Supporting Information

Design, Synthesis, Mode of Action and Herbicidal Evaluation of Quinazolin-4(3*H*)-one Derivatives Based on Aryloxyphenoxypropionate Motif

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Inhibition of the root growth of *Brassica campestris*

Emulsions of target compounds and quizalofop-P-ethyl were prepared by dissolving them in 100 μL of DMF adding a few drops of Tween-80 and dispersing in water. A mixture of the same amount of water, DMF and Tween-80 was used as control. Rape seeds were soaked in distilled water for 4 h before being placed on a filter paper in a 6 cm petri plate, to which 2 mL of inhibitor solution had been added in advance. Usually, 15 seeds were used on each plate. The plate was placed in a dark room and allowed to germinate for 65 h at 28 ± 1 ℃. The lengths of ten *B. campestris* roots randomly selected from each plate were measured, and the means were calculated. Each treatment was performed triplicate. Formulas used in these tests are as follows: Control effect (%) = (the root length of *B. campestris* of the control − the root length of *B. campestris* treated by tested compound)/the root length of *B. campestris* of the control × 100%. The data represented the percent displaying herbicidal damage as compared to the control, where complete control of the target is 100 and no control is 0.

Inhibition of the seedling growth of *Echinochloa crusgalli*

Emulsions of target compounds and quizalofop-P-ethyl were prepared according to above method. A mixture of the same amount of water, DMF and Tween-80 was used as control. 10 *E. crusgalli* seeds were placed into a 25 mL cup covered with a layer of glass beads and a piece of filter paper at the bottom, to which 2.5 mL of inhibitor solution had been added in advance. The cup was placed in a bright room, and the seeds were allowed to germinate for 72 h at 28 ± 1 ℃. The heights of the above-ground parts of the seedlings in each cup were measured, and the means were calculated. Formulas used in these tests are as follows: Control effect (%) = (the height of *E. crusgalli* of the control − the height of *E. crusgalli* treated by tested compound)/the height of *E. crusgalli* of the control × 100%. The percentage inhibition was used to describe the control efficiency of the compounds. The data represented the percent displaying herbicidal damage as compared to the control, where complete control of the target is 100 and no control is 0. Each test was performed in triplicate.

Greenhouse Tests

The greenhouse herbicidal activities of target compounds and control compounds were evaluated using a standard procedure at Nankai University. Two dicotyledonous species mustard (*Brassica campestris*) and amaranth pigweed (*Amaranthus retroflexus*), and two monocotyledonous species

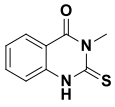
barnyard grass (*Echinochloa crusgalli*) and crabgrass (*Digitaria sanguinalis*) were used to test the herbicidal activities of the compounds. For pre-emergence tests, sandy clay (100 g) in a 7-cm-diameter test pot was wetted by water. Then 15 sprouting seeds of the weed were planted to 0.6 cm depth and placed in a greenhouse. All the tested compounds were dissolved in 100 % DMF and then diluted with Tween-80 (concentration: 100 g/L). The resulting solutions were diluted with water to the appropriate concentrations before use. The solutions of the compounds evaluated were sprayed immediately after seed planting. The mixture of same amount of water, *N*, *N*-dimethylformamide and Tween 80 was sprayed as the control. For post-emergence tests, the same solution of the compounds was applied at the same rate as for the pre-emergence tests. Compounds were sprayed immediately after the expansion of the first true leaf. After 14 days, the fresh weight of the above-ground tissues in each pot was weighed and the percentage of inhibition calculated. Each treatment was done in triplicate, all the experiments were performed under natural light conditions at 18 – 28 ℃. Additionally, adverse weather lighting was provided using sodium vapour lamps with a 12 : 12 h light : dark photo period.

Formulas used in these tests are as follows: Control effect (%) = (the weight of live weeds in the control pots − the weight of live weeds in the treated pots)/the weight of live weeds in the control pots × 100%. The data represented the percent displaying herbicidal damage as compared to the control, where complete control of the target is 100 and no control is 0.

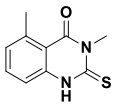
Crop selectivity

The crops were planted in flowerpots (12 cm diameter) and grown at room temperature in the test soil. Crop safety experiments were conducted at the dosage of 375 g ha^{-1} when the crops had reached the four-leaf stage. After 14 days of treatment by compound **QPP-7**, the crop selectivity was evaluated with three duplicates per experiment.

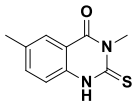
The ^{1}H NMR and ^{13}C NMR Data of Compounds 2a-2o



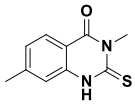
3-Methyl-2-thioxo-2,3-dihydroquinazolin-4(1*H*)-one (**2a**): white solid, yield 92.7%, m.p. 244-247 ^{o}C; ^{1}H NMR (500 MHz, DMSO) δ: 12.94 (s, 1H), 7.96 (dd, J = 8.0, 1.3 Hz, 1H), 7.75 – 7.72 (m, 1H), 7.39 (d, J = 8.2 Hz, 1H), 7.36 – 7.30 (m, 1H), 3.66 (s, 3H); ^{13}C NMR (125 MHz, DMSO) δ: 175.8, 160.1, 139.5, 135.8, 127.7, 124.8, 116.0, 115.7, 33.7.



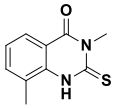
3,5-Dimethyl-2-thioxo-2,3-dihydroquinazolin-4(1*H*)-one (**2b**): white solid, yield 71.3%, m.p. 243-246 °C; ^{1}H NMR (500 MHz, DMSO) δ: 12.78 (s, 1H), 7.56 (t, J = 7.8 Hz, 1H), 7.26 (d, J = 8.2 Hz, 1H), 7.11 (d, J = 7.3 Hz, 1H), 3.63 (s, 3H), 2.69 (s, 3H); ^{13}C NMR (125 MHz, DMSO) δ: 175.3, 160.5, 141.5, 140.7, 134.8, 127.4, 114.2, 114.1, 33.8, 22.7.



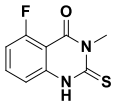
3,6-Dimethyl-2-thioxo-2,3-dihydroquinazolin-4(1*H*)-one (**2c**): white solid, yield 95.0%, m.p. 237-240 °C; ^{1}H NMR (500 MHz, DMSO) δ: 12.89 (s, 1H), 7.76 (s, 1H), 7.56 (d, J = 8.3 Hz, 1H), 7.30 (d, J = 8.3 Hz, 1H), 3.65 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (125 MHz, DMSO) δ: 175.3, 160.1, 137.5, 136.9, 134.4, 127.0, 116.0, 115.6, 33.7, 20.9.



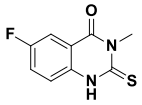
3,7-Dimethyl-2-thioxo-2,3-dihydroquinazolin-4(1*H*)-one (**2d**): white solid, yield 89.7%, m.p. 258-260 °C; ^{1}H NMR (500 MHz, DMSO) δ: 12.86 (s, 1H), 7.84 (d, J = 8.0 Hz, 1H), 7.16 (d, J = 8.7 Hz, 2H), 3.64 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (125 MHz, DMSO) δ: 175.8, 159.9, 146.6, 139.5, 127.7, 126.3, 115.6, 113.5, 33.7, 22.1



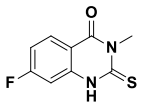
3,8-Dimethyl-2-thioxo-2,3-dihydroquinazolin-4(1*H*)-one (**2e**): white solid, yield 89.8%, m.p. 228-230 °C; ^{1}H NMR (500 MHz, DMSO) δ: 11.68 (s, 1H), 7.92 – 7.75 (m, 1H), 7.56 (d, J = 7.2 Hz, 1H), 7.23 (t, J = 7.6 Hz, 1H), 3.67 (s, 3H), 2.47 (s, 3H); ^{13}C NMR (125 MHz, DMSO) δ: 176.2, 160.1, 137.9, 136.9, 125.6, 124.8, 124.7, 116.1, 34.0, 17.7.



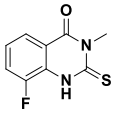
5-Fluoro-3-methyl-2-thioxo-2,3-dihydroquinazolin-4(1*H*)-one (**2f**): white solid, yield 81.1%, m.p. 280-283 °C; ^{1}H NMR (500 MHz, DMSO) δ: 12.98 (s, 1H), 7.74 – 7.69 (m, 1H), 7.20 (d, J = 8.3 Hz, 1H), 7.10 – 7.06 (m, 1H), 3.61 (s, 3H); ^{13}C NMR (125 MHz, DMSO) δ: 175.9, 161.22 (d, J = 262.1 Hz), 156.9 (d, J = 4.0 Hz), 141.1 (d, J = 2.2 Hz), 136.8 (d, J = 10.8 Hz), 112.1 (d, J = 4.2 Hz), 111.3 (d, J = 20.4 Hz), 105.6 (d, J = 9.4 Hz), 33.5.



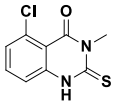
6-Fluoro-3-methyl-2-thioxo-2,3-dihydroquinazolin-4(1*H*)-one (**2g**): white solid, yield 82.5%, m.p. 266-269 °C; ^{1}H NMR (500 MHz, DMSO) δ: 12.98 (s, 1H), 7.69 – 7.56 (m, 2H), 7.43 – 7.40 (m, 1H), 3.64 (s, 3H); ^{13}C NMR (125 MHz, DMSO) δ: 175.3, 158.7 (d, J = 241.1 Hz), 159.4 (d, J = 3.2 Hz), 136.3, 123.9 (d, J = 24.5 Hz), 118.7 (d, J = 8.2 Hz), 116.9 (d, J = 8.2 Hz), 112.5 (d, J = 24.3 Hz), 33.8.



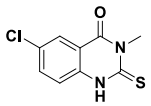
7-Fluoro-3-methyl-2-thioxo-2,3-dihydroquinazolin-4(1*H*)-one (**2h**): white solid, yield 59.8%, m.p. 241-244 °C; ^{1}H NMR (500 MHz, DMSO) δ: 12.97 (s, 1H), 8.03 – 8.00 (m, 1H), 7.19 – 7.15 (m, 1H), 7.13 – 7.07 (m, 1H), 3.63 (s, 3H); ^{13}C NMR (125 MHz, DMSO) δ: 176.3, 166.2 (d, J = 252.5 Hz), 159.3, 141.2 (d, J = 13.1 Hz), 131.2 (d, J = 11.3 Hz), 113.0 (d, J = 23.4 Hz), 112.8, 102.0 (d, J = 26.3 Hz), 33.7.



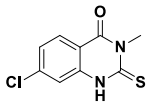
8-Fluoro-3-methyl-2-thioxo-2,3-dihydroquinazolin-4(1*H*)-one (**2i**): white solid, yield 75.0%, m.p. 217-219 °C; ^{1}H NMR (500 MHz, DMSO) δ: 12.88 (s, 1H), 7.78 (d, J = 8.0 Hz, 1H), 7.66 – 7.62 (m, 1H), 7.33 – 7.29 (m, 1H), 3.66 (s, 3H); ^{13}C NMR (125 MHz, DMSO) δ: 176.2, 159.11 (d, J = 3.0 Hz), 148.6 (d, J = 250.9 Hz), 128.6 (d, J = 14.4 Hz), 124.8 (d, J = 6.6 Hz), 123.4 (d, J = 3.7 Hz), 121.1 (d, J = 16.9 Hz), 117.9 (d, J = 1.5 Hz), 33.9.



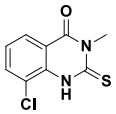
5-Chloro-3-methyl-2-thioxo-2,3-dihydroquinazolin-4(1*H*)-one (**2j**): white solid, yield 72.8%, m.p. 250-253 °C; ^{1}H NMR (500 MHz, DMSO) δ: 12.94 (s, 1H), 7.76 – 7.48 (m, 1H), 7.35 – 7.31 (m, 2H), 3.62 (s, 3H); ^{13}C NMR (125 MHz, DMSO) δ: 175.5, 157.8, 141.8, 135.5, 134.1, 127.2, 115.4, 112.6, 33.9.



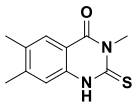
6-Chloro-3-methyl-2-thioxo-2,3-dihydroquinazolin-4(1*H*)-one (**2k**): white solid, yield 92.4%, m.p. 246-249 °C; ^{1}H NMR (500 MHz, DMSO) δ: 13.01 (s, 1H), 7.83 (d, J = 2.4 Hz, 1H), 7.75 (dd, J = 8.8, 2.5 Hz, 1H), 7.37 (d, J = 8.8 Hz, 1H), 3.63 (s, 3H); ^{13}C NMR (125 MHz, DMSO) δ: 175.7, 159.1, 138.2, 135.6, 128.7, 126.5, 118.3, 117.0, 33.8.



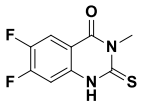
7-Chloro-3-methyl-2-thioxo-2,3-dihydroquinazolin-4(1*H*)-one (**2l**): white solid, yield 88.1%, m.p. 260-263 °C; ^{11}H NMR (500 MHz, DMSO) δ: 12.97 (s, 1H), 7.96 (d, J = 8.5 Hz, 1H), 7.40 (d, J = 1.8 Hz, 1H), 7.36 (dd, J = 8.5, 1.9 Hz, 1H), 3.64 (s, 3H); ^{13}C NMR (125 MHz, DMSO) δ: 176.3, 159.5, 140.4, 140.1, 129.9, 124.9, 115.4, 114.7, 33.8.



8-Chloro-3-methyl-2-thioxo-2,3-dihydroquinazolin-4(1*H*)-one (**2m**): white solid, yield 72.5%, m.p. 174-176 °C; ^{1}H NMR (500 MHz, DMSO) δ: 11.51 (s, 1H), 7.93 (dd, J = 7.9, 1.3 Hz, 1H), 7.86 (dd, J = 7.9, 1.3 Hz, 1H), 7.33 (t, J = 7.9 Hz, 1H), 3.66 (s, 3H); ^{13}C NMR (125 MHz, DMSO) δ: 176.4, 159.2, 136.1, 135.8, 127.0, 125.4, 118.7, 117.6, 34.2.

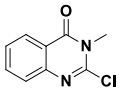


3,6,7-Trimethyl-2-thioxo-2,3-dihydroquinazolin-4(1*H*)-one (**2n**): white solid, yield 85.5%, m.p. 260-263 °C; ^{1}H NMR (500 MHz, DMSO) δ: 7.73 (s, 1H), 7.16 (s, 1H), 3.64 (s, 3H), 2.31 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (125 MHz, DMSO) δ: 175.3, 159.9, 145.9, 137.9, 133.9, 127.4, 116.2, 113.6, 33.7, 20.7, 19.4.

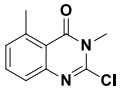


6,7-Difluoro-3-methyl-2-thioxo-2,3-dihydroquinazolin-4(1*H*)-one (**2o**): white solid, yield 53.4%, m.p. 275-276 °C; ^{1}H NMR (500 MHz, DMSO) *δ*: 13.00 (s, 1H), 7.90 (dd, *J* = 10.1, 8.4 Hz, 1H), 7.30 (dd, *J* = 10.9, 6.7 Hz, 1H), 3.62 (s, 3H); ^{13}C NMR (125 MHz, DMSO) *δ*: 175.9, 158.8, 154.3 (dd, *J* = 255.2, 14.7 Hz), 147.0 (dd, *J* = 245.6, 13.9 Hz), 137.2 (d, *J* = 11.0 Hz), 115.9 (d, *J* = 19.5 Hz), 112.8 (d, *J* = 6.5 Hz), 104.9 (d, *J* = 21.9 Hz), 33.8.

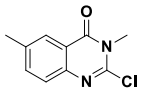
The ^{1}H NMR and ^{13}C NMR Data of Compounds 3a-3o



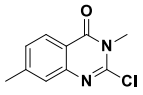
2-Chloro-3-methylquinazolin-4(3*H*)-one (**3a**): white solid, yield 60.3%, m.p. 109-110 °C; ^{1}H NMR (500 MHz, DMSO) *δ*: 8.12 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.85 (ddd, *J* = 8.5, 7.2, 1.5 Hz, 1H), 7.62 (d, *J* = 8.1 Hz, 1H), 7.59 – 7.55 (m, 1H), 3.63 (s, 3H); ^{13}C NMR (125 MHz, DMSO) *δ*: 161.8, 146.6, 145.8, 135.5, 127.9, 127.2, 126.8, 120.3, 33.6.



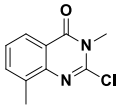
2-Chloro-3,5-dimethylquinazolin-4(3*H*)-one (**3b**): white solid, yield 48.9%, m.p. 118-119 °C; ^{1}H NMR (500 MHz, $CDCl_3$) *δ*: 7.58 (t, *J* = 7.8 Hz, 1H), 7.47 (d, *J* = 8.1 Hz, 1H), 7.25 (d, *J* = 7.4 Hz, 1H), 3.71 (s, 3H), 2.84 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) *δ*: 162.4, 147.7, 144.8, 141.6, 133.9, 130.1, 124.8, 118.5, 33.2, 22.9.



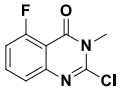
2-Chloro-3,6-dimethylquinazolin-4(3*H*)-one (**3c**): white solid, yield 52.6%, m.p. 130-133 °C; ^{1}H NMR (500 MHz, DMSO) *δ*: 7.89 (s, 1H), 7.66 (dd, *J* = 8.3, 1.9 Hz, 1H), 7.50 (d, *J* = 8.3 Hz, 1H), 3.61 (s, 3H), 2.44 (s, 3H); ^{13}C NMR (125 MHz, DMSO) *δ*: 161.7, 144.8, 144.6, 137.7, 136.7, 126.7, 126.4, 120.0, 33.5, 21.3.



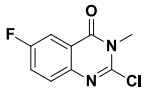
2-Chloro-3,7-dimethylquinazolin-4(3*H*)-one (**3d**): white solid, yield 54.2%, m.p. 90-92 °C; ^{1}H NMR (500 MHz, DMSO) *δ*: 7.99 (d, *J* = 8.1 Hz, 1H), 7.41 (s, 1H), 7.39 (d, *J* = 8.2 Hz, 1H), 3.61 (s, 3H), 2.46 (s, 3H); ^{13}C NMR (125 MHz, DMSO) *δ*: 161.7, 146.7, 146.2, 145.7, 129.3, 127.0, 126.4, 117.9, 33.5, 21.8.



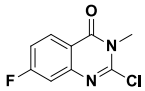
2-Chloro-3,8-dimethylquinazolin-4(3*H*)-one (**3e**): white solid, yield 49.8%, m.p. 107-108 °C; ^{1}H NMR (500 MHz, DMSO) δ: 7.94 (dd, J = 7.9, 0.7 Hz, 1H), 7.78 – 7.65 (m, 1H), 7.44 (t, J = 7.6 Hz, 1H), 3.62 (s, 3H), 2.48 (s, 3H); ^{13}C NMR (125 MHz, DMSO) δ: 162.1, 145.2, 144.8, 135.8, 135.0, 127.4, 124.8, 120.2, 33.6, 17.2.



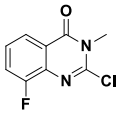
2-Chloro-5-fluoro-3-methylquinazolin-4(3*H*)-one (**3f**): white solid, yield 50.2%, m.p. 155-156 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.69 (td, J = 8.2, 5.4 Hz, 1H), 7.41 (d, J = 8.2 Hz, 1H), 7.18 – 7.10 (m, 1H), 3.73 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 161.2 (d, J = 266.7 Hz), 158.8 (d, J = 4.5 Hz), 148.1, 146.2, 135.3 (d, J = 10.3 Hz), 122.7 (d, J = 4.4 Hz), 114.1 (d, J = 20.9 Hz), 109.8 (d, J = 6.5 Hz), 33.2.



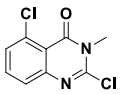
2-Chloro-6-fluoro-3-methylquinazolin-4(3*H*)-one (**3g**): white solid, yield 48.9%, m.p. 110-111 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.84 (dd, J = 8.3, 2.9 Hz, 1H), 7.63 (dd, J = 8.9, 4.8 Hz, 1H), 7.47 (ddd, J = 8.9, 8.1, 3.0 Hz, 1H), 3.76 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 161.3 (d, J = 3.6 Hz), 161.0 (d, J = 249.4 Hz), 144.5 (d, J = 2.3 Hz), 143.1 (d, J = 1.6 Hz), 129.1 (d, J = 8.3 Hz), 123.5 (d, J = 24.4 Hz), 121.4 (d, J = 9.1 Hz), 112.2 (d, J = 24.2 Hz), 33.5.



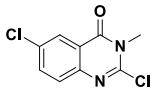
2-Chloro-7-fluoro-3-methylquinazolin-4(3*H*)-one (**3h**): white solid, yield 49.2%, m.p. 115-116 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.25 (dd, J = 8.9, 6.0 Hz, 1H), 7.30 – 7.27 (m, 1H), 7.22 (td, J = 8.5, 2.5 Hz, 1H), 3.76 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 166.69 (d, J = 255.8 Hz), 161.2, 148.4 (d, J = 13.5 Hz), 146.6, 130.1 (d, J = 10.8 Hz), 116.8 (d, J = 2.1 Hz), 116.3 (d, J = 23.7 Hz), 112.3 (d, J = 22.4 Hz), 33.4.



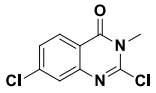
2-Chloro-8-fluoro-3-methylquinazolin-4(3*H*)-one (**3i**): white solid, yield 53.0%, m.p. 159-162 °C; ^{1}H NMR (500 MHz, DMSO) δ: 7.93 (d, J = 8.0 Hz, 1H), 7.74 (ddd, J = 10.4, 8.1, 1.3 Hz, 1H), 7.56 (td, J = 8.0, 4.8 Hz, 1H), 3.63 (s, 3H); ^{13}C NMR (125 MHz, DMSO) δ: 161.0, 155.9 (d, J = 254.1 Hz), 146.8, 135.8 (d, J = 12.7 Hz), 128.3 (d, J = 7.7 Hz), 122.9 (d, J = 4.2 Hz), 122.4 (s), 120.8 (d, J = 18.4 Hz), 33.8.



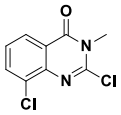
2,5-Dichloro-3-methylquinazolin-4(3*H*)-one (**3j**): white solid, yield 53.2%, m.p. 149-152 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.59 (t, J = 8.0 Hz, 1H), 7.51 – 7.47 (m, 2H), 3.73 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 159.8, 148.7, 145.8, 134.6, 134.2, 130.2, 125.9, 117.2, 33.6.



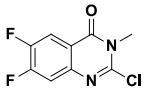
2,6-Dichloro-3-methylquinazolin-4(3*H*)-one (**3k**): white solid, yield 54.1%, m.p. 152-155 °C; ^{1}H NMR (500 MHz, DMSO) δ: 8.02 (d, J = 2.5 Hz, 1H), 7.87 (dd, J = 8.7, 2.5 Hz, 1H), 7.63 (d, J = 8.7 Hz, 1H), 3.62 (s, 3H); ^{13}C NMR (125 MHz, DMSO) δ: 160.8, 146.4, 145.3, 135.5, 132.0, 129.1, 126.1, 121.6, 33.8.



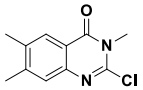
2,7-Dichloro-3-methylquinazolin-4(3*H*)-one (**3l**): white solid, yield 50.5%, m.p. 102-106 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.15 (d, J = 8.6 Hz, 1H), 7.60 (d, J = 1.9 Hz, 1H), 7.44 (dd, J = 8.6, 2.0 Hz, 1H), 3.75 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 161.4, 147.3, 146.4, 141.2, 128.7, 128.1, 126.3, 118.5, 33.4.



2,8-Dichloro-3-methylquinazolin-4(3*H*)-one (**3m**): white solid, yield 62.2%, m.p. 118-121 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.14 (d, J = 8.0 Hz, 1H), 7.82 (d, J = 7.8 Hz, 1H), 7.41 (t, J = 7.9 Hz, 1H), 3.77 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 161.5, 146.2, 143.4, 135.1, 131.1, 127.5, 126.0, 121.6, 33.6.

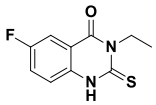


2-Chloro-6,7-difluoro-3-methylquinazolin-4(3*H*)-one (**3n**): white solid, yield 59.8%, m.p. 162-163 °C; ^{1}H NMR (500 MHz, DMSO) δ: 8.06 (dd, J = 10.3, 8.6 Hz, 1H), 7.78 (dd, J = 11.2, 7.2 Hz, 1H), 3.62 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 160.6, 155.2 (dd, J = 259.2, 14.7 Hz), 150.0 (dd, J = 253.3, 14.1 Hz), 145.9, 144.1 (d, J = 9.2 Hz), 117.1 (d, J = 6.5 Hz), 114.8 (d, J = 17.6 Hz), 114.7 (dd, J = 20.2, 2.5 Hz), 33.5.

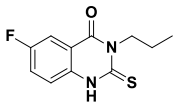


2-Chloro-3,6,7-trimethylquinazolin-4(3*H*)-one (**3o**): white solid, yield 50.6%, m.p. 164-166 °C; ^{1}H NMR (500 MHz, DMSO) δ: 7.86 (s, 1H), 7.40 (s, 1H), 3.61 (s, 3H), 2.37 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (125 MHz, DMSO) δ: 161.6, 145.6, 145.0, 144.8, 137.3, 126.8, 126.7, 118.0, 33.5, 20.3, 19.7.

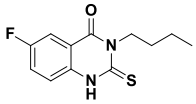
The ^{1}H NMR and ^{13}C NMR Data of Compounds 5a-5n



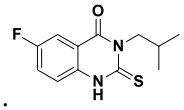
3-Ethyl-6-fluoro-2-thioxo-2,3-dihydroquinazolin-4(1*H*)-one (**5a**): white solid, yield 83.5%, m.p. 246-247 °C; ^{1}H NMR (500 MHz, DMSO) δ: 12.99 (s, 1H), 7.82 – 7.55 (m, 2H), 7.53 – 7.37 (m, 1H), 4.44 (q, J = 7.0 Hz, 2H), 1.23 (t, J = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, DMSO) δ: 174.8, 158.9 (d, J = 3.2 Hz), 158.8 (d, J = 243.2 Hz), 136.4, 124.1 (d, J = 24.6 Hz), 118.7 (d, J = 8.2 Hz), 117.3 (d, J = 8.3 Hz), 112.6 (d, J = 24.3 Hz), 41.6, 12.3.



6-Fluoro-3-propyl-2-thioxo-2,3-dihydroquinazolin-4(1*H*)-one (**5b**): white solid, yield 76.0%, m.p. 232-235 ºC; ^{1}H NMR (500 MHz, DMSO) *δ*: 13.00 (s, 1H), 7.78 – 7.56 (m, 2H), 7.48 – 7.32 (m, 1H), 4.42 – 4.19 (m, 2H), 1.77 – 1.57 (m, 2H), 0.91 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (125 MHz, DMSO) *δ*: 175.1, 159.1 (d, *J* = 2.8 Hz), 158.8 (d, *J* = 243.2 Hz), 136.4, 124.1 (d, *J* = 24.7 Hz), 118.8 (d, *J* = 8.2 Hz), 117.2 (d, *J* = 8.2 Hz), 112.7 (d, *J* = 24.1 Hz), 47.7, 20.1, 11.6.



3-Butyl-6-fluoro-2-thioxo-2,3-dihydroquinazolin-4(1*H*)-one (**5c**): white solid, yield 71.5%, m.p. 203-204 ºC; ^{1}H NMR (500 MHz, DMSO) *δ*: 12.99 (s, 1H), 7.73 – 7.55 (m, 2H), 7.43 (dd, *J* = 9.9, 4.4 Hz, 1H), 4.46 – 4.27 (m, 2H), 1.66 (dt, *J* = 15.2, 7.6 Hz, 2H), 1.43 – 1.25 (m, 2H), 0.93 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (125 MHz, DMSO) *δ*: 174.9, 159.0 (d, *J* = 3.0 Hz), 158.8 (d, *J* = 243.2 Hz), 136.4, 124.1 (d, *J* = 24.6 Hz), 118.7 (d, *J* = 8.2 Hz), 117.2 (d, *J* = 8.2 Hz), 112.6 (d, *J* = 24.1 Hz), 46.0, 28.8, 20.1, 14.1.



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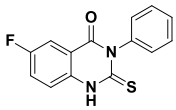
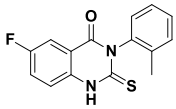
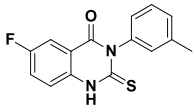
6-Fluoro-3-isobutyl-2-thioxo-2,3-dihydroquinazolin-4(1*H*)-one (**5d**): white solid, yield 37.5%, m.p. 217-219 ºC; ^{1}H NMR (500 MHz, DMSO) *δ*: 13.00 (s, 1H), 7.75 – 7.56 (m, 2H), 7.46 – 7.43 (m, 1H), 4.27 (d, *J* = 7.4 Hz, 2H), 2.39 – 2.31 (m, 1H), 0.90 (s, 3H), 0.88 (s, 3H); ^{13}C NMR (125 MHz, DMSO) *δ*: 175.6, 159.6 (d, *J* = 2.8 Hz), 158.8 (d, *J* = 243.2 Hz), 136.5, 124.1 (d, *J* = 24.6 Hz), 118.8 (d, *J* = 8.1 Hz), 117.1 (d, *J* = 8.2 Hz), 112.8 (d, *J* = 24.3 Hz), 52.4, 26.7, 20.5.



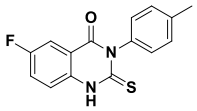
6-Fluoro-3-phenyl-2-thioxo-2,3-dihydroquinazolin-4(1*H*)-one (**5e**): white solid, yield 84.0%, m.p. 264-267 ºC; ^{1}H NMR (500 MHz, DMSO) *δ*: 13.12 (s, 1H), 7.76 – 7.64 (m, 2H), 7.55 – 7.45 (m, 3H), 7.43 – 7.38 (m, 1H), 7.29 – 7.27 (m, 2H); ^{13}C NMR (125 MHz, DMSO) *δ*: 176.1, 159.7, 158.7 (d, *J* = 239.2 Hz), 139.6, 137.0, 129.4, 128.7, 124.2 (d, *J* = 24.6 Hz), 118.9 (d, *J* = 7.8 Hz), 118.0 (d, *J* = 8.1 Hz), 112.9 (d, *J* = 24.2 Hz).



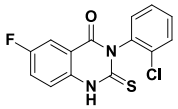
6-Fluoro-2-thioxo-3-(*o*-tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (**5f**): white solid, yield 80.9%, m.p. 271-274 ºC; ^{1}H NMR (500 MHz, DMSO) *δ*: 13.19 (s, 1H), 7.78 – 7.64 (m, 2H), 7.52 (dd, *J* = 9.0, 4.5 Hz, 1H), 7.36 – 7.27 (m, 3H), 7.22 – 7.18 (m, 1H), 2.05 (s, 3H); ^{13}C NMR (125 MHz, DMSO) *δ*: 175.3, 159.2 (d, *J* = 2.7 Hz), 158.5 (d, *J* = 243.2 Hz), 138.6, 137.1, 135.7, 130.9, 129.2, 128.9, 127.3, 124.4 (d, *J* = 24.6 Hz), 118.9 (d, *J* = 8.1 Hz), 117.6 (d, *J* = 8.1 Hz), 112.9 (d, *J* = 24.1 Hz), 17.4.



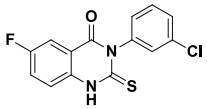
6-Fluoro-2-thioxo-3-(*m*-tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (**5g**): white solid, yield 83.3%, m.p. 267-270 °C; ^{1}H NMR (500 MHz, DMSO) δ: 13.10 (s, 1H), 7.71 (td, *J* = 8.7, 3.0 Hz, 1H), 7.66 (dd, *J* = 8.4, 2.9 Hz, 1H), 7.50 (dd, *J* = 9.0, 4.5 Hz, 1H), 7.36 (t, *J* = 7.7 Hz, 1H), 7.22 (d, *J* = 7.6 Hz, 1H), 7.08 – 7.06 (m, 2H), 2.34 (s, 3H); ^{13}C NMR (125 MHz, DMSO) δ: 176.1, 159.6 (d, *J* = 2.8 Hz), 158.7 (d, *J* = 243.2 Hz), 139.5, 138.7, 136.9, 129.7, 129.3 (d, *J* = 16.3 Hz), 126.4, 124.2 (d, *J* = 24.4 Hz), 118.8 (d, *J* = 8.0 Hz), 117.9 (d, *J* = 8.2 Hz), 112.9 (d, *J* = 24.0 Hz), 21.3.



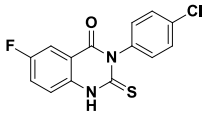
6-Fluoro-2-thioxo-3-(*p*-tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (**5h**): white solid, yield 81.7%, m.p. 276-279 °C; ^{1}H NMR (500 MHz, DMSO) δ: 13.09 (s, 1H), 7.74 – 7.63 (m, 2H), 7.49 (dd, *J* = 9.0, 4.5 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.14 (d, *J* = 8.2 Hz, 2H), 2.37 (s, 3H); ^{13}C NMR (125 MHz, DMSO) δ: 176.2, 159.7 (d, *J* = 3.2 Hz), 158.7 (d, *J* = 243.0 Hz), 137.9, 137.0 (d, *J* = 10.2 Hz), 129.9, 129.1, 124.2 (d, *J* = 24.8 Hz), 118.8 (d, *J* = 8.1 Hz), 117.9 (d, *J* = 8.2 Hz), 112.9 (d, *J* = 24.1 Hz), 21.3.



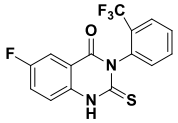
3-(2-Chlorophenyl)-6-fluoro-2-thioxo-2,3-dihydroquinazolin-4(1*H*)-one (**5i**): white solid, yield 69.9%, m.p. 273-276 °C; ^{1}H NMR (500 MHz, DMSO) δ: 13.30 (s, 1H), 7.78 – 7.69 (m, 2H), 7.64 – 7.61 (m, 1H), 7.55 – 7.45 (m, 4H); ^{13}C NMR (125 MHz, DMSO) δ: 175.1, 158.9 (d, *J* = 2.7 Hz), 158.8 (d, *J* = 243.0 Hz), 137.1, 136.8, 131.9, 131.7, 130.8, 130.2, 128.6, 124.7 (d, *J* = 24.6 Hz), 119.1 (d, *J* = 8.0 Hz), 117.4 (d, *J* = 8.2 Hz), 113.0 (d, *J* = 24.2 Hz).



3-(3-Chlorophenyl)-6-fluoro-2-thioxo-2,3-dihydroquinazolin-4(1*H*)-one (**5j**): white solid, yield 70.9%, m.p. 250-253 °C; ^{1}H NMR (500 MHz, DMSO) δ: 13.13 (s, 1H), 7.75 – 7.65 (m, 2H), 7.55 – 7.45 (m, 4H), 7.31 – 7.29 (m, 1H); ^{13}C NMR (125 MHz, DMSO) δ: 175.8, 159.6 (d, *J* = 2.9 Hz), 158.7 (d, *J* = 243.0 Hz), 140.9, 137.1, 133.4, 130.9, 129.7, 128.8, 128.5, 124.3 (d, *J* = 24.3 Hz), 118.9 (d, *J* = 8.1 Hz), 118.1 (d, *J* = 8.0 Hz), 112.9 (d, *J* = 24.1 Hz).

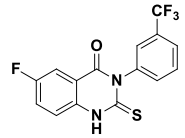


3-(4-Chlorophenyl)-6-fluoro-2-thioxo-2,3-dihydroquinazolin-4(1*H*)-one (**5k**): white solid, yield 86.6%, m.p. 269-272 °C; ^{1}H NMR (500 MHz, DMSO) δ: 13.16 (s, 1H), 7.74 – 7.65 (m, 2H), 7.59 – 7.53 (m, 2H), 7.50 (dd, *J* = 9.0, 4.4 Hz, 1H), 7.37 – 7.31 (m, 2H); ^{13}C NMR (125 MHz, DMSO) δ: 175.9, 159.6 (d, *J* = 2.7 Hz), 158.7 (d, *J* = 243.0 Hz), 138.6, 136.9, 133.3, 131.5, 129.5, 124.3 (d, *J* = 24.6 Hz), 118.9 (d, *J* = 8.0 Hz), 118.1 (d, *J* = 8.2 Hz), 112.9 (d, *J* = 24.3 Hz).



6-Fluoro-2-thioxo-3-(2-(trifluoromethyl)phenyl)-2,3-dihydroquinazolin-4(1*H*)-one (**5l**): white solid, yield 68.2%, m.p. 131-134 °C; ^{1}H NMR (500 MHz, DMSO) δ: 13.29 (s, 1H), 7.91 – 7.81 (m,

2H), 7.79 – 7.66 (m, 3H), 7.60 (d, *J* = 7.9 Hz, 1H), 7.53 (dd, *J* = 9.0, 4.4 Hz, 1H); ^{13}C NMR (125 MHz, DMSO) *δ*: 175.9, 159.6 (d, *J* = 3.0 Hz), 158.8 (d, *J* = 244.4 Hz), 137.1, 136.9, 134.1, 132.6, 130.0, 127.6 (q, *J* = 4.4 Hz), 126.6 (q, *J* = 30.4 Hz), 124.7 (d, *J* = 24.6 Hz), 122.6, 119.1 (d, *J* = 8.1 Hz), 117.4 (d, *J* = 8.2 Hz), 112.9 (d, *J* = 24.2 Hz).



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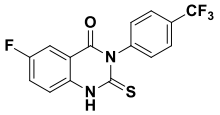
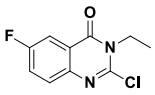
6-Fluoro-2-thioxo-3-(3-(trifluoromethyl)phenyl)-2,3-dihydroquinazolin-4(1*H*)-one (**5m**): white solid, yield 48.9%, m.p. 244-247 °C; ^{1}H NMR (500 MHz, DMSO) *δ*: 13.21 (s, 1H), 7.80 – 7.79 (m, 2H), 7.73 (td, *J* = 8.6, 3.0 Hz, 2H), 7.68 (dd, *J* = 8.4, 2.9 Hz, 1H), 7.64 (d, *J* = 7.9 Hz, 1H), 7.51 (dd, *J* = 9.0, 4.5 Hz, 1H); ^{13}C NMR (125 MHz, DMSO) *δ*: 175.9, 159.7 (d, *J* = 3.4 Hz), 158.7 (d, *J* = 243.7 Hz), 140.4, 137.0, 134.0, 130.2 (q, *J* = 16.4 Hz), 127.7, 126.8 (q, *J* = 3.8 Hz), 125.6 (d, *J* = 3.7 Hz), 125.5 (d, *J* = 3.7 Hz), 124.3 (d, *J* = 24.5 Hz), 121.2, 118.9 (d, *J* = 8.1 Hz), 118.2 (d, *J* = 8.2 Hz), 112.9 (d, *J* = 24.2 Hz).

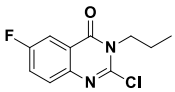


6-Fluoro-2-thioxo-3-(4-(trifluoromethyl)phenyl)-2,3-dihydroquinazolin-4(1*H*)-one (**5n**): white solid, yield 87.1%, m.p. 269-272 °C; ^{1}H NMR (500 MHz, DMSO) *δ*: 13.22 (s, 1H), 7.88 (d, *J* = 8.4 Hz, 2H), 7.76 – 7.66 (m, 2H), 7.57 (d, *J* = 8.2 Hz, 2H), 7.51 (dd, *J* = 9.0, 4.4 Hz, 1H); ^{13}C NMR (125 MHz, DMSO) *δ*: 175.7, 159.6 (d, *J* = 3.1 Hz), 158.7 (d, *J* = 243.2 Hz), 143.4, 137.1, 130.8, 129.2 (d, *J* = 31.7 Hz), 126.6 (d, *J* = 3.6 Hz), 125.7, 124.3 (d, *J* = 24.4 Hz), 123.5, 118.9 (d, *J* = 7.9 Hz), 118.1 (d, *J* = 8.2 Hz), 112.9 (d, *J* = 24.3 Hz).

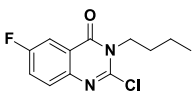
The ^{1}H NMR, ^{13}C NMR Data of Compounds 6a-6n



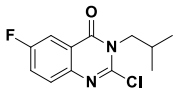
2-Chloro-3-ethyl-6-fluoroquinazolin-4(3*H*)-one (**6a**): white solid, yield 60.6%, m.p. 79-80 °C; ^{1}H NMR (500 MHz, $CDCl_3$) *δ*: 7.86 (dd, *J* = 8.3, 2.9 Hz, 1H), 7.63 (dd, *J* = 8.9, 4.8 Hz, 1H), 7.49 – 7.45 (m, 1H), 4.37 (q, *J* = 7.1 Hz, 2H), 1.41 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) *δ*: 160.9 (d, *J* = 3.5 Hz), 144.0, 143.2 (d, *J* = 1.7 Hz), 129.1 (d, *J* = 8.4 Hz), 123.5 (d, *J* = 24.1 Hz), 121.7 (d, *J* = 8.8 Hz), 112.2 (d, *J* = 24.0 Hz), 42.3, 13.6.



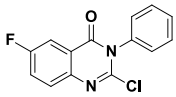
2-Chloro-6-fluoro-3-propylquinazolin-4(3*H*)-one (**6b**): white solid, yield 76.3%, m.p. 70-72 °C; ^{1}H NMR (500 MHz, $CDCl_3$) *δ*: 7.86 (dd, *J* = 8.3, 2.9 Hz, 1H), 7.63 (dd, *J* = 8.9, 4.8 Hz, 1H), 7.49 – 7.45 (m, 1H), 4.30 – 4.20 (m, 2H), 1.89 – 1.73 (m, 2H), 1.03 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) *δ*: 161.1 (d, *J* = 3.4 Hz), 161.0 (d, *J* = 249.5 Hz), 144.2 (d, *J* = 2.0 Hz), 143.1 (d, *J* = 1.7 Hz), 129.1 (d, *J* = 8.3 Hz), 123.4 (d, *J* = 24.3 Hz), 121.7 (d, *J* = 8.6 Hz), 112.3 (d, *J* = 24.1 Hz), 48.4, 21.8, 11.1.



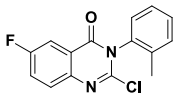
3-Butyl-2-chloro-6-fluoroquinazolin-4(3*H*)-one (**6c**): white solid, yield 65.0%, m.p. 61-62 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.85 (dd, *J* = 8.3, 2.9 Hz, 1H), 7.63 (dd, *J* = 8.9, 4.8 Hz, 1H), 7.47 (td, *J* = 8.5, 3.0 Hz, 1H), 4.36 – 4.20 (m, 2H), 1.77 (dt, *J* = 12.7, 7.7 Hz, 2H), 1.56 – 1.36 (m, 2H), 1.00 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 161.1 (d, *J* = 3.5 Hz), 161.0 (d, *J* = 249.5 Hz), 144.2 (d, *J* = 2.4 Hz), 143.1 (d, *J* = 1.7 Hz), 129.1 (d, *J* = 8.3 Hz), 123.4 (d, *J* = 24.4 Hz), 121.7 (d, *J* = 8.6 Hz), 112.2 (d, *J* = 23.9 Hz), 46.8, 30.4, 20.0, 13.7.



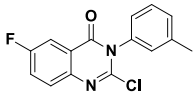
2-Chloro-6-fluoro-3-isobutylquinazolin-4(3*H*)-one (**6d**): white solid, yield 53.4%, m.p. 77-78 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.90 – 7.82 (m, 1H), 7.67 – 7.61 (m, 1H), 7.52 – 7.43 (m, 1H), 4.15 (d, *J* = 7.5 Hz, 2H), 2.32 – 2.24 (m, 1H), 1.01 (s, 3H), 0.99 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 161.4 (d, *J* = 3.3 Hz), 161.1 (d, *J* = 249.5 Hz), 144.5 (d, *J* = 2.2 Hz), 143.1 (d, *J* = 1.6 Hz), 129.1 (d, *J* = 8.3 Hz), 123.5 (d, *J* = 24.2 Hz), 121.7 (d, *J* = 8.7 Hz), 112.4 (d, *J* = 24.0 Hz), 53.3, 28.1, 19.9.



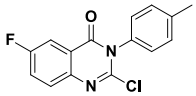
2-Chloro-6-fluoro-3-phenylquinazolin-4(3*H*)-one (**6e**): white solid, yield 74.1%, m.p. 167-168 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.87 (dd, *J* = 8.2, 2.9 Hz, 1H), 7.71 (dd, *J* = 8.9, 4.7 Hz, 1H), 7.60 – 7.47 (m, 4H), 7.32 – 7.28 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 161.3 (d, *J* = 3.2 Hz), 161.2 (d, *J* = 250.7 Hz), 143.7 (d, *J* = 2.2 Hz), 143.3 (d, *J* = 1.9 Hz), 137.0, 129.8, 129.4 (d, *J* = 8.3 Hz), 128.2, 123.7 (d, *J* = 24.1 Hz), 122.1 (d, *J* = 9.0 Hz), 112.6 (d, *J* = 24.0 Hz).



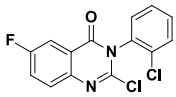
2-Chloro-6-fluoro-3-(*o*-tolyl)quinazolin-4(3*H*)-one (**6f**): white solid, yield 66.0%, m.p. 152-154 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.91 (dd, *J* = 8.2, 2.9 Hz, 1H), 7.73 (dd, *J* = 8.9, 4.7 Hz, 1H), 7.55 – 7.51 (m, 1H), 7.47 – 7.34 (m, 3H), 7.20 – 7.16 (m, 1H), 2.17 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 161.3 (d, *J* = 249.5 Hz), 160.8 (d, *J* = 3.2 Hz), 143.9 (d, *J* = 1.9 Hz), 143.5 (d, *J* = 1.8 Hz), 136.3, 135.6, 131.4, 130.1, 129.4 (d, *J* = 8.3 Hz), 128.2, 127.5, 123.8 (d, *J* = 24.1 Hz), 122.0 (d, *J* = 8.9 Hz), 112.7 (d, *J* = 23.9 Hz), 17.4.



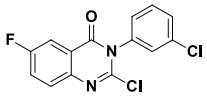
2-Chloro-6-fluoro-3-(*m*-tolyl)quinazolin-4(3*H*)-one (**6g**): white solid, yield 52.8%, m.p. 157-158 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.89 (dd, *J* = 8.2, 2.9 Hz, 1H), 7.71 (dd, *J* = 8.9, 4.7 Hz, 1H), 7.55 – 7.49 (m, 1H), 7.44 (t, *J* = 7.6 Hz, 1H), 7.34 (d, *J* = 7.7 Hz, 1H), 7.09 (d, *J* = 8.1 Hz, 2H), 2.44 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 161.4 (d, *J* = 3.5 Hz), 161.2 (d, *J* = 250.7 Hz), 143.8 (d, *J* = 2.4 Hz), 143.3 (d, *J* = 1.5 Hz), 140.0, 136.9, 130.7, 129.6, 129.4 (d, *J* = 8.3 Hz), 128.6, 125.1, 123.7 (d, *J* = 24.1 Hz), 122.1 (d, *J* = 9.1 Hz), 112.6 (d, *J* = 24.1 Hz), 21.3.



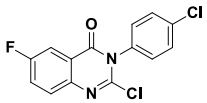
2-Chloro-6-fluoro-3-(*p*-tolyl)quinazolin-4(3*H*)-one (**6h**): white solid, yield 65.4%, m.p. 159-160 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.90 – 7.86 (m, 1H), 7.70 (dd, *J* = 8.9, 4.8 Hz, 1H), 7.54 – 7.48 (m, 1H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.16 (d, *J* = 8.3 Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 161.4 (d, *J* = 3.1 Hz), 161.2 (d, *J* = 250.7 Hz), 144.0 (d, *J* = 2.3 Hz), 143.3 (d, *J* = 2.1 Hz), 140.0, 134.5, 130.5, 129.4 (d, *J* = 8.3 Hz), 127.9, 123.7 (d, *J* = 24.2 Hz), 122.1 (d, *J* = 9.0 Hz), 112.6 (d, *J* = 24.0 Hz), 21.3.



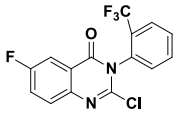
2-Chloro-3-(2-chlorophenyl)-6-fluoroquinazolin-4(3*H*)-one (**6i**): white solid, yield 45.5%, m.p. 158-160 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.91 (dd, *J* = 8.1, 2.9 Hz, 1H), 7.74 (dd, *J* = 8.9, 4.7 Hz, 1H), 7.62 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.58 – 7.45 (m, 3H), 7.37 (dd, *J* = 7.6, 1.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 161.3 (d, *J* = 250.7 Hz), 160.5 (d, *J* = 3.4 Hz), 143.4 (d, *J* = 1.9 Hz), 143.0 (d, *J* = 2.2 Hz), 134.8, 132.8, 131.3, 130.6, 130.0, 129.5 (d, *J* = 8.3 Hz), 128.2, 123.9 (d, *J* = 24.0 Hz), 121.9 (d, *J* = 8.7 Hz), 112.8 (d, *J* = 24.1 Hz).



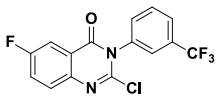
2-Chloro-3-(3-chlorophenyl)-6-fluoroquinazolin-4(3*H*)-one (**6j**): white solid, yield 53.4%, m.p. 172-175 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.88 (dd, *J* = 8.1, 2.9 Hz, 1H), 7.72 (dd, *J* = 8.9, 4.7 Hz, 1H), 7.57 – 7.48 (m, 3H), 7.33 (t, *J* = 1.8 Hz, 1H), 7.21 (dt, *J* = 7.1, 1.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 161.3 (d, *J* = 250.7 Hz), 161.1 (d, *J* = 3.4 Hz), 143.2 (d, *J* = 1.8 Hz), 142.9 (d, *J* = 2.3 Hz), 137.9, 135.4, 130.8, 130.2, 129.5 (d, *J* = 8.3 Hz), 128.8, 126.7, 123.9 (d, *J* = 24.3 Hz), 121.9 (d, *J* = 8.5 Hz), 112.7 (d, *J* = 24.0 Hz).



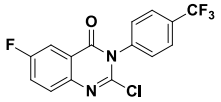
2-Chloro-3-(4-chlorophenyl)-6-fluoroquinazolin-4(3*H*)-one (**6k**): white solid, yield 36.8%, m.p. 165-166 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.88 (dd, *J* = 8.1, 2.9 Hz, 1H), 7.72 (dd, *J* = 8.9, 4.7 Hz, 1H), 7.57 – 7.51 (m, 3H), 7.25 – 7.21 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 161.3 (d, *J* = 250.7 Hz), 161.2 (d, *J* = 3.5 Hz), 143.2 (d, *J* = 2.3 Hz), 143.1 (d, *J* = 2.5 Hz), 136.0, 135.4, 130.1, 129.7, 129.5 (d, *J* = 8.3 Hz), 123.9 (d, *J* = 24.1 Hz), 121.9 (d, *J* = 8.9 Hz), 112.7 (d, *J* = 24.0 Hz).



2-Chloro-6-fluoro-3-(2-(trifluoromethyl)phenyl)quinazolin-4(3*H*)-one (**6l**): white solid, yield 37.0%, m.p. 166-169 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.91 – 7.86 (m, 2H), 7.80 – 7.77 (m, 1H), 7.75 – 7.68 (m, 2H), 7.56 – 7.52 (m, 1H), 7.41 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 161.4 (d, *J* = 250.7 Hz), 161.1 (d, *J* = 3.2 Hz), 143.3 (d, *J* = 1.8 Hz), 142.9 (d, *J* = 2.1 Hz), 134.7 (d, *J* = 1.6 Hz), 133.6, 130.9, 130.6, 129.6 (d, *J* = 8.3 Hz), 128.4, 128.2, 127.9 (dd, *J* = 9.3, 4.6 Hz), 127.7, 126.0, 123.9 (d, *J* = 24.0 Hz), 123.8, 121.7, 121.7 (d, *J* = 3.6 Hz), 119.5, 112.8 (d, *J* = 24.4 Hz).

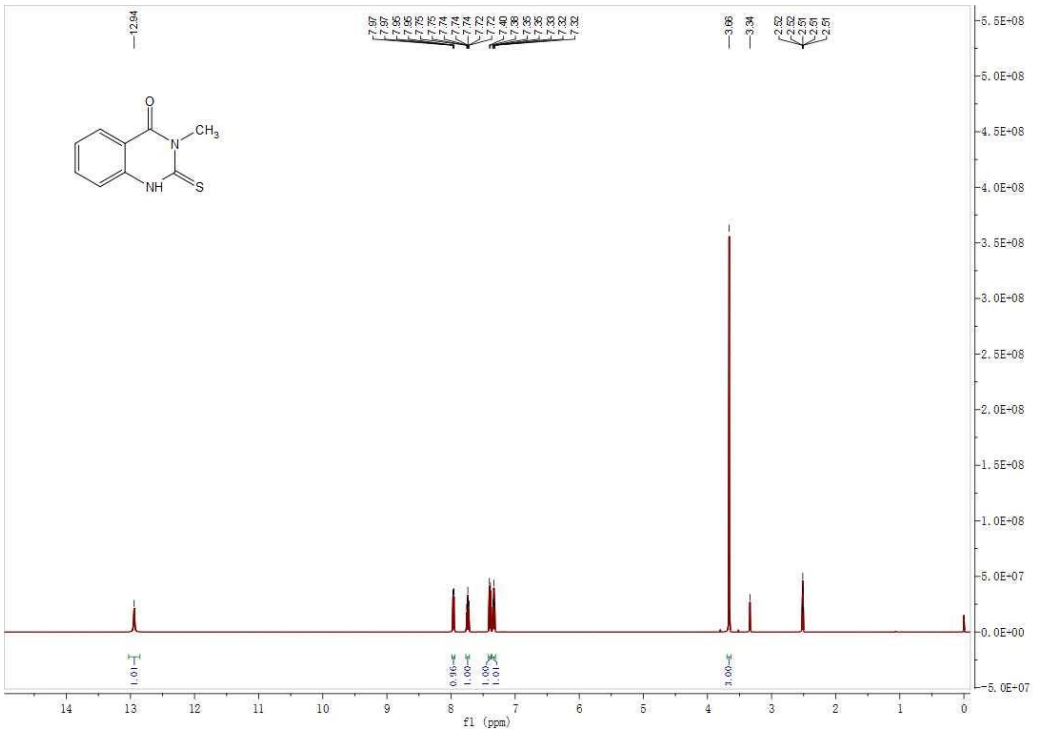


2-Chloro-6-fluoro-3-(3-(trifluoromethyl)phenyl)quinazolin-4(3*H*)-one (**6m**): white solid, yield 60.6%, m.p. 155-158 ºC; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.88 (dd, J = 8.1, 2.9 Hz, 1H), 7.82 (d, J = 7.9 Hz, 1H), 7.76 – 7.70 (m, 2H), 7.60 (s, 1H), 7.58 – 7.49 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 161.4 (d, J = 252.0 Hz), 161.1 (d, J = 3.4 Hz), 143.2 (d, J = 1.8 Hz), 142.7 (d, J = 2.2 Hz), 137.4, 132.5 (q, J = 33.4 Hz), 131.9, 130.5, 129.6 (d, J = 8.3 Hz), 126.8 (q, J = 3.6 Hz), 125.7 (q, J = 3.7 Hz), 124.1 (d, J = 24.3 Hz), 123.3 (q, J = 273.4 Hz), 121.9 (d, J = 9.0 Hz), 112.7 (d, J = 24.0 Hz).



2-Chloro-6-fluoro-3-(4-(trifluoromethyl)phenyl)quinazolin-4(3*H*)-one (**6n**): white solid, yield 50.3%, m.p. 180-182 ºC; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.90 – 7.83 (m, 3H), 7.73 (dd, J = 8.9, 4.7 Hz, 1H), 7.57 – 7.52 (m, 1H), 7.45 (d, J = 8.3 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 161.4 (d, J = 250.7 Hz), 161.1 (d, J = 3.4 Hz), 143.2 (d, J = 2.2 Hz), 142.5 (d, J = 2.4 Hz), 139.9, 132.1 (q, J = 33.1 Hz), 129.6 (d, J = 8.4 Hz), 129.1, 127.1 (q, J = 3.6 Hz), 124.1 (d, J = 24.3 Hz), 123.5 (q, J = 273.4 Hz), 121.9 (d, J = 9.0 Hz), 112.7 (d, J = 24.0 Hz).

The ^{1}H NMR and ^{13}C NMR Spectrum of intermediates 2a-2o, 3a-3o, 5a-5n, and 6a-6n


