J_1 = 10.0 Hz, J_2 = 14.4 Hz, 1H), 3.60 (dd,J_1 = 3.0 Hz, J_2 = 14.4 Hz, 1H), 3.56 (s, 3H), 2.17(s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.4, 153.9, 144.2, 138.6, 136.3, 133.0, 132.1, 130.2, 130.0, 129.4, 128.8, 128.4, 128.3, 127.5, 123.5, 113.4, 59.4, 42.1, 29.1, 21.4; ESI HRMS: calculated for $C_{24}H_{23}N_2O_3S$ $[M+H]^+$ 419.1429, found 419.1438.



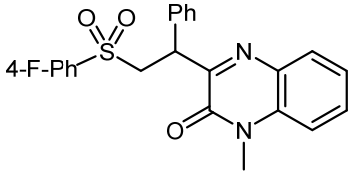
1-methyl-3-(1-phenyl-2-(m-tolylsulfonyl)ethyl)quinoxalin-2(1H)-one (5c), ^{1}H NMR(500 MHz, $CDCl_3$): δ 7.76 - 7.74 (m, 1H), 7.62 (d, J = 7.8 Hz, 1H), 7.55 (s, 1H), 7.52 - 7.49 (m, 1H), 7.34 (d, J = 7.3 Hz, 2H), 7.33 - 7.30(m, 1H), 7.23 - 7.19 (m, 3H), 7.17 - 7.15 (m, 2H), 7.08 (d, J = 7.6 Hz, 1H), 5.27 (dd,J_1 = 3.4 Hz, J_2 = 10.0 Hz, 1H), 4.78 (dd,J_1 = 10.2 Hz, J_2 = 14.4 Hz, 1H), 3.62 (dd,J_1 = 3.0 Hz, J_2 = 14.4 Hz, 1H),3.55 (s, 3H), 2.18 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.4, 153.8, 139.2, 139.0, 138.5, 133.8, 133.0, 132.1, 130.3, 130.0, 128.8, 128.7, 128.6, 128.3, 127.5, 125.5, 123.5, 113.4, 59.4, 42.2, 29.1, 21.0; ESI HRMS: calculated for $C_{24}H_{23}N_2O_3S$ $[M+H]^+$ 419.1429, found 419.1464.



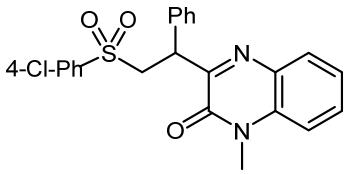
1-methyl-3-(1-phenyl-2-(o-tolylsulfonyl)ethyl)quinoxalin-2(1H)-one (5d), ^{1}HNMR(500 MHz, $CDCl_3$): δ 7.89 - 7.87(m, 1H), 7.76 (d, J = 7.9 Hz, 1H), 7.50 (t, J = 7.8 Hz, 1H), 7.36 (d, J = 7.4 Hz, 2H), 7.31 (t, J = 7.6 Hz, 1H), 7.22 (t, J = 7.6 Hz, 2H), 7.16 (t, J = 7.8 Hz, 2H),7.13 - 7.10 (m, 2H), 6.89 - 6.88 (m, 1H), 5.28 (dd,J_1 = 3.4 Hz, J_2 = 10.0 Hz, 1H), 4.88 (dd,J_1 = 10.0 Hz, J_2 = 14.4 Hz, 1H), 3.62 (dd,J_1 = 3.0 Hz, J_2 = 14.4 Hz, 1H),3.59 (s, 3H), 2.67 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ157.4, 153.7, 138.6, 138.5, 137.1, 133.1, 132.9, 132.2, 131.9, 130.5, 130.3, 129.8, 128.8, 128.3, 127.5, 126.0, 123.5, 113.5, 58.3, 42.0, 29.0, 20.5; ESI HRMS: calculated for $C_{24}H_{22}N_2NaO_3S$ $[M+Na]^+$ 441.1249, found 441.1283.



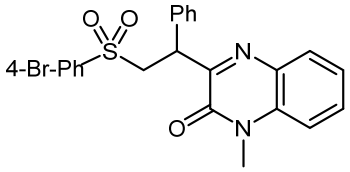
3-(2-((4-methoxyphenyl)sulfonyl)-1-phenylethyl)-1-methylquinoxalin-2(1H)-one (5e),^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 - 7.76 (m, 1H), 7.71 (d, J = 8.8 Hz, 2H), 7.53 - 7.49(m, 1H), 7.35 - 7.30(m, 3H), 7.24 - 7.14(m, 4H), 6.69 (d, J = 8.8 Hz, 2H), 5.27 (dd,J_1 = 3.4 Hz, J_2 = 10.0 Hz, 1H), 4.78 (dd,J_1 = 10.2 Hz, J_2 = 14.4 Hz, 1H), 3.64(s, 3H), 3.62 (dd,J_1 = 3.0 Hz, J_2 = 14.4 Hz, 1H), 3.56 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.2, 157.5, 153.8, 138.6, 133.0, 132.2, 130.7, 130.6, 130.1, 130.0, 128.8, 128.3, 127.5, 123.5, 113.9, 113.4, 59.6, 55.4, 42.2, 29.0; ESI HRMS: calculated for $C_{24}H_{23}N_2O_4S$ $[M+H]^+$ 435.1379, found 435.1415.



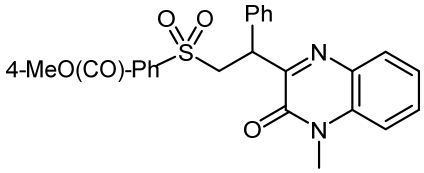
3-(2-((4-fluorophenyl)sulfonyl)-1-phenylethyl)-1-methylquinoxalin-2(1H)-one (5f),^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 - 7.77 (m, 3H), 7.55 - 7.51(m, 1H), 7.36 - 7.32(m, 3H), 7.23 - 7.16(m, 4H), 6.96 (t, J = 8.6 Hz, 2H), 6.69 (d, J = 8.8 Hz, 2H), 5.27 (dd,J_1 = 3.8 Hz, J_2 = 10.0 Hz, 1H), 4.75 (dd, J_1 = 10.0 Hz, J_2 = 14.4 Hz, 1H), 3.67 (dd,J_1 = 3.8 Hz, J_2 = 14.4 Hz, 1H), 3.58 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.4 (d, J = 254.6 Hz), 157.4, 153.8, 138.2, 135.4 (d, J = 3.2 Hz), 133.0, 132.1, 131.2 (d, J = 9.5 Hz), 130.5, 130.0, 128.8, 128.3,127.6, 123.7, 116.0 (d, J = 22.5 Hz), 113.6, 59.5,42.1, 29.1; ESI HRMS: calculated for $C_{23}H_{20}FN_2O_3S$ $[M+H]^+$ 423.1179, found 423.1202.



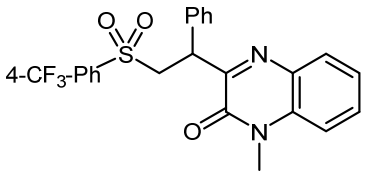
3-(2-((4-chlorophenyl)sulfonyl)-1-phenylethyl)-1-methylquinoxalin-2(1H)-one (5g), ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76 - 7.74 (m, 1H), 7.70 (d, J = 8.6 Hz, 2H), 7.55 - 7.50 (m, 1H), 7.36 - 7.33 (m, 3H), 7.23 - 7.15 (m, 6H), 6.69 (d, J = 8.8 Hz, 2H), 5.24 (dd,J_1 = 3.4 Hz, J_2 = 10.0 Hz, 1H), 4.76 (dd,J_1 = 10.2 Hz, J_2 = 14.4 Hz, 1H), 3.66 (dd,J_1 = 3.4 Hz, J_2 = 14.4 Hz, 1H), 3.57(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.2, 153.7, 140.0, 138.2, 137.7, 133.0, 132.0, 130.5, 129.9, 129.0, 128.8, 128.3, 127.6, 123.7, 113.6, 59.5, 42.2, 29.1; ESI HRMS: calculated for $C_{23}H_{20}ClN_2O_3S$ $[M+H]^+$ 439.0883, found 439.0901.



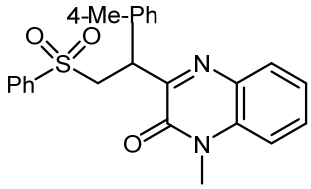
3-(2-((4-bromophenyl)sulfonyl)-1-phenylethyl)-1-methylquinoxalin-2(1H)-one (5h), ^{1}H NMR (400MHz, $CDCl_3$): δ 7.76 - 7.74 (m, 1H), 7.63 (d, J = 8.6 Hz, 2H), 7.56 - 7.51 (m, 1H), 7.38 - 7.33 (m, 5H), 7.24 - 7.17 (m, 4H), 6.69 (d, J = 8.8 Hz, 2H), 5.24 (dd,J_1= 3.4 Hz, J_2 = 10.0 Hz, 1H), 4.77 (dd,J_1 = 10.0 Hz, J_2 = 14.4 Hz, 1H), 3.64 (dd,J_1 = 3.4 Hz, J_2 = 14.4 Hz, 1H),3.58(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.2, 153.7, 138.2, 138.1, 132.9, 132.0, 130.5, 130.0, 129.9, 128.8, 128.6, 128.3, 127.6, 123.8, 113.7, 59.4, 42.2, 29.1; ESI HRMS: calculated for $C_{23}H_{20}BrN_2O_3S$ $[M+H]^+$ 483.0378, found 483.0412.



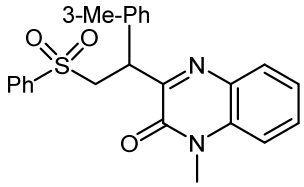
Methyl4-((2-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)-2-phenylethyl)sulfonyl) benzoate (5i),^{1}H NMR(400MHz, $CDCl_3$): δ 7.91 - 7.84 (m, 4H), 7.71 - 7.69 (m, 1), 7.51 - 7.47 (m, 1H), 7.34 - 7.29 (m, 3H), 7.23 - 7.14 (m, 4H), 5.28 (dd,J_1 = 3.4 Hz, J_2 = 10.0 Hz, 1H), 4.77 (dd,J_1 = 10.1 Hz, J_2 = 14.4 Hz, 1H), 3.89 (s, 3H), 3.67 (dd,J_1 = 3.4 Hz, J_2 = 14.4 Hz, 1H),3.57 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.2, 157.1, 153.8, 143.1, 138.1, 134.1, 132.9, 131.9, 130.3, 129.9, 129.9, 128.8, 128.4, 128.3, 127.7, 123.6, 113.5, 59.4, 52.5, 42.1, 29.1; ESI HRMS: calculated for $C_{25}H_{23}N_2O_5S$ $[M+H]^+$ 463.1328, found 463.1306.



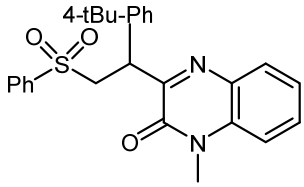
1-methyl-3-(1-phenyl-2-((4-(trifluoromethyl)phenyl)sulfonyl)ethyl)quinoxalin-2(1H)-one (5j),[1]H NMR (400 MHz, $CDCl_3$): δ 7.90 (d, J = 8.2 Hz, 2H), 7.72 - 7.70 (m, 1H), 7.54 - 7.49 (m, 3H), 7.34 - 7.31 (m, 3H), 7.22 - 7.16 (m, 4H), 5.28 (dd,J_1 = 3.4 Hz, J_2 = 10.0 Hz, 1H), 4.77 (dd,J_1 = 10.1 Hz, J_2 = 14.4 Hz, 1H), 3.73 (dd,J_1 = 3.4 Hz, J_2 = 14.4 Hz, 1H),3.55 (s, 3H); [13]C NMR (100 MHz, $CDCl_3$): δ 157.0, 153.7, 142.8, 137.9, 134.7 (q, J = 33.9 Hz), 132.9, 131.8, 130.6, 129.8, 129.0, 128.8, 128.3, 127.7, 125.8(q, J = 3.6 Hz), 123.8, 113.6, 59.3, 42.2, 29.0; ESI HRMS: calculated for $C_{24}H_{23}F_3N_2O_3S$ $[M+H]^+$473.1147, found 473.1150.



1-methyl-3-(2-(phenylsulfonyl)-1-(p-tolyl)ethyl)quinoxalin-2(1H)-one (5k), [1]H NMR (400 MHz, $CDCl_3$): δ 7.82 - 7.80 (m, 2H), 7.77 - 7.75 (m, 1H), 7.52 - 7.48 (m, 1H), 7.38 - 7.29 (m, 4H), 7.20 (t, J = 8.3 Hz, 3H), 7.01 (d, J = 8.0 Hz, 2H), 5.24 (dd,J_1 = 3.4 Hz, J_2 = 10.0 Hz, 1H), 4.77 (dd,J_1 = 10.0 Hz, J_2 = 14.4 Hz, 1H), 3.63 (dd,J_1 = 3.4 Hz, J_2 = 14.4 Hz, 1H), 3.56 (s, 3H), 2.23 (s, 3H); [13]C NMR (100 MHz, $CDCl_3$): δ 157.5, 153.9, 139.4, 137.3, 135.4, 133.0, 132.1, 130.2, 130.0, 129.5, 128.8, 128.3, 128.2, 123.5, 113.5, 59.4, 41.8, 29.1, 21.0; ESI HRMS: calculated for $C_{24}H_{23}N_2O_3S$ $[M+H]^+$ 419.1429, found 419.1436.

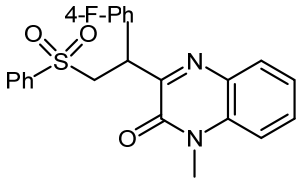


1-methyl-3-(2-(phenylsulfonyl)-1-(m-tolyl)ethyl)quinoxalin-2(1H)-one (5l), [1]H NMR (400 MHz, $CDCl_3$): δ 7.82 - 7.76 (m, 3H), 7.53 - 7.49 (m, 1H), 7.38 - 7.29 (m, 4H), 7.20 (d, J = 8.2 Hz, 1H), 7.13 - 7.07 (m, 3H) 6.96 (d, J = 7.0 Hz, 1H), 5.24 (dd,J_1 = 3.4Hz, J_2 = 10.0 Hz, 1H), 4.78 (dd,J_1 = 10.0 Hz, J_2 = 14.4 Hz, 1H), 3.63 (dd,J_1 = 3.4 Hz, J_2 = 14.4 Hz, 1H),3.57 (s, 3H), 2.23 (s, 3H); [13]C NMR (100 MHz, $CDCl_3$): δ 157.5, 153.9, 139.4, 138.4, 138.3, 133.0, 133.0, 132.1, 130.2, 130.1, 129.0, 128.8, 128.6, 128.3, 125.3, 123.5, 113.5, 59.4, 42.0, 29.1, 21.4. ESI HRMS: calculated for $C_{24}H_{23}N_2O_3S$ $[M+H]^+$ 419.1429, found 419.1416.

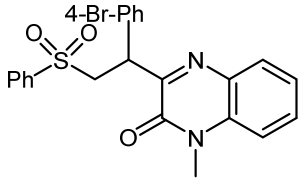


3-(1-(4-(tert-butyl)phenyl)-2-(phenylsulfonyl)ethyl)-1,6-dimethyl-5-vinylpyrazin-2(1H)-one (5m),[1]H NMR (400 MHz, $CDCl_3$): δ 7.82 - 7.76 (m, 3H), 7.52 -7.48 (m, 1H), 7.35 - 7.28 (m, 4H), 7.24 - 7.18 (m, 5H), 5.26 (dd,J_1 = 3.4 Hz, J_2 = 10.0 Hz, 1H), 4.78 (dd,J_1 = 10.0 Hz, J_2 = 14.4 Hz, 1H), 3.66 (dd,J_1 = 3.4 Hz, J_2 = 14.4 Hz, 1H),3.57 (s, 3H), 1.22 (s, 9H); [13]C NMR (100 MHz, $CDCl_3$): δ 157.6, 153.9, 150.3, 139.4,

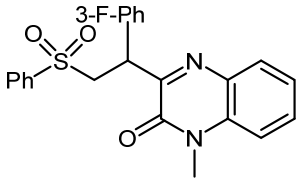
135.3, 133.0, 132.2, 130.2, 130.0, 128.8, 128.3, 127.9, 125.7, 123.5, 113.4, 59.3, 41.6, 34.4, 31.2, 29.1; ESI HRMS: calculated for $C_{27}H_{29}N_2O_3S$ $[M+H]^+$ 461.1899, found 461.1967.



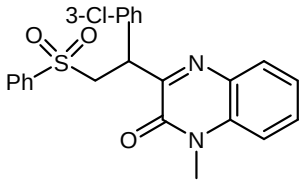
3-(1-(4-fluorophenyl)-2-(phenylsulfonyl)ethyl)-1-methylquinoxalin-2(1H)-one (5n), ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 - 7.76 (m, 3H), 7.55 - 7.51 (m, 1H), 7.40 - 7.28 (m, 6H), 7.22 (d, J = 8.3 Hz, 1H), 6.88 (t, J = 8.7 Hz, 2H), 5.27 (dd,J_1 = 4.1 Hz, J_2 = 10.0 Hz, 1H), 4.69 (dd,J_1 = 10.0 Hz, J_2 = 14.4 Hz, 1H), 3.65 (dd,J_1 = 4.1 Hz, J_2 = 14.4 Hz, 1H),3.58 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.1 (d, J = 245.1 Hz), 157.3, 153.8, 139.3, 134.0(d, J = 3.2 Hz), 133.1, 133.0, 132.1, 130.4, 130.0 (d, J = 9.3 Hz), 128.9, 128.3, 123.6, 115.6 (d, J = 21.4 Hz), 113.5, 59.3, 41.4, 29.1; ESI HRMS: calculated for $C_{23}H_{20}FN_2O_3S$ $[M+H]^+$ 423.1179, found 423.1196.



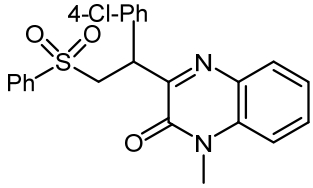
3-(1-(4-bromophenyl)-2-(phenylsulfonyl)ethyl)-1-methylquinoxalin-2(1H)-one (5o), ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80 - 7.76 (m, 3H), 7.55 - 7.51 (m, 1H), 7.41 - 7.38 (m, 1H), 7.35 - 7.30 (m, 5H), 7.21 (t, J = 8.1 Hz, 3H), 5.24 (dd,J_1 = 4.3 Hz, J_2 = 9.2 Hz, 1H), 4.67 (dd,J_1 = 9.2 Hz, J_2 = 14.4 Hz, 1H), 3.66 (dd,J_1 = 4.3 Hz, J_2 = 14.4 Hz, 1H),3.58 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.0, 153.8, 139.3, 137.3, 133.2, 133.0, 132.1, 131.8, 130.5, 130.1, 130.1, 128.9, 128.2, 123.7, 121.7, 113.6, 59.1, 41.7, 29.1; ESI HRMS: calculated for $C_{23}H_{20}BrN_2O_3S$ $[M+H]^+$ 483.0378, found 483.0392.



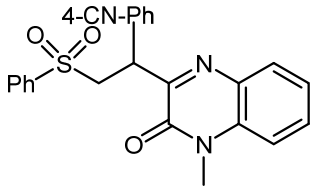
3-(1-(3-fluorophenyl)-2-(phenylsulfonyl)ethyl)-1-methylquinoxalin-2(1H)-one (5p),^{1}H NMR (500 MHz, $CDCl_3$): δ 7.81 (d, J = 7.3 Hz, 2H), 7.77 (d, J = 7.9 Hz, 1H), 7.53 (t, J = 7.8 Hz, 1H), 7.39 - 7.37 (m, 1H), 7.34 - 7.32 (m, 3H), 7.22 (d, J = 8.4 Hz, 1H), 7.19 - 7.13 (m, 2H), 7.01 (d, J = 9.8 Hz, 1H), 6.87 - 6.83 (m, 1H), 5.28 (dd,J_1 = 3.8 Hz, J_2 = 10.0 Hz, 1H), 4.71 (dd,J_1 = 10.0 Hz, J_2 = 14.4 Hz, 1H), 3.64 (dd,J_1 = 3.8 Hz, J_2 = 14.4 Hz, 1H),3.58 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 162.8 (d, J = 245.3 Hz), 156.9, 153.8, 140.8 (d, J = 7.2 Hz), 139.2, 133.2, 133.1, 132.1, 130.6, 130.3 (d, J = 8.2 Hz), 130.1, 128.9, 128.3, 124.2 (d, J = 2.8 Hz), 123.7, 115.2 (d, J = 21.9 Hz), 114.6 (d, J = 20.9 Hz), 113.6, 59.2, 41.8, 29.2; ESI HRMS: calculated for $C_{23}H_{20}FN_2O_3S$ $[M+H]^+$ 423.1179, found 423.1222.



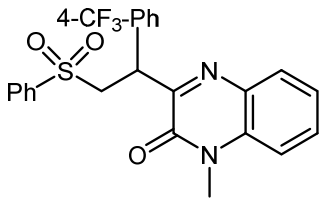
3-(1-(3-chlorophenyl)-2-(phenylsulfonyl)ethyl)-1-methylquinoxalin-2(1H)-one(5q), ^{1}H NMR (400 Hz, $CDCl_3$): δ 7.81 - 7.78 (m, 3H), 7.53 (t, J = 7.3 Hz, 2H), 7.39 - 7.32 (m, 4H), 7.26 - 7.21 (m, 3H), 7.17 - 7.11 (m, 2H), 5.25 (dd,J_1 = 4.1 Hz, J_2 = 10.0 Hz, 1H), 4.69 (dd,J_1 = 10.0 Hz, J_2 = 14.4 Hz, 1H), 3.65 (dd,J_1 = 4.1 Hz, J_2 = 14.4 Hz, 1H),3.59 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.9, 153.8, 140.3, 139.3, 134.5, 133.2, 132.1, 130.6, 130.2, 130.0, 128.9, 128.3, 128.3, 127.8, 126.8, 123.7, 113.6, 59.1, 41.8, 29.2; ESI HRMS: calculated for $C_{23}H_{20}ClN_2O_3S$ $[M+H]^+$ 439.0883, found 439.0920.



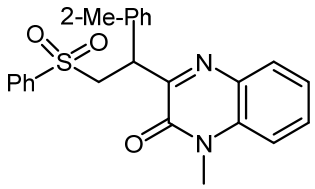
3-(1-(4-chlorophenyl)-2-(phenylsulfonyl)ethyl)-1-methylquinoxalin-2(1H)-one(5r), ^{1}H NMR (500 Hz, $CDCl_3$): δ 7.79 - 7.75 (m, 3H), 7.54- 7.51 (m, 1H), 7.40 - 7.37 (m, 1H), 7.34 - 7.31 (m, 3H), 7.26 (d, J = 8.5 Hz, 2H), 7.21 (d, J = 8.4 Hz, 1H), 7.16 (d, J = 8.5 Hz, 2H), 5.25 (dd,J_1 = 4.3 Hz, J_2 = 9.2 Hz, 1H), 4.67 (dd,J_1 = 9.2 Hz, J_2 = 14.4 Hz, 1H), 3.66 (dd,J_1 = 4.3 Hz, J_2 = 14.4 Hz, 1H),3.57 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.1, 153.8, 139.3, 136.8, 133.5, 133.2, 133.0, 132.1, 130.5, 130.1, 129.8, 128.9, 128.9, 128.3, 123.7, 113.6, 59.2, 41.6, 29.2; ESI HRMS: calculated for $C_{23}H_{20}ClN_2O_3S$ $[M+H]^+$ 439.0883, found 439.0854.



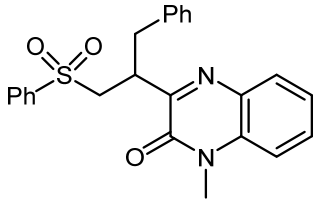
4-(1-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)-2-(phenylsulfonyl)ethyl)benzon itrile(5s),^{1}H NMR (400 Hz, $CDCl_3$): δ 7.81 - 7.77 (m, 3H), 7.58 - 7.54 (m, 1H), 7.51 - 7.45 (m, 4H), 7.44 - 7.40 (m, 1H), 7.37 - 7.33 (m, 3H), 7.24 (d, J = 8.5 Hz, 1H), 5.33 (dd,J_1 = 4.7 Hz, J_2 = 8.8 Hz, 1H), 4.64 (dd,J_1 = 8.8 Hz, J_2 = 14.4 Hz, 1H), 3.69 (dd,J_1 = 4.7 Hz, J_2 = 14.4 Hz, 1H),3.59 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.4, 153.7, 143.6, 139.2, 133.4, 133.1, 132.5, 132.0, 130.9, 130.1, 129.3, 129.0, 128.2, 123.9, 118.5, 113.7, 111.5, 58.8, 42.3, 29.2; ESI HRMS: calculated for $C_{24}H_{20}N_3O_3S$ $[M+H]^+$ 430.1225, found 430.1237.



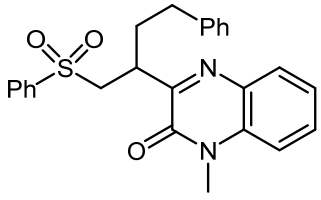
1-methyl-3-(2-(phenylsulfonyl)-1-(4-trifluoromethyl)phenyl)ethyl)quinoxalin-2(1H)-one(5t), ^{1}H NMR (400Hz, $CDCl_3$): δ 7.80 - 7.77 (m, 3H), 7.56 - 7.52 (m, 1H), 7.47 - 7.43 (m, 4H), 7.41 - 7.30 (m, 4H), 7.23 (d, J = 8.3 Hz, 1H),5.35 (dd,J_1 = 4.6 Hz, J_2 = 8.9 Hz, 1H), 4.68 (dd,J_1 = 8.9 Hz, J_2 = 14.4 Hz, 1H), 3.72 (dd,J_1 = 4.6 Hz, J_2 = 14.4 Hz, 1H), 3.59 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.8, 153.8, 142.2, 139.2, 133.3, 133.1, 132.1, 130.7, 130.1, 129.8 (d, J = 32.3 Hz), 128.9, 128.8, 128.2, 125.6 (q, J = 3.7 Hz), 123.9 (d, J = 270.5 Hz), 123.8, 113.6, 59.0, 42.1, 29.2; ESI HRMS: calculated for $C_{24}H_{23}F_3N_2O_3S$ $[M+H]^+$ 473.1147, found 473.1121.



1-methyl-3-(2-(phenylsulfonyl)-1-(o-tolyl)ethyl)quinoxalin-2(1H)-one(5u), ^{1}H NMR (400 Hz, $CDCl_3$): δ 7.87 - 7.81 (m, 3H), 7.55 - 7.51 (m, 1H), 7.41 - 7.32 (m, 4H), 7.22 (d, J = 8.3 Hz, 1H),7.13 (d, J = 7.3 Hz, 1H), 7.08 - 7.03 (m, 2H), 6.96 (t, J = 7.4 Hz, 1H), 5.48 (dd,J_1 = 2.6 Hz, J_2 = 10.3 Hz, 1H), 4.79 (dd,J_1 = 10.3 Hz, J_2 = 14.4 Hz, 1H), 3.58 (s, 3H), 3.41 (dd,J_1 = 2.6 Hz, J_2 = 14.4 Hz, 1H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.6, 154.1, 139.1, 136.9, 136.8, 133.1, 133.0, 132.0, 131.0, 130.3, 130.1, 128.9, 128.4, 127.4, 127.1, 126.1, 123.6, 113.5, 59.2, 37.4, 29.1, 19.5; ESI HRMS: calculated for $C_{24}H_{23}N_2O_3S$ $[M+H]^+$ 419.1429, found 419.1413.

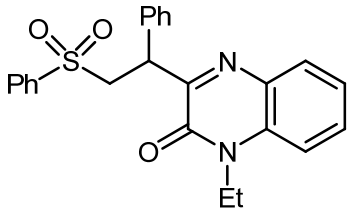


1-methyl-3-(1-phenyl-3-(phenylsulfonyl)propan-2-yl)quinoxalin-2(1H)-one(5v), ^{1}H NMR (400 Hz, $CDCl_3$): δ 7.77 - 7.74 (m, 1H), 7.70 - 7.68 (m, 2H), 7.56 - 7.52 (m, 1H), 7.39 - 7.31 (m, 2H), 7.30 - 7.24 (m, 3H), 7.19 - 7.15 (m, 3H), 7.08 - 7.06 (m, 2H), 4.33 - 4.27 (m, 1H), 4.25 - 4.21 (m, 1H), 3.64 (s, 3H), 3.28 (dd,J_1 = 1.8 Hz, J_2 = 13.9 Hz, 1H), 3.13 (dd,J_1 = 5.1 Hz, J_2 = 13.9 Hz, 1H), 2.69 (d,J_1 = 9.7 Hz, J_2 = 13.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.9, 154.1, 133.0, 132.9, 132.3, 130.3, 129.9, 129.1, 128.7, 128.6, 128.3, 126.7, 123.6, 113.5, 56.1, 39.0, 38.9, 29.1; ESI HRMS: calculated for $C_{24}H_{23}N_2O_3S$ $[M+H]^+$ 419.1429, found 419.1397.