12.94
7.97
7.96
7.75
7.74
7.72
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3.34
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2.51
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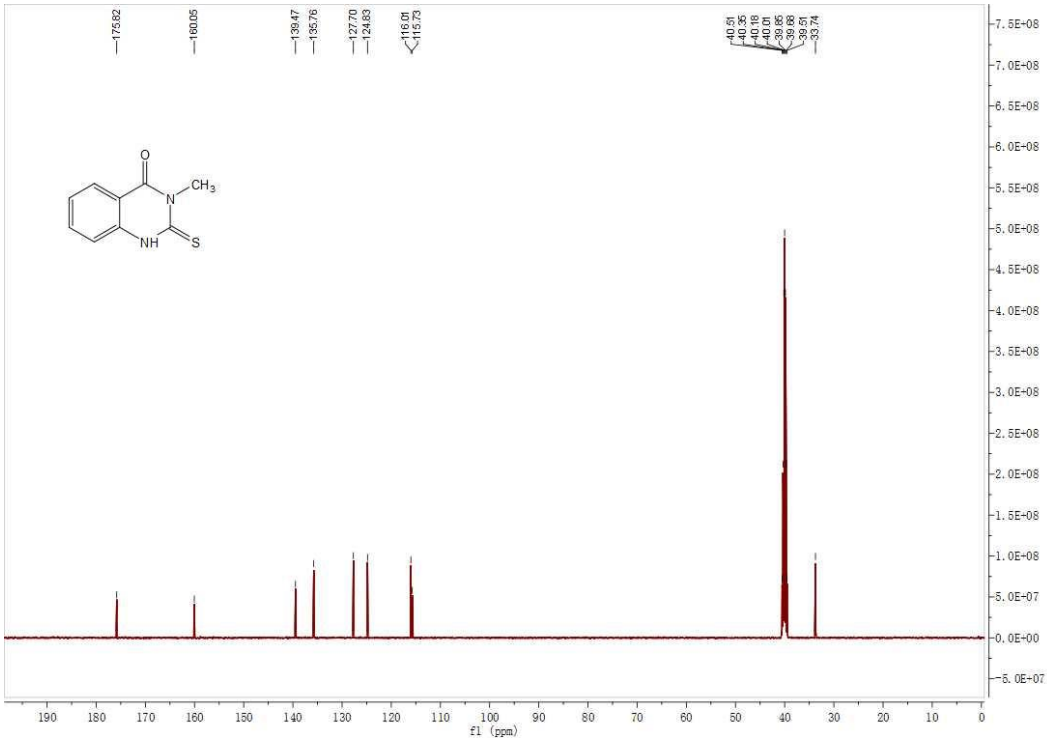
CH3
NH
S
f1 (ppm)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124.63
116.01
115.73
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40.01
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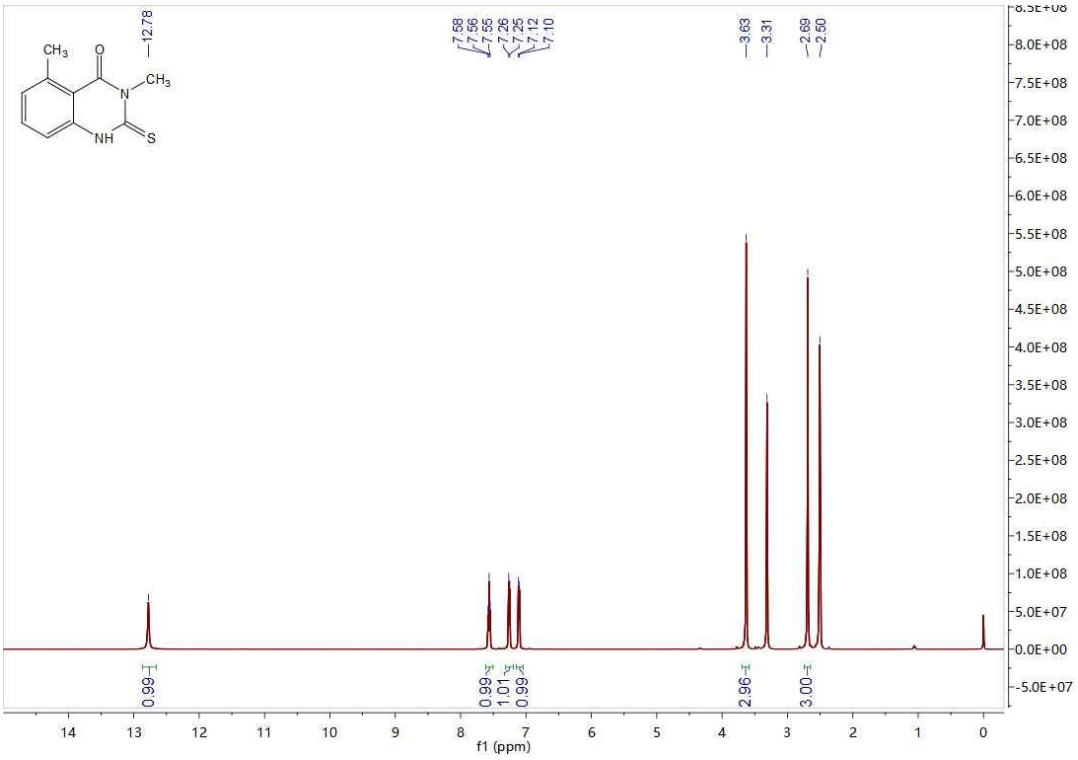
39.68
39.51
33.74
O
N
CH3
NH
S
f1 (ppm)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7.25
7.12
7.10
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2.69
2.50
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0.99
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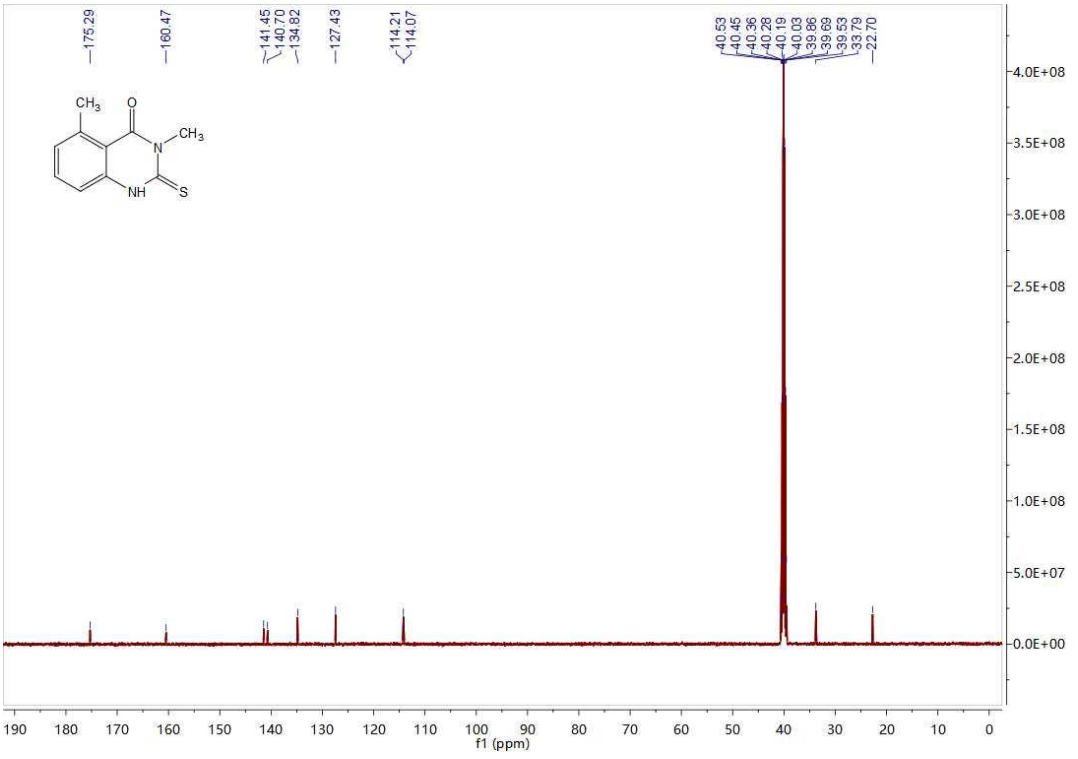
0.99
2.96
3.00
f1 (ppm)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114.21
114.07
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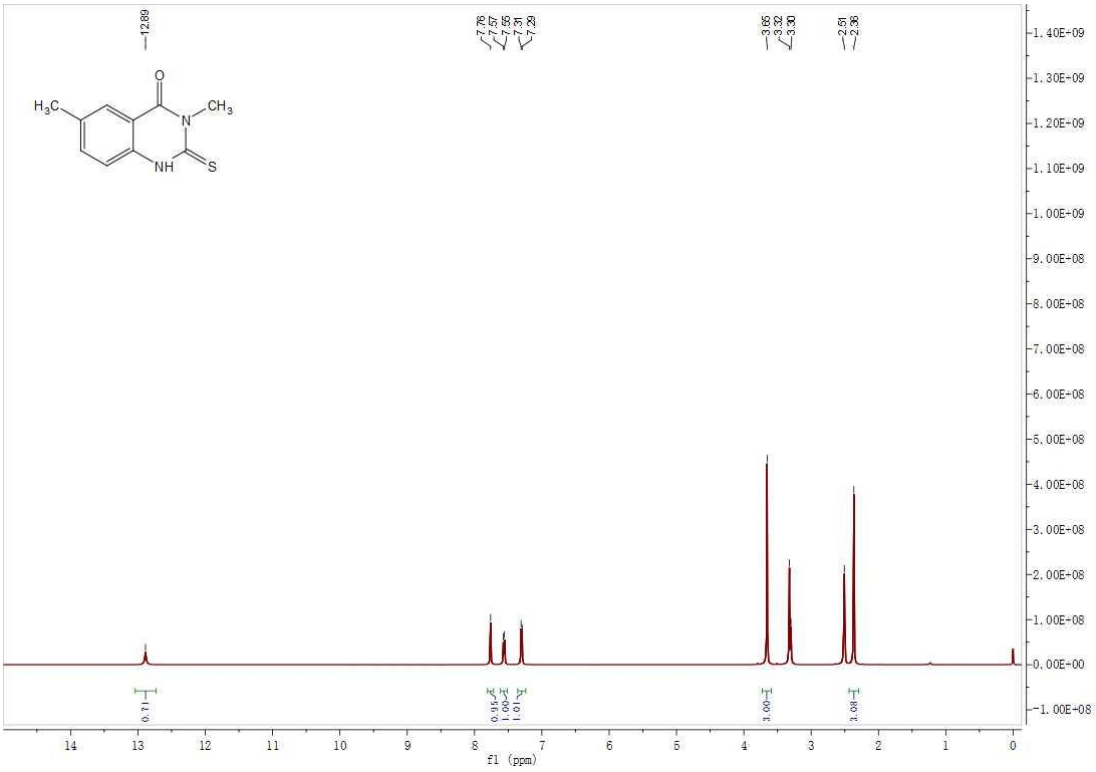
39.69
39.53
33.79
22.70
f1 (ppm)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7.29
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3.32
3.30
2.51
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H3C
NH
S
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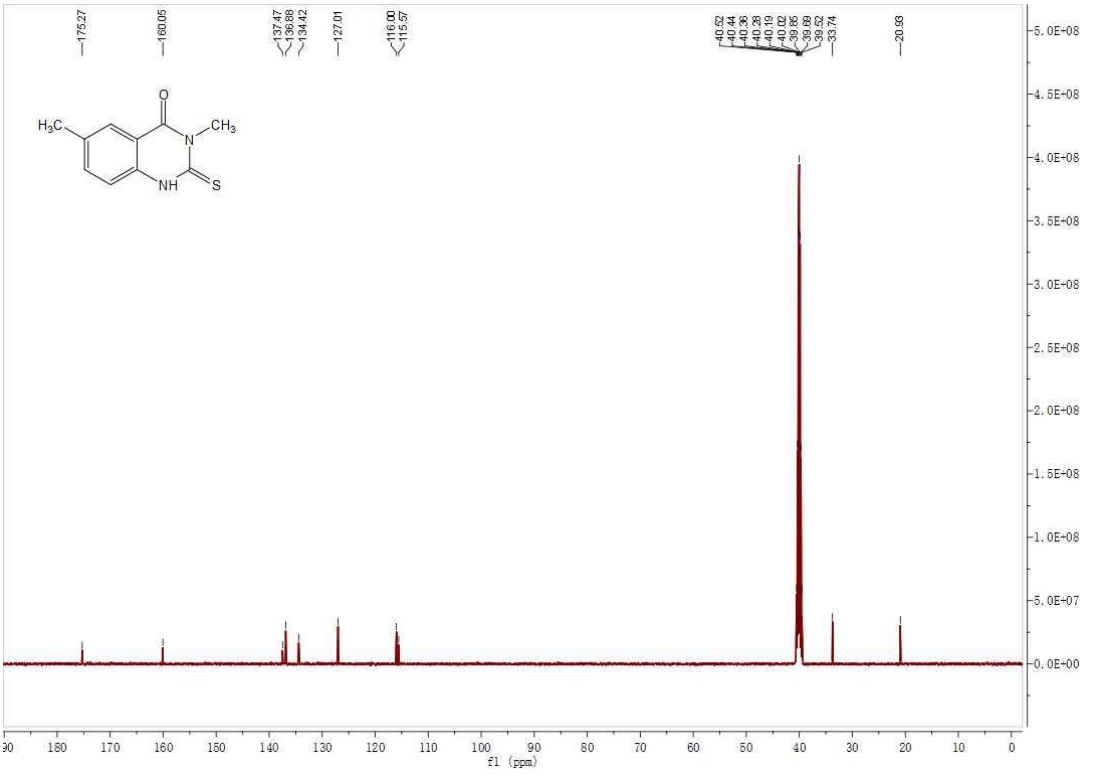
0.95
1.00
1.01
3.00
3.08
f1 (ppm)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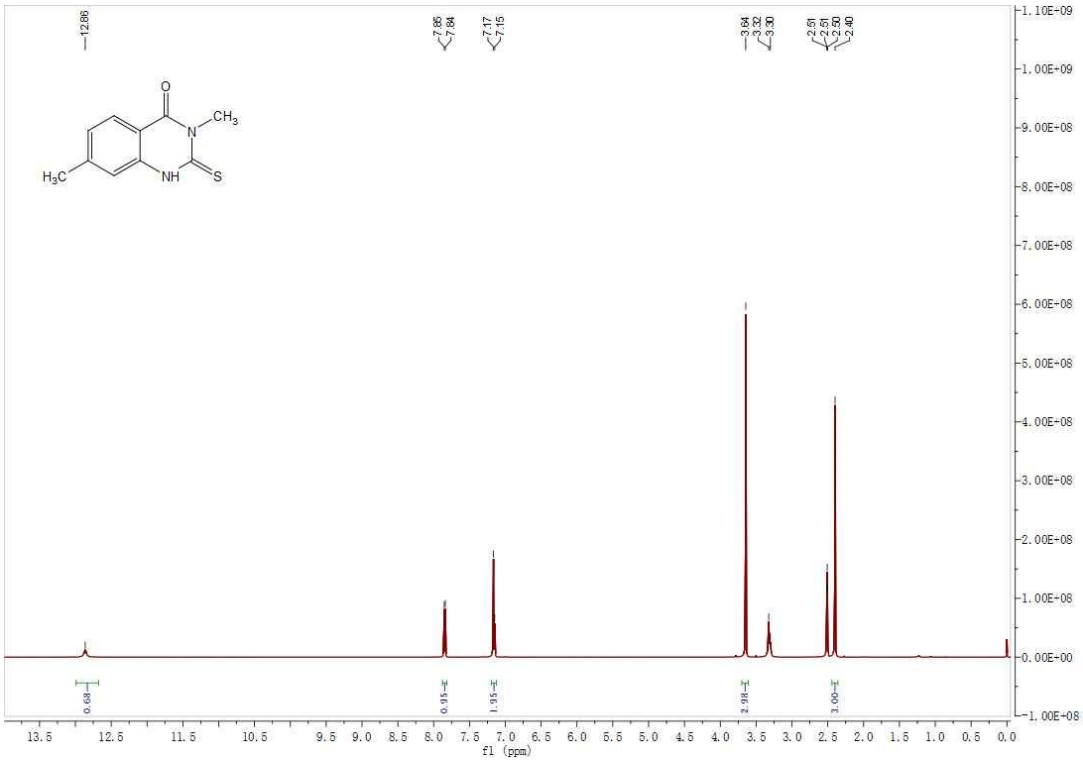
CH3
H3C
NH
S
f1 (ppm)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3.30
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H3C
NH
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1.95
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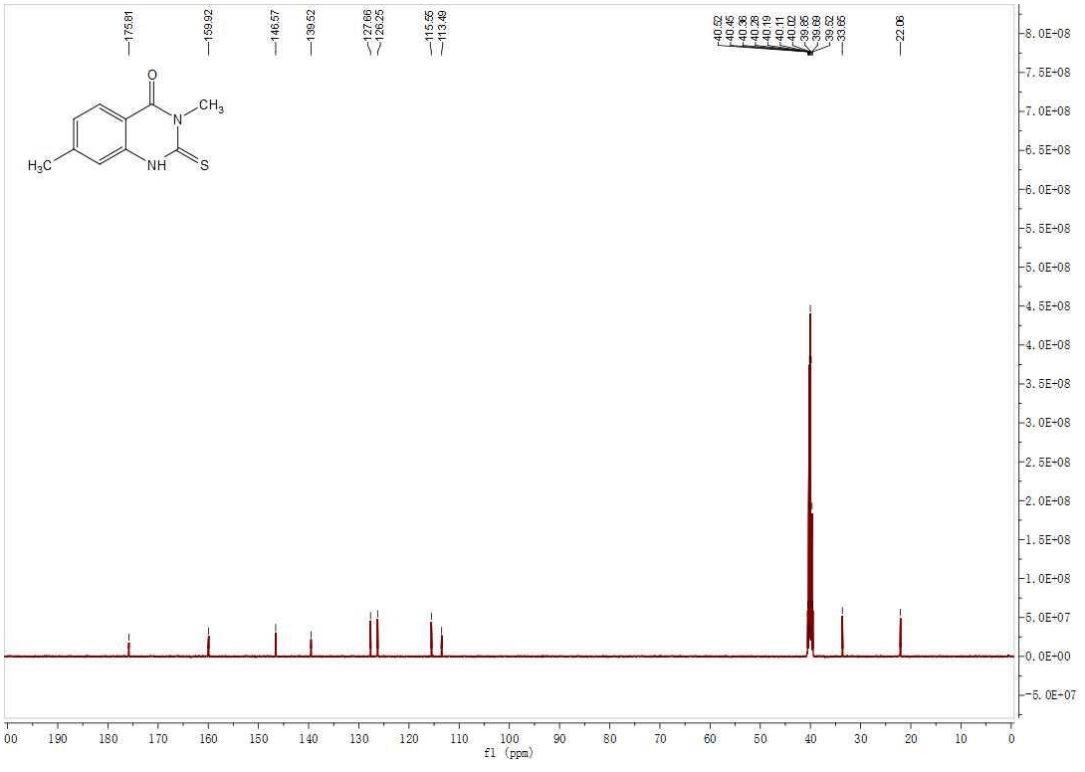
3.00
f1 (ppm)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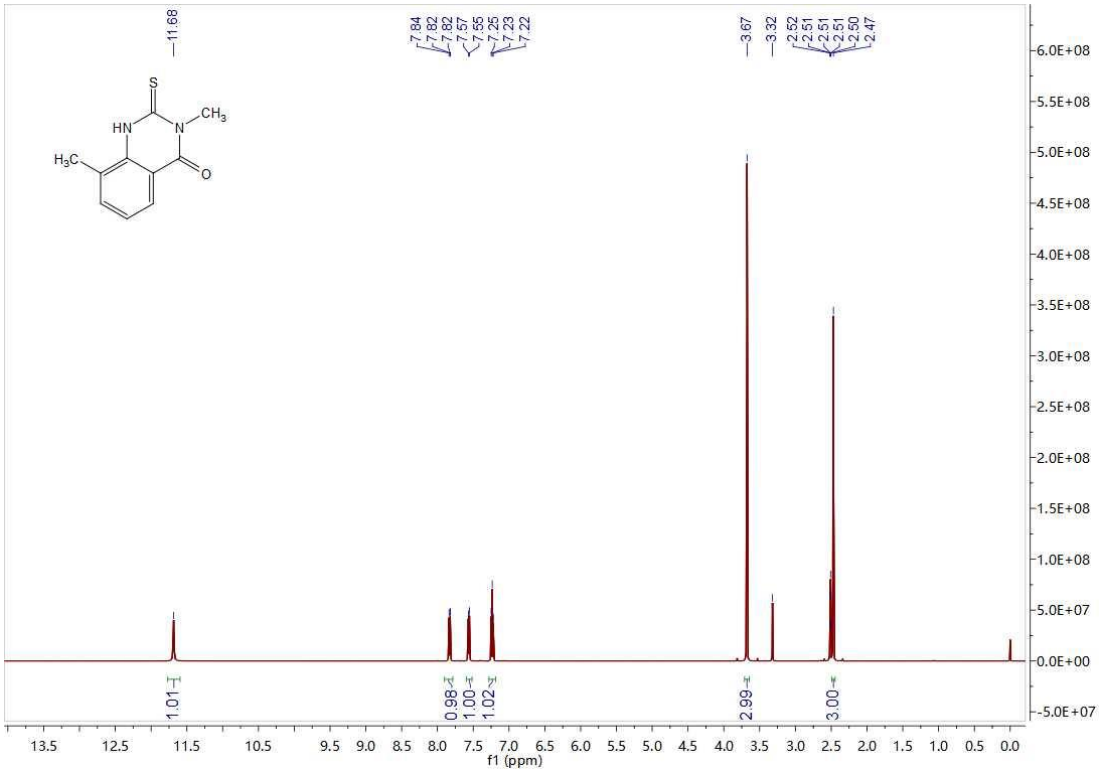
CH3
H3C
NH
S
f1 (ppm)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7.55
7.25
7.23
7.22
3.67
3.32
2.52
2.51
2.51
2.51
2.50
2.47
S
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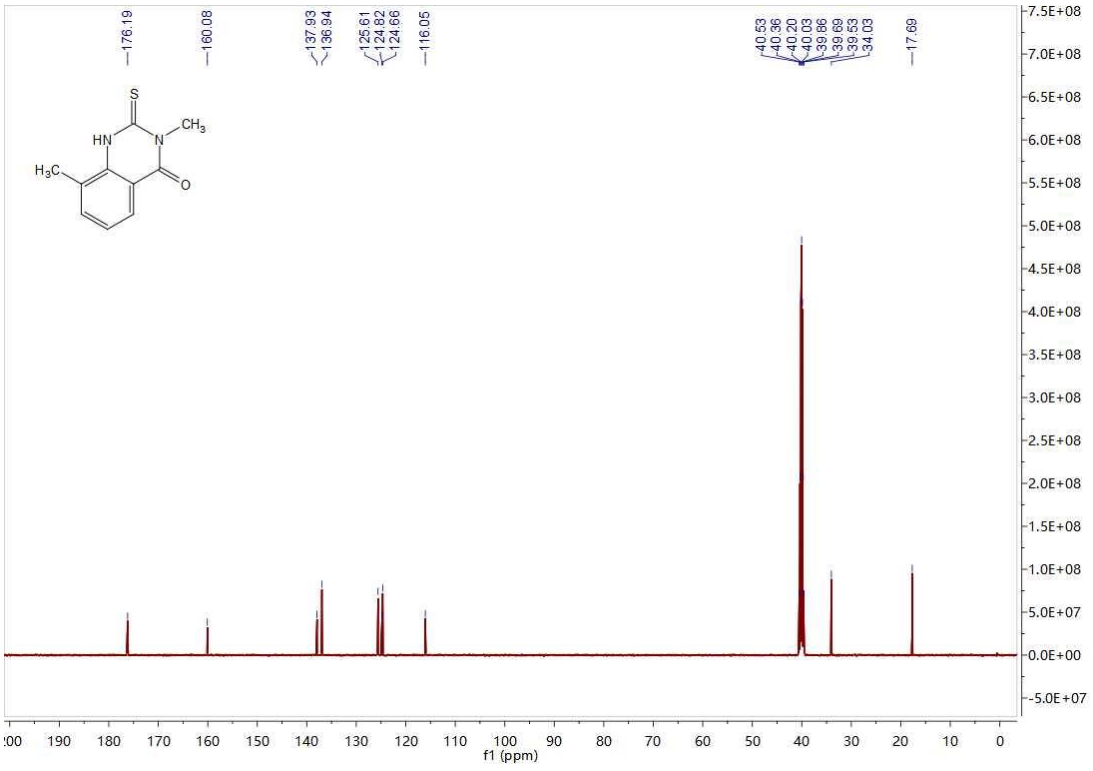
N
CH3
H3C
O
1.01
0.98
1.00
1.02
2.99
3.00
f1 (ppm)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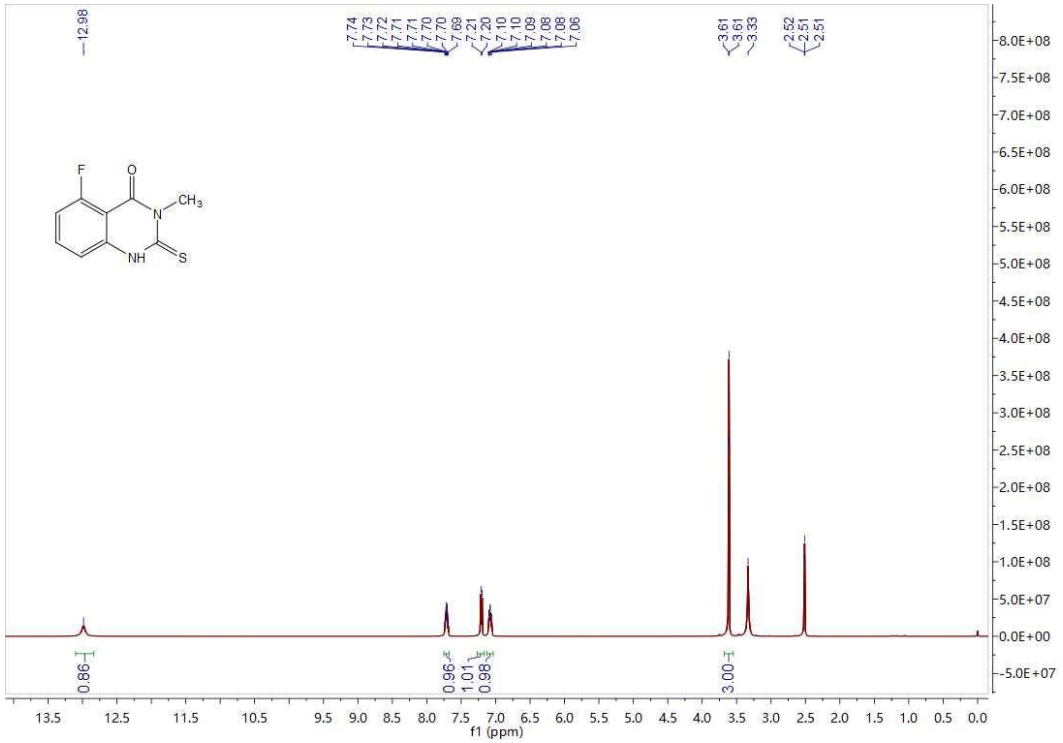
17.69
S
HN
N
CH3
H3C
O
f1 (ppm)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7.69
7.21
7.20
7.10
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7.09
7.08
7.08
7.06
3.61
3.61
3.33
2.52
2.51
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O
N
CH3
NH
S
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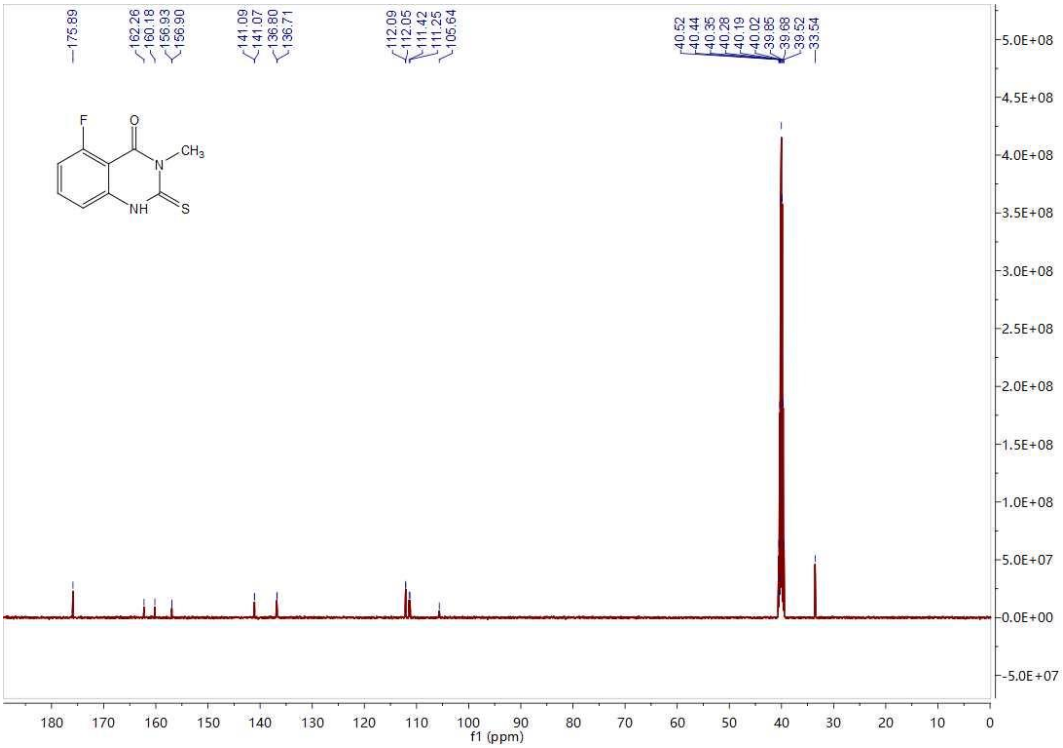
0.96
1.01
0.98
3.00
f1 (ppm)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112.05
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40.44
40.35
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33.54
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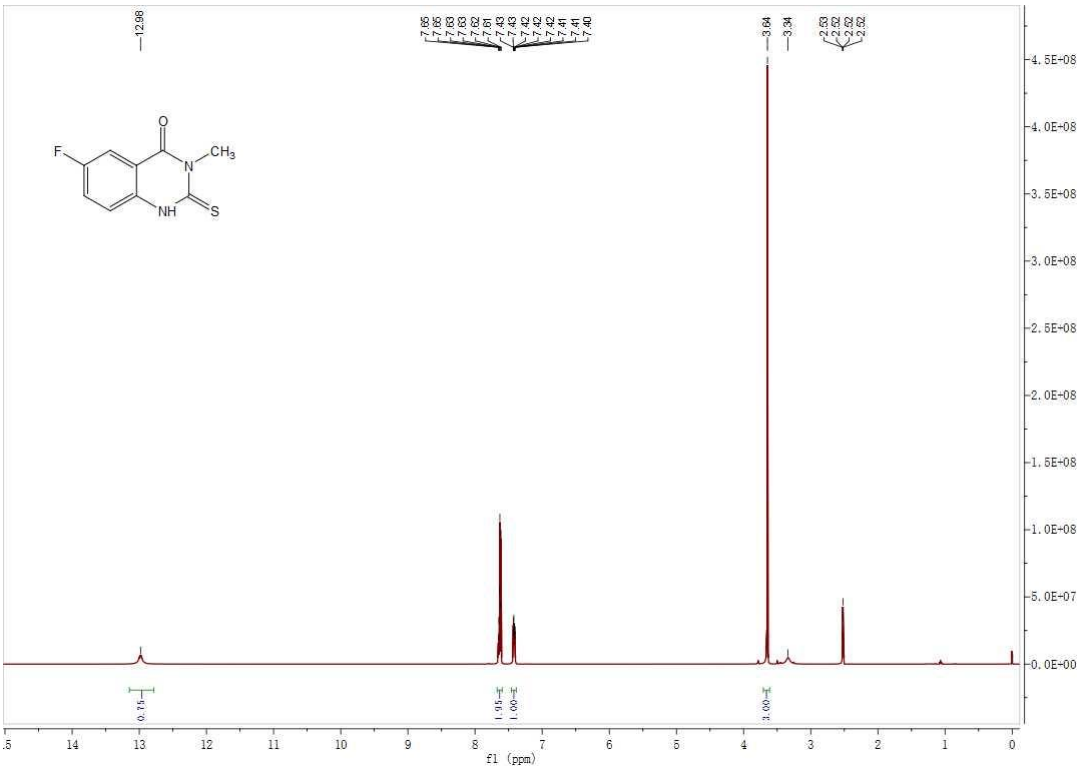
O
N
CH3
NH
S
f1 (ppm)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3.34
2.53
2.52
2.52
2.52
F
O
N
CH3
NH
S
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4.0E-08
3.5E-08
3.0E-08
2.5E-08
2.0E-08
1.5E-08
1.0E-08
5.0E-07
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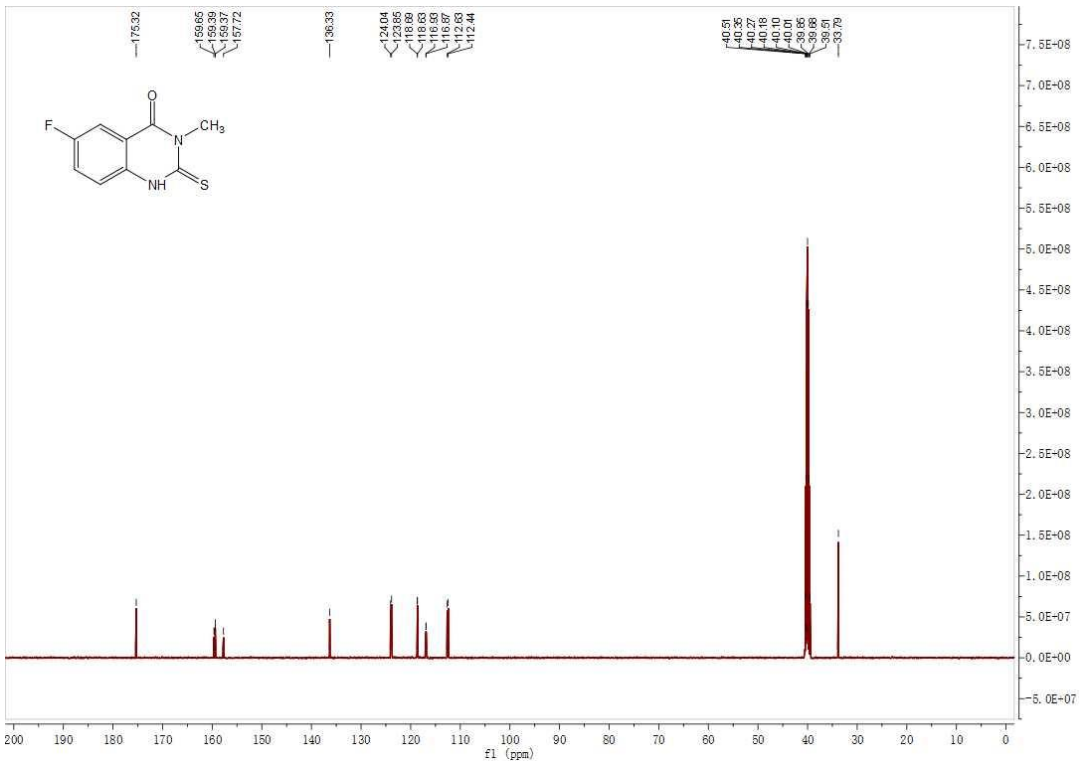
0.15
1.95
1.00
3.00
f1 (ppm)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112.44
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40.35
40.27
40.18
40.10
40.01
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39.68
39.51
33.79
F
O
N
CH3
NH
S
7.5E-08
7.0E-08
6.5E-08
6.0E-08
5.5E-08
5.0E-08
4.5E-08
4.0E-08
3.5E-08
3.0E-08
2.5E-08
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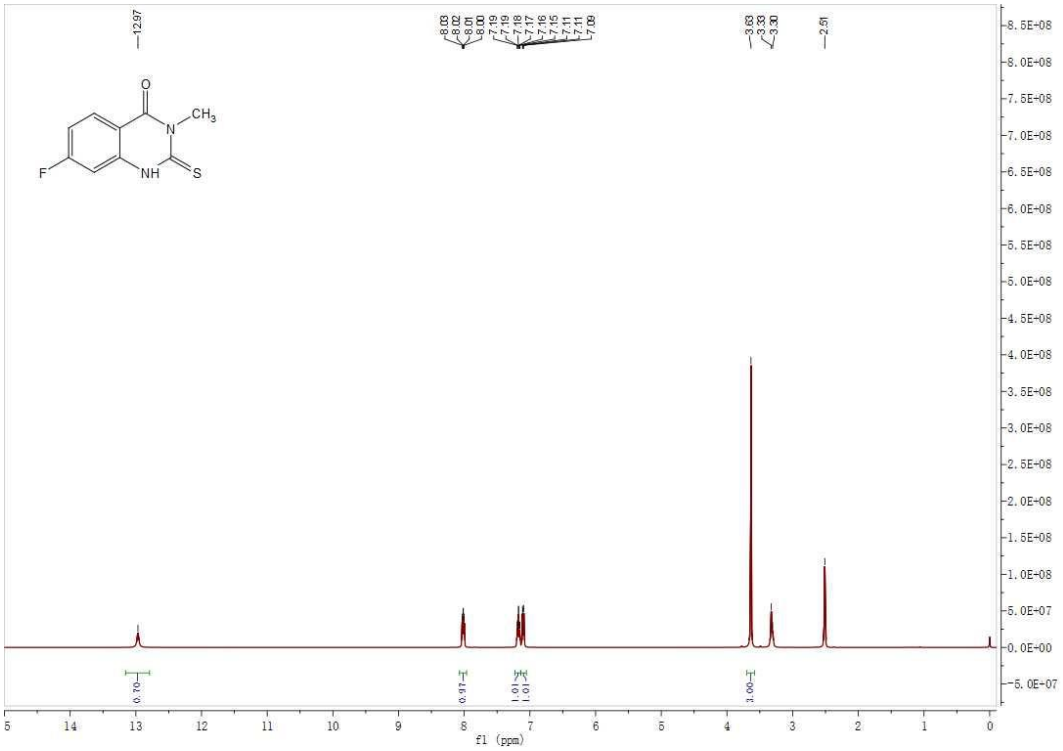
1.5E-08
1.0E-08
5.0E-07
0.0E-00
-5.0E-07
f1 (ppm)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8.01
8.00
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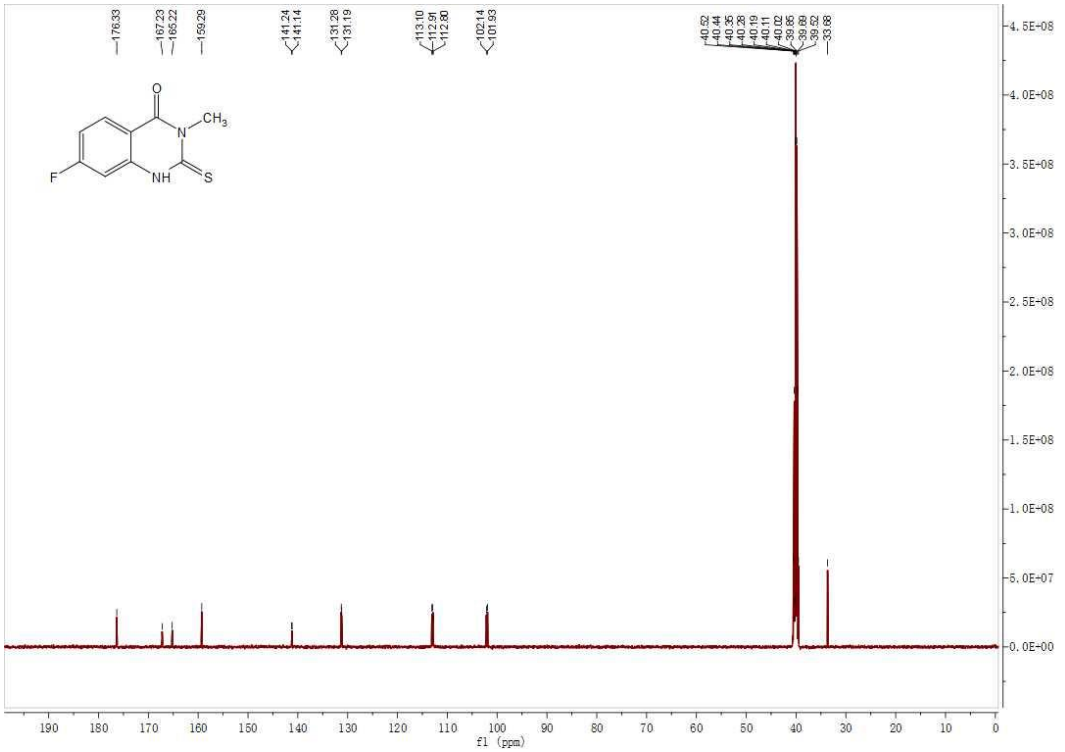
7.18
7.17
7.16
7.15
7.11
7.09
3.63
3.33
3.30
2.51
O
N
CH3
F
NH
S
0.70
0.97
1.01
1.01
3.00
f1 (ppm)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40.44
40.35
40.28
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39.52
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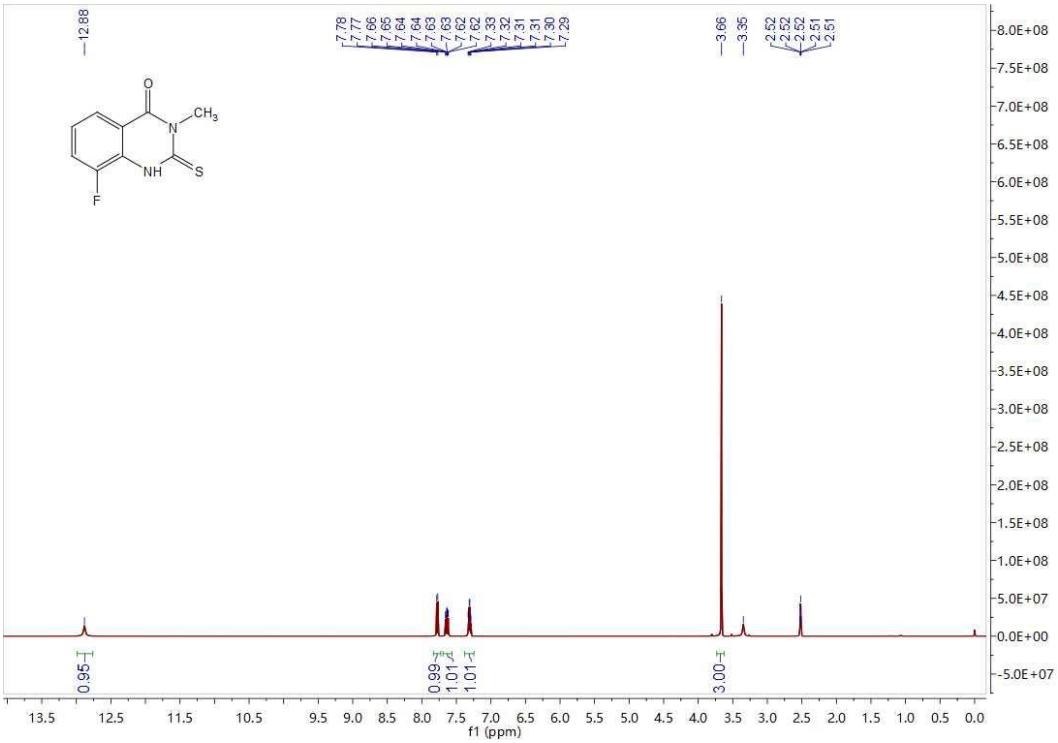
O
N
CH3
F
NH
S
f1 (ppm)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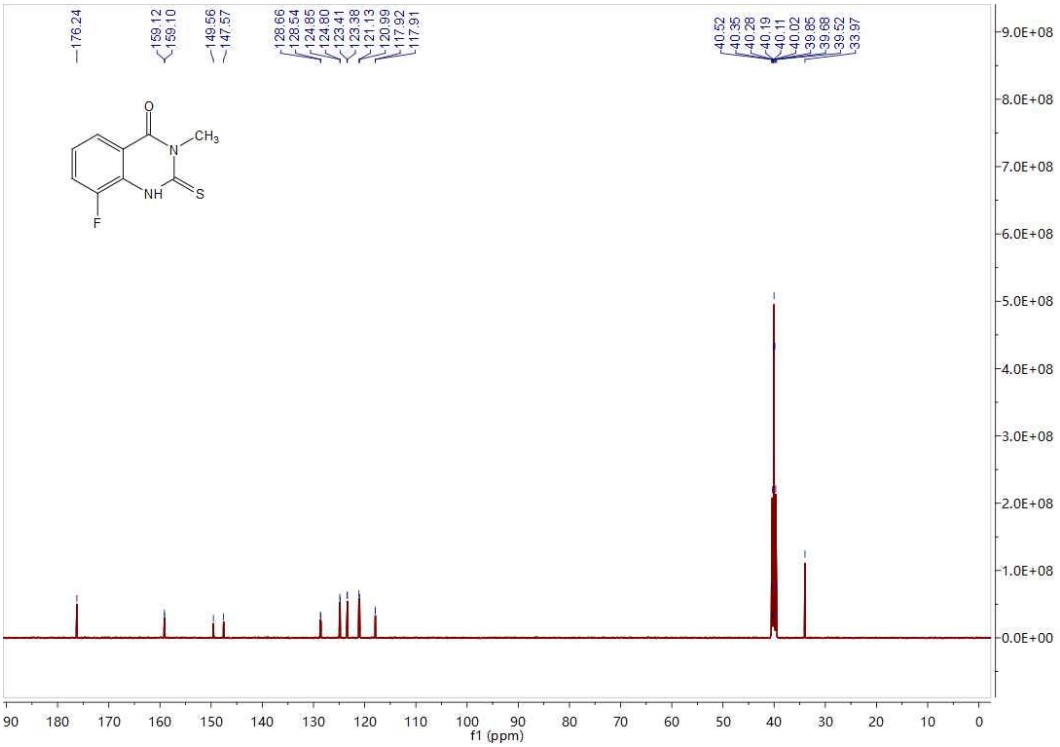
7.64
7.63
7.63
7.62
7.62
7.33
7.32
7.31
7.31
7.30
7.29
3.66
3.36
2.52
2.52
2.52
2.51
2.51
O
N
CH3
NH
S
F
0.95
0.99
1.01
1.01
3.00
f1 (ppm)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121.13
120.99
117.92
117.91
40.52
40.35
40.28
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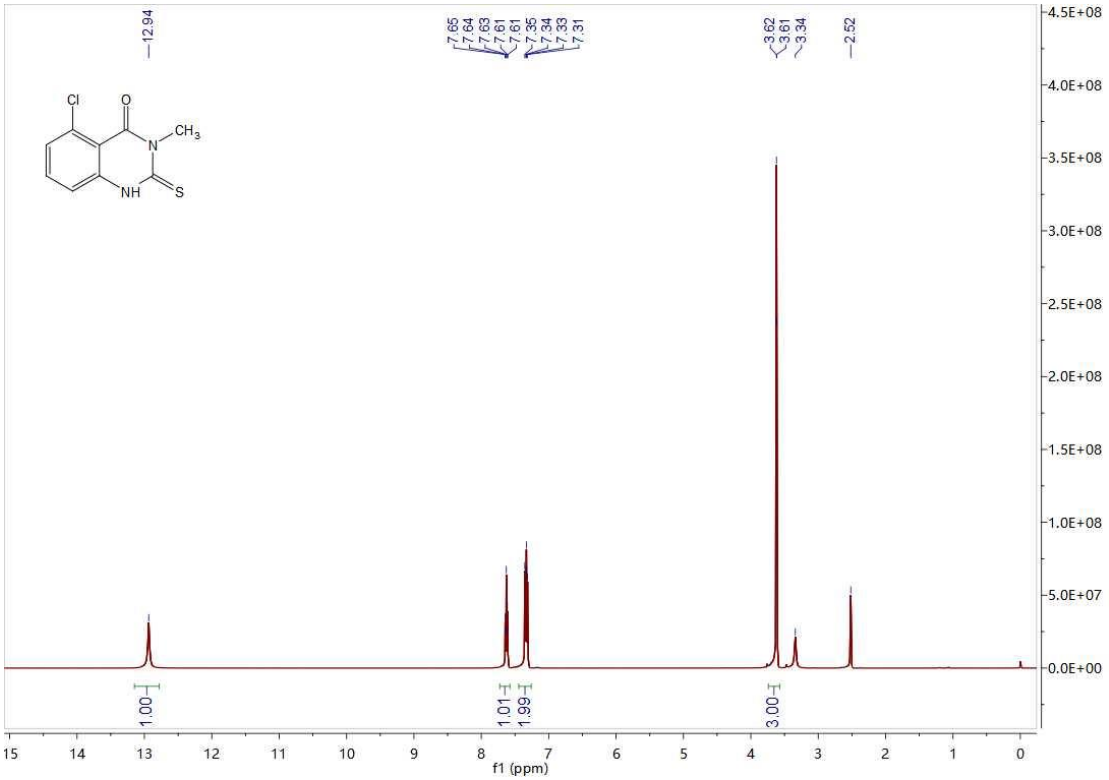
39.52
33.97
O
N
CH3
NH
S
F
f1 (ppm)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7.33
7.31
3.62
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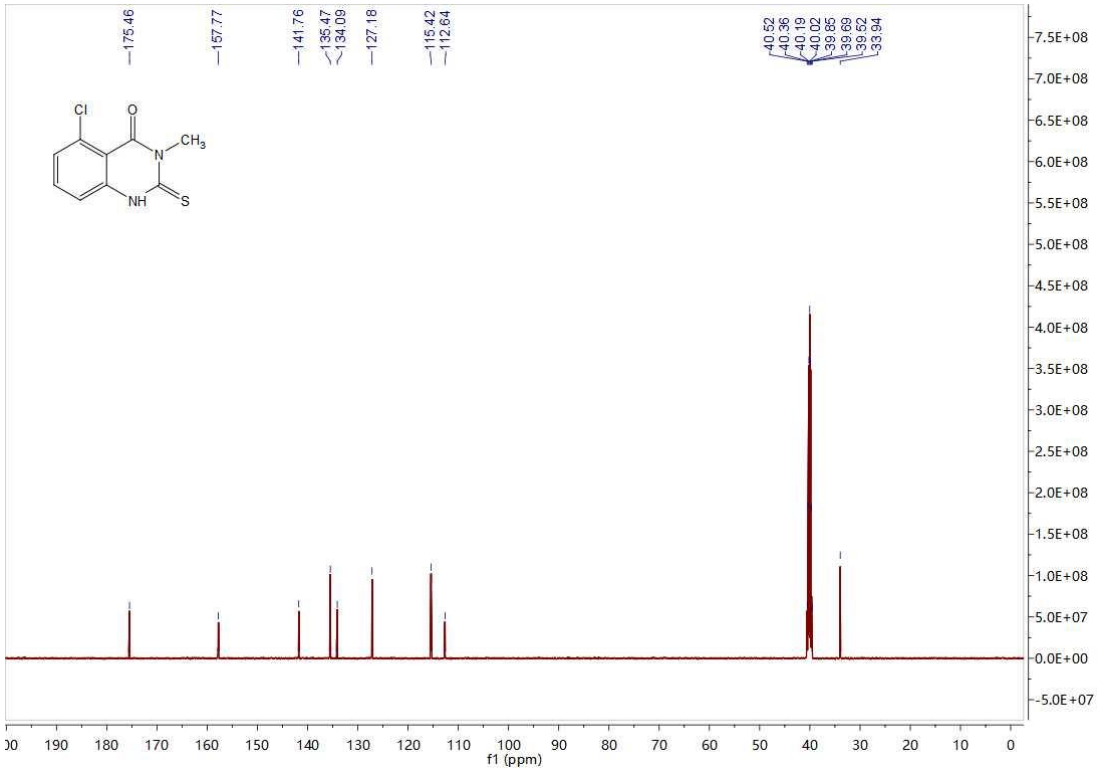
S
1.00
1.01
1.99
3.00
f1 (ppm)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O
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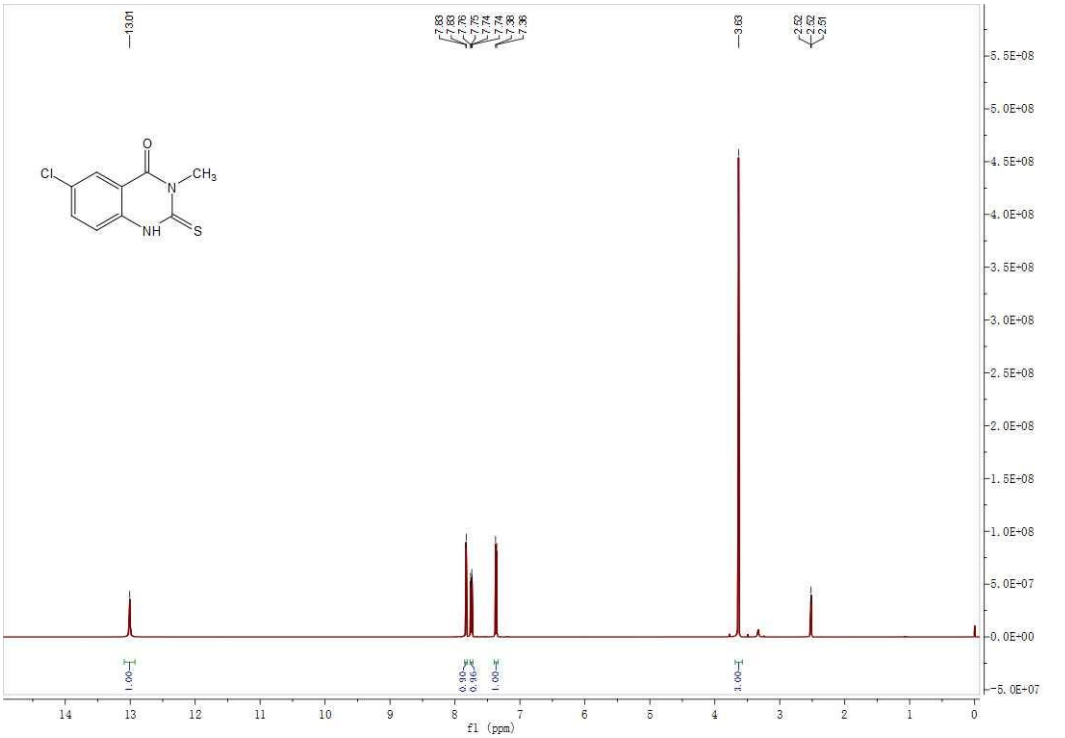
CH3
NH
S
f1 (ppm)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3.63
2.52
2.52
2.51
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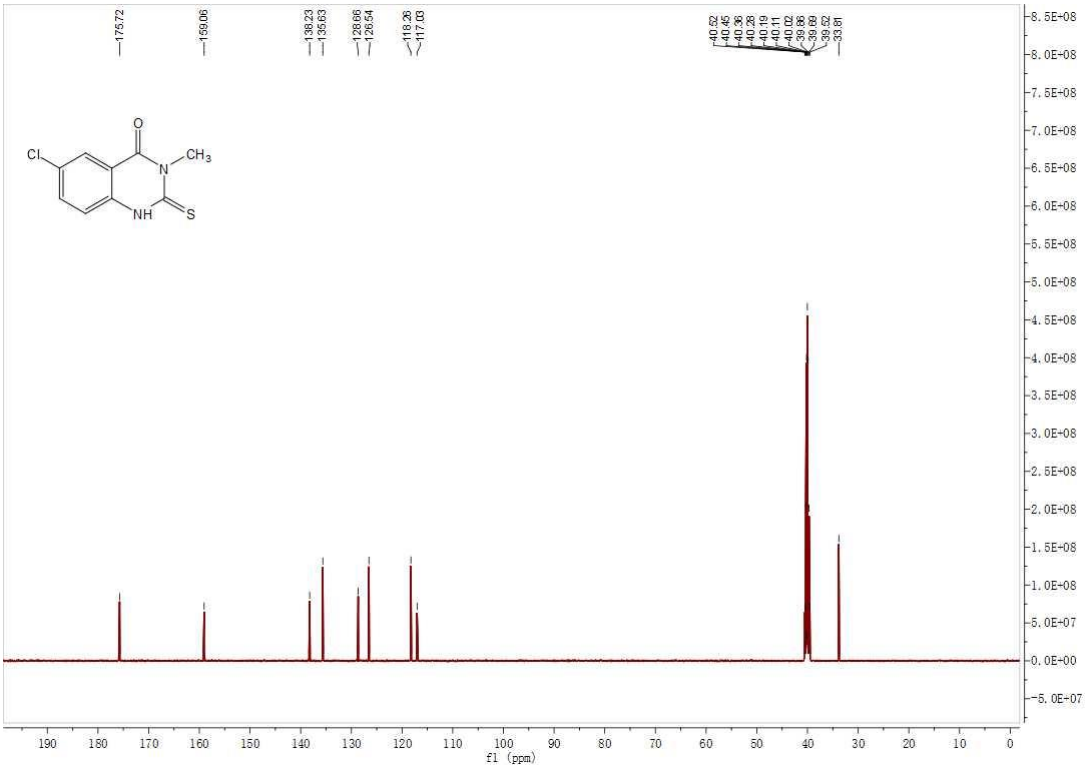
O
N
CH3
NH
S
1.00
0.93
0.96
1.00
3.00
f1 (ppm)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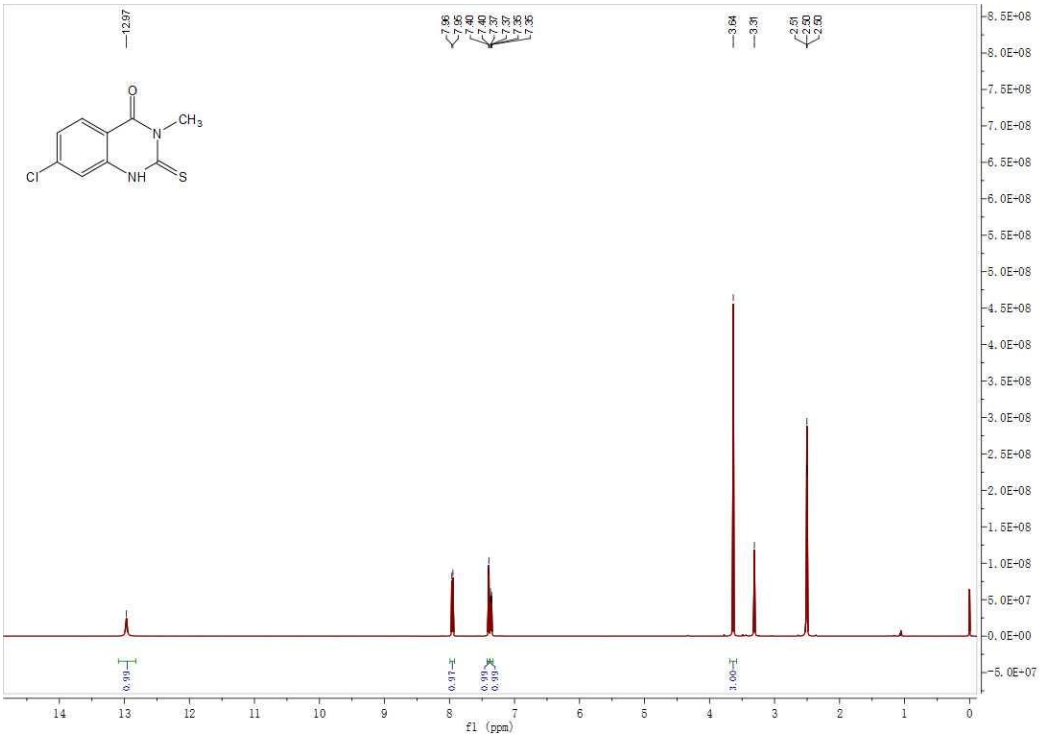
CH3
NH
S
f1 (ppm)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7.37
7.35
7.35
3.64
3.31
2.51
2.50
2.50
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N
CH3
Cl
NH
S
0.99
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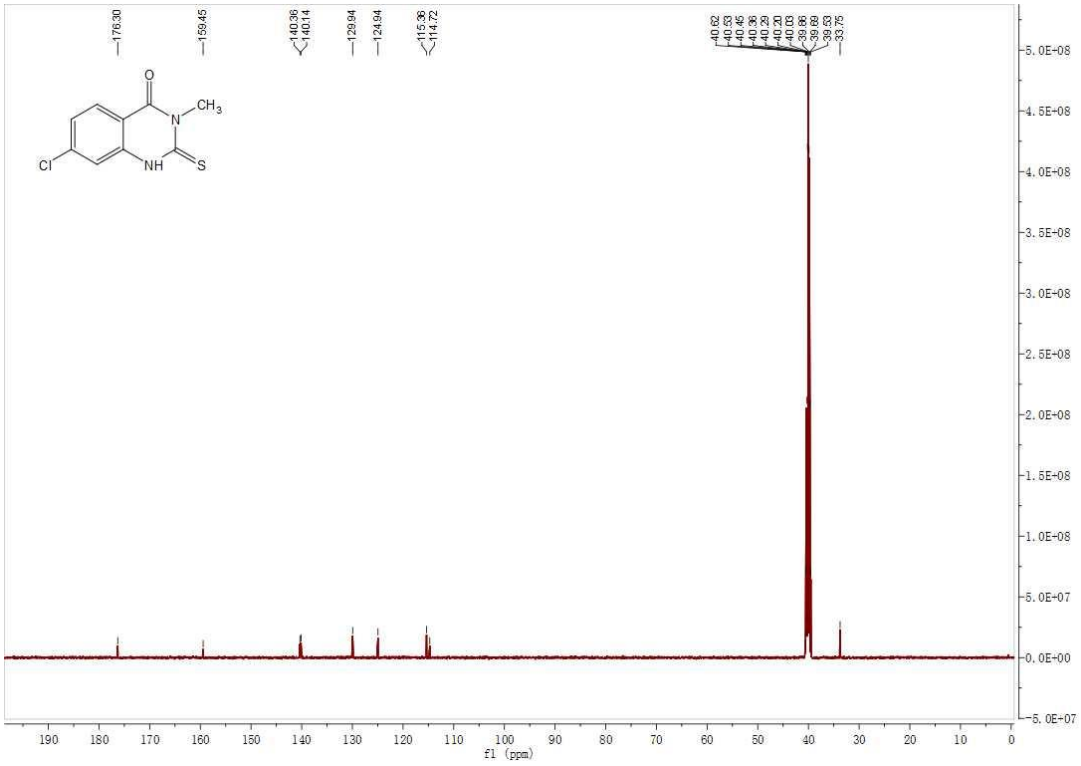
0.99
0.99
3.06
f1 (ppm)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40.53
40.45
40.36
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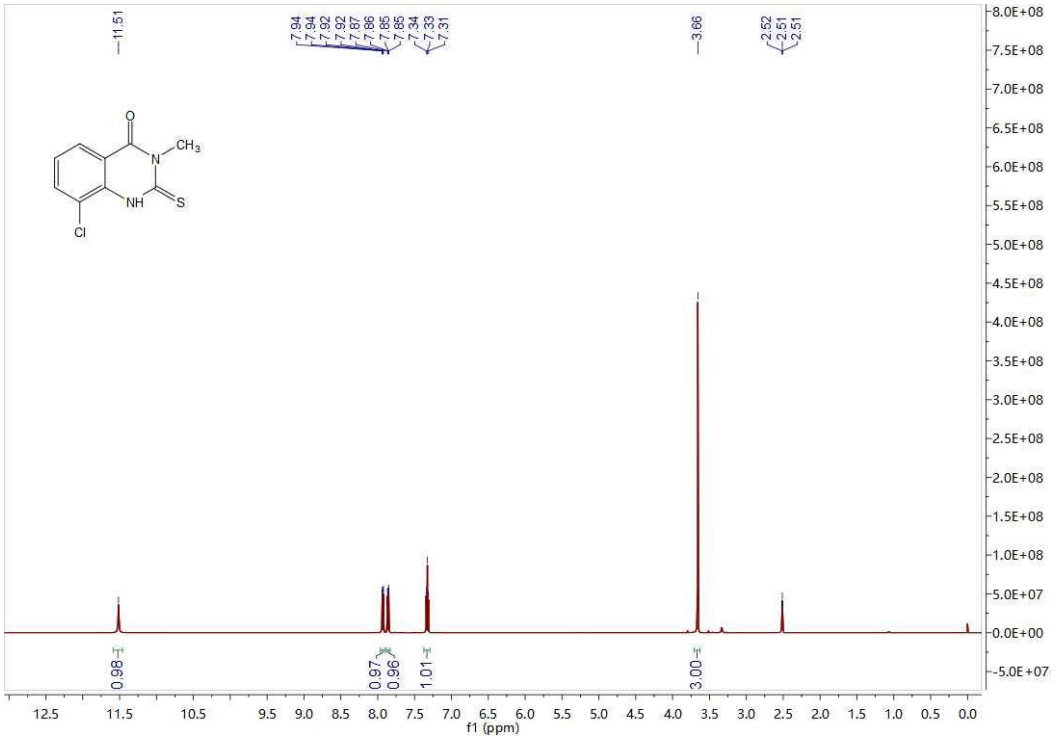
39.53
33.75
O
N
CH3
Cl
NH
S
f1 (ppm)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7.34
7.33
7.31
3.66
2.52
2.51
2.51
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N
CH3
NH
S
Cl
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0.96
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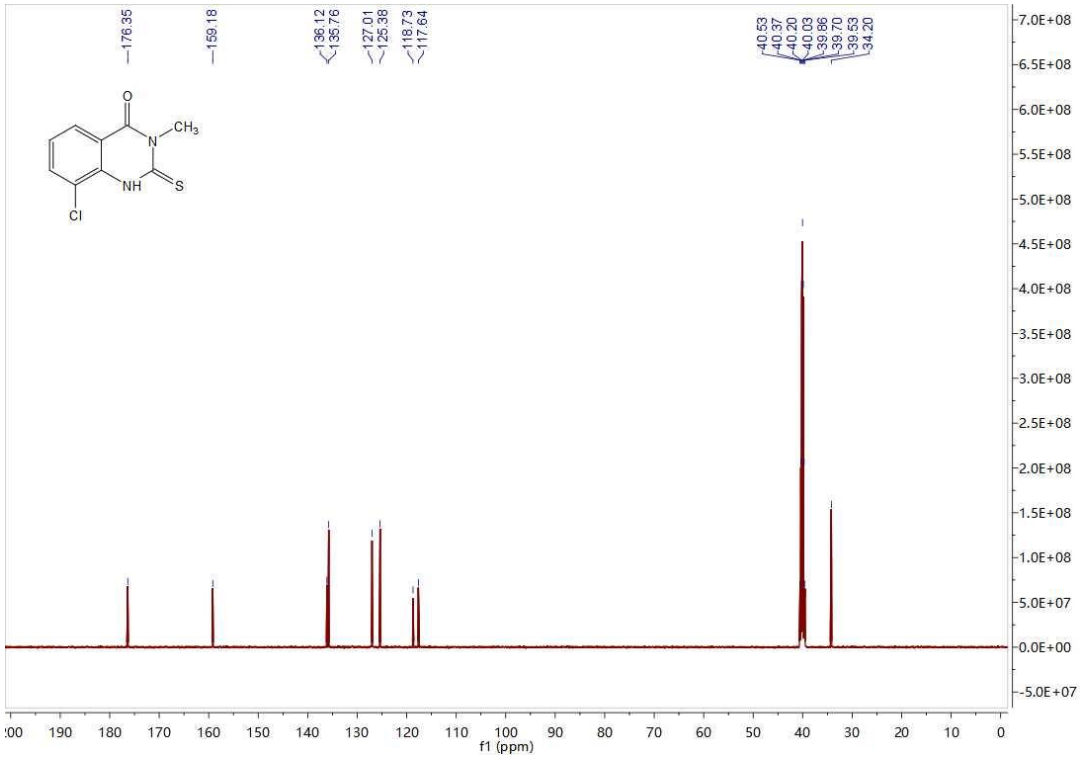
3.00
f1 (ppm)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34.20
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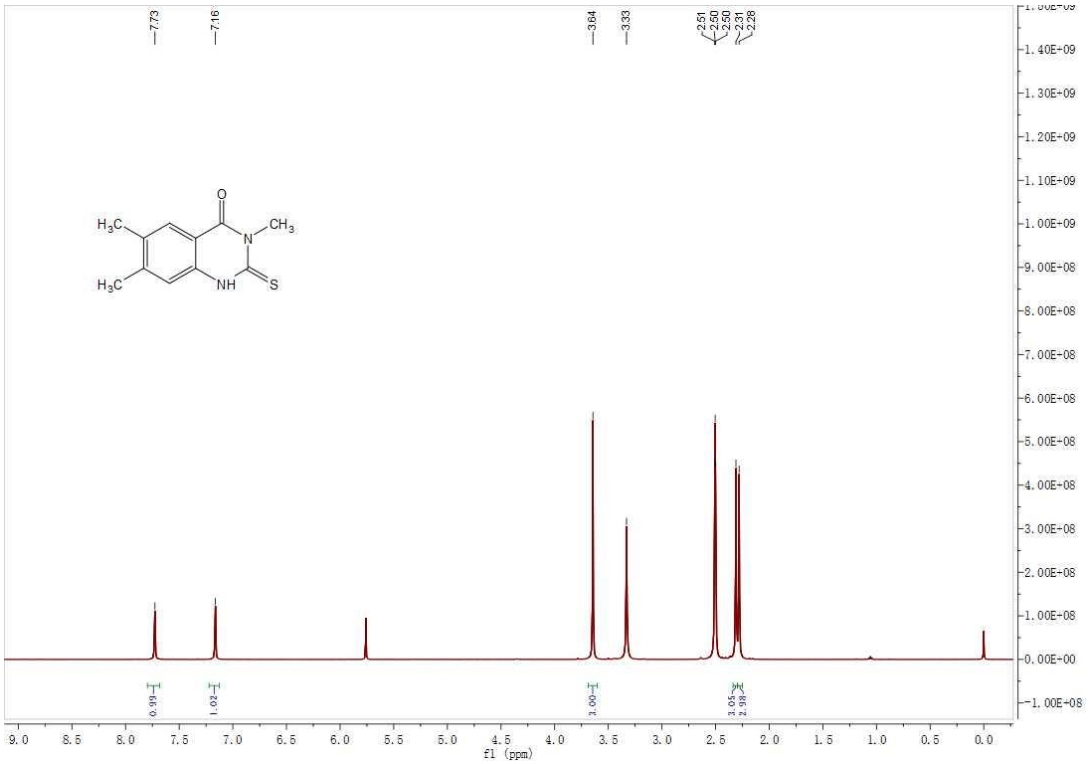
N
CH3
NH
S
Cl
f1 (ppm)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2.50
2.31
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H3C
H3C
NH
S
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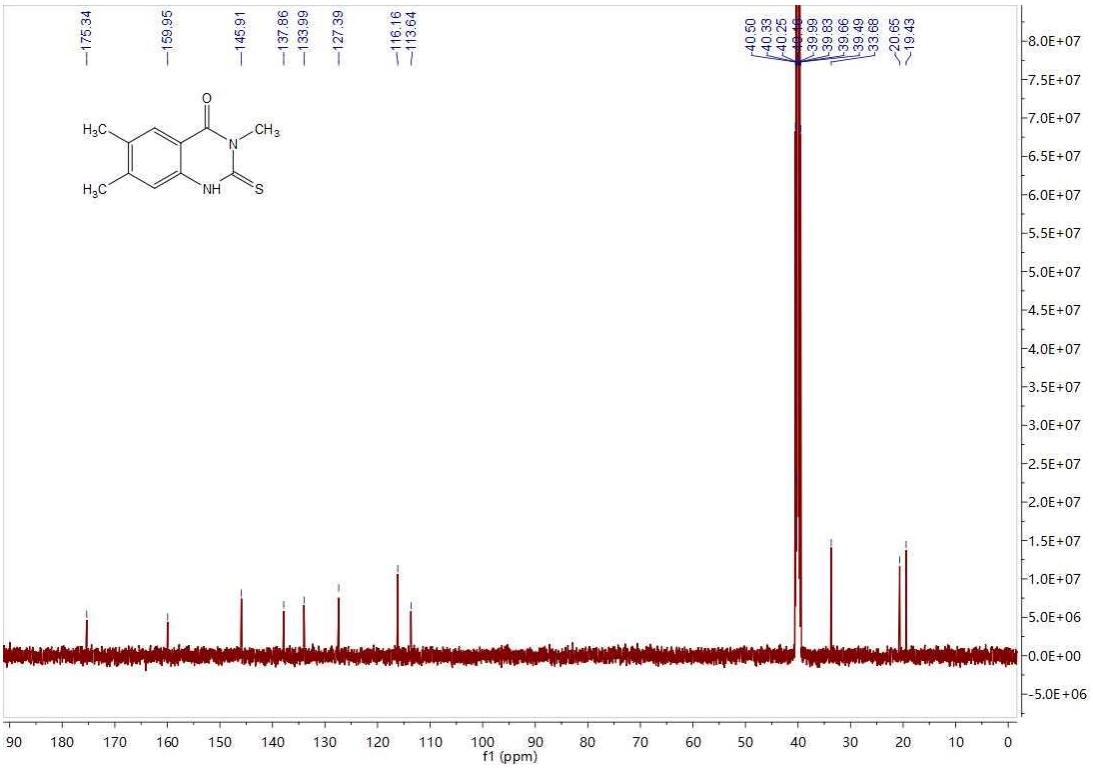
3.00
3.05
2.98
f1 (ppm)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40.25
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20.65
19.43
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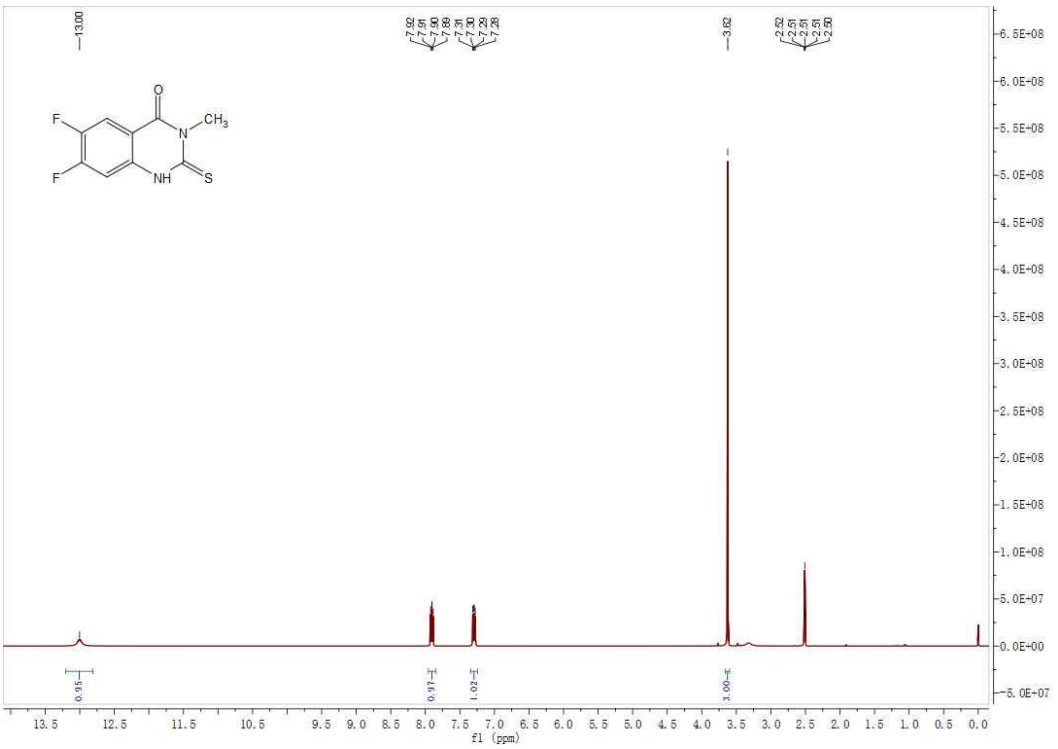
CH3
H3C
H3C
NH
S
f1 (ppm)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7.29
7.28
3.62
2.52
2.51
2.51
2.51
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F
F
O
N
CH3
NH
S
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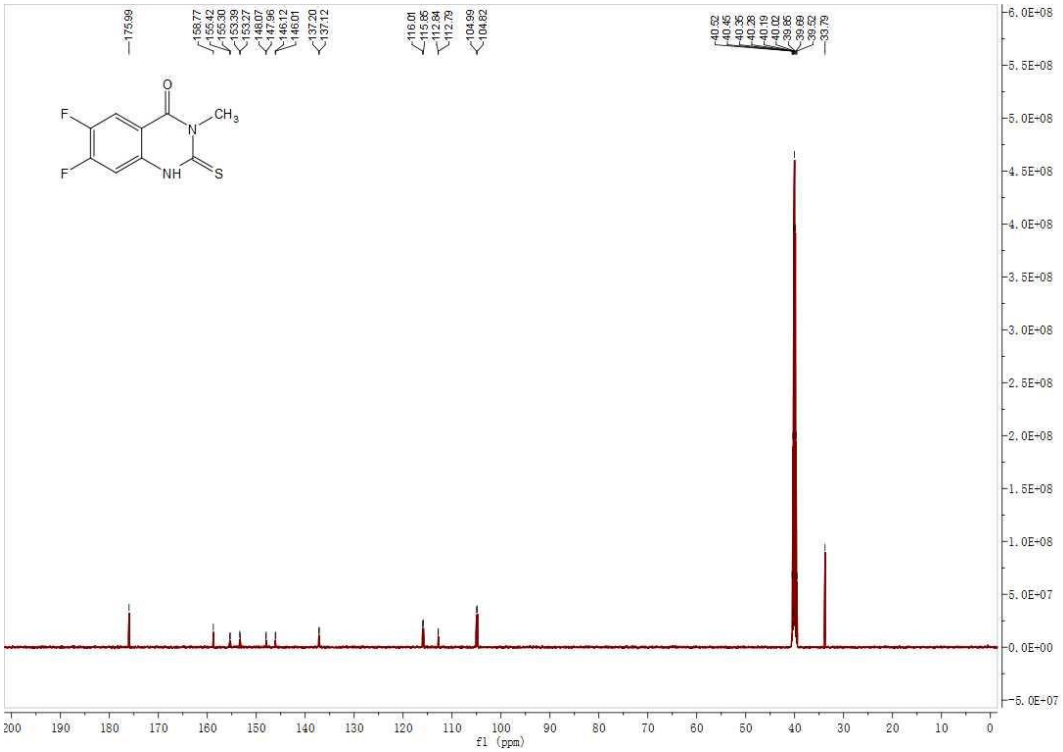
0.97
1.02
3.00
f1 (ppm)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146.01
137.20
137.12
116.01
115.85
112.84
112.79
104.99
104.82
40.52
40.45
40.36
40.28
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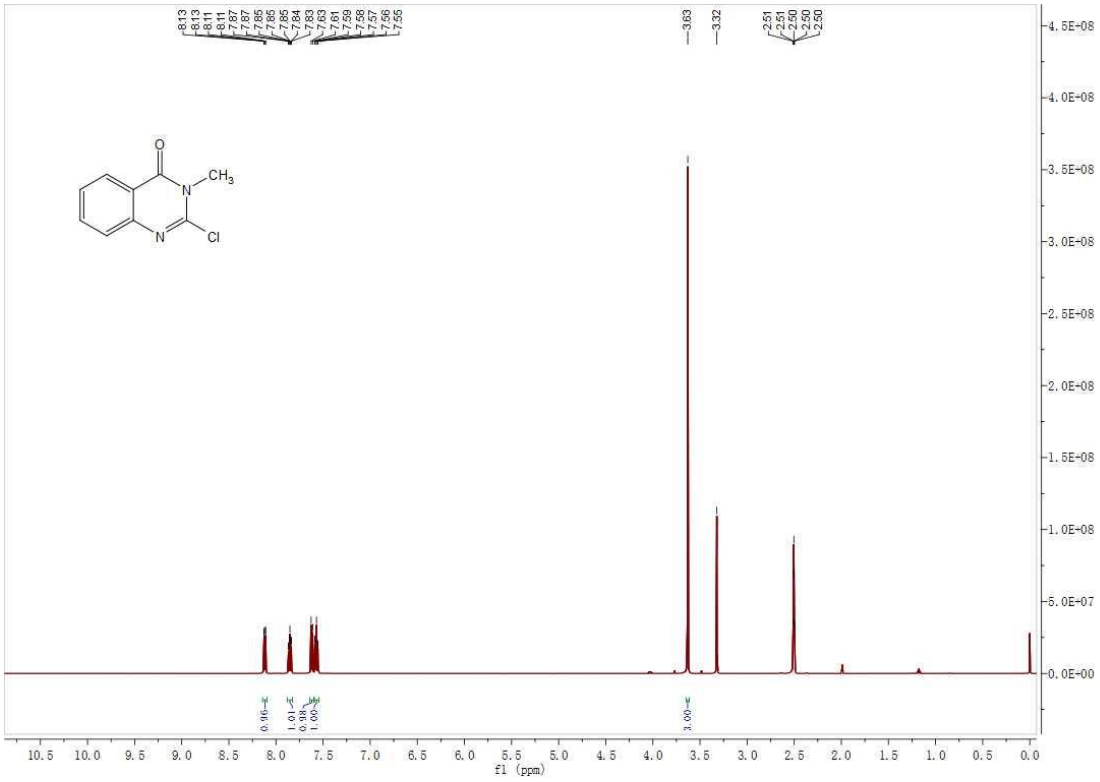
39.86
39.69
39.52
33.79
F
F
O
N
CH3
NH
S
f1 (ppm)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7.59
7.58
7.57
7.56
7.55
3.63
3.32
2.51
2.51
2.50
2.50
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O
N
CH3
N
Cl
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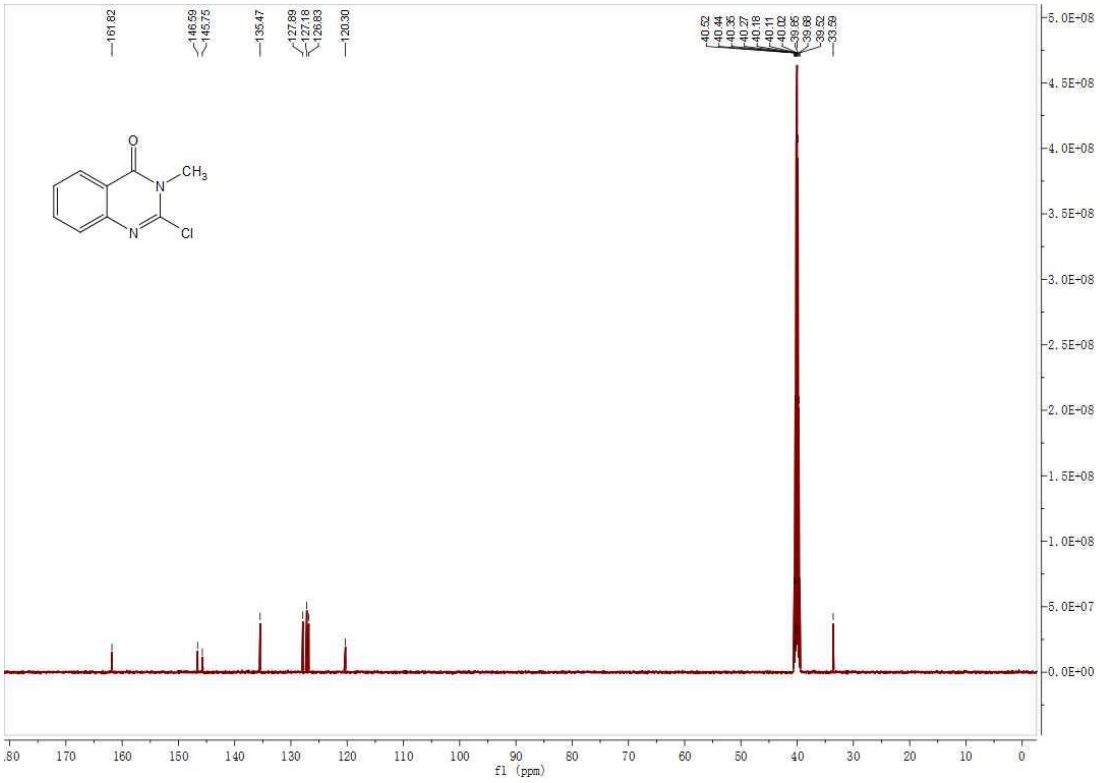
0.98
1.00
3.00
f1 (ppm)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40.35
40.27
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40.02
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39.68
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O
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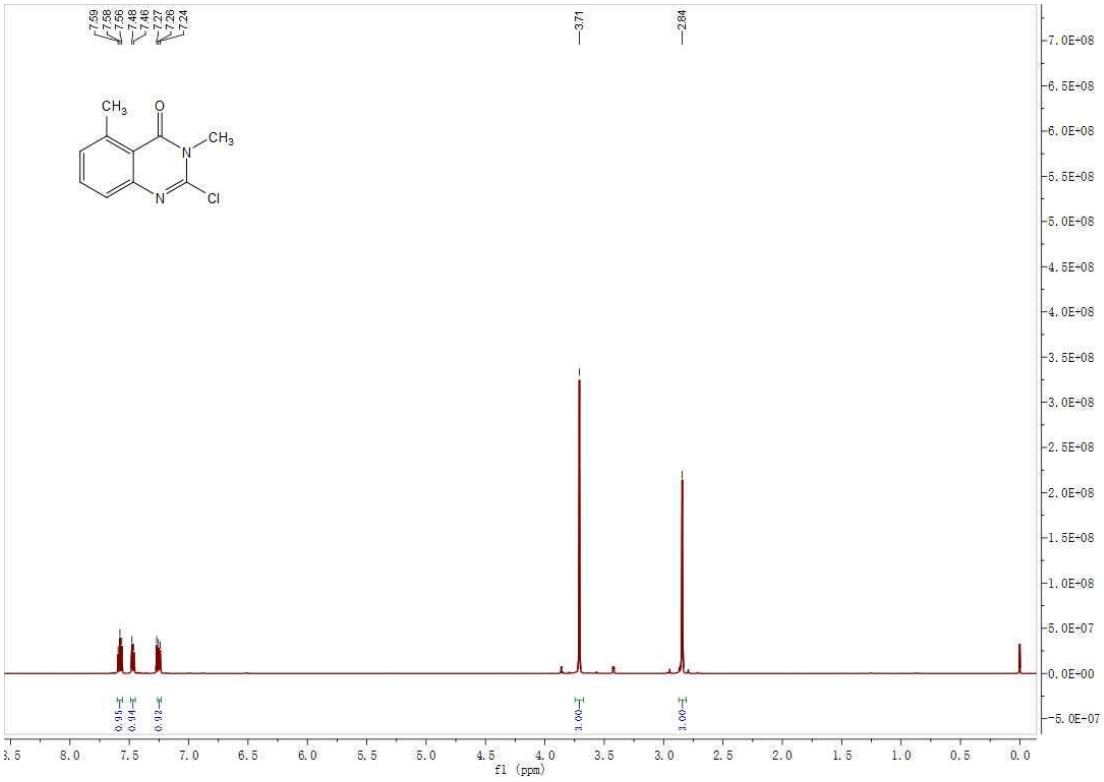
CH3
N
Cl
f1 (ppm)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7.58
7.56
7.48
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7.27
7.26
7.24
3.71
2.84
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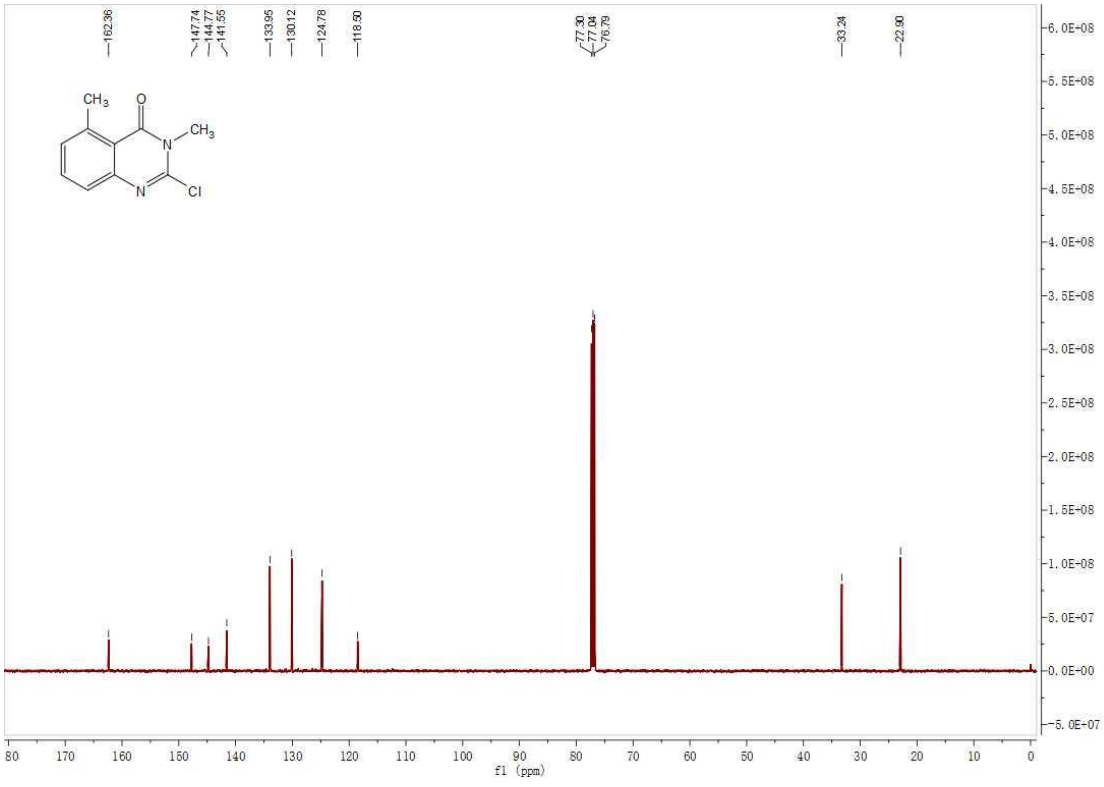
N
CH3
N
Cl
0.95
0.94
0.92
1.00
1.00
f1 (ppm)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141.55
133.95
130.12
124.78
118.50
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77.04
76.79
33.24
22.90
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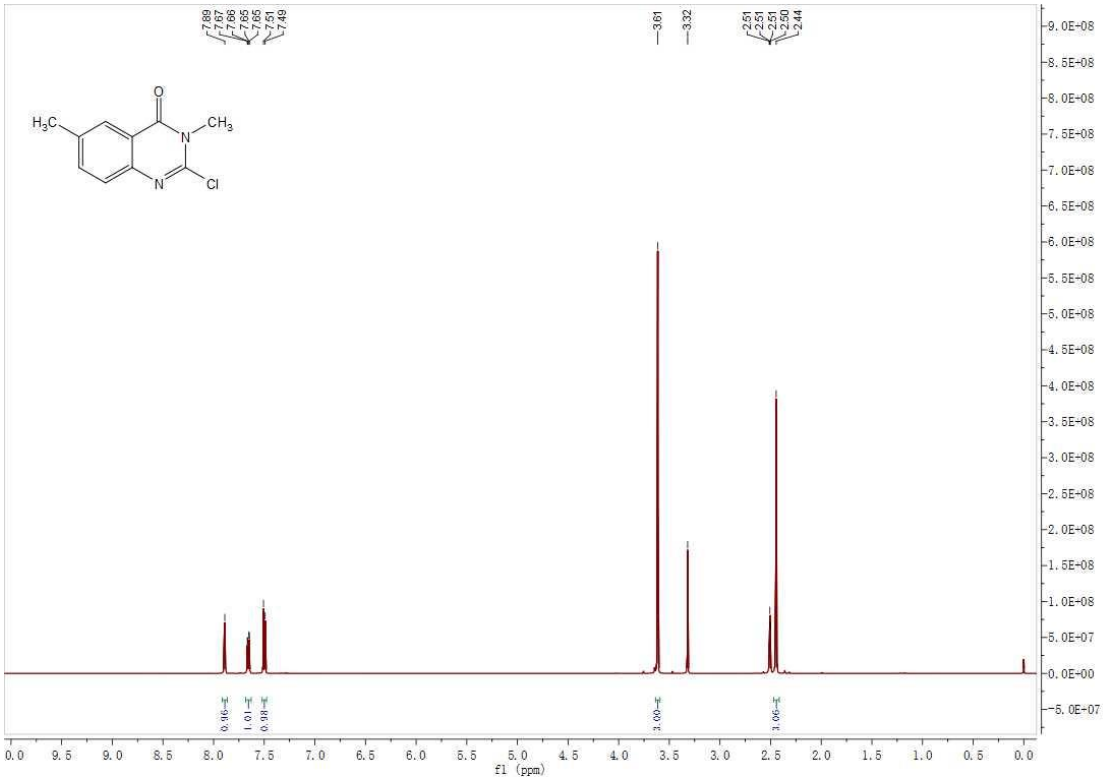
N
CH3
N
Cl
f1 (ppm)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7.67
7.66
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7.65
7.51
7.49
3.61
3.32
2.51
2.51
2.51
2.50
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H3C
N
CH3
N
Cl
0.96
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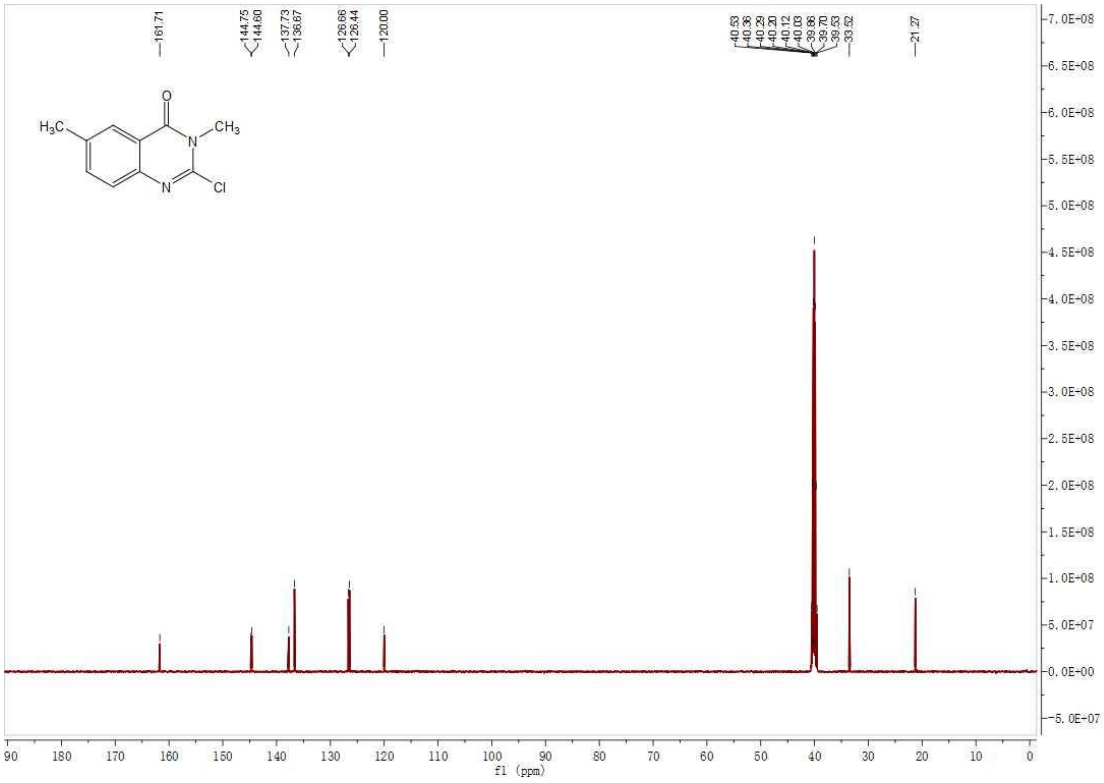
0.98
3.00
3.06
f1 (ppm)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144.75
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136.67
126.66
126.44
120.00
40.53
40.36
40.20
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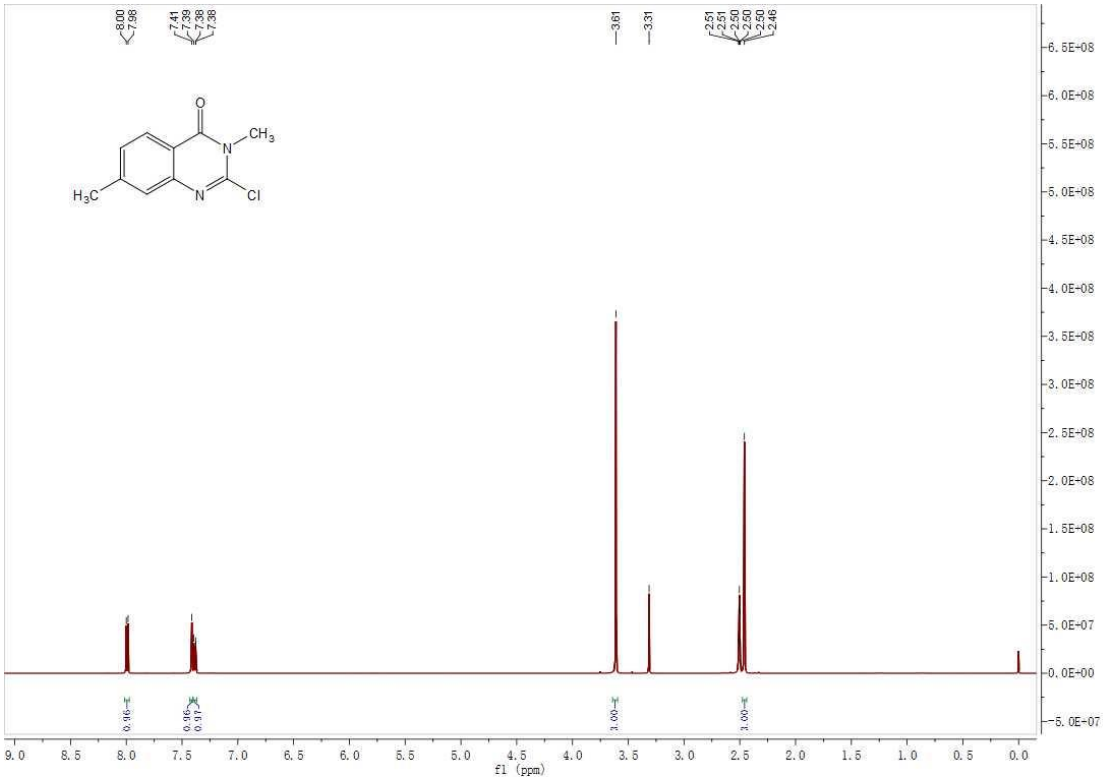
39.70
39.53
33.52
21.27
O
H3C
N
CH3
N
Cl
f1 (ppm)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7.98
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7.38
7.38
3.61
3.31
2.51
2.51
2.50
2.50
2.50
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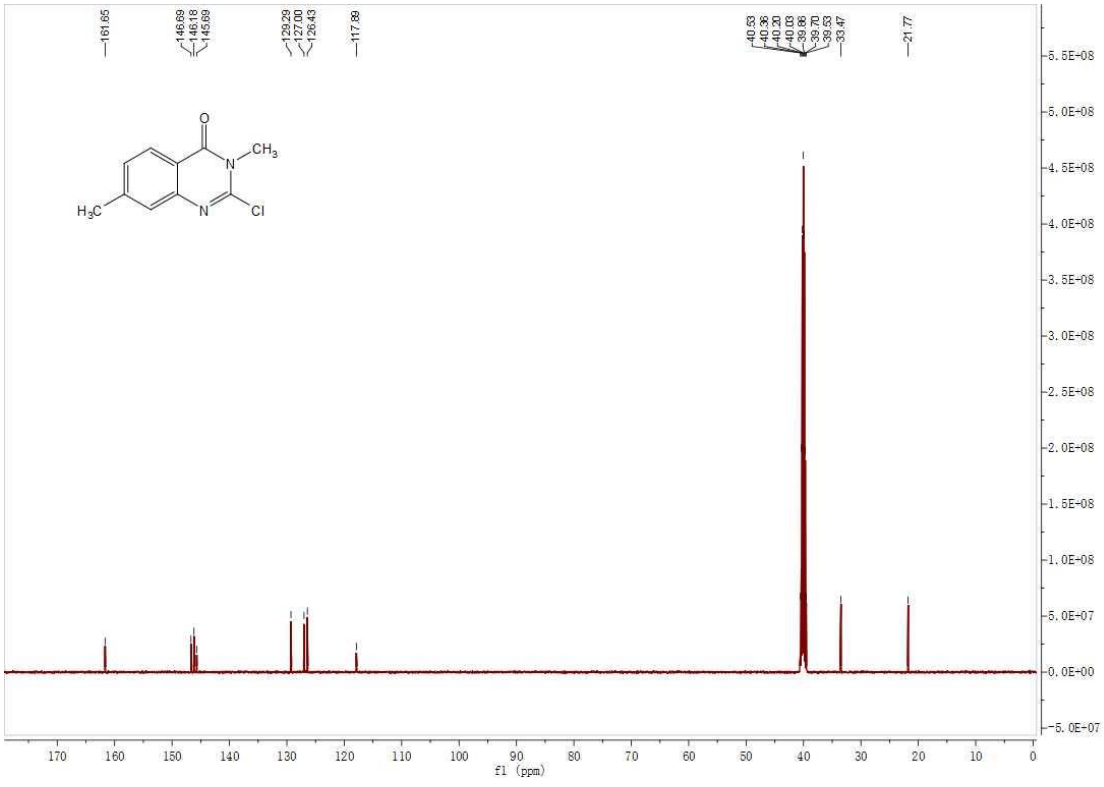
O
CH3
N
H3C
N
Cl
0.96
0.97
3.00
3.00
f1 (ppm)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126.43
117.89
40.53
40.36
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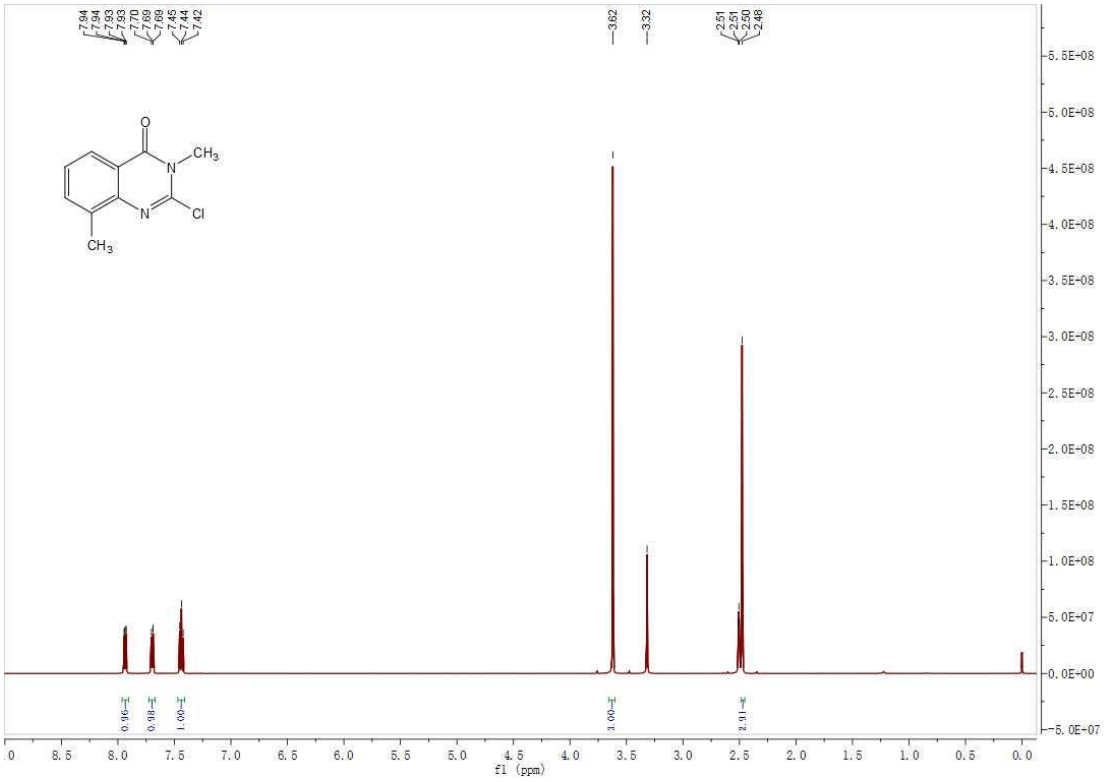
39.70
39.53
33.47
21.77
O
CH3
N
H3C
N
Cl
f1 (ppm)


7.94
7.94
7.93
7.93
7.70
7.69
7.69
7.45
7.44
7.42
3.62
3.32
2.51
2.51
2.50
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N
CH3
N
Cl
CH3
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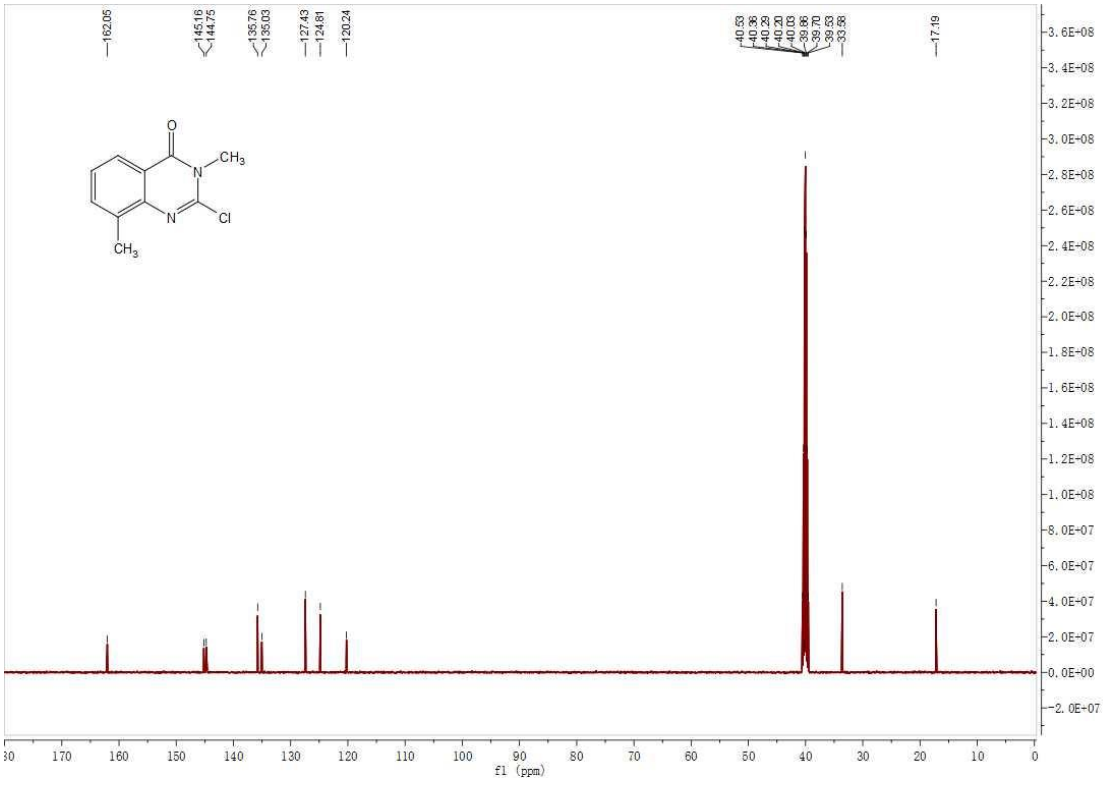
0.98
1.00
3.00
2.91
f1 (ppm)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145.16
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135.76
135.03
127.43
124.81
120.24
40.53
40.36
40.29
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39.70
39.53
39.36
17.19
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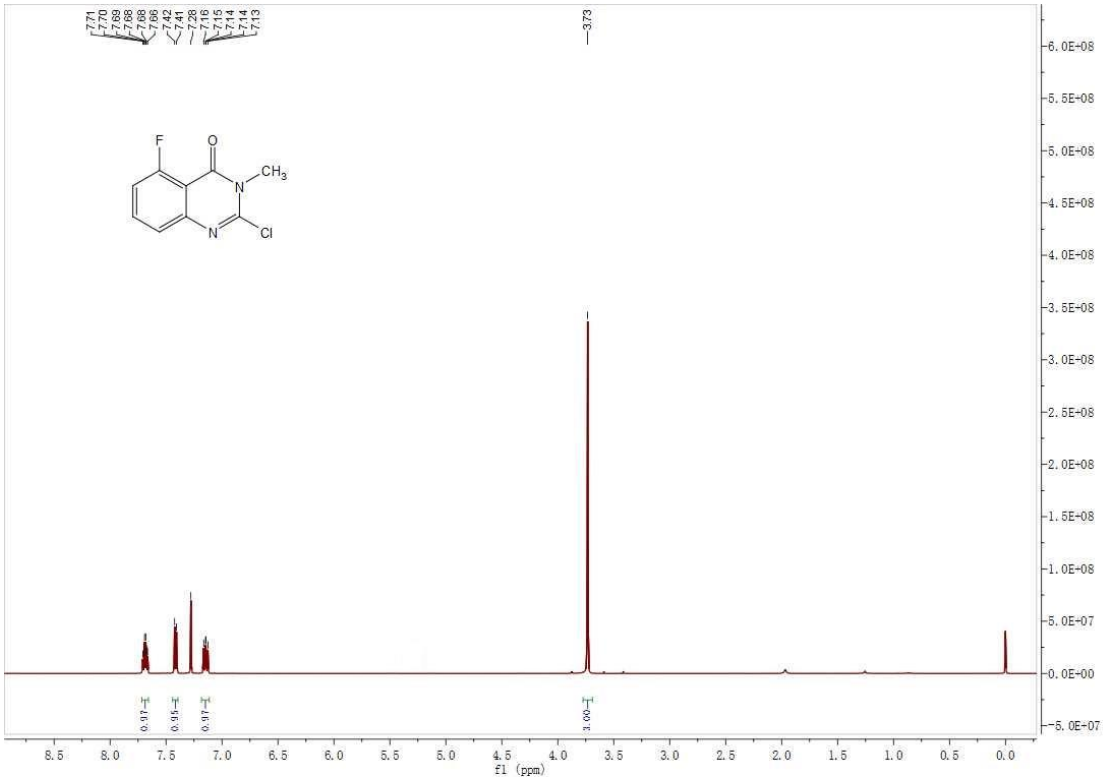
N
CH3
N
Cl
CH3
f1 (ppm)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7.70
7.69
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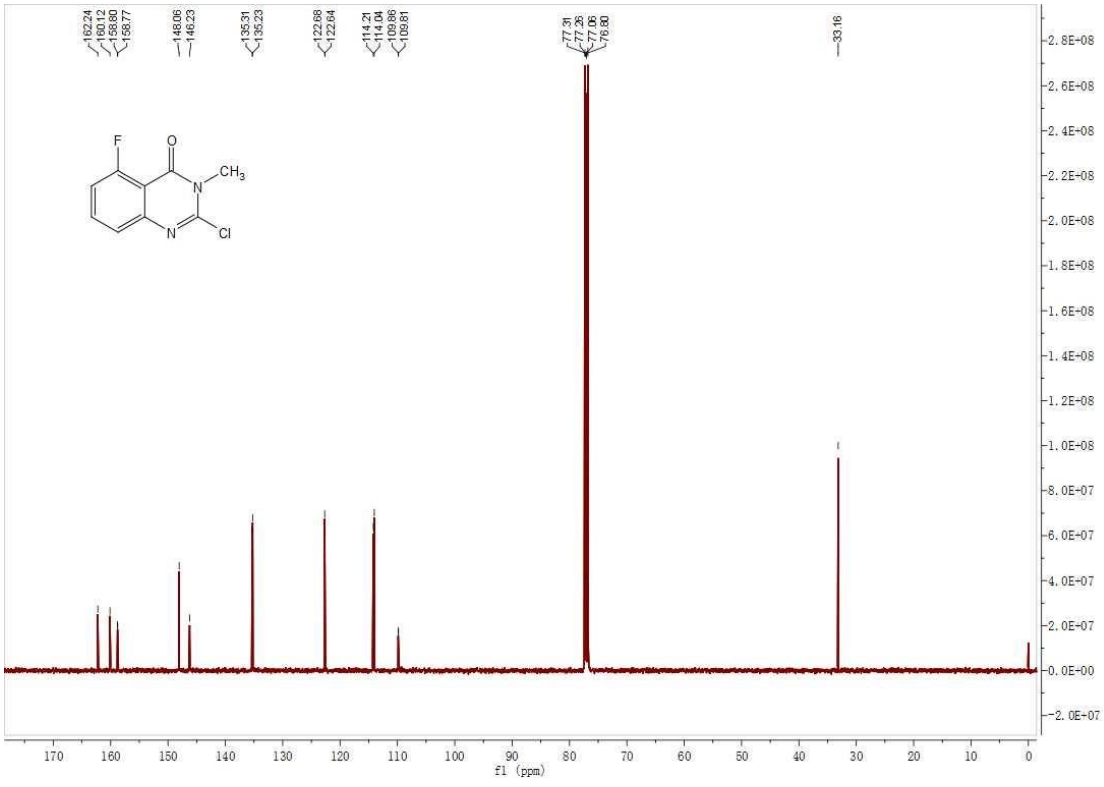
7.68
7.66
7.42
7.41
7.28
7.16
7.15
7.14
7.14
7.13
3.73
F
O
N
CH3
N
Cl
0.97
0.95
0.97
3.00
f1 (ppm)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146.23
135.31
135.23
122.68
122.64
114.21
114.04
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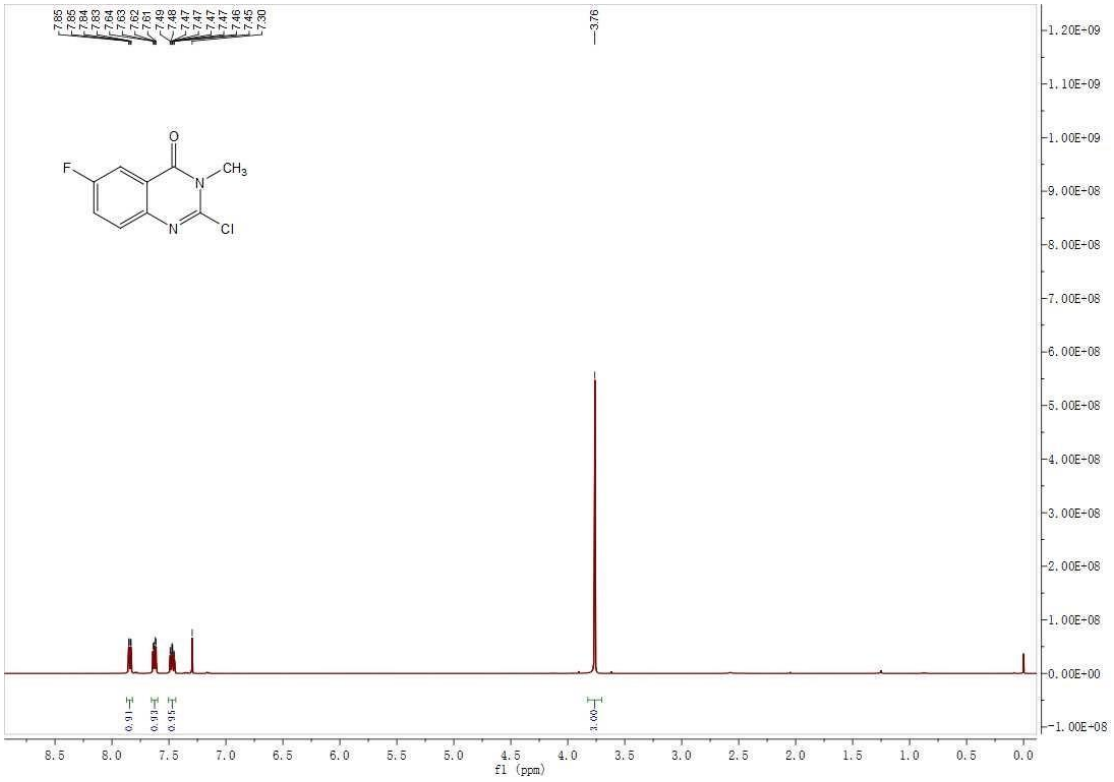
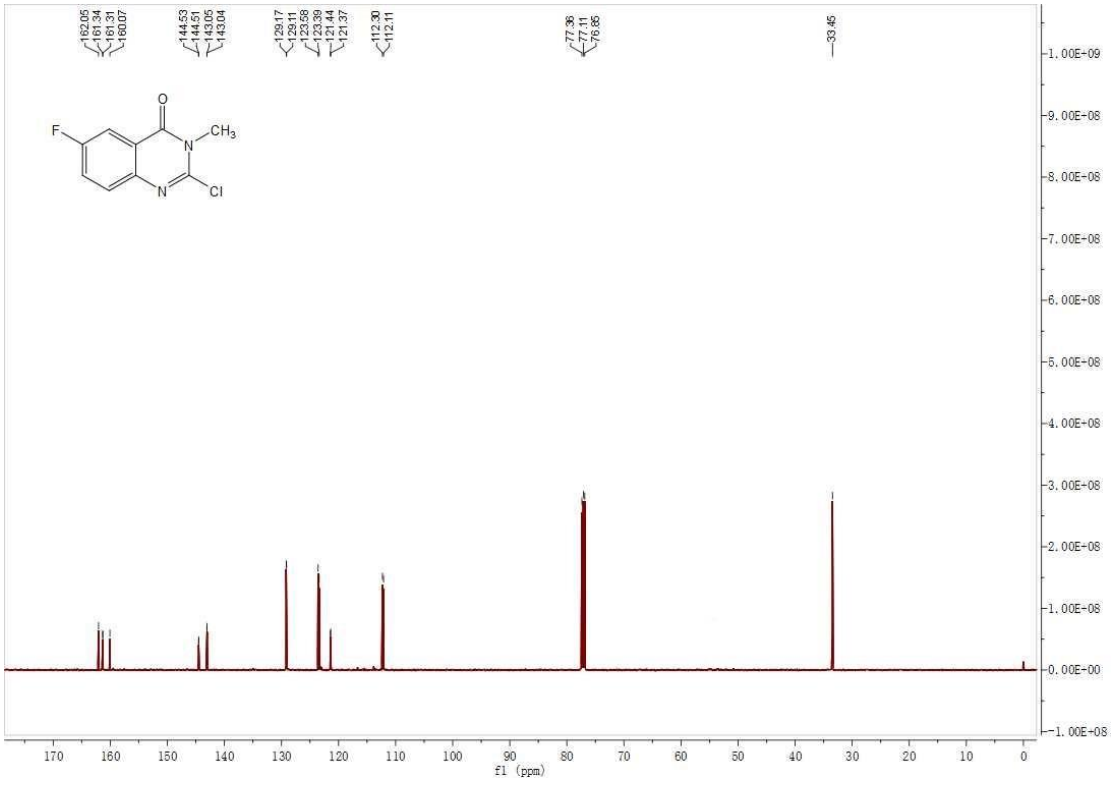
77.25
77.06
76.80
33.16
F
O
N
CH3
N
Cl
f1 (ppm)


7.85
7.85
7.84
7.84
7.83
7.64
7.63
7.62
7.61
7.49
7.48
7.47
7.47
7.47
7.47
7.46
7.45
7.30
3.76
O
F
CH3
N
N
Cl
0.91
0.93
0.95
3.00
f1 (ppm)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161.31
160.07
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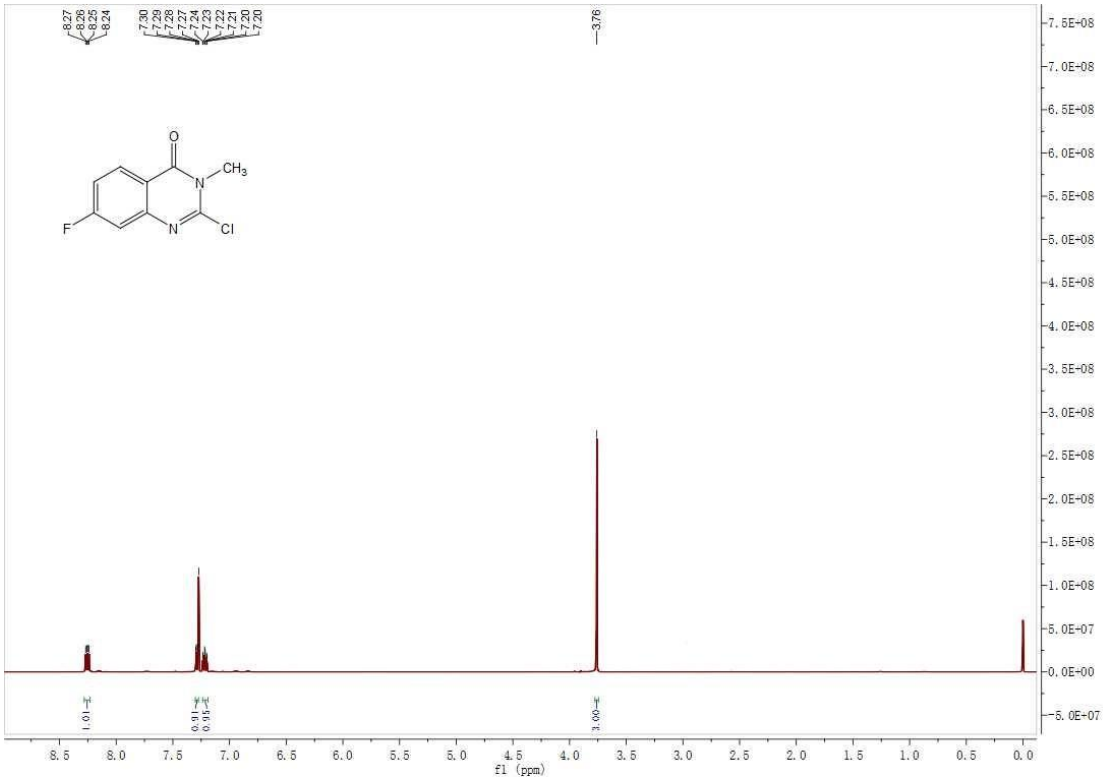
144.51
143.05
143.04
129.17
129.11
123.58
123.39
121.44
121.37
112.30
112.11
77.36
77.11
76.86
33.45
O
F
CH3
N
N
Cl
f1 (ppm)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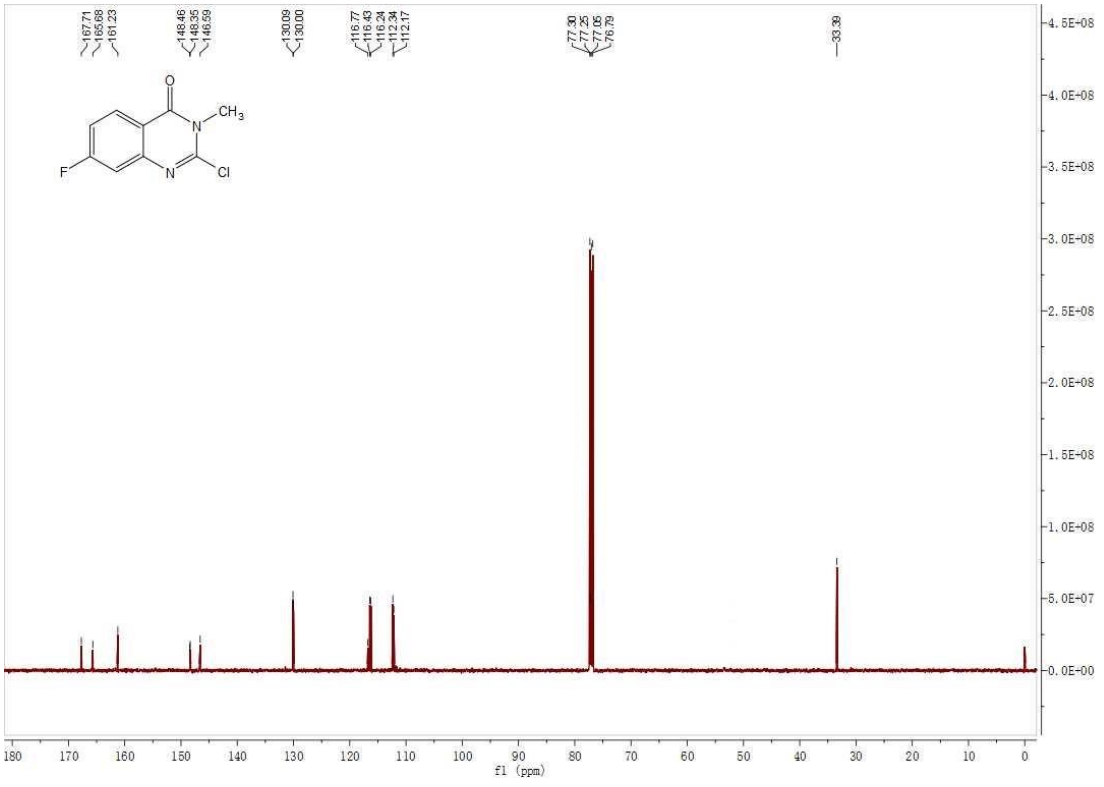
8.26
8.25
8.24
7.30
7.29
7.28
7.27
7.24
7.23
7.22
7.21
7.20
3.76
O
N
CH3
F
N
Cl
1.01
0.91
0.95
3.00
f1 (ppm)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130.09
130.00
116.77
116.43
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77.25
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76.79
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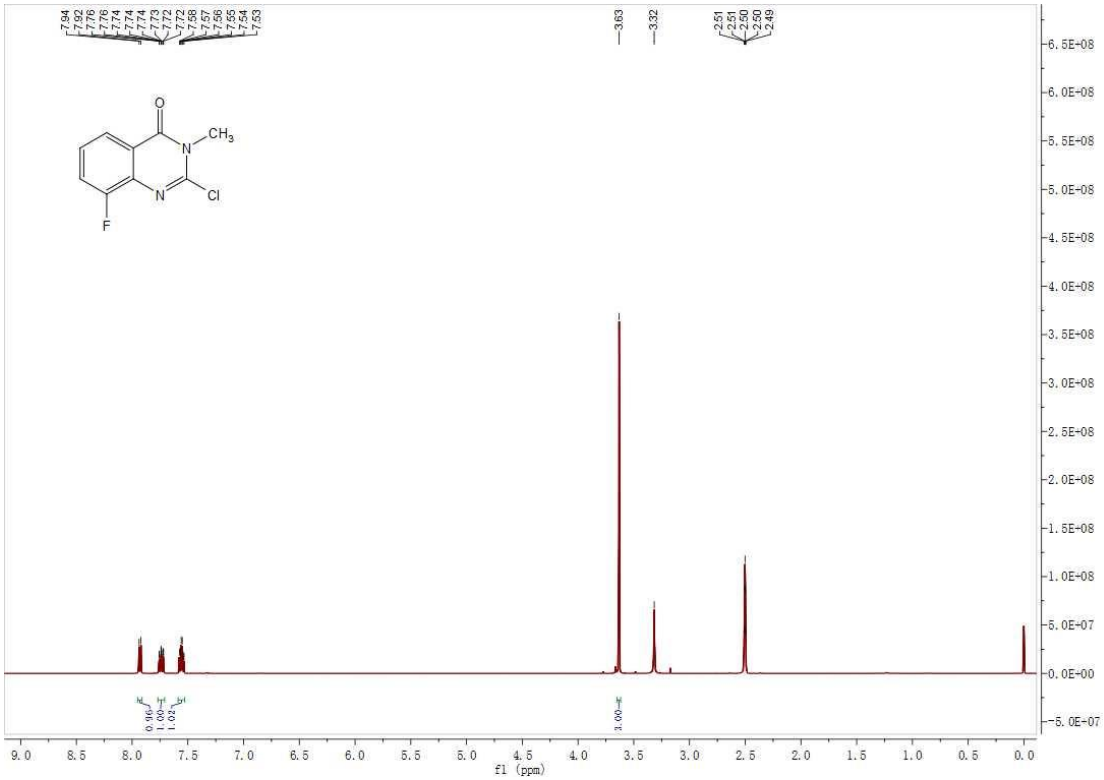
O
N
CH3
F
N
Cl
f1 (ppm)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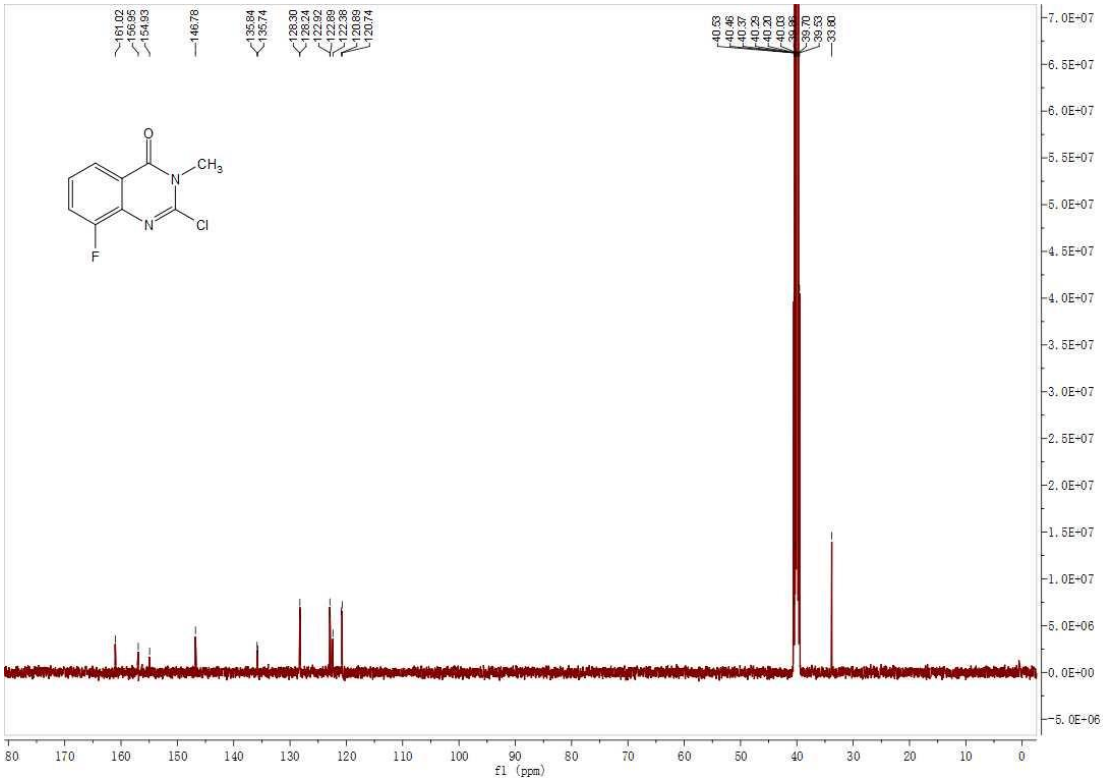
7.92
7.76
7.76
7.74
7.74
7.74
7.73
7.72
7.72
7.58
7.57
7.56
7.55
7.54
7.53
3.63
3.32
2.51
2.51
2.50
2.50
2.49
O
N
CH3
N
Cl
F
0.96
1.00
1.02
3.00
f1 (ppm)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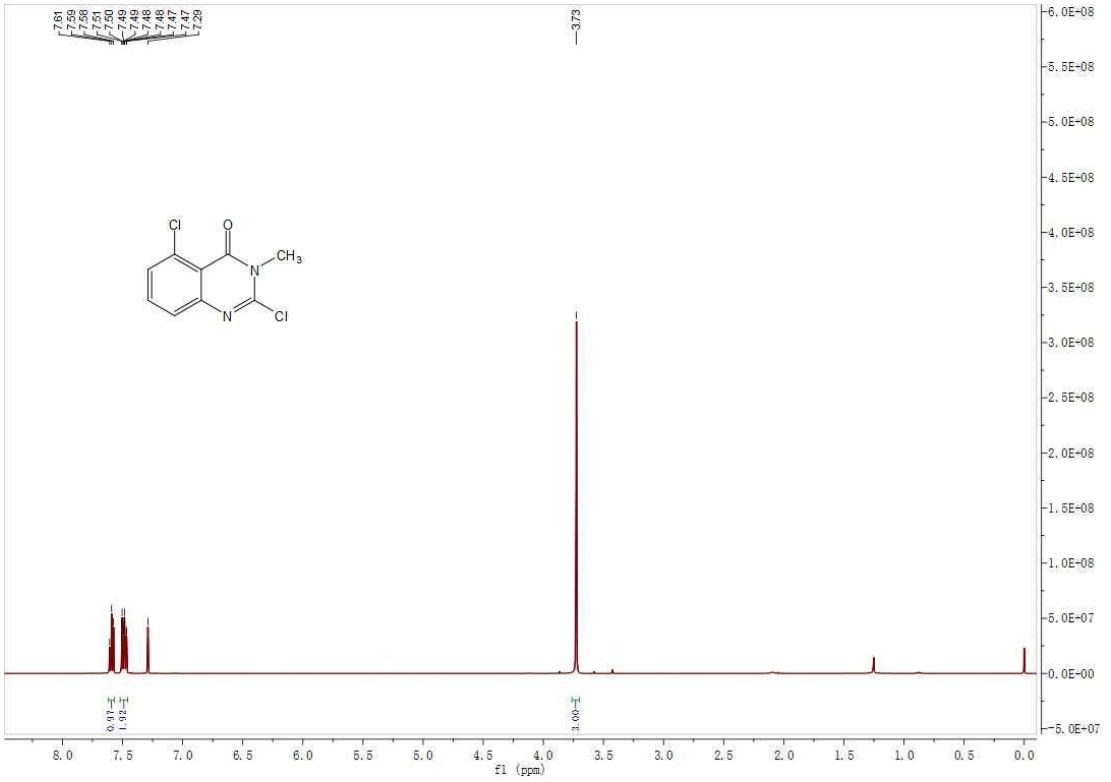
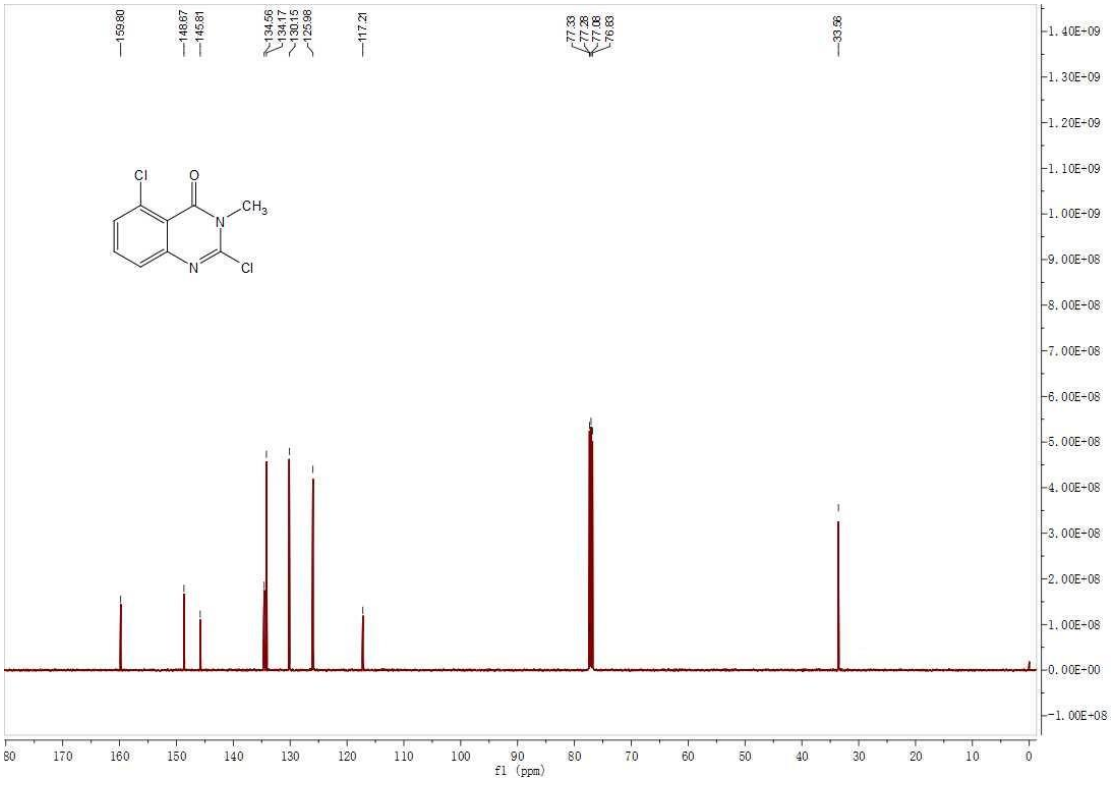
135.84
135.74
128.30
128.24
122.92
122.89
122.38
120.89
120.74
40.53
40.46
40.37
40.29
40.20
40.03
39.86
39.70
39.53
33.90
O
N
CH3
N
Cl
F
f1 (ppm)


7.61
7.59
7.58
7.51
7.50
7.49
7.49
7.48
7.48
7.47
7.47
7.29
3.73
Cl
O
N
CH3
N
Cl
0.97
1.92
3.00
f1 (ppm)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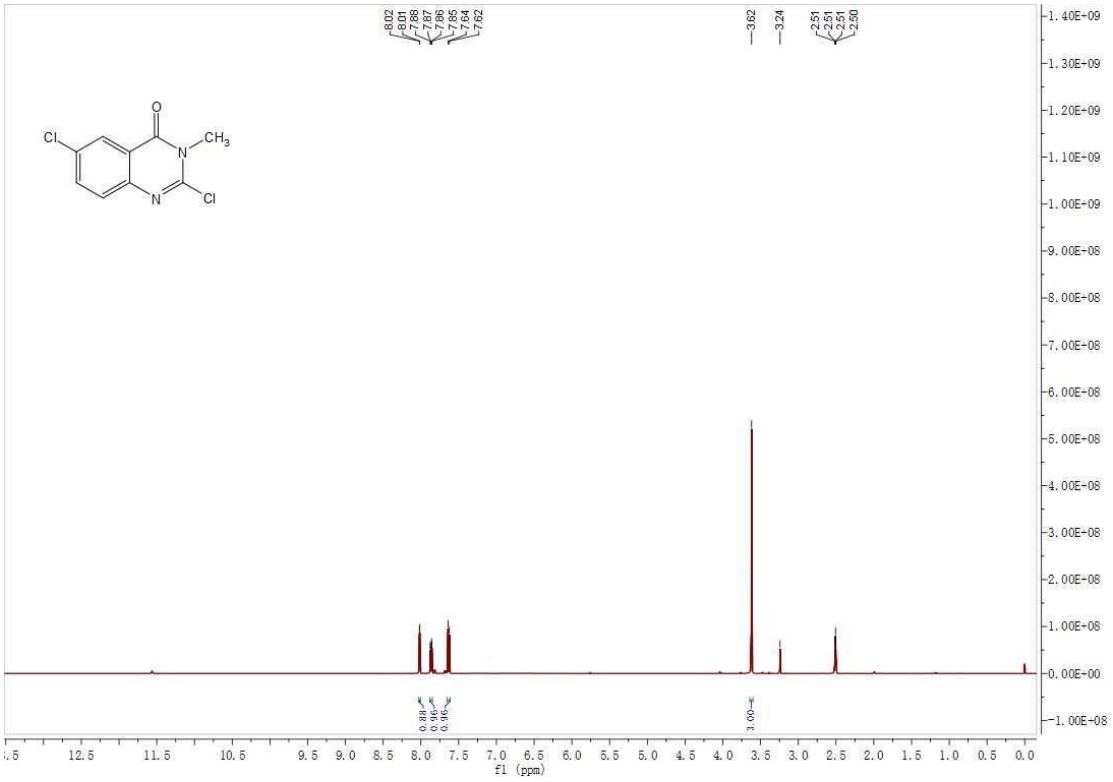
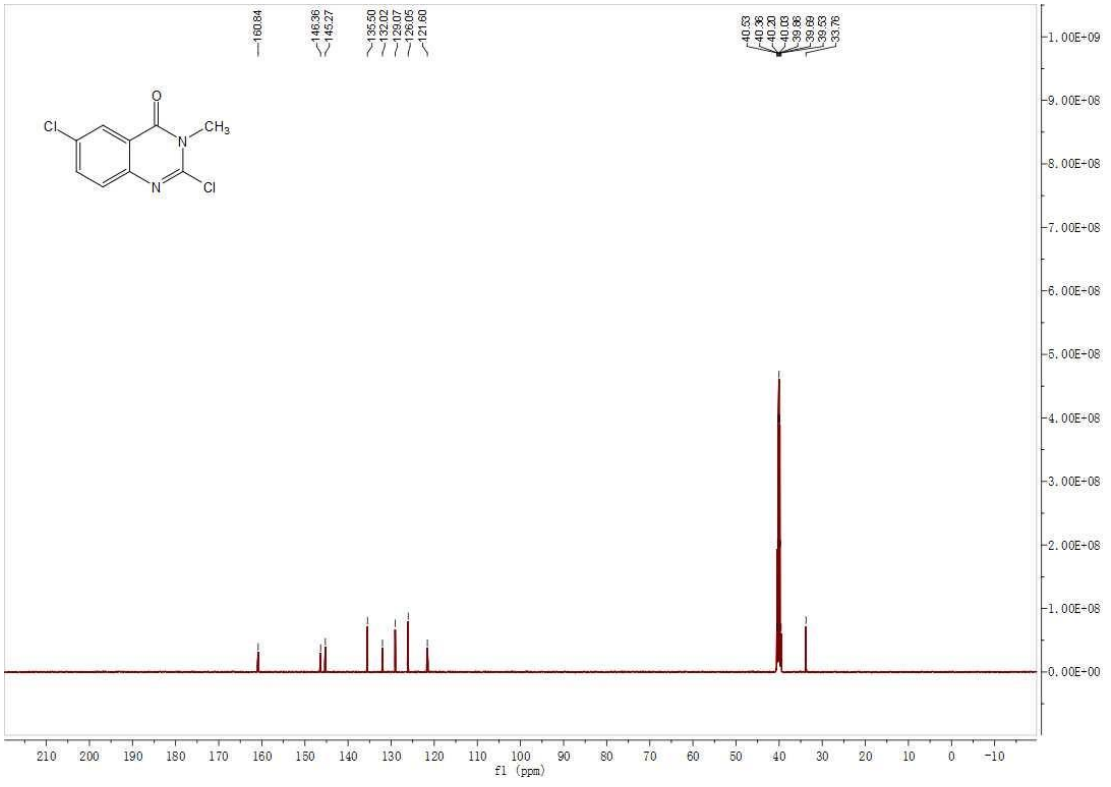
148.67
145.81
134.56
134.17
130.15
125.98
117.21
77.33
77.28
77.08
76.83
33.56
Cl
O
N
CH3
N
Cl
f1 (ppm)


8.02
8.01
7.88
7.87
7.86
7.85
7.84
7.82
3.62
3.24
2.51
2.51
2.51
2.50
O
Cl
N
CH3
N
Cl
0.81
0.91
0.96
3.00
fl (ppm)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129.07
126.05
121.60
40.53
40.36
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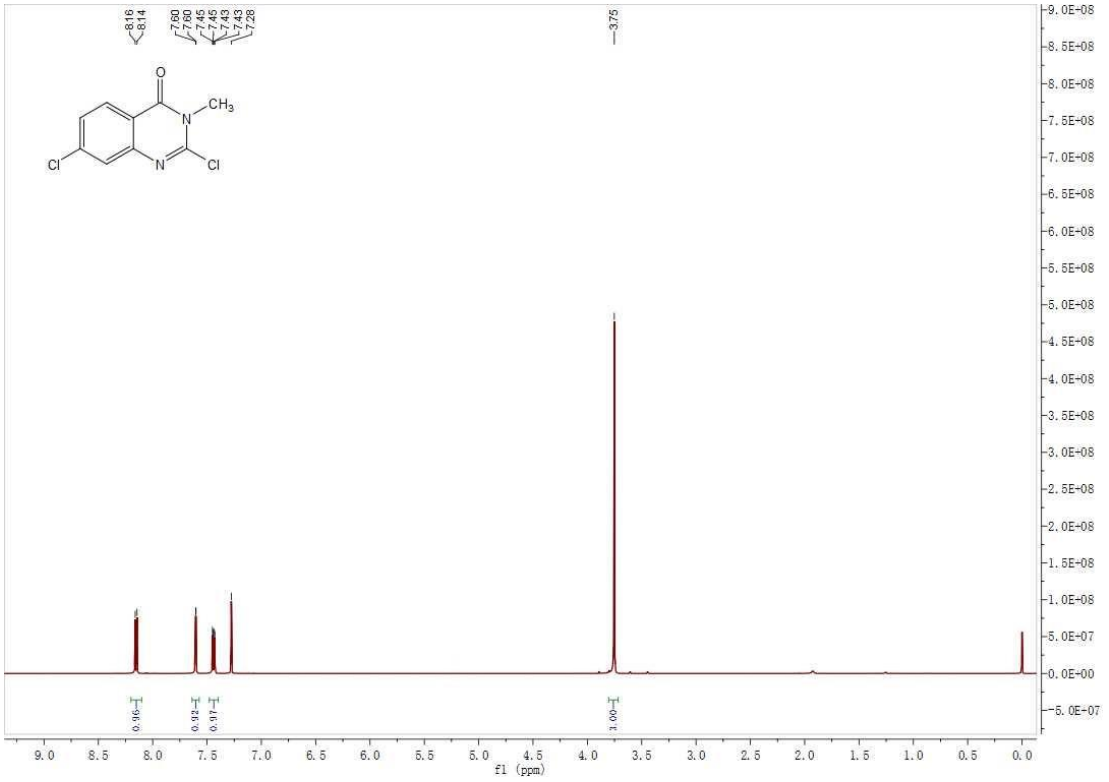
40.03
39.86
39.69
39.53
33.76
O
Cl
N
CH3
N
Cl
fl (ppm)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8.14
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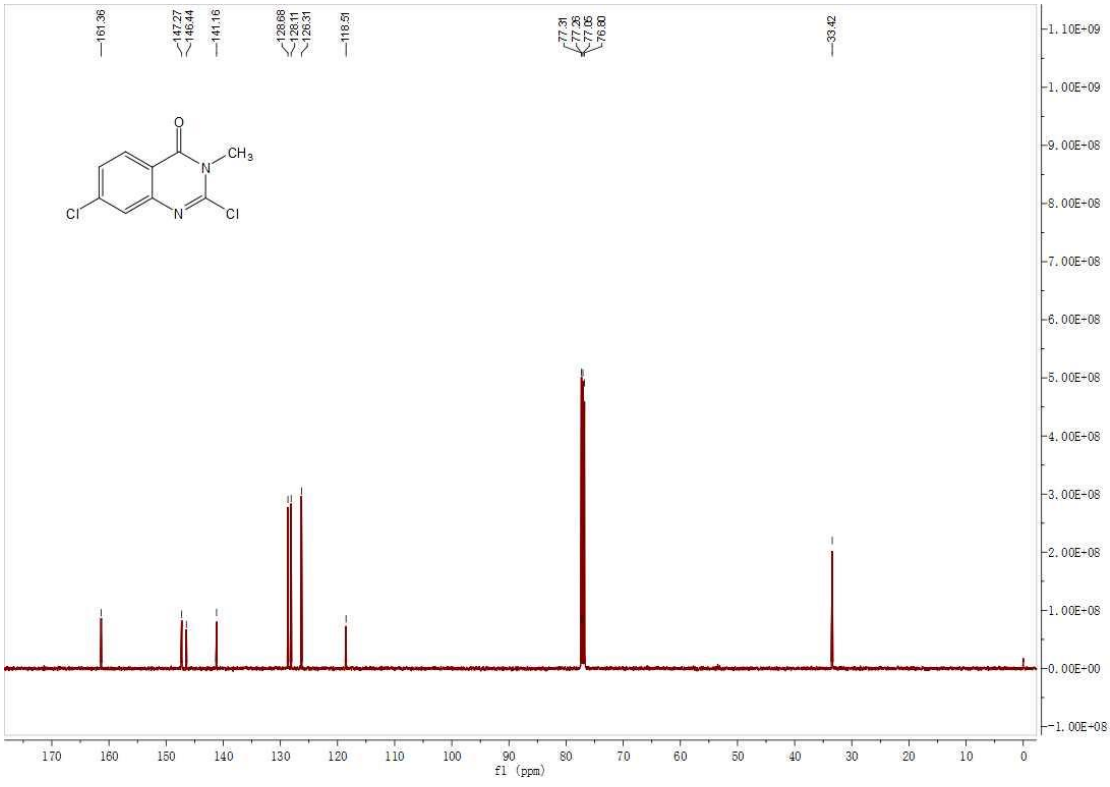
7.60
7.45
7.45
7.43
7.43
7.28
3.75
O
CH3
N
Cl
N
Cl
0.96
0.92
0.97
3.00
9.0E-08
8.5E-08
8.0E-08
7.5E-08
7.0E-08
6.5E-08
6.0E-08
5.5E-08
5.0E-08
4.5E-08
4.0E-08
3.5E-08
3.0E-08
2.5E-08
2.0E-08
1.5E-08
1.0E-08
5.0E-07
0.0E+00
-5.0E-07
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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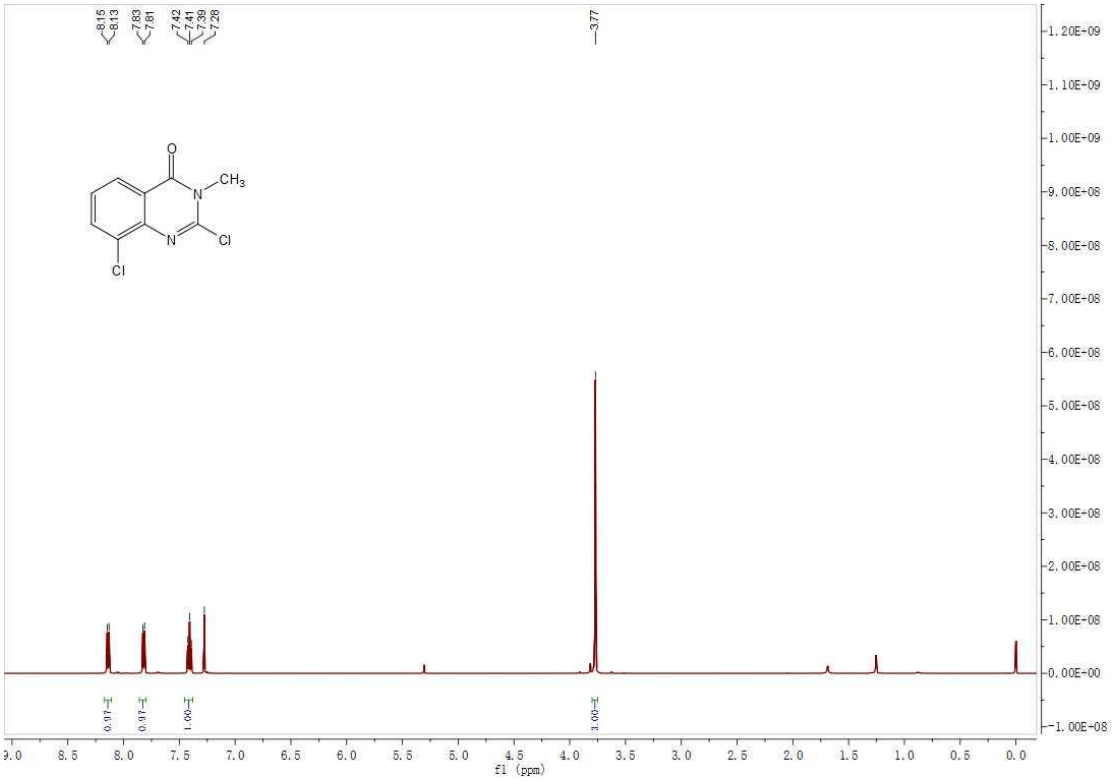
128.68
128.11
126.31
118.51
77.31
77.26
77.05
76.80
33.42
O
CH3
N
Cl
N
Cl
1.10E-09
1.00E-09
9.00E-08
8.00E-08
7.00E-08
6.00E-08
5.00E-08
4.00E-08
3.00E-08
2.00E-08
1.00E-08
0.00E+00
-1.00E-08
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.13
7.83
7.81
7.42
7.41
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7.28
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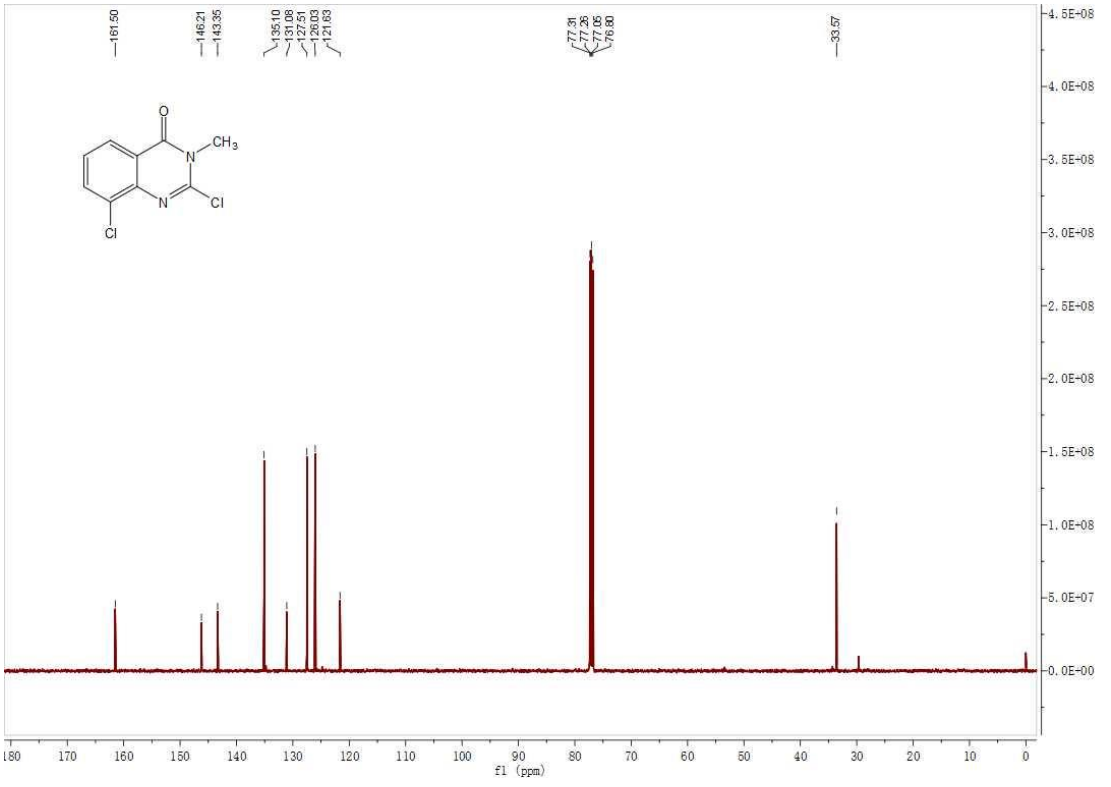
O
N
CH3
N
Cl
Cl
0.97
0.97
1.00
3.00
f1 (ppm)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146.21
143.35
135.10
131.08
127.51
126.03
121.63
77.31
77.36
77.05
76.80
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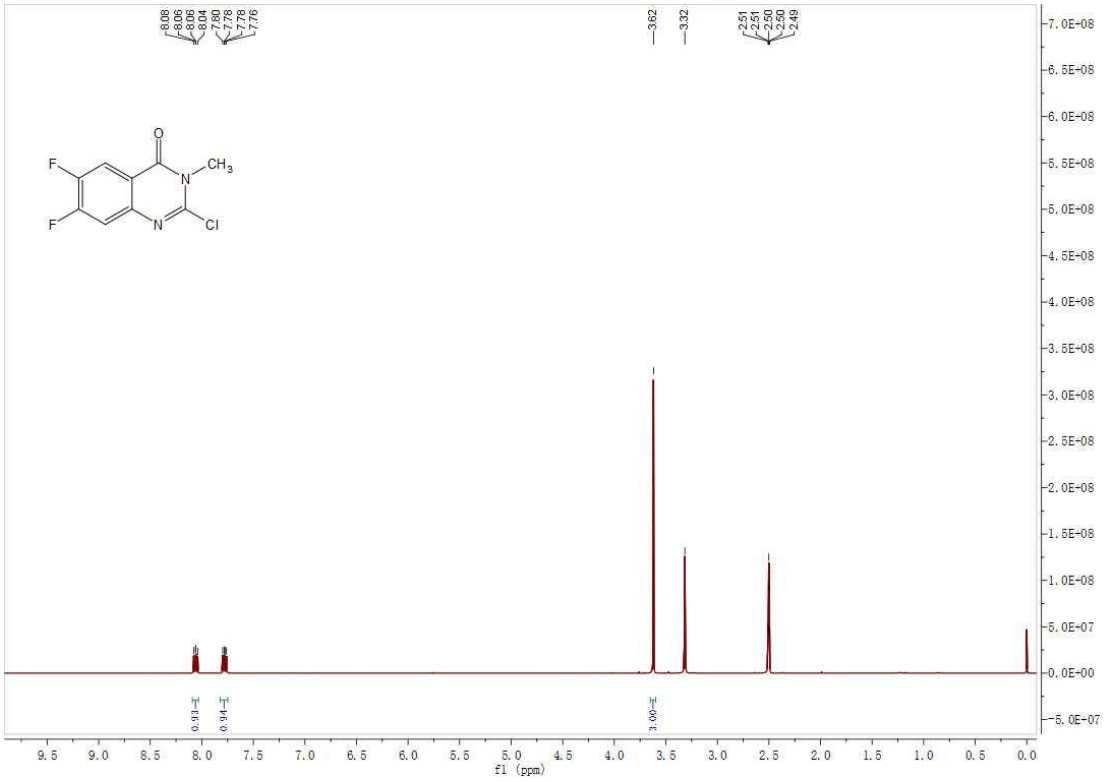
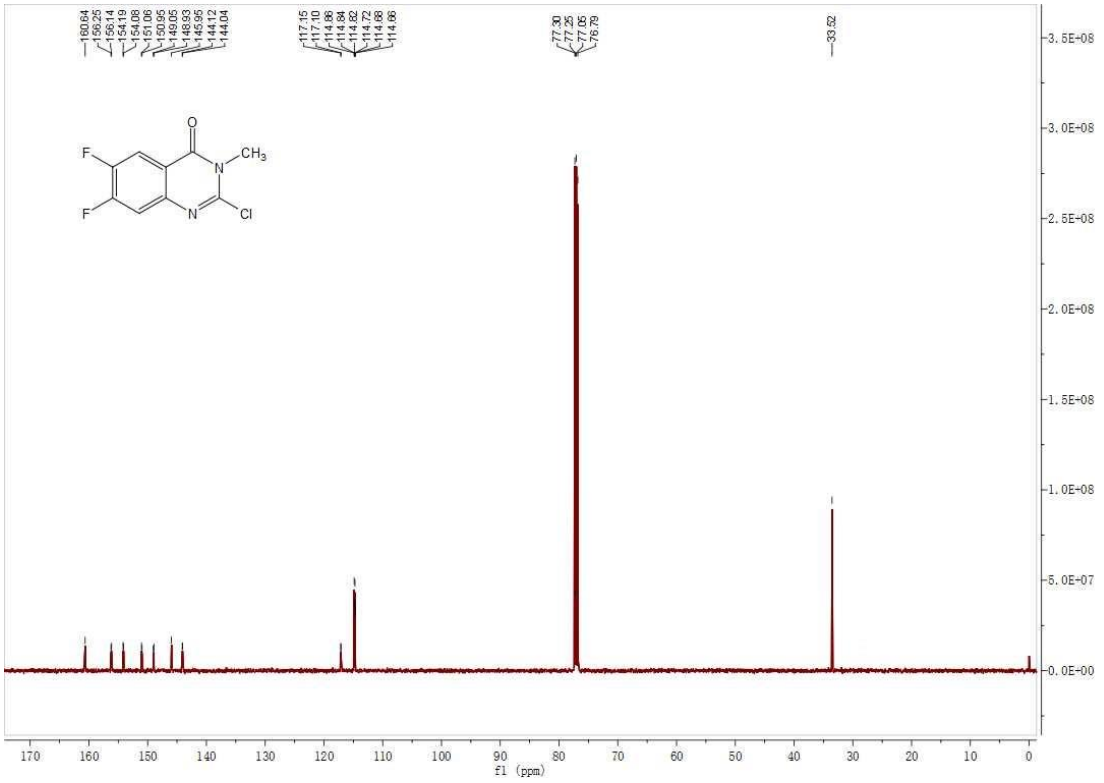
O
N
CH3
N
Cl
Cl
f1 (ppm)