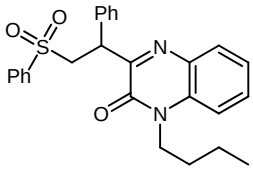


1-methyl-3-(4-phenyl-1-(phenylsulfonyl)butan-2-yl)quinoxalin-2(1H)-one(5w), ^{1}H NMR (400 Hz, $CDCl_3$): δ 7.81 - 7.79 (m, 2H), 7.76 - 7.74 (m, 1H), 7.55 - 7.50 (m, 1H), 7.41 - 7.37 (m, 1H), 7.32 (t, J = 7.4 Hz, 3H), 7.21 (d, J = 8.4 Hz, 1H), 7.15 (t, J = 7.2 Hz, 2H), 7.09 - 7.07 (m, 1H), 7.04 (d, J = 8.2 Hz, 2H), 4.31 (dd,J_1 = 10.0 Hz, J_2 = 14.4 Hz, 1H), 4.06 - 4.02 (m, 1H), 3.58 (s, 3H), 3.40 (dd,J_1 = 3.1 Hz, J_2 = 14.4 Hz, 1H), 2.68 - 2.60 (m, 1H), 2.53 - 2.46 (m, 1H), 2.23 - 2.15 (m, 1H), 2.02 - 1.93 (m, 1H);

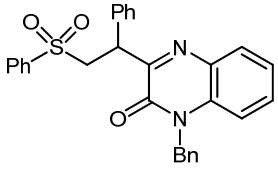
^{13}C NMR (100 MHz, $CDCl_3$): δ 159.2, 154.2, 140.9, 139.1, 133.1, 133.0, 132.2, 130.2, 129.9, 128.8, 128.4, 128.3, 128.2, 125.9, 123.5, 113.4, 58.3, 37.5, 35.2, 33.1, 29.0; ESI HRMS: calculated for $C_{25}H_{25}N_2O_3S$ $[M+H]^+$ 433.1586, found 433.1580.



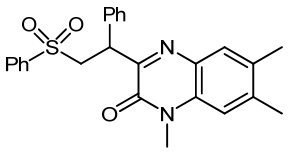
1-ethyl-3-(1-phenyl-2-(phenylsulfonyl)ethyl)quinoxalin-2(1H)-one(5x), ^{1}H NMR (500 Hz, $CDCl_3$): δ 7.81 - 7.80 (m, 2H), 7.77 - 7.75 (m, 1H), 7.52 - 7.48 (m, 1H), 7.34 - 7.26 (m, 6H), 7.21 (t, J = 7.3 Hz, 3H), 7.16 (t, J = 7.2 Hz, 1H), 5.30 - 5.27 (m, 1H), 4.82 - 4.77 (m, 1H), 4.26 - 4.18 (m, 1H), 4.16 - 4.08 (m, 1H), 3.66 - 3.63 (m, 1H), 1.29 (t, J = 7.2 Hz, 3H) ; ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.4, 153.3, 139.3, 138.6, 133.1, 132.4, 131.9, 130.3, 130.3, 128.9, 128.8, 128.3, 127.5, 123.3, 113.3, 59.4, 42.0, 37.5, 12.3; ESI HRMS: calculated for $C_{24}H_{23}N_2O_3S$ $[M+H]^+$ 419.1429, found 429.1426.



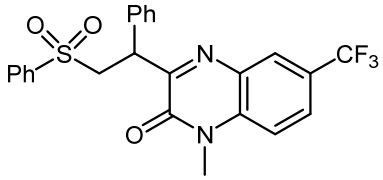
1-butyl-3-(1-phenyl-2-(phenylsulfonyl)ethyl)quinoxalin-2(1H)-one (5y), ^{1}H NMR (400 Hz, $CDCl_3$): δ7.95-7.89 (m ,1H),7.82-7.79 (m, 2H), 7.76 (dd, J_1 = 1.3 Hz,J_2 = 8.0 Hz,1H), 7.52-7.46 (m, 1H), 7.34 - 7.26 (m, 6H), 7.22-7.15 (m, 3H), 5.28 (dd, J_1 = 3.4 Hz,J_2 = 10.0 Hz,1H), 4.78 (dd, J_1 = 10.0 Hz,J_2 = 14.4 Hz,1H), 4.20-4.12 (m, H), 4.07-3.99 (m, 1H), 3.64 (dd, J_1 = 3.4 Hz,J_2 = 14.4 Hz,1H), 1.69-1.61 (m, 2H), 1.47-1.40 (m, 2H), 0.97 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.4, 153.6, 139.4, 138.6, 133.0, 132.4, 132.2, 130.3, 130.2, 128.9, 128.8, 128.8, 128.3, 127.4, 123.3, 113.5, 59.4, 42.3, 42.0, 29.2, 20.3, 13.8. ESI HRMS: calculated for $C_{26}H_{27}N_2O_3S$ $[M+H]^+$ 447.1742, found 447.1750.



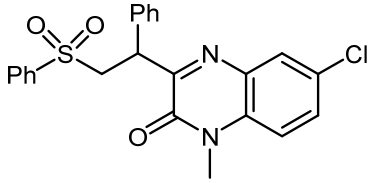
1-benzyl-3-(1-phenyl-2-(phenylsulfonyl)ethyl)quinoxalin-2(1H)-one(5z), ^{1}H NMR (400 Hz, $CDCl_3$): δ 7.82 (d, J = 7.1 Hz, 2H), 7.74 (dd, J_1 = 1.4 Hz,J_2 = 8.0 Hz,1H), 7.38-7.33 (m, 3H), 7.26 - 7.23 (m, 9H), 7.18-7.15 (m, 4H), 5.46 (d, J = 15.6 Hz, 1H), 5.35 (dd, J_1 = 3.4 Hz,J_2 = 10.0 Hz,1H), 5.22 (d, J = 15.6 Hz, 1H), 4.81 (dd, J_1 = 10.0 Hz,J_2 = 14.4 Hz,1H), 3.66 (dd, J_1 = 3.4 Hz,J_2 = 14.4 Hz,1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.6, 154.1, 139.4, 138.5, 135.1, 133.2, 132.4, 132.3, 130.3, 130.2, 128.9, 128.9, 128.8, 128.3, 128.3, 127.8, 127.6, 127.0, 123.6, 114.3, 59.4, 46.0, 42.2. ESI HRMS: calculated for $C_{29}H_{25}N_2O_3S$ $[M+H]^+$ 481.1586, found 481.1595.



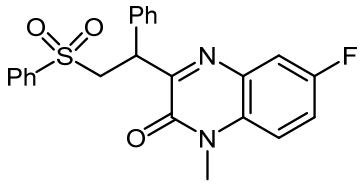
1,6,7-trimethyl-3-(1-phenyl-2-(phenylsulfonyl)ethyl)quinoxalin-2(1H)-one(5a'), ^{1}H NMR (400 Hz, $CDCl_3$): δ 7.82 - 7.80 (m, 2H), 7.54 (s, 1H), 7.39 - 7.36 (m, 1H), 7.34 - 7.30 (m, 4H), 7.21 - 7.14 (m, 3H), 6.96 (s, 1H), 5.24 (dd,J_1 = 3.7 Hz, J_2 = 9.8 Hz, 1H), 4.75 (dd,J_1 = 10.0 Hz, J_2 = 14.4 Hz, 1H), 3.64 (dd,J_1 = 3.7 Hz, J_2 = 14.4 Hz, 1H), 3.54 (s, 3H), 2.40 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.1, 153.9, 140.1, 139.4, 138.7, 133.0, 132.4, 131.1, 130.6, 130.1, 128.8, 128.7, 128.3, 128.3, 127.4, 114.0, 59.4, 42.0, 29.0, 20.6, 19.1; ESI HRMS: calculated for $C_{25}H_{25}N_2O_3S$ $[M+H]^+$ 433.1586, found 433.1596.



1-methyl-3-(1-phenyl-2-(phenylsulfonyl)ethyl)-6-(trifluoromethyl)quinoxalin-2(1H)-one(5b'), ^{1}H NMR (400 Hz, $CDCl_3$): δ 8.04 (s, 1H), 7.84 - 7.82 (m, 2H), 7.75 - 7.72 (m, 1H), 7.44 - 7.30 (m, 6H), 7.25 - 7.15 (m, 4H), 5.31 (dd,J_1 = 3.2 Hz, J_2 = 10.4 Hz, 1H), 4.75 (dd,J_1 = 10.4 Hz, J_2 = 14.4 Hz, 1H), 3.64(dd,J_1 = 3.2 Hz, J_2 = 14.4 Hz, 1H), 3.62 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.4, 153.8, 139.5, 137.8, 135.4, 133.3, 131.4, 128.9 (q, J = 9.9 Hz), 128.3, 128.3, 127.8, 127.5, 127.4 (q, J = 3.8 Hz), 126.6 (q, J = 3.4 Hz), 125.8 (q, J = 45.6 Hz), 122.3, 114.2, 59.2, 42.1, 29.4; ESI HRMS: calculated for $C_{24}H_{23}F_3N_2O_3S$ $[M+H]^+$ 473.1147, found 473.1177.



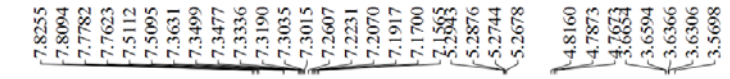
6-**chloro-1-methyl-3-(1-phenyl-2-(phenylsulfonyl)ethyl)quinoxalin-2(1H)-one(5c'),** ^{1}H NMR (400 Hz, $CDCl_3$): δ 7.81 (d, J = 7.4 Hz, 2H), 7.68 (d, J = 8.4 Hz, 1H), 7.46 - 7.28 (m, 6H), 7.23-7.15 (m, 4H), 5.25 (d, J = 9.9 Hz, 1H), 4.77 - 4.71 (dd, J_1 =10.5Hz, J_2 =14.4Hz, 1H), 3.62 (d, J = 14.4 Hz, 1H), 3.53 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.6, 153.6, 139.3, 138.2, 136.3, 133.9, 133.2, 131.1, 130.6, 128.9, 128.8, 128.3, 128.3, 127.7, 124.0, 113.6, 59.2, 42.0, 29.3. ESI HRMS: calculated for $C_{23}H_{20}ClN_2O_3S$ $[M+H]^+$ 439.0883, found 439.0883.

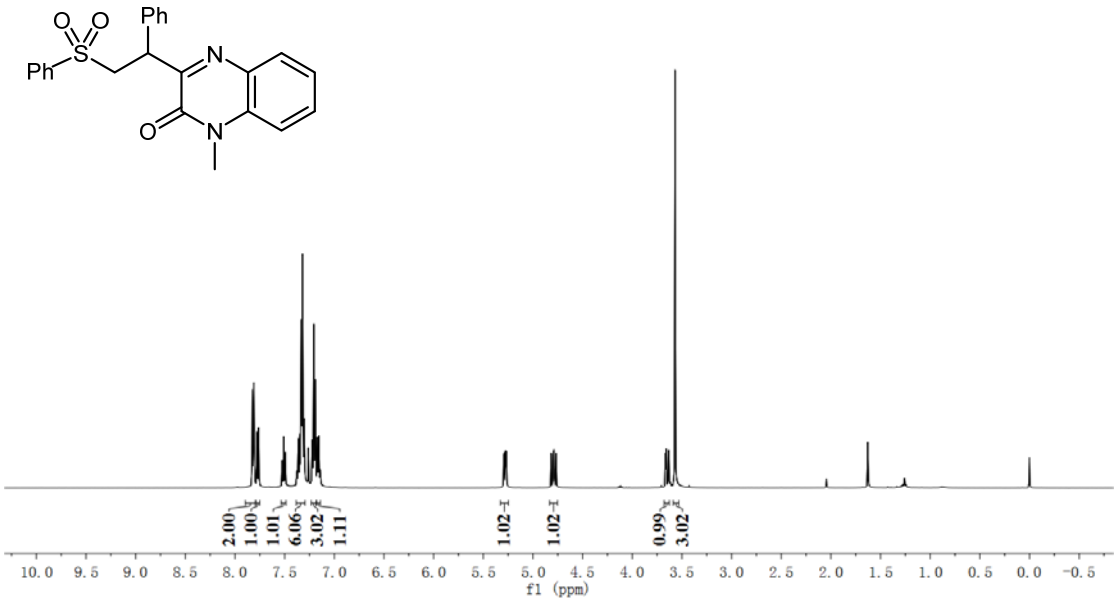


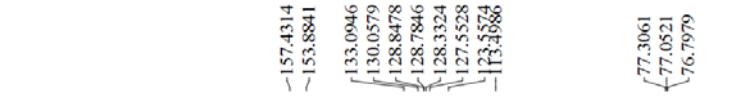
6-fluoro-1-methyl-3-(1-phenyl-2-(phenylsulfonyl)ethyl)quinoxalin-2(1H)-one(5d'), ^{1}H NMR (400Hz, $CDCl_3$): δ 7.84 - 7.82 (m, 2H), 7.49 - 7.46 (m, 1H), 7.41 - 7.31 (m, 5H), 7.27 - 7.15 (m, 5H), 5.29 (dd, J_1 = 3.3 Hz, J_2 = 10.2 Hz, 1H), 4.75 (dd,J_1 =10.2

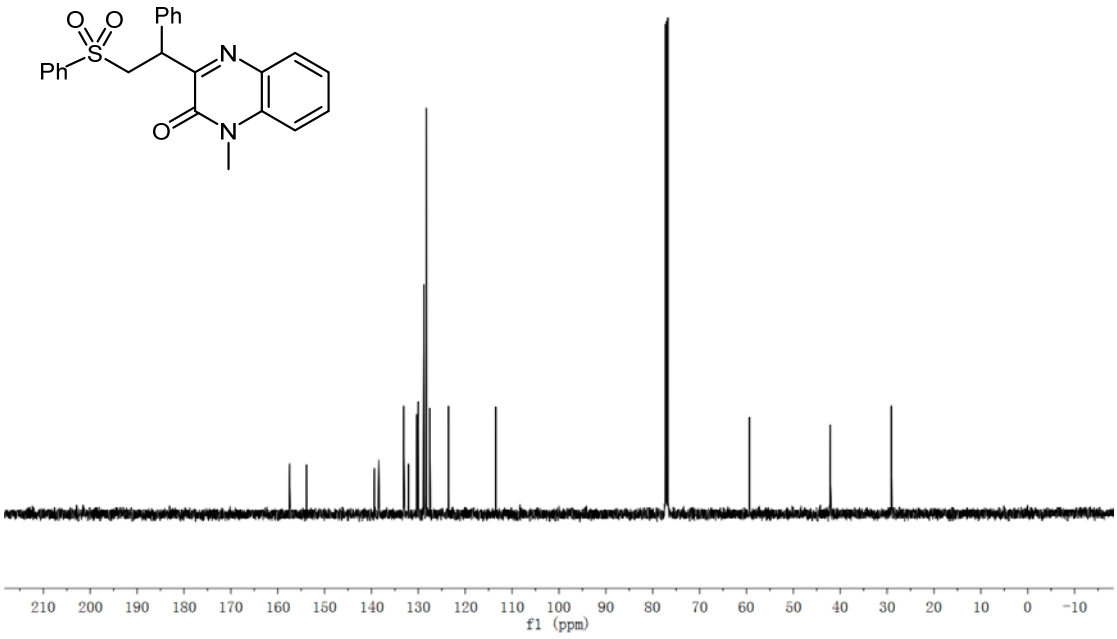
Hz, J_2 = 14.4 Hz, 1H), 3.63 (dd,J_1 = 3.3 Hz, J_2 = 14.4 Hz, 1H), 3.58 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.1, 158.6 (d, J = 242.5 Hz), 153.6, 139.4, 138.1, 133.2, 132.6 (d, J = 11.2 Hz), 129.7 (d, J = 2.0 Hz), 128.9, 128.8, 128.3, 128.3, 127.7, 118.0 (d, J = 23.8 Hz), 115.4 (d, J = 22.3 Hz), 114.6 (d, J = 8.7 Hz), 59.2, 42.1, 29.4; ESI HRMS: calculated for $C_{23}H_{20}FN_2O_3S$ $[M+H]^+$ 423.1179, found 423.1186.

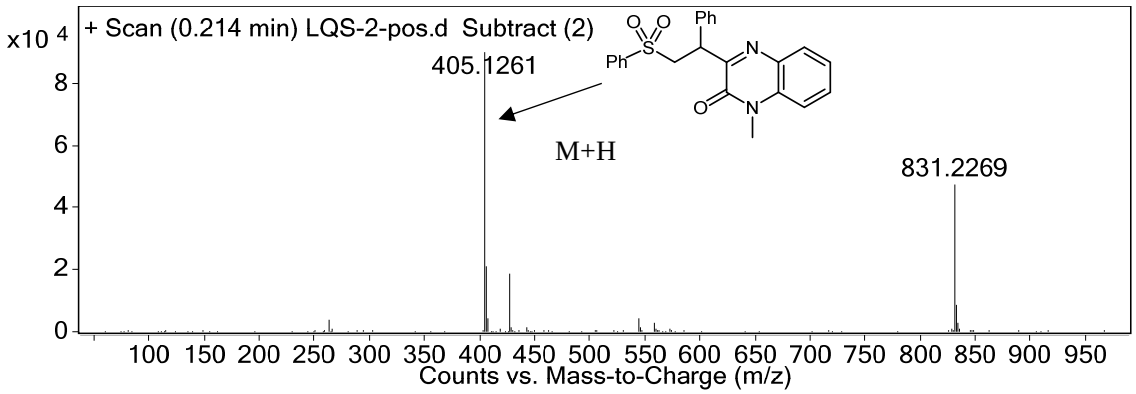
5. Copies of NMR and HRMS spectra

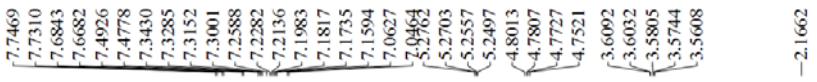









+ Scan (0.214 min) LQS-2-pos.d Subtract (2)
x10 4
405.1261
M+H
831.2269
Counts vs. Mass-to-Charge (m/z)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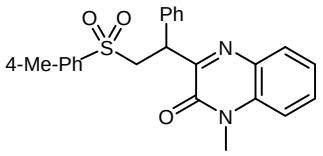
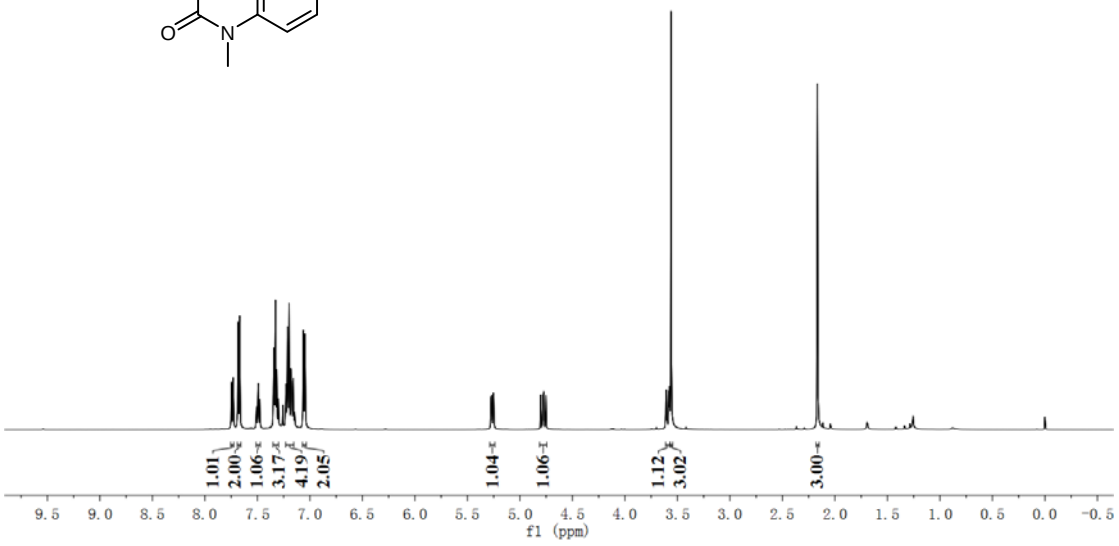
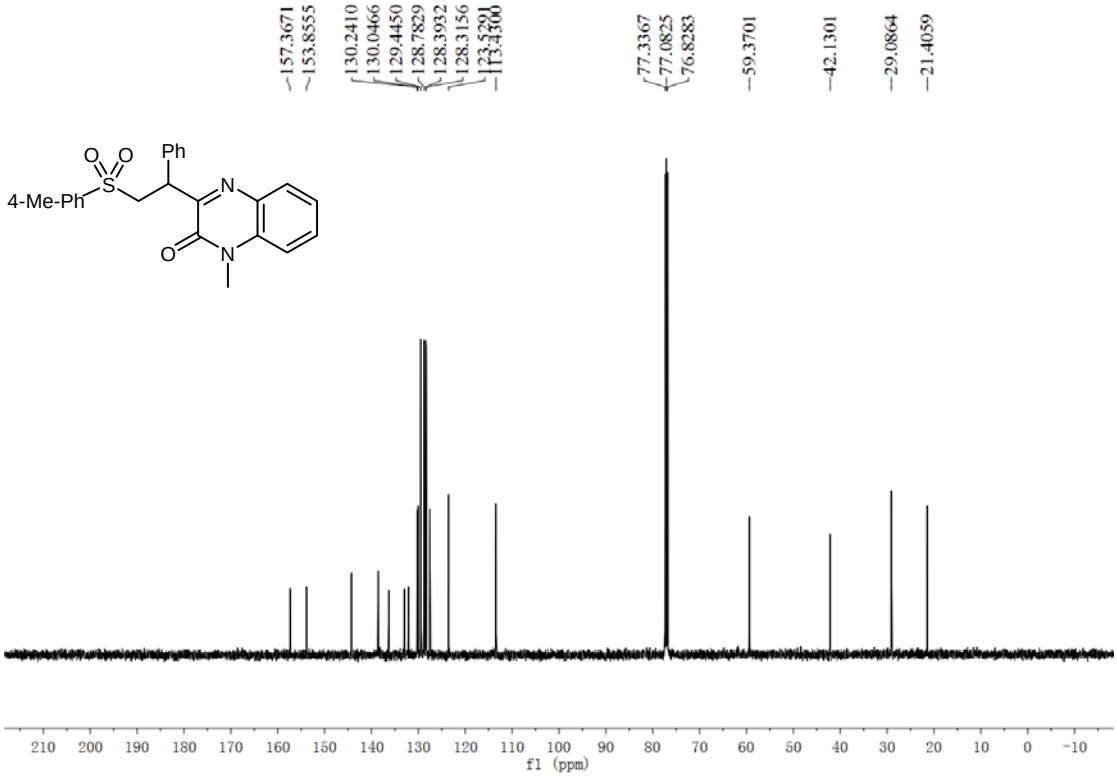
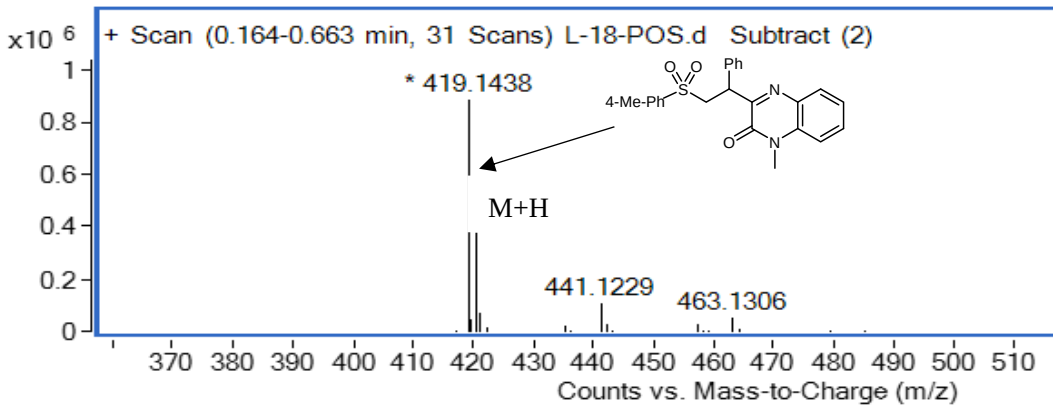
7.7310
7.6843
7.6682
7.4926
7.4778
7.3430
7.3285
7.3152
7.3001
7.2588
7.2282
7.2136
7.1983
7.1817
7.1735
7.1594
7.0627
5.2762
5.2703
5.2557
5.2497
4.8013
4.7807
4.7727
4.7521
3.6092
3.6032
3.5805
3.5744
3.5608
2.1662

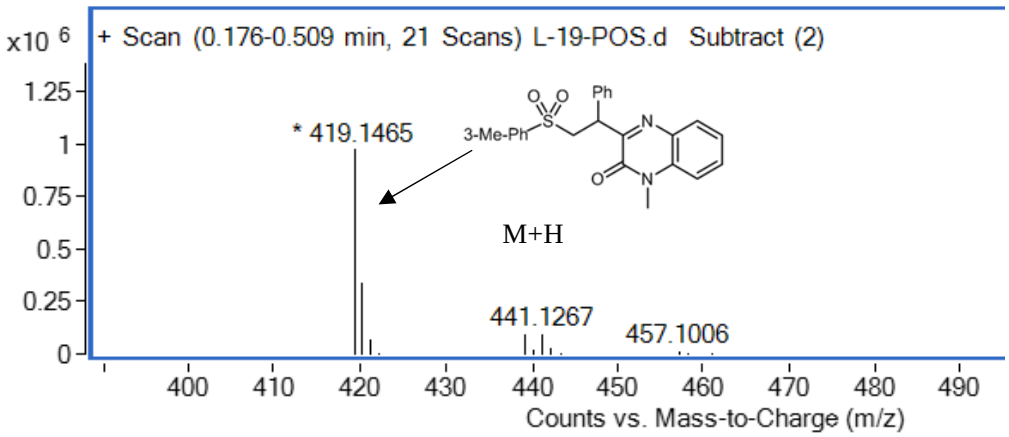

4-Me-Ph
Ph


1.01
2.00
1.06
3.17
4.19
2.05
1.04
1.06
1.12
3.02
3.00
f1 (ppm)

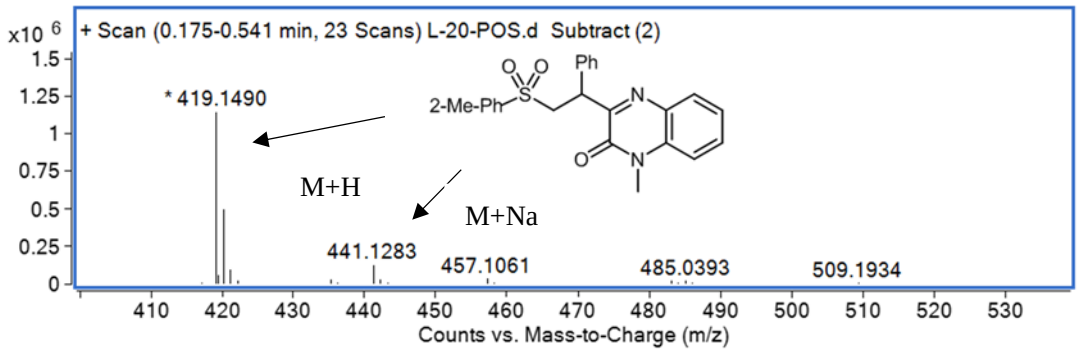

157.3671
153.8555
130.2410
130.0466
129.4450
128.7829
128.3932
128.3156
123.5291
113.4300
77.3367
77.0825
76.8283
59.3701
42.1301
29.0864
21.4059
4-Me-Ph
Ph
f1 (ppm)


x10 6
+ Scan (0.164-0.663 min, 31 Scans) L-18-POS.d Subtract (2)
* 419.1438
M+H
441.1229
463.1306
Counts vs. Mass-to-Charge (m/z)


7.7562
7.7427
7.7402
7.5526
7.5033
7.3496
7.3350
7.3099
7.2583
7.2262
7.2119
7.1965
7.1893
7.1711
7.1610
7.1562
7.1455
5.2789
5.2653
5.2587
4.8084
4.7881
4.7797
4.7595
3.6504
3.6438
3.6217
3.6151
3.5476
2.1760
Ph
3-Me-Ph
O
O
S
N
N
O
1.00
1.00
1.01
1.10
2.08
1.13
2.98
2.11
1.06
0.99
1.04
1.02
3.04
3.00
f1 (ppm)
157.3751
153.7840
130.0103
128.7526
128.7133
128.6449
128.3427
125.5359
77.3150
77.0610
76.8069
59.3737
42.1812
29.0752
21.0379
f1 (ppm)


x10 6
+ Scan (0.176-0.509 min, 21 Scans) L-19-POS.d Subtract (2)
1.25
1
0.75
0.5
0.25
0
* 419.1465
3-Me-Ph
Ph
M+H
441.1267
457.1006
400
410
420
430
440
450
460
470
480
490
Counts vs. Mass-to-Charge (m/z)


7.8903
7.8719
7.7646
7.7488
7.4989
7.3648
7.3500
7.3148
7.2582
7.2344
7.2197
7.2041
7.1760
7.1617
7.1448
7.1301
7.1232
5.2885
5.2734
5.2679
4.9050
4.8844
4.8765
4.8559
3.6176
3.6120
3.5890
3.5835
3.5035
2.6684
Ph
2-Me-Ph
O
S
N
1.00
1.00
1.07
2.10
1.18
2.09
2.10
1.97
1.02
1.03
1.04
1.03
2.99
3.00
f1 (ppm)
157.4403
153.7188
132.2165
130.4689
129.8331
128.7981
128.2694
126.0298
123.5010
113.4368
77.3067
76.7985
58.3288
41.9902
29.0245
20.5377
f1 (ppm)


x10 6
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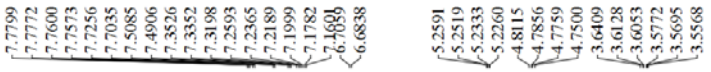
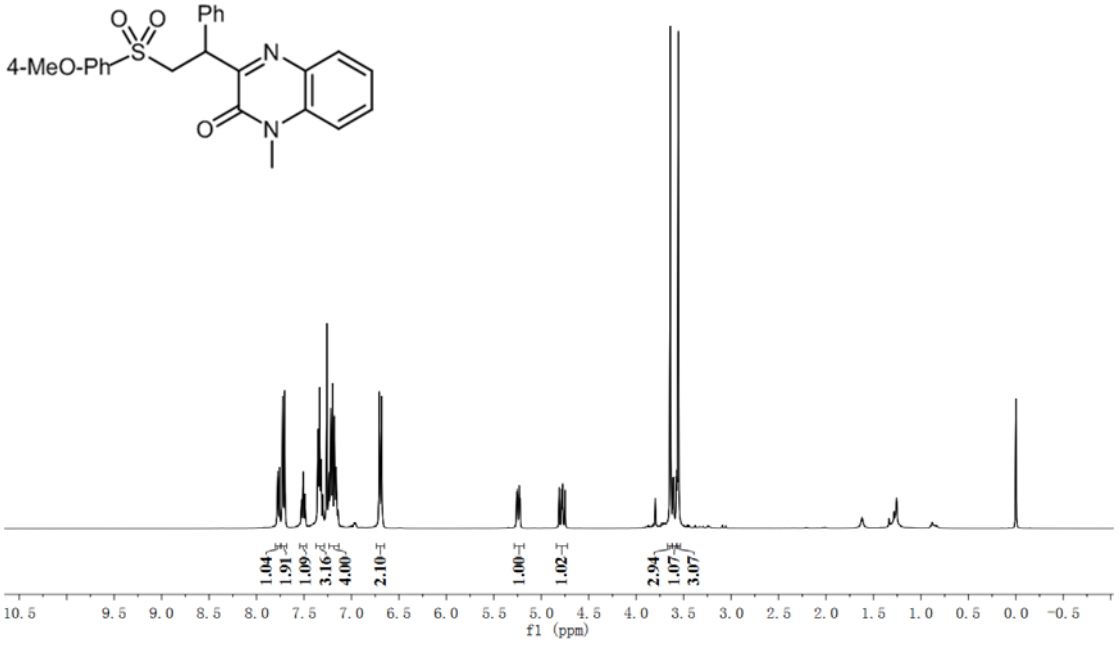
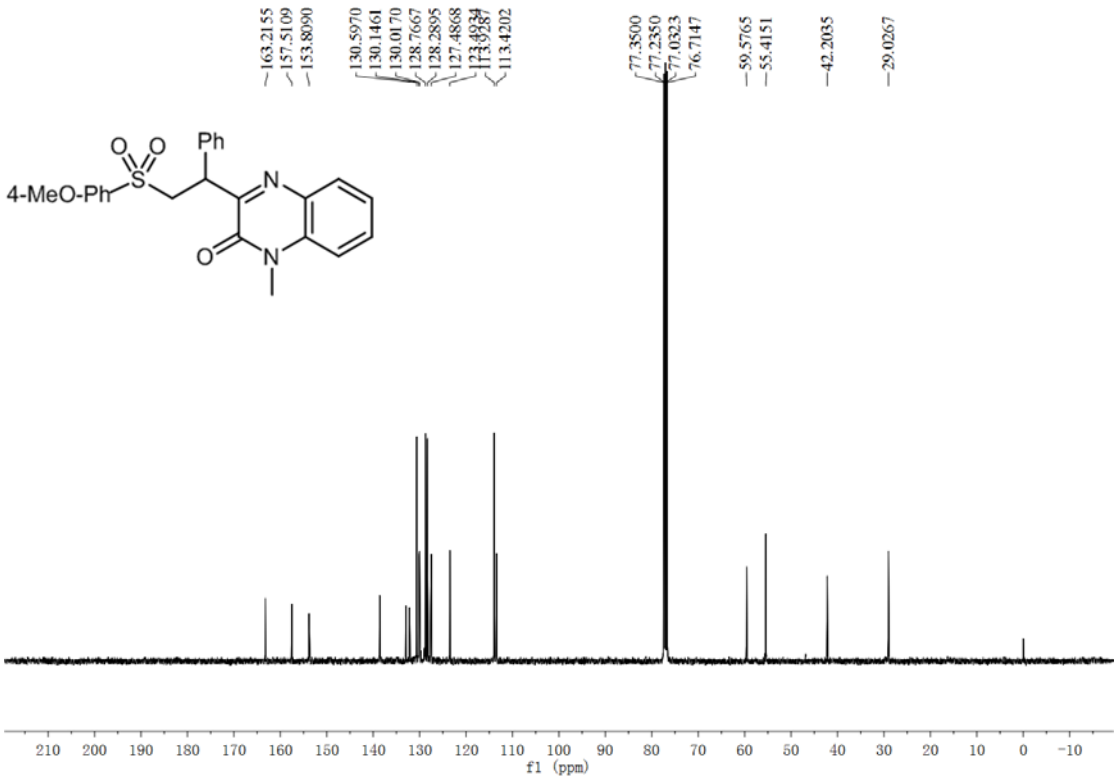
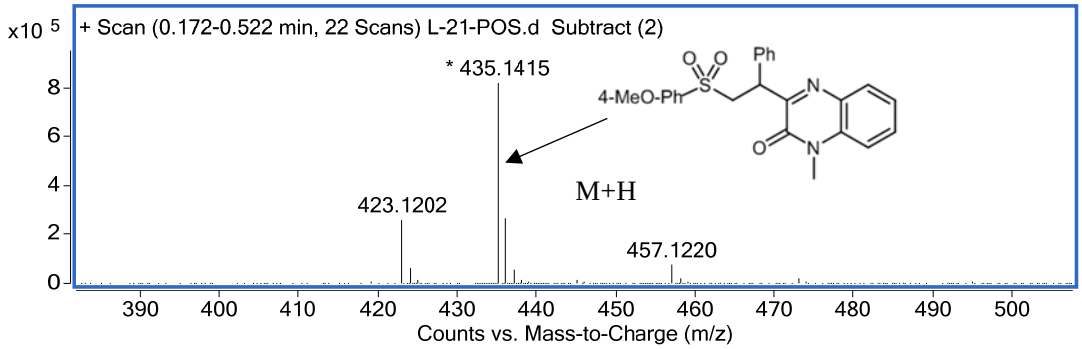
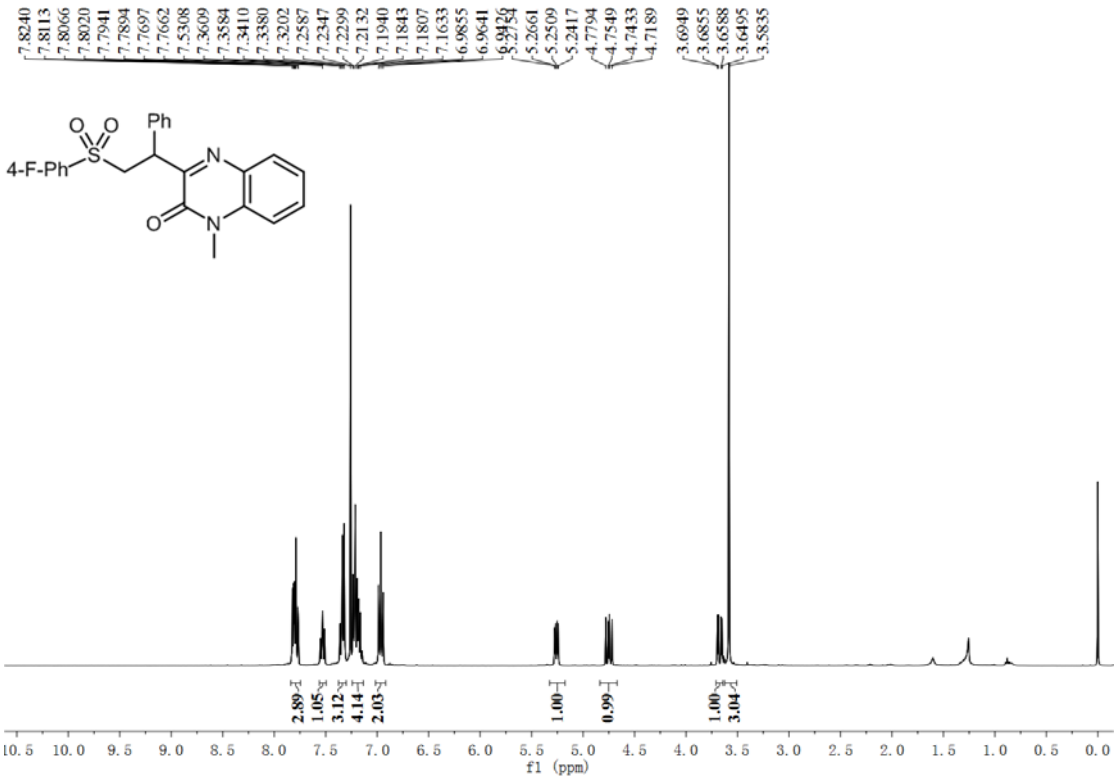
* 419.1490
2-Me-Ph
Ph
M+H
M+Na
441.1283
457.1061
485.0393
509.1934
Counts vs. Mass-to-Charge (m/z)




4-MeO-Ph
Ph
f1 (ppm)


163.2155
157.5109
153.8090
130.5970
130.1461
130.0170
128.7667
128.2895
127.4868
123.4834
113.4202
77.3500
77.2350
77.0323
76.7147
59.5765
55.4151
42.2035
29.0267
4-MeO-Ph
Ph
O
O
S
N
O
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


x10 5
+ Scan (0.172-0.522 min, 22 Scans) L-21-POS.d Subtract (2)
* 435.1415
423.1202
457.1220
M+H
4-MeO-Ph
Ph
8
6
4
2
0
390 400 410 420 430 440 450 460 470 480 490 500
Counts vs. Mass-to-Charge (m/z)


7.8240
7.8113
7.8066
7.8020
7.7941
7.7894
7.7697
7.7662
7.5308
7.3609
7.3584
7.3410
7.3380
7.3202
7.2587
7.2347
7.2299
7.2132
7.1940
7.1843
7.1807
7.1633
6.9855
6.9641
5.2661
5.2509
5.2417
4.7794
4.7549
4.7433
4.7189
3.6949
3.6855
3.6588
3.6495
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Ph
4-F-Ph
O
O
S
N
O
N
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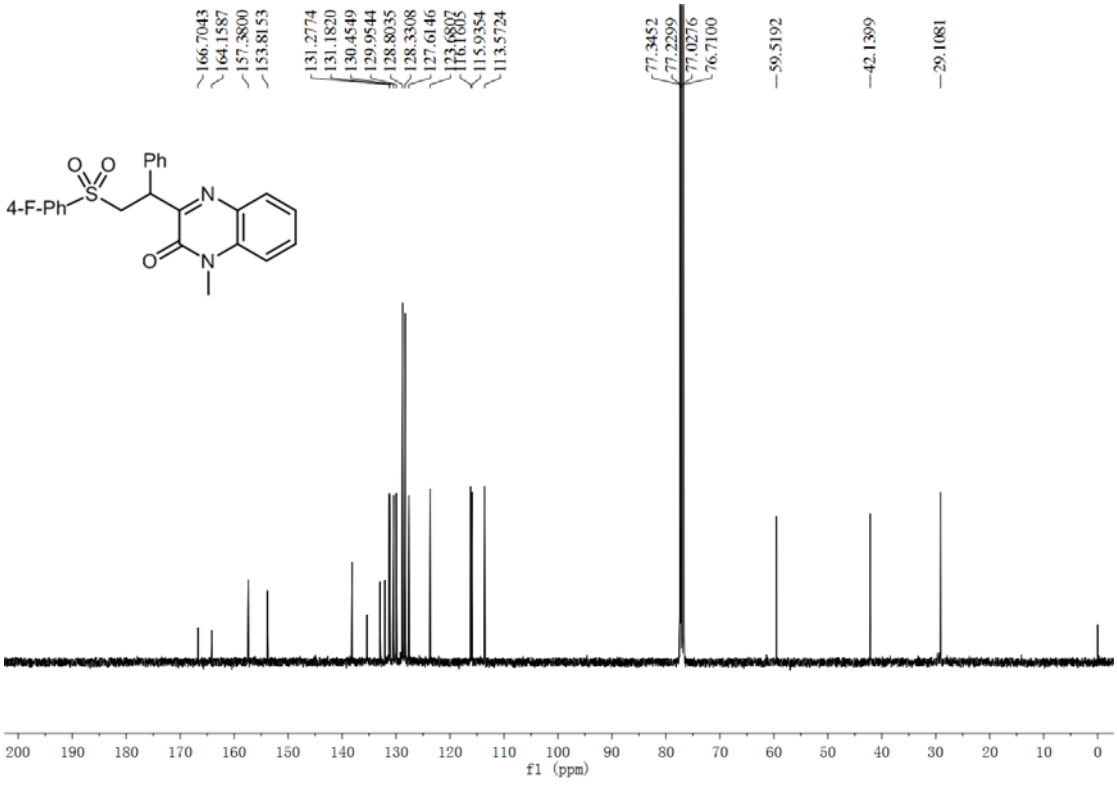
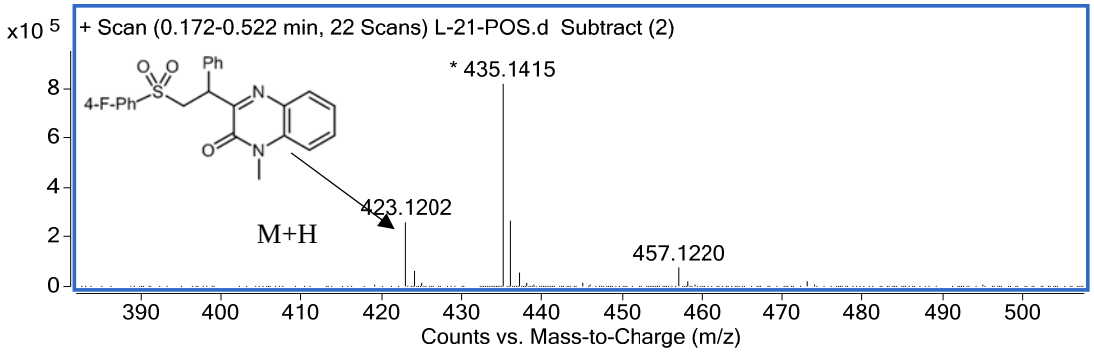
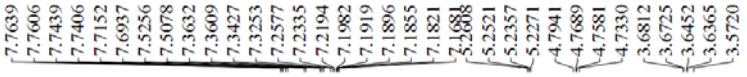
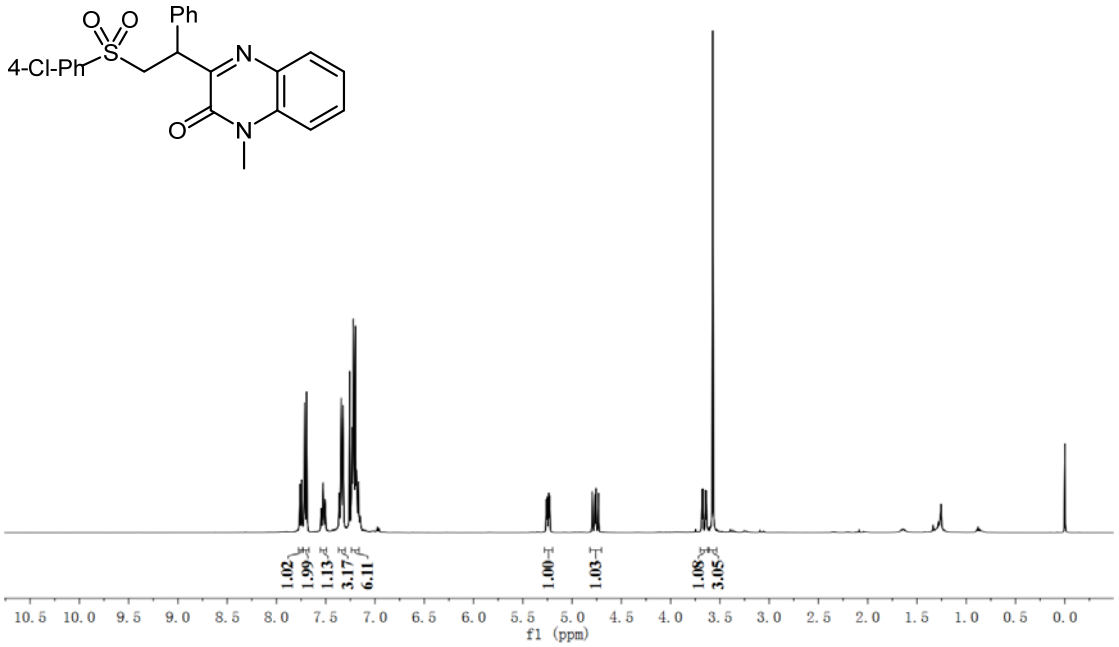
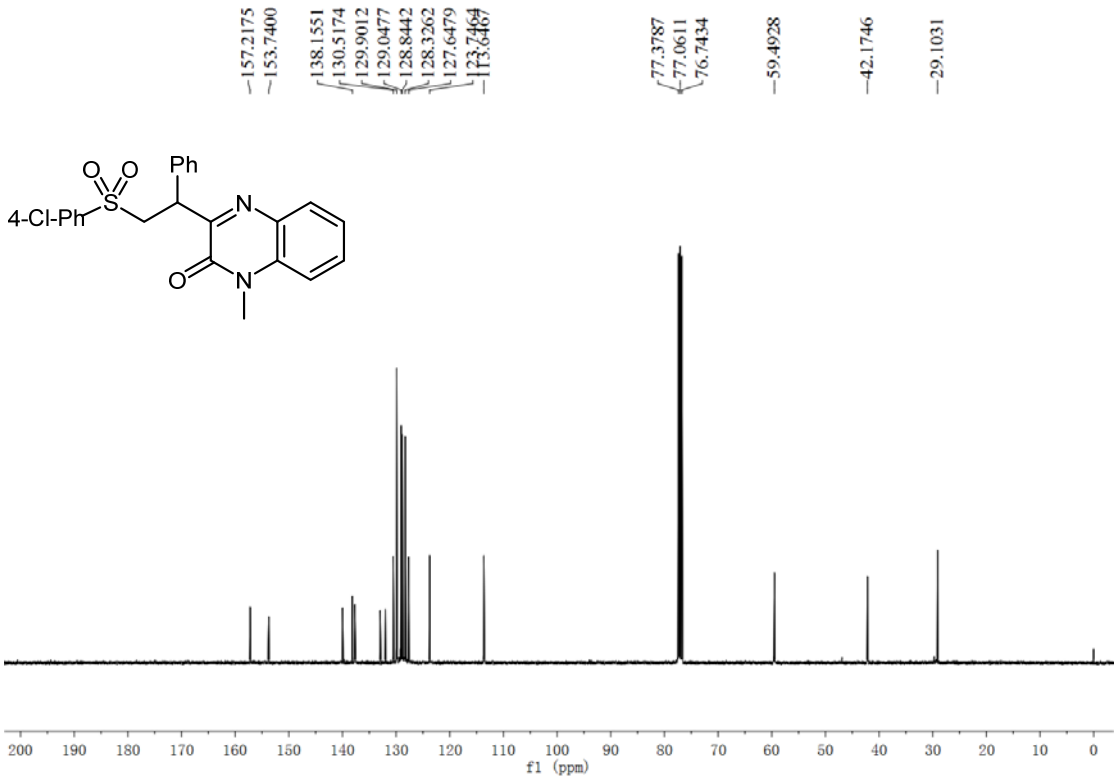
1.05
3.12
4.14
2.03
1.00
0.99
1.00
3.04
f1 (ppm)


166.7043
164.1587
157.3800
153.8153
131.2774
131.1820
130.4549
129.9544
128.8035
128.3308
127.6146
115.9354
113.5724
77.3452
77.2299
77.0276
76.7100
59.5192
42.1399
29.1081
Ph
4-F-Ph
O
O
S
N
O
N
f1 (ppm)


x10 5
+ Scan (0.172-0.522 min, 22 Scans) L-21-POS.d Subtract (2)
4-F-Ph
Ph
* 435.1415
423.1202
M+H
457.1220
Counts vs. Mass-to-Charge (m/z)




4-Cl-Ph
Ph
f1 (ppm)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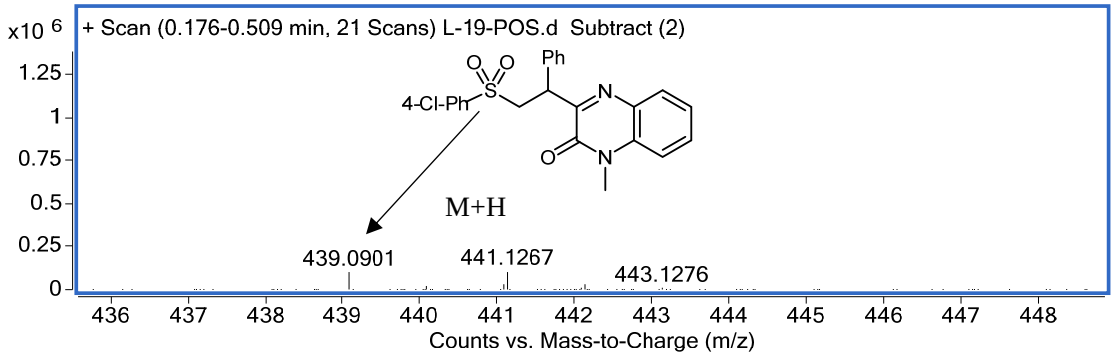
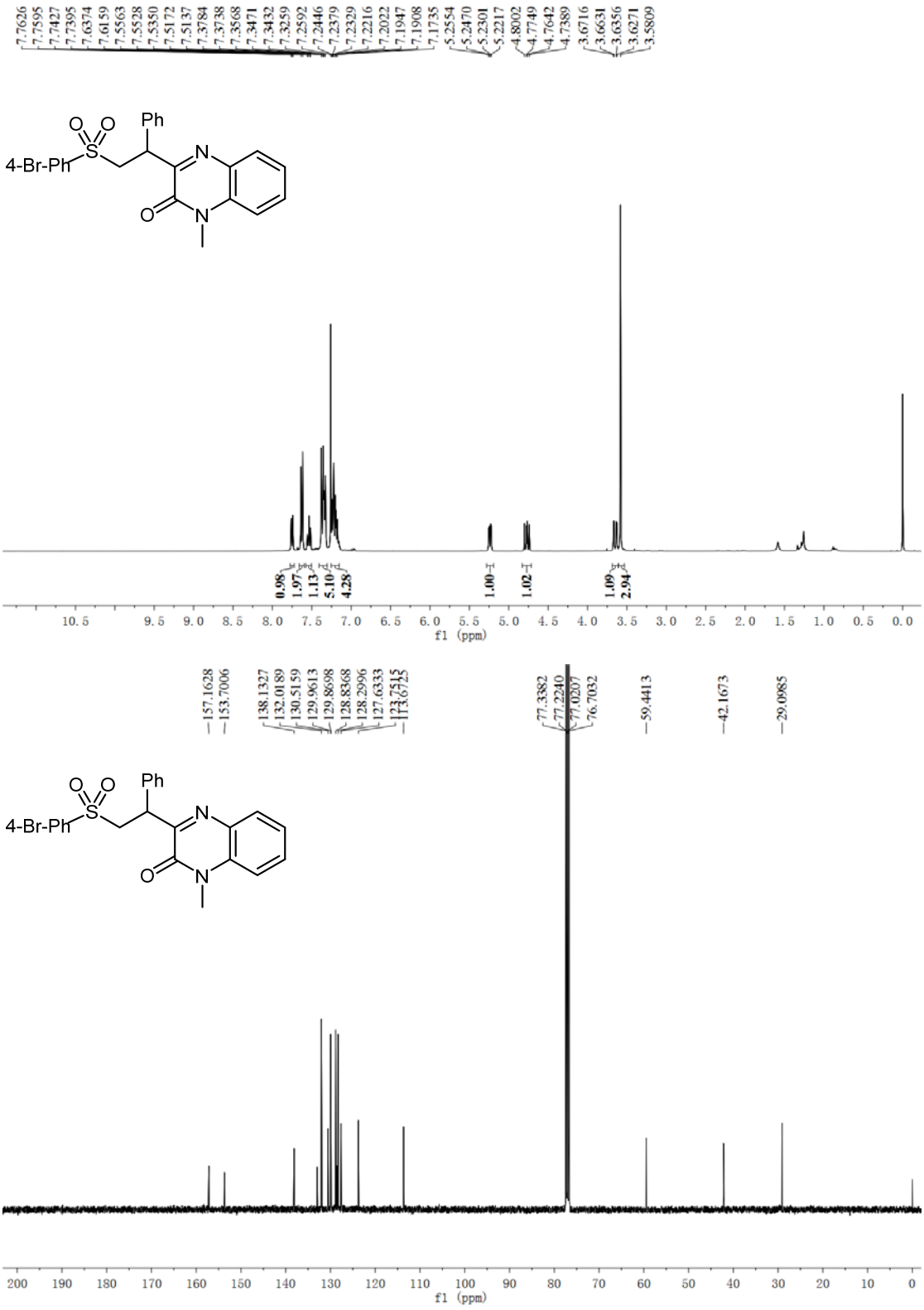
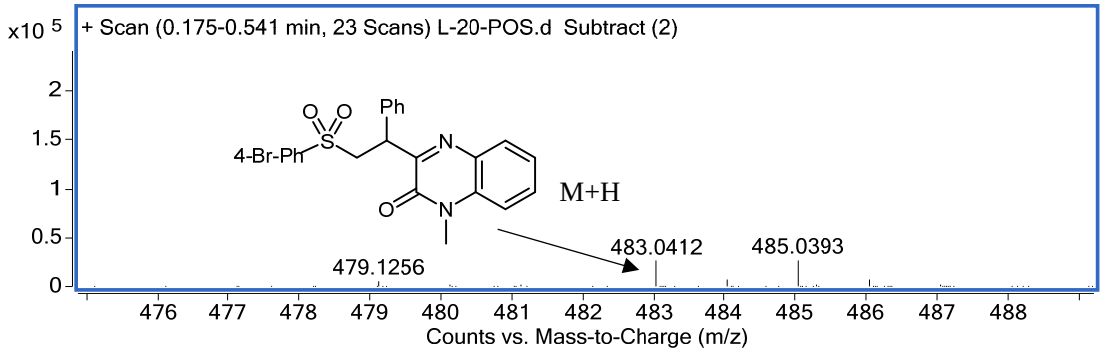
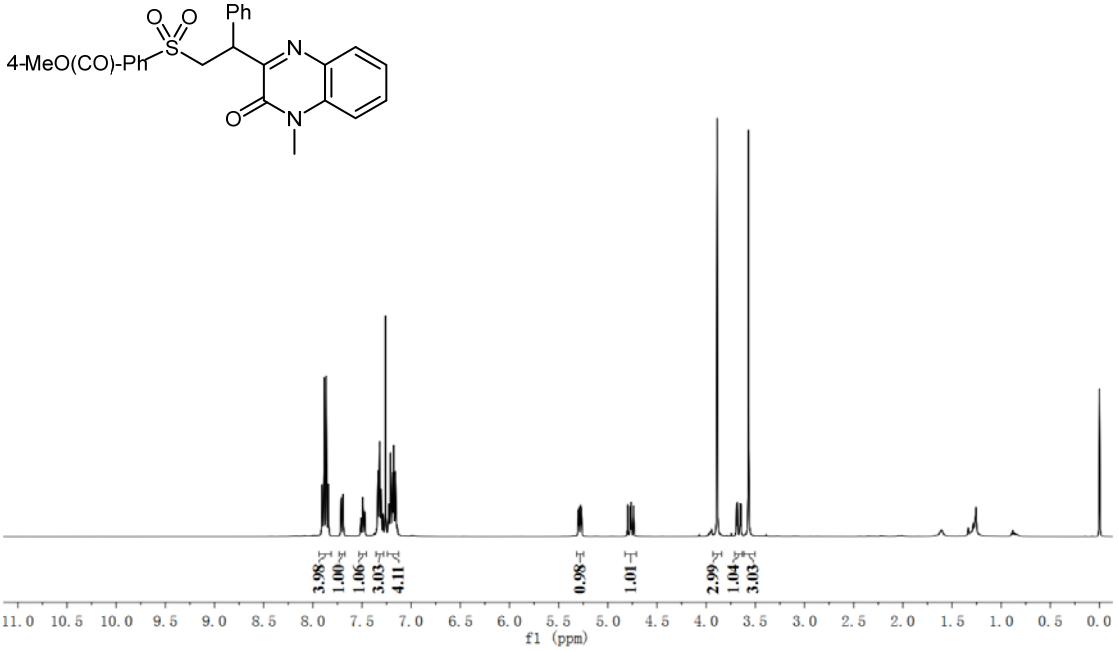
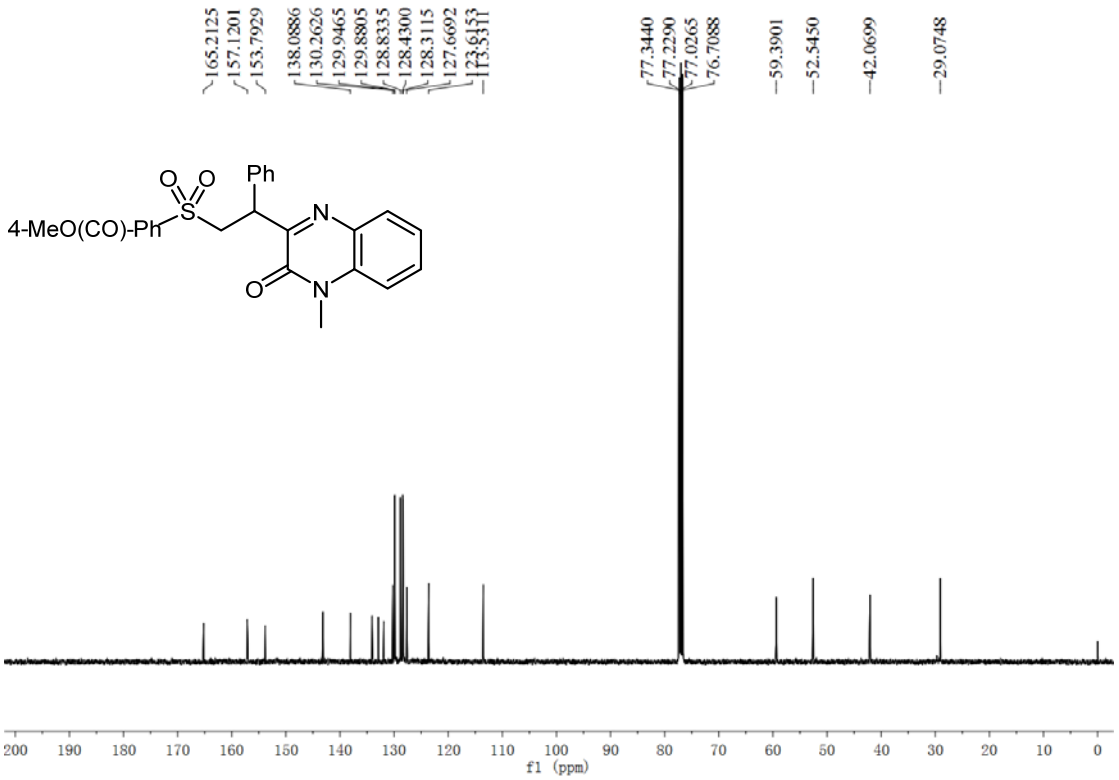
153.7400
138.1551
130.5174
129.9012
129.0477
128.8442
128.3262
127.6479
123.7464
123.6467
77.3787
77.0611
76.7434
59.4928
42.1746
29.1031
4-Cl-Ph
Ph
O
O
S
N
O
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