8.08
8.06
8.06
8.04
7.80
7.78
7.78
7.76
3.62
3.32
2.51
2.51
2.50
2.50
2.49
F
F
O
N
CH3
N
Cl
0.93
0.94
3.00
f1 (ppm)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149.05
148.93
145.95
144.12
144.04
117.15
117.10
114.86
114.84
114.82
114.72
114.68
114.66
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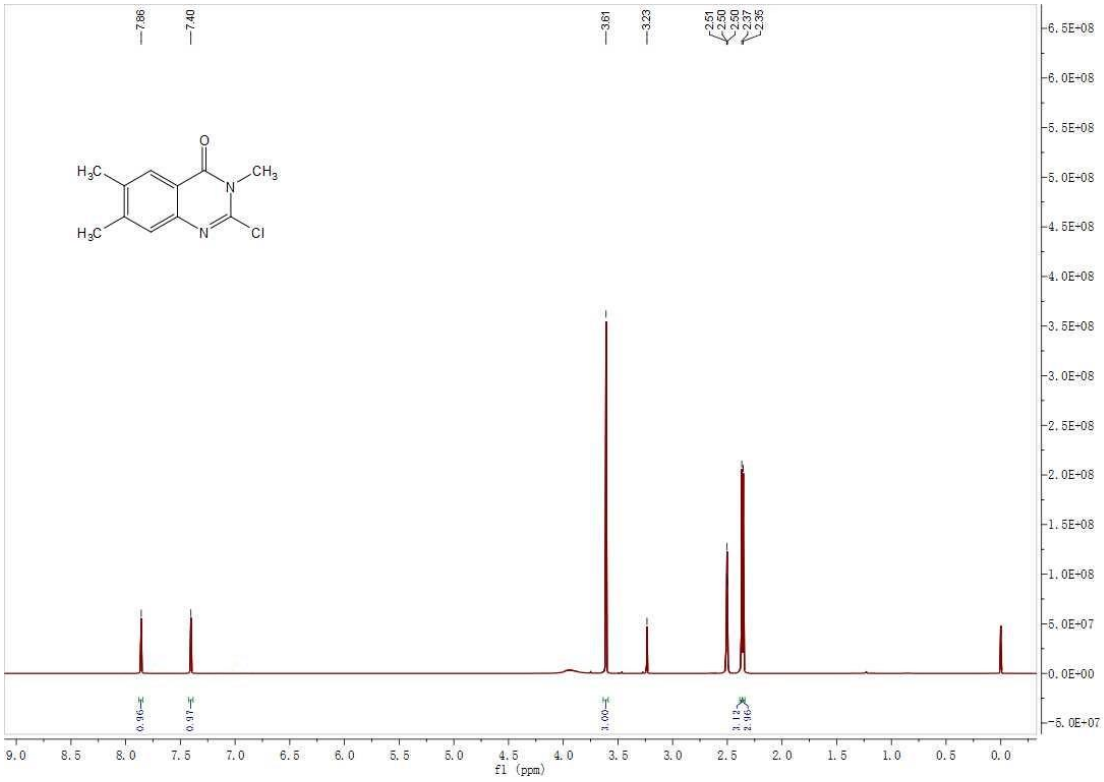
77.25
77.05
76.79
33.52
F
F
O
N
CH3
N
Cl
f1 (ppm)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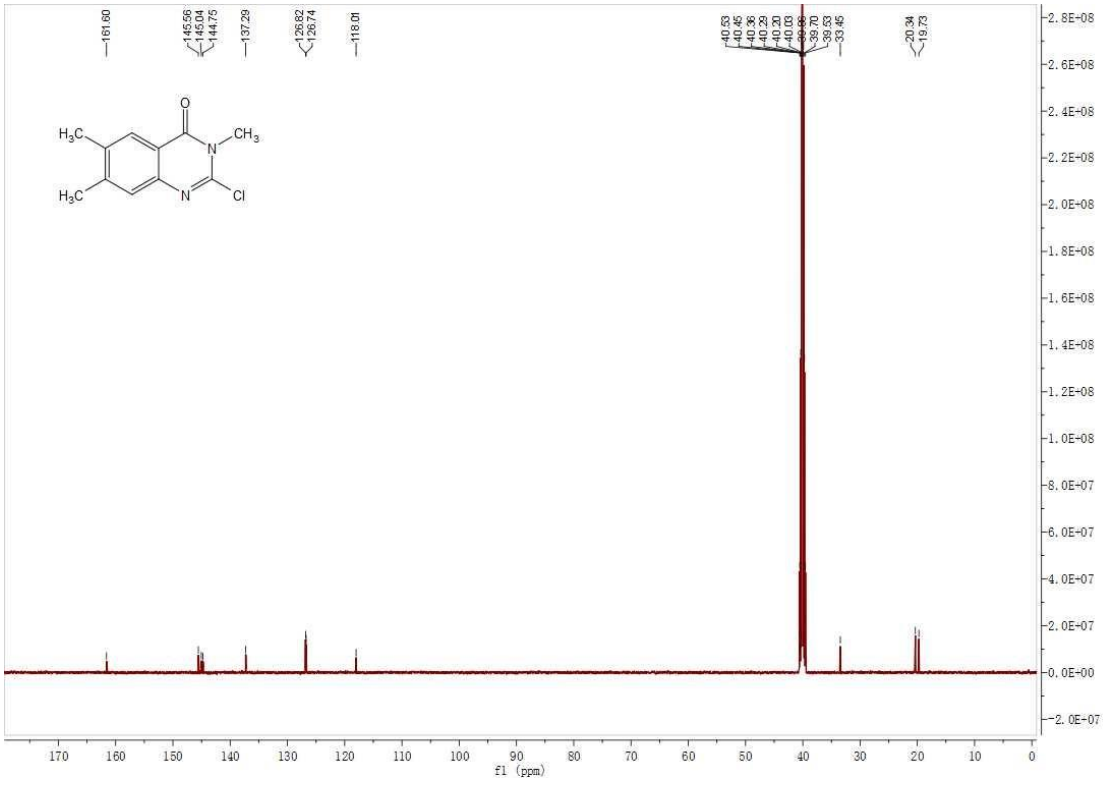
7.40
3.61
3.23
2.51
2.50
2.50
2.37
2.35
O
N
CH3
H3C
H3C
N
Cl
0.96
0.97
1.00
3.12
2.96
f1 (ppm)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126.74
118.01
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40.45
40.36
40.29
40.20
40.03
39.86
39.70
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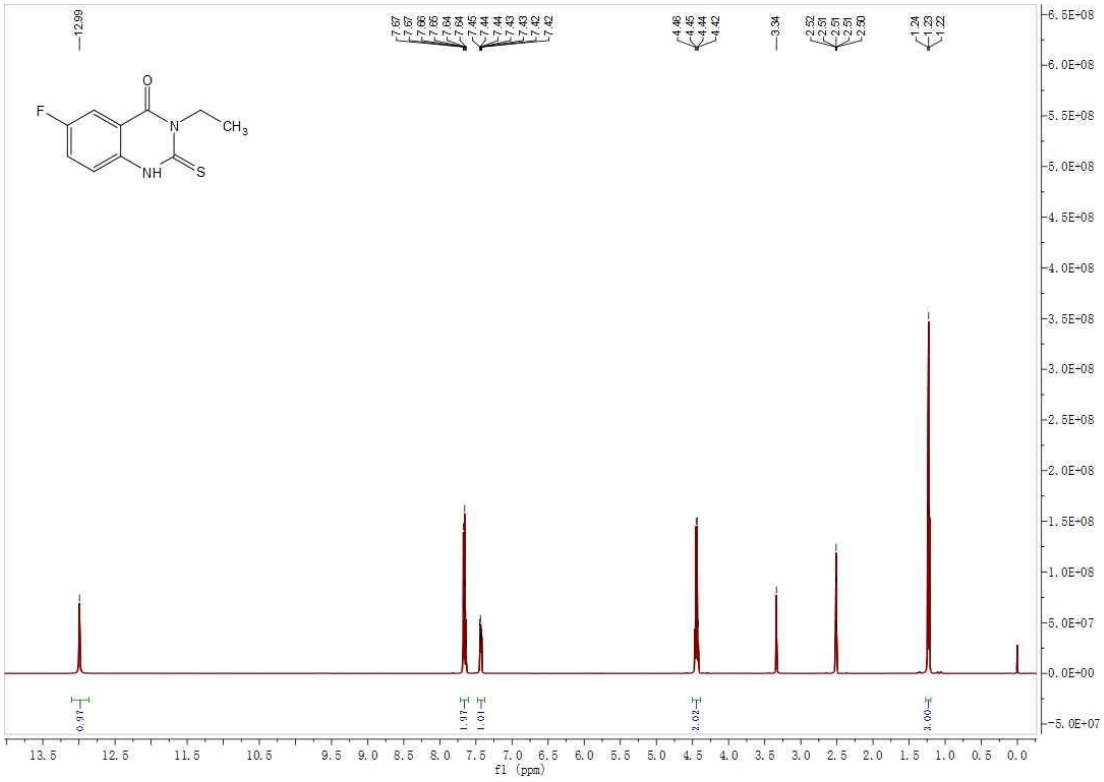
33.45
20.34
19.73
O
N
CH3
H3C
H3C
N
Cl
f1 (ppm)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7.67
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7.64
7.64
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7.44
7.44
7.43
7.43
7.42
7.42
4.46
4.45
4.44
4.42
3.34
2.52
2.51
2.51
2.51
2.50
1.24
1.23
1.22
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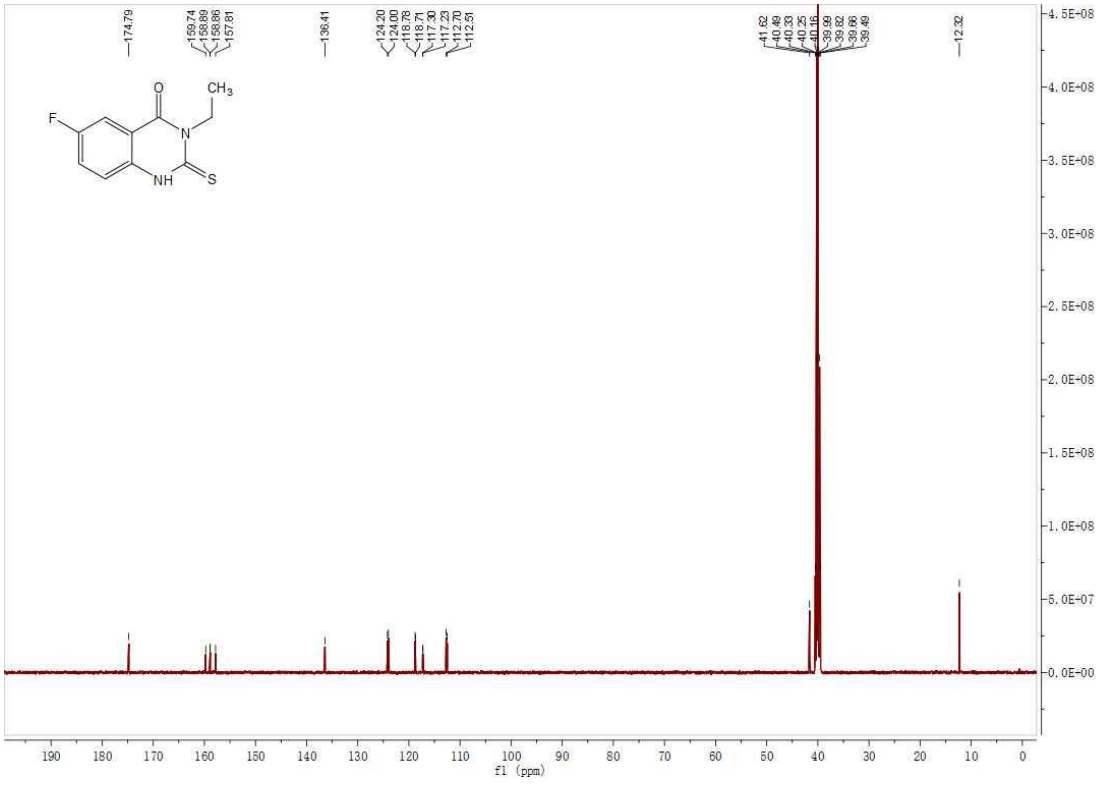
O
N
CH3
NH
S
0.97
1.97
1.01
2.02
3.00
f1 (ppm)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124.20
124.00
118.78
118.71
117.30
117.23
112.70
112.51
41.62
40.49
40.33
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40.16
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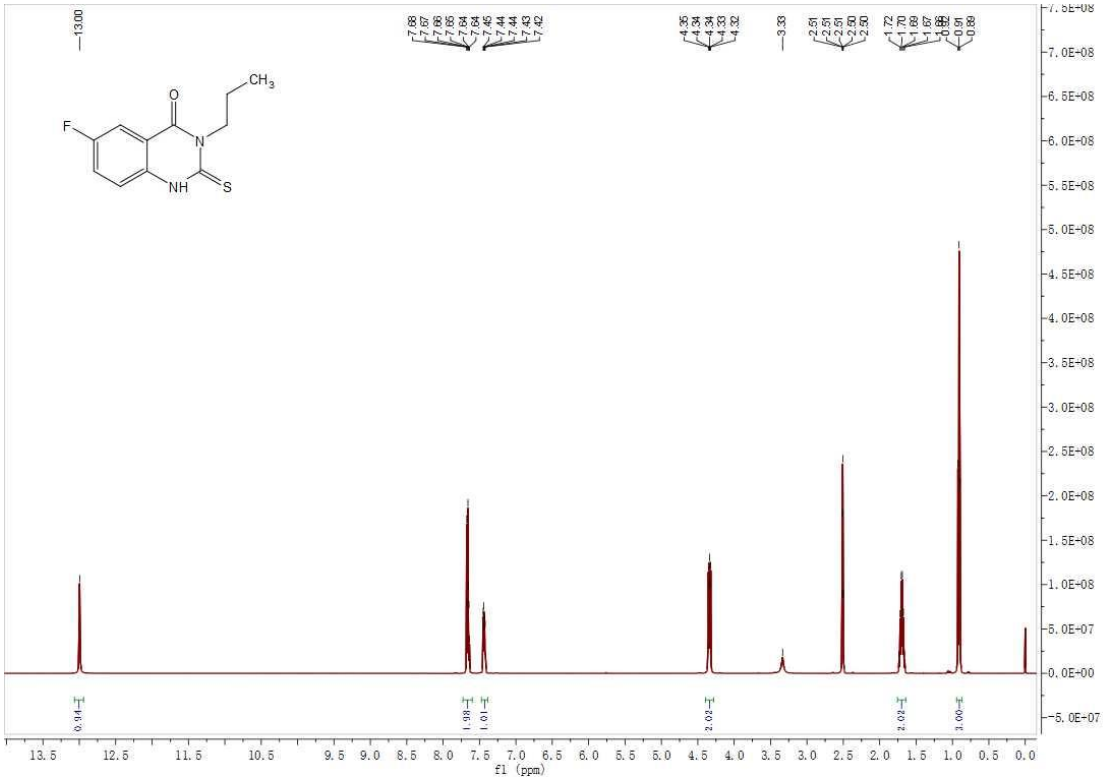
39.82
39.66
39.49
12.32
F
O
N
CH3
NH
S
f1 (ppm)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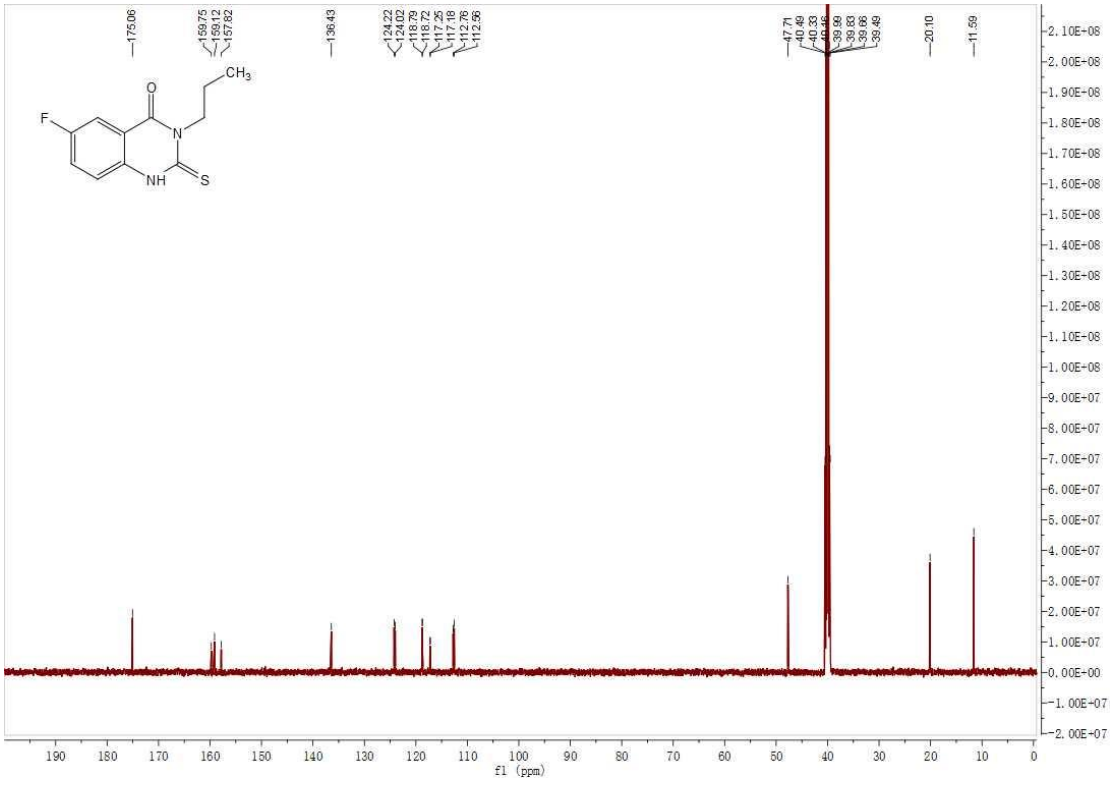
7.44
7.43
7.42
4.35
4.34
4.34
4.33
4.32
3.33
2.51
2.51
2.51
2.50
2.50
1.72
1.70
1.69
1.67
0.92
0.91
0.89
O
F
N
NH
S
CH3
0.94
1.98
1.01
2.02
2.02
3.00
f1 (ppm)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20.10
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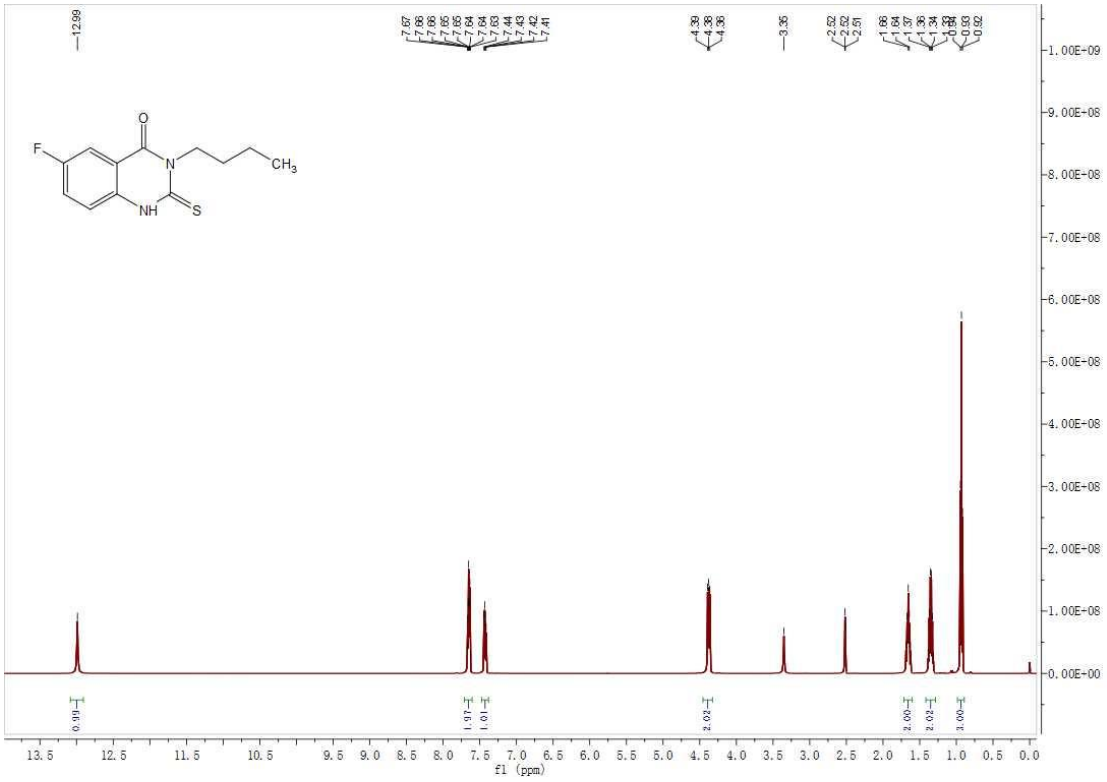
F
N
NH
S
CH3
f1 (ppm)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4.36
3.35
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2.52
2.51
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1.36
1.34
1.33
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0.93
0.92
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S
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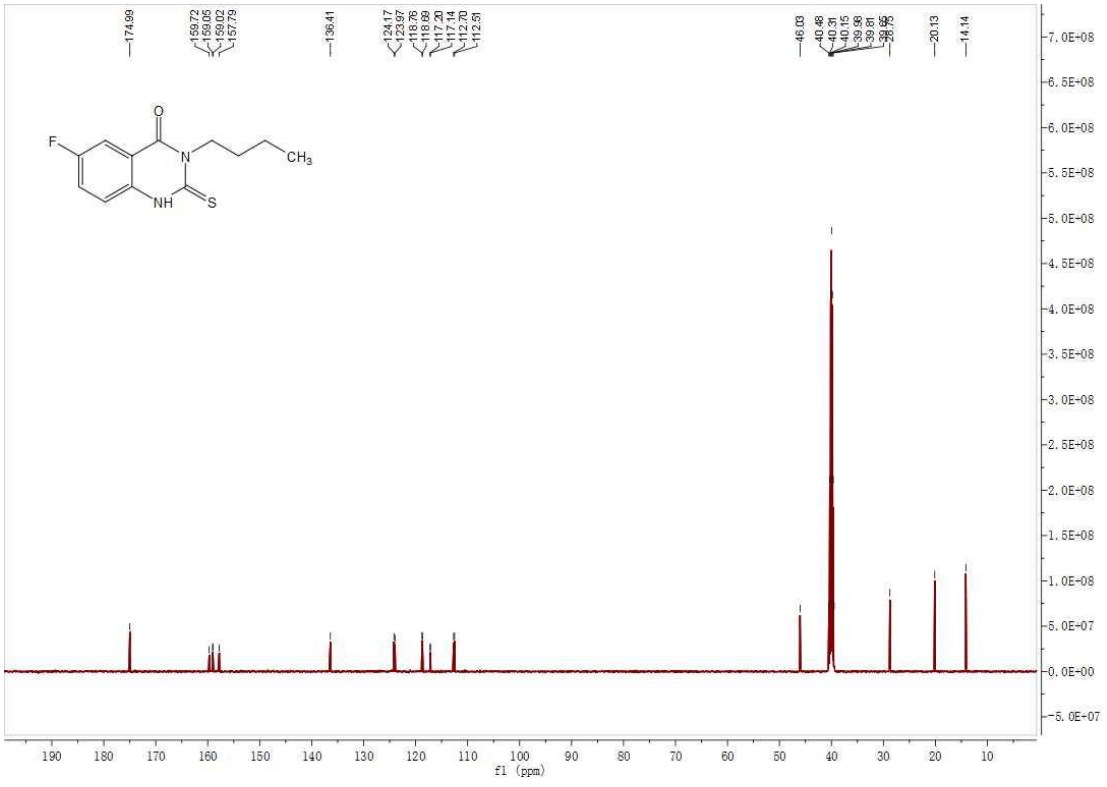
2.02
3.00
f1 (ppm)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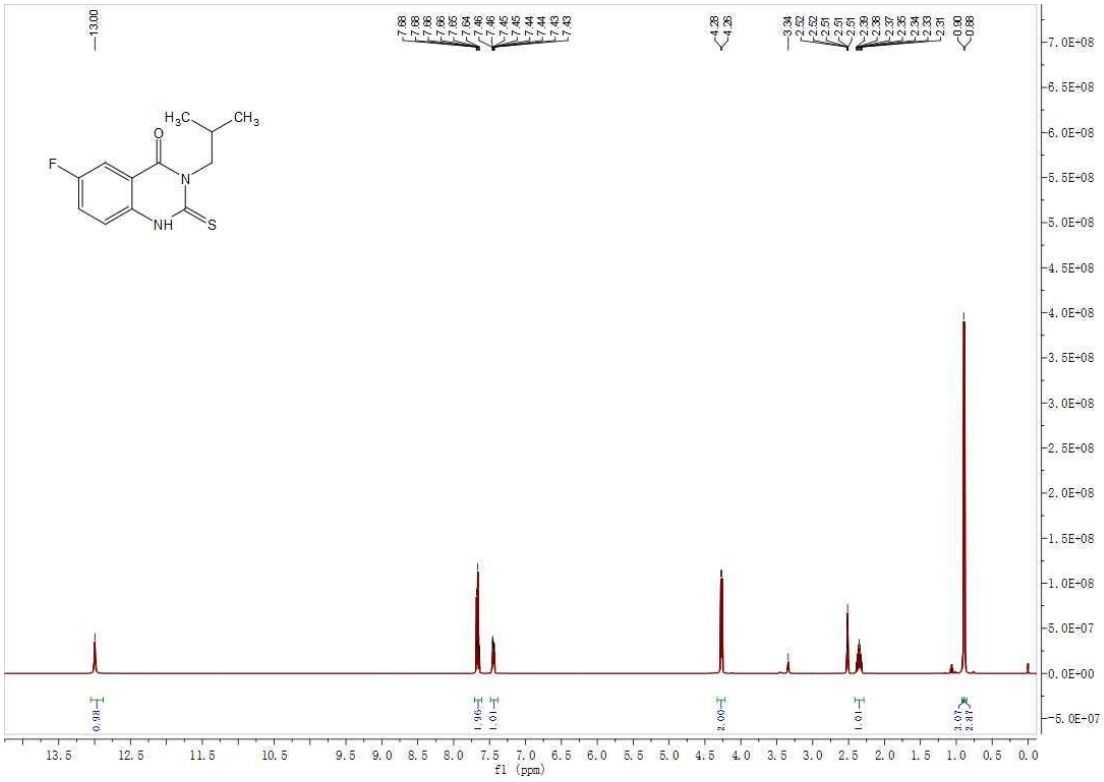
F
N
CH3
NH
S
f1 (ppm)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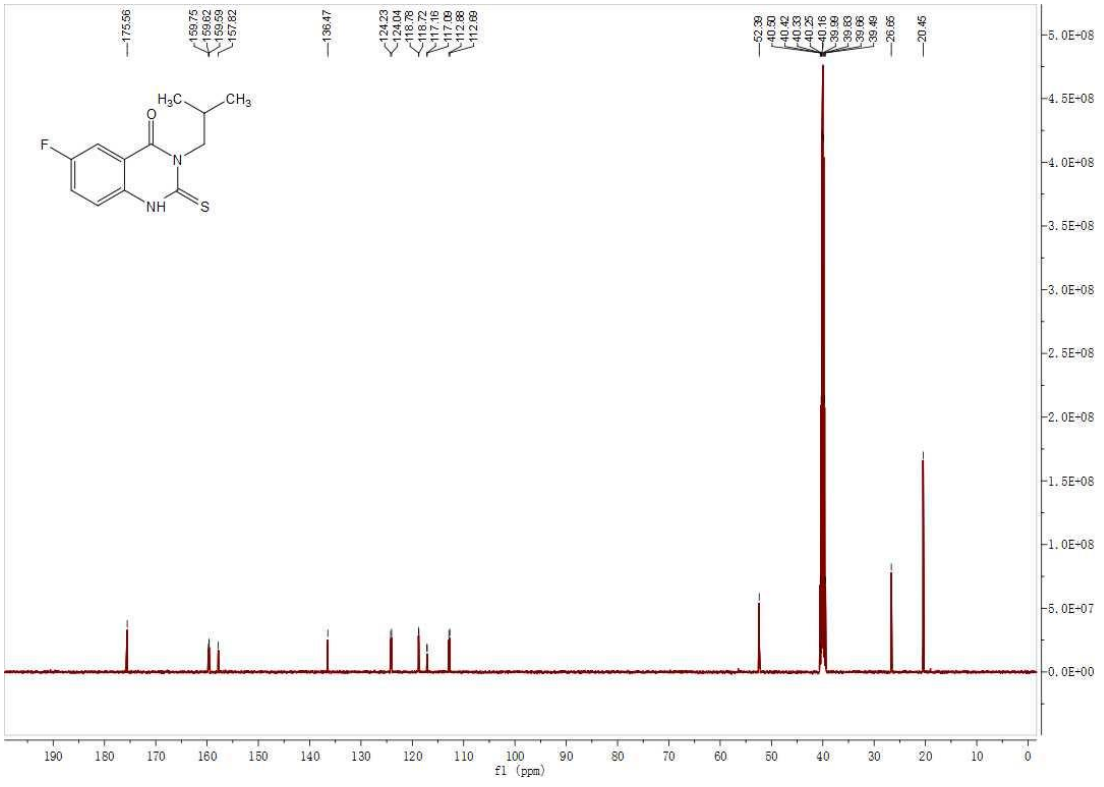
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CH3
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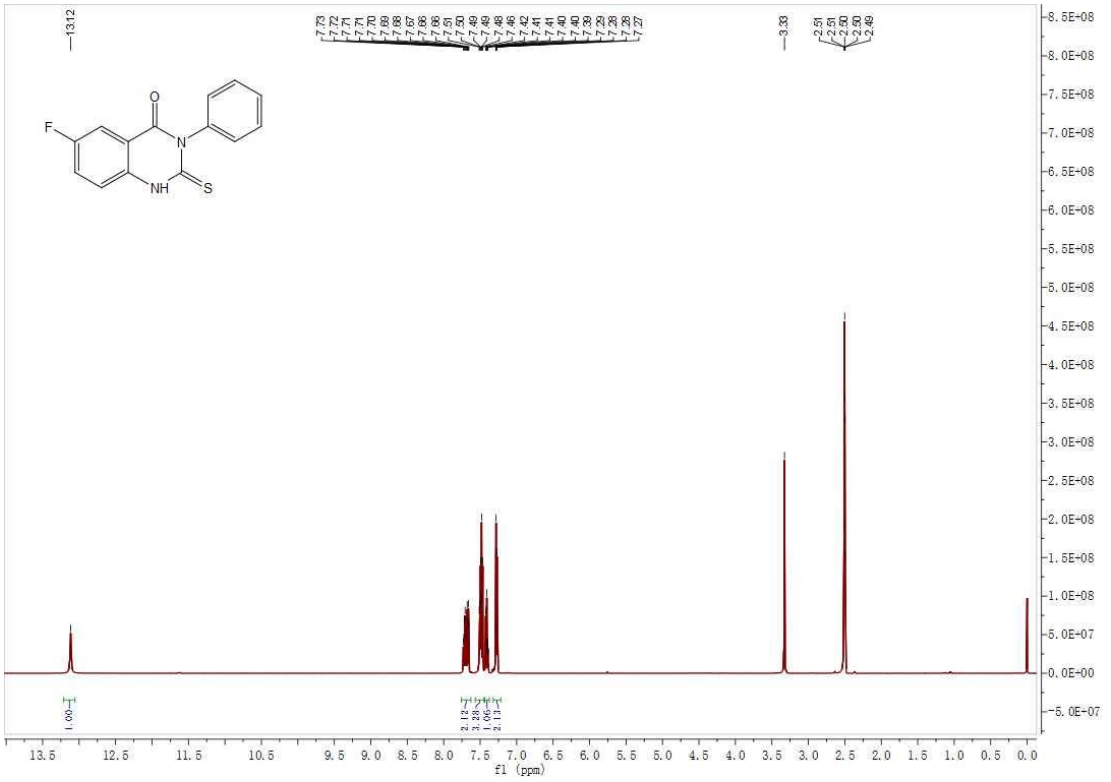
N
NH
S
f1 (ppm)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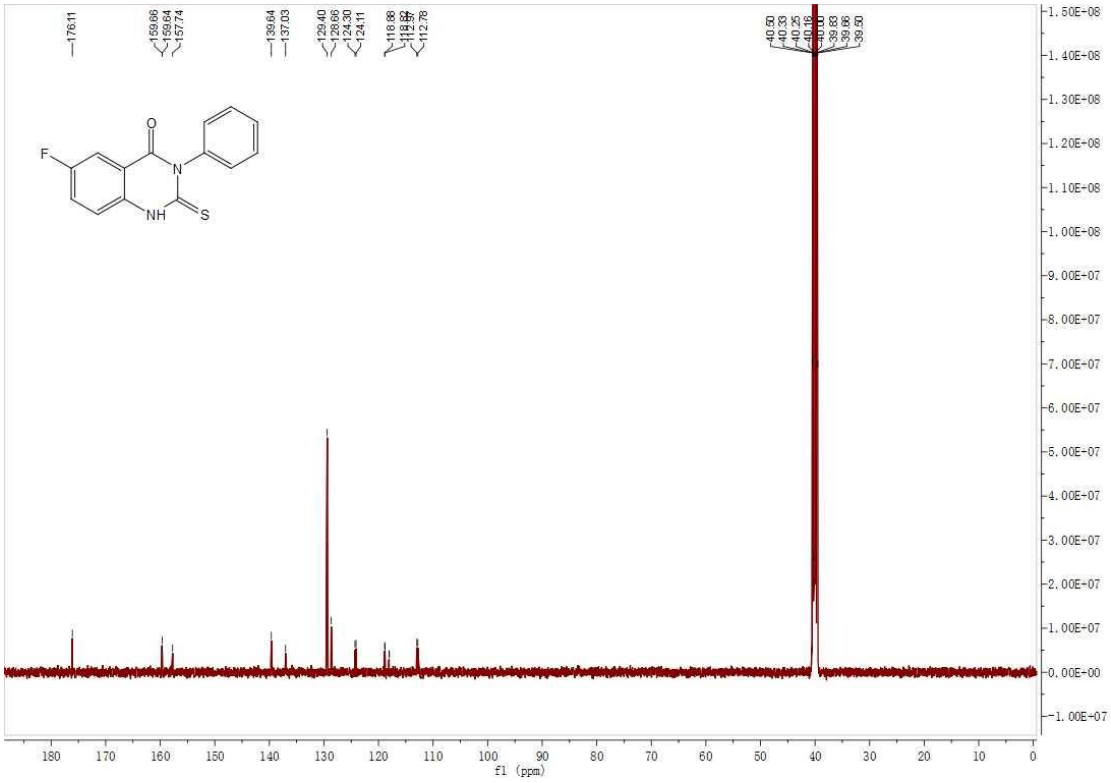
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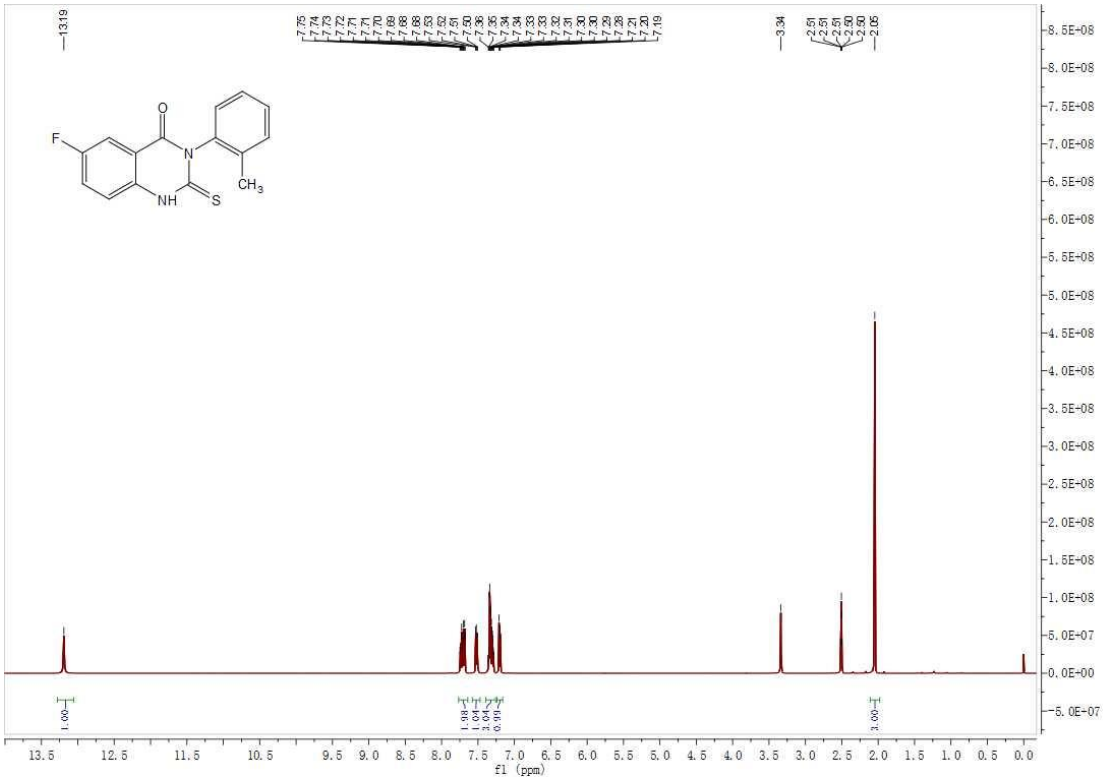
O
F
N
NH
S
f1 (ppm)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7.33
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7.31
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7.21
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7.19
3.34
2.51
2.51
2.51
2.50
2.50
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CH3
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1.04
1.04
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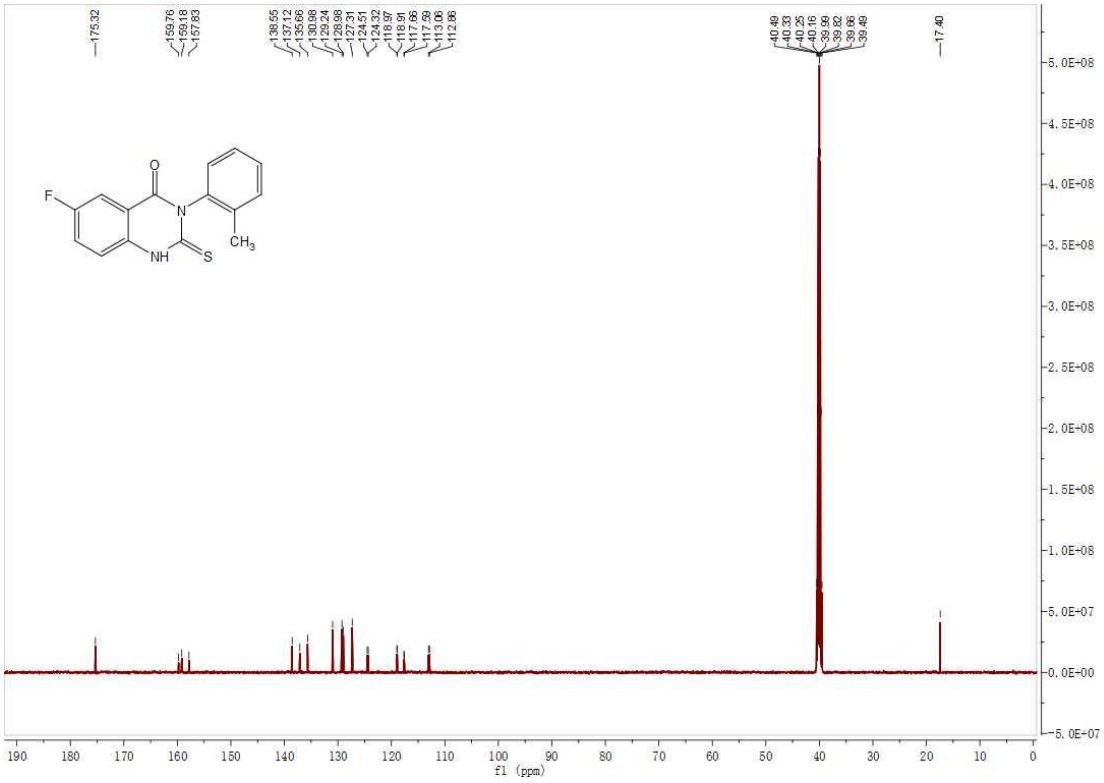
3.00
fl (ppm)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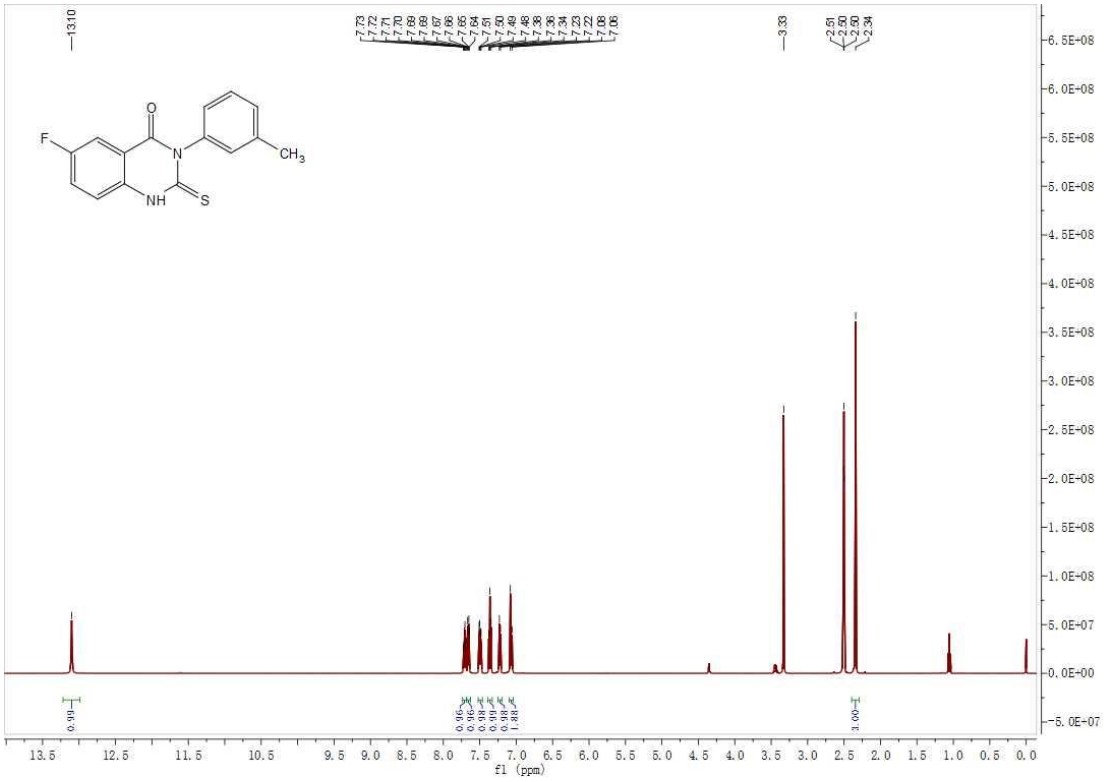
CH3
NH
S
fl (ppm)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7.22
7.08
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2.50
2.49
2.34
F
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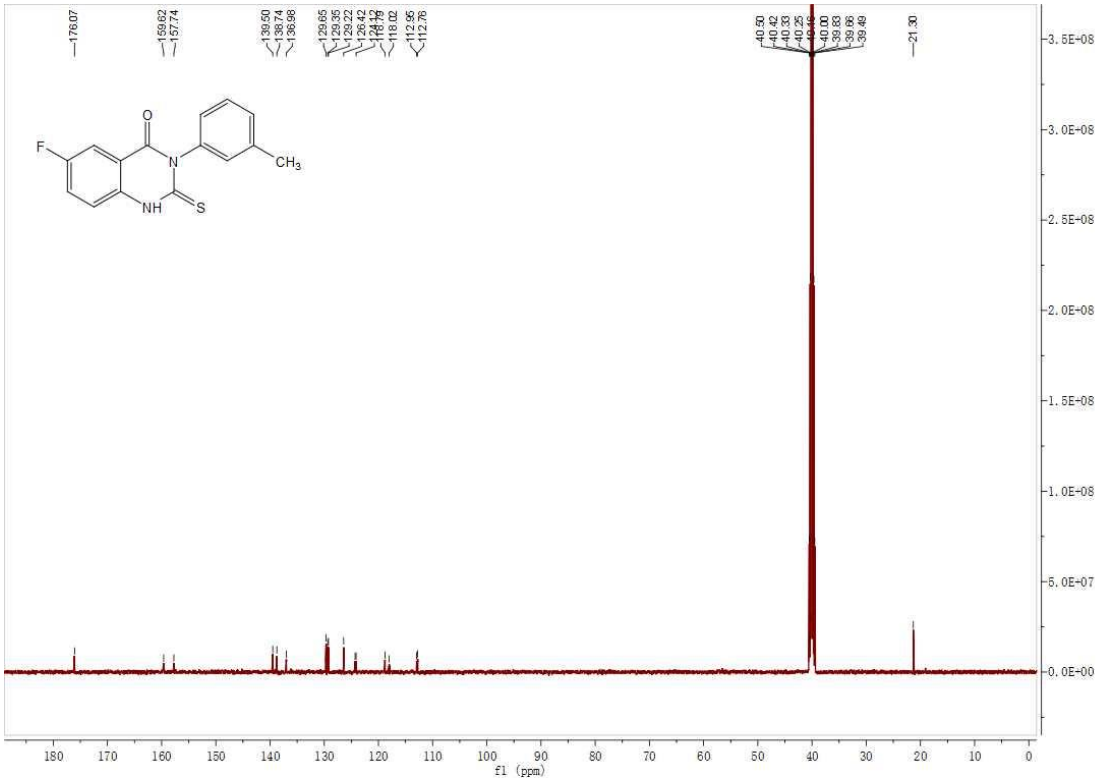
3.00
f1 (ppm)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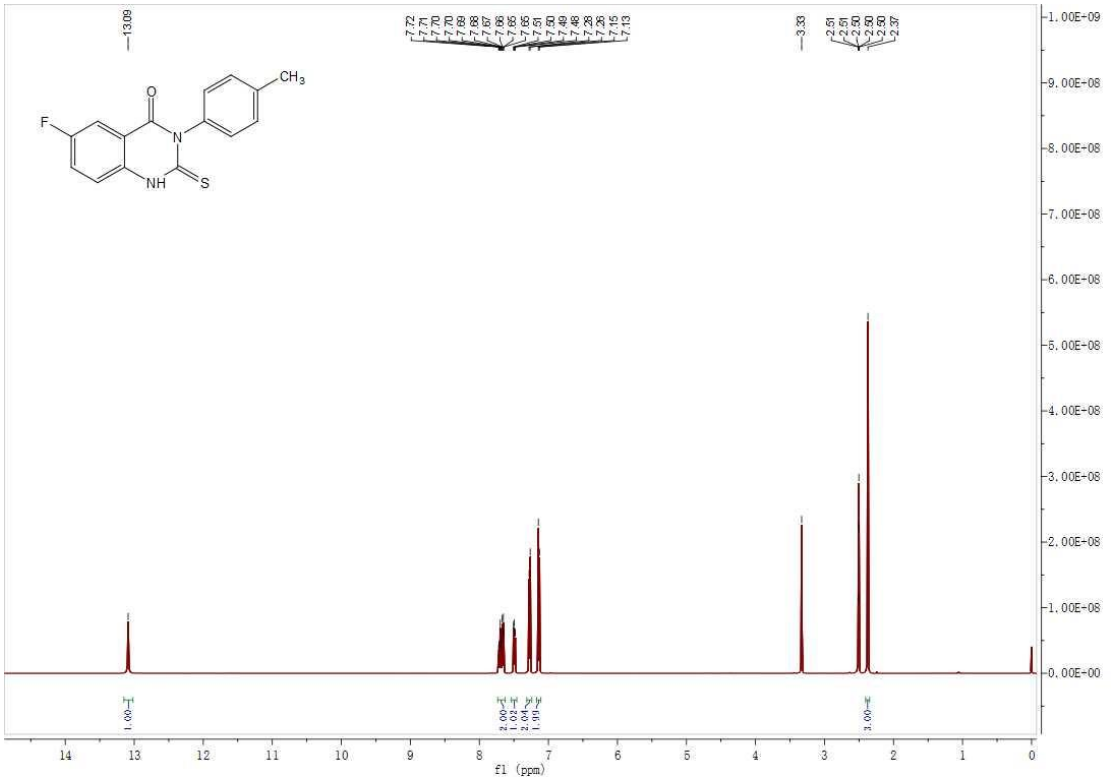
O
N
NH
S
CH3
f1 (ppm)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3.00
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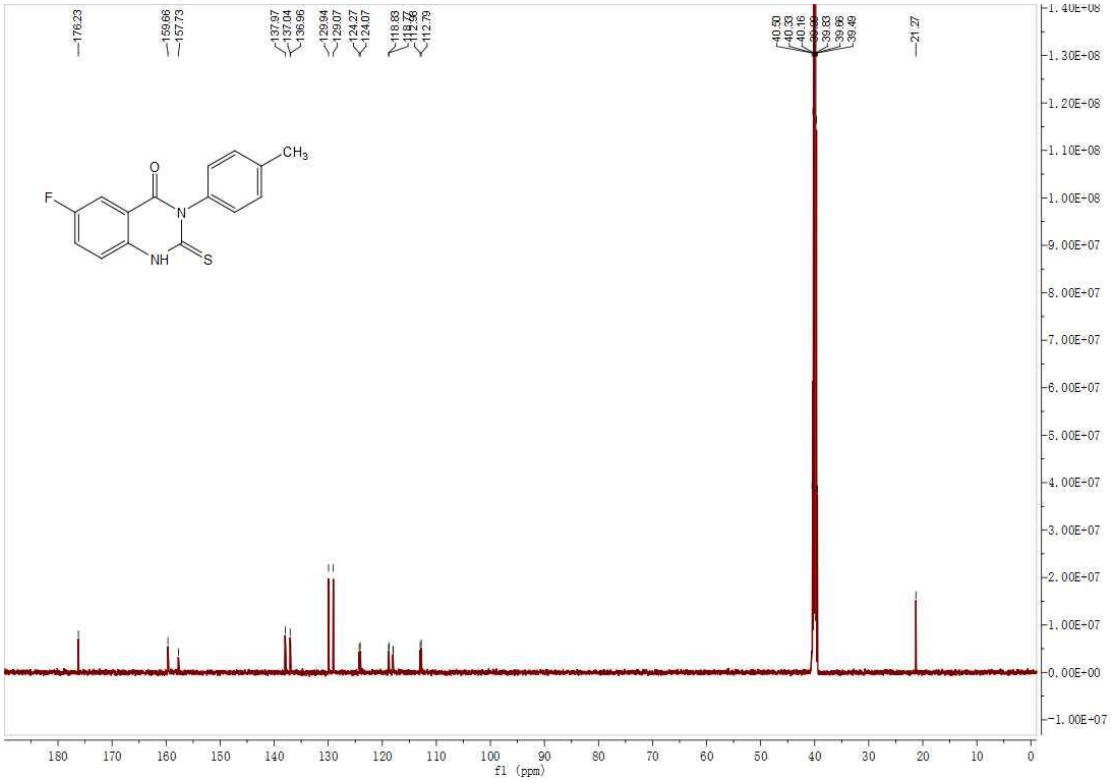
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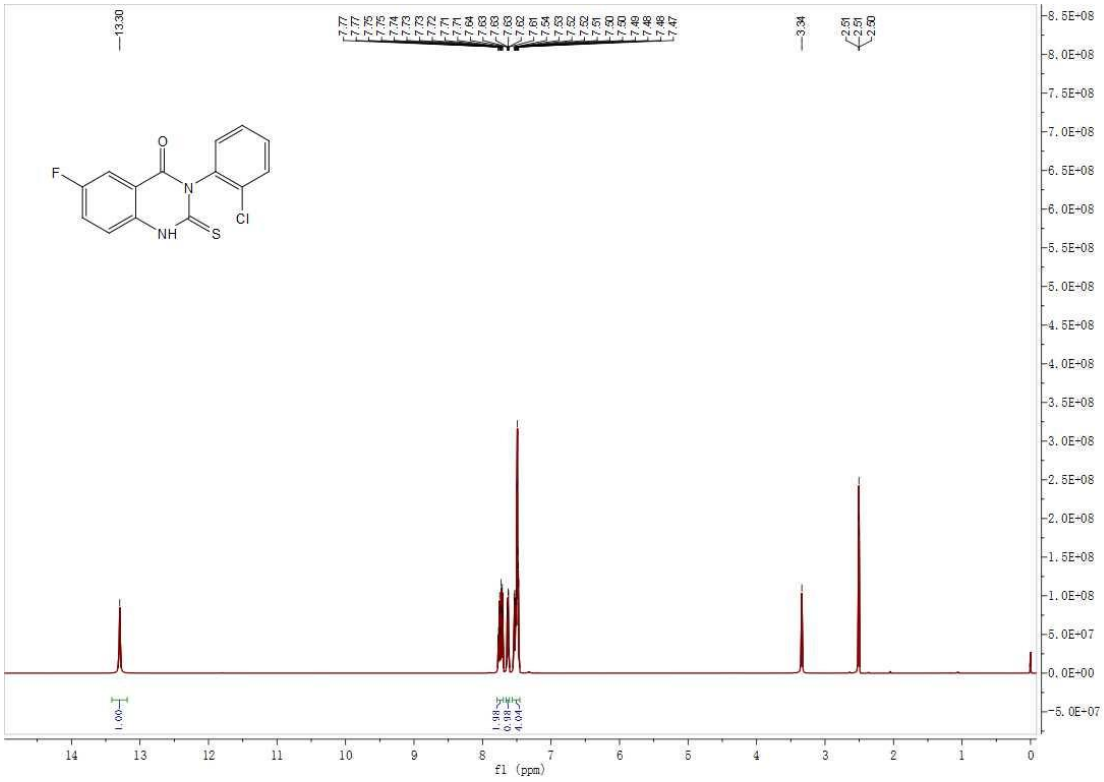
f1 (ppm)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Cl
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4.04
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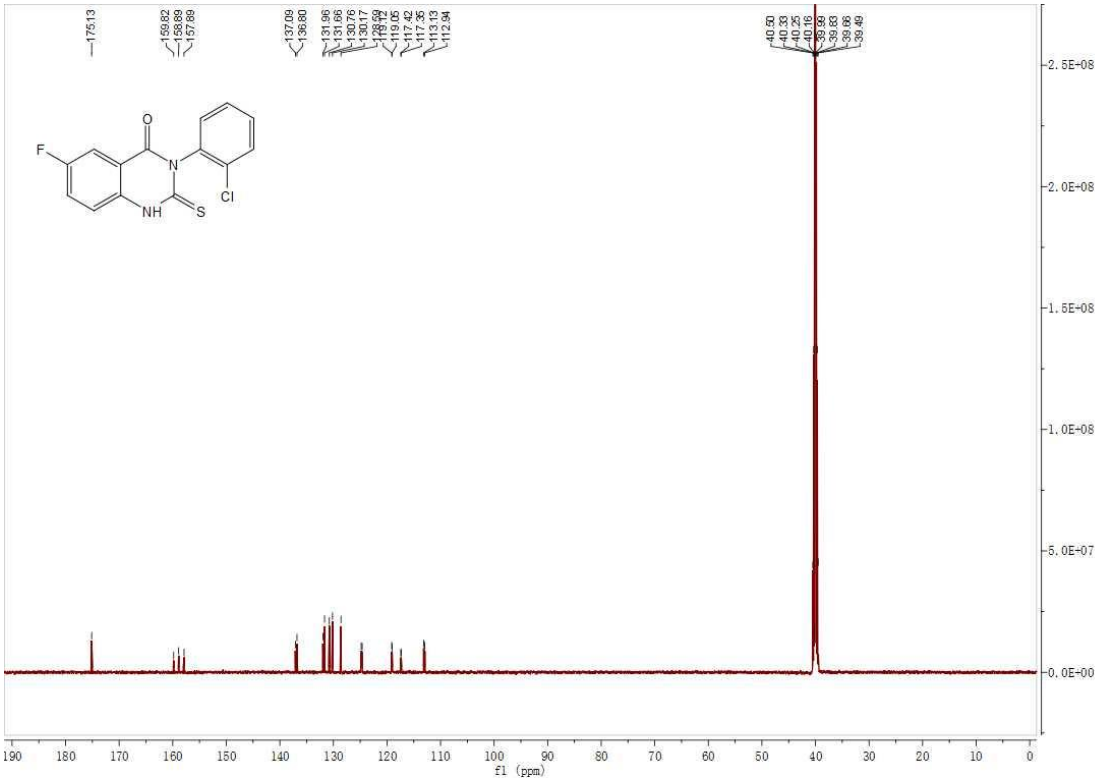
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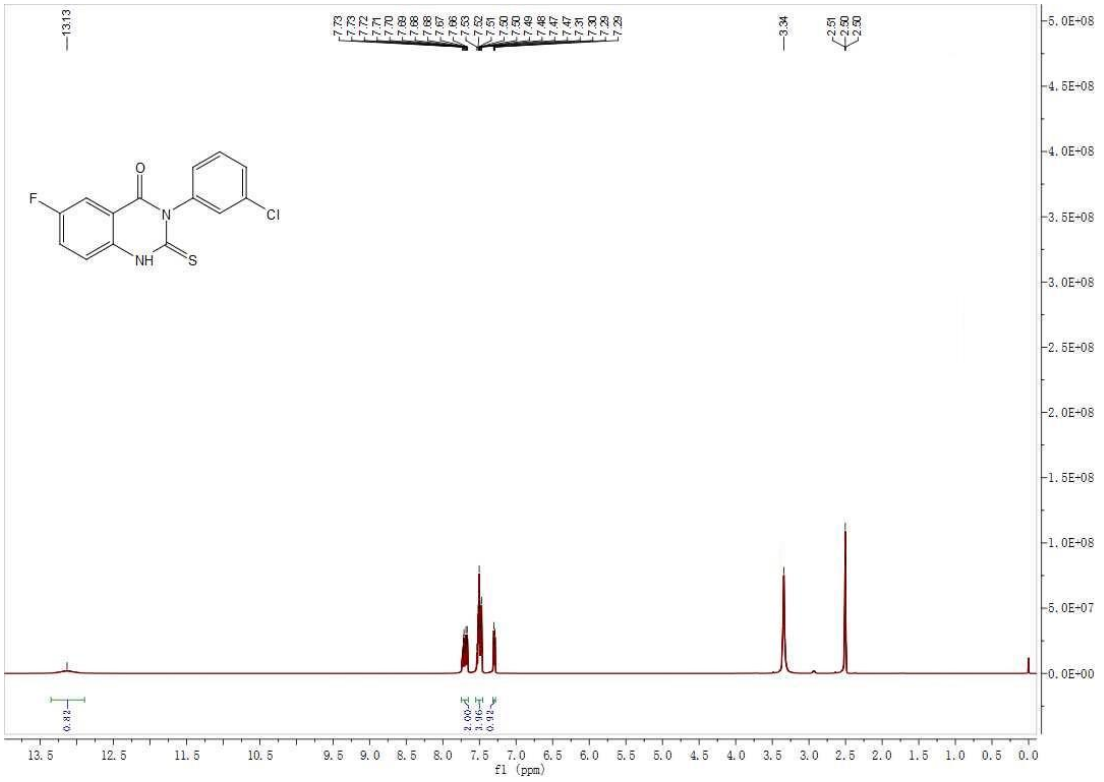
f1 (ppm)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7.29
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Cl
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S
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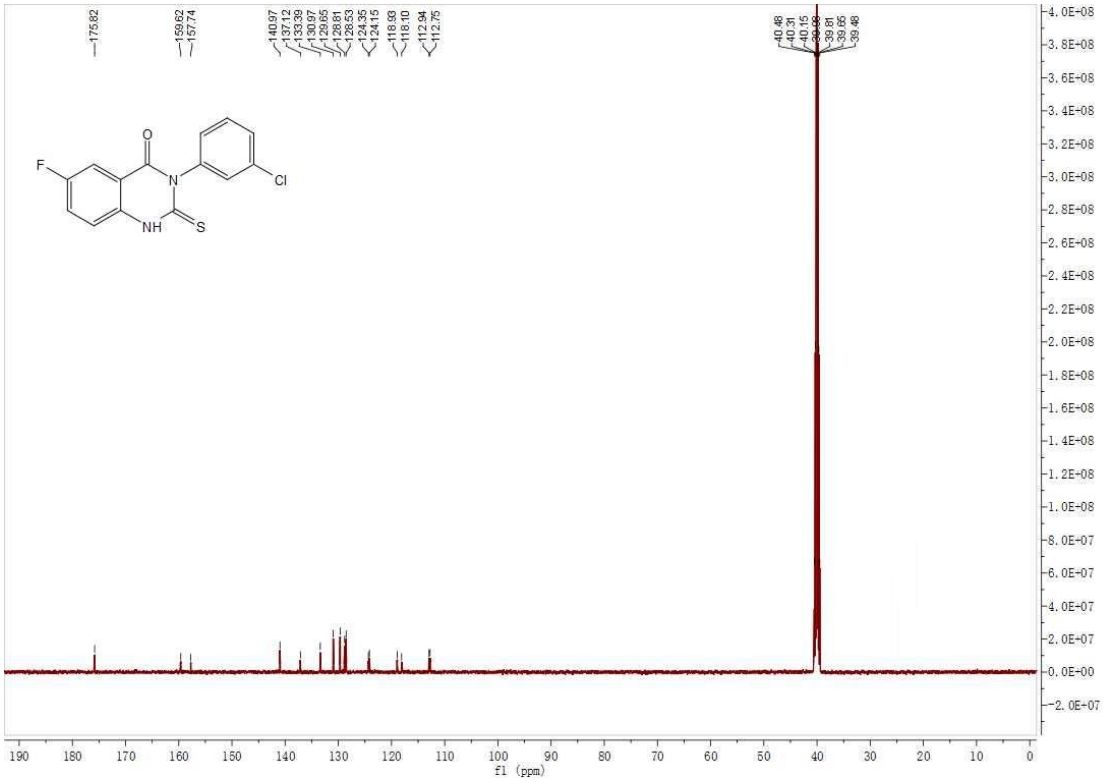
f1 (ppm)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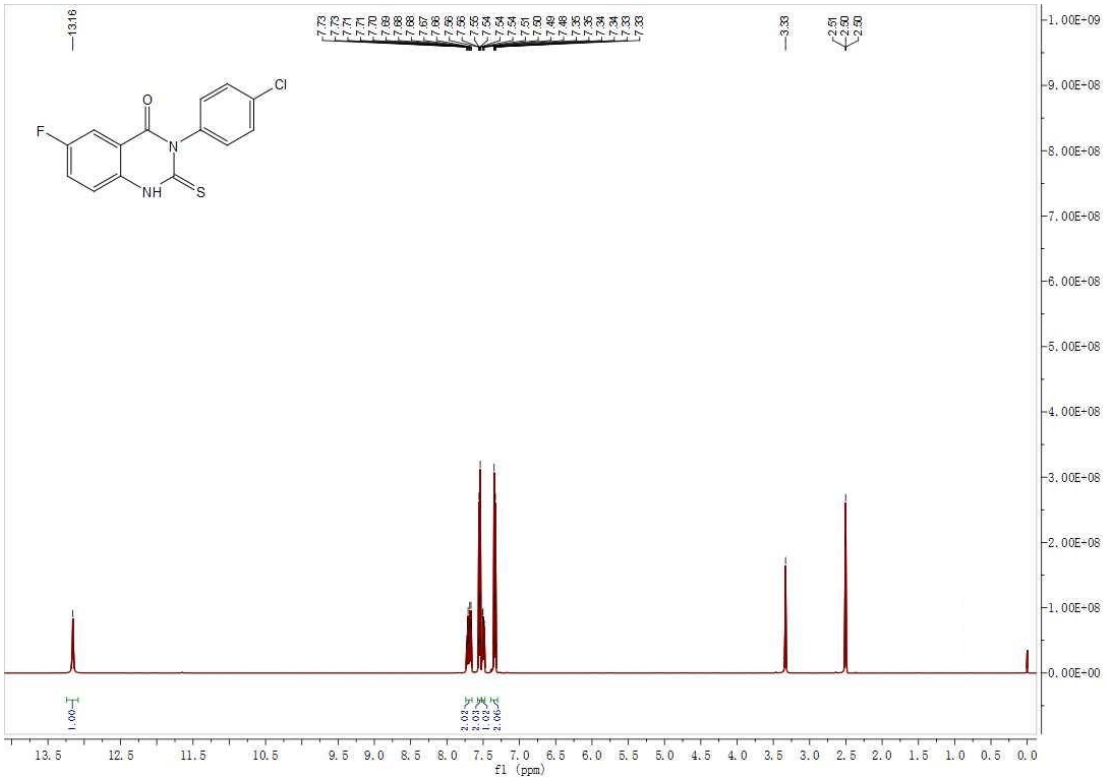
F
Cl
NH
S
f1 (ppm)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N
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2.03
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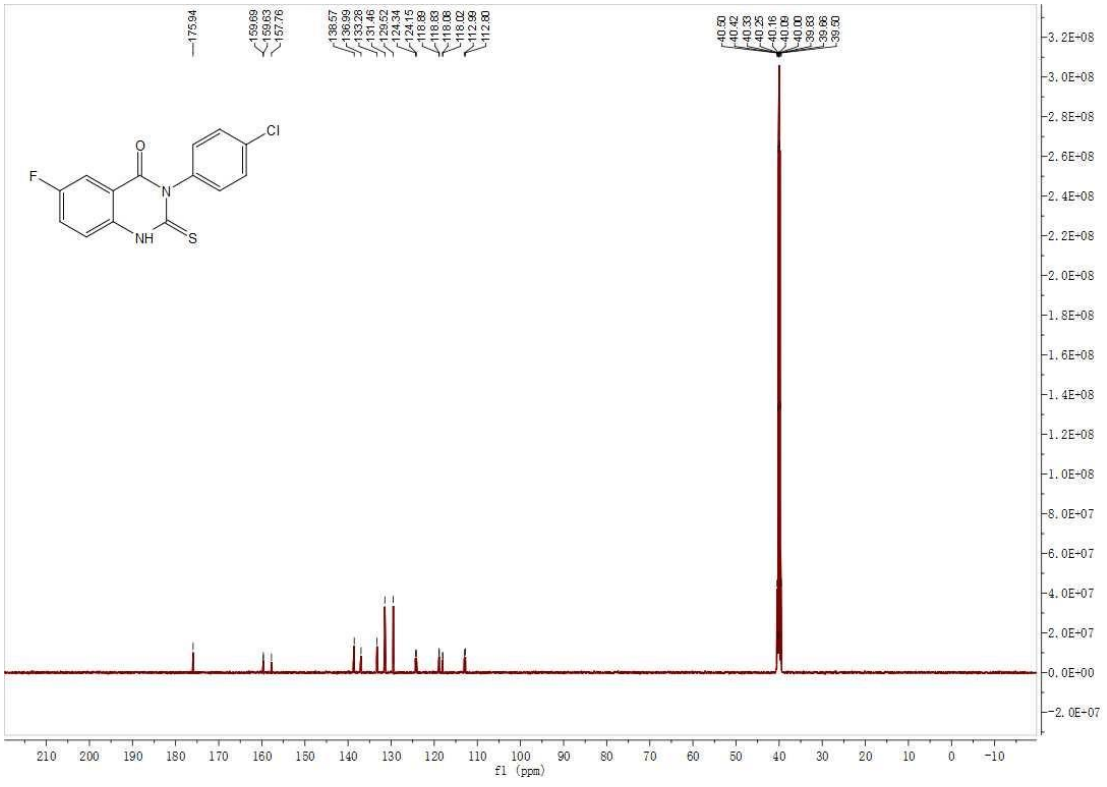
2.06
f1 (ppm)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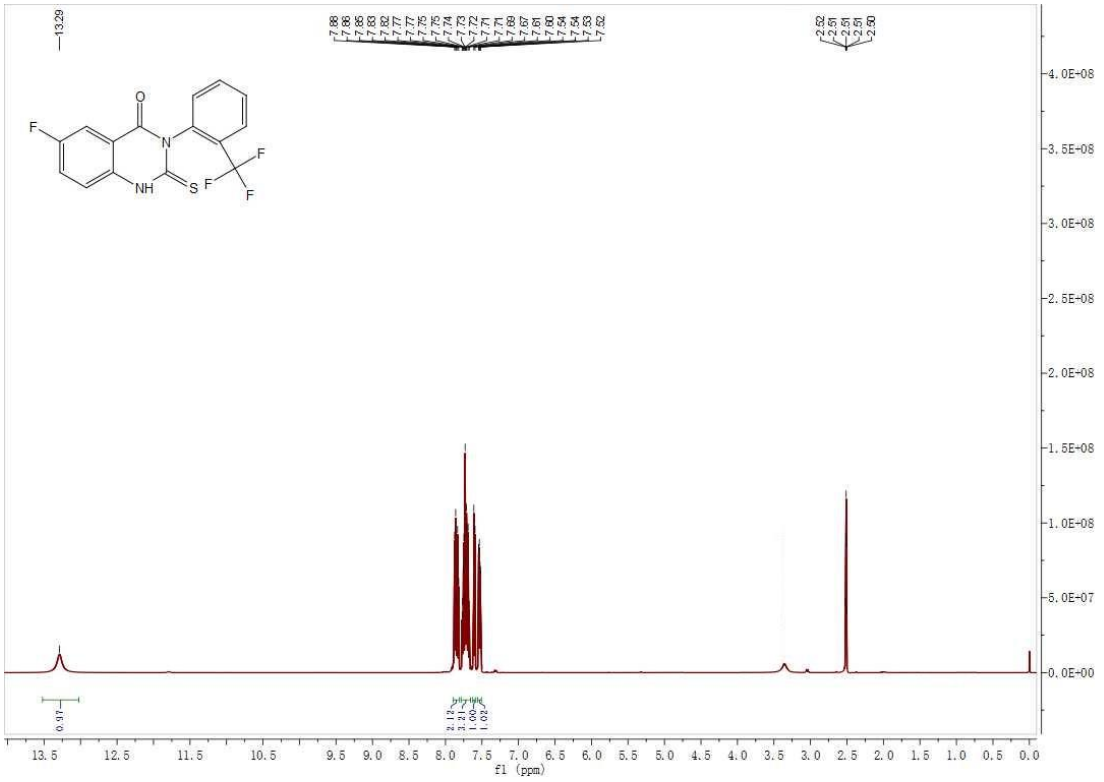
O
F
N
Cl
NH
S
f1 (ppm)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F
F
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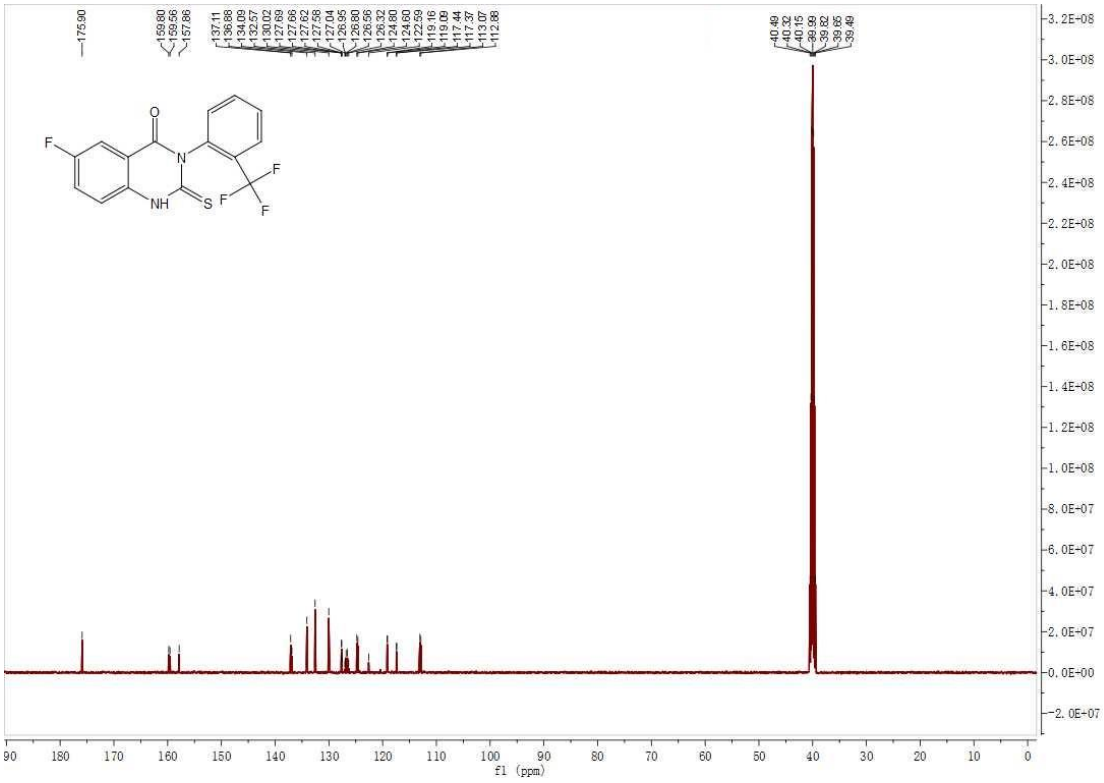
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NH
S
F
F
F
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0.0E+00
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180
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110
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90
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50
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10
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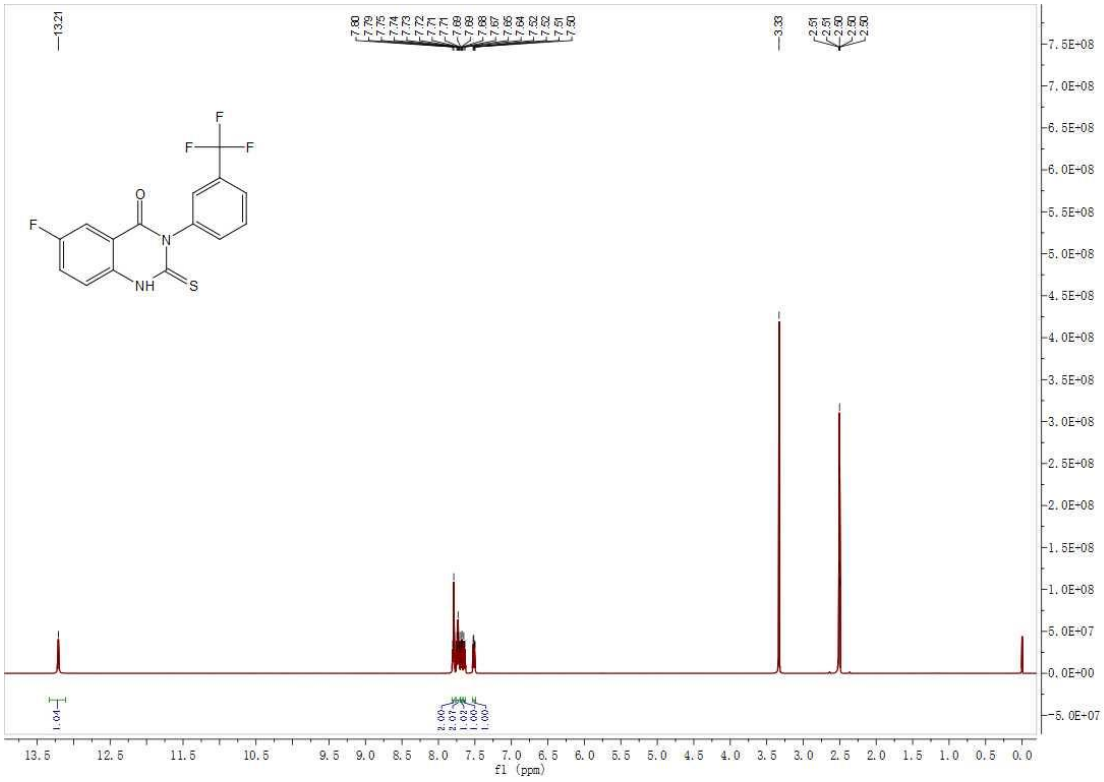
f1 (ppm)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7.50
3.33
2.51
2.51
2.50
2.50
2.50
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F
NH
S
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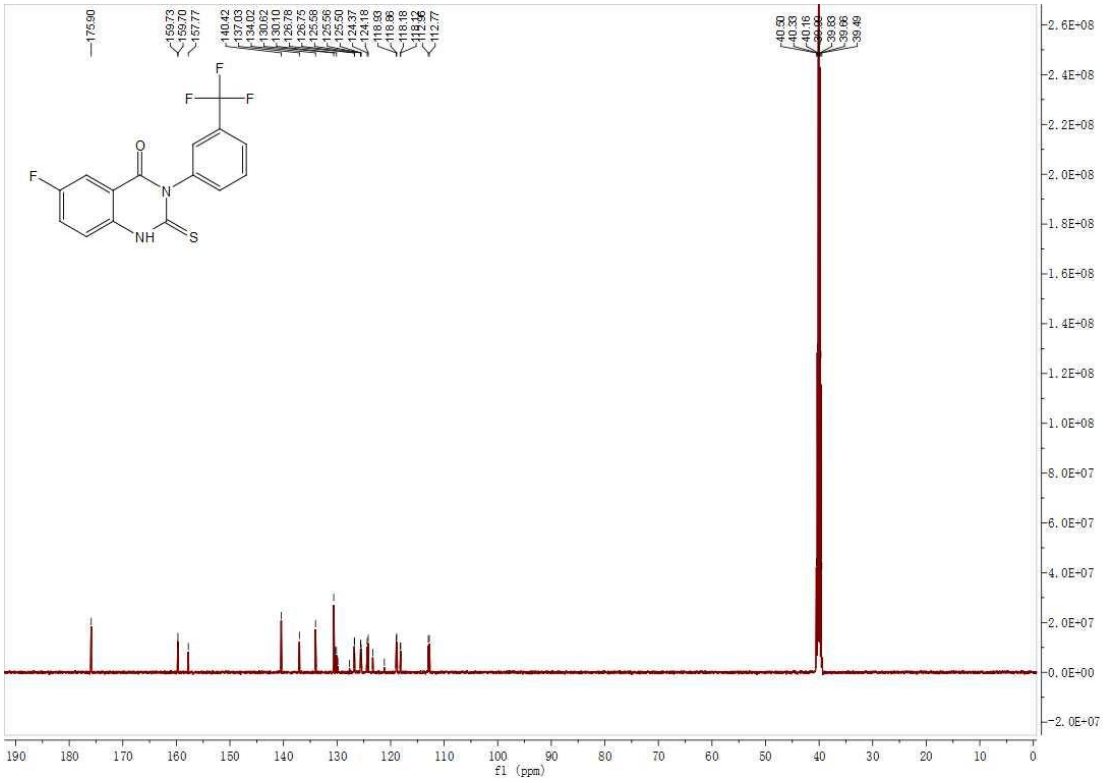
2.00
2.07
2.07
1.00
1.00
fl (ppm)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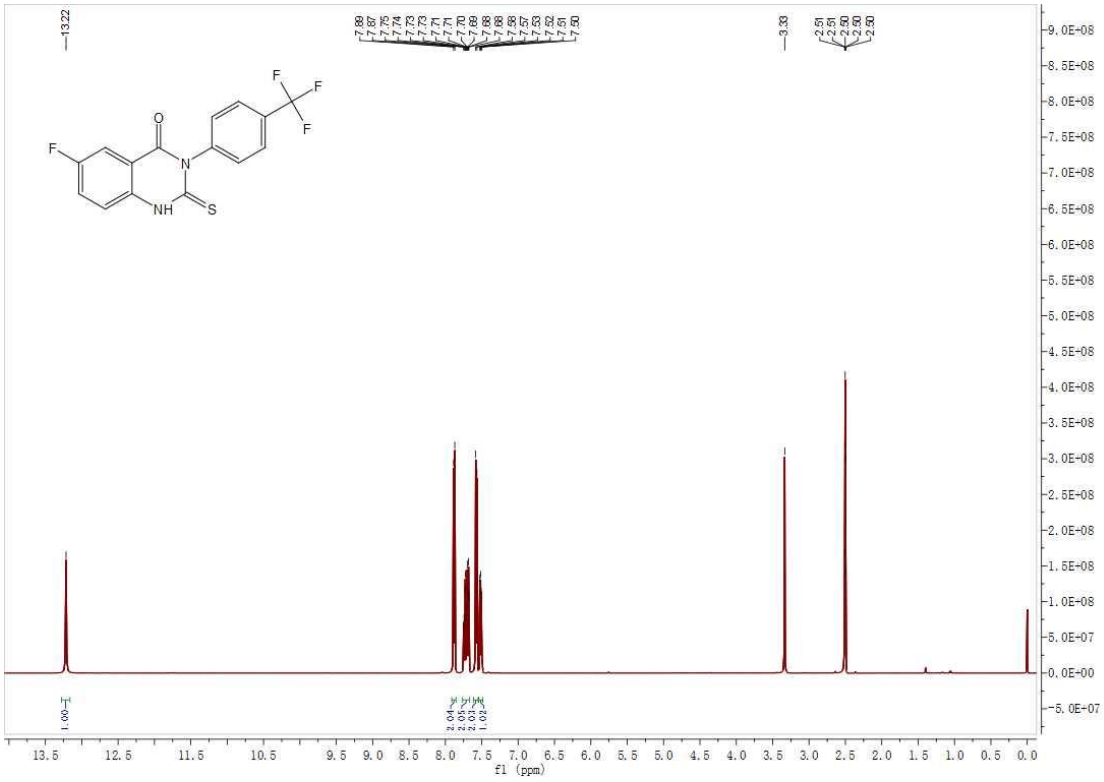
NH
S
fl (ppm)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3.33
2.51
2.51
2.50
2.50
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NH
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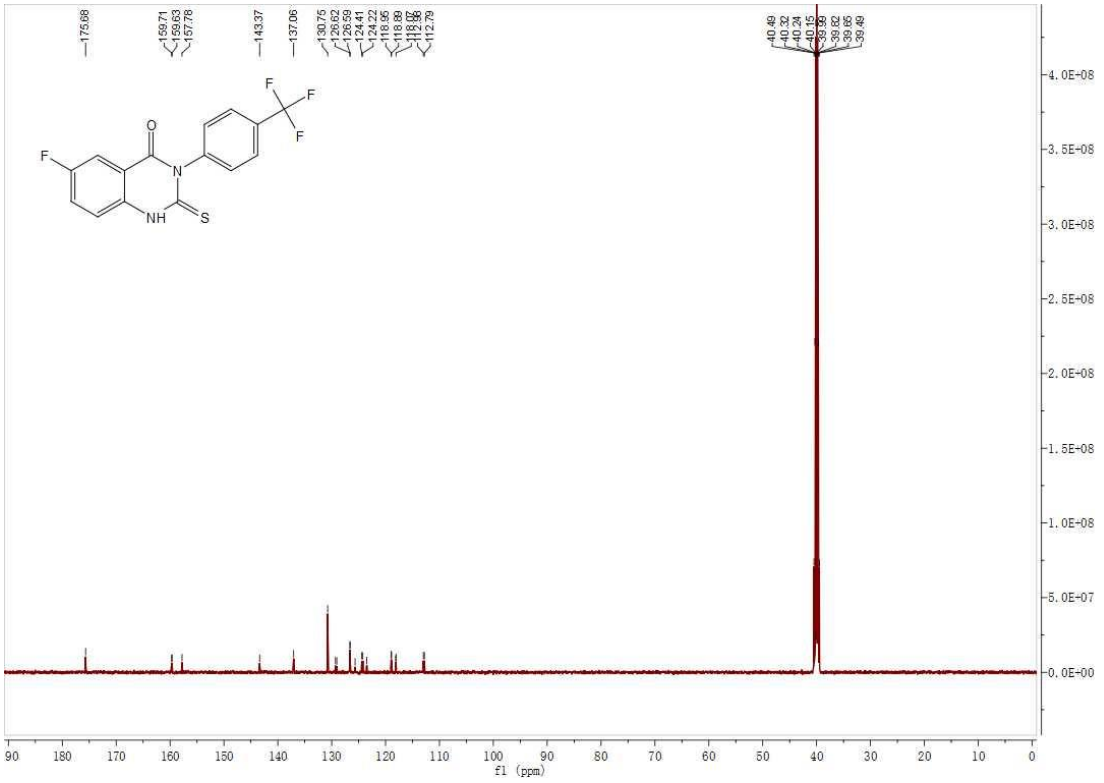
2.23
2.03
1.02
f1 (ppm)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39.82
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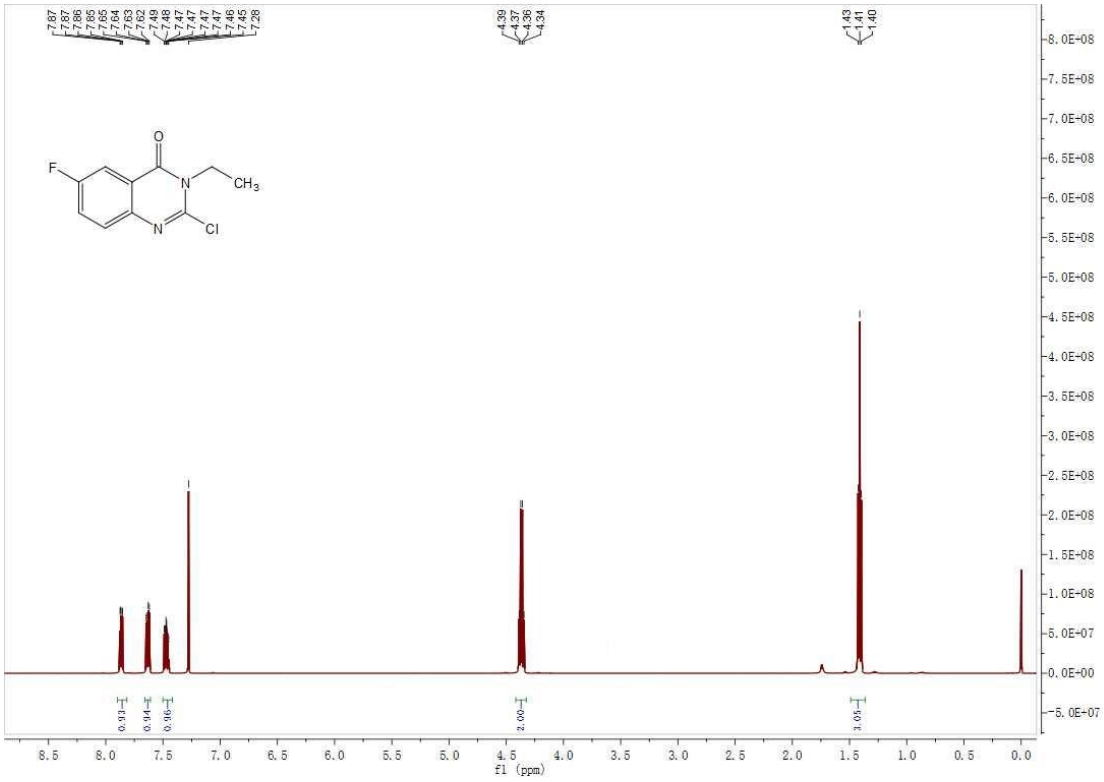
F
F
F
O
N
NH
S
f1 (ppm)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1.43
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N
CH3
N
Cl
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0.96
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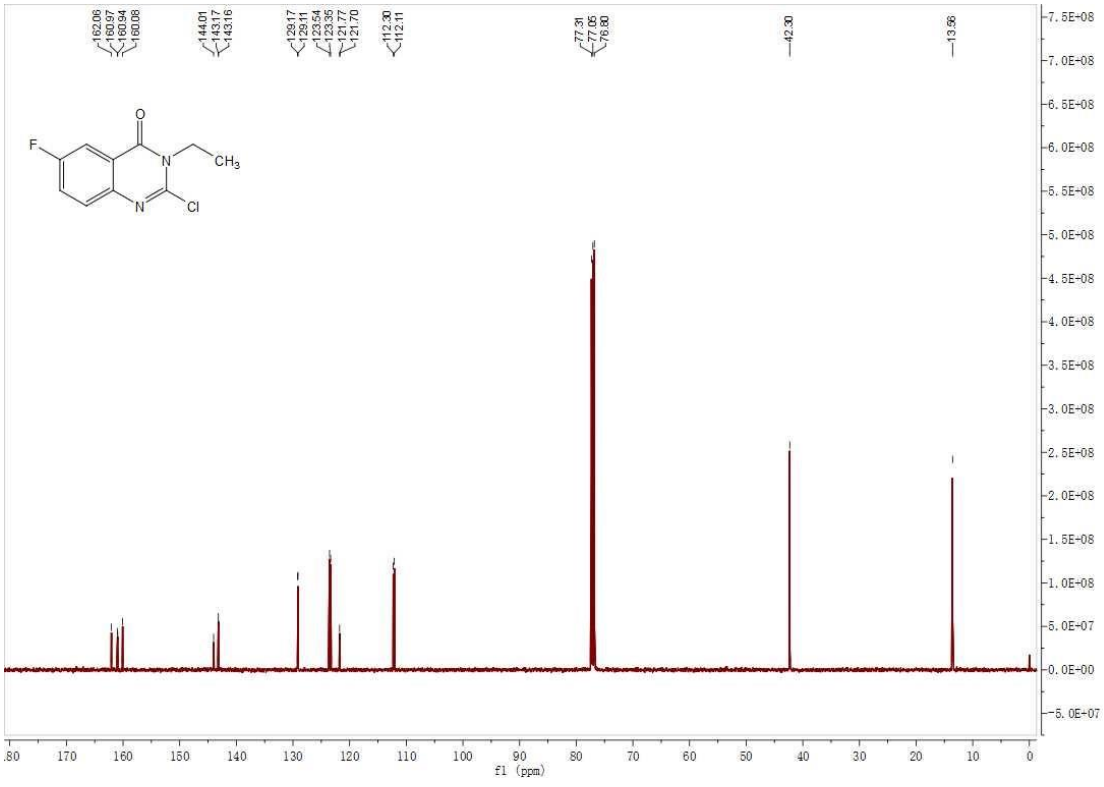
3.05
f1 (ppm)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121.70
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77.05
76.80
42.30
13.56
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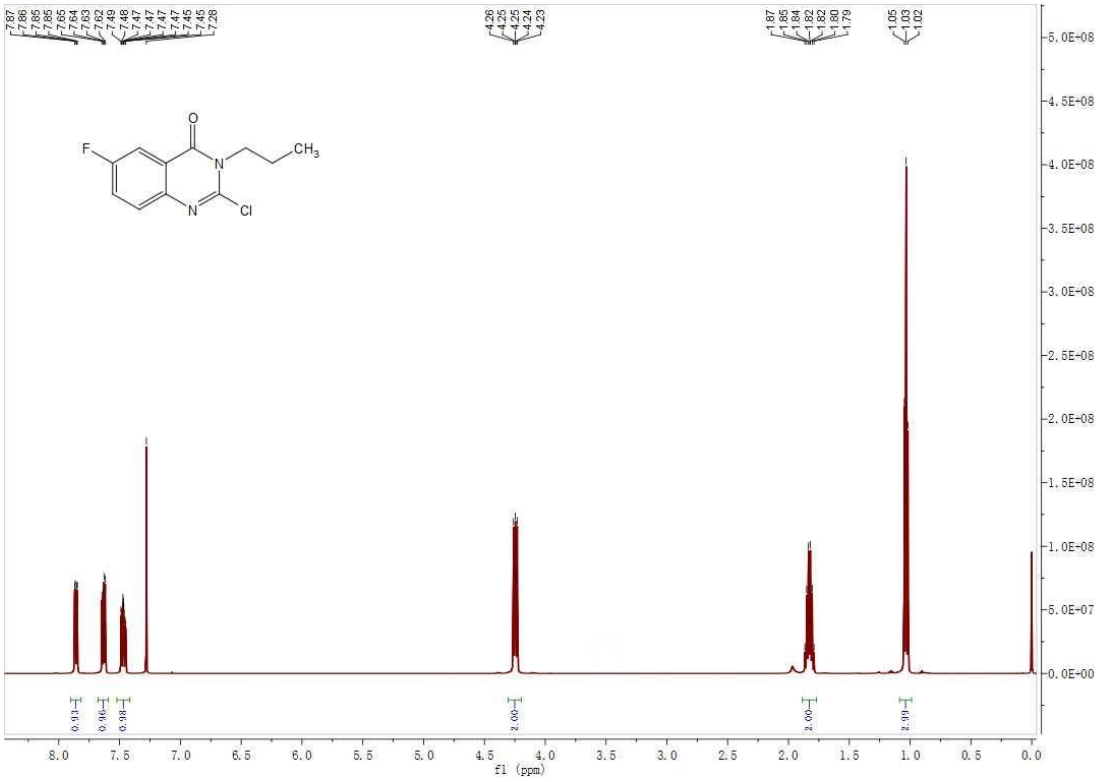
O
N
CH3
N
Cl
f1 (ppm)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7.83
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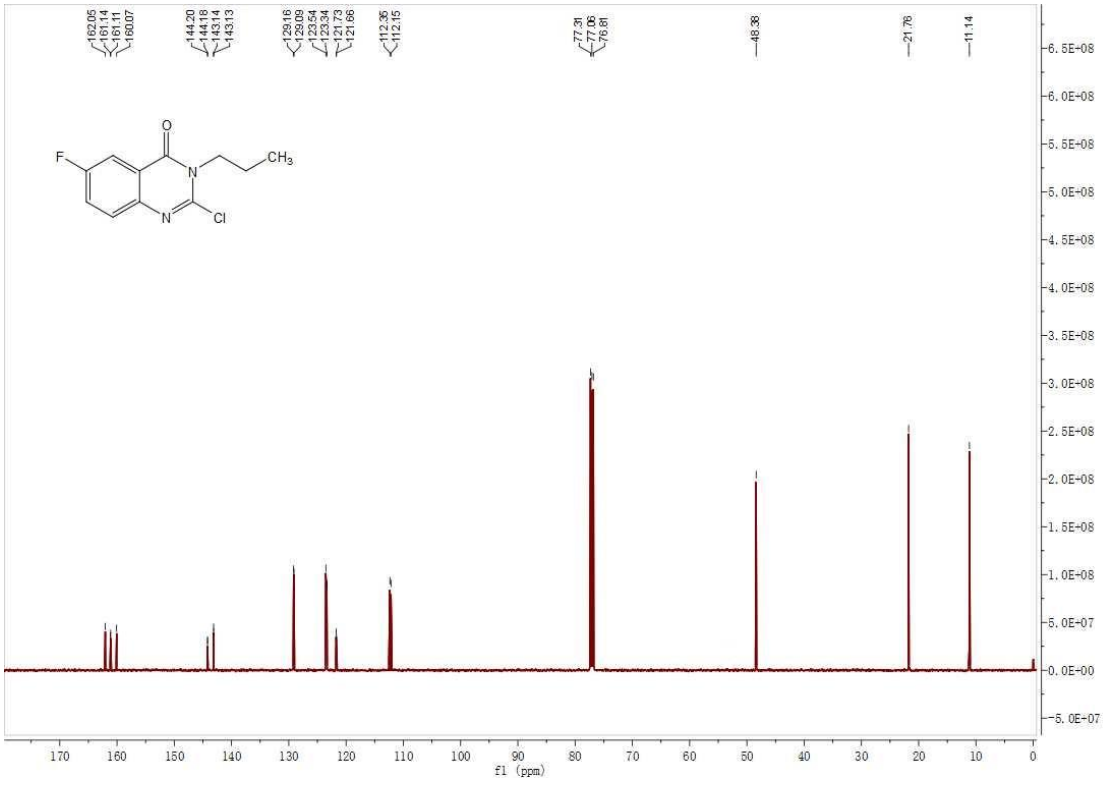
7.47
7.47
7.47
7.47
7.45
7.45
7.28
4.26
4.25
4.25
4.24
4.23
1.87
1.85
1.84
1.82
1.82
1.80
1.79
1.05
1.03
1.02
O
F
N
CH3
N
Cl
0.93
0.96
0.98
2.00
2.00
2.91
f1 (ppm)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143.13
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129.09
123.54
123.34
121.73
121.68
112.36
112.15
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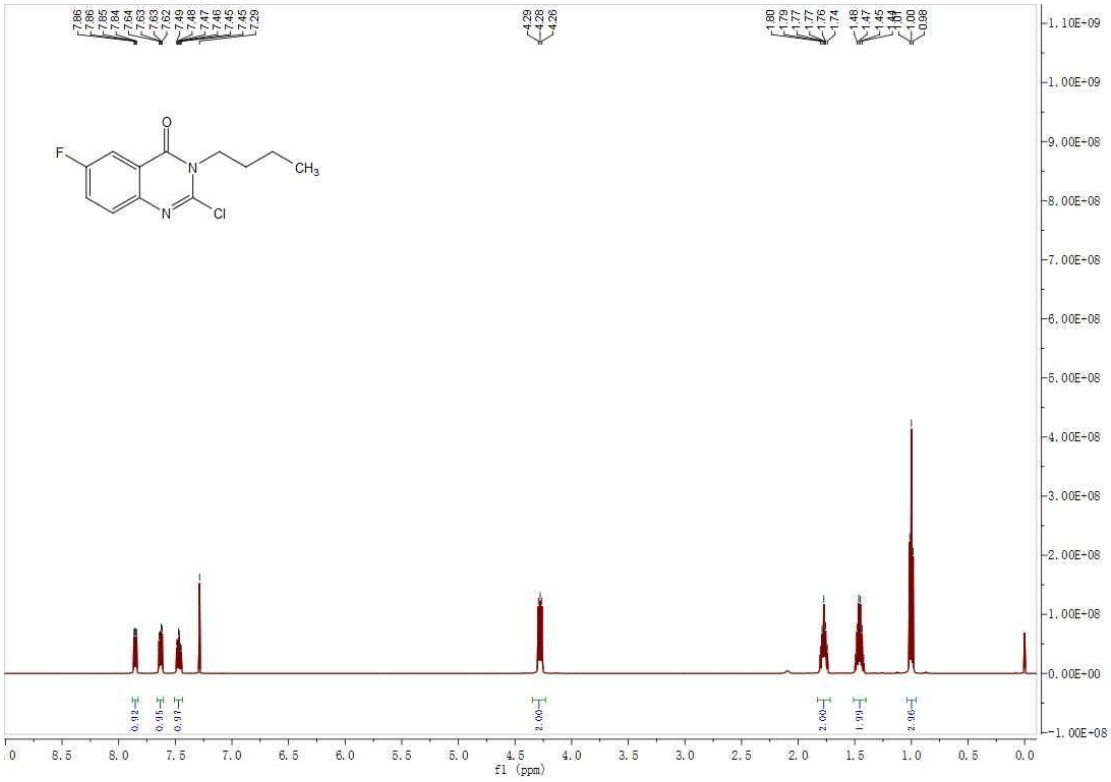
76.81
48.38
21.76
11.14
O
F
N
CH3
N
Cl
f1 (ppm)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7.62
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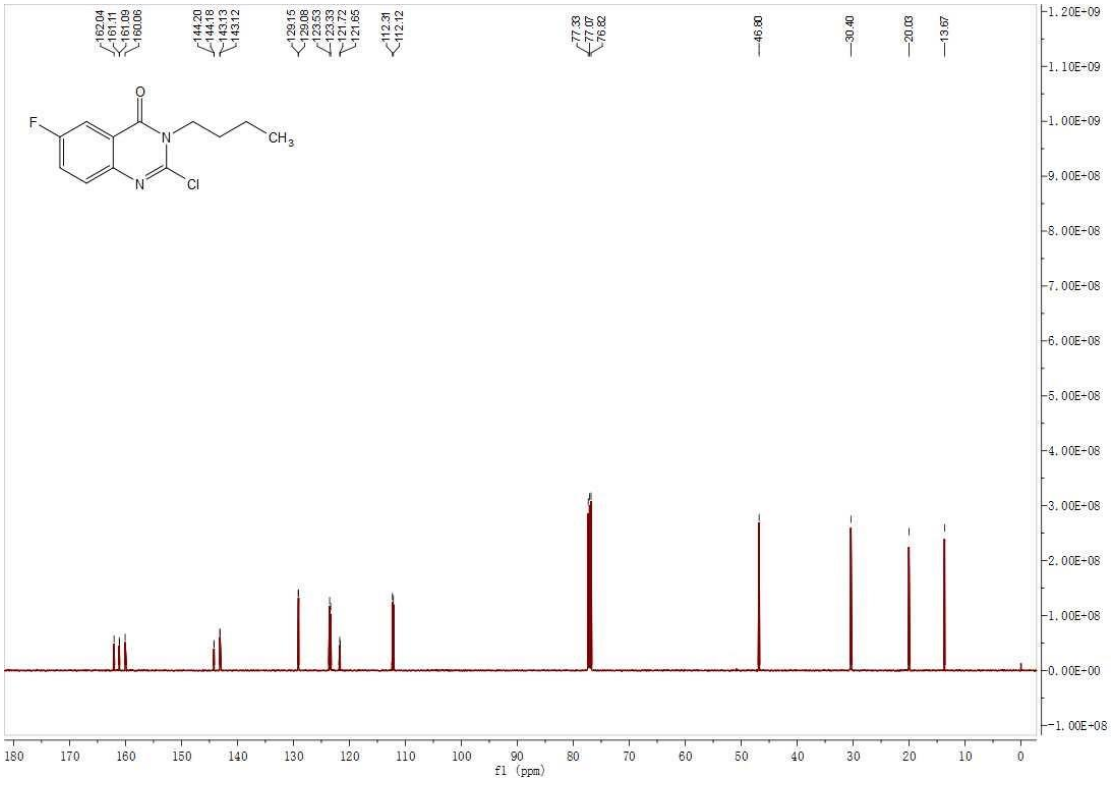
7.47
7.46
7.45
7.45
7.29
4.29
4.28
4.26
1.80
1.79
1.77
1.77
1.76
1.74
1.48
1.47
1.45
1.44
1.01
1.00
0.98
O
F
N
CH3
N
Cl
0.92
0.91
0.97
2.00
2.00
1.90
2.96
f1 (ppm)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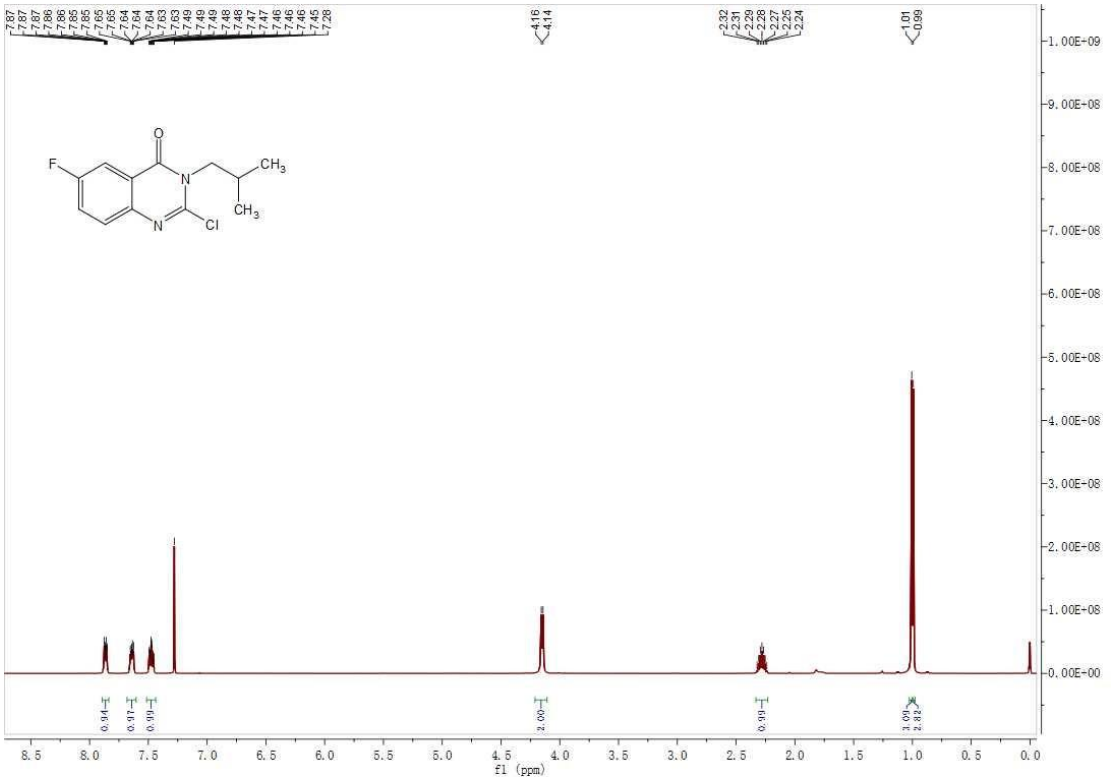
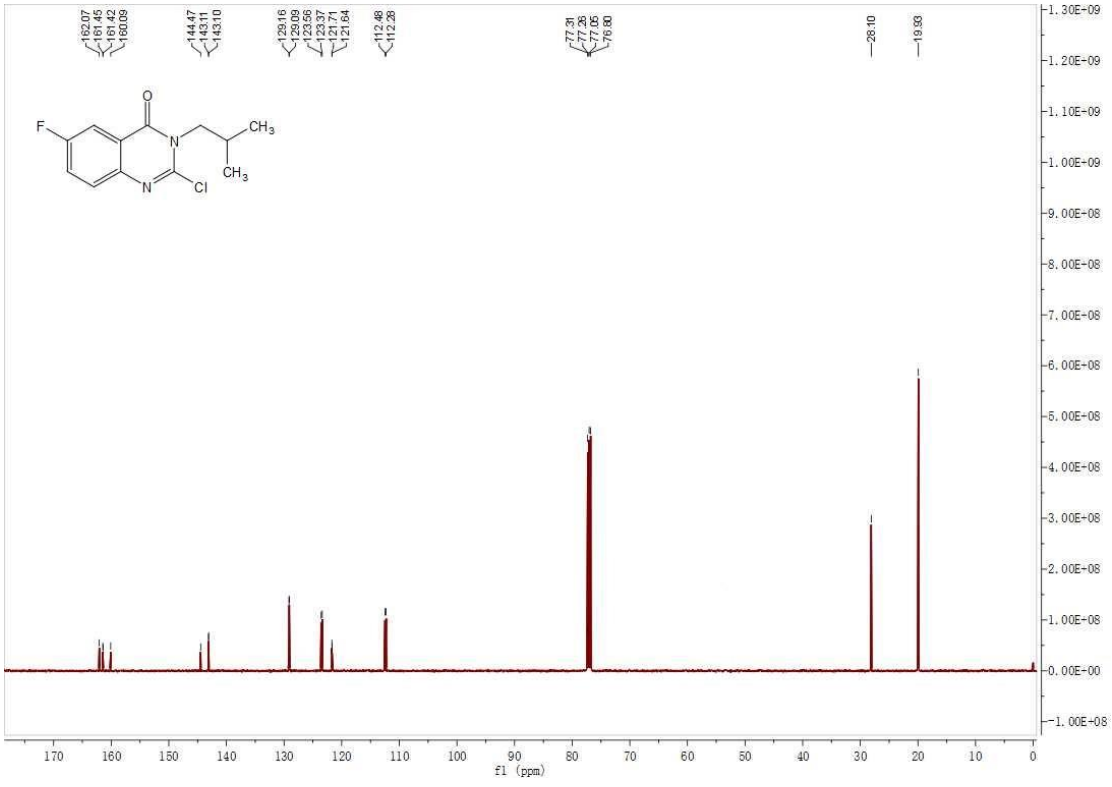
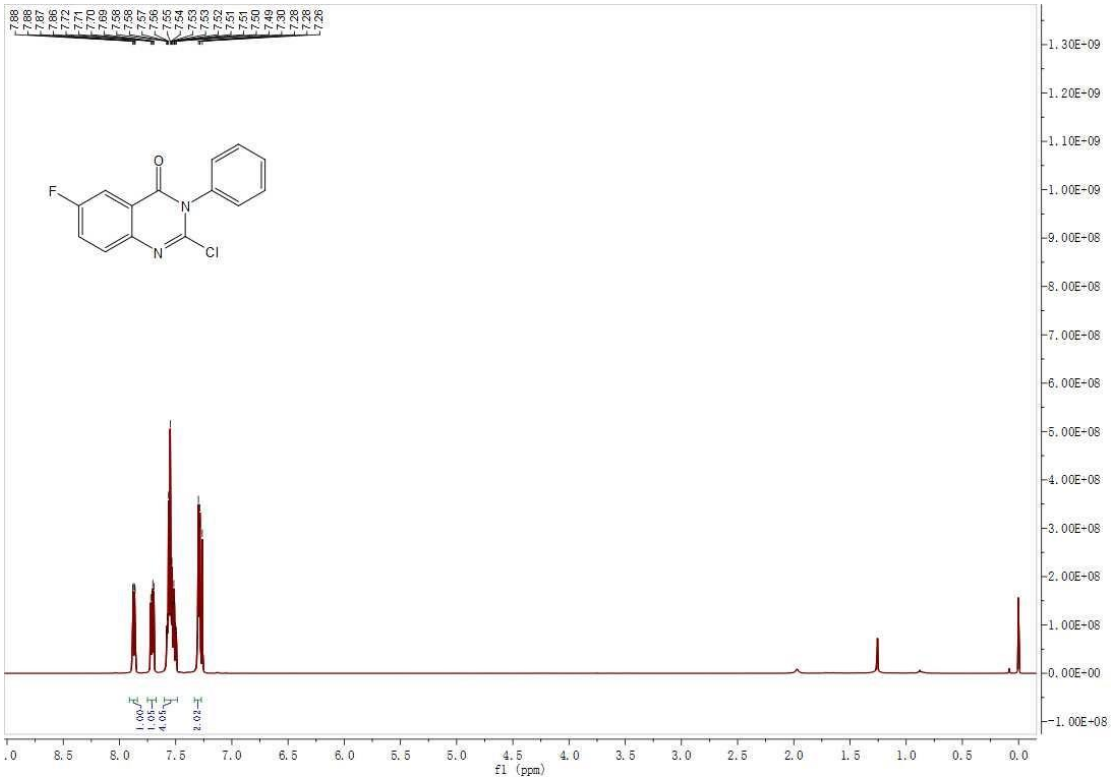
143.12
129.15
129.08
123.53
123.33
121.72
121.65
112.31
112.12
77.33
77.07
76.82
46.80
30.40
20.03
13.67
O
F
N
CH3
N
Cl
f1 (ppm)