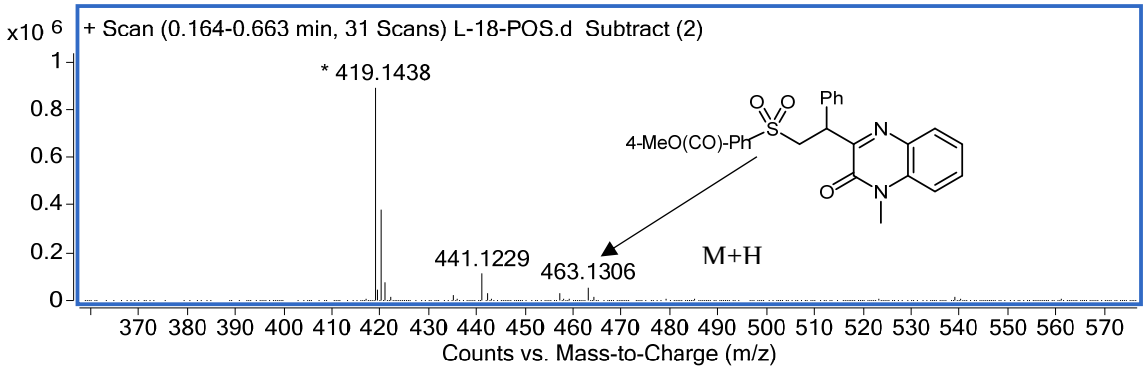

x10 6
+ Scan (0.176-0.509 min, 21 Scans) L-19-POS.d Subtract (2)
1.25
1
0.75
0.5
0.25
0
4-Cl-Ph
Ph
M+H
439.0901
441.1267
443.1276
436 437 438 439 440 441 442 443 444 445 446 447 448
Counts vs. Mass-to-Charge (m/z)

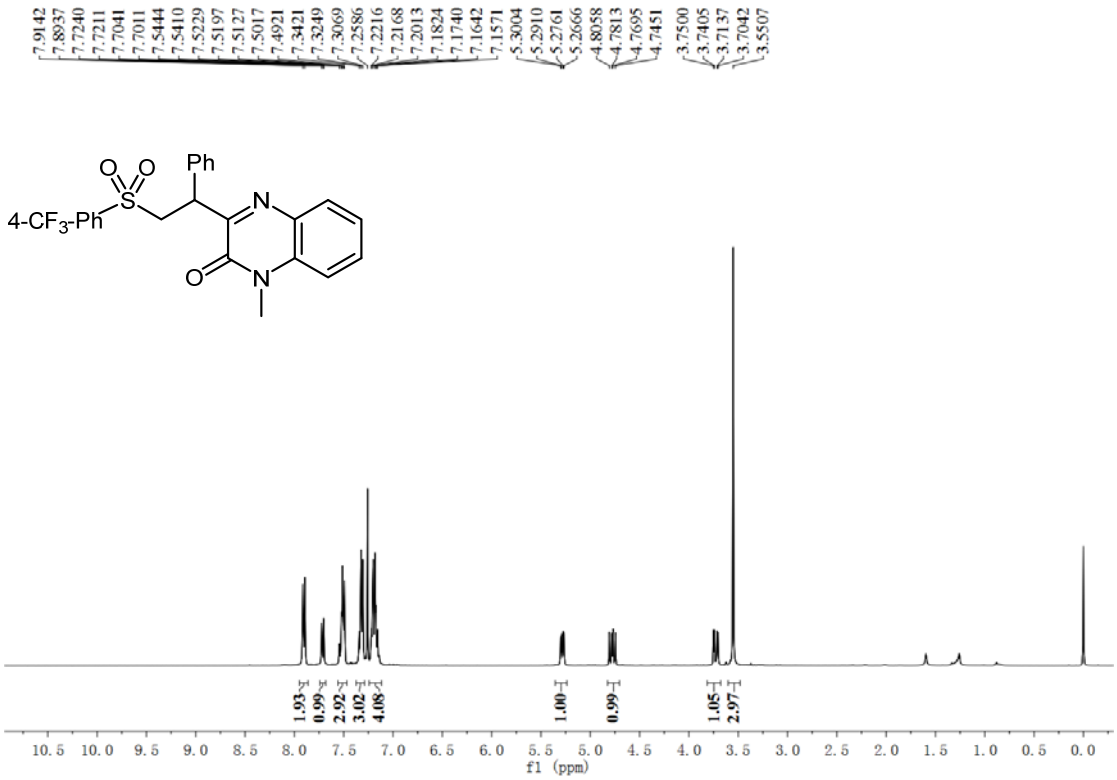

7.7626
7.7595
7.7427
7.7395
7.6374
7.6159
7.5563
7.5528
7.5350
7.5172
7.5137
7.3784
7.3738
7.3568
7.3471
7.3432
7.3259
7.2592
7.2446
7.2379
7.2329
7.2216
7.2022
7.1947
7.1908
7.1735
5.2554
5.2470
5.2301
5.2217
4.8002
4.7749
4.7642
4.7389
3.6716
3.6631
3.6356
3.6271
3.5809
Ph
4-Br-Ph
O
O
S
N
O
N
0.98
1.97
1.13
5.10
4.28
1.00
1.02
1.09
2.94
f1 (ppm)
157.1628
153.7006
138.1327
132.0189
130.5159
129.9613
129.8698
128.8368
128.2996
127.6333
123.7515
123.6725
77.3382
77.2240
77.0207
76.7032
59.4413
42.1673
29.0985
f1 (ppm)

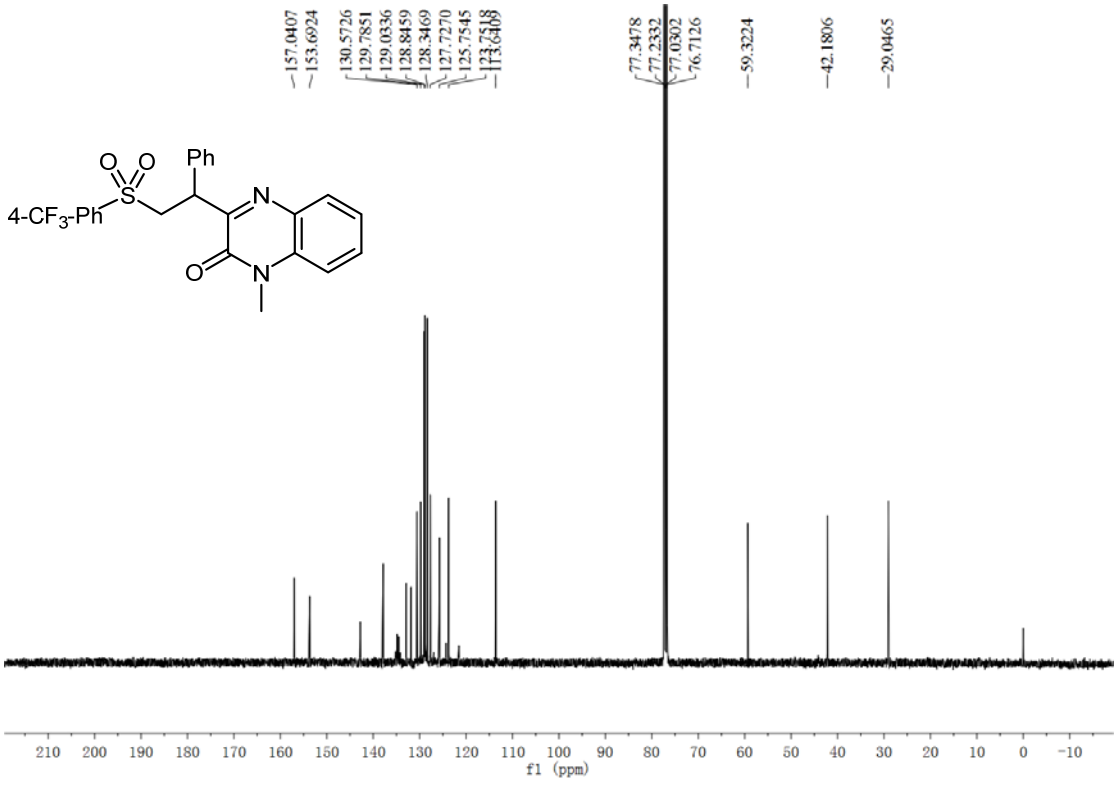

x10 5
+ Scan (0.175-0.541 min, 23 Scans) L-20-POS.d Subtract (2)
4-Br-Ph
Ph
M+H
479.1256
483.0412
485.0393
Counts vs. Mass-to-Charge (m/z)

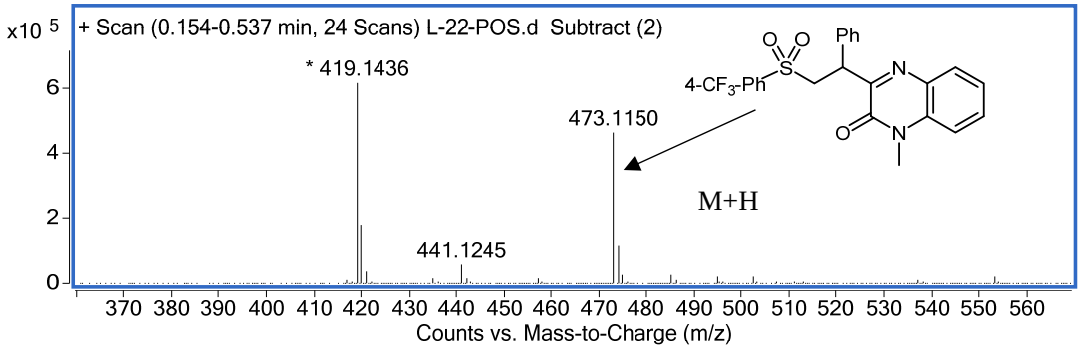

4-MeO(CO)-Ph
Ph
f1 (ppm)

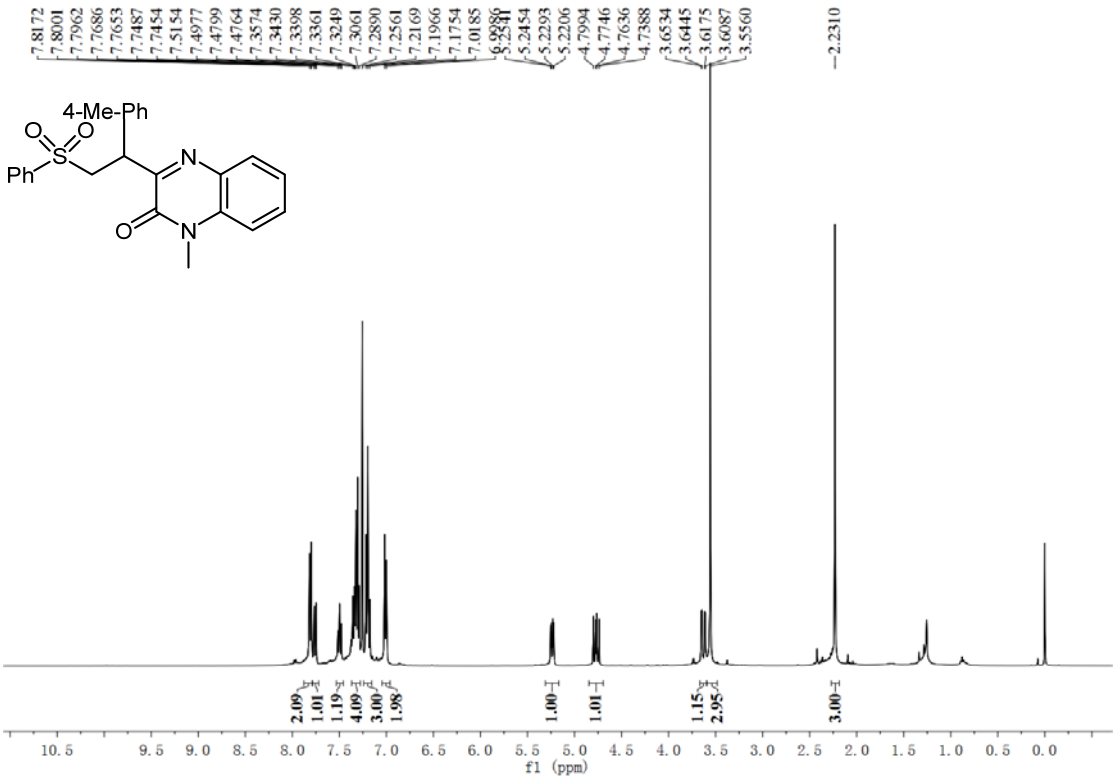

165.2125
157.1201
153.7929
138.0886
130.2626
129.9465
129.8805
128.8335
128.4300
128.3115
127.6692
123.6153
123.3311
77.3440
77.2290
77.0265
76.7088
59.3901
52.5450
42.0699
29.0748
4-MeO(CO)-Ph
Ph
O
O
S
N
O
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

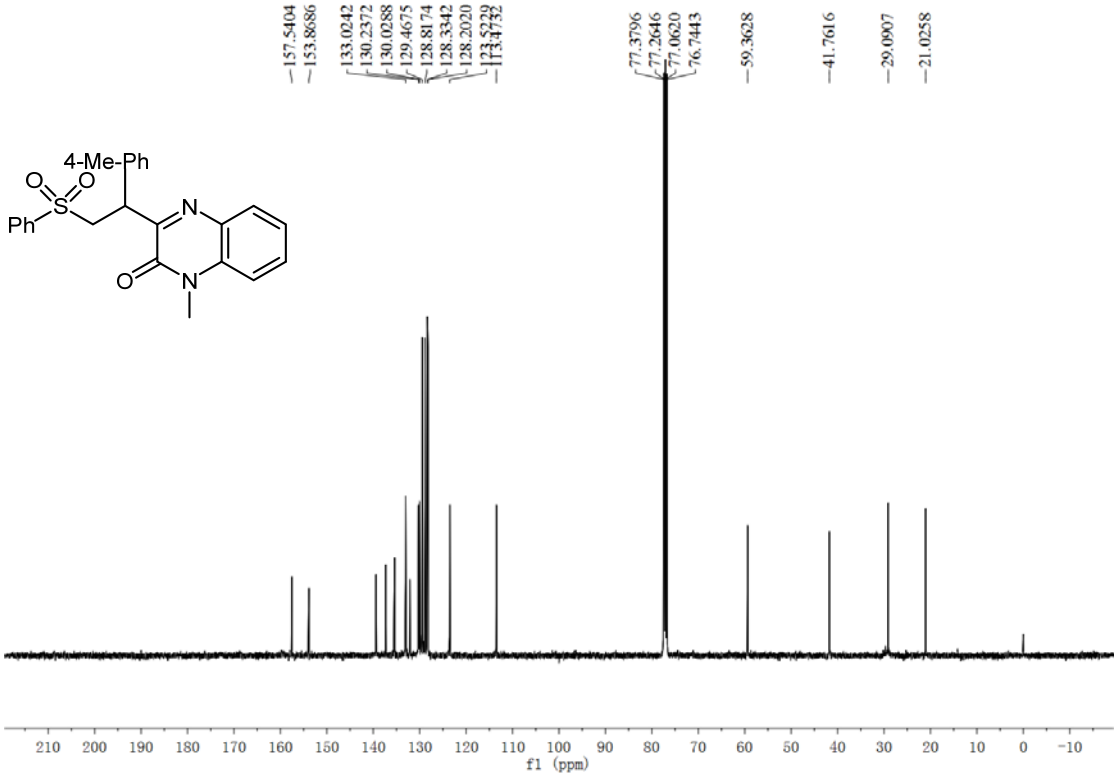

x10 6
+ Scan (0.164-0.663 min, 31 Scans) L-18-POS.d Subtract (2)
1
0.8
0.6
0.4
0.2
0
* 419.1438
441.1229
463.1306
M+H
4-MeO(CO)-Ph
Ph
O
O
S
N
O
N
370 380 390 400 410 420 430 440 450 460 470 480 490 500 510 520 530 540 550 560 570
Counts vs. Mass-to-Charge (m/z)

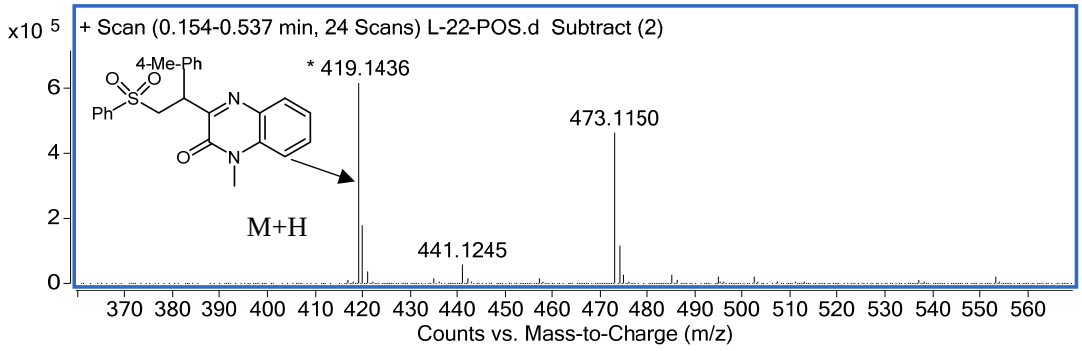

7.9142
7.8937
7.7240
7.7211
7.7041
7.7011
7.5444
7.5410
7.5229
7.5197
7.5127
7.5017
7.4921
7.3421
7.3249
7.3069
7.2586
7.2216
7.2168
7.2013
7.1824
7.1740
7.1642
7.1571
5.3004
5.2910
5.2761
5.2666
4.8058
4.7813
4.7695
4.7451
3.7500
3.7405
3.7137
3.7042
3.5507
Ph
O
O
S
4-CF3-Ph
N
O
N
1.93
0.99
2.92
3.02
4.08
1.00
0.99
1.05
2.97
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)

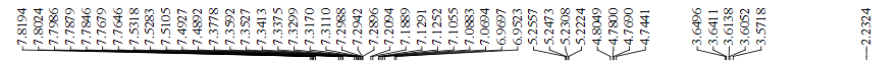

157.0407
153.6924
130.5726
129.7851
129.0336
128.8459
128.3469
127.7270
125.7545
123.7518
113.6409
77.3478
77.2332
77.0302
76.7126
59.3224
42.1806
29.0465
Ph
O
O
S
4-CF3-Ph
N
O
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

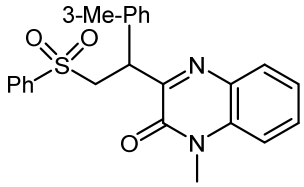

x10 5
+ Scan (0.154-0.537 min, 24 Scans) L-22-POS.d Subtract (2)
* 419.1436
473.1150
441.1245
4-CF3-Ph
Ph
M+H
Counts vs. Mass-to-Charge (m/z)

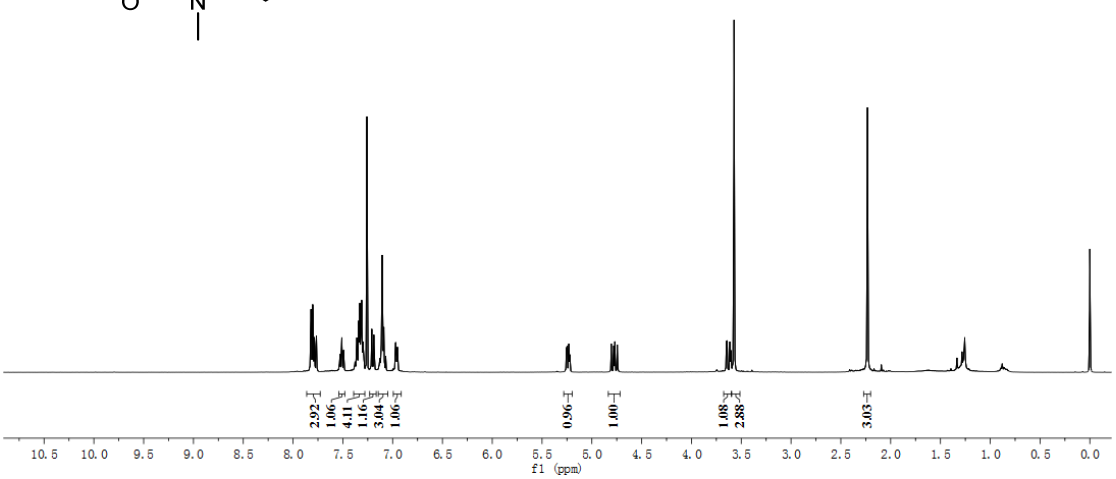

4-Me-Ph
Ph
f1 (ppm)


157.5404
153.8686
133.0242
130.2372
130.0288
129.4675
128.8174
128.3342
128.2020
123.5229
113.4732
77.3796
77.2646
77.0620
76.7443
59.3628
41.7616
29.0907
21.0258
4-Me-Ph
O
O
S
Ph
N
O
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

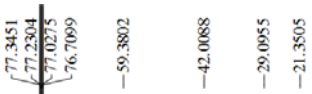

x10 5
+ Scan (0.154-0.537 min, 24 Scans) L-22-POS.d Subtract (2)
4-Me-Ph
O
O
S
Ph
N
O
N
* 419.1436
473.1150
M+H
441.1245
6
4
2
0
370 380 390 400 410 420 430 440 450 460 470 480 490 500 510 520 530 540 550 560
Counts vs. Mass-to-Charge (m/z)

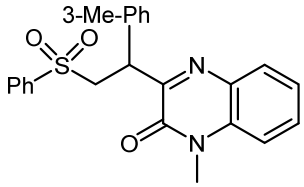

7.8194
7.8024
7.7986
7.7879
7.7846
7.7679
7.7646
7.5318
7.5283
7.5105
7.4927
7.4892
7.3778
7.3592
7.3527
7.3413
7.3375
7.3299
7.3170
7.3110
7.2988
7.2942
7.2896
7.2094
7.1889
7.1291
7.1252
7.1055
7.0883
7.0694
6.9697
6.9523
5.2557
5.2473
5.2308
5.2224
4.8049
4.7800
4.7690
4.7441
3.6496
3.6411
3.6138
3.6052
3.5718
2.2324


3-Me-Ph
O
O
S
Ph
N
O
N

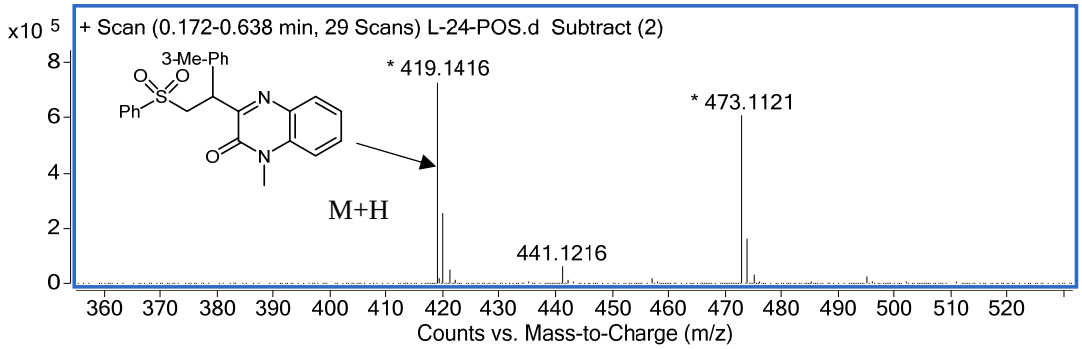

2.92
1.06
4.11
1.16
3.04
1.06
0.96
1.00
1.08
2.88
3.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

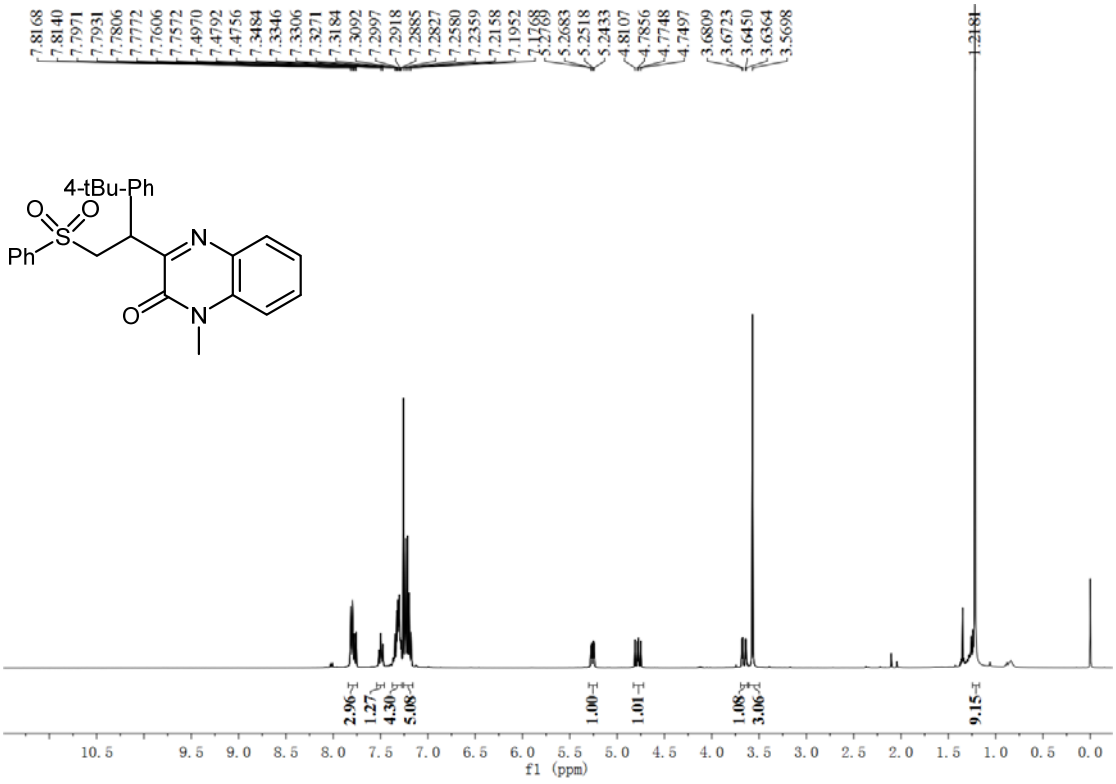

157.4607
153.8824
133.0263
130.0595
129.0014
128.7785
128.6364
128.3184
125.2891
123.5038
113.4618

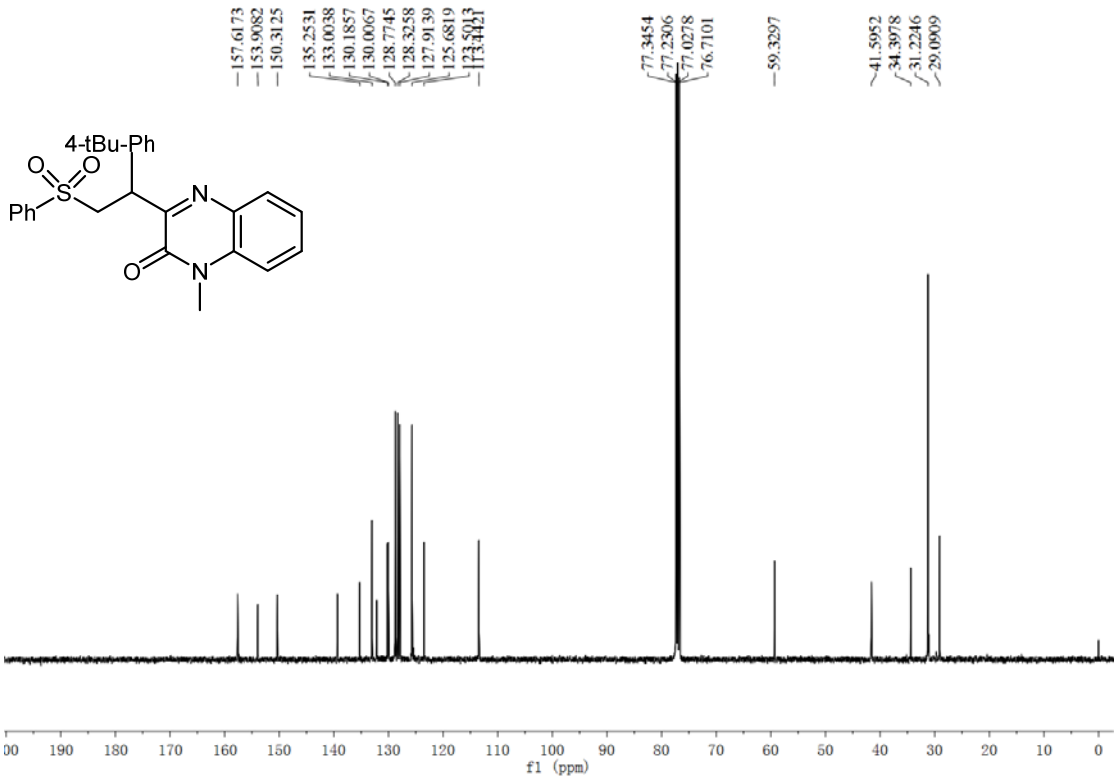

77.3451
77.2304
77.0275
76.7099
59.3802
42.0088
29.0955
21.3505

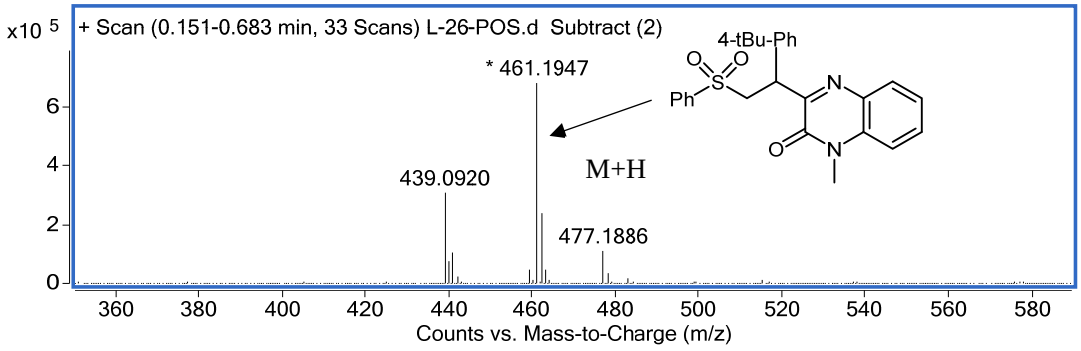

3-Me-Ph
O
O
S
Ph
N
O
N

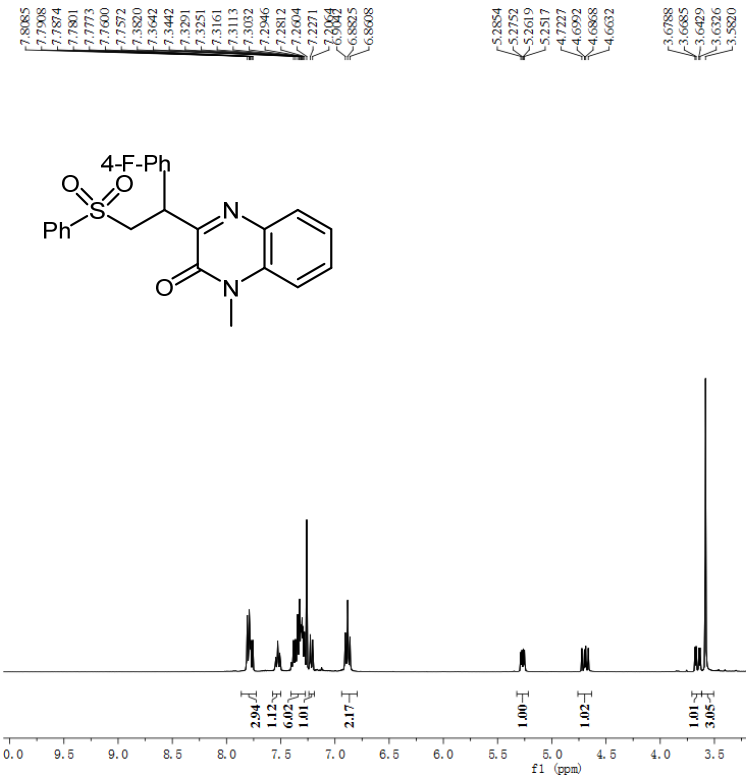
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

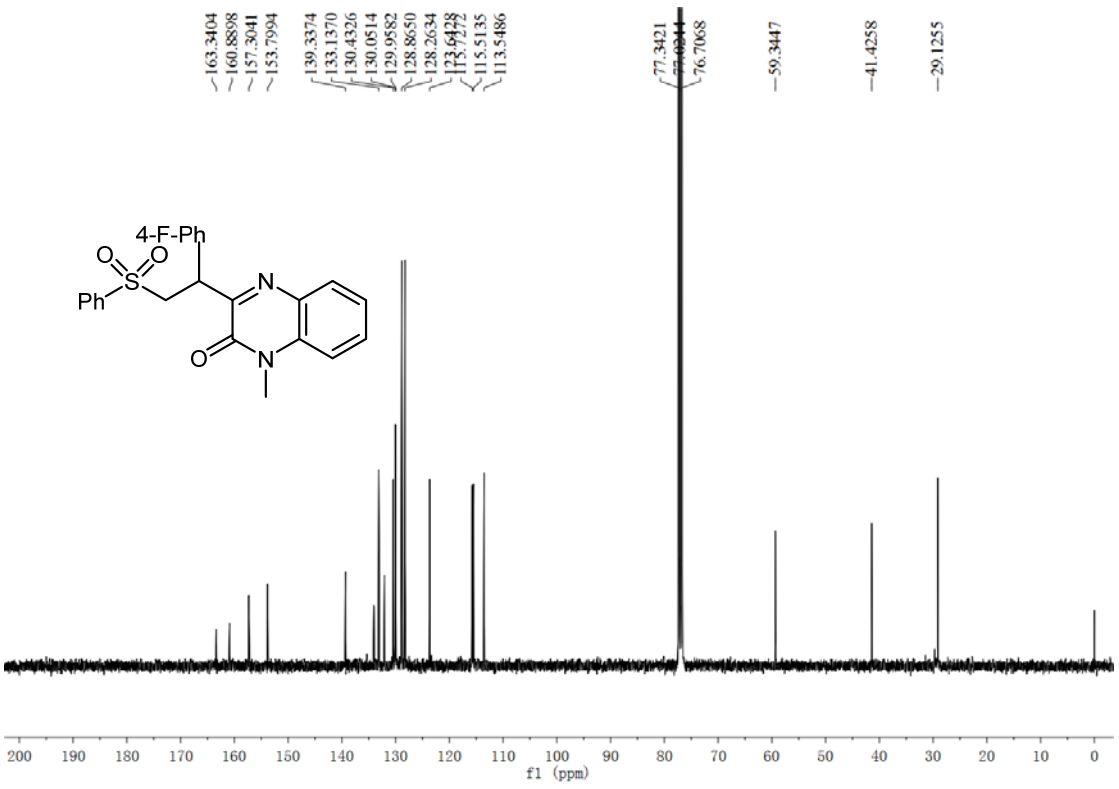

x10 5
+ Scan (0.172-0.638 min, 29 Scans) L-24-POS.d Subtract (2)
3-Me-Ph
Ph
* 419.1416
* 473.1121
M+H
441.1216
Counts vs. Mass-to-Charge (m/z)

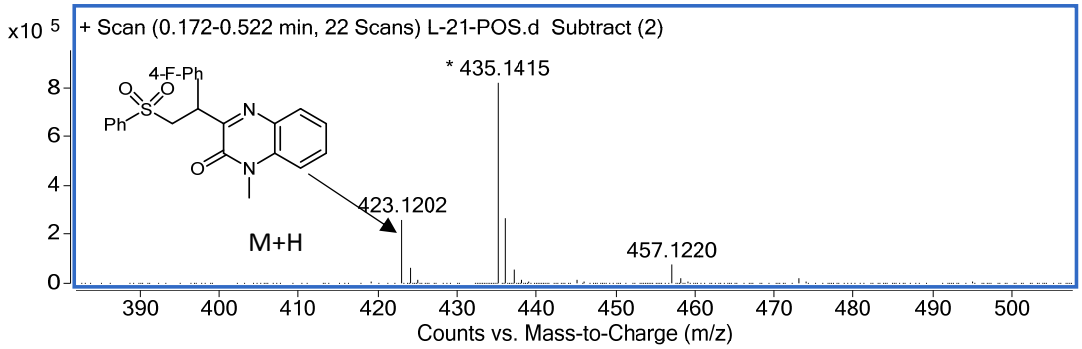

4-tBu-Ph
Ph
f1 (ppm)

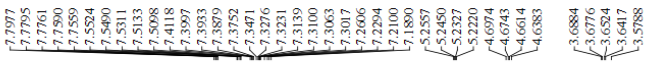

157.6173
153.9082
150.3125
135.2531
133.0038
130.1857
130.0067
128.7745
128.3258
127.9139
125.6819
77.3454
77.2306
77.0278
76.7101
59.3297
41.5952
34.3978
31.2246
29.0909
4-tBu-Ph
Ph
O
S
N
f1 (ppm)

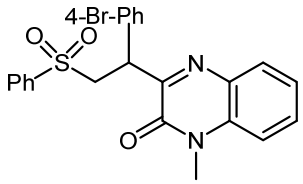

x10 5
+ Scan (0.151-0.683 min, 33 Scans) L-26-POS.d Subtract (2)
* 461.1947
439.0920
477.1886
M+H
4-tBu-Ph
Ph
Counts vs. Mass-to-Charge (m/z)

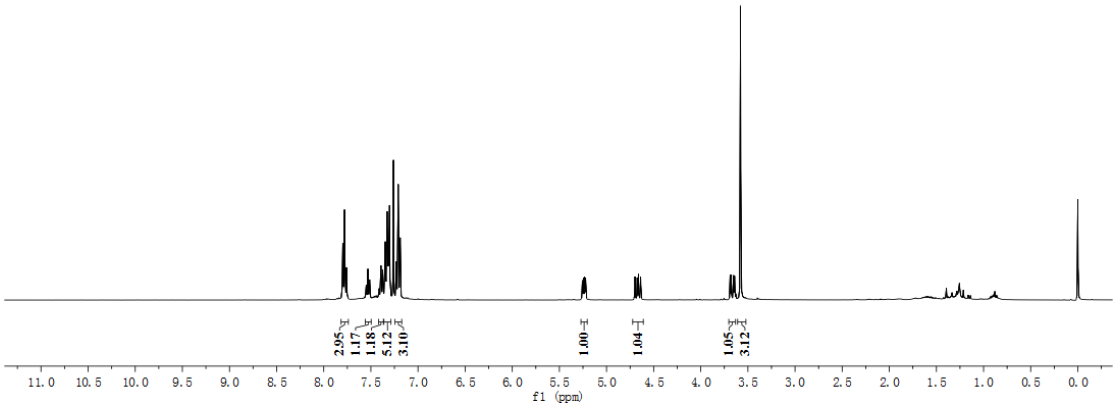

7.8085
7.7908
7.7874
7.7801
7.7773
7.7600
7.7572
7.3820
7.3642
7.3442
7.3291
7.3251
7.3161
7.3113
7.3032
7.2946
7.2812
7.2604
7.2271
6.8825
6.8608
5.2854
5.2752
5.2619
5.2517
4.7227
4.6992
4.6858
4.6632
3.6788
3.6685
3.6429
3.6326
3.5820
4-F-Ph
Ph
O
S
N
O
N
2.94
1.12
6.02
1.01
2.17
1.00
1.02
1.01
3.05
f1 (ppm)

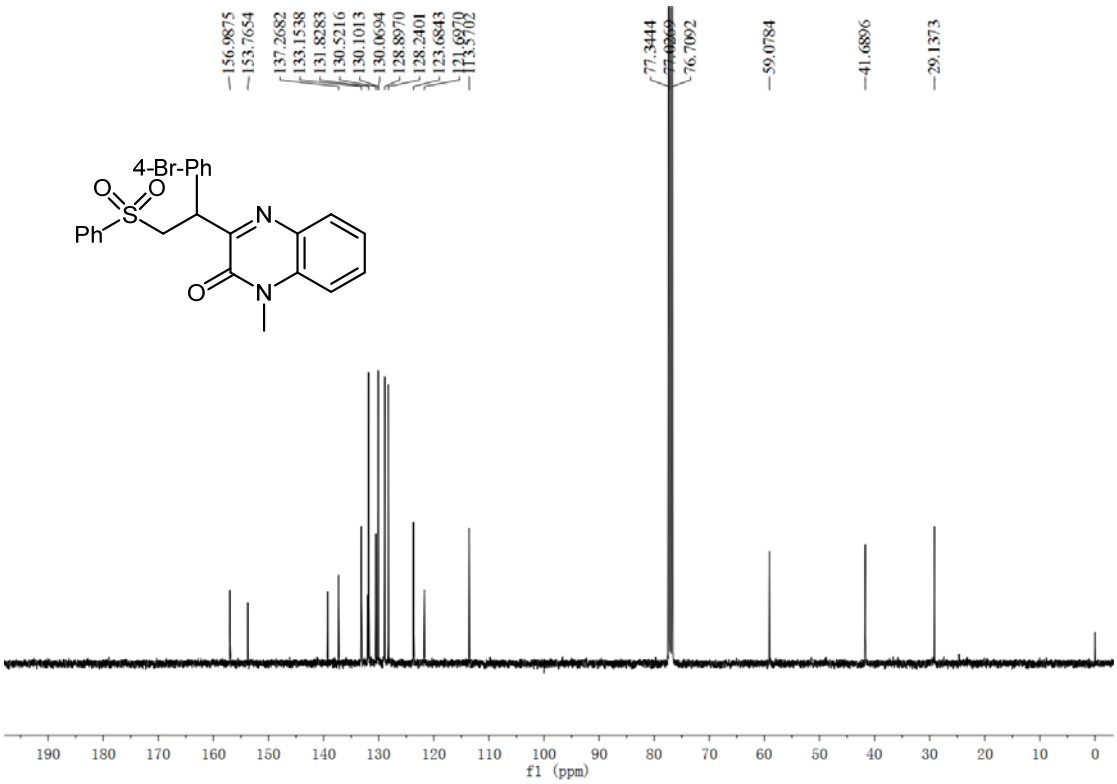

163.3404
160.8898
157.3041
153.7994
139.3374
133.1370
130.4326
130.0514
129.9582
128.8650
128.2634
115.5135
113.5486
77.3421
76.7068
59.3447
41.4258
29.1255
4-F-Ph
Ph
O
S
N
O
N
f1 (ppm)

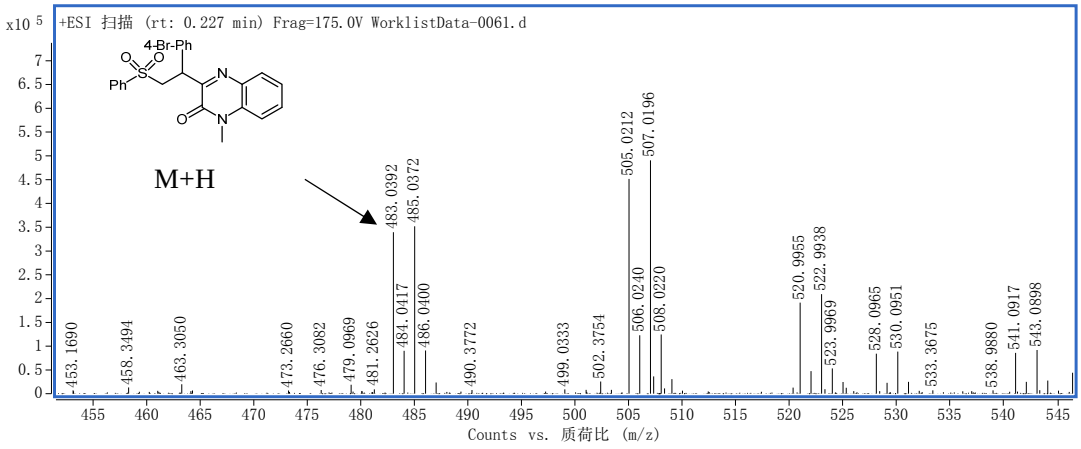

x10 5
+ Scan (0.172-0.522 min, 22 Scans) L-21-POS.d Subtract (2)
4-F-Ph
Ph
* 435.1415
423.1202
M+H
457.1220
Counts vs. Mass-to-Charge (m/z)

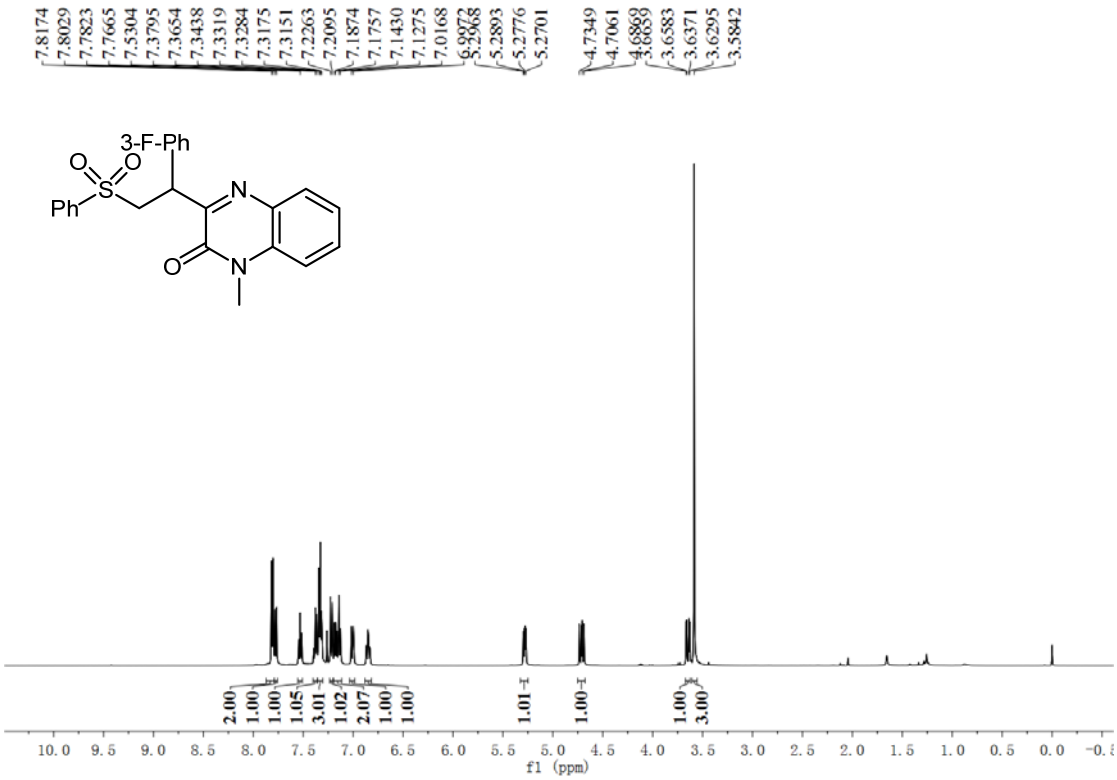


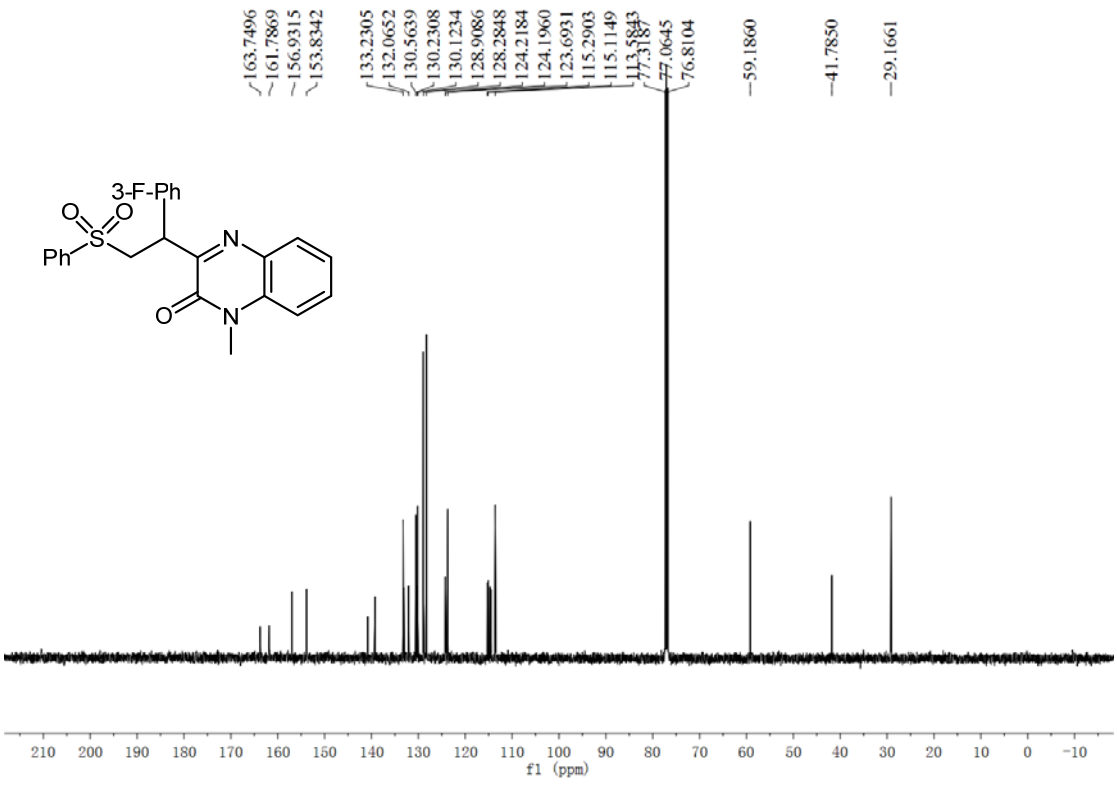

4-Br-Ph
Ph

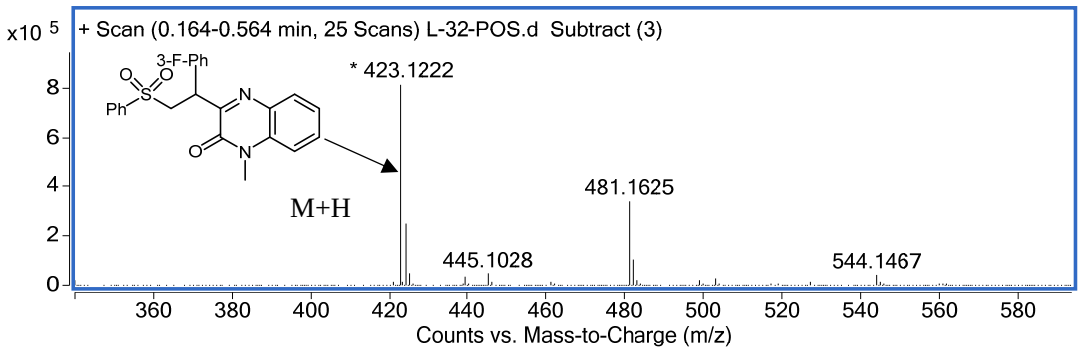

2.95
1.17
1.18
5.12
3.10
1.00
1.04
1.05
3.12
f1 (ppm)

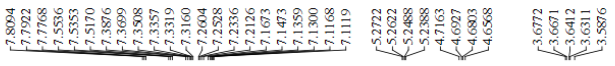

156.9875
153.7654
137.2682
133.1538
131.8283
130.5216
130.1013
130.0694
128.8970
128.2401
123.6843
121.6870
113.5702
77.3444
76.7092
59.0784
41.6896
29.1373
4-Br-Ph
O
O
S
Ph
N
O
N
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

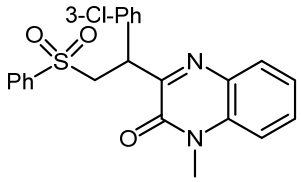

x10 5
+ESI 扫描 (rt: 0.227 min) Frag=175.0V WorklistData-0061.d
4-Br-Ph
Ph
M+H
453.1690
458.3494
463.3050
473.2660
476.3082
479.0969
481.2626
483.0392
484.0417
485.0372
486.0400
490.3772
499.0333
502.3754
505.0212
506.0240
507.0196
508.0220
520.9955
522.9938
523.9969
528.0965
530.0951
533.3675
538.9880
541.0917
543.0898
Counts vs. 质荷比 (m/z)

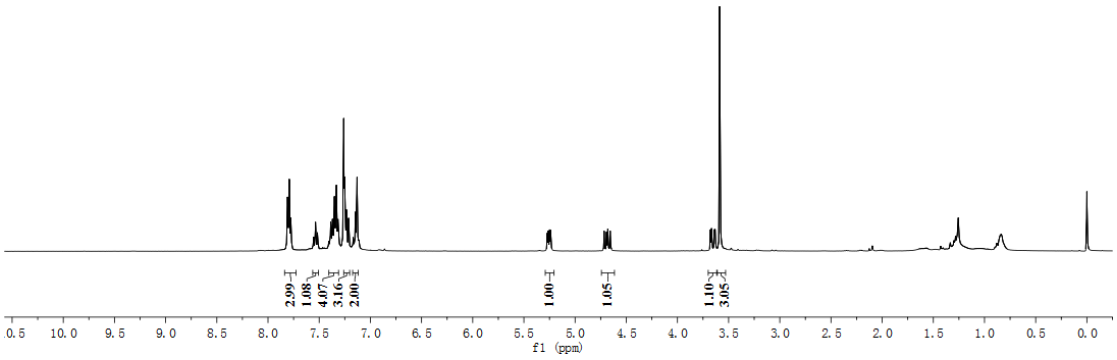

7.8174
7.8029
7.7823
7.7665
7.5304
7.3795
7.3654
7.3438
7.3319
7.3284
7.3175
7.3151
7.2263
7.2095
7.1874
7.1757
7.1430
7.1275
7.0168
6.9972
6.9868
5.2893
5.2776
5.2701
4.7349
4.7061
4.6869
4.6639
3.6583
3.6371
3.6295
3.5842
3-F-Ph
O
O
S
Ph
N
O
N
2.00
1.00
1.00
1.05
3.01
1.02
2.07
1.00
1.00
1.01
1.00
1.00
3.00
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)