F
O
N
CH3
CH3
N
Cl
fl (ppm)


F
O
N
CH3
CH3
N
Cl
fl (ppm)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7.57
7.56
7.55
7.54
7.53
7.53
7.52
7.51
7.51
7.50
7.49
7.30
7.28
7.28
7.26
O
F
N
N
Cl
1.00
1.05
4.05
2.02
1.30E-09
1.20E-09
1.10E-09
1.00E-09
9.00E-08
8.00E-08
7.00E-08
6.00E-08
5.00E-08
4.00E-08
3.00E-08
2.00E-08
1.00E-08
0.00E-00
-1.00E-08
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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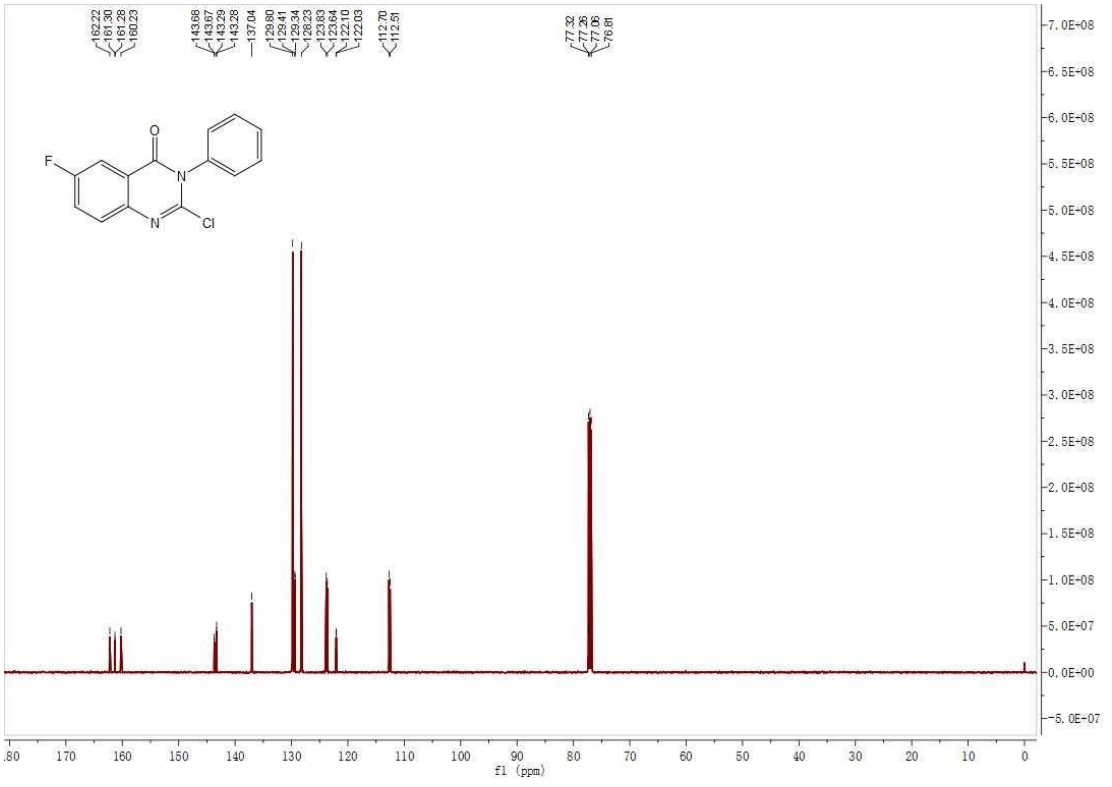
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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137.04
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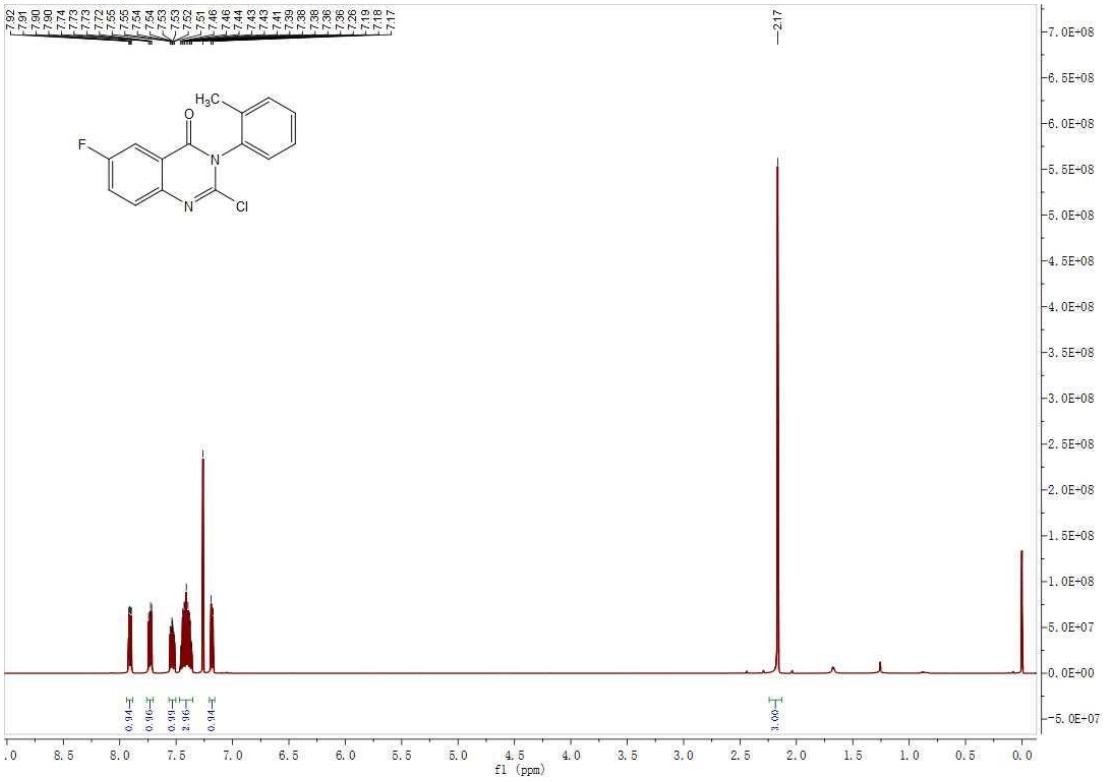
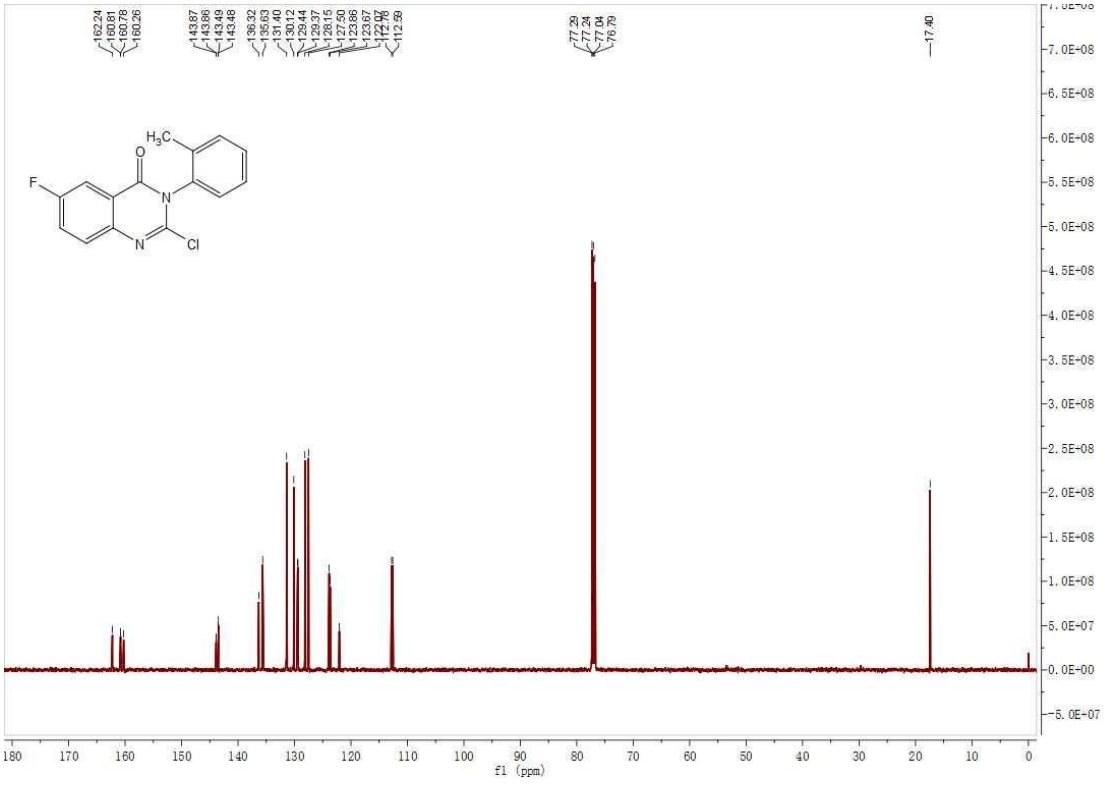
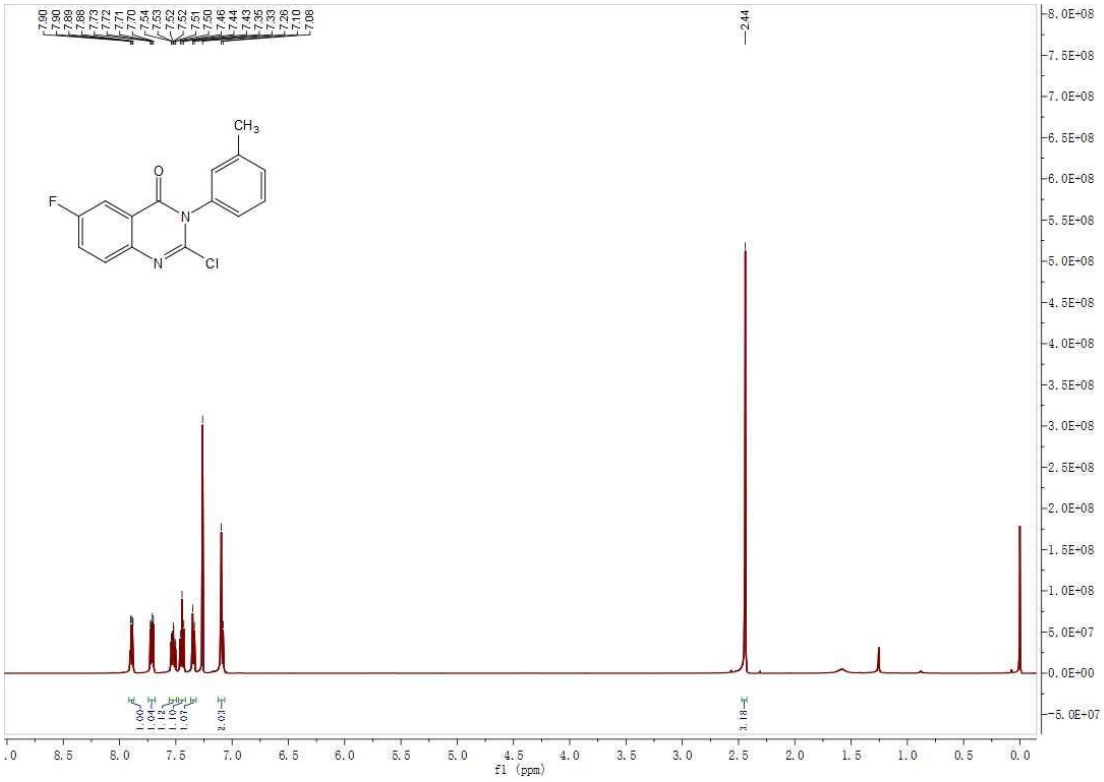
128.34
128.23
123.83
123.64
122.10
122.03
112.70
112.51
77.32
77.26
77.06
76.81
O
F
N
N
Cl
7.0E-08
6.5E-08
6.0E-08
5.5E-08
5.0E-08
4.5E-08
4.0E-08
3.5E-08
3.0E-08
2.5E-08
2.0E-08
1.5E-08
1.0E-08
5.0E-07
0.0E-00
-5.0E-07
.80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


F
O
N
N
Cl
H3C
fl (ppm)


F
O
N
N
Cl
H3C
fl (ppm)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7.71
7.70
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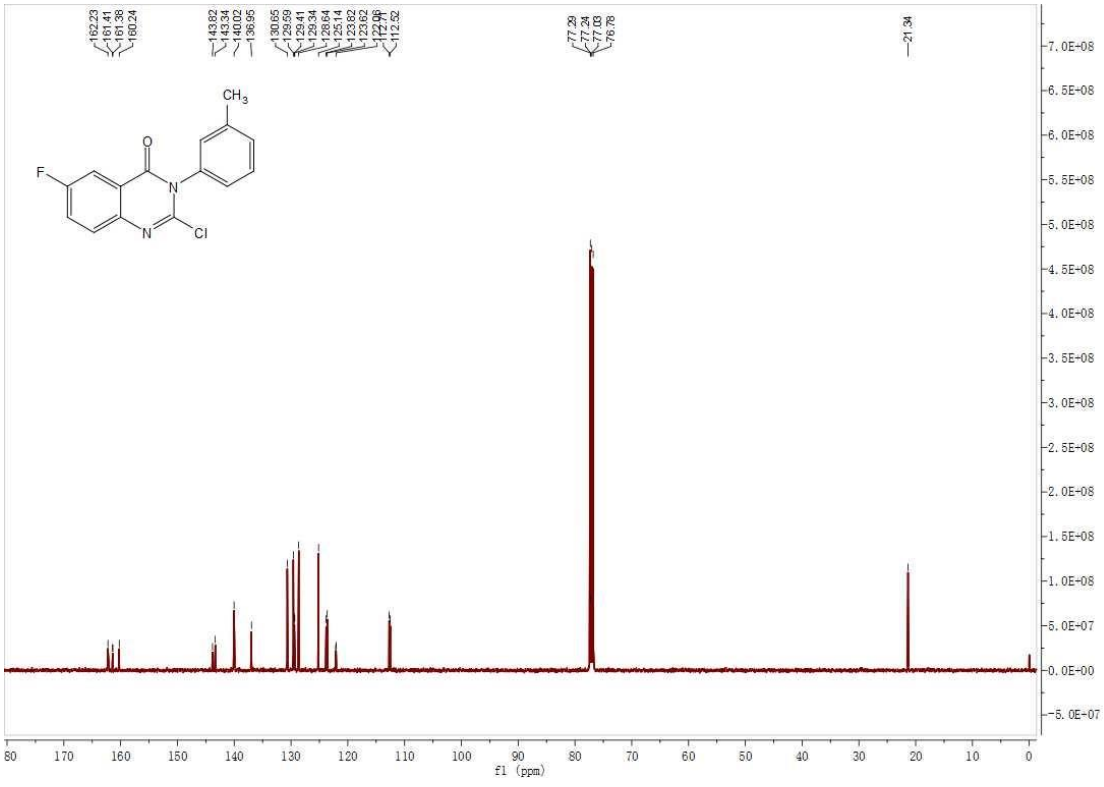
7.52
7.52
7.51
7.51
7.50
7.46
7.44
7.43
7.35
7.33
7.26
7.10
7.08
2.44
CH3
O
F
N
N
Cl
1.00
1.04
1.12
1.10
1.07
2.03
3.10
f1 (ppm)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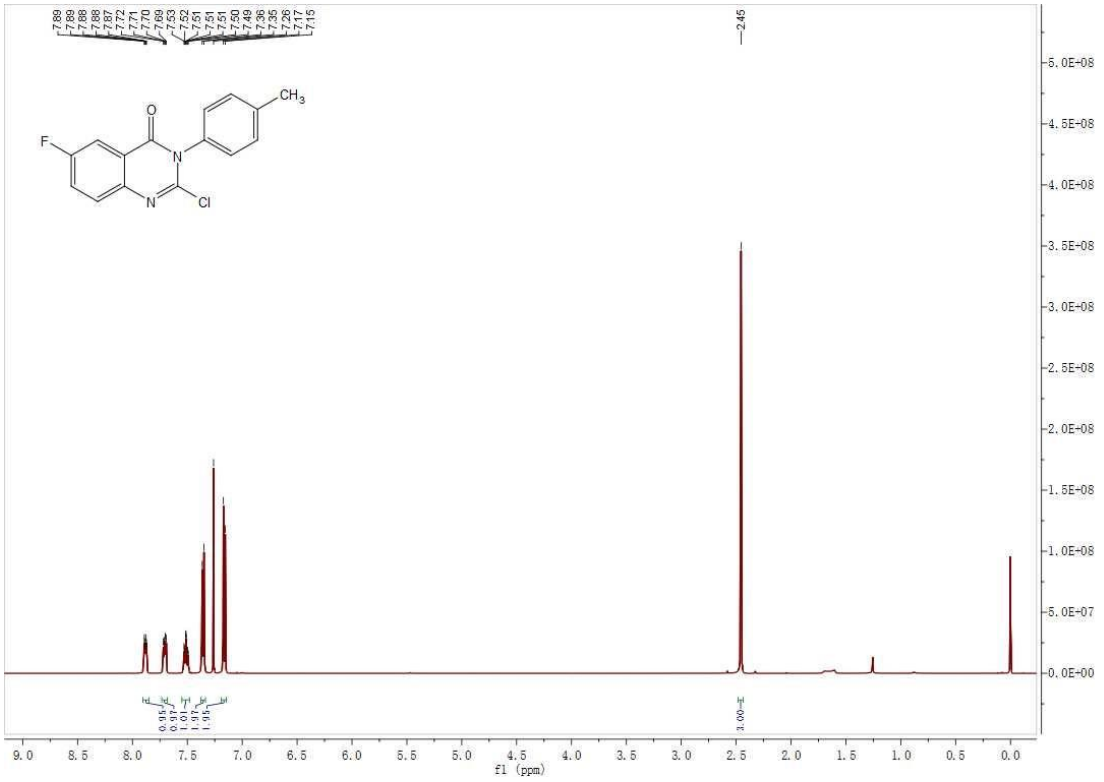
161.38
160.24
143.82
143.34
140.02
136.95
130.65
129.59
129.41
129.34
128.64
125.14
123.82
123.62
122.06
112.71
112.52
77.29
77.24
77.03
76.78
21.34
CH3
O
F
N
N
Cl
f1 (ppm)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7.89
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7.88
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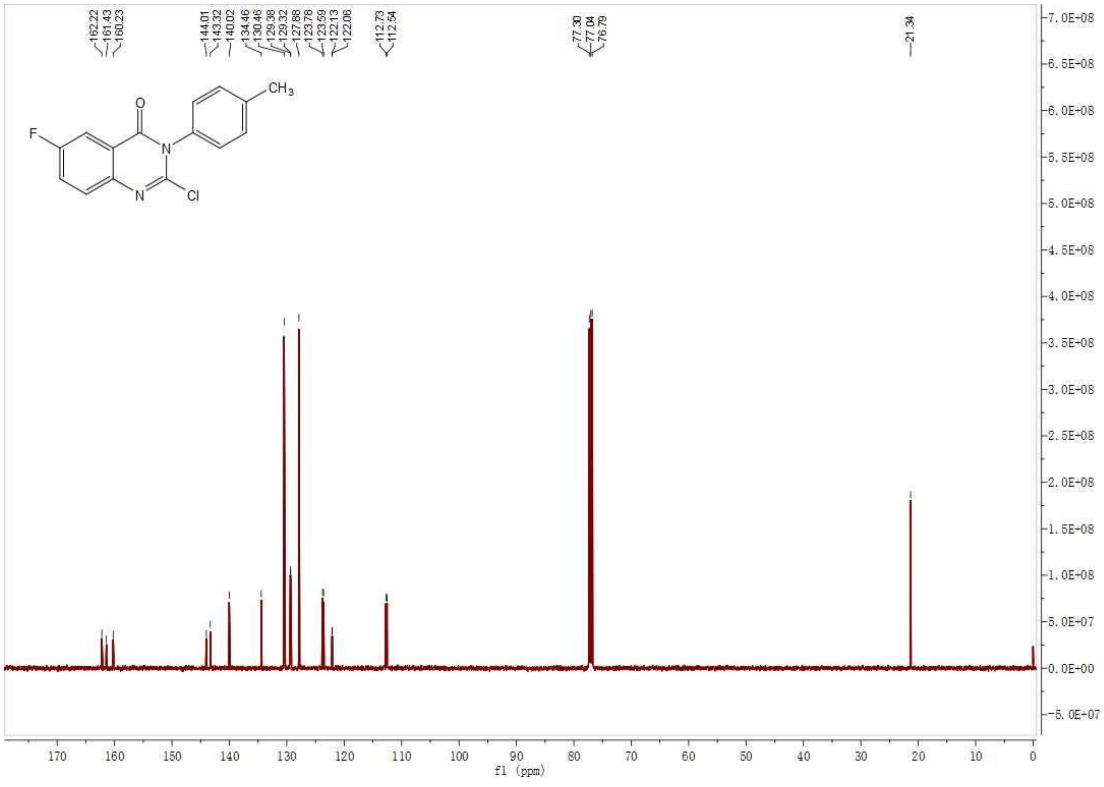
7.71
7.70
7.69
7.53
7.52
7.51
7.51
7.51
7.50
7.49
7.36
7.35
7.26
7.17
7.15
2.45
CH3
O
F
N
N
Cl
0.91
0.97
1.07
1.97
1.91
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
5.0E-08
4.5E-08
4.0E-08
3.5E-08
3.0E-08
2.5E-08
2.0E-08
1.5E-08
1.0E-08
5.0E-07
0.0E+00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161.43
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143.32
140.02
134.46
130.46
129.36
129.32
127.78
123.76
123.59
122.13
122.06
112.73
112.54
77.30
77.04
76.79
21.34
CH3
O
F
N
N
Cl
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
7.0E-08
6.5E-08
6.0E-08
5.5E-08
5.0E-08
4.5E-08
4.0E-08
3.5E-08
3.0E-08
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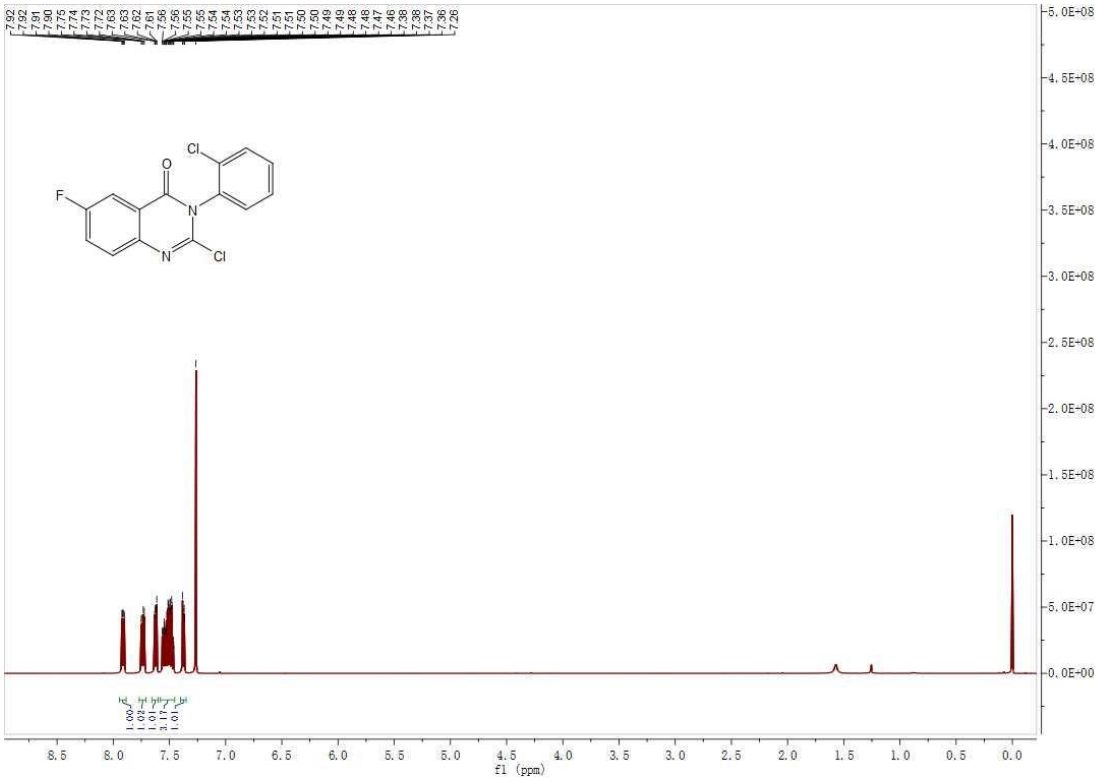
2.0E-08
1.5E-08
1.0E-08
5.0E-07
0.0E+00
-5.0E-07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7.73
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7.62
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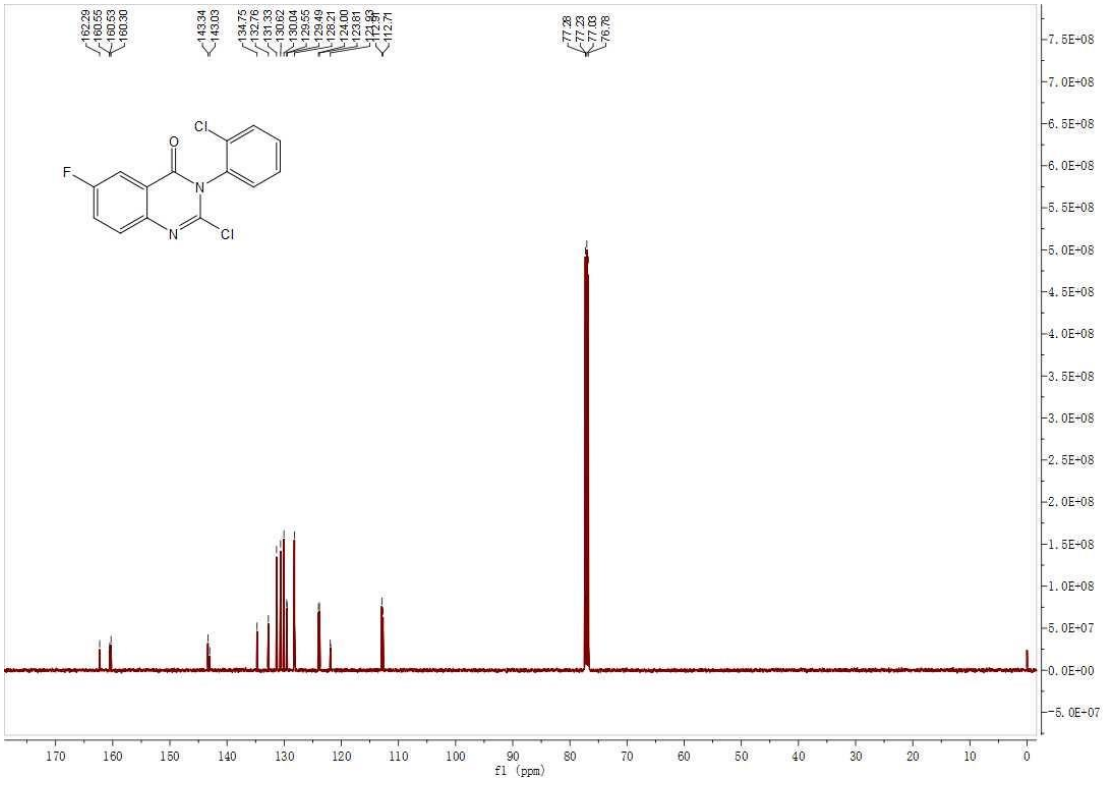
7.56
7.55
7.55
7.54
7.54
7.53
7.53
7.52
7.51
7.51
7.50
7.50
7.49
7.49
7.48
7.48
7.47
7.46
7.38
7.38
7.37
7.36
7.26
Cl
O
F
N
N
Cl
1.00
1.02
1.01
3.11
1.01
f1 (ppm)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160.53
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143.34
143.03
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131.33
130.62
130.04
129.55
129.49
128.21
124.00
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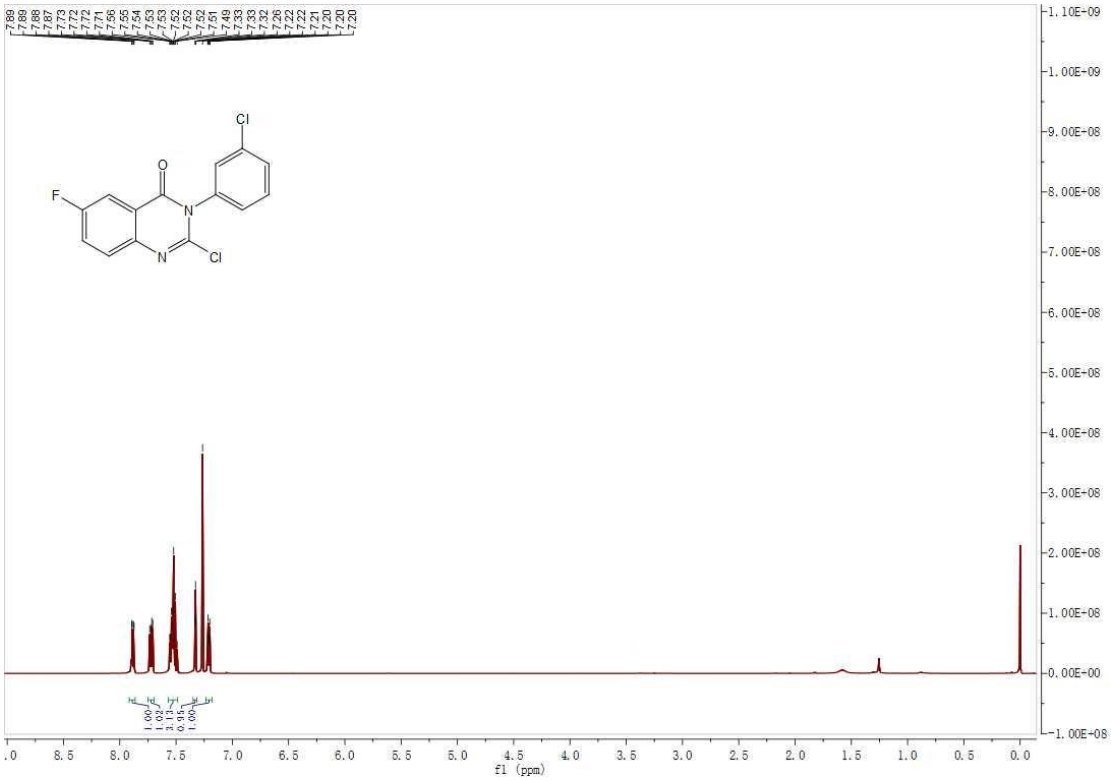
112.71
77.28
77.23
77.03
76.78
Cl
O
F
N
N
Cl
f1 (ppm)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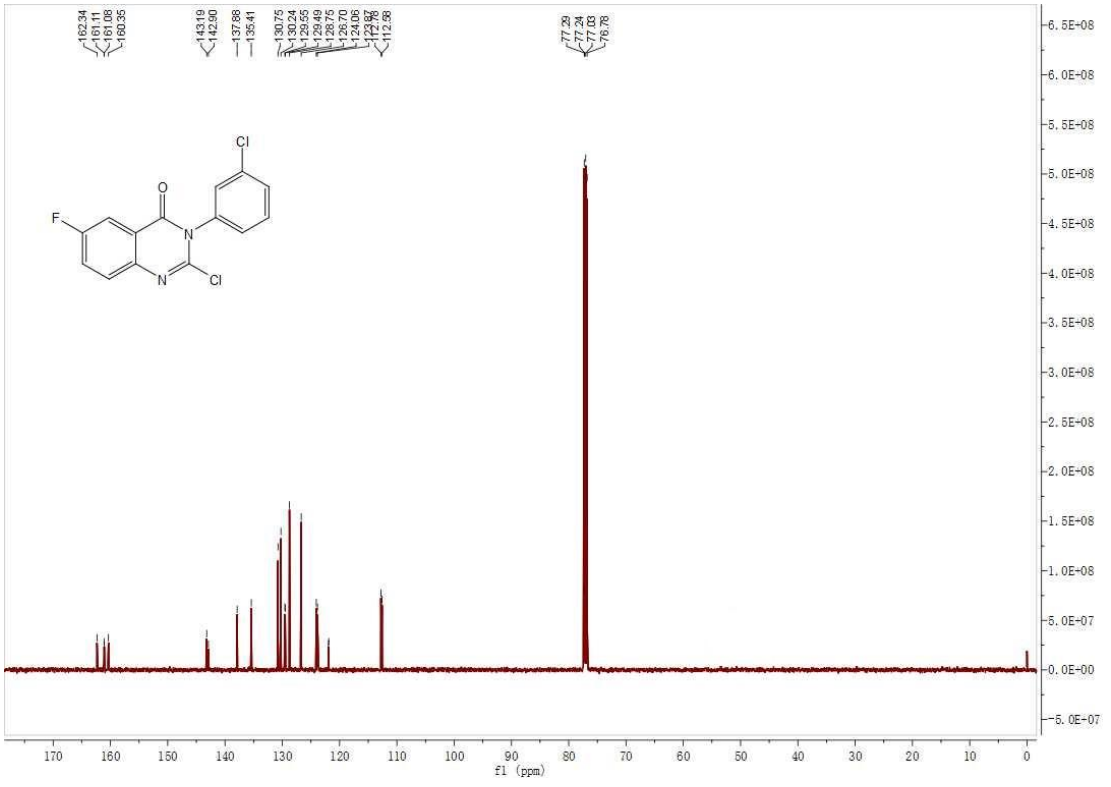
7.55
7.54
7.53
7.52
7.52
7.52
7.51
7.49
7.33
7.32
7.26
7.22
7.21
7.20
7.20
7.20
Cl
O
F
N
N
Cl
1.00
1.02
1.13
0.91
1.00
f1 (ppm)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135.41
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130.24
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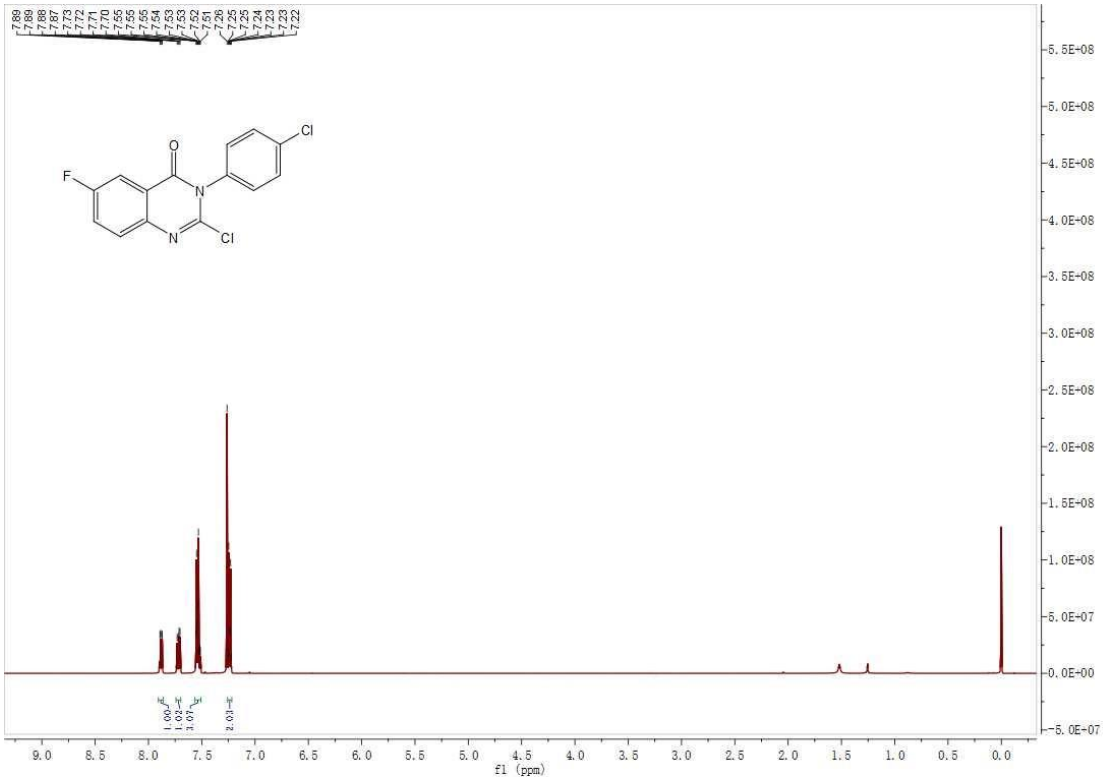
129.49
128.75
128.70
124.06
112.89
77.29
77.24
77.03
76.78
Cl
O
F
N
N
Cl
f1 (ppm)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7.88
7.88
7.87
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7.71
7.70
7.55
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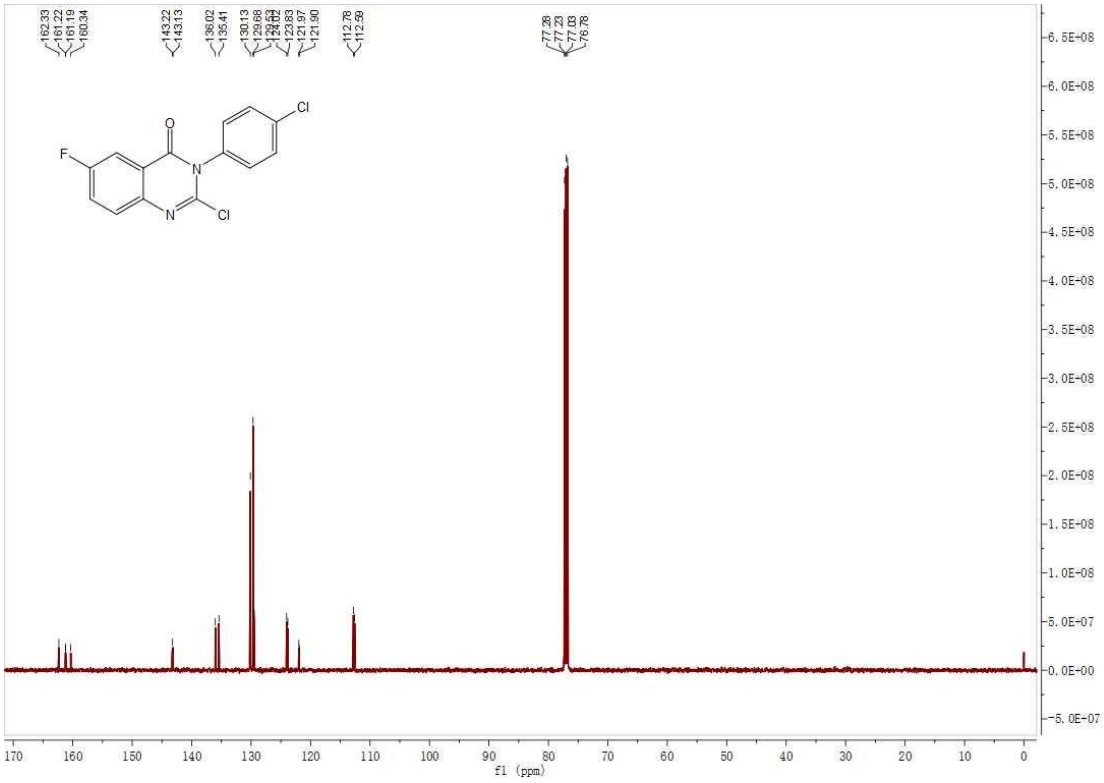
7.54
7.54
7.53
7.53
7.52
7.51
7.26
7.25
7.24
7.23
7.23
7.22
O
N
N
F
Cl
Cl
1.00
1.02
3.07
2.01
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
5.5E-08
5.0E-08
4.5E-08
4.0E-08
3.5E-08
3.0E-08
2.5E-08
2.0E-08
1.5E-08
1.0E-08
5.0E-07
0.0E+00
-5.0E-07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161.72
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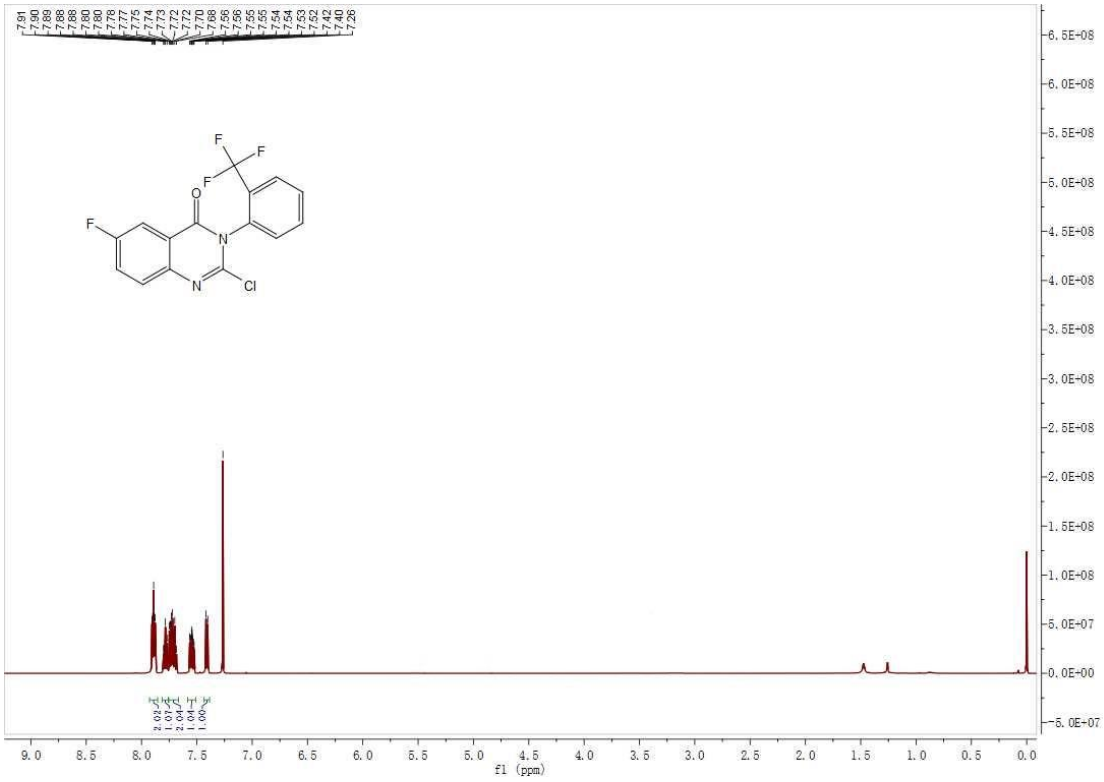
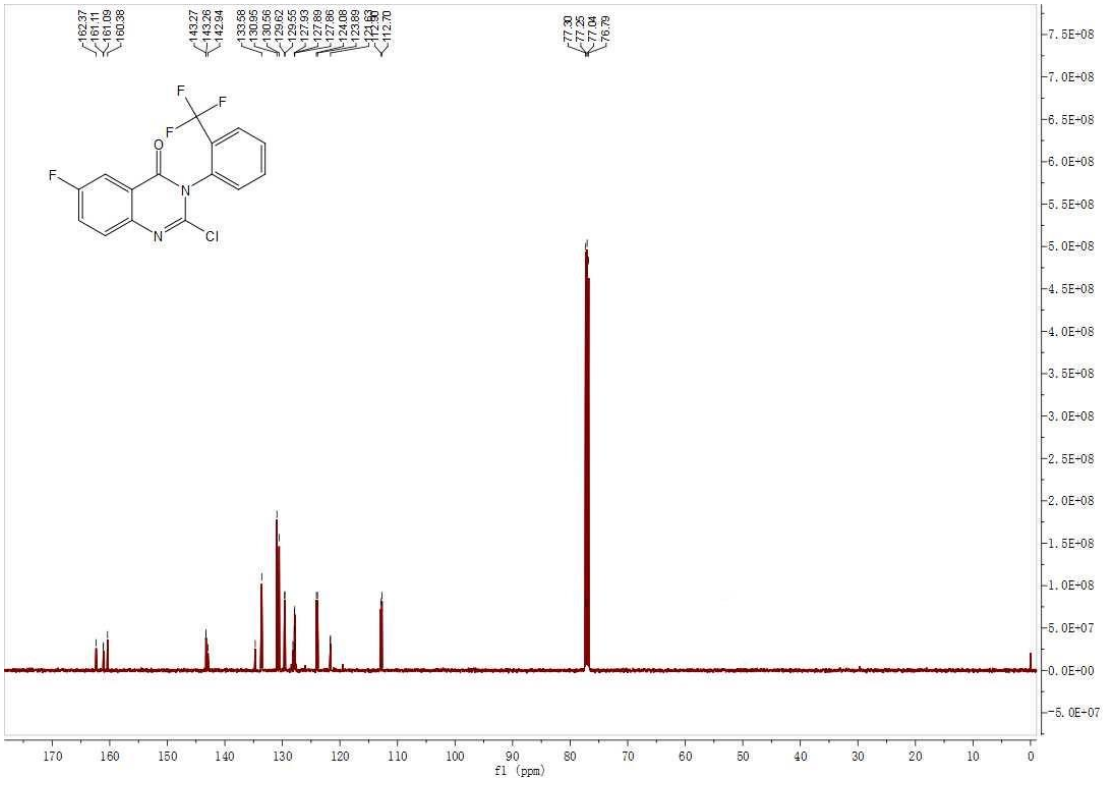
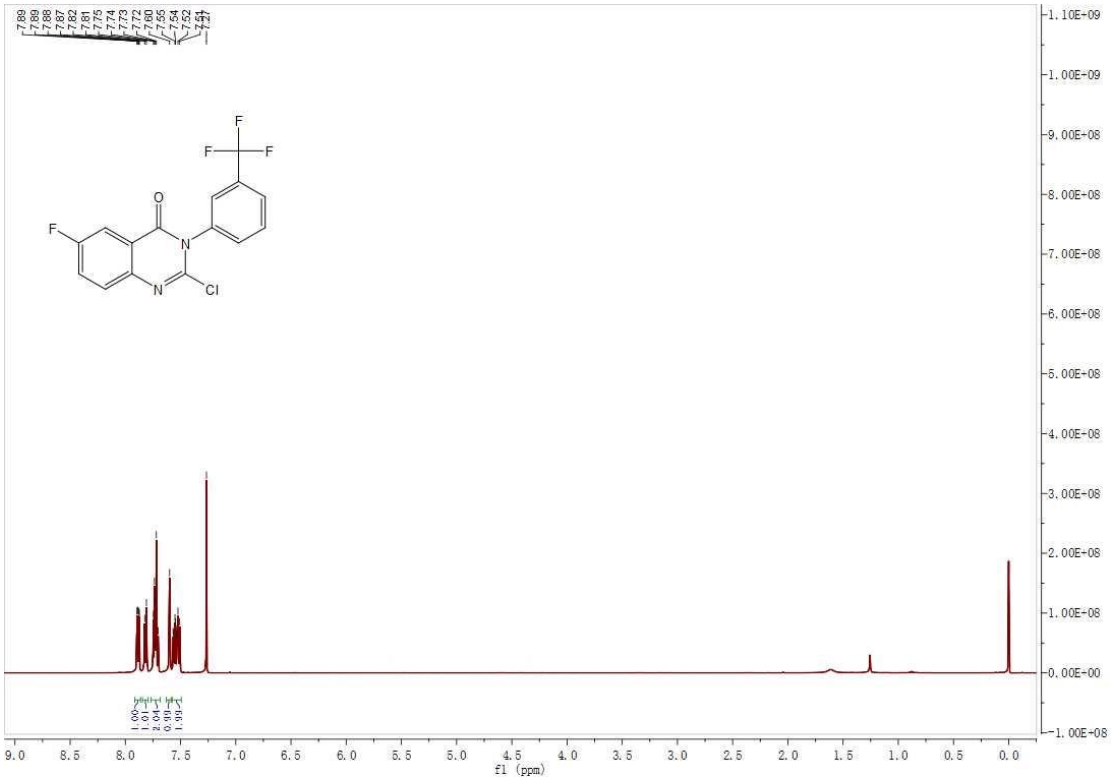
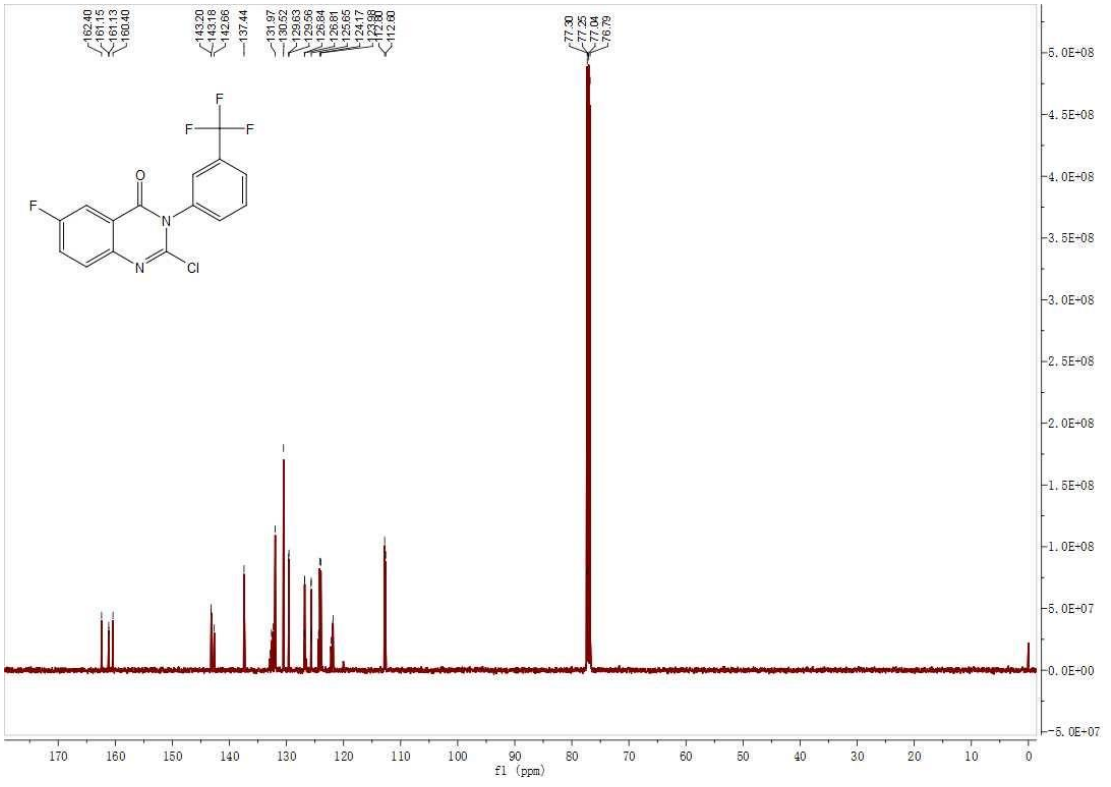
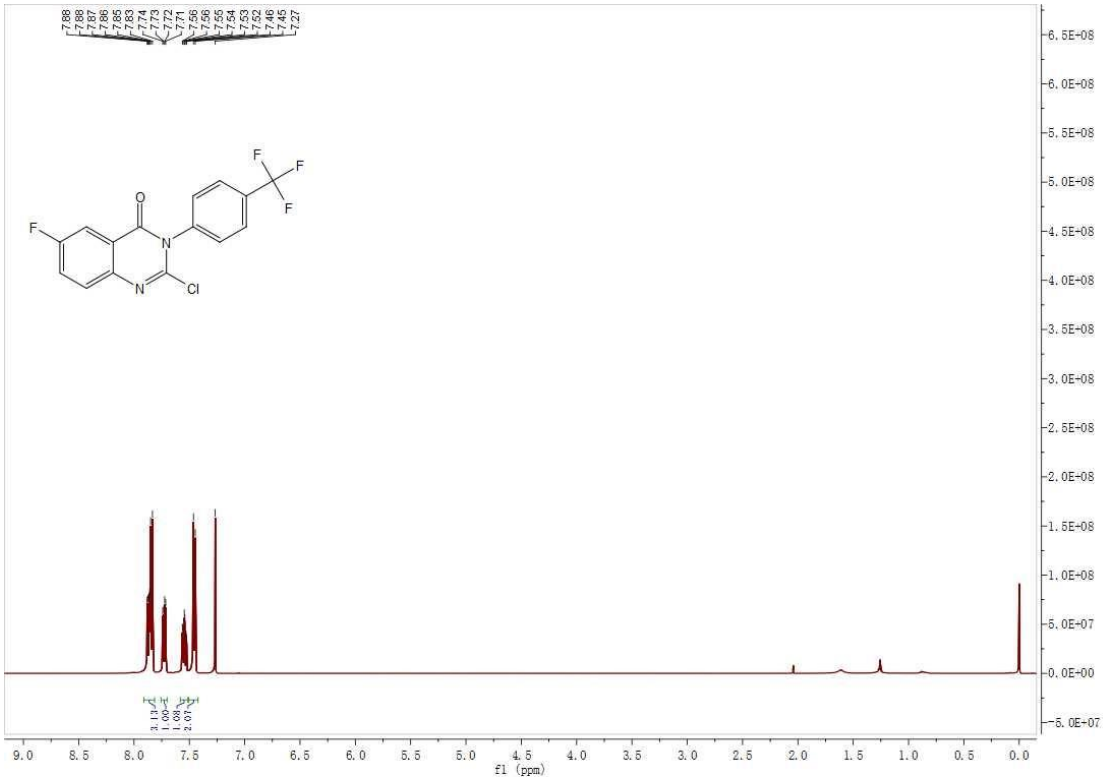
160.34
143.22
143.13
136.02
135.41
130.13
129.68
123.83
121.97
121.90
112.78
112.59
77.28
77.23
77.03
76.78
O
N
N
F
Cl
Cl
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
6.5E-08
6.0E-08
5.5E-08
5.0E-08
4.5E-08
4.0E-08
3.5E-08
3.0E-08
2.5E-08
2.0E-08
1.5E-08
1.0E-08
5.0E-07
0.0E+00
-5.0E-07

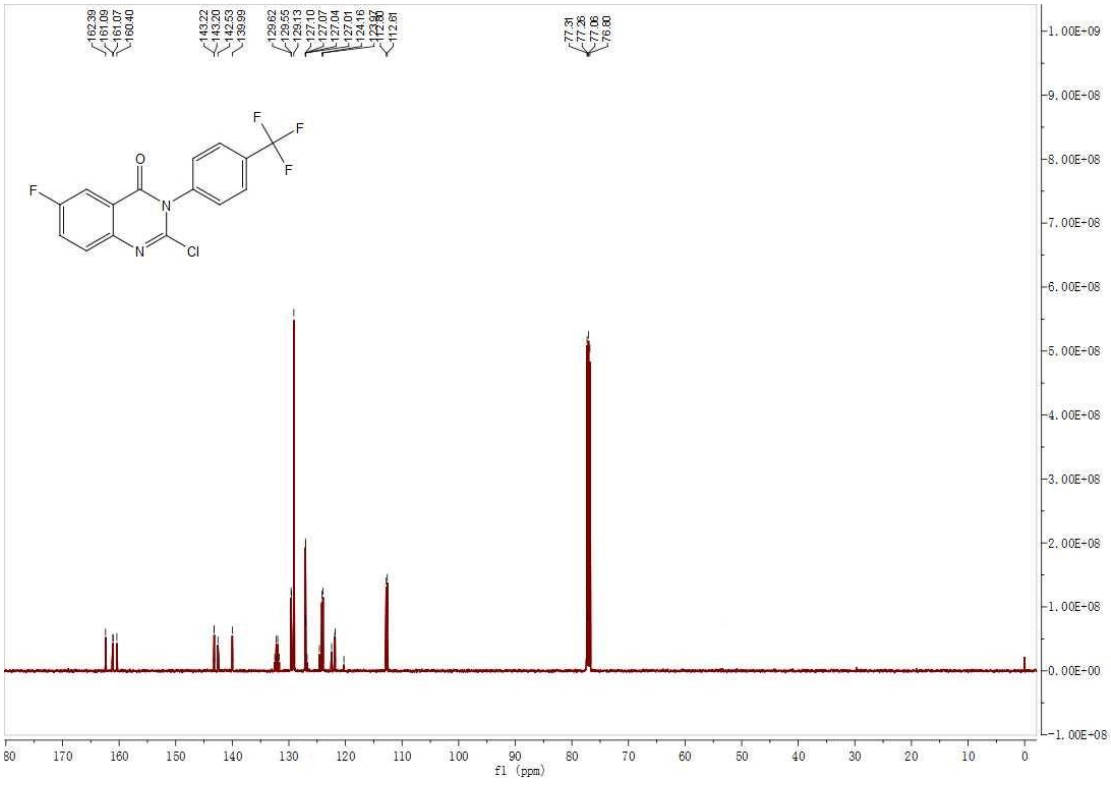

F
F
F
O
N
F
N
Cl
f1 (ppm)


F
F
F
O
N
F
N
Cl
f1 (ppm)

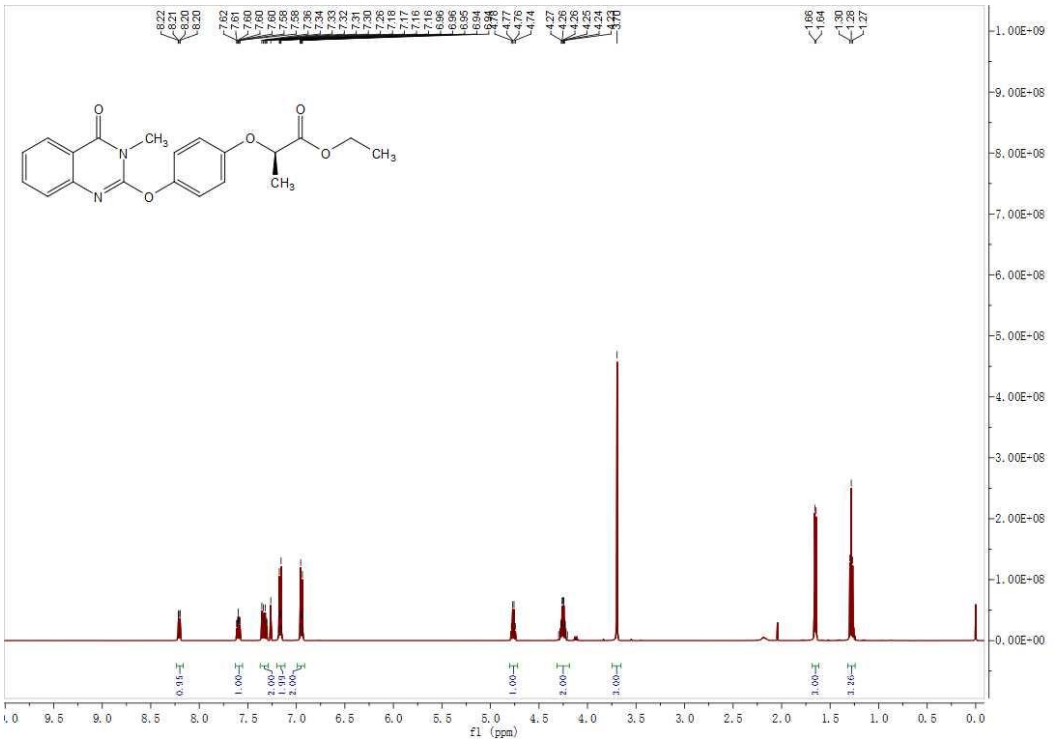

F
F
F
O
F
N
N
Cl
f1 (ppm)


F
F
F
O
F
N
N
Cl
f1 (ppm)





The ^{1}H NMR, ^{13}C NMR and HRMS Spectrum of Target Compounds QPP-1 to QPP-29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8.21
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8.20
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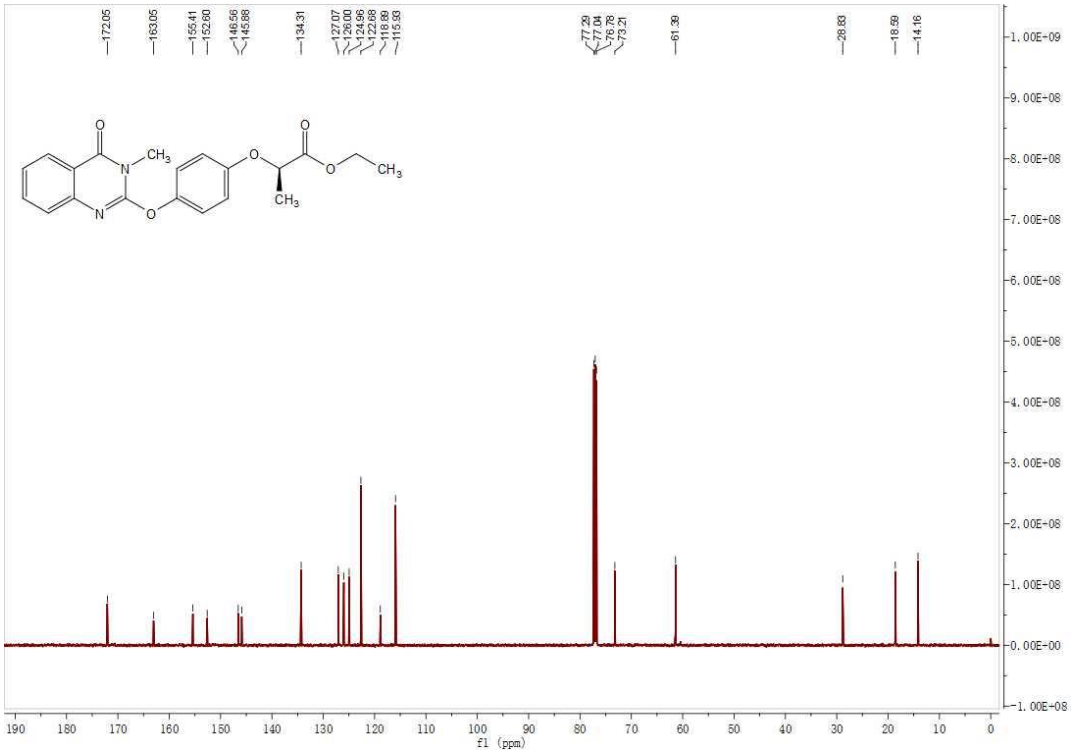
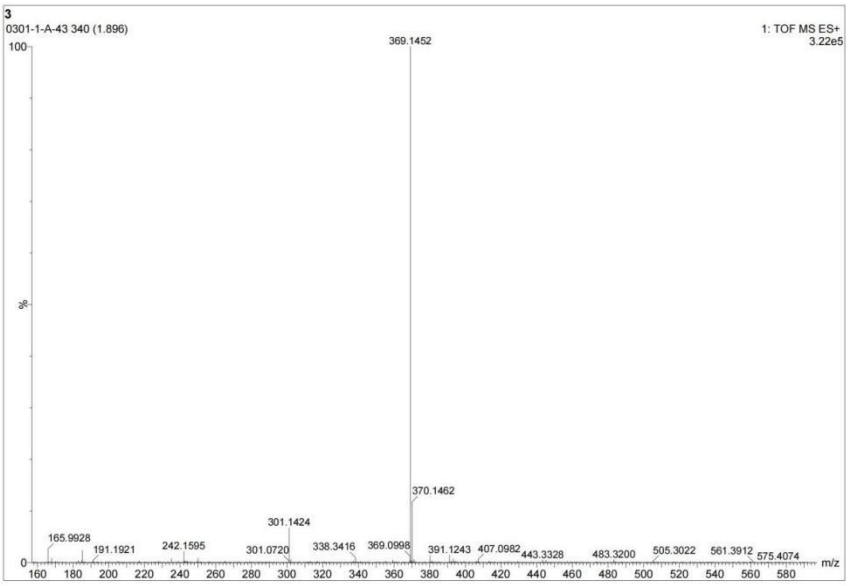
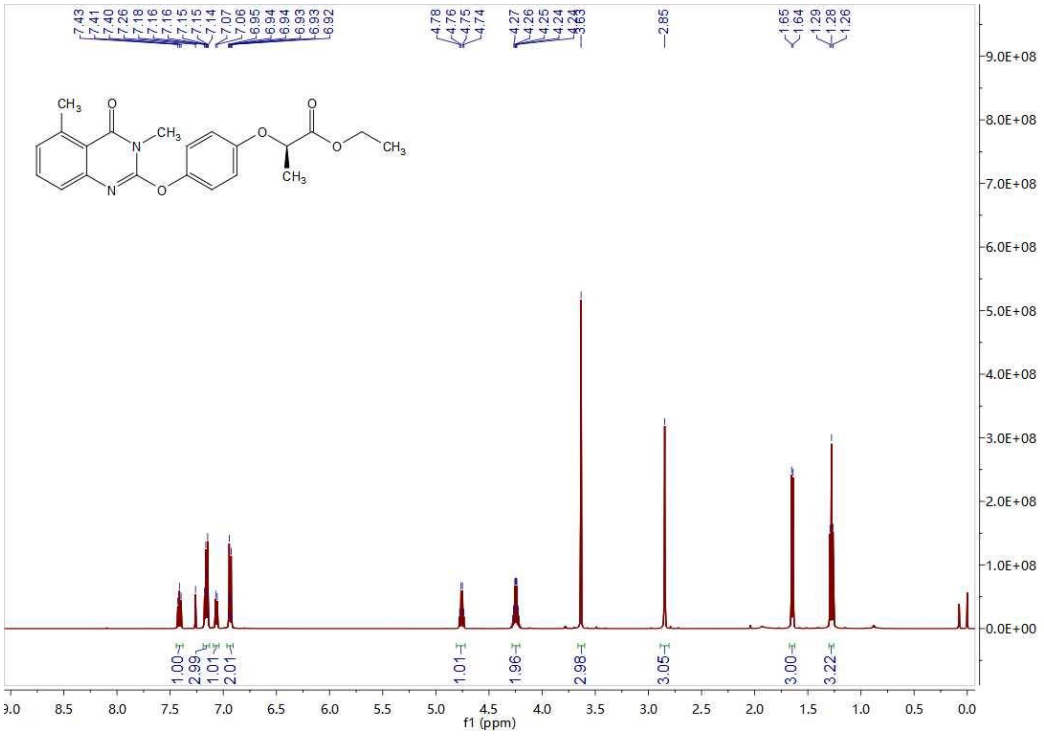
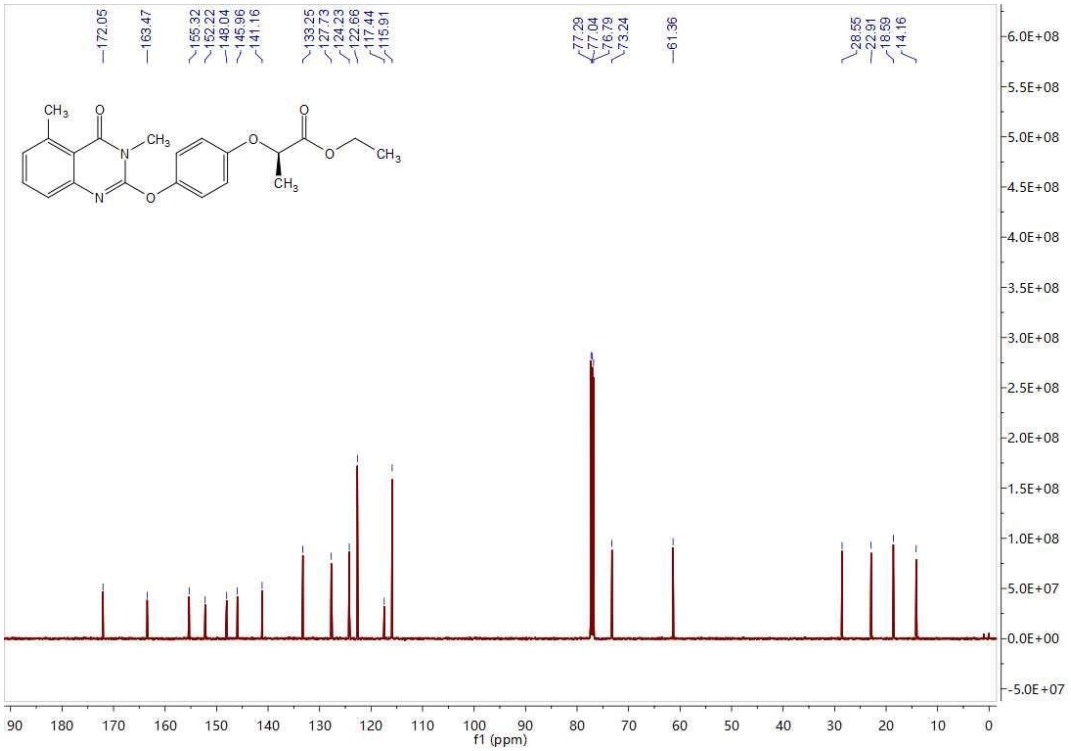
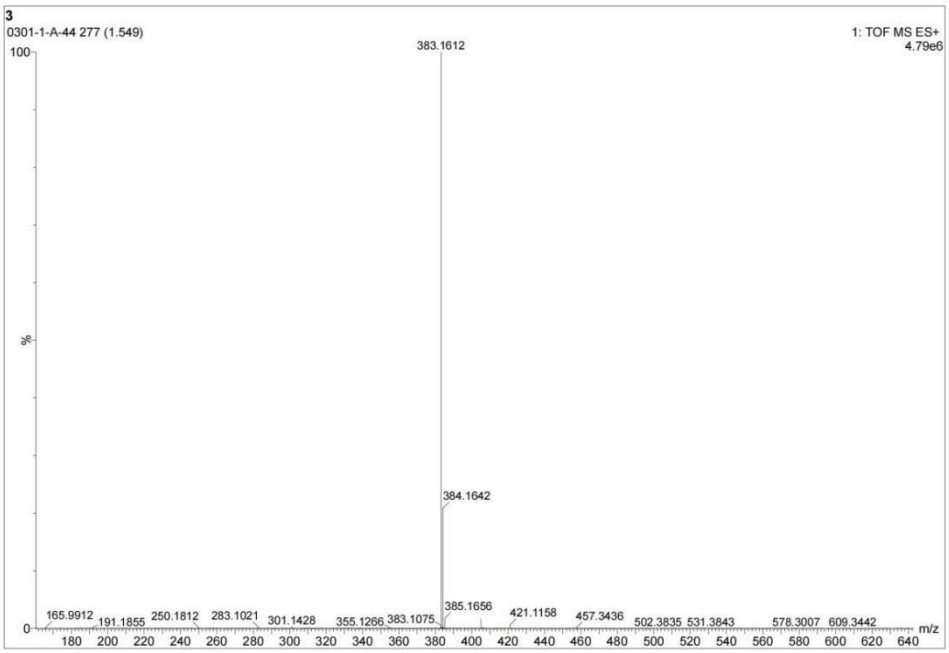
7.60
7.60
7.60
7.58
7.58
7.36
7.34
7.33
7.32
7.31
7.30
7.28
7.18
7.17
7.16
7.16
6.96
6.95
6.94
6.94
4.77
4.76
4.74
4.27
4.26
4.26
4.25
4.24
1.66
1.64
1.30
1.28
1.27
O
N
CH3
O
O
O
CH3
CH3
N
O
0.91
1.00
2.00
1.01
2.05
1.00
2.00
3.00
3.00
3.26
1.00E-09
9.00E-08
8.00E-08
7.00E-08
6.00E-08
5.00E-08
4.00E-08
3.00E-08
2.00E-08
1.00E-08
0.00E+00
f1 (ppm)

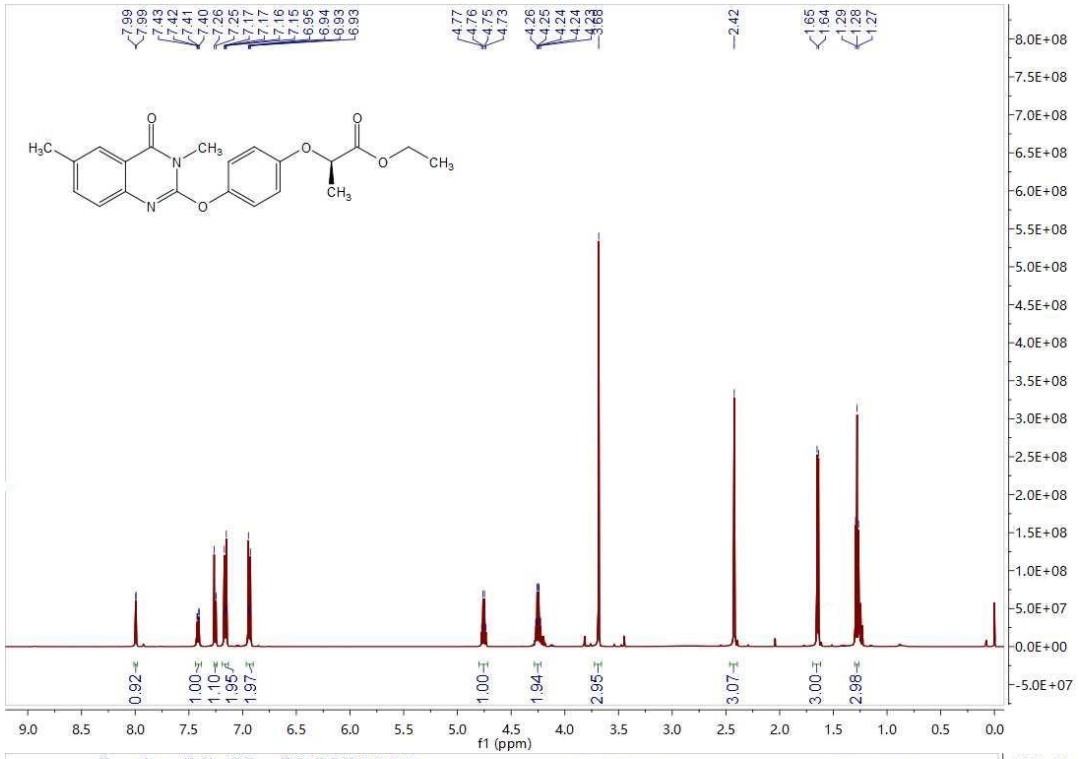

172.05
163.05
155.41
152.60
146.56
145.88
134.31
127.07
126.60
124.96
122.68
118.89
115.93
77.29
77.04
76.78
73.21
61.39
28.83
18.59
14.16
O
N
CH3
O
O
O
CH3
CH3
N
O
1.00E-09
9.00E-08
8.00E-08
7.00E-08
6.00E-08
5.00E-08
4.00E-08
3.00E-08
2.00E-08
1.00E-08
0.00E+00
-1.00E-08
f1 (ppm)

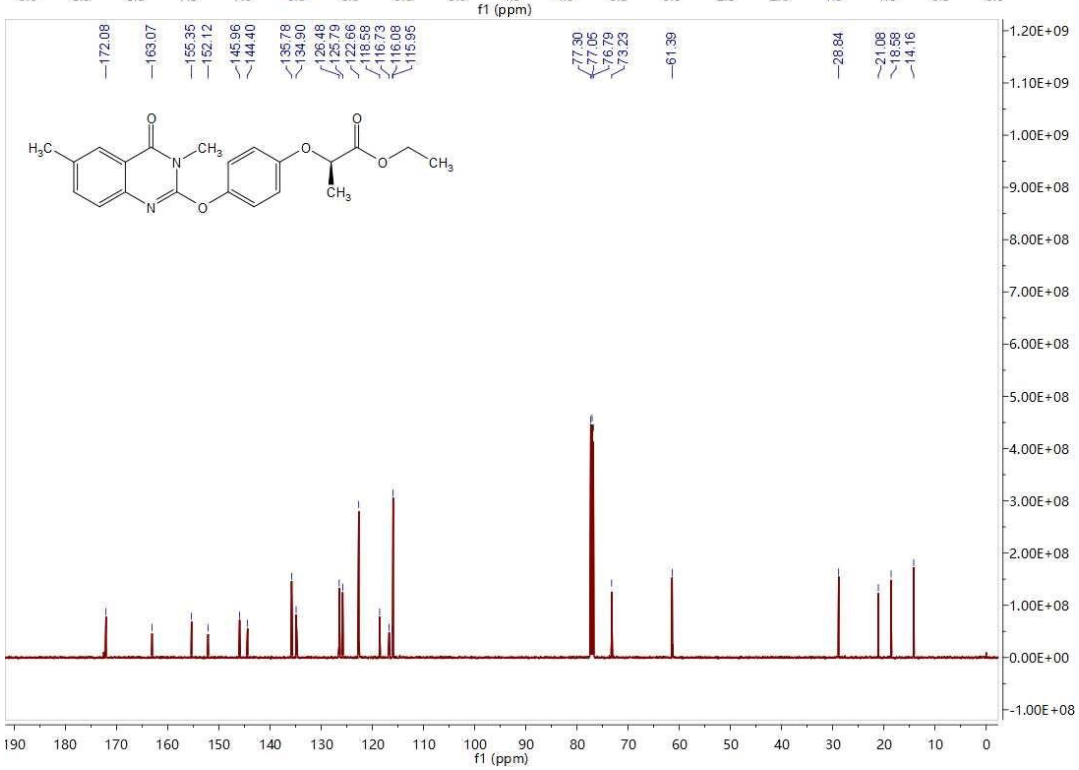

3
0301-1-A-43 340 (1.896)
1: TOF MS ES+
3.22e5
100
%
0
369.1452
370.1462
301.1424
165.9928
191.1921
242.1595
301.0720
338.3416
369.0998
391.1243
407.0982
443.3328
483.3200
505.3022
561.3912
575.4074
m/z
160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580

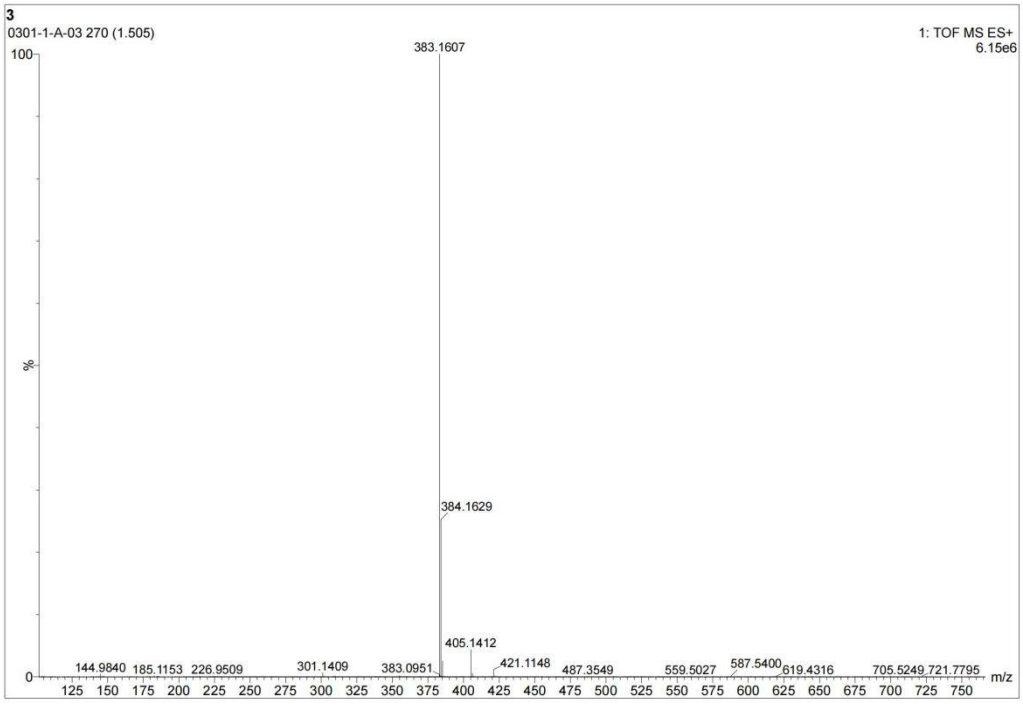

7.43
7.41
7.40
7.26
7.18
7.16
7.16
7.15
7.15
7.14
7.07
7.06
6.95
6.94
6.94
6.93
6.93
6.92
4.78
4.76
4.75
4.74
4.27
4.26
4.25
4.24
4.23
4.22
2.85
1.65
1.64
1.29
1.28
1.26
CH3
O
N
CH3
O
O
O
CH3
N
O
CH3
9.0E+08
8.0E+08
7.0E+08
6.0E+08
5.0E+08
4.0E+08
3.0E+08
2.0E+08
1.0E+08
0.0E+00
1.00
2.99
1.01
2.01
1.01
1.96
2.98
3.05
3.00
3.22
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)

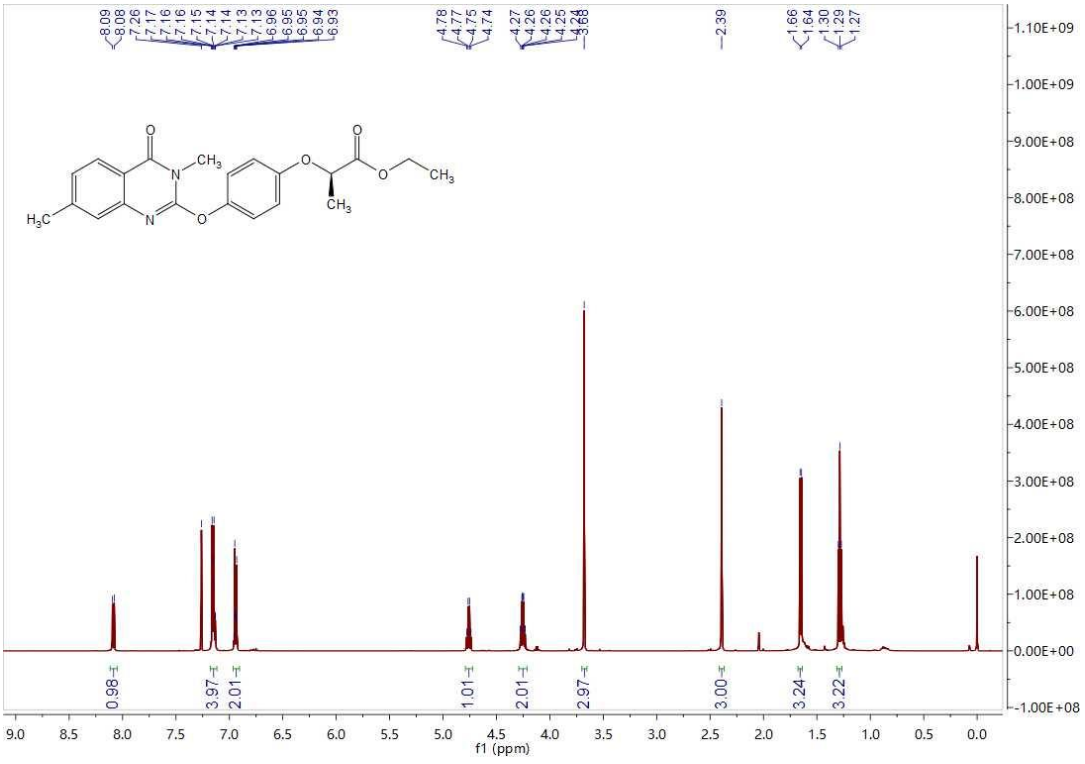

172.05
163.47
155.32
152.22
148.04
145.96
141.16
133.25
127.73
124.23
122.66
117.44
115.91
77.29
77.04
76.79
73.24
61.36
28.55
22.91
18.59
14.16
CH3
O
N
CH3
O
O
O
CH3
CH3
N
O
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

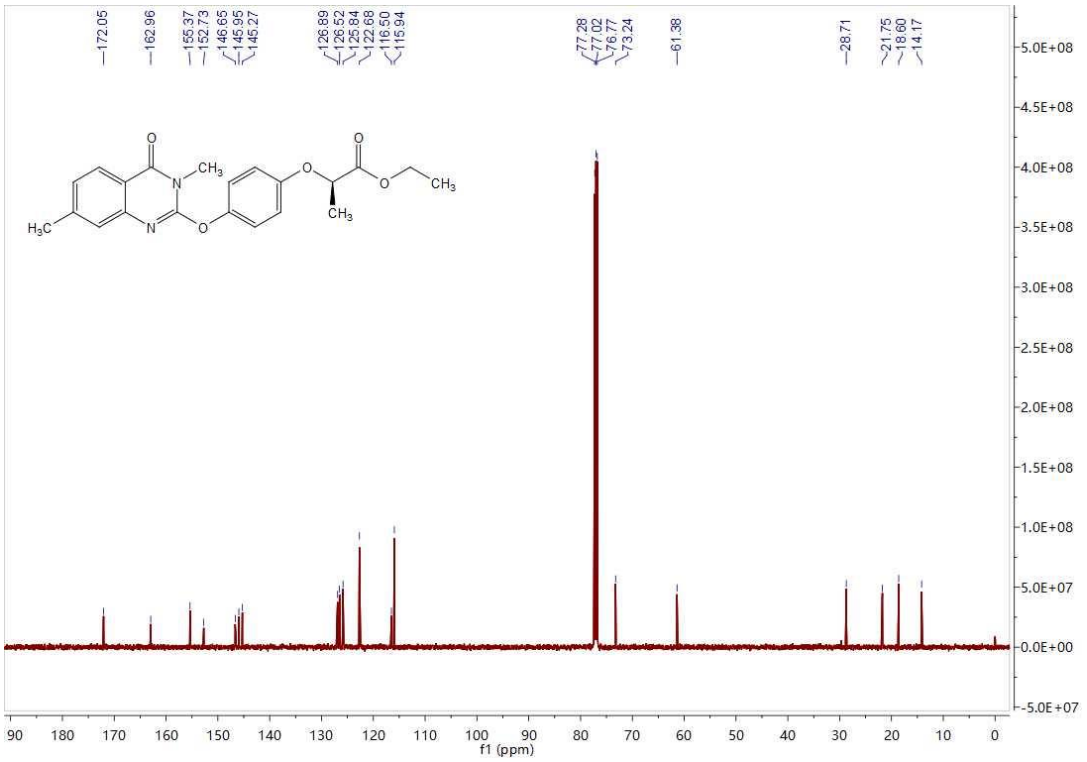

3
0301-1-A-44 277 (1.549)
1: TOF MS ES+
4.79e6
100
%
0
383.1612
384.1642
385.1656
165.9912
191.1855
250.1812
283.1021
301.1428
355.1266
383.1075
421.1158
457.3436
502.3835
531.3843
578.3007
609.3442
180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600 620 640
m/z

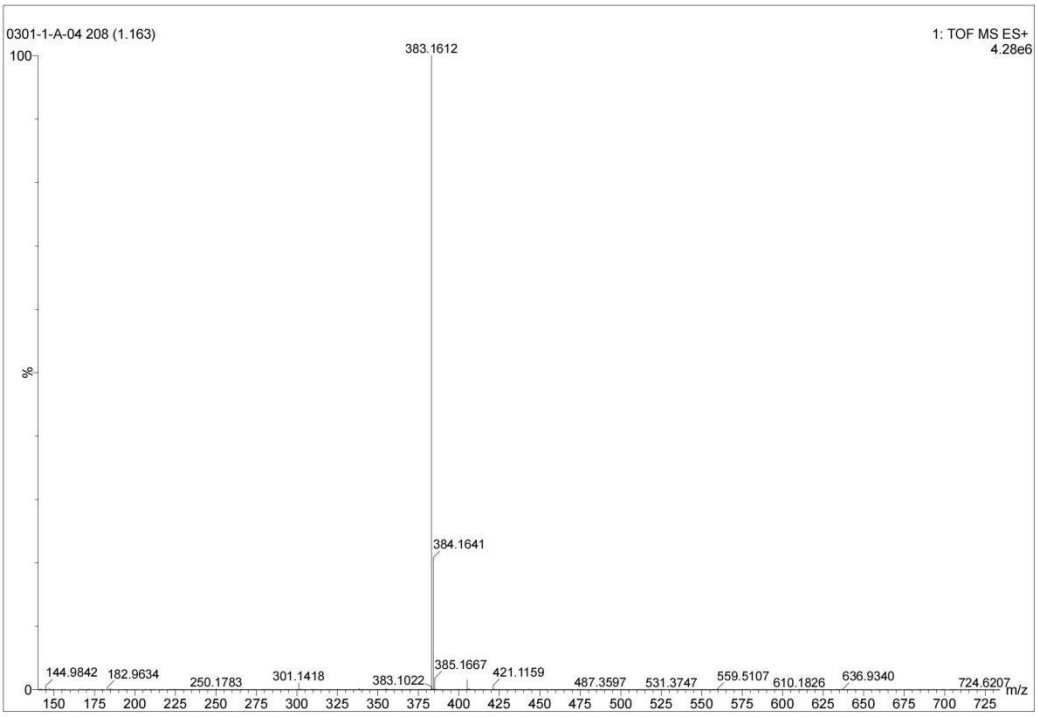

7.99
7.99
7.43
7.42
7.41
7.40
7.26
7.25
7.17
7.17
7.16
7.15
6.95
6.94
6.93
6.93
4.77
4.76
4.75
4.73
4.26
4.25
4.24
4.24
4.23
4.22
2.42
1.65
1.64
1.29
1.28
1.27
0.92
1.00
1.10
1.95
1.97
1.00
1.94
2.95
3.07
3.00
2.98
f1 (ppm)

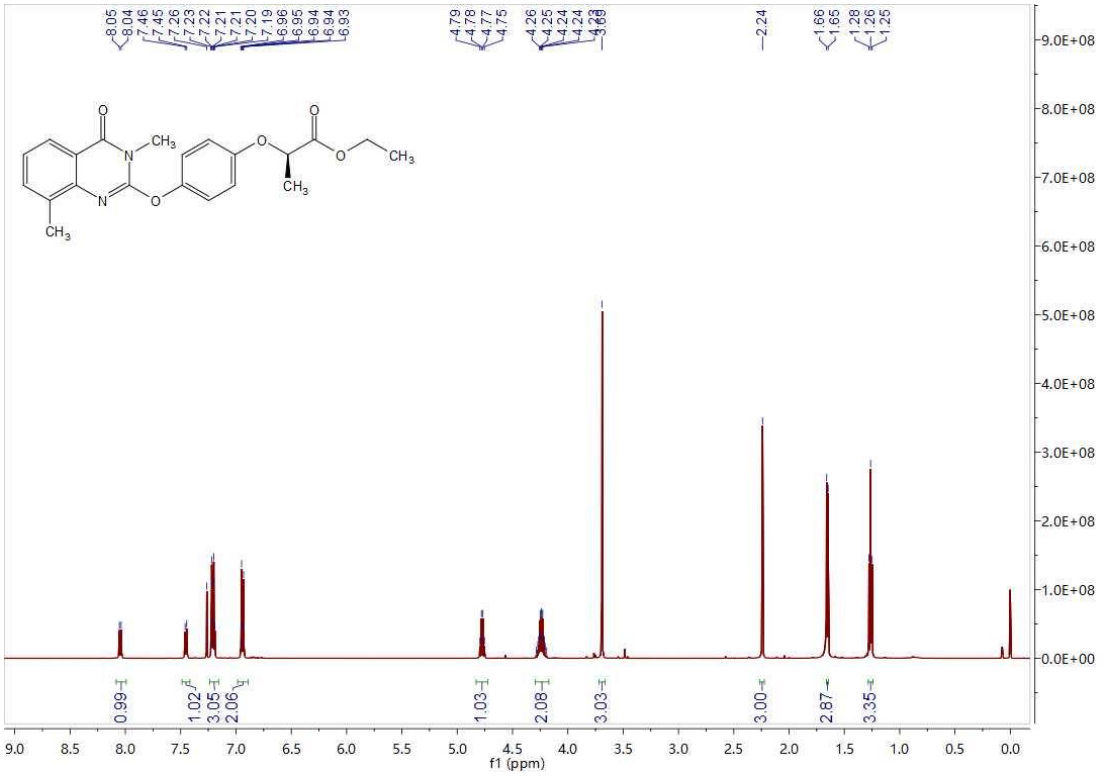

172.08
163.07
155.35
152.12
145.96
144.40
135.78
134.90
126.48
125.79
122.66
118.58
116.73
116.08
115.95
77.30
77.05
76.79
73.23
61.39
28.84
21.08
18.58
14.16
f1 (ppm)

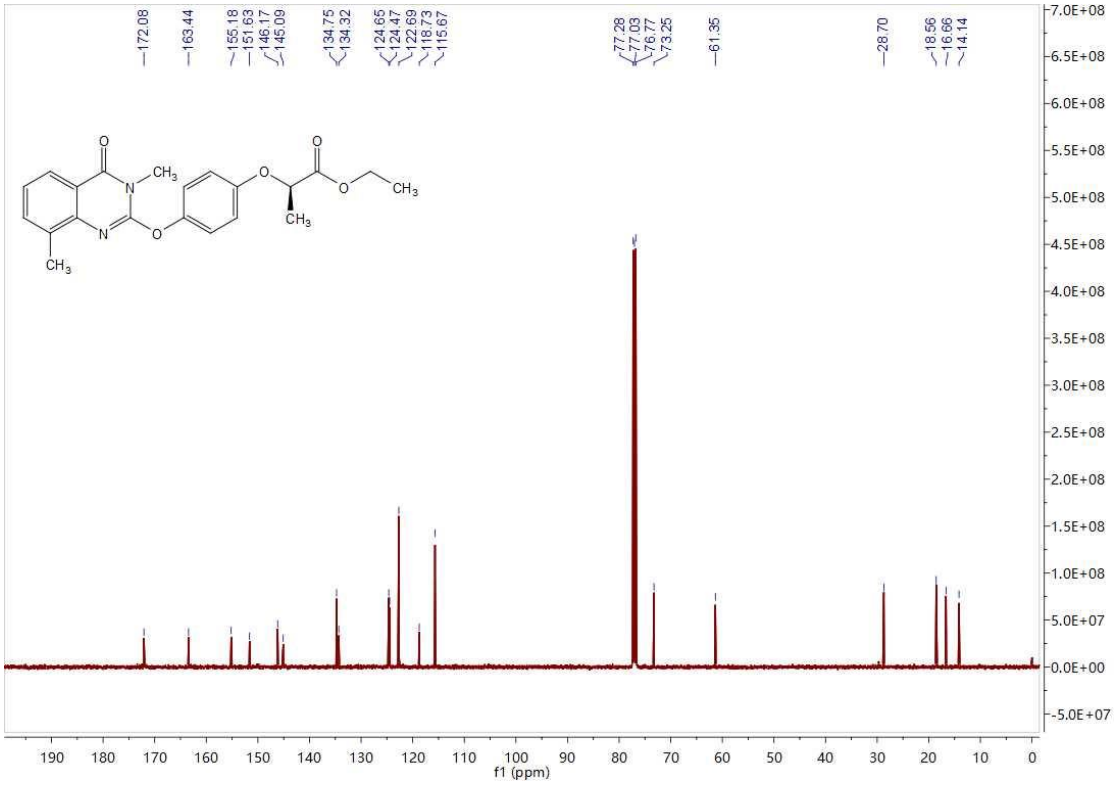

3
0301-1-A-03 270 (1.505)
1: TOF MS ES+
6.15e6
100
%
0
383.1607
384.1629
405.1412
144.9840
185.1153
226.9509
301.1409
383.0951
421.1148
487.3549
559.5027
587.5400
619.4316
705.5249
721.7795
m/z
125 150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 625 650 675 700 725 750