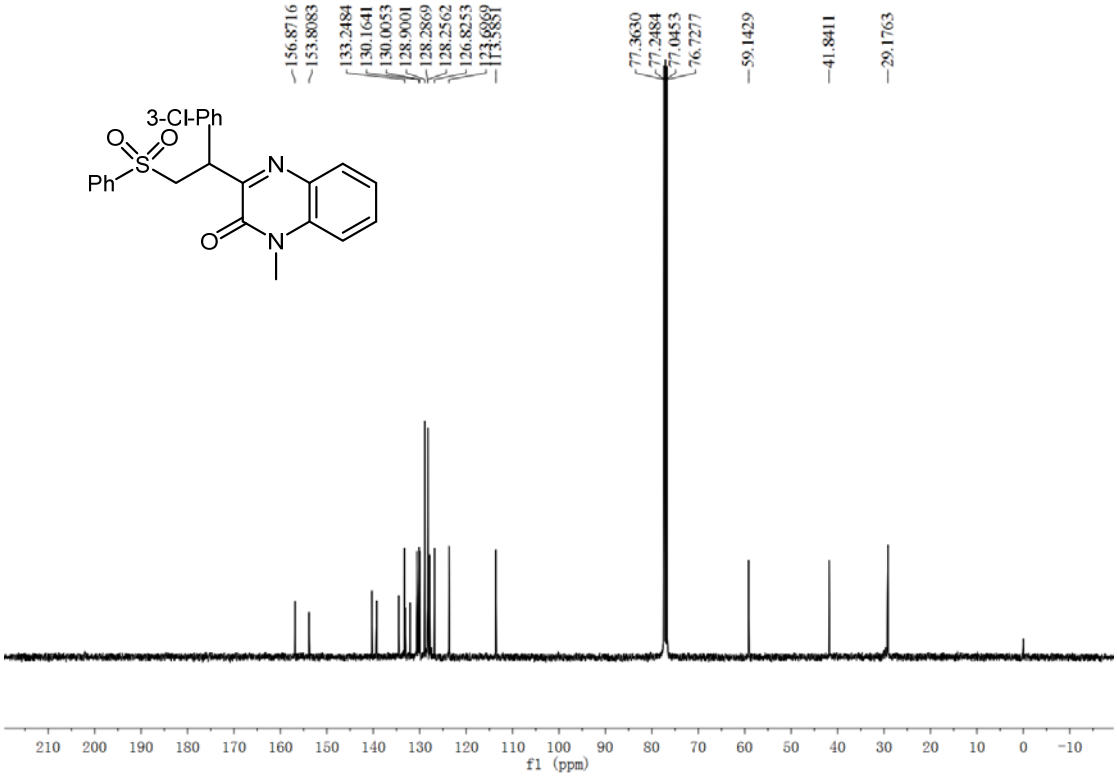

163.7496
161.7869
156.9315
153.8342
133.2305
132.0652
130.5639
130.2308
130.1234
128.9086
128.2848
124.2184
124.1960
123.6931
115.2903
115.1149
113.5843
77.3187
77.0645
76.8104
59.1860
41.7850
29.1661
3-F-Ph
O
O
S
Ph
N
O
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

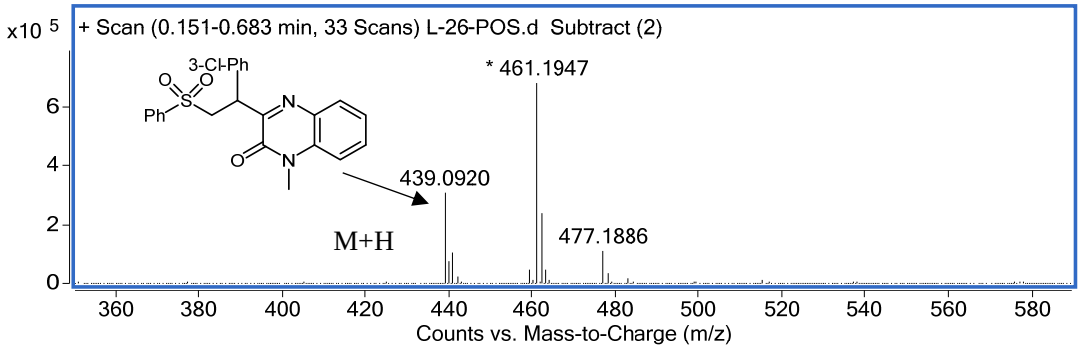

x10 5
+ Scan (0.164-0.564 min, 25 Scans) L-32-POS.d Subtract (3)
3-F-Ph
* 423.1222
481.1625
445.1028
544.1467
M+H
Counts vs. Mass-to-Charge (m/z)

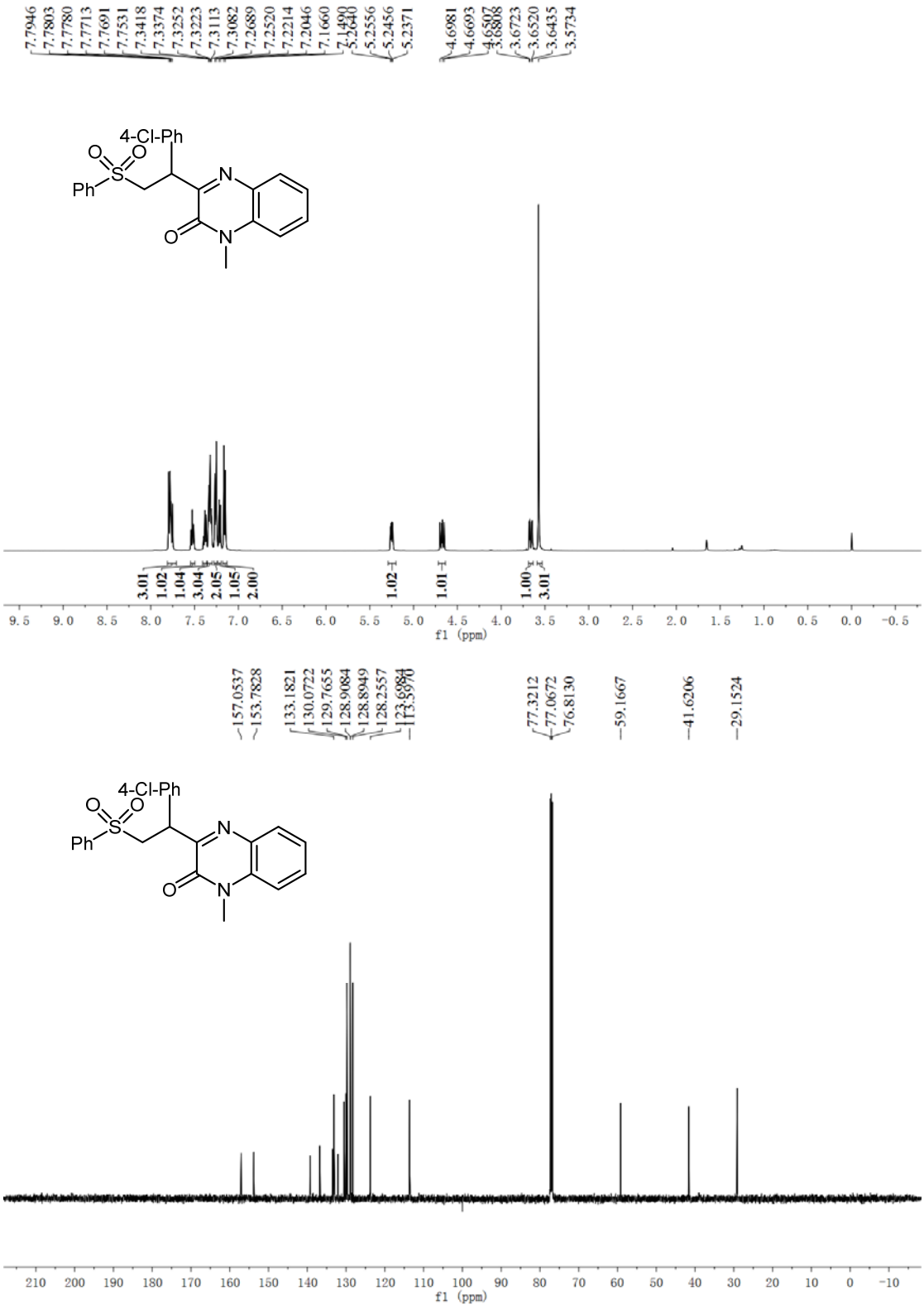


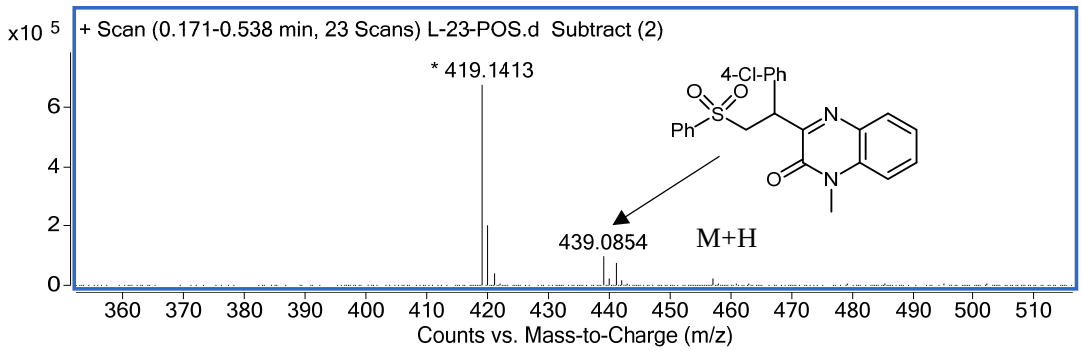

3-Cl-Ph

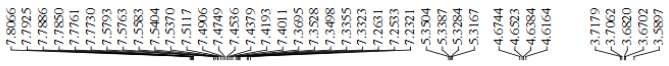

f1 (ppm)

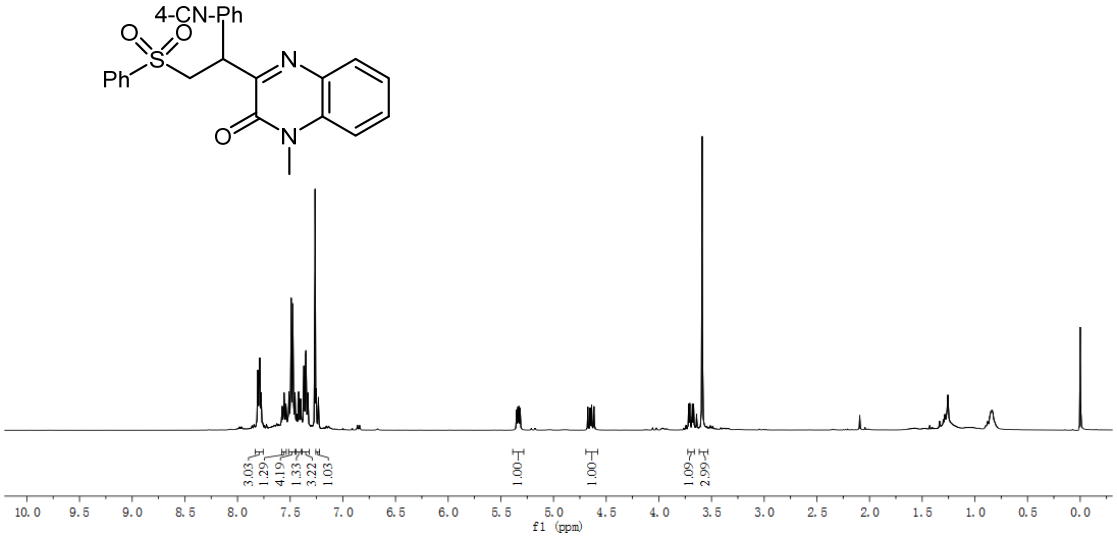

156.8716
153.8083
133.2484
130.1641
130.0053
128.9001
128.2869
128.2562
126.8253
123.6869
113.5851
77.3630
77.2484
77.0453
76.7277
59.1429
41.8411
29.1763
3-Cl-Ph
Ph
O
S
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

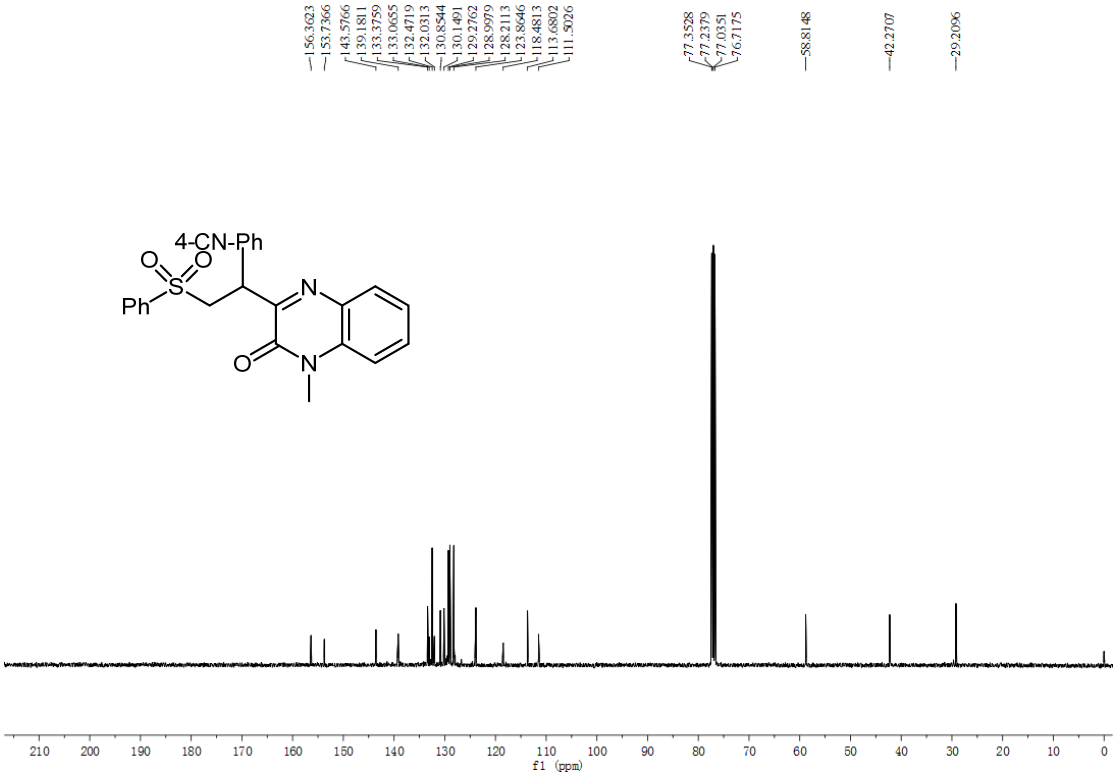

x10 5
+ Scan (0.151-0.683 min, 33 Scans) L-26-POS.d Subtract (2)
3-Cl-Ph
Ph
* 461.1947
439.0920
M+H
477.1886
6
4
2
0
360 380 400 420 440 460 480 500 520 540 560 580
Counts vs. Mass-to-Charge (m/z)

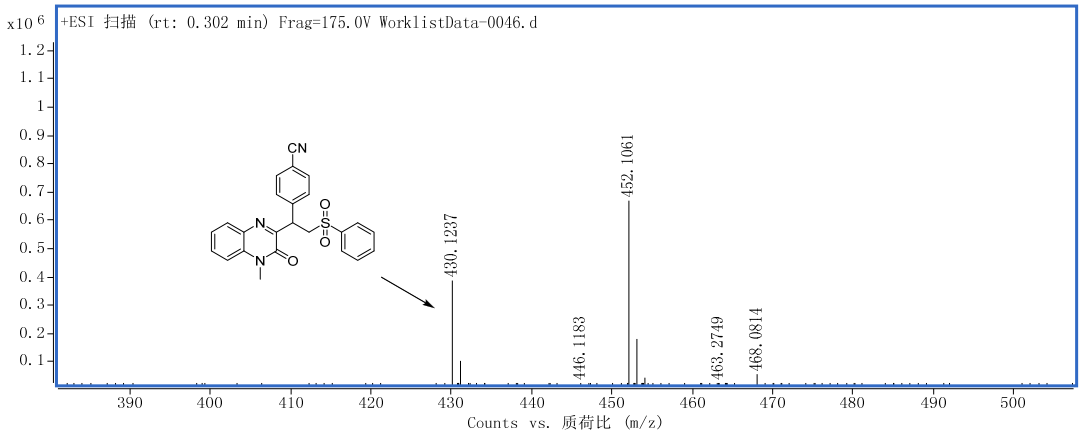

7.7946
7.7803
7.7780
7.7713
7.7691
7.7531
7.3418
7.3374
7.3252
7.3223
7.3113
7.3082
7.2689
7.2520
7.2214
7.2046
7.1660
7.1490
5.2640
5.2556
5.2456
5.2371
4.6981
4.6693
4.6507
4.6308
3.6723
3.6520
3.6435
3.5734
4-Cl-Ph
Ph
O
S
N
O
N
3.01
1.02
1.04
3.04
2.05
1.05
2.00
1.02
1.01
1.00
3.01
f1 (ppm)
157.0537
153.7828
133.1821
130.0722
129.7655
128.9084
128.8949
128.2557
123.6984
123.5970
77.3212
77.0672
76.8130
59.1667
41.6206
29.1524
4-Cl-Ph
Ph
O
S
N
O
N
f1 (ppm)

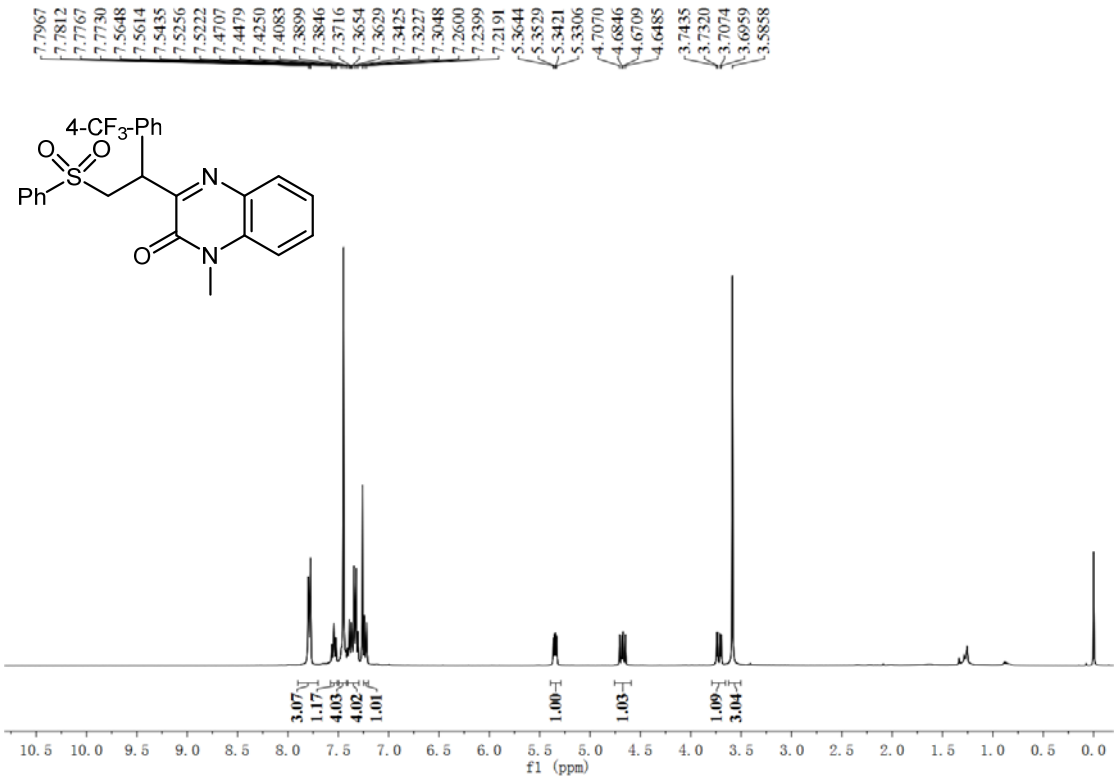

x10 5
+ Scan (0.171-0.538 min, 23 Scans) L-23-POS.d Subtract (2)
* 419.1413
4-Cl-Ph
Ph
439.0854
M+H
Counts vs. Mass-to-Charge (m/z)

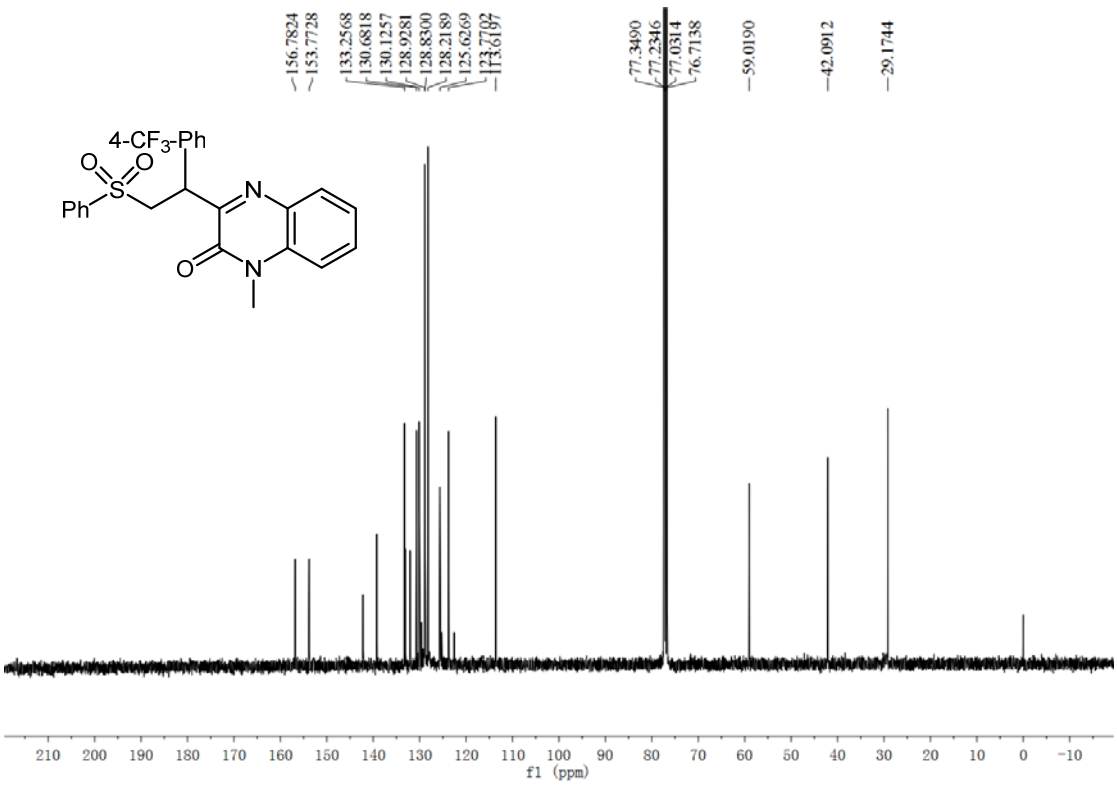


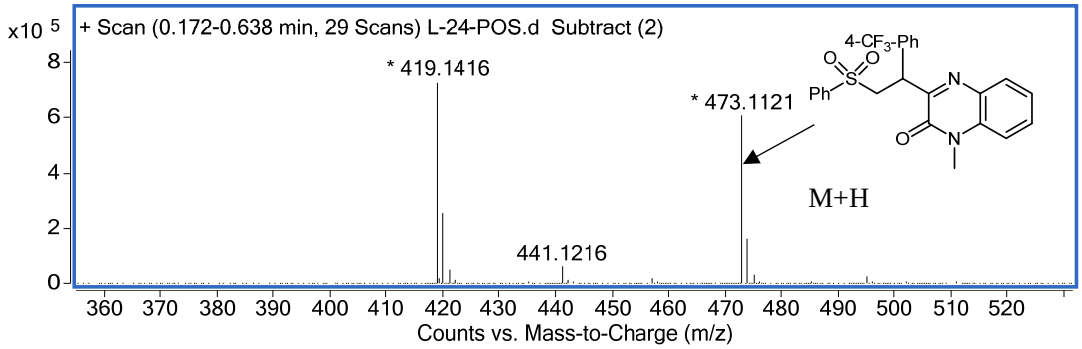

4-CN-Ph
Ph
f1 (ppm)

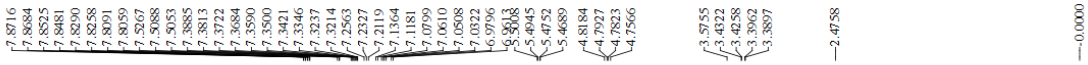

156.3623
153.7366
143.5766
139.1811
133.3759
133.0655
132.4719
132.0313
130.8544
130.1491
129.2762
128.9979
128.2113
123.8646
118.4813
113.6802
111.5026
77.3528
77.2379
77.0351
76.7175
58.8148
42.2707
29.2096
4-CN-Ph
O
O
S
Ph
N
O
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

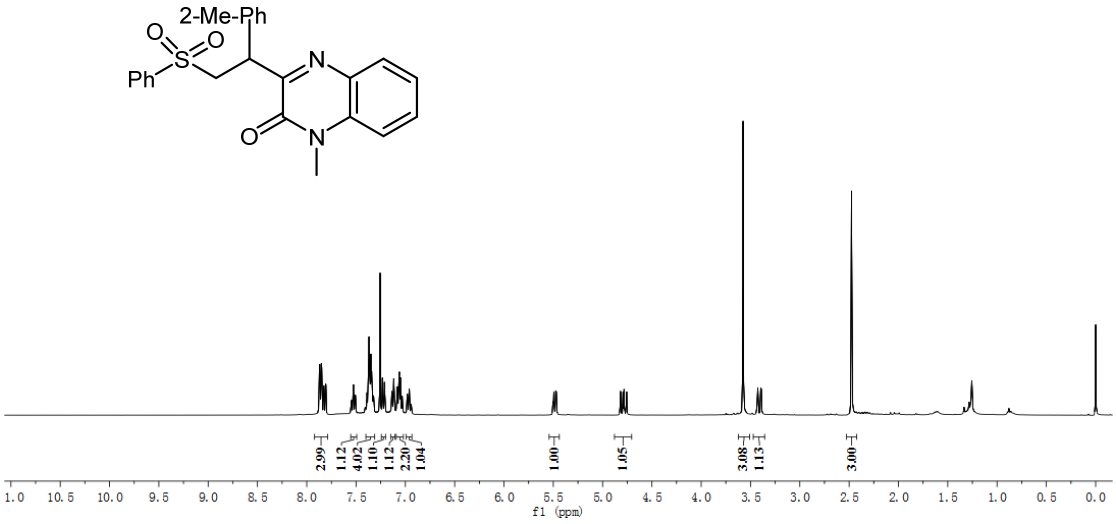

x10 6
+ESI 扫描 (rt: 0.302 min) Frag=175.0V WorklistData-0046.d
1.2
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
CN
O
S
O
N
O
N
430.1237
446.1183
452.1061
463.2749
468.0814
390 400 410 420 430 440 450 460 470 480 490 500
Counts vs. 质荷比 (m/z)

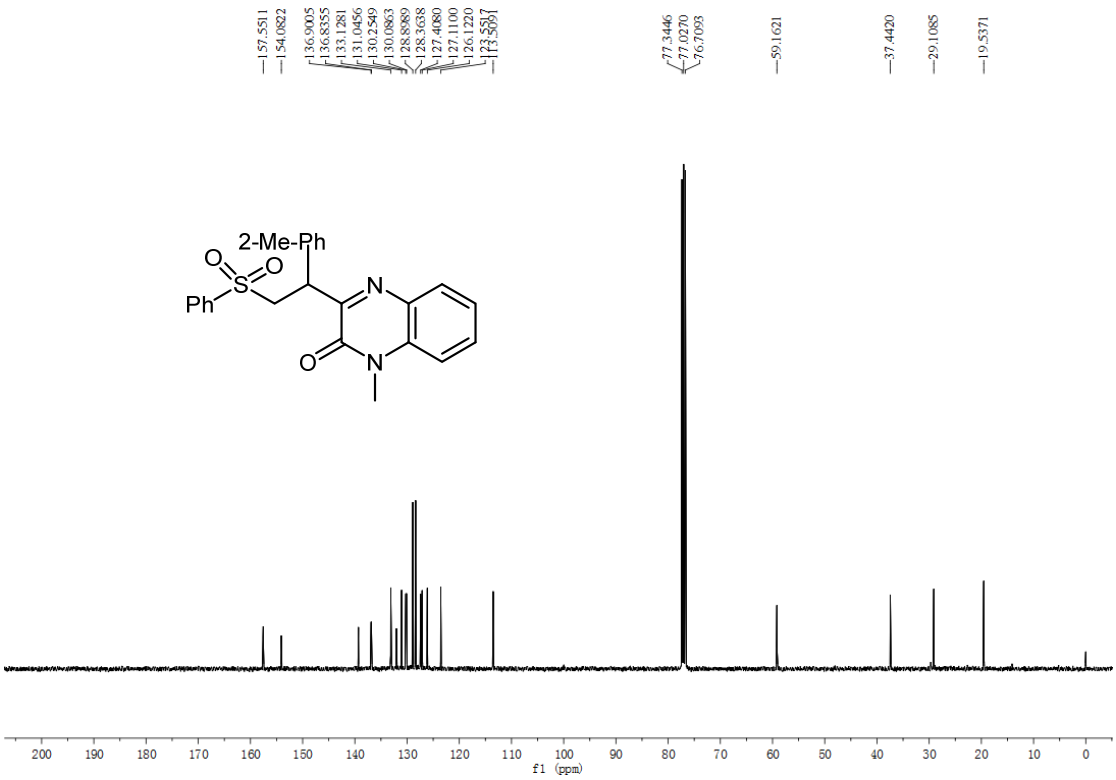

7.7967
7.7812
7.7767
7.7730
7.5648
7.5614
7.5435
7.5256
7.5222
7.4707
7.4479
7.4250
7.4083
7.3899
7.3846
7.3716
7.3654
7.3629
7.3425
7.3227
7.3048
7.2600
7.2399
7.2191
5.3644
5.3529
5.3421
5.3306
4.7070
4.6846
4.6709
4.6485
3.7435
3.7320
3.7074
3.6959
3.5858
4-CF3-Ph
Ph
3.07
1.17
4.03
4.02
1.01
1.00
1.03
1.09
3.04
f1 (ppm)