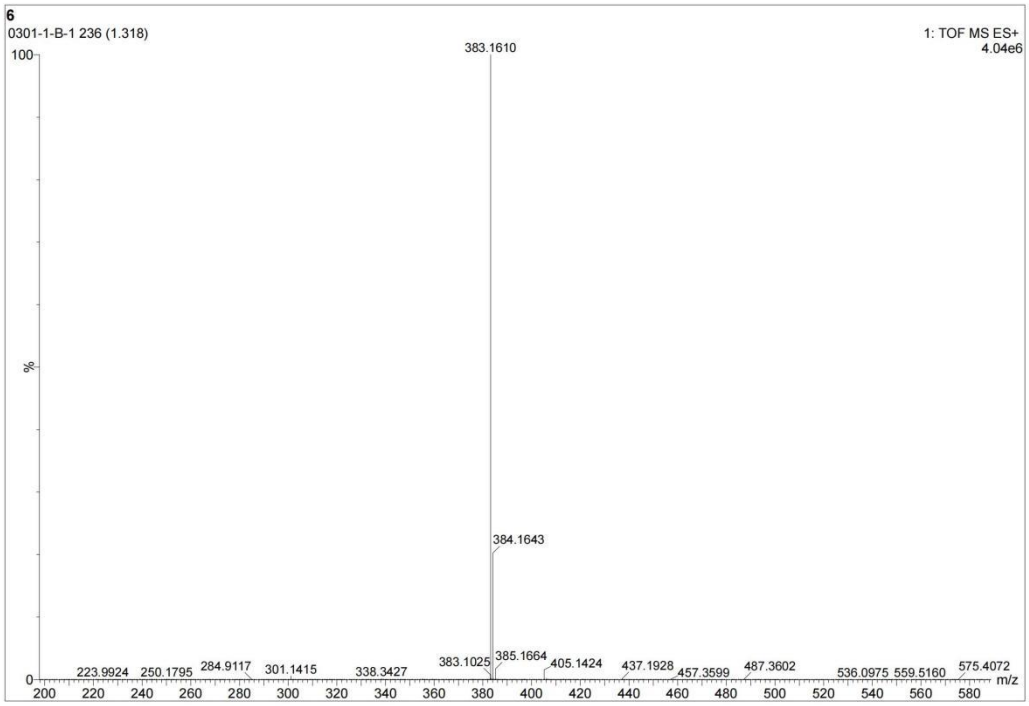

8.09
8.08
7.26
7.17
7.16
7.15
7.14
7.13
6.96
6.95
6.94
6.93
4.78
4.77
4.75
4.74
4.27
4.26
4.25
4.24
4.23
2.39
1.66
1.64
1.30
1.29
1.27
1.10E+09
1.00E+09
9.00E+08
8.00E+08
7.00E+08
6.00E+08
5.00E+08
4.00E+08
3.00E+08
2.00E+08
1.00E+08
0.00E+00
-1.00E+08
0.98
3.97
2.01
1.01
2.01
2.97
3.00
3.24
3.22
9.0 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)

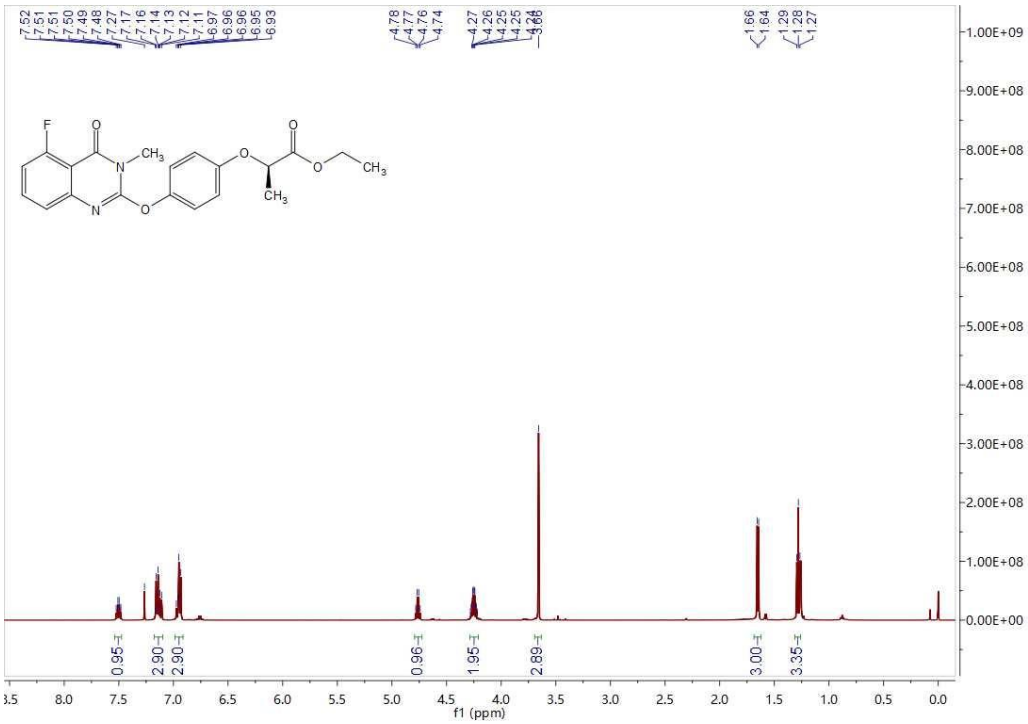

172.05
162.96
155.37
152.73
146.65
145.95
145.27
126.89
126.52
125.84
122.68
116.50
115.94
77.28
77.02
76.77
73.24
61.38
28.71
21.75
18.60
14.17
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

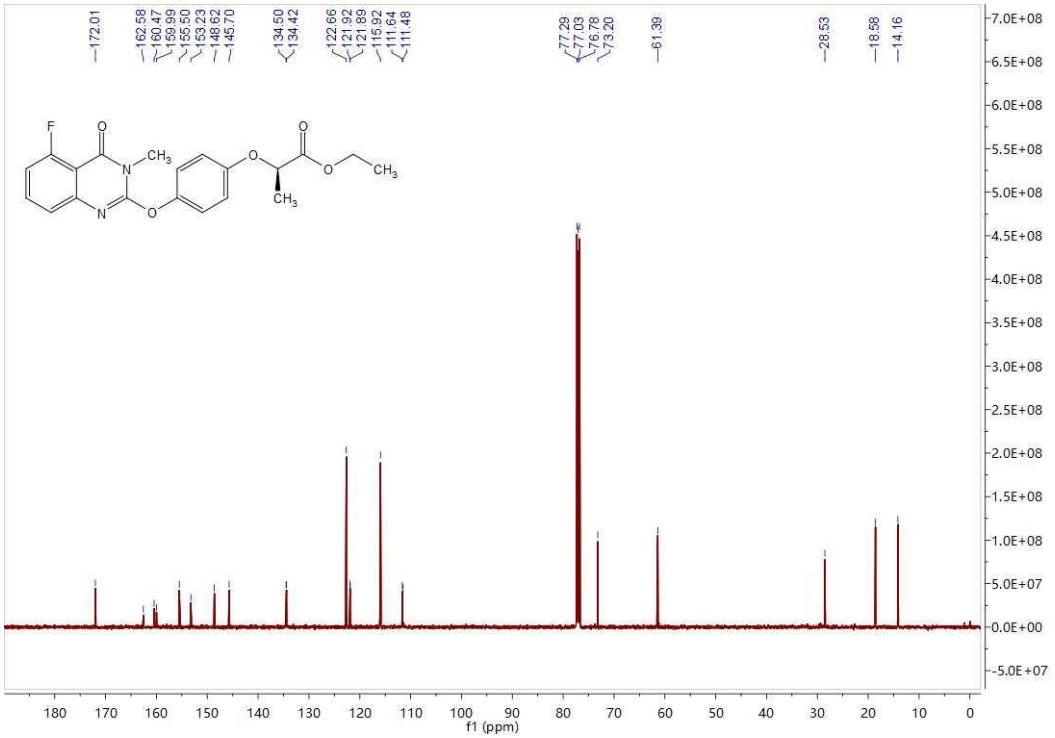

0301-1-A-04 208 (1.163)
1: TOF MS ES+
4.28e6
100
%
0
383.1612
384.1641
385.1667
144.9842
182.9634
250.1783
301.1418
383.1022
421.1159
487.3597
531.3747
559.5107
610.1826
636.9340
724.6207
150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 625 650 675 700 725
m/z

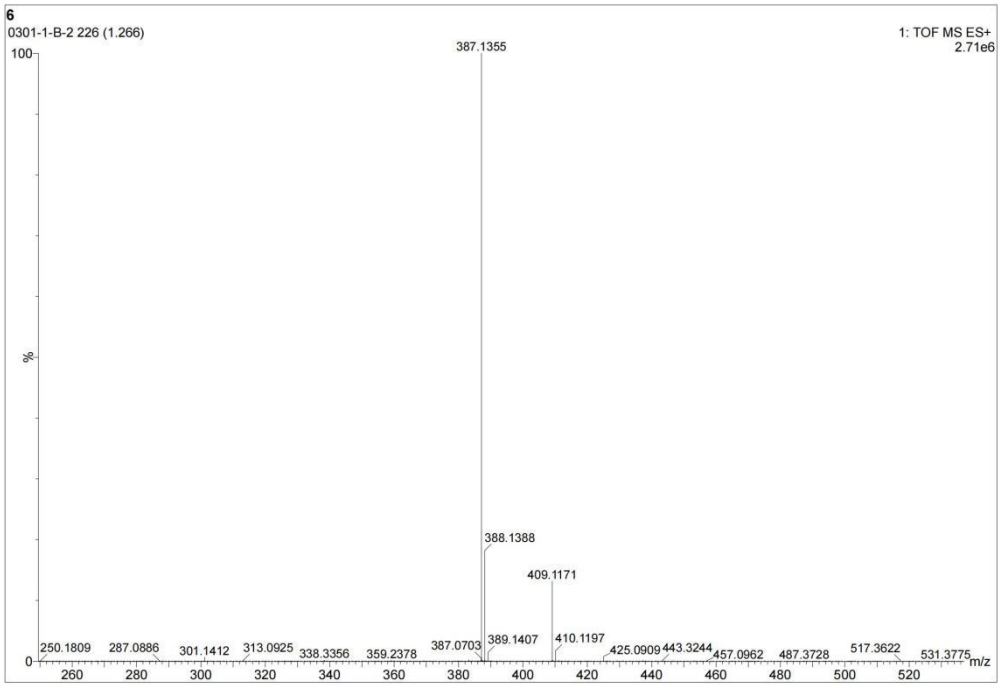

8.05
8.04
7.46
7.45
7.26
7.23
7.22
7.21
7.21
7.20
7.19
6.96
6.95
6.94
6.94
6.93
4.79
4.78
4.77
4.75
4.26
4.25
4.24
4.24
3.03
2.24
1.66
1.65
1.28
1.26
1.25
0.99
1.02
3.05
2.06
1.03
2.08
3.03
3.00
2.87
3.35
f1 (ppm)

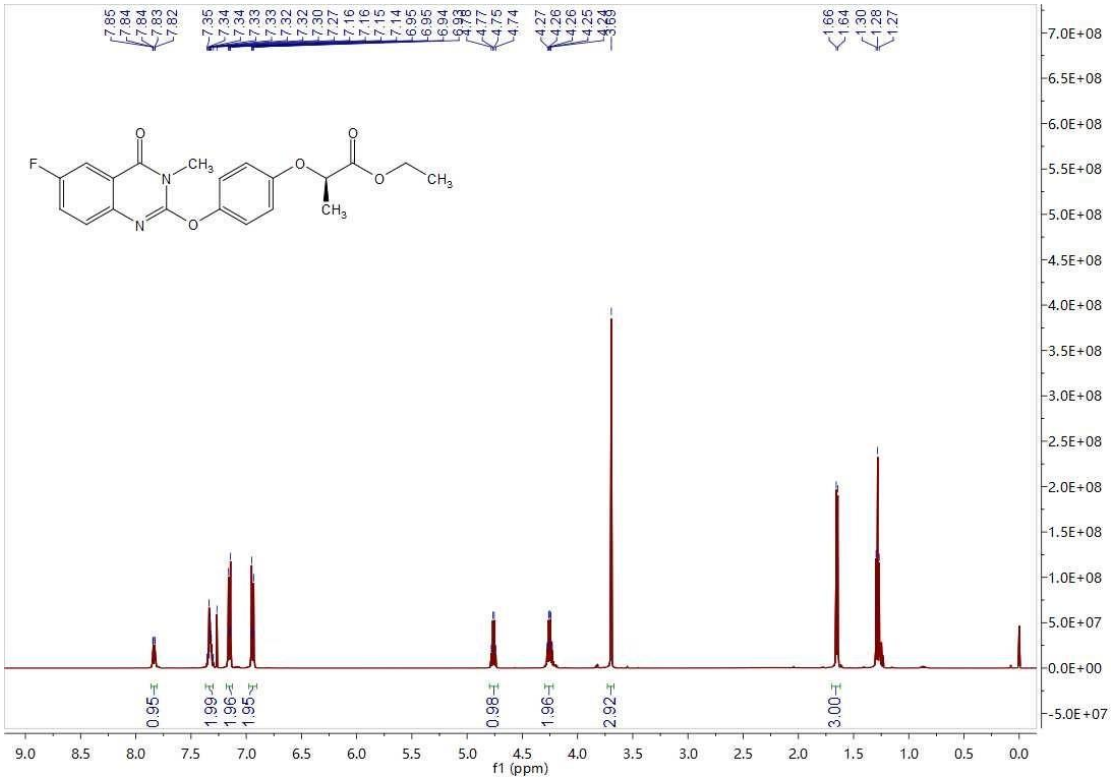

172.08
163.44
155.18
151.63
146.17
145.09
134.75
134.32
124.65
124.47
122.69
118.73
115.67
77.28
77.03
76.77
73.25
61.35
28.70
18.56
16.66
14.14
f1 (ppm)

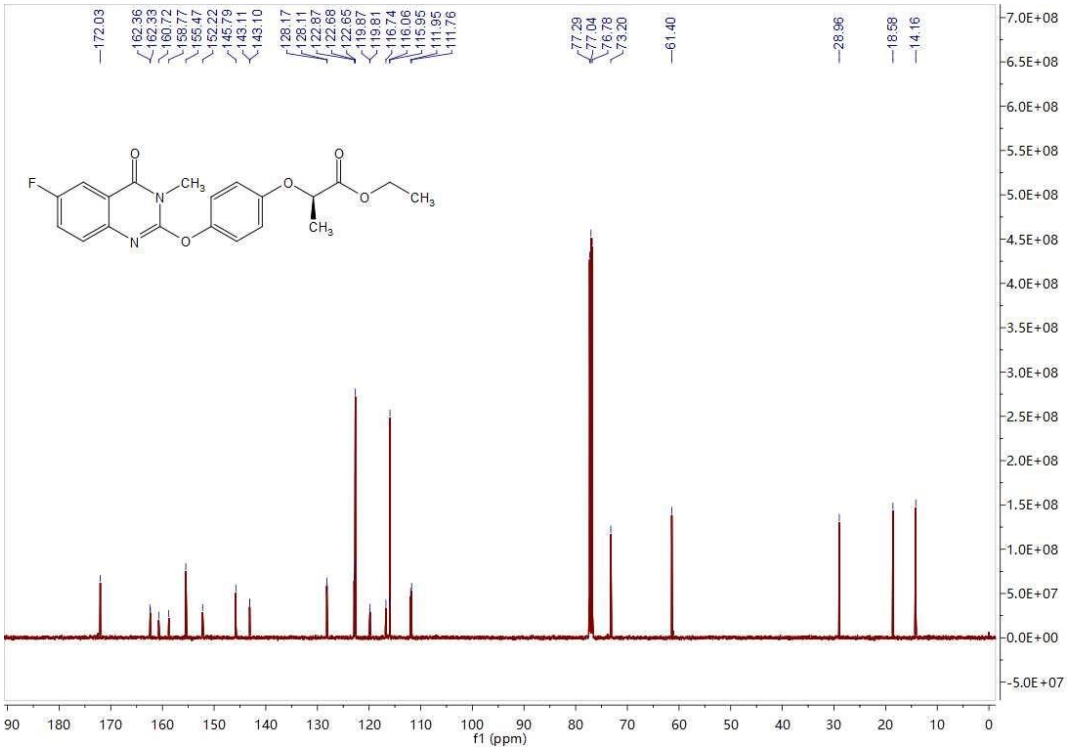

6
0301-1-B-1 236 (1.318)
1: TOF MS ES+
4.04e6
100
%
0
383.1610
384.1643
223.9924
250.1795
284.9117
301.1415
338.3427
383.1025
385.1664
405.1424
437.1928
457.3599
487.3602
536.0975
559.5160
575.4072
m/z

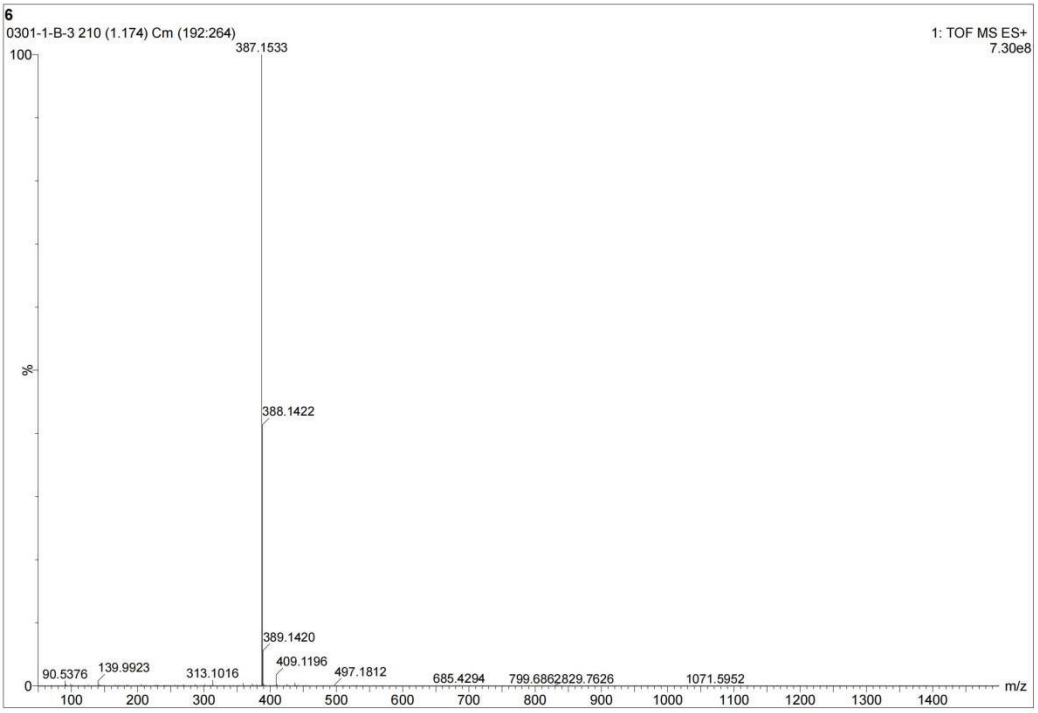

7.52
7.51
7.51
7.50
7.49
7.48
7.27
7.17
7.16
7.14
7.13
7.12
7.11
6.97
6.96
6.96
6.95
6.93
4.78
4.77
4.76
4.74
4.27
4.26
4.25
4.25
4.24
3.68
1.66
1.64
1.29
1.28
1.27
F
O
N
CH3
O
O
O
CH3
CH3
N
1.00E+09
9.00E+08
8.00E+08
7.00E+08
6.00E+08
5.00E+08
4.00E+08
3.00E+08
2.00E+08
1.00E+08
0.00E+00
0.95
2.90
2.90
0.96
1.95
2.89
3.00
3.35
f1 (ppm)

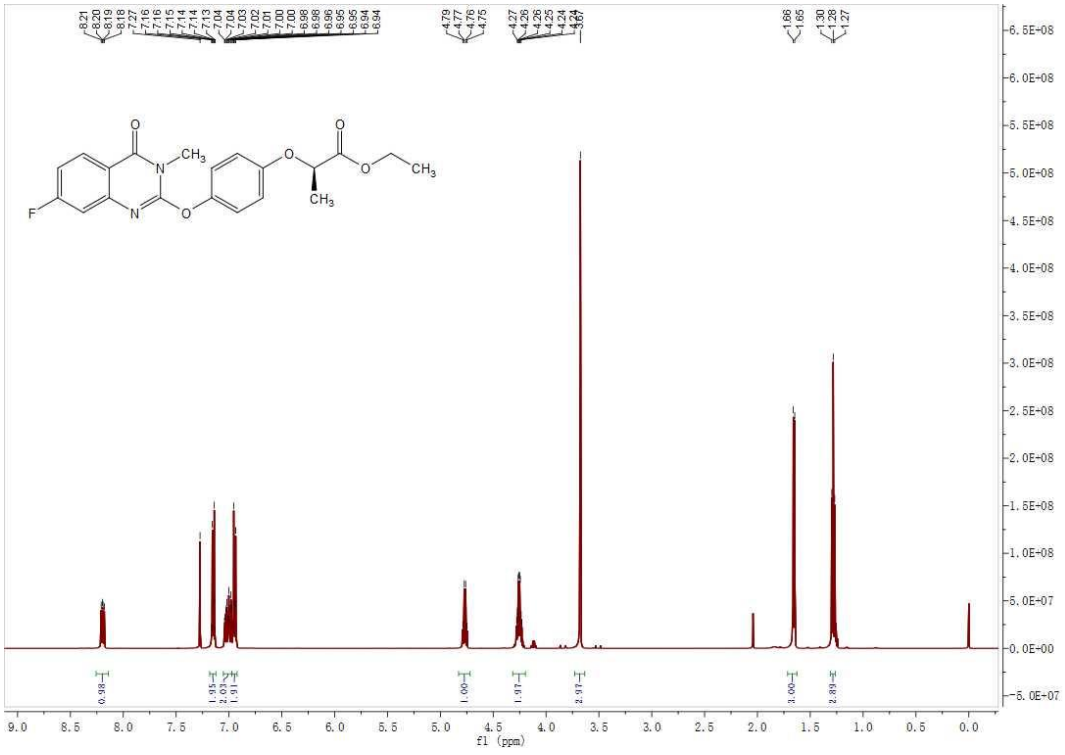

172.01
162.58
160.47
159.99
155.50
153.23
148.62
145.70
134.50
134.42
122.66
121.92
121.89
115.92
111.64
111.48
77.29
77.03
76.78
73.20
61.39
28.53
18.58
14.16
F
O
N
CH3
O
O
O
O
CH3
CH3
N
7.0E+08
6.5E+08
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

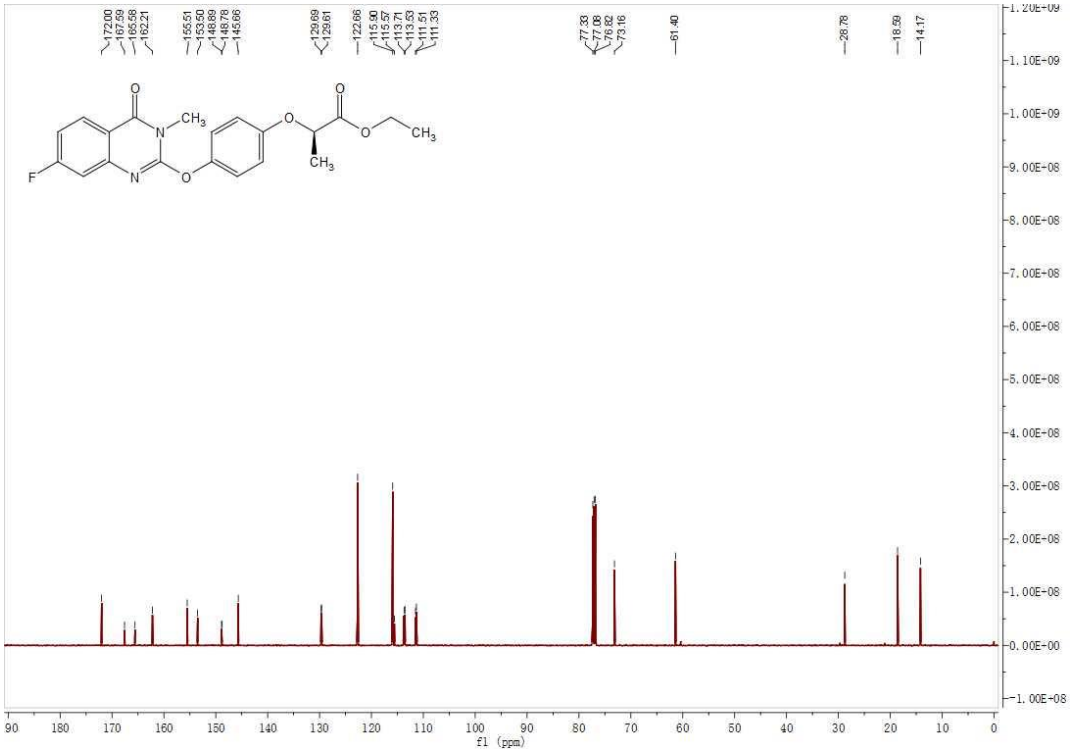

6
0301-1-B-2 226 (1.266)
1: TOF MS ES+
2.71e6
100
%
0
387.1355
388.1388
409.1171
250.1809
287.0886
301.1412
313.0925
338.3356
359.2378
387.0703
389.1407
410.1197
425.0909
443.3244
457.0962
487.3728
517.3622
531.3775
m/z
260 280 300 320 340 360 380 400 420 440 460 480 500 520

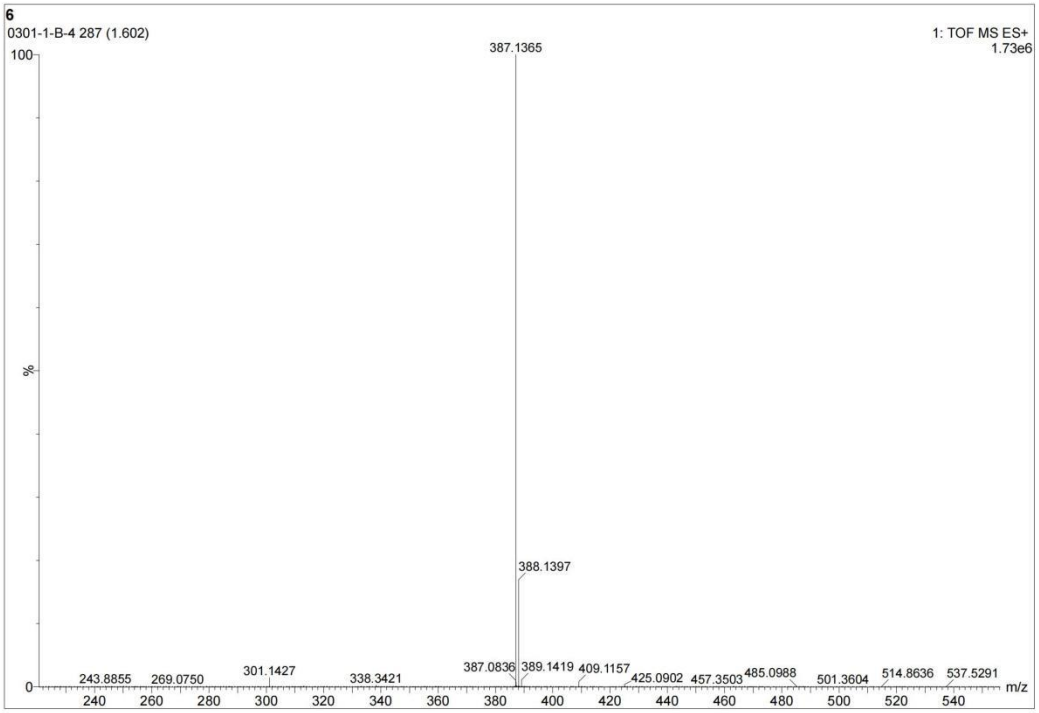

7.85
7.84
7.84
7.83
7.82
7.35
7.34
7.34
7.33
7.33
7.32
7.32
7.30
7.27
7.16
7.16
7.15
7.14
6.95
6.95
6.94
6.93
4.78
4.77
4.75
4.74
4.27
4.26
4.26
4.25
4.24
3.69
1.66
1.64
1.30
1.28
1.27
F
O
N
CH3
O
O
O
CH3
CH3
N
O
0.95
1.99
1.96
1.95
0.98
1.96
2.92
3.00
f1 (ppm)

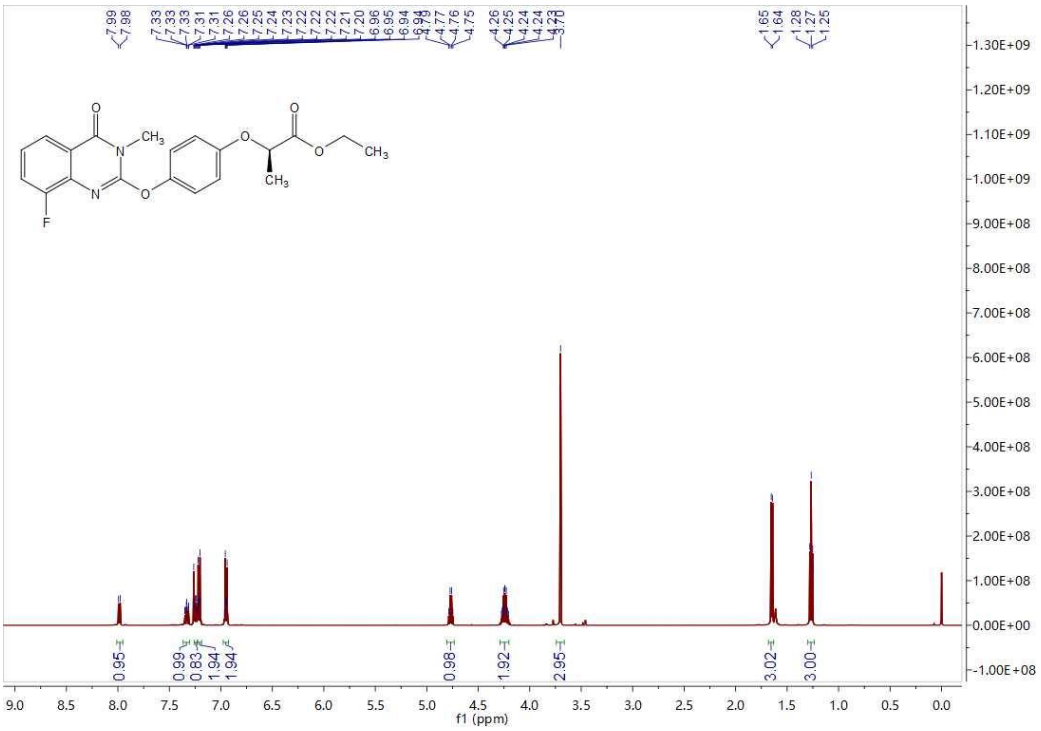

172.03
162.36
162.33
160.72
158.77
155.47
152.22
145.79
143.11
143.10
128.17
128.11
122.87
122.68
122.65
119.87
119.81
116.74
116.06
115.95
111.95
111.76
77.29
77.04
76.78
73.20
61.40
28.96
18.58
14.16
F
O
N
CH3
O
O
O
CH3
CH3
N
O
f1 (ppm)

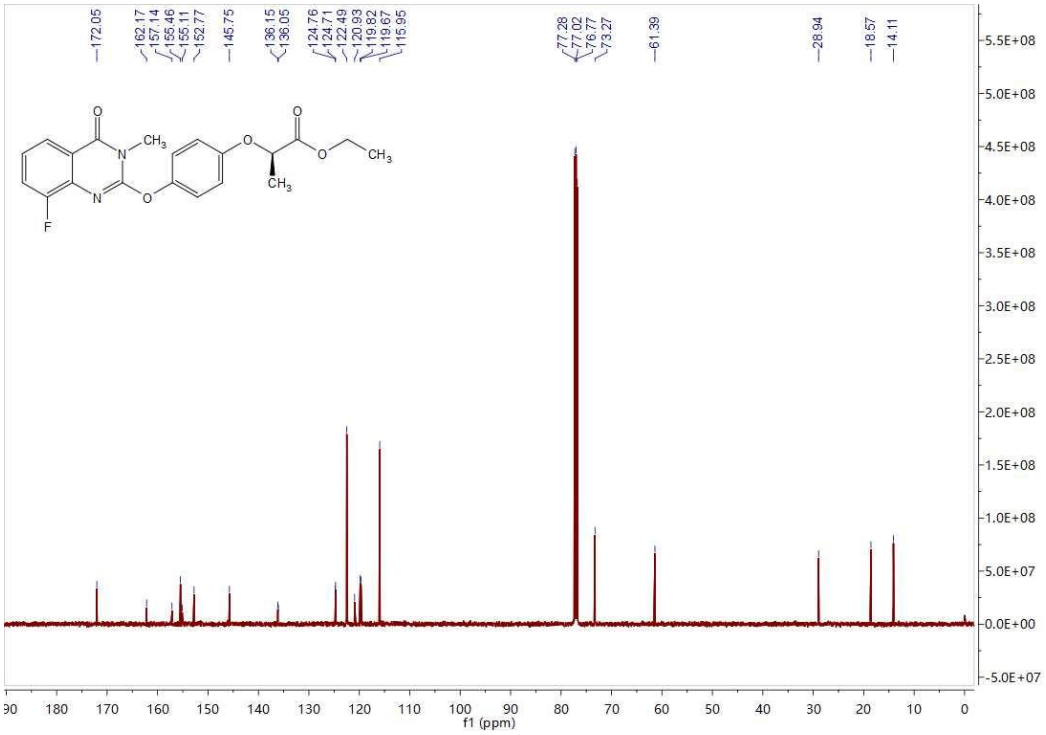

6
0301-1-B-3 210 (1.174) Cm (192:264)
1: TOF MS ES+
7.30e8
100
%
0
387.1533
388.1422
389.1420
409.1196
90.5376
139.9923
313.1016
497.1812
685.4294
799.6862829.7626
1071.5952
m/z
100
200
300
400
500
600
700
800
900
1000
1100
1200
1300
1400

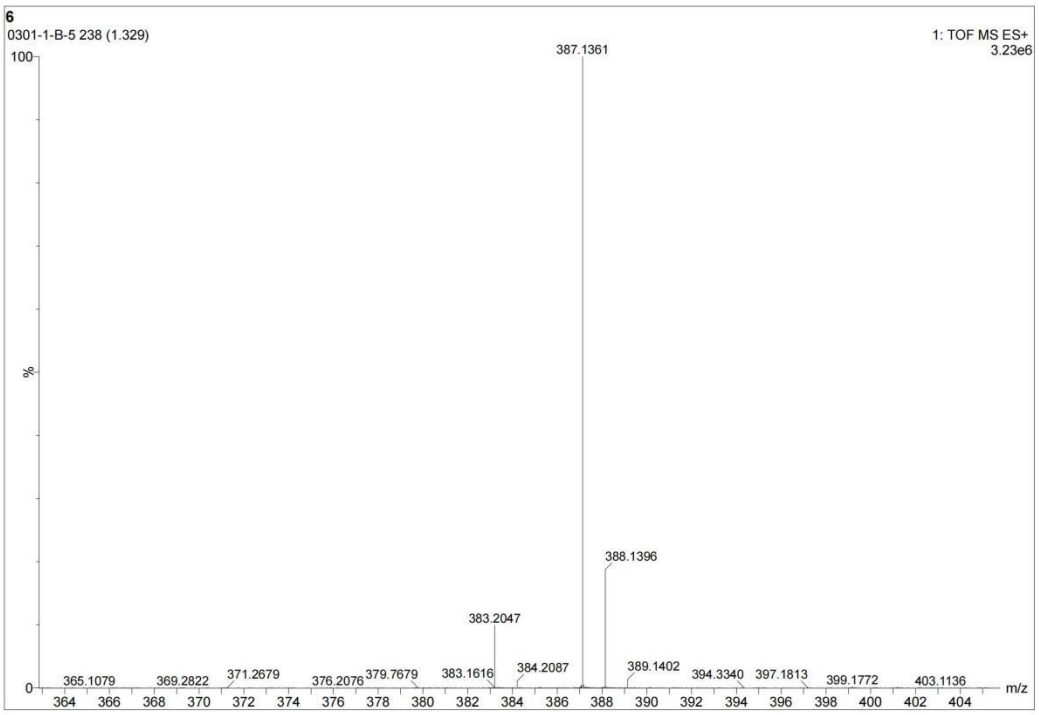

8.21
8.20
8.19
8.18
7.27
7.16
7.16
7.15
7.14
7.14
7.13
7.04
7.04
7.03
7.02
7.01
7.00
7.00
6.98
6.98
6.96
6.95
6.95
6.94
6.94
4.79
4.77
4.76
4.75
4.27
4.26
4.26
4.25
4.24
4.24
1.66
1.65
1.30
1.28
1.27
O
N
CH3
O
O
O
CH3
F
N
O
CH3
6.5E+08
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
0.98
1.95
2.03
1.91
1.00
1.97
2.97
3.00
2.89
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)

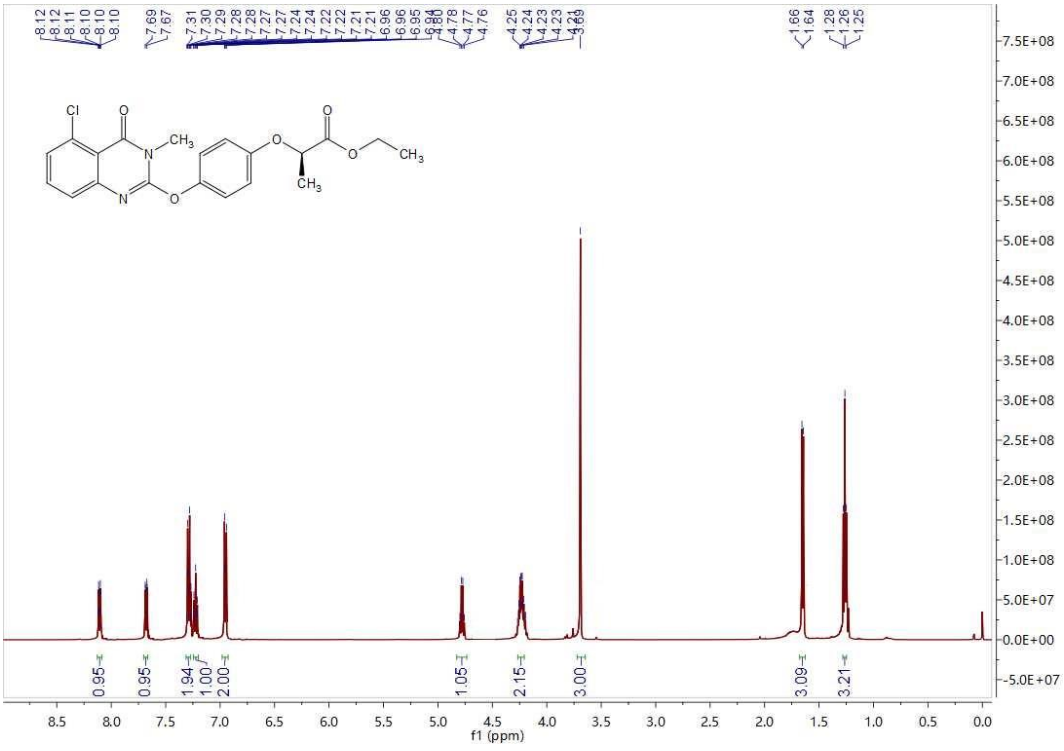

172.00
167.59
165.58
162.21
155.51
153.50
148.89
148.78
145.66
129.69
129.61
122.66
115.90
115.57
113.71
113.53
111.51
111.33
77.33
77.08
76.82
73.16
61.40
28.78
18.59
14.17
O
N
CH3
O
O
O
CH3
CH3
F
N
O
1.20E+09
1.10E+09
1.00E+09
9.00E+08
8.00E+08
7.00E+08
6.00E+08
5.00E+08
4.00E+08
3.00E+08
2.00E+08
1.00E+08
0.00E+00
-1.00E+08
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

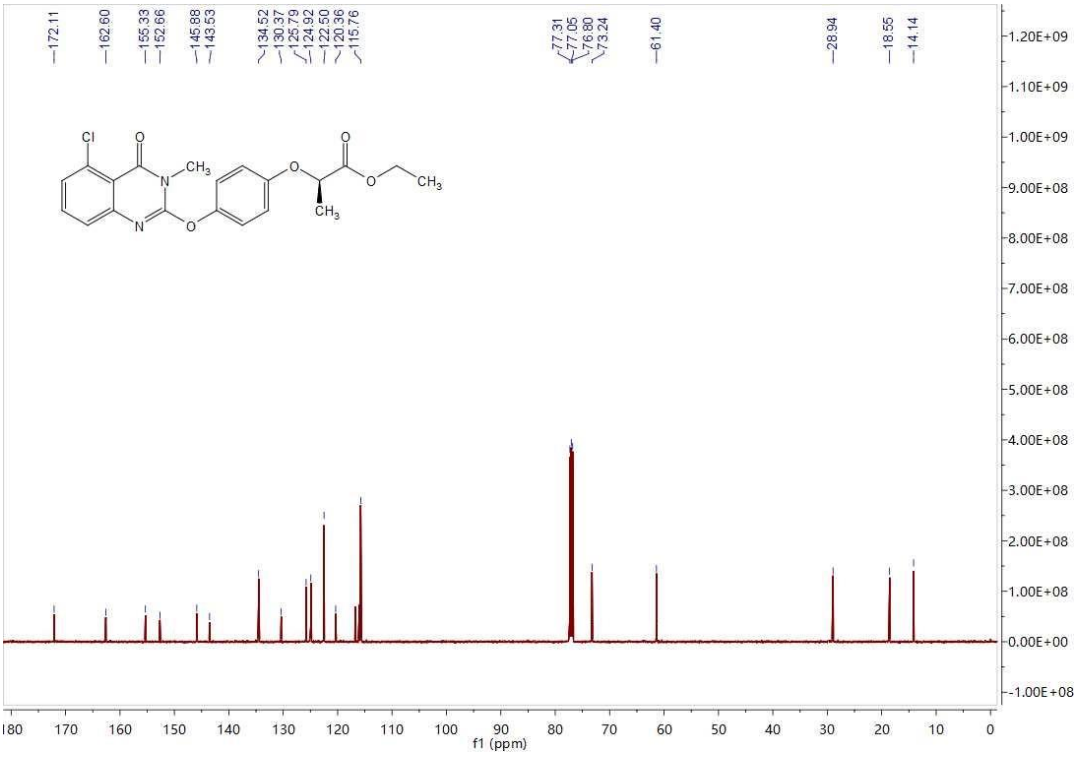

6
0301-1-B-4 287 (1.602)
1: TOF MS ES+
1.73e6
100
%
0
387.1365
388.1397
243.8855
269.0750
301.1427
338.3421
387.0836
389.1419
409.1157
425.0902
457.3503
485.0988
501.3604
514.8636
537.5291
240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540
m/z

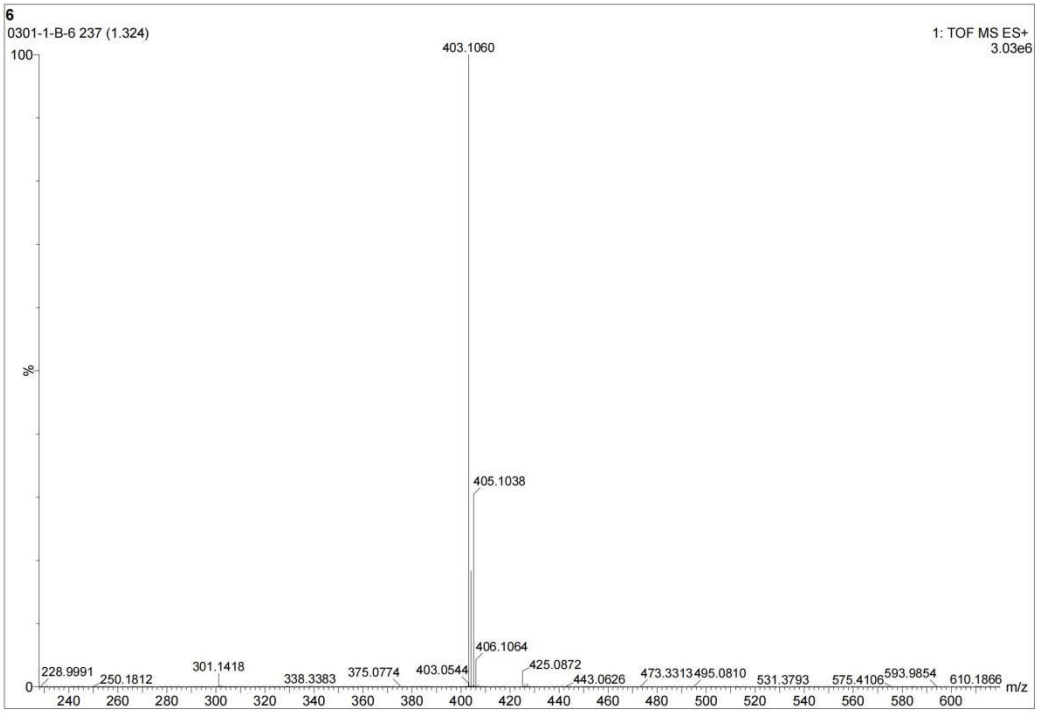

7.99
7.98
7.33
7.33
7.33
7.31
7.26
7.25
7.24
7.23
7.22
7.22
7.21
7.20
6.96
6.95
6.94
6.94
4.77
4.76
4.75
4.26
4.25
4.24
4.24
4.23
1.65
1.64
1.28
1.27
1.25
0.95
0.99
0.83
1.94
1.94
0.98
1.92
2.95
3.02
3.00
f1 (ppm)

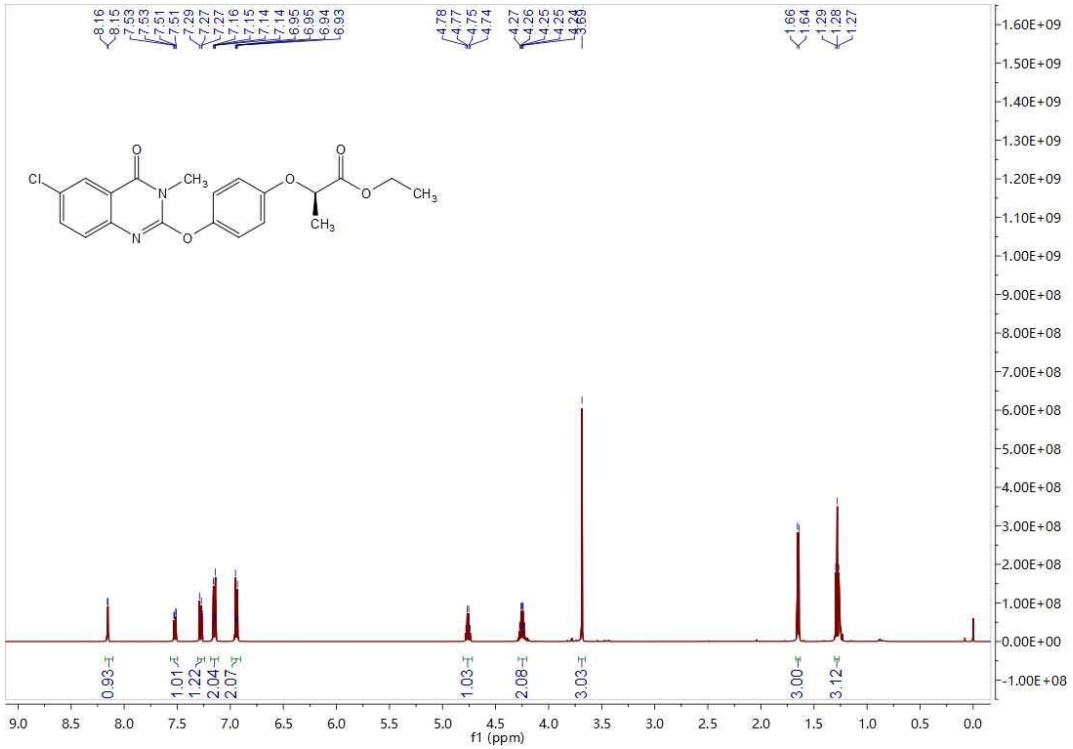

172.05
162.17
157.14
155.46
155.11
152.77
145.75
138.15
136.05
124.76
124.71
122.49
120.93
119.82
119.67
115.95
77.28
77.02
76.77
73.27
61.39
28.94
18.57
14.11
f1 (ppm)

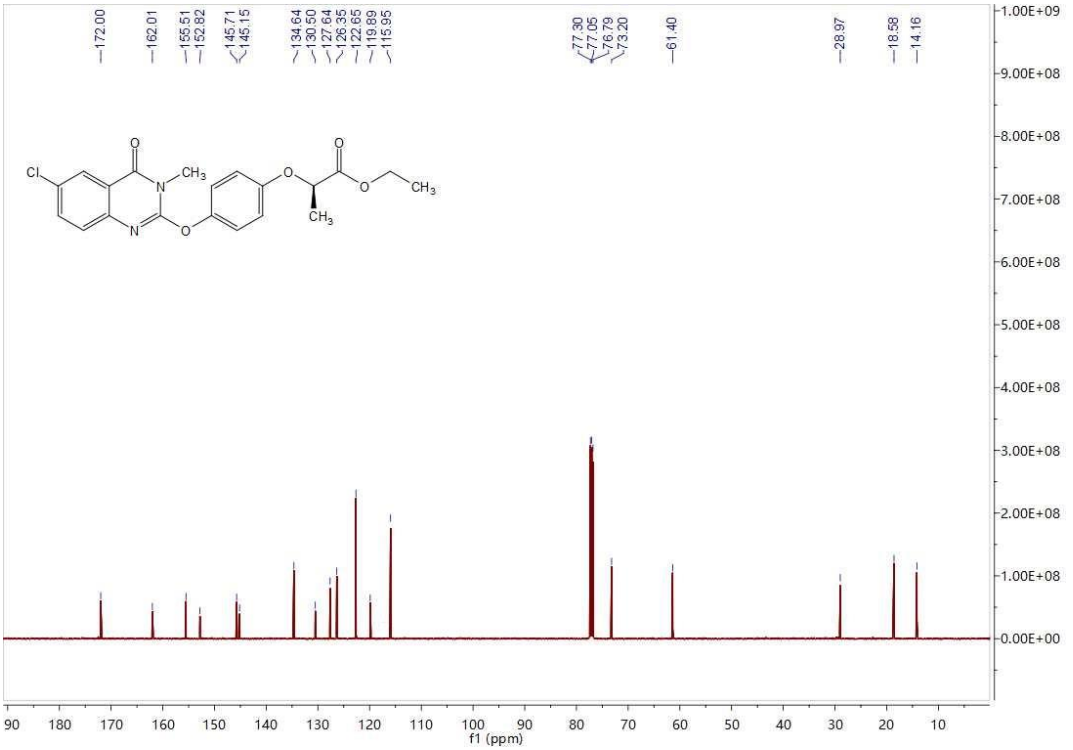

6
0301-1-B-5 238 (1.329)
1: TOF MS ES+
3.23e6
100
%
0
387.1361
388.1396
383.2047
365.1079
369.2822
371.2679
376.2076
379.7679
383.1616
384.2087
389.1402
394.3340
397.1813
399.1772
403.1136
m/z
364 366 368 370 372 374 376 378 380 382 384 386 388 390 392 394 396 398 400 402 404

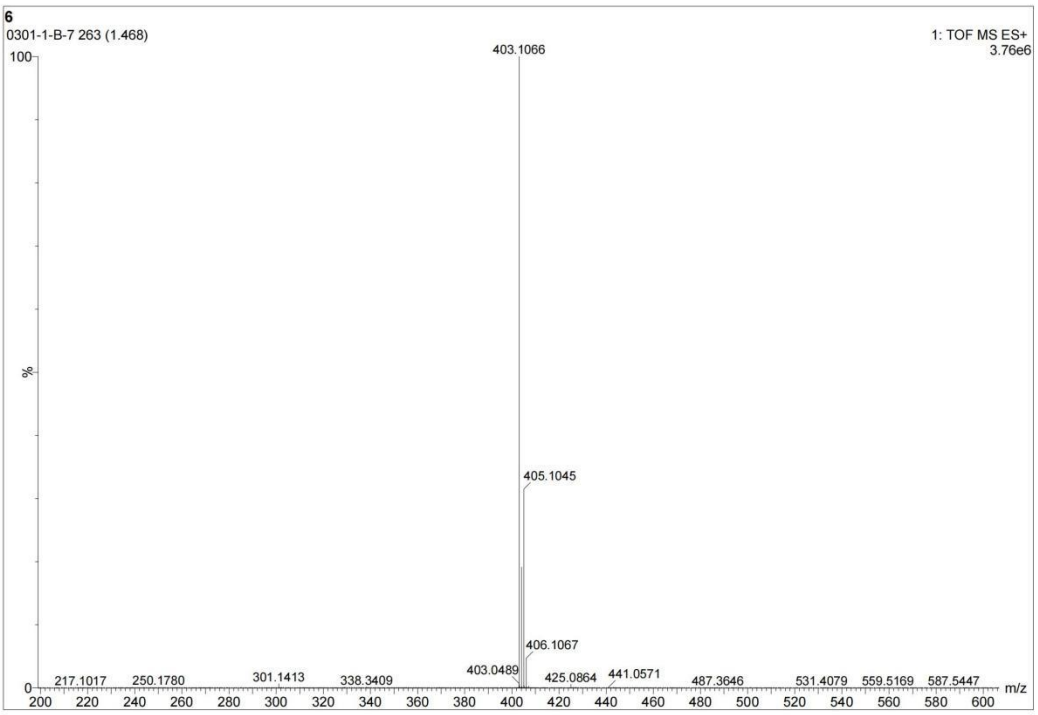

8.12 8.12 8.11 8.10 8.10 8.10
7.69 7.67
7.31 7.30 7.29 7.28 7.28 7.27 7.27 7.24 7.24 7.22 7.21 7.21 6.96 6.96 6.95
4.78 4.77 4.76
4.25 4.24 4.23 4.23
1.66 1.64
1.28 1.26 1.25
Cl
O
N
CH3
O
O
O
CH3
CH3
N
O
7.5E+08
7.0E+08
6.5E+08
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
0.95 0.95 1.94 1.00 2.00 1.05 2.15 3.00 3.09 3.21
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)

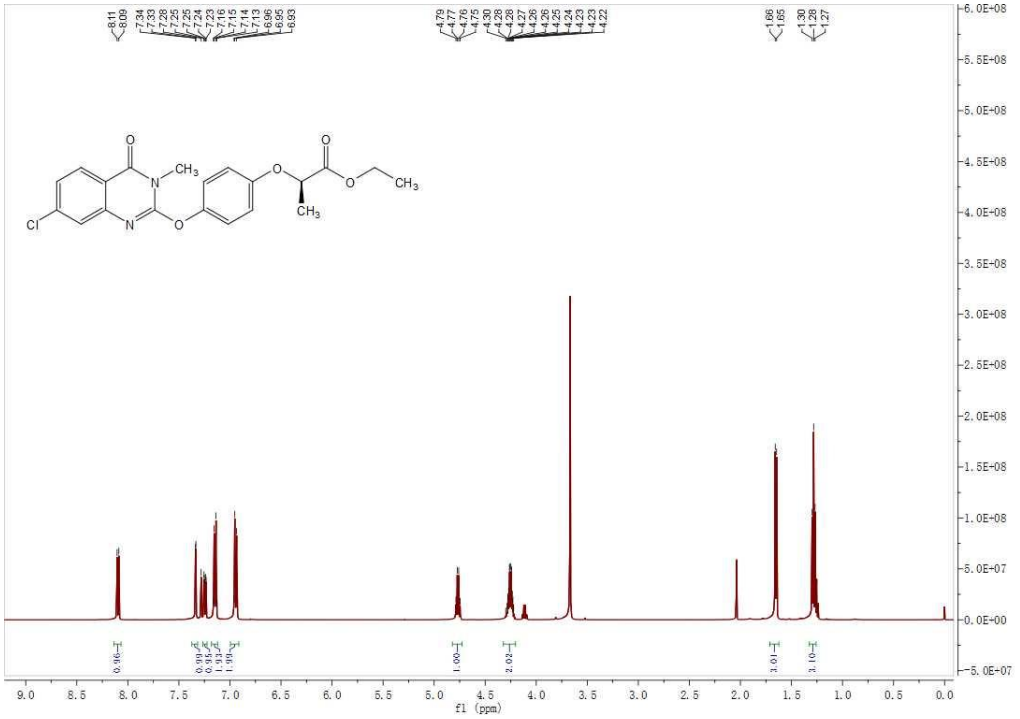

172.11
162.60
155.33
152.66
145.88
143.53
134.52
130.37
125.79
124.92
122.50
120.36
115.76
77.31
77.05
76.80
73.24
61.40
28.94
18.55
14.14
Cl
O
N
CH3
O
O
O
CH3
CH3
N
O
1.20E+09
1.10E+09
1.00E+09
9.00E+08
8.00E+08
7.00E+08
6.00E+08
5.00E+08
4.00E+08
3.00E+08
2.00E+08
1.00E+08
0.00E+00
-1.00E+08
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

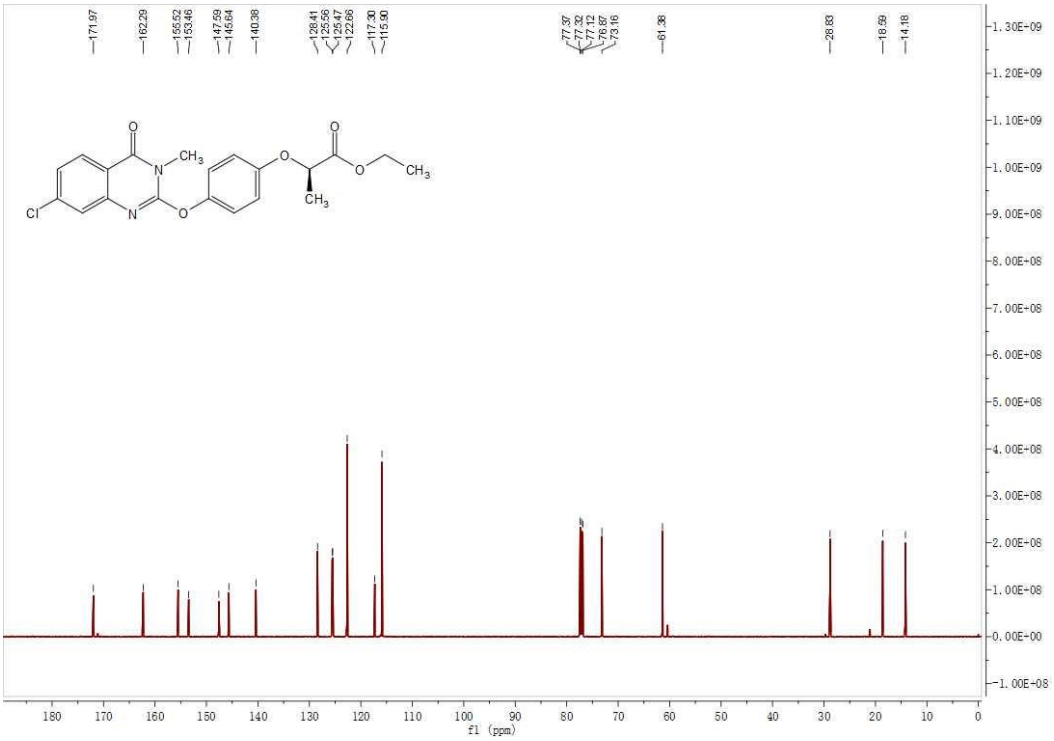

6
0301-1-B-6 237 (1.324)
1: TOF MS ES+
3.03e6
100
%
0
403.1060
405.1038
406.1064
425.0872
228.9991
250.1812
301.1418
338.3383
375.0774
403.0544
443.0626
473.3313
495.0810
531.3793
575.4106
593.9854
610.1866
240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600
m/z

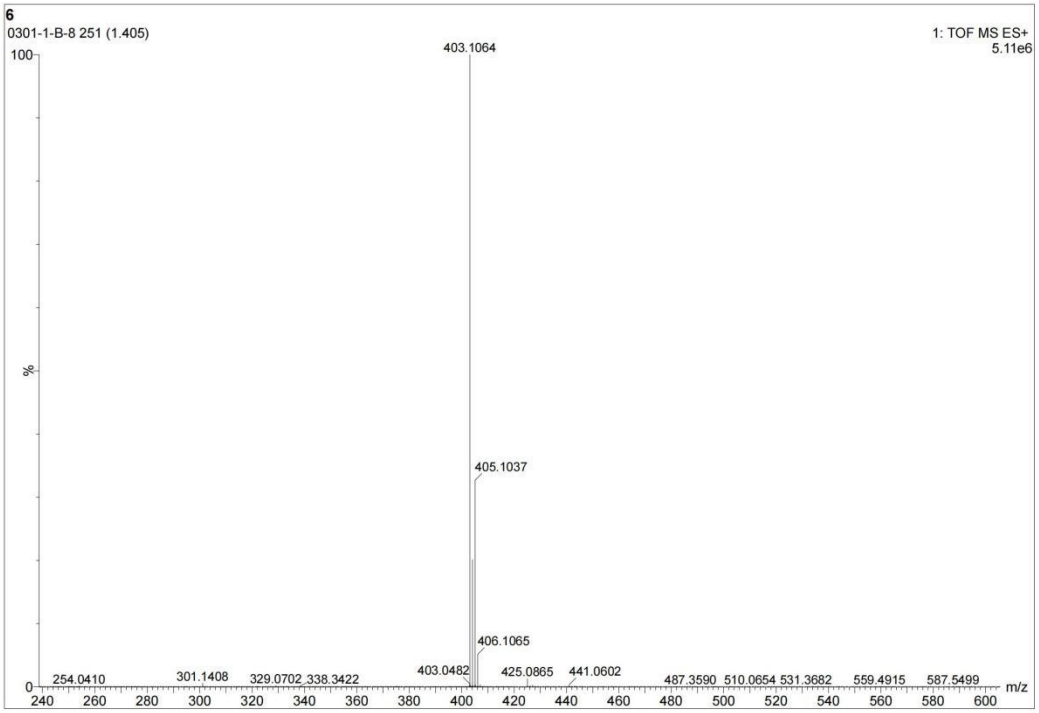

8.16
8.15
7.53
7.51
7.51
7.29
7.27
7.27
7.16
7.15
7.14
6.95
6.95
6.94
6.93
4.78
4.77
4.75
4.74
4.27
4.26
4.25
4.25
3.69
1.66
1.64
1.29
1.28
1.27
Cl
O
N
CH3
O
O
O
O
CH3
CH3
N
O
0.93
1.01
1.22
2.04
2.07
1.03
2.08
3.03
3.00
3.12
f1 (ppm)

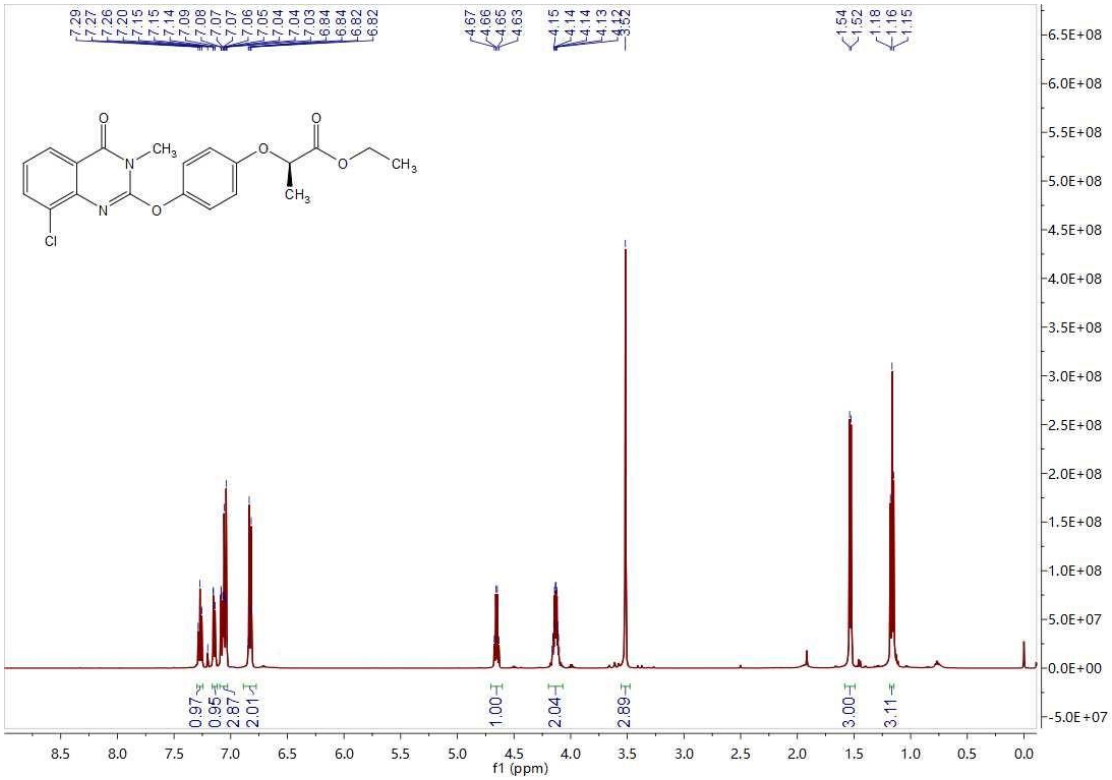

172.00
162.01
155.51
152.82
145.71
145.15
134.64
130.50
127.64
126.35
122.65
119.89
115.95
77.30
77.05
76.79
73.20
61.40
28.97
18.58
14.16
Cl
O
N
CH3
O
O
O
O
CH3
CH3
N
O
f1 (ppm)

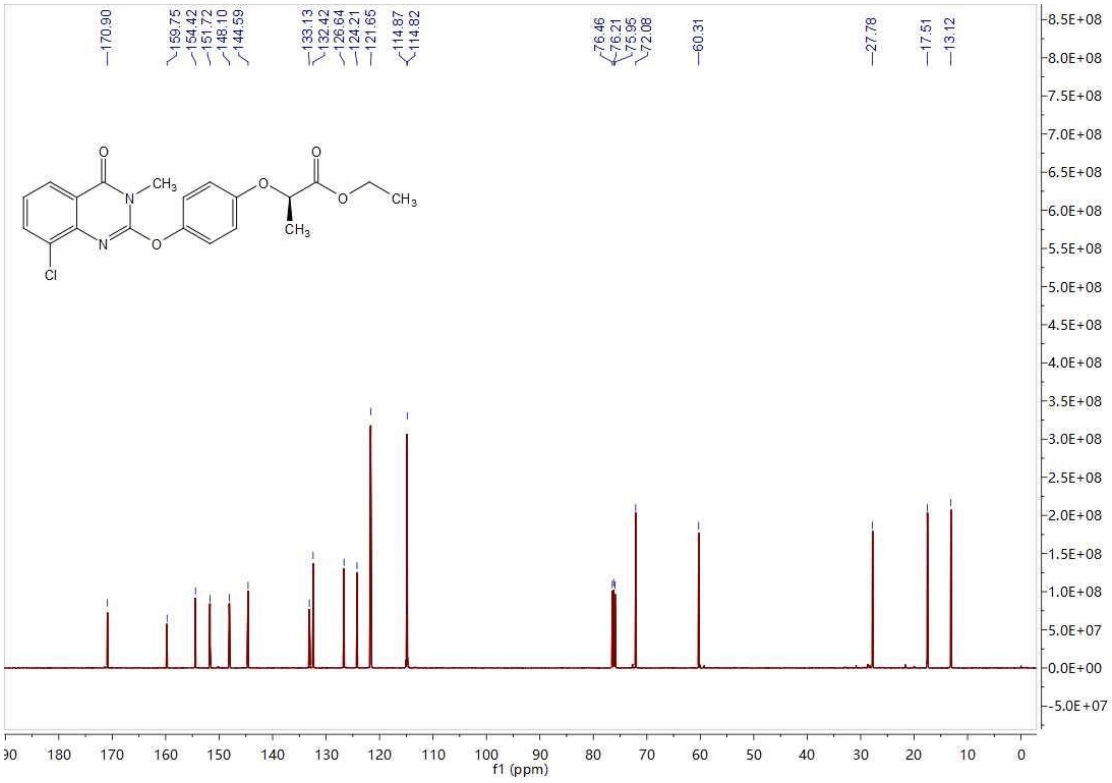

6
0301-1-B-7 263 (1.468)
1: TOF MS ES+
3.76e6
100
%
0
403.1066
405.1045
406.1067
403.0489
217.1017
250.1780
301.1413
338.3409
425.0864
441.0571
487.3646
531.4079
559.5169
587.5447
m/z
200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600

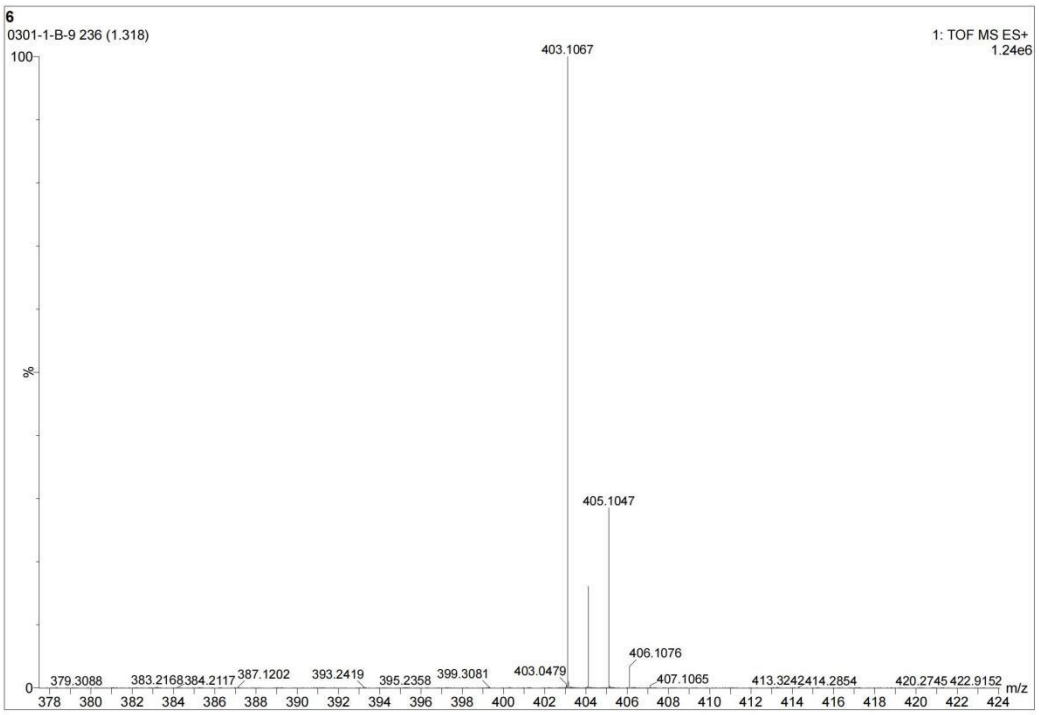

8.11
8.09
7.34
7.33
7.28
7.25
7.25
7.24
7.23
7.16
7.15
7.14
7.13
6.96
6.95
6.93
4.79
4.77
4.76
4.75
4.30
4.28
4.28
4.27
4.26
4.26
4.25
4.24
4.23
4.23
4.22
1.66
1.65
1.30
1.29
1.27
O
N
CH3
Cl
O
O
O
CH3
CH3
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E-07
0.96
0.99
0.95
1.93
1.99
1.00
2.02
3.01
3.10
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)