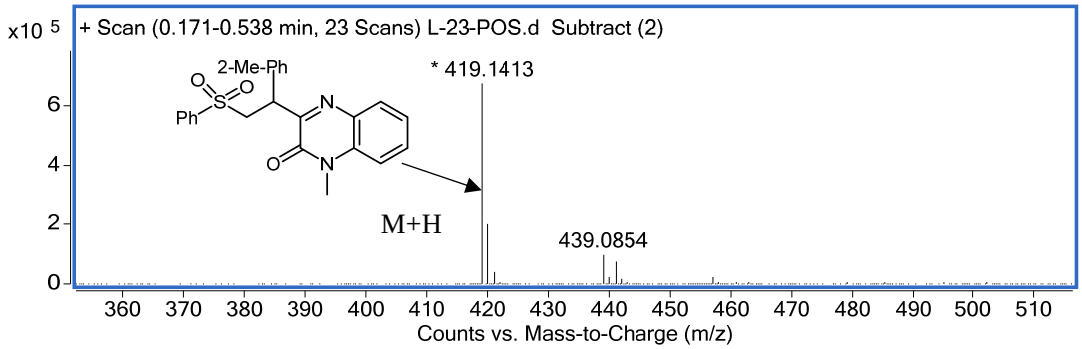

156.7824
153.7728
133.2568
130.6818
130.1257
128.9281
128.8300
128.2189
125.6269
123.7702
113.6197
77.3490
77.2346
77.0314
76.7138
59.0190
42.0912
29.1744
4-CF3-Ph
Ph
f1 (ppm)

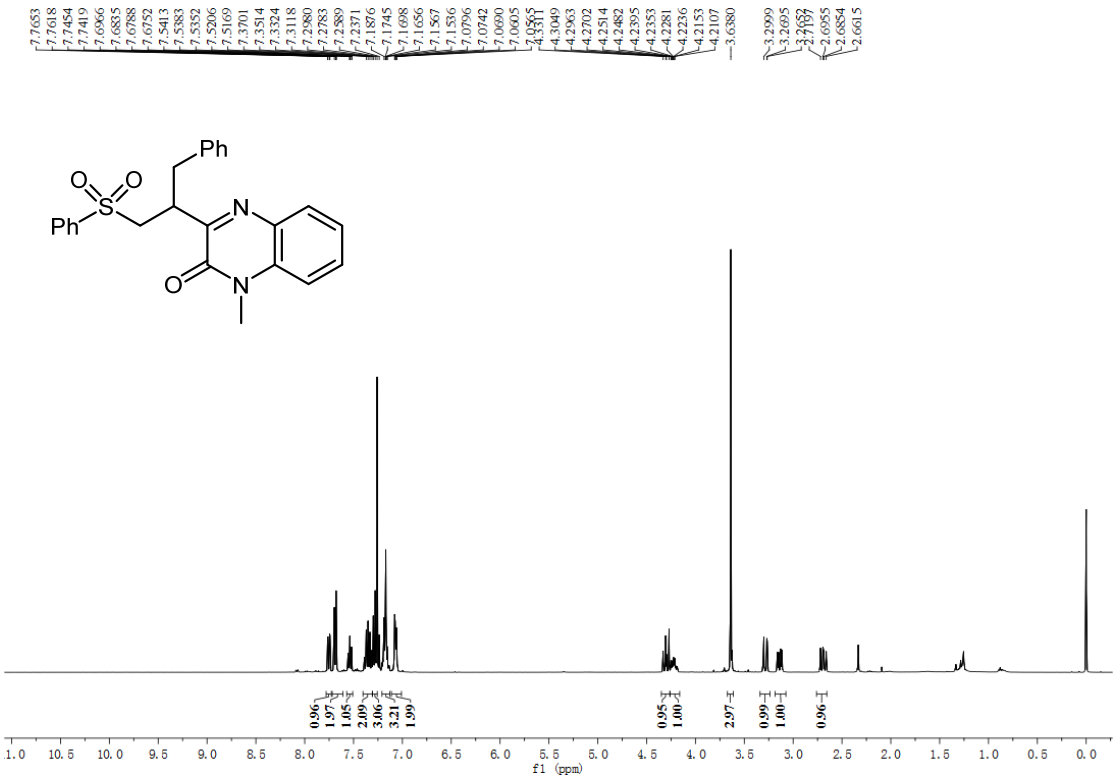

x10 5
+ Scan (0.172-0.638 min, 29 Scans) L-24-POS.d Subtract (2)
* 419.1416
* 473.1121
441.1216
4-CF3-Ph
Ph
M+H
Counts vs. Mass-to-Charge (m/z)

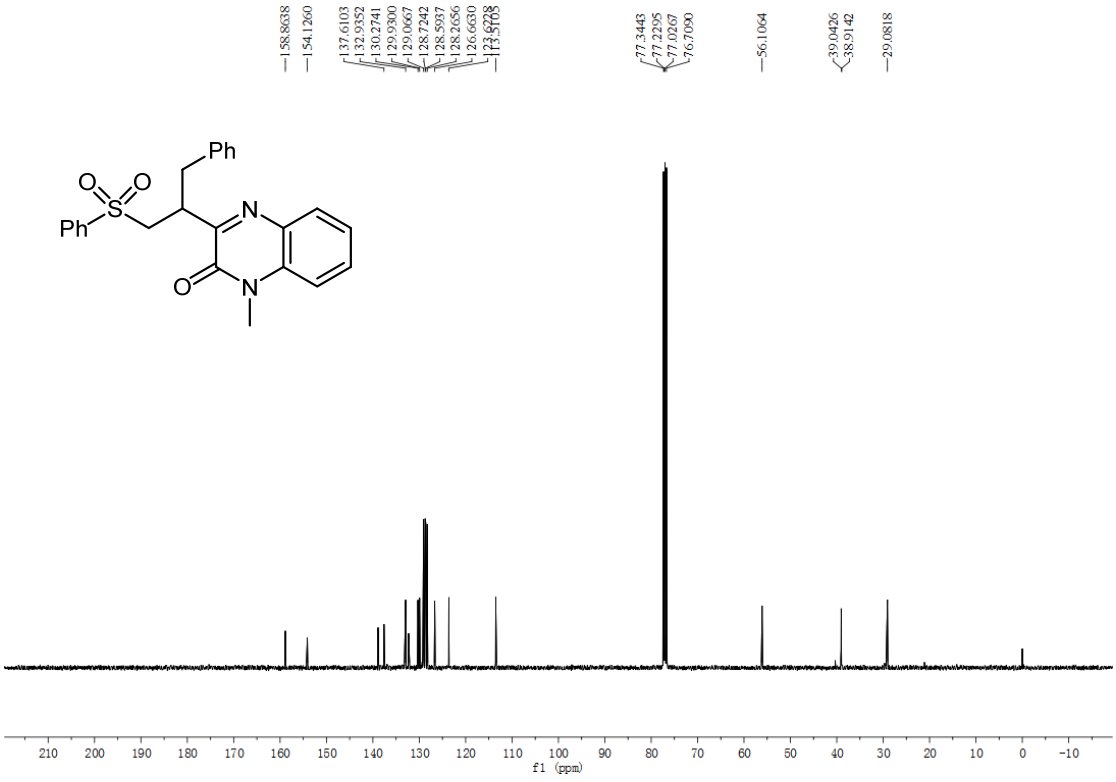


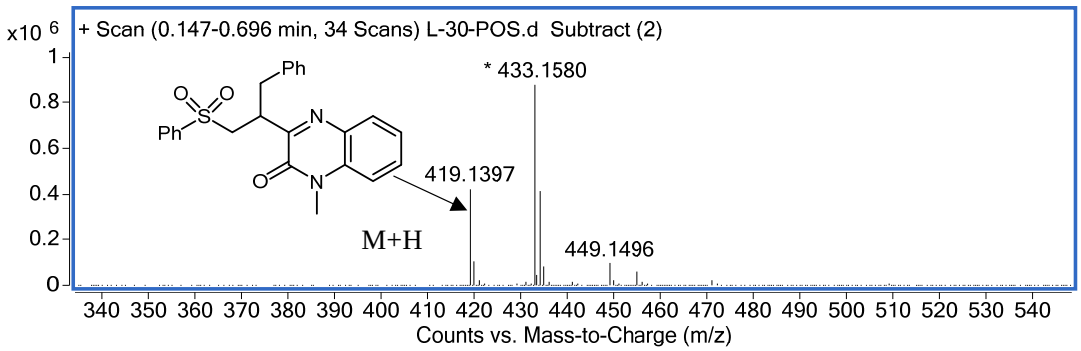

2-Me-Ph
Ph
f1 (ppm)

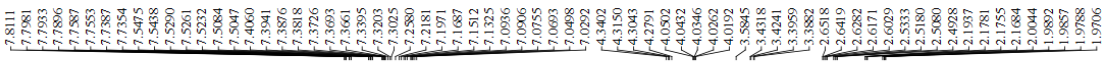

157.5511
154.0822
136.9005
136.8355
133.1281
131.0456
130.2549
130.0863
128.8889
128.3638
127.4080
127.1100
126.1220
123.5517
123.5091
77.3446
77.0270
76.7093
59.1621
37.4420
29.1085
19.5371
2-Me-Ph
Ph
O
S
N
N
f1 (ppm)

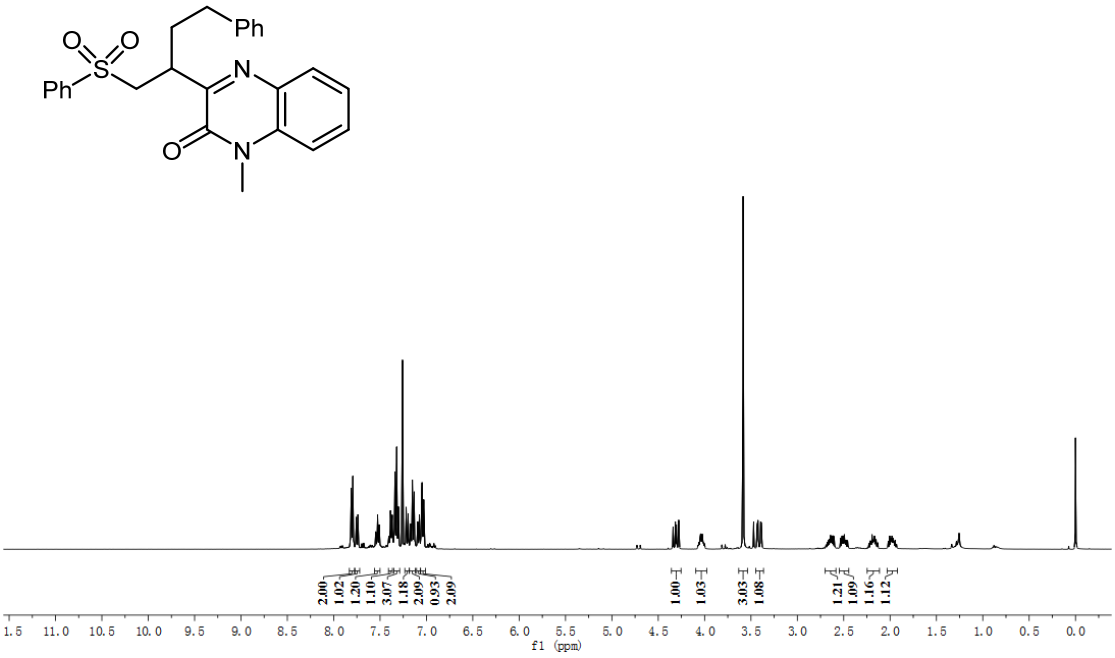

x10 5
+ Scan (0.171-0.538 min, 23 Scans) L-23-POS.d Subtract (2)
2-Me-Ph
* 419.1413
M+H
439.0854
Counts vs. Mass-to-Charge (m/z)

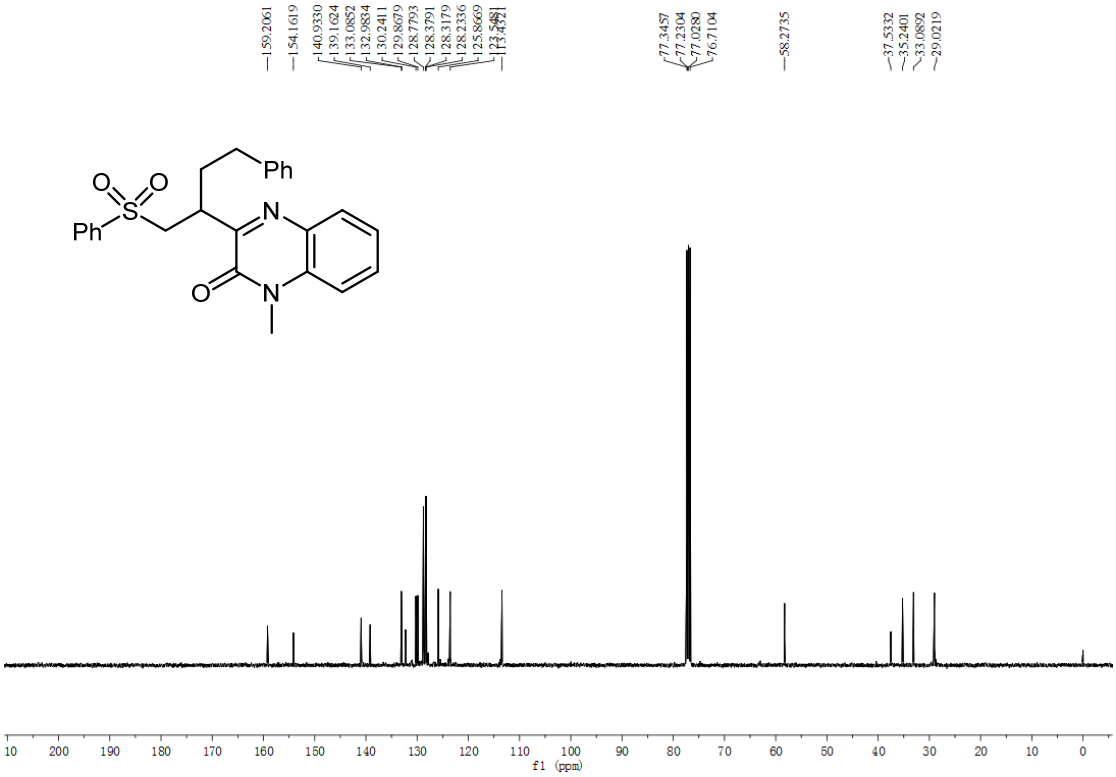

Ph
O
O
S
Ph
N
O
N
0.96
1.97
1.05
2.09
3.06
3.21
1.99
0.95
1.00
2.97
0.99
1.00
0.96
f1 (ppm)

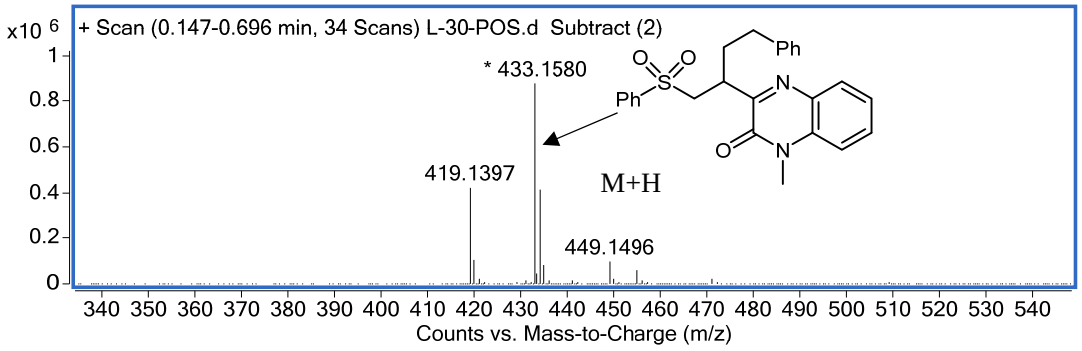

Ph
O
O
S
Ph
N
O
N
f1 (ppm)

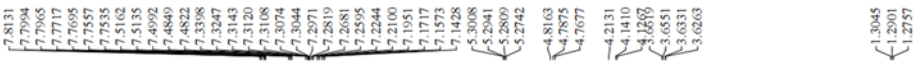

x10 6
+ Scan (0.147-0.696 min, 34 Scans) L-30-POS.d Subtract (2)
* 433.1580
419.1397
449.1496
M+H
Counts vs. Mass-to-Charge (m/z)

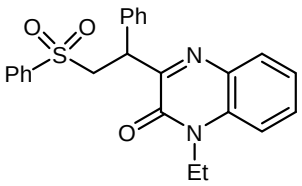


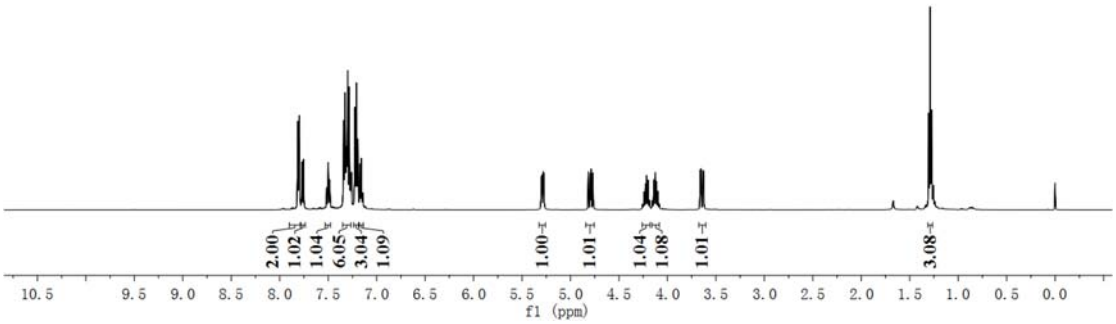

f1 (ppm)

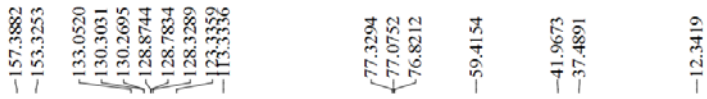

159.2061
154.1619
140.9330
139.1624
133.0852
132.9834
130.2411
129.8679
128.7793
128.3791
128.3179
128.2336
125.8669
77.3457
77.2304
77.0280
76.7104
58.2735
37.5332
35.2401
33.0892
29.0219
Ph
O
O
S
Ph
N
O
N
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

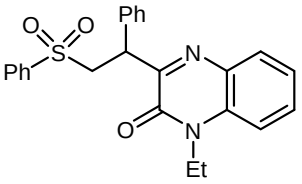

x10 6
+ Scan (0.147-0.696 min, 34 Scans) L-30-POS.d Subtract (2)
* 433.1580
419.1397
449.1496
M+H
Ph
O
O
S
Ph
N
O
N
1
0.8
0.6
0.4
0.2
0
340 350 360 370 380 390 400 410 420 430 440 450 460 470 480 490 500 510 520 530 540
Counts vs. Mass-to-Charge (m/z)



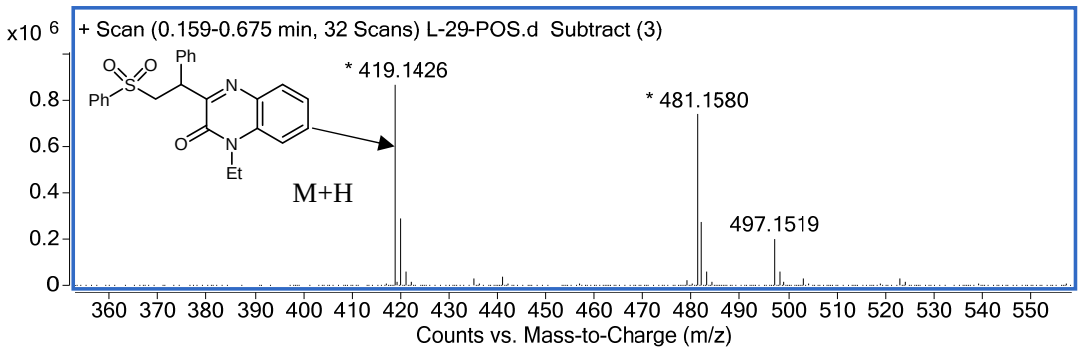

O
O
S
Ph
Ph
N
O
N
Et

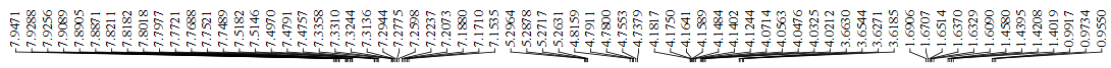

2.00
1.02
1.04
6.05
3.04
1.09
1.00
1.01
1.04
1.08
1.01
3.08
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

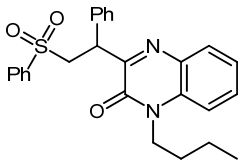


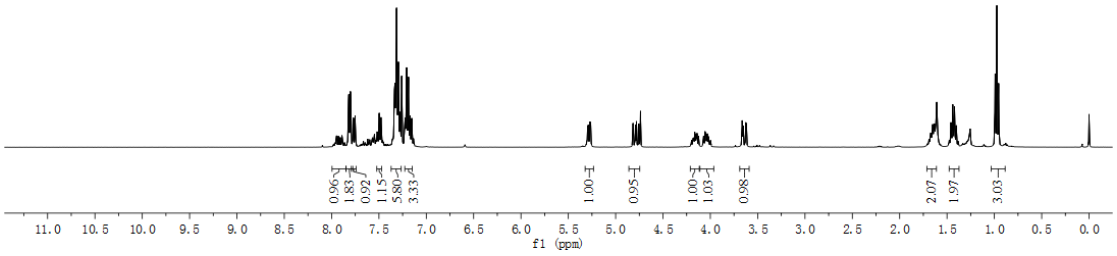

O
O
S
Ph
Ph
N
O
N
Et

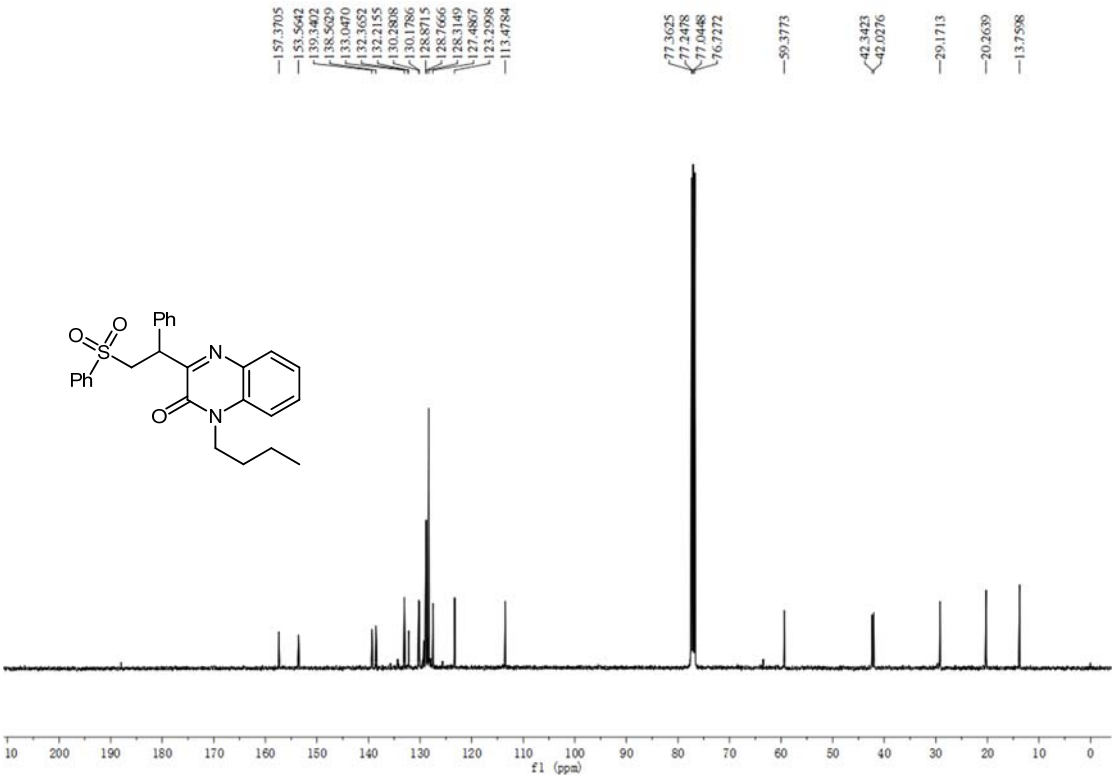
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

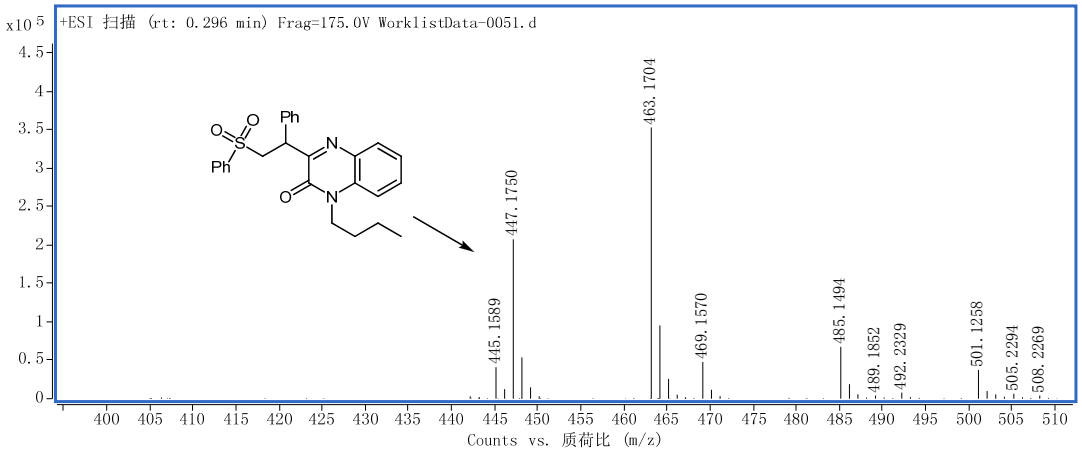

x10 6
+ Scan (0.159-0.675 min, 32 Scans) L-29-POS.d Subtract (3)
* 419.1426
* 481.1580
497.1519
M+H
Counts vs. Mass-to-Charge (m/z)

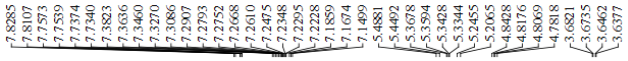


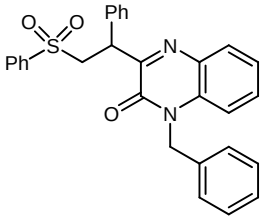


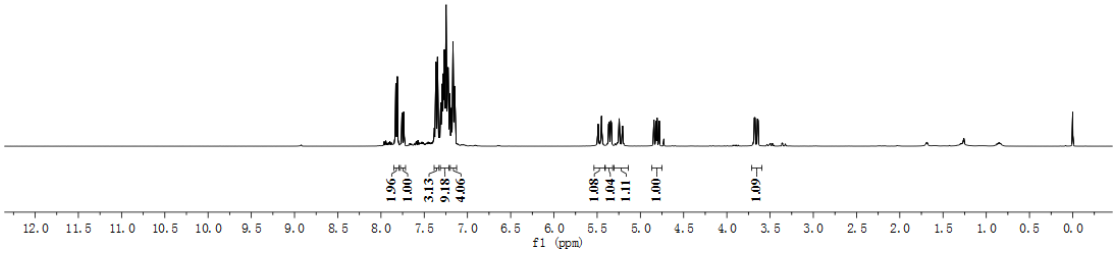

f1 (ppm)


157.3705
153.5642
139.3402
138.5029
133.0470
132.3652
132.2155
130.2808
130.1786
128.8715
128.7666
128.3149
127.4867
123.2998
113.4784
77.3625
77.2478
77.0448
76.7272
59.3773
42.3423
42.0276
29.1713
20.2639
13.7598
Ph
O
O
S
Ph
N
O
N
f1 (ppm)

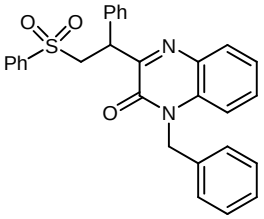

x10 5
+ESI 扫描 (rt: 0.296 min) Frag=175.0V WorklistData-0051.d
463.1704
447.1750
445.1589
469.1570
485.1494
489.1852
492.2329
501.1258
505.2294
508.2269
Counts vs. 质荷比 (m/z)

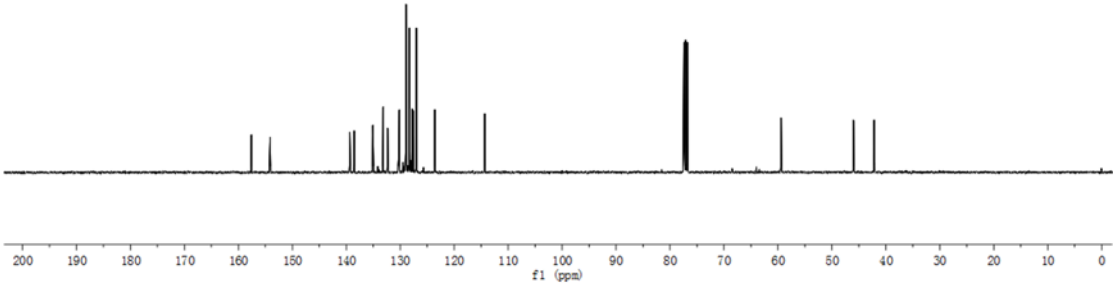

7.8285
7.8107
7.7573
7.7539
7.7374
7.7340
7.3823
7.3636
7.3460
7.3270
7.3086
7.2907
7.2793
7.2752
7.2668
7.2610
7.2475
7.2348
7.2295
7.2228
7.1859
7.1674
7.1499
5.4881
5.4492
5.3678
5.3594
5.3428
5.3344
5.2455
5.2065
4.8428
4.8176
4.8069
4.7818
3.6821
3.6735
3.6462
3.6377

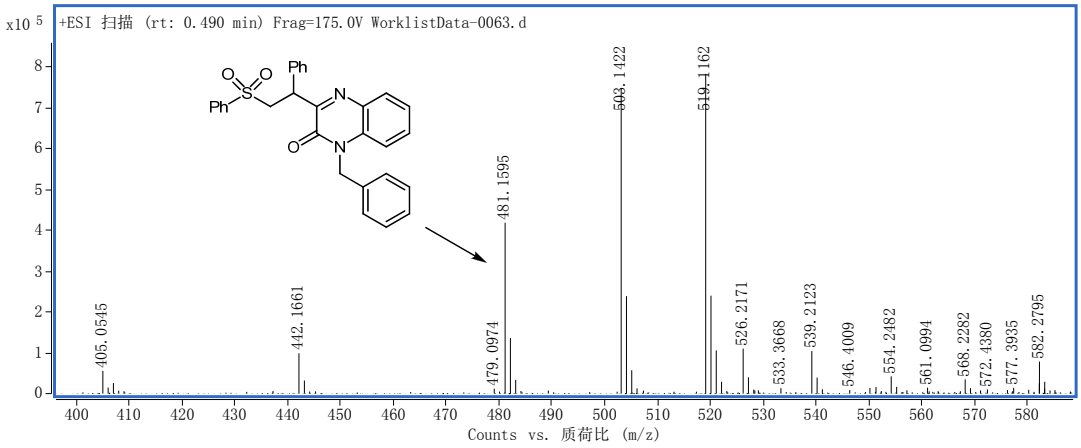

O
O
S
Ph
Ph
N
O
N

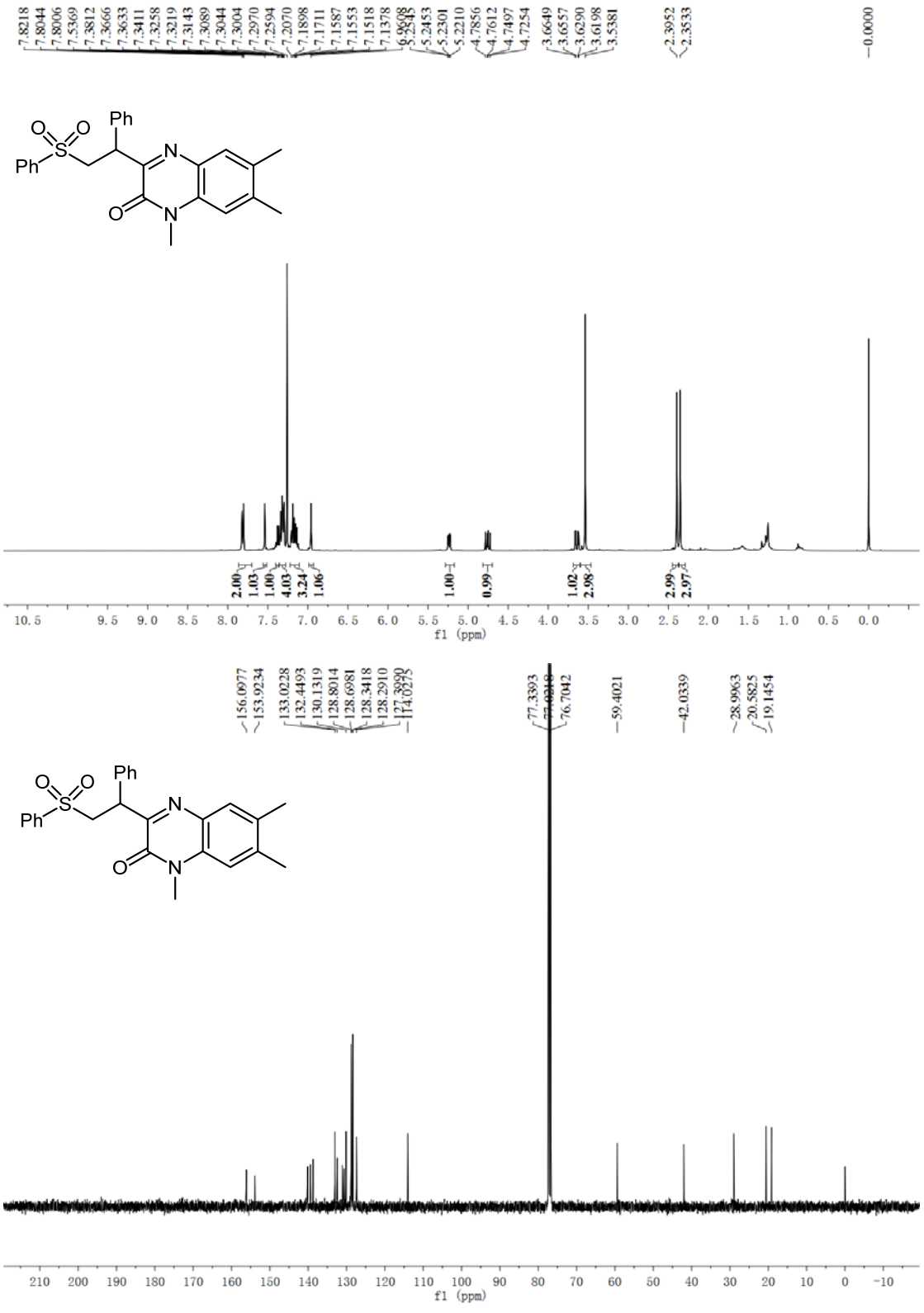

1.96
1.00
3.13
9.18
4.06
1.08
1.04
1.11
1.00
1.09
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

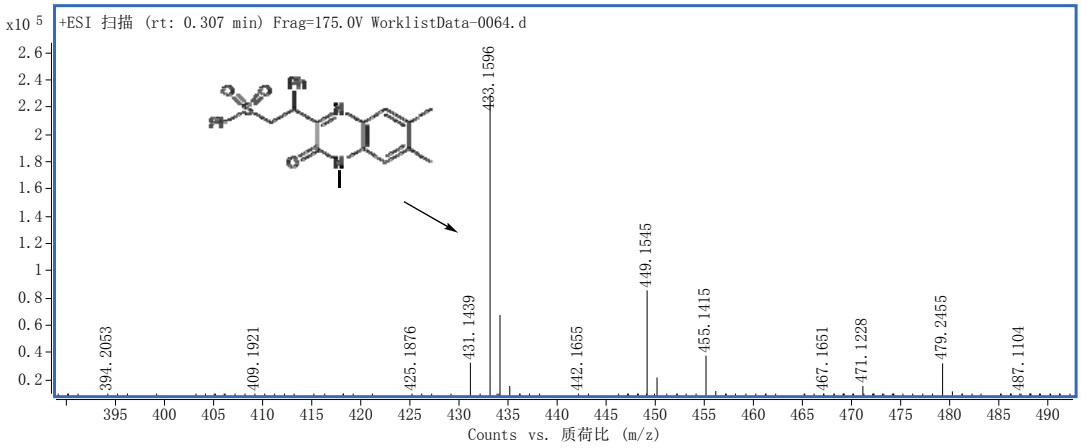

157.5822
154.1025
133.1677
130.2809
130.1666
128.9462
128.9279
128.8483
128.3362
128.2584
127.7715
127.5981
127.0210
123.5911
114.3436
77.4216
77.1036
76.7857
59.4233
46.0046
42.1697

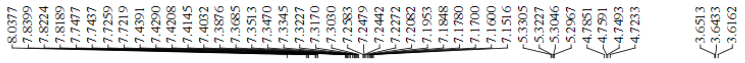

O
O
S
Ph
Ph
N
O
N

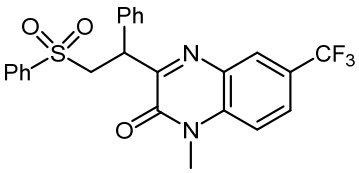

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

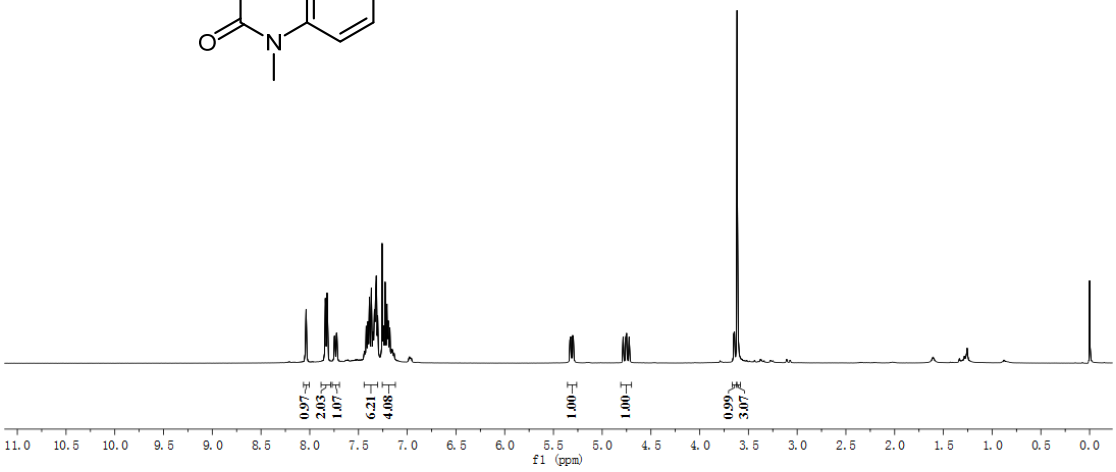

x10 5
+ESI 扫描 (rt: 0.490 min) Frag=175.0V WorklistData-0063.d
405.0545
442.1661
479.0974
481.1595
503.1422
519.1162
526.2171
533.3668
539.2123
546.4009
554.2482
561.0994
568.2282
572.4380
577.3935
582.2795
Counts vs. 质荷比 (m/z)

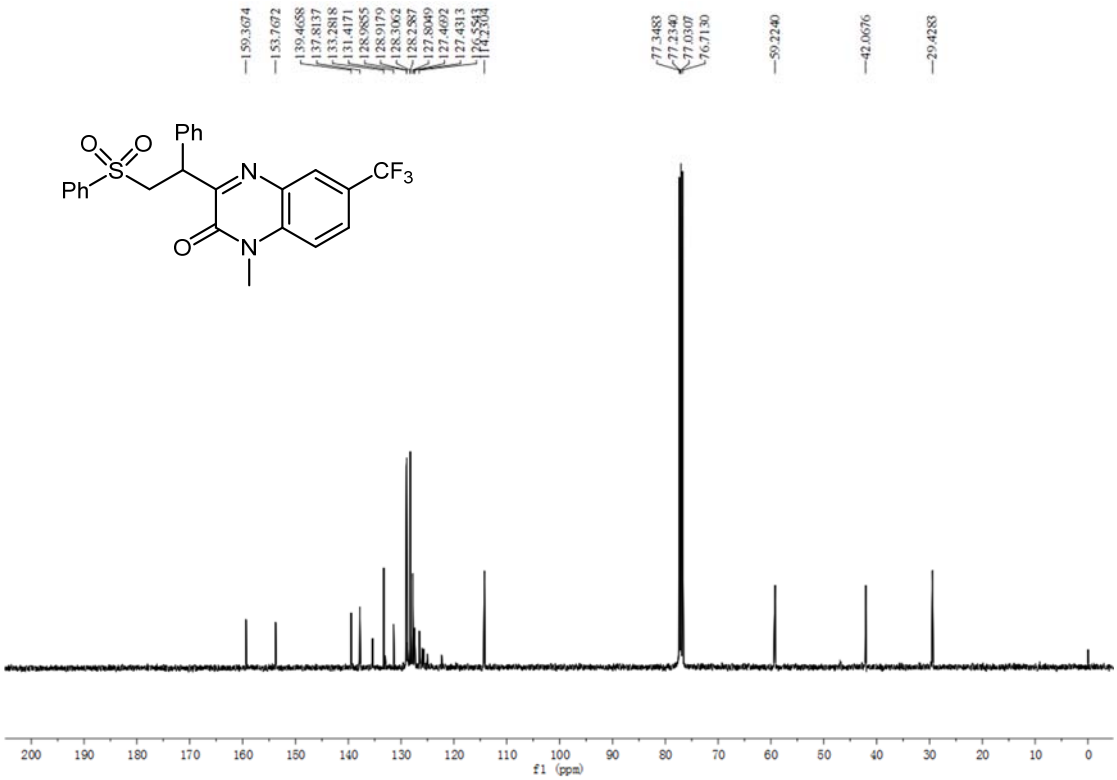

7.8218
7.8044
7.8006
7.5369
7.3812
7.3666
7.3633
7.3411
7.3258
7.3219
7.3143
7.3089
7.3044
7.3004
7.2970
7.2594
7.2070
7.1898
7.1711
7.1587
7.1553
7.1518
7.1378
6.9608
5.2545
5.2453
5.2301
5.2210
4.7856
4.7612
4.7497
4.7254
3.6649
3.6557
3.6290
3.6198
3.5381
2.3952
2.3533
0.0000
Ph
O
O
S
Ph
N
O
N
2.00
1.03
1.00
4.03
3.24
1.06
1.00
0.99
1.02
2.98
2.99
2.97
10.5 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)
156.0977
153.9234
133.0228
132.4493
130.1319
128.8014
128.6981
128.3418
128.2910
127.3990
114.0275
77.3393
77.0818
76.7042
59.4021
42.0339
28.9963
20.5825
19.1454
Ph
O
O
S
Ph
N
O
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

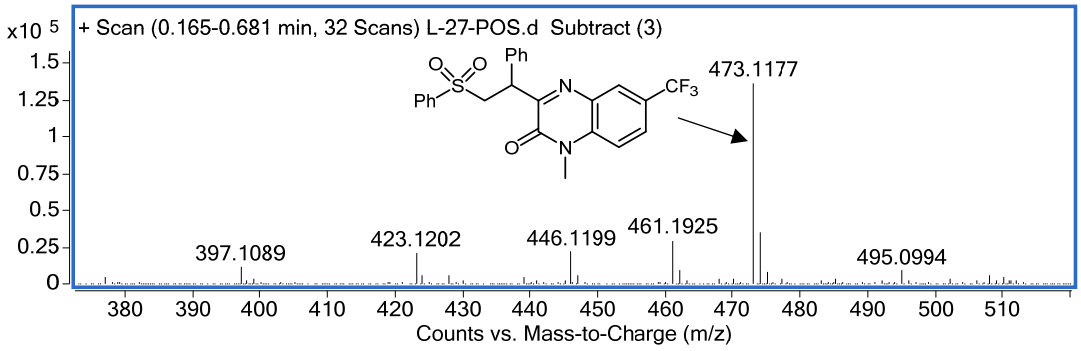

x10 5
+ESI 扫描 (rt: 0.307 min) Frag=175.0V WorklistData-0064.d
433.1596
449.1545
431.1439
455.1415
394.2053
409.1921
425.1876
442.1655
467.1651
471.1228
479.2455
487.1104
Counts vs. 质荷比 (m/z)

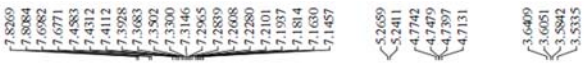

8.0377
7.8399
7.8224
7.8189
7.7477
7.7437
7.7259
7.7219
7.4391
7.4290
7.4208
7.4145
7.4032
7.3876
7.3685
7.3513
7.3470
7.3345
7.3227
7.3170
7.3080
7.2983
7.2479
7.2442
7.2272
7.2082
7.1953
7.1848
7.1780
7.1700
7.1600
7.1516
5.3305
5.3227
5.3046
5.2967
4.7851
4.7591
4.7493
4.7233
3.6513
3.6433
3.6162

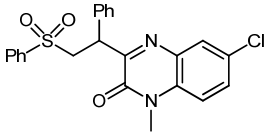

Ph
O
O
S
Ph
N
CF3
O
N

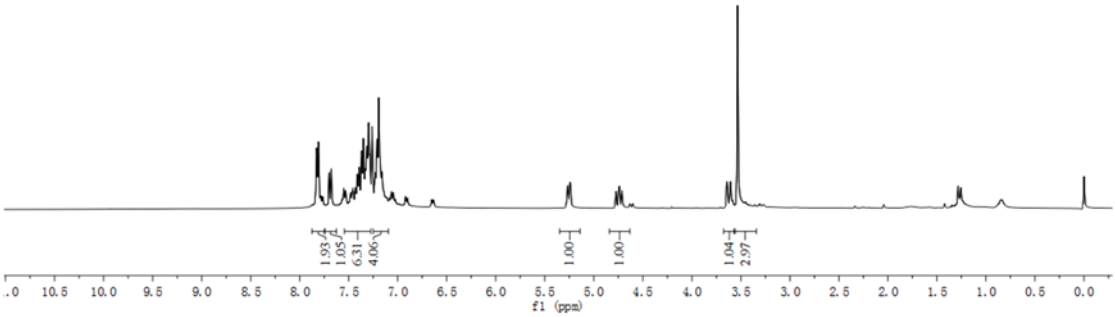

0.97
2.03
1.07
6.21
4.08
1.00
1.00
0.99
3.07
f1 (ppm)


159.3674
153.7672
139.4658
137.8137
133.2818
131.4171
128.9855
128.9179
128.3062
128.2587
127.8049
127.4692
127.4313
126.5543
124.2304
77.3483
77.2340
77.0307
76.7130
59.2240
42.0676
29.4283
Ph
O
O
S
Ph
N
CF3
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

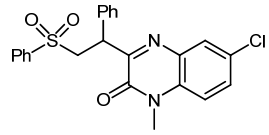

x10 5
+ Scan (0.165-0.681 min, 32 Scans) L-27-POS.d Subtract (3)
1.5
1.25
1
0.75
0.5
0.25
0
Ph
O
O
S
Ph
N
CF3
O
N
473.1177
397.1089
423.1202
446.1199
461.1925
495.0994
380
390
400
410
420
430
440
450
460
470
480
490
500
510
Counts vs. Mass-to-Charge (m/z)


7.8269
7.8084
7.6982
7.6771
7.4583
7.4312
7.4112
7.3928
7.3683
7.3502
7.3300
7.3146
7.2965
7.2859
7.2608
7.2280
7.2101
7.1937
7.1814
7.1630
7.1457
5.2659
5.2411
4.7742
4.7479
4.7397
4.7131
3.6409
3.6051
3.5842
3.5335

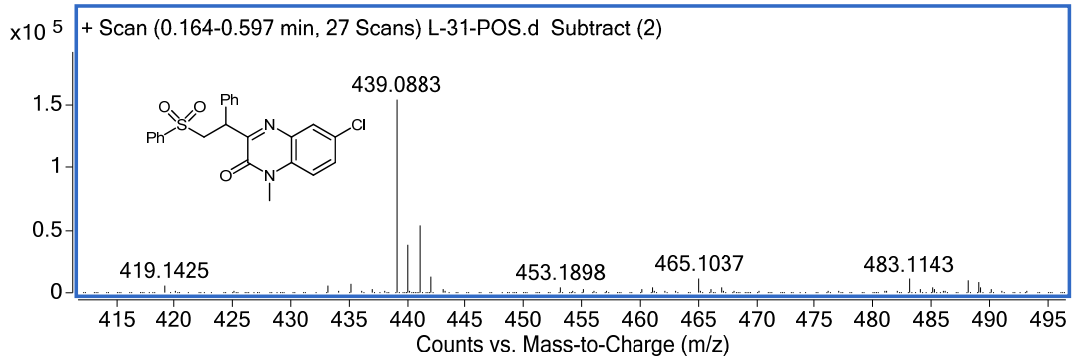

Ph
O
O
S
Ph
N
Cl
O
N

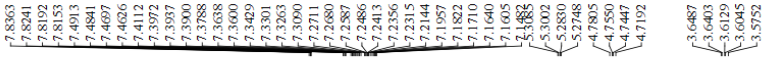

1.93
1.05
6.31
4.06
1.00
1.00
1.04
2.97
f1 (ppm)

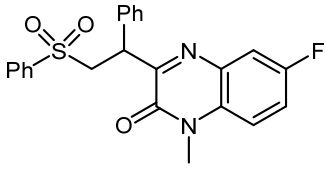

157.6367
153.6324
139.3298
138.1550
136.2744
133.9179
133.2442
131.0730
128.9315
128.8485
128.3179
128.2583
127.6748
77.3818
77.0640
76.7462
59.2350
42.0635
29.2635

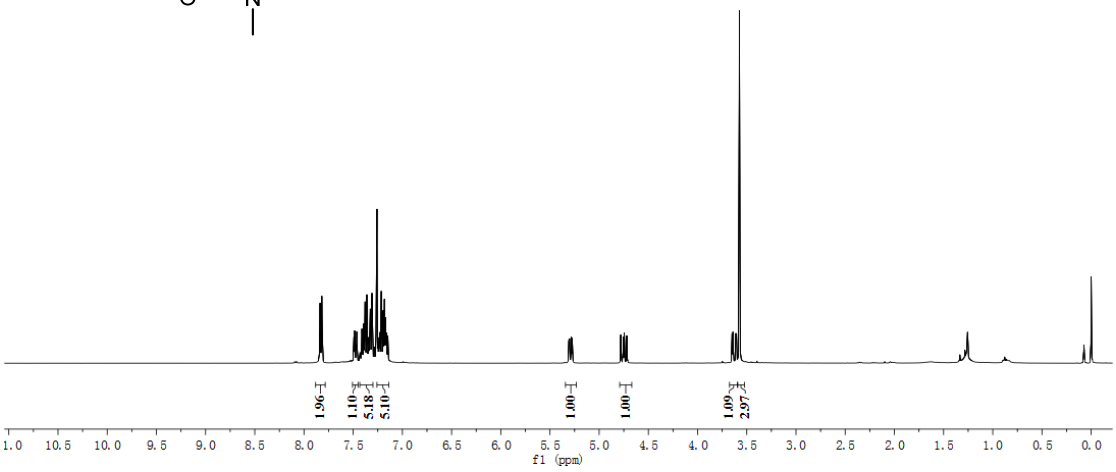

Ph
O
O
S
Ph
N
Cl
O
N

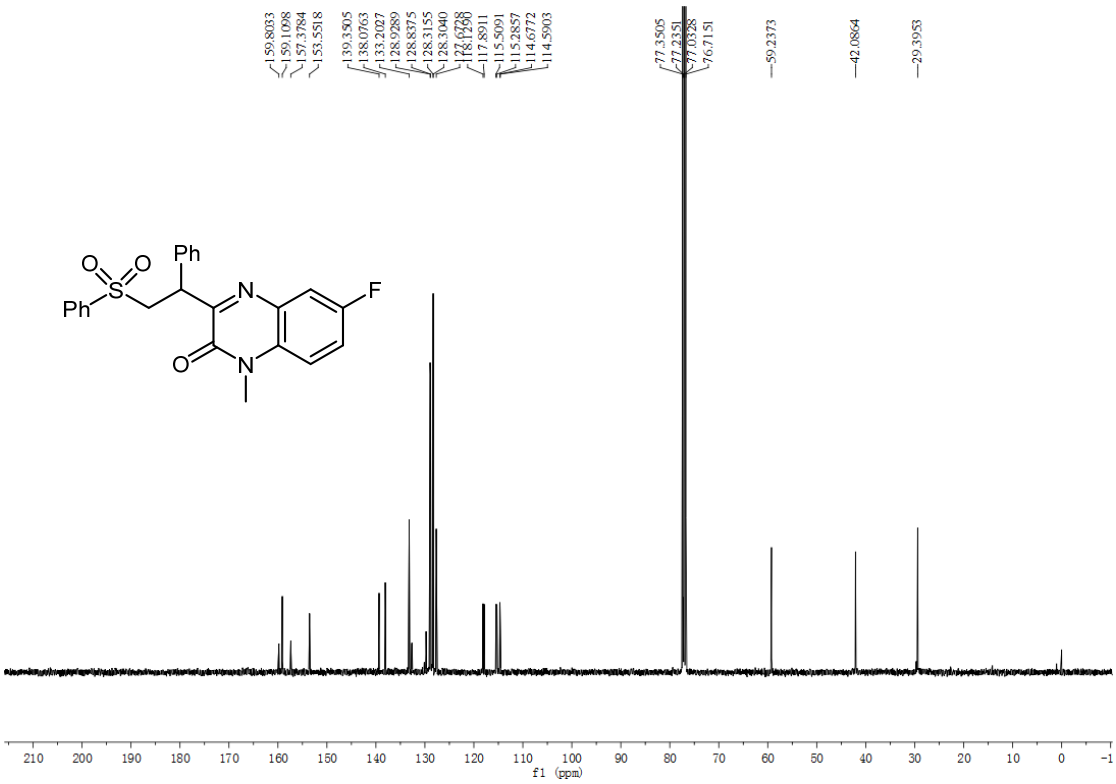
f1 (ppm)

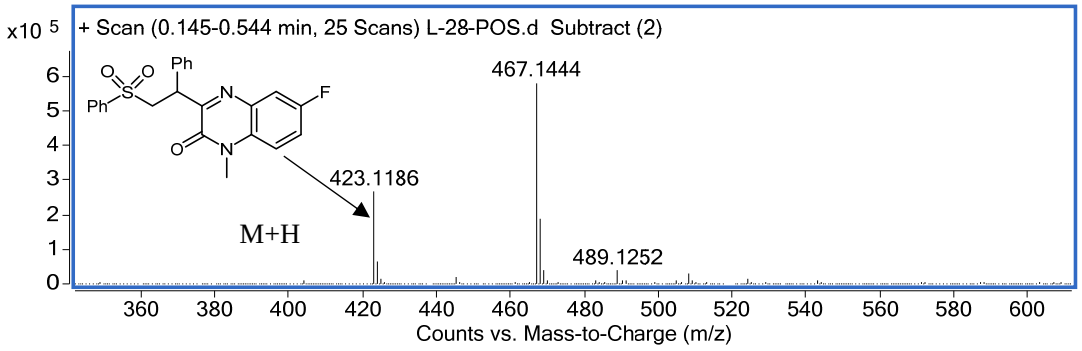

x10 5
+ Scan (0.164-0.597 min, 27 Scans) L-31-POS.d Subtract (2)
439.0883
419.1425
453.1898
465.1037
483.1143
Counts vs. Mass-to-Charge (m/z)






f1 (ppm)


159.8033
159.1098
157.3784
153.5518
139.3505
138.0763
133.2027
128.9289
128.8375
128.3155
128.3040
117.8911
115.5091
115.2857
114.6772
114.5903
77.3505
77.2351
77.0328
76.7151
59.2373
42.0864
29.3953
Ph
Ph
O
O
S
N
F
O
N
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


x10 5
+ Scan (0.145-0.544 min, 25 Scans) L-28-POS.d Subtract (2)
Ph
Ph
O
O
S
N
F
O
N
467.1444
423.1186
M+H
489.1252
6
5
4
3
2
1
0
360
380
400
420
440
460
480
500
520
540
560
580
600
Counts vs. Mass-to-Charge (m/z)