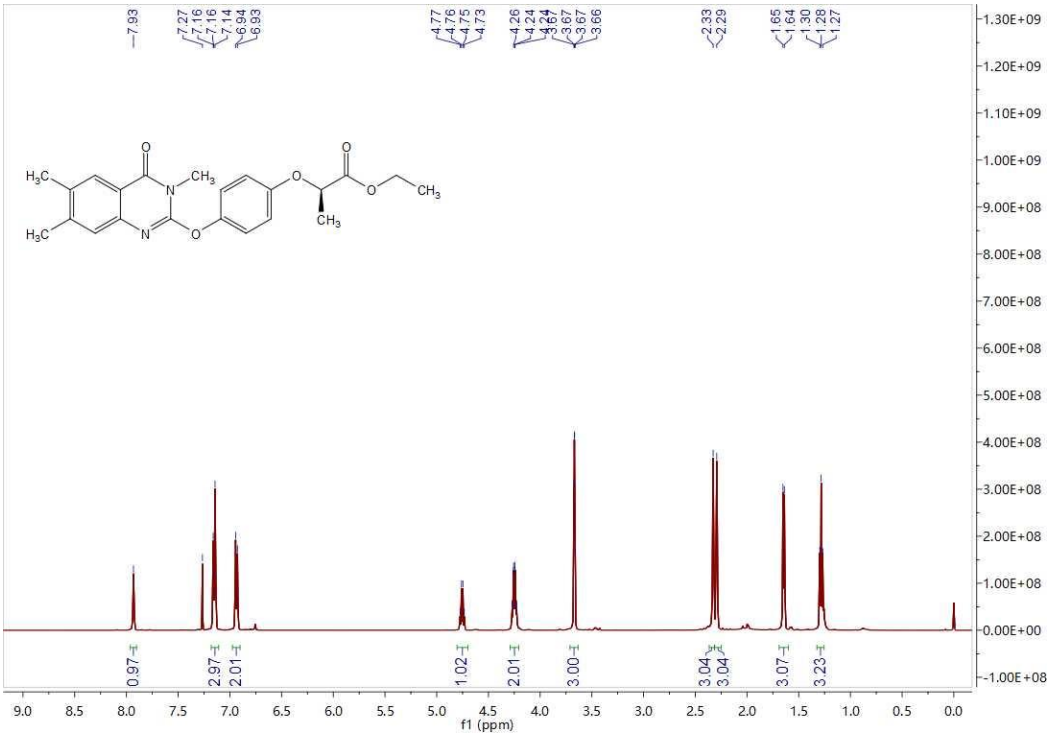

171.97
162.29
155.52
153.46
147.59
145.64
140.38
128.41
125.56
123.47
122.66
117.30
115.90
77.37
77.32
77.12
76.87
73.16
61.38
28.83
18.59
14.18
f1 (ppm)

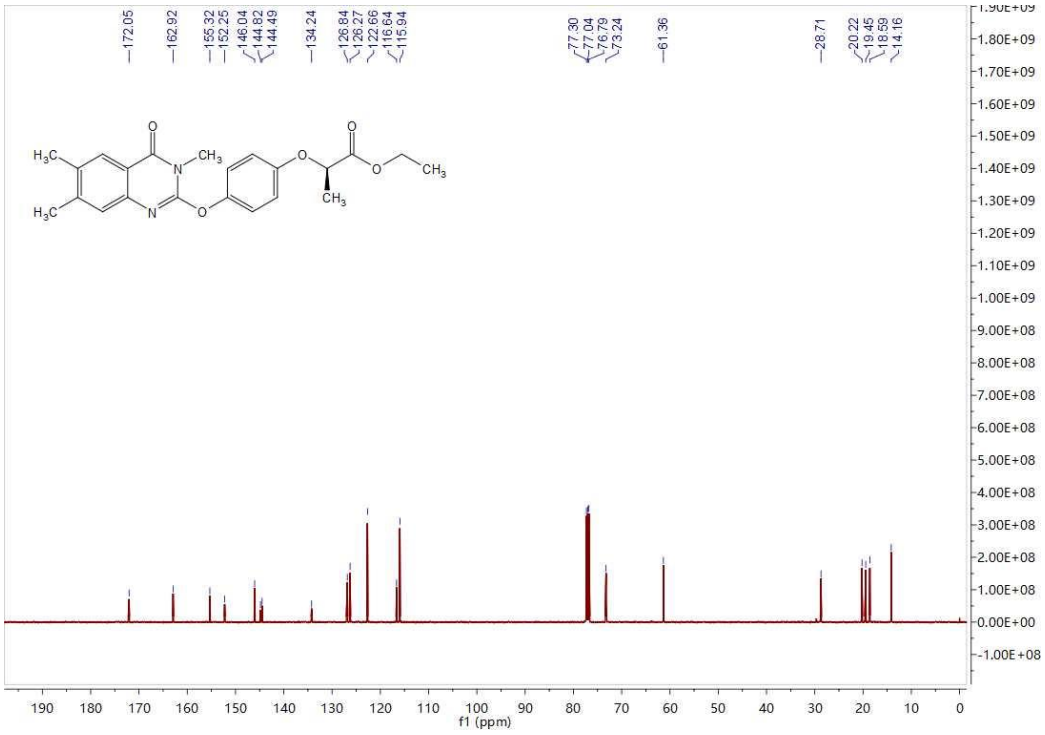

6
0301-1-B-8 251 (1.405)
1: TOF MS ES+
5.11e6
403.1064
405.1037
406.1065
254.0410
301.1408
329.0702
338.3422
403.0482
425.0865
441.0602
487.3590
510.0654
531.3682
559.4915
587.5499
%
m/z

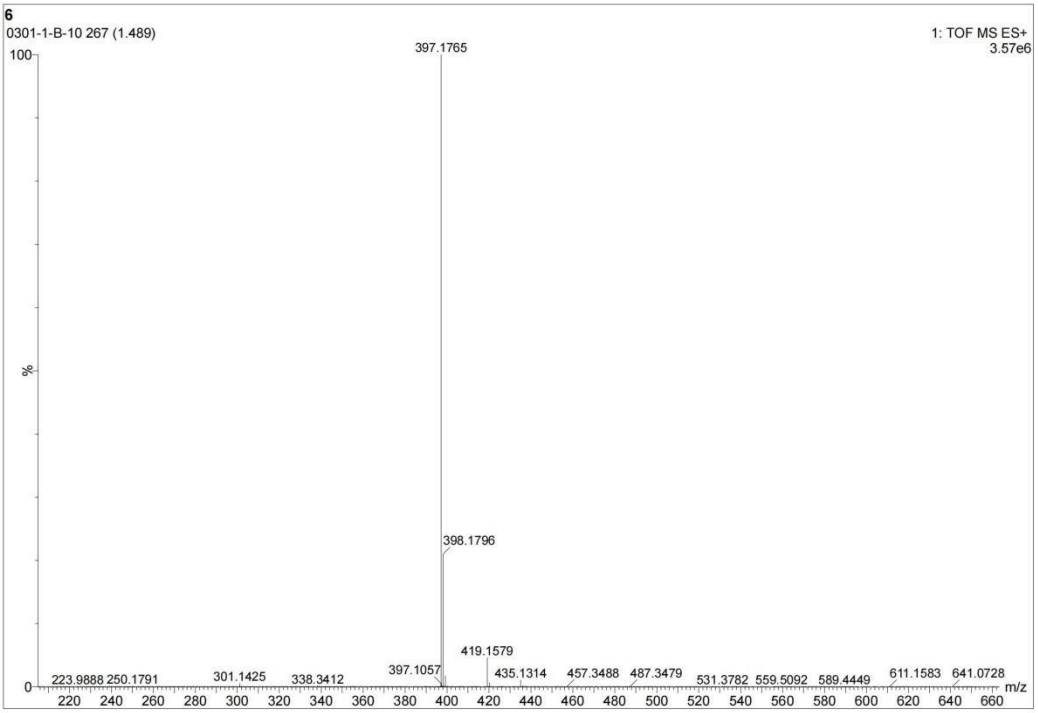

7.29
7.27
7.26
7.20
7.15
7.15
7.14
7.09
7.08
7.07
7.07
7.06
7.05
7.04
7.04
7.03
6.84
6.84
6.82
6.82
4.67
4.66
4.65
4.63
4.15
4.14
4.14
4.13
4.12
3.52
1.54
1.52
1.18
1.16
1.15
O
N
CH3
O
O
O
CH3
CH3
N
O
Cl
0.97
0.95
2.87
2.01
1.00
2.04
2.89
3.00
3.11
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
6.5E+08
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07

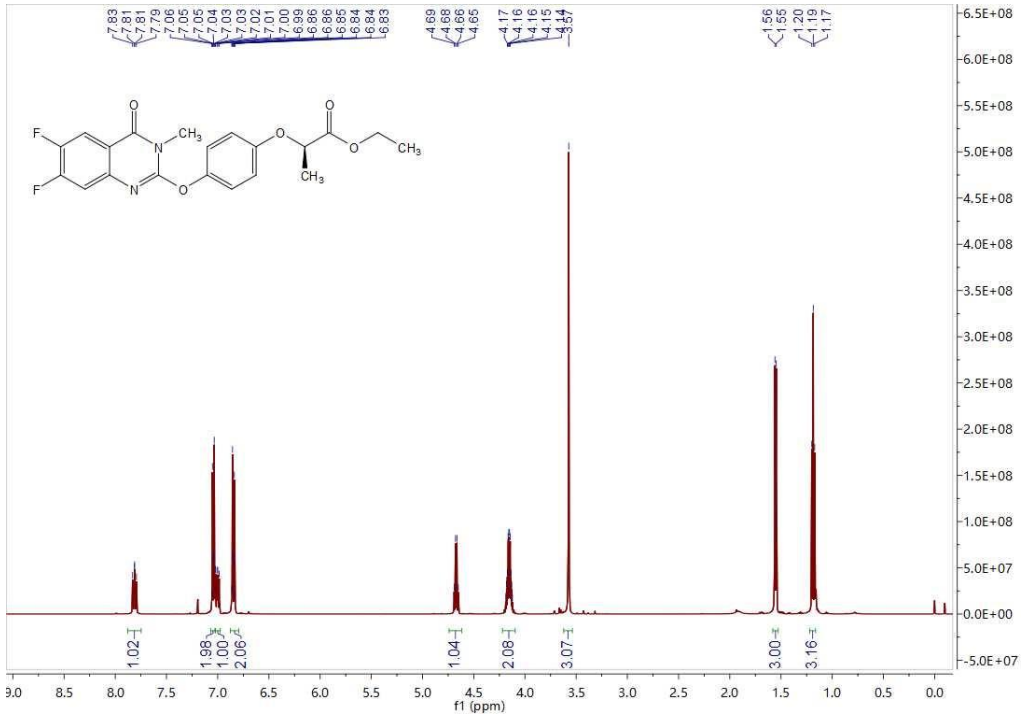

170.90
159.75
154.42
151.72
148.10
144.59
133.13
132.42
126.64
124.21
121.65
114.87
114.82
76.46
76.21
75.95
72.08
60.31
27.78
17.51
13.12
O
N
CH3
O
O
O
CH3
CH3
N
O
Cl
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
8.5E+08
8.0E+08
7.5E+08
7.0E+08
6.5E+08
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07

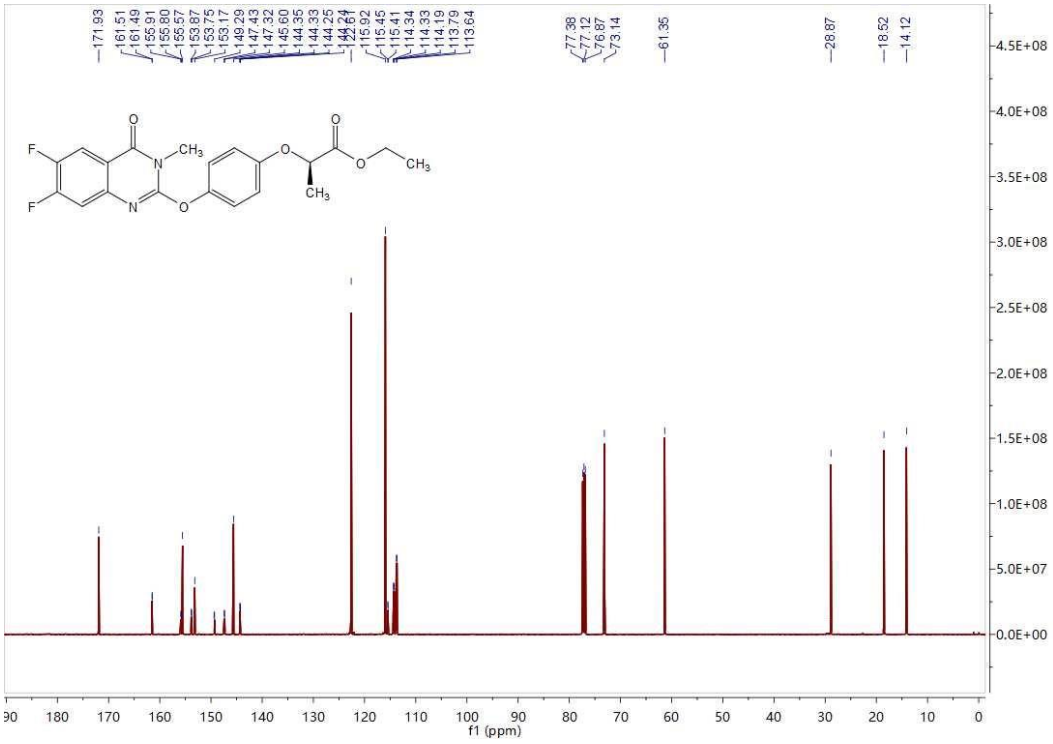

6
0301-1-B-9 236 (1.318)
1: TOF MS ES+
1.24e6
100
%
0
403.1067
405.1047
406.1076
379.3088
383.2168
384.2117
387.1202
393.2419
395.2358
399.3081
403.0479
407.1065
413.3242
414.2854
420.2745
422.9152
m/z
378 380 382 384 386 388 390 392 394 396 398 400 402 404 406 408 410 412 414 416 418 420 422 424

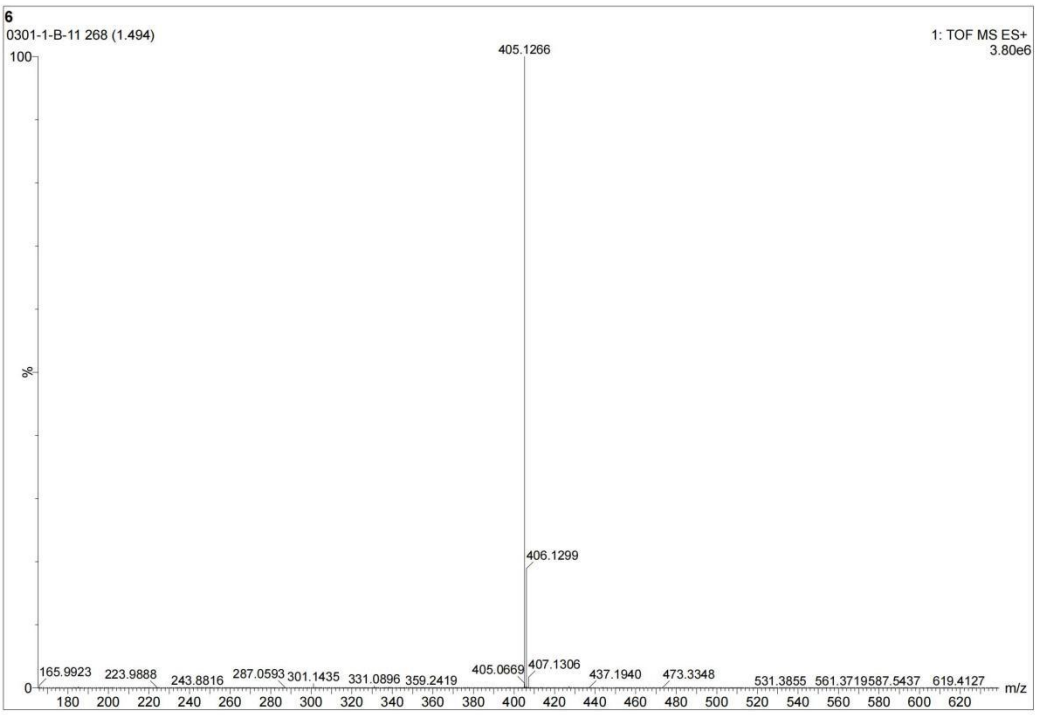

7.93
7.27
7.16
7.16
7.14
6.94
6.93
4.77
4.76
4.75
4.73
4.26
4.24
4.24
3.67
3.67
3.67
3.66
2.33
2.29
1.65
1.64
1.30
1.28
1.27
H3C
CH3
N
O
O
O
O
CH3
CH3
H3C
1.30E+09
1.20E+09
1.10E+09
1.00E+09
9.00E+08
8.00E+08
7.00E+08
6.00E+08
5.00E+08
4.00E+08
3.00E+08
2.00E+08
1.00E+08
0.00E+00
-1.00E+08
0.97
2.97
2.01
1.02
2.01
3.00
3.04
3.04
3.07
3.23
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)

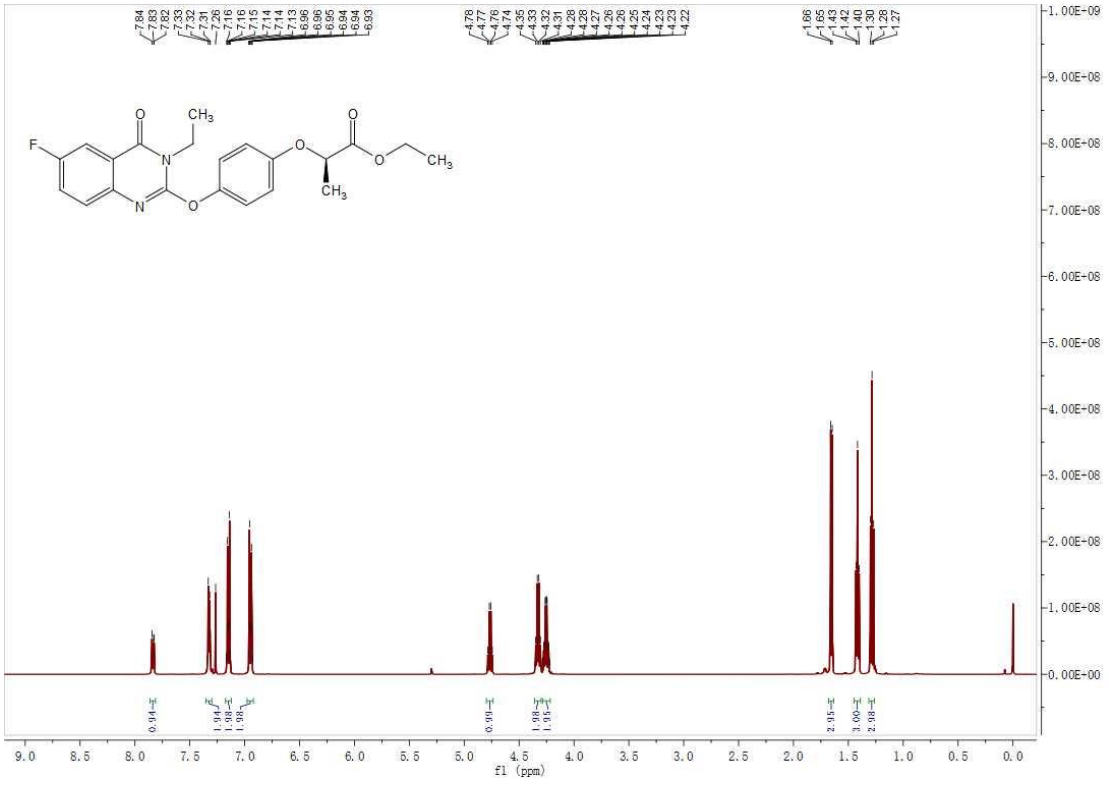

172.05
162.92
155.32
152.25
146.04
144.82
144.49
134.24
126.84
126.27
122.66
116.64
115.94
77.30
77.04
76.79
73.24
61.36
28.71
20.22
19.45
18.59
14.16
f1 (ppm)

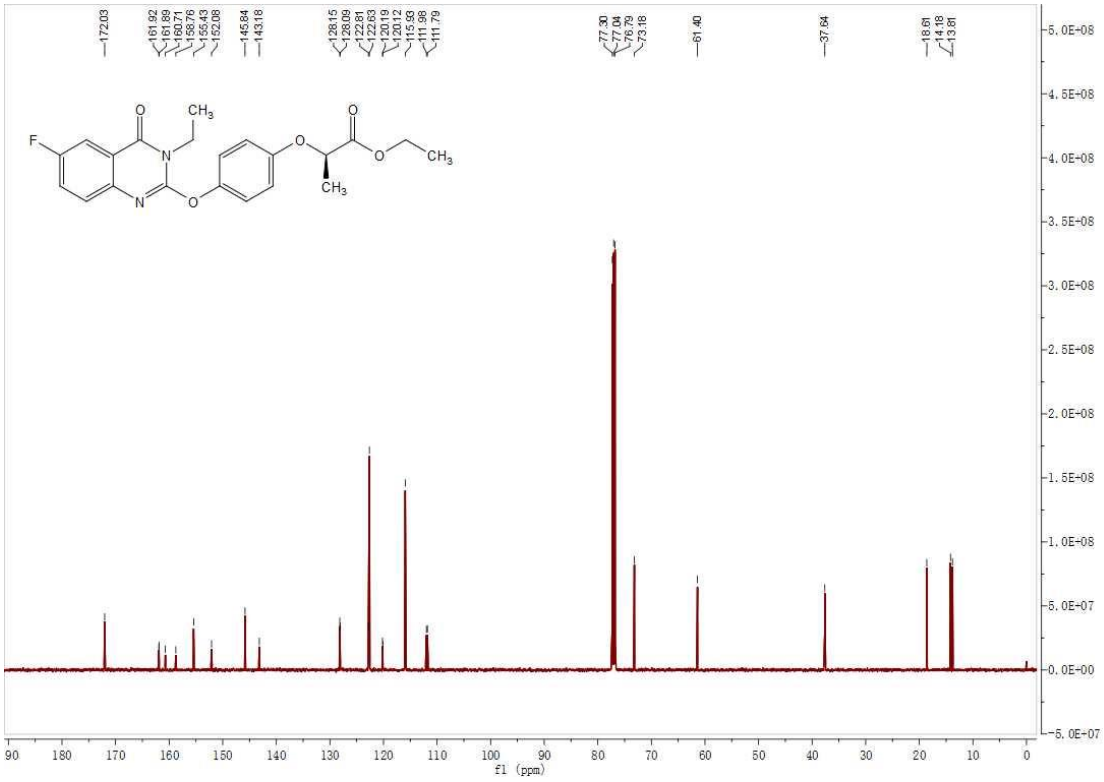

6
0301-1-B-10 267 (1.489)
1: TOF MS ES+
3.57e6
397.1765
398.1796
419.1579
%
m/z

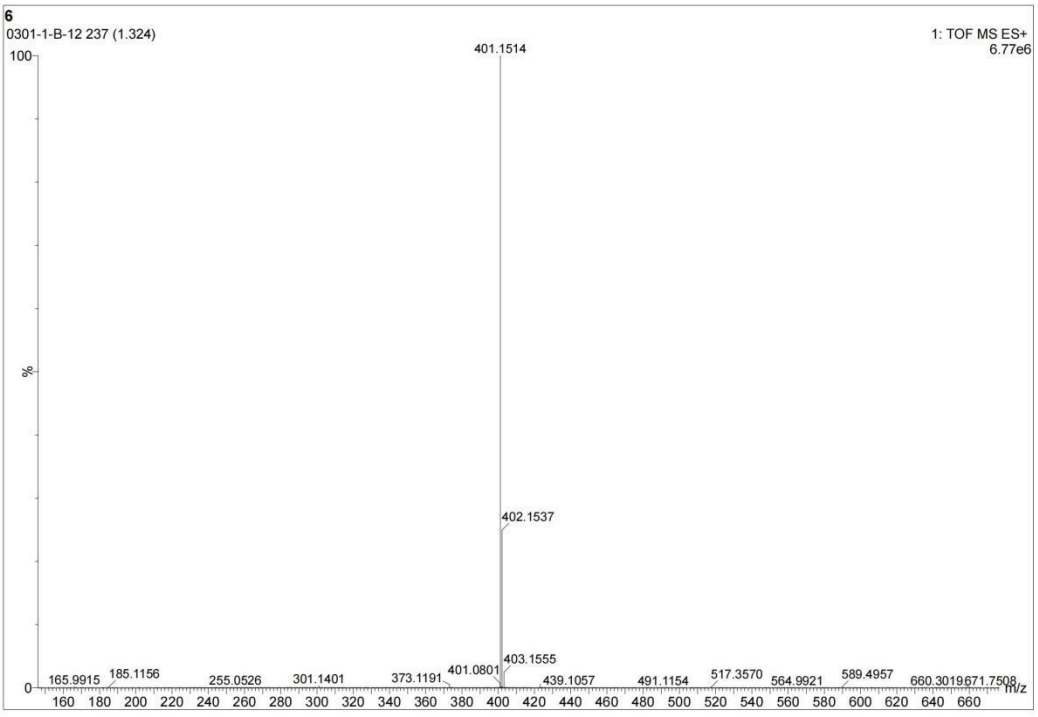

7.83
7.81
7.81
7.79
7.06
7.05
7.05
7.04
7.03
7.03
7.02
7.01
7.00
6.99
6.86
6.86
6.85
6.84
6.84
6.83
4.69
4.68
4.66
4.65
4.17
4.16
4.16
4.15
4.15
3.54
1.56
1.55
1.20
1.19
1.17
F
F
O
N
CH3
O
O
O
CH3
CH3
N
O
1.02
1.98
1.00
2.06
1.04
2.08
3.07
3.00
3.16
6.5E+08
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
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)

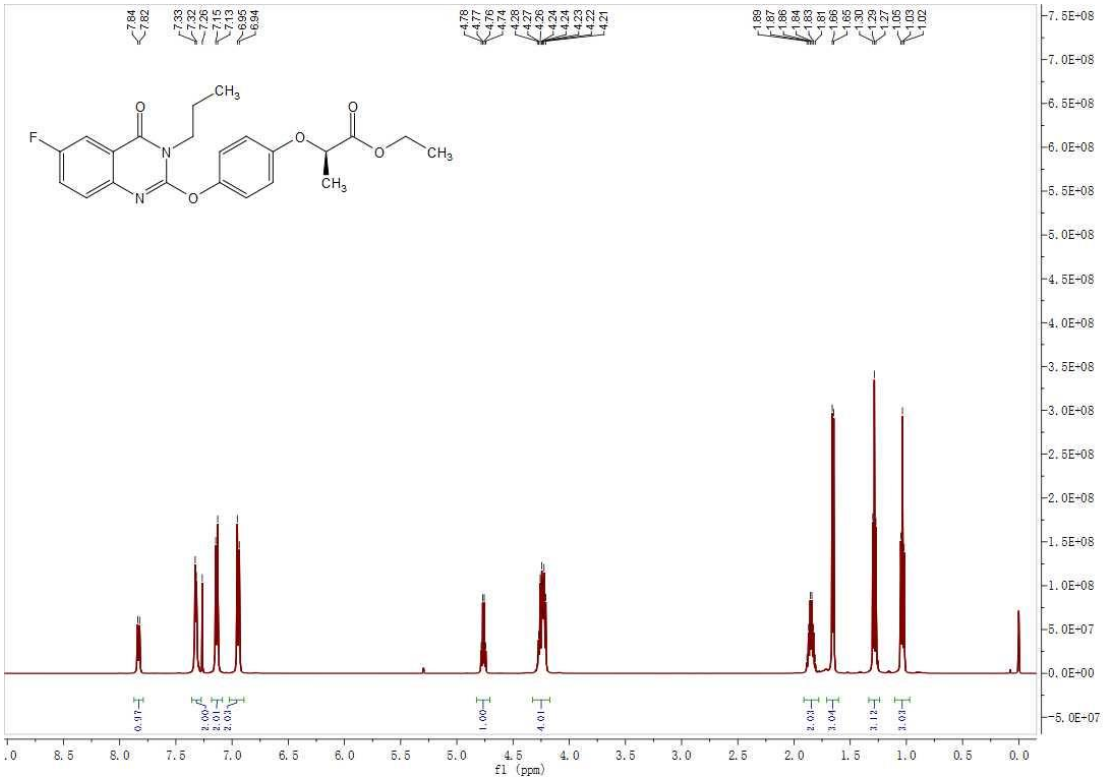

171.93
161.51
161.49
155.91
155.80
155.57
153.87
153.75
153.17
149.29
147.43
147.32
145.60
144.35
144.33
144.25
115.92
115.45
115.41
114.34
114.33
114.19
113.79
113.64
77.38
77.12
76.87
73.14
61.35
28.87
18.52
14.12
F
F
O
N
CH3
O
O
O
CH3
CH3
N
O
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

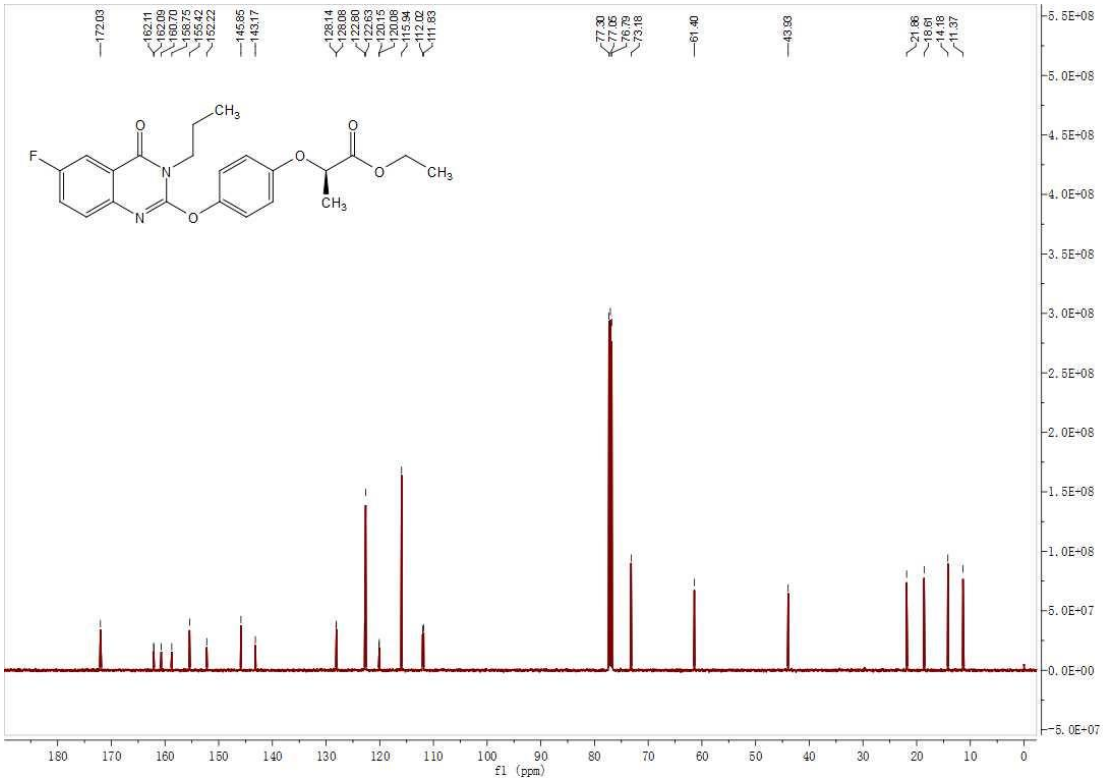

6
0301-1-B-11 268 (1.494)
1: TOF MS ES+
3.80e6
100
%
0
405.1266
406.1299
407.1306
165.9923
223.9888
243.8816
287.0593
301.1435
331.0896
359.2419
405.0669
437.1940
473.3348
531.3855
561.3719
587.5437
619.4127
m/z

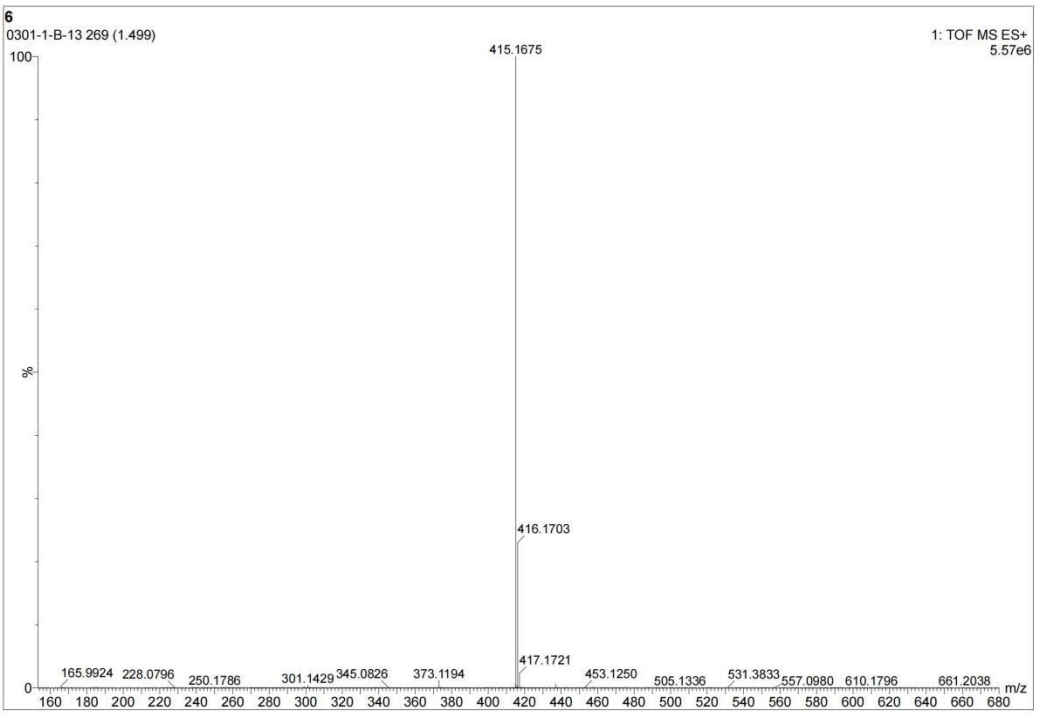

F
O
N
CH3
O
O
O
CH3
CH3
f1 (ppm)

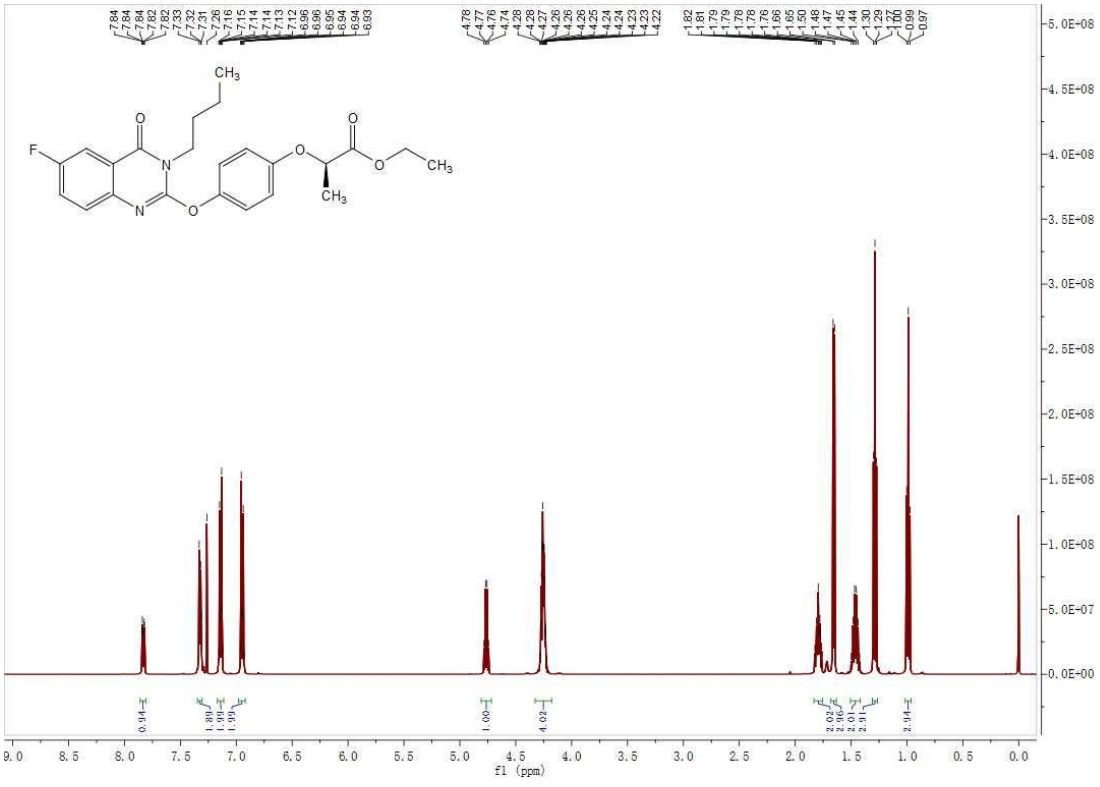

172.03
161.92
161.89
160.71
158.76
155.43
152.08
145.84
143.18
128.15
128.09
122.81
122.63
120.19
120.12
115.83
111.98
111.79
77.30
77.04
76.79
73.18
61.40
37.64
18.61
14.18
13.81
F
O
N
O
CH3
O
O
O
CH3
CH3
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
f1 (ppm)

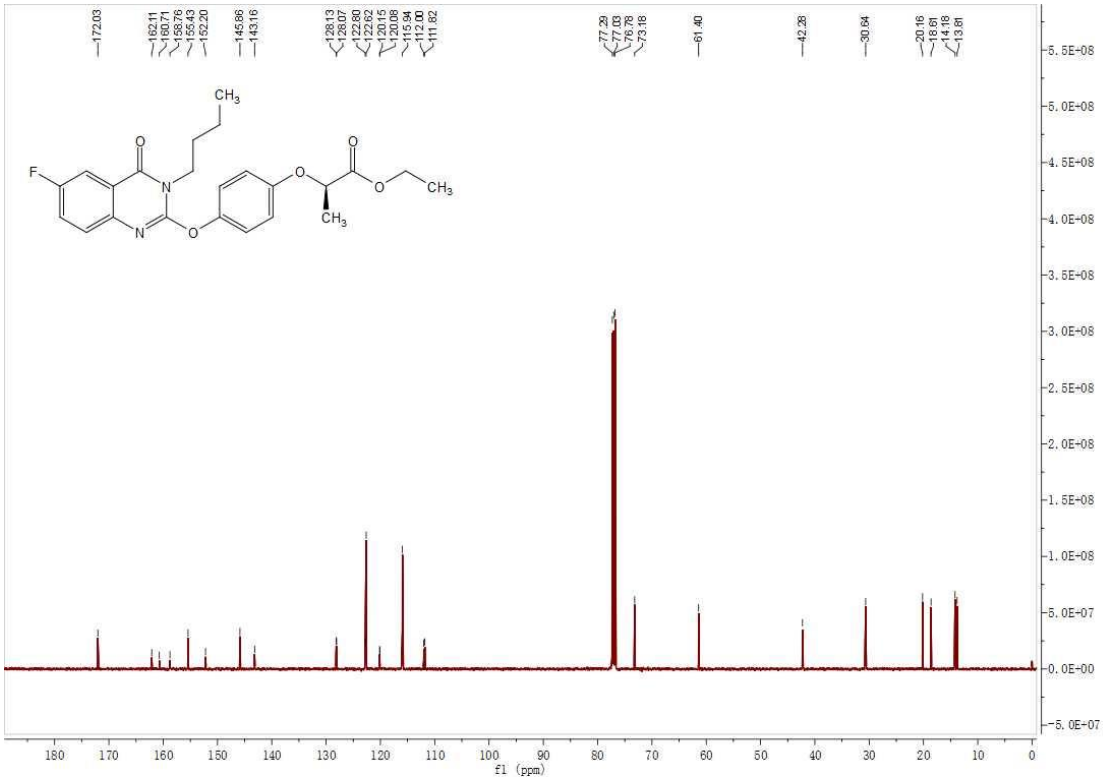

6
0301-1-B-12 237 (1.324)
1: TOF MS ES+
6.77e6
100
%
0
401.1514
402.1537
403.1555
165.9915
185.1156
255.0526
301.1401
373.1191
401.0801
439.1057
491.1154
517.3570
564.9921
589.4957
660.3019
671.7508
m/z

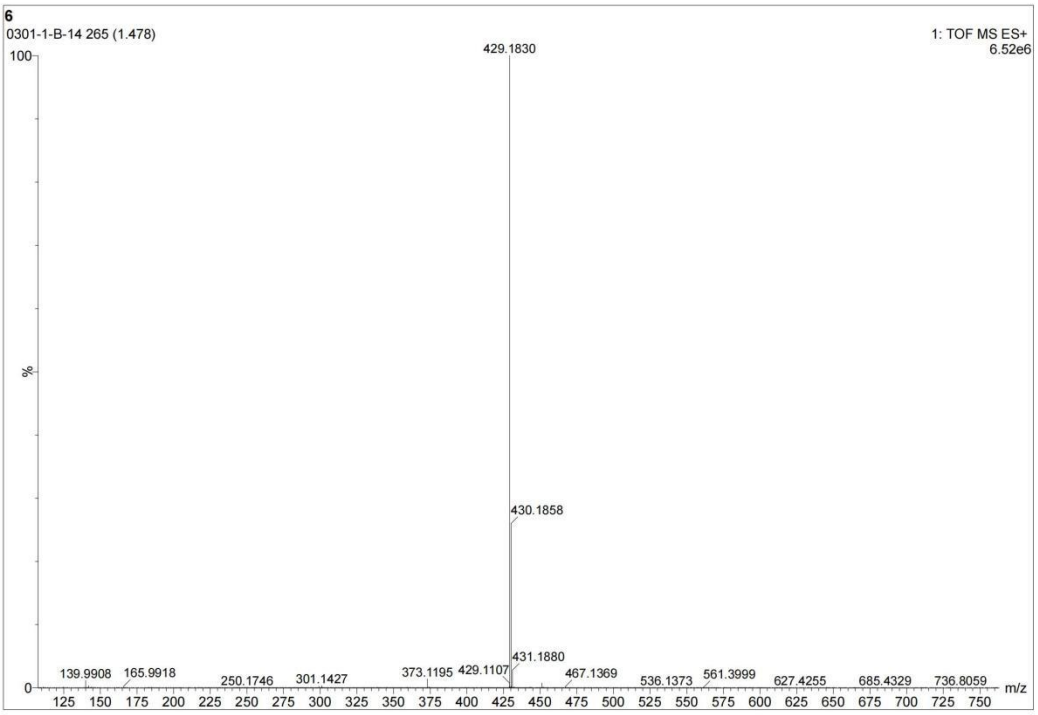

7.84
7.82
7.33
7.32
7.26
7.15
7.13
6.95
6.94
4.78
4.77
4.76
4.74
4.28
4.27
4.26
4.24
4.24
4.23
4.22
4.21
1.89
1.87
1.86
1.84
1.83
1.81
1.66
1.65
1.30
1.29
1.27
1.05
1.03
1.02
CH3
O
F
N
O
O
O
CH3
CH3
0.97
2.00
2.01
2.03
1.00
4.01
2.03
3.04
3.12
3.03
f1 (ppm)

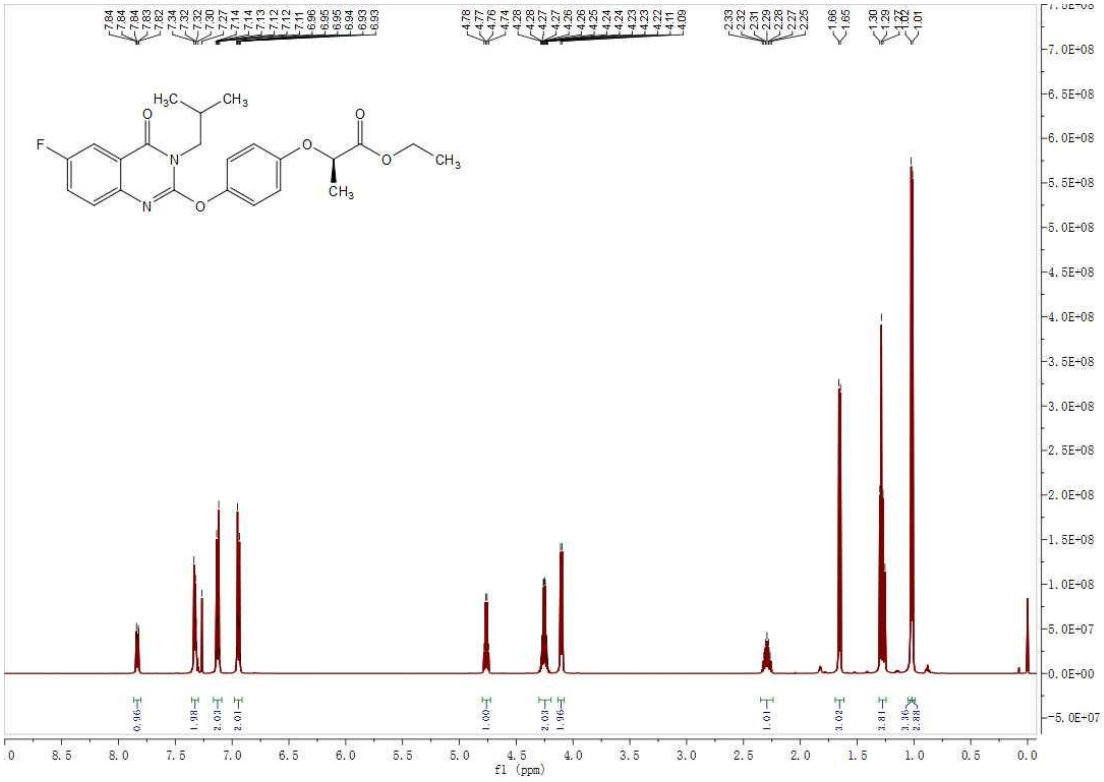

172.03
162.11
162.09
160.70
158.75
155.42
152.22
145.65
143.17
128.14
128.08
122.80
122.63
120.15
120.08
115.94
112.02
111.83
77.30
77.05
76.79
73.18
61.40
43.93
21.86
18.61
14.18
11.37
CH3
O
F
N
O
O
O
CH3
CH3
f1 (ppm)

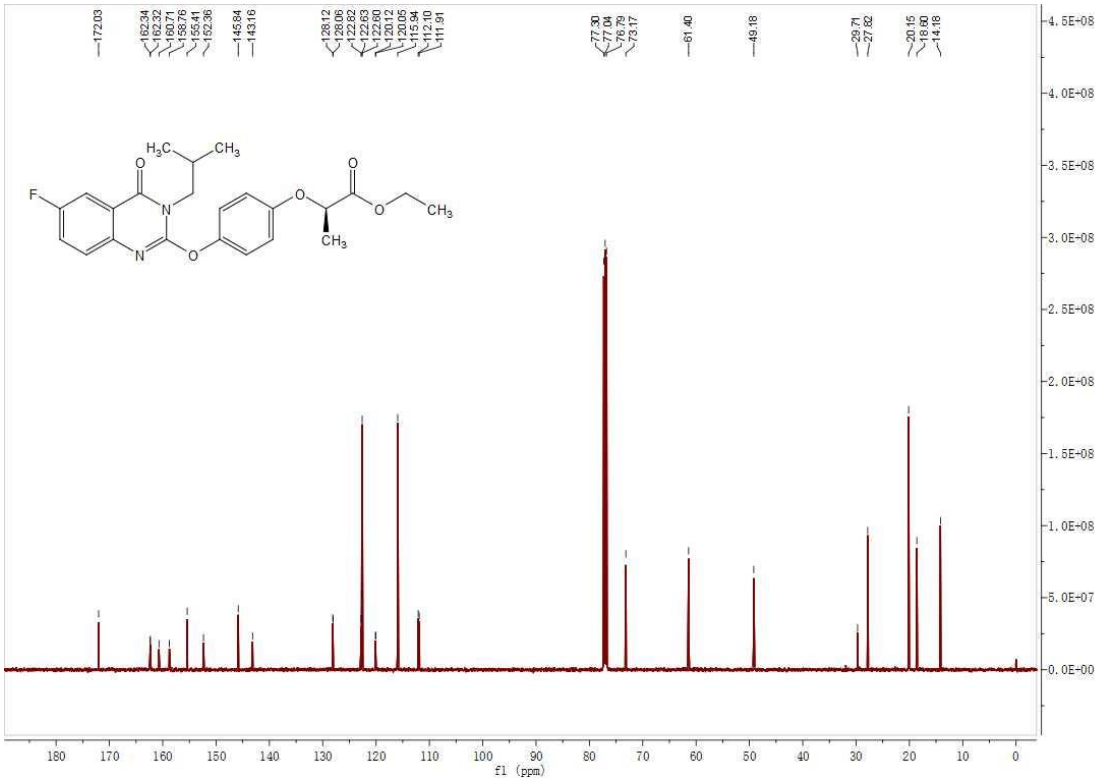

6
0301-1-B-13 269 (1.499)
1: TOF MS ES+
5.57e6
100
%
0
415.1675
416.1703
417.1721
165.9924
228.0796
250.1786
301.1429
345.0826
373.1194
453.1250
505.1336
531.3833
557.0980
610.1796
661.2038
m/z
160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600 620 640 660 680

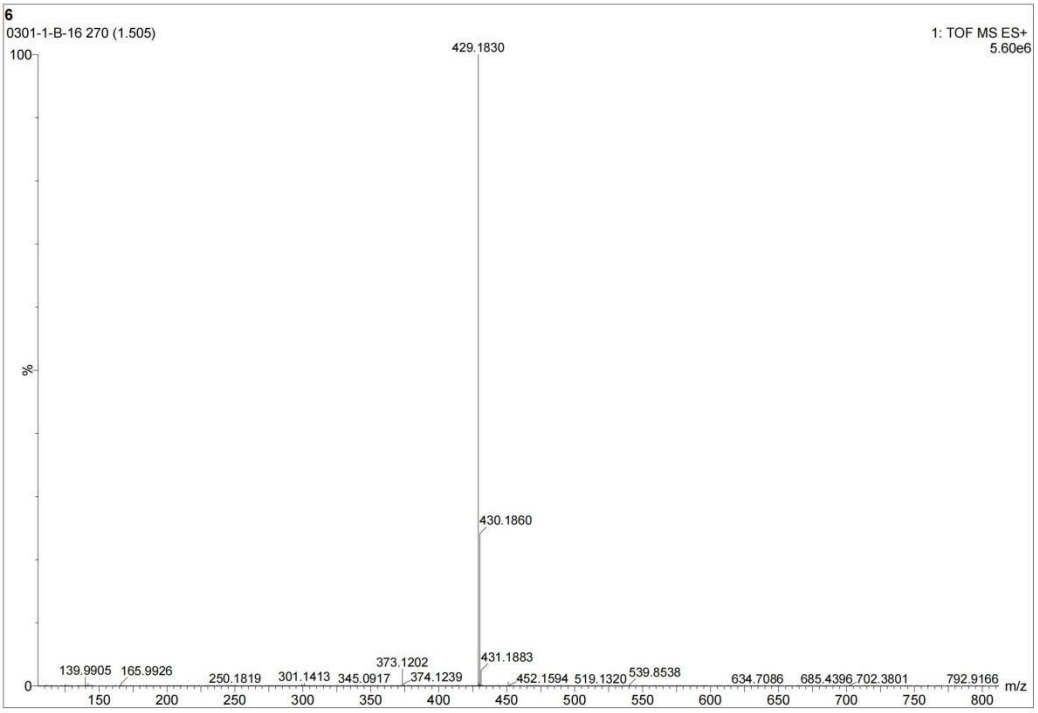

F
O
N
N
O
O
O
O
CH3
CH3
CH3
5.0E-08
4.5E-08
4.0E-08
3.5E-08
3.0E-08
2.5E-08
2.0E-08
1.5E-08
1.0E-08
5.0E-07
0.0E+00
0.94
1.89
1.99
1.99
1.00
4.02
2.02
2.06
2.01
2.91
2.94
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

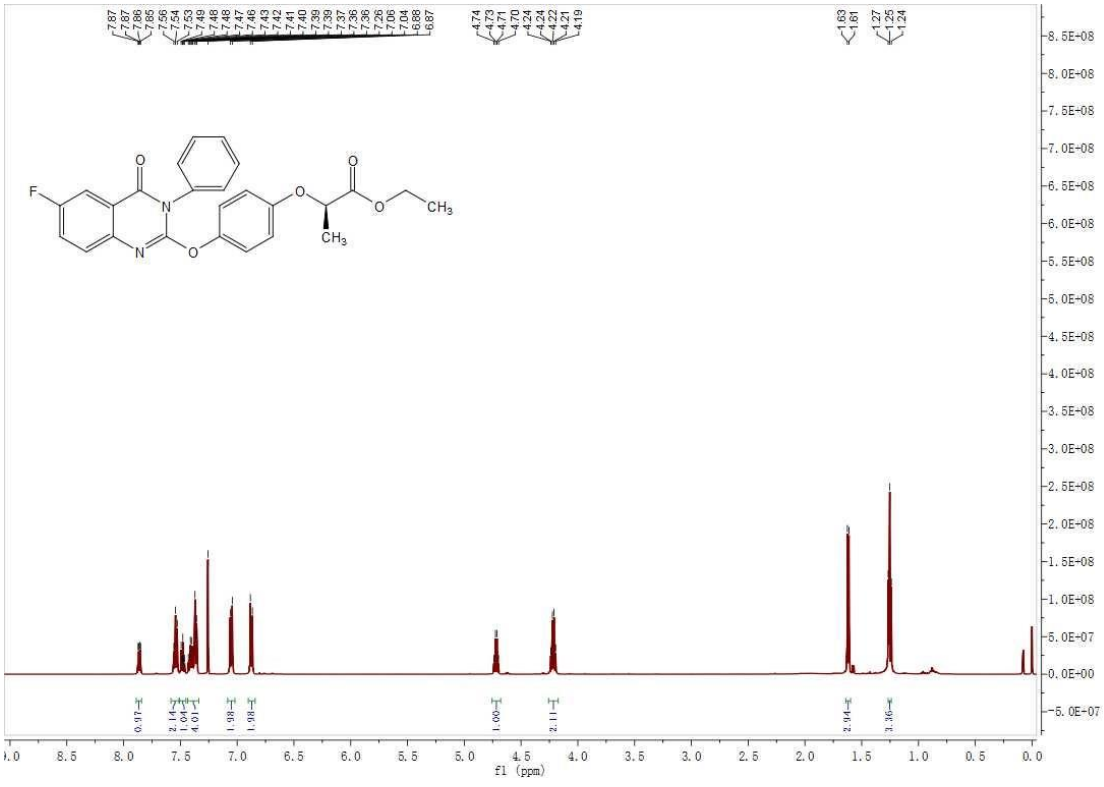

172.03
162.11
160.71
158.76
155.43
152.20
145.86
143.16
128.13
128.07
122.80
122.62
120.15
120.08
115.94
112.06
111.82
77.29
77.00
76.78
73.18
61.40
42.28
30.64
20.16
18.61
14.18
13.81
F
O
N
O
O
O
O
CH3
CH3
CH3
f1 (ppm)

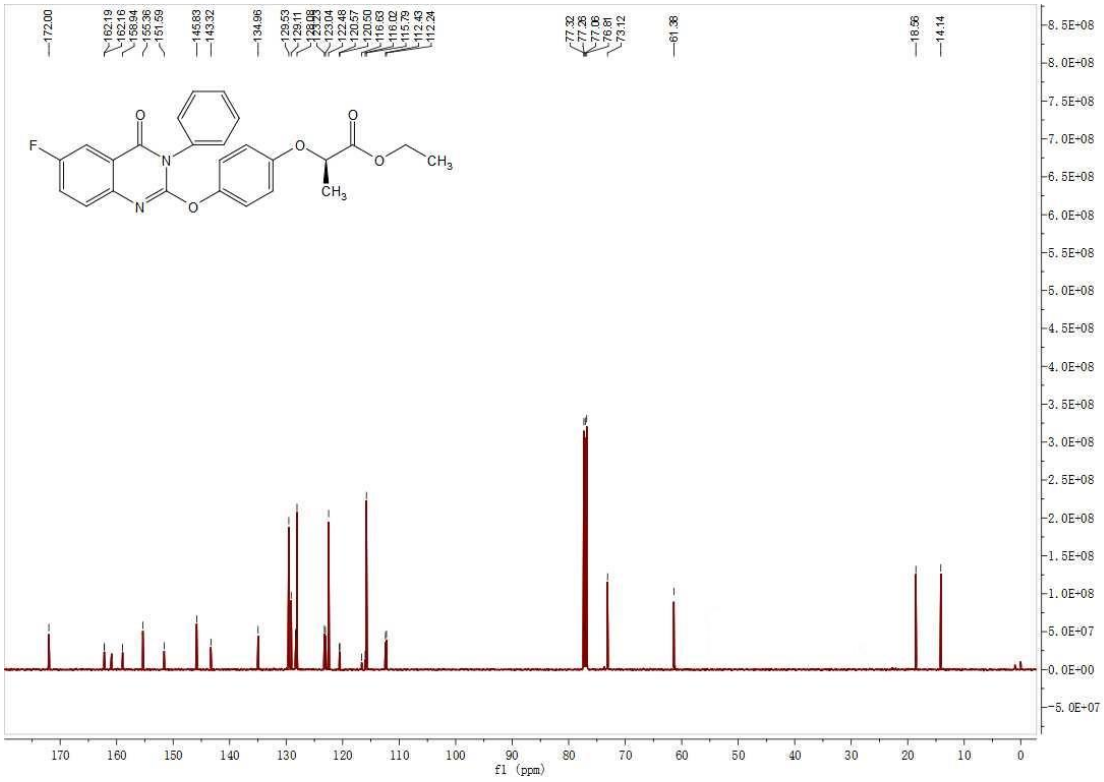

6
0301-1-B-14 265 (1.478)
1: TOF MS ES+
6.52e6
100
%
0
429.1830
430.1858
431.1880
139.9908
165.9918
250.1746
301.1427
373.1195
429.1107
467.1369
536.1373
561.3999
627.4255
685.4329
736.8059
m/z

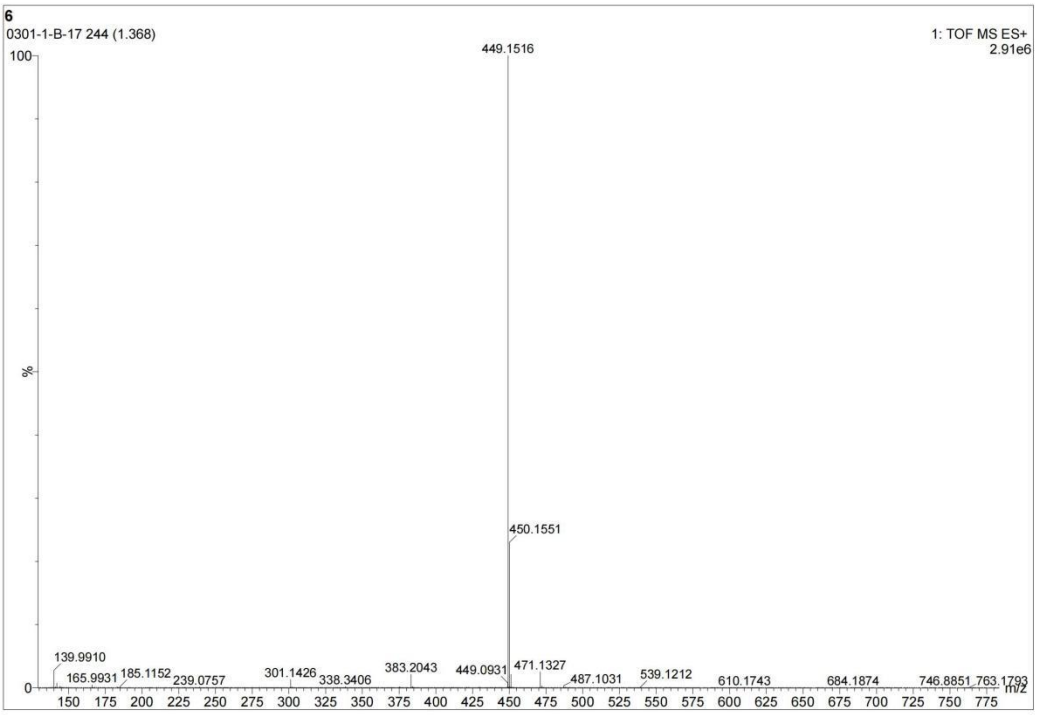

7.84
7.84
7.84
7.83
7.82
7.34
7.32
7.30
7.27
7.14
7.14
7.13
7.12
7.12
7.11
6.96
6.95
6.95
6.94
6.93
6.93
4.78
4.77
4.76
4.74
4.28
4.28
4.27
4.26
4.26
4.25
4.24
4.24
4.23
4.23
4.22
4.11
4.09
2.33
2.32
2.31
2.29
2.28
2.27
2.25
1.66
1.65
1.30
1.29
1.02
1.02
1.01
0.96
1.98
2.03
2.01
1.00
2.03
1.96
1.01
3.02
3.81
3.36
2.88
f1 (ppm)

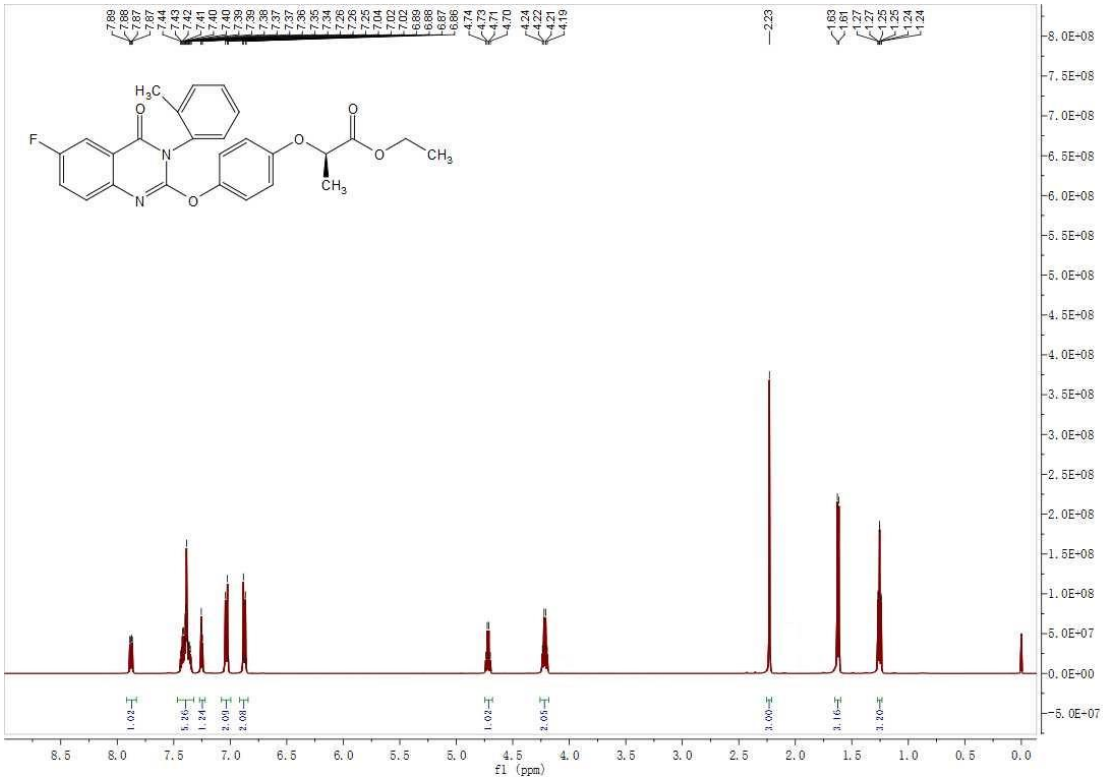

172.03
162.34
162.32
160.71
158.76
155.41
152.36
145.84
143.16
128.12
128.06
122.82
122.63
122.60
120.12
120.05
115.94
112.10
111.91
77.30
77.04
76.79
73.17
61.40
49.18
29.71
27.62
20.15
18.90
14.18
f1 (ppm)

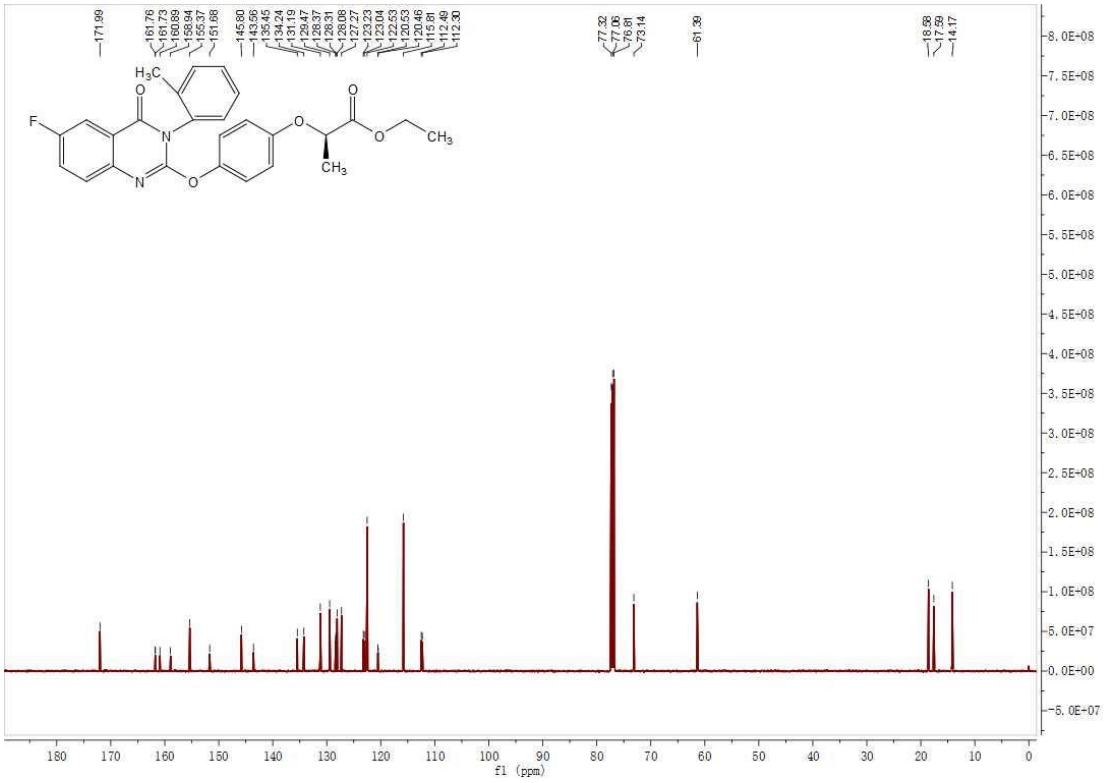

6
0301-1-B-16 270 (1.505)
1: TOF MS ES+
5.60e6
100
%
0
429.1830
430.1860
431.1883
373.1202
139.9905
165.9926
250.1819
301.1413
345.0917
374.1239
452.1594
519.1320
539.8538
634.7086
685.4396
702.3801
792.9166
m/z
150
200
250
300
350
400
450
500
550
600
650
700
750
800

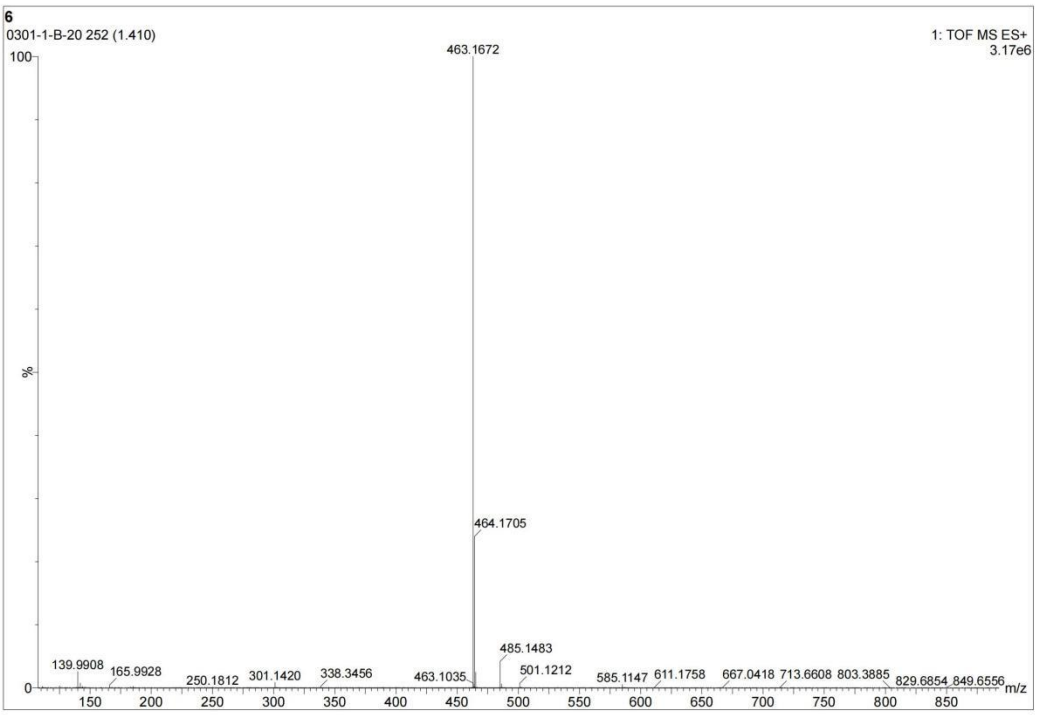

F
O
N
O
O
O
CH3
CH3
f1 (ppm)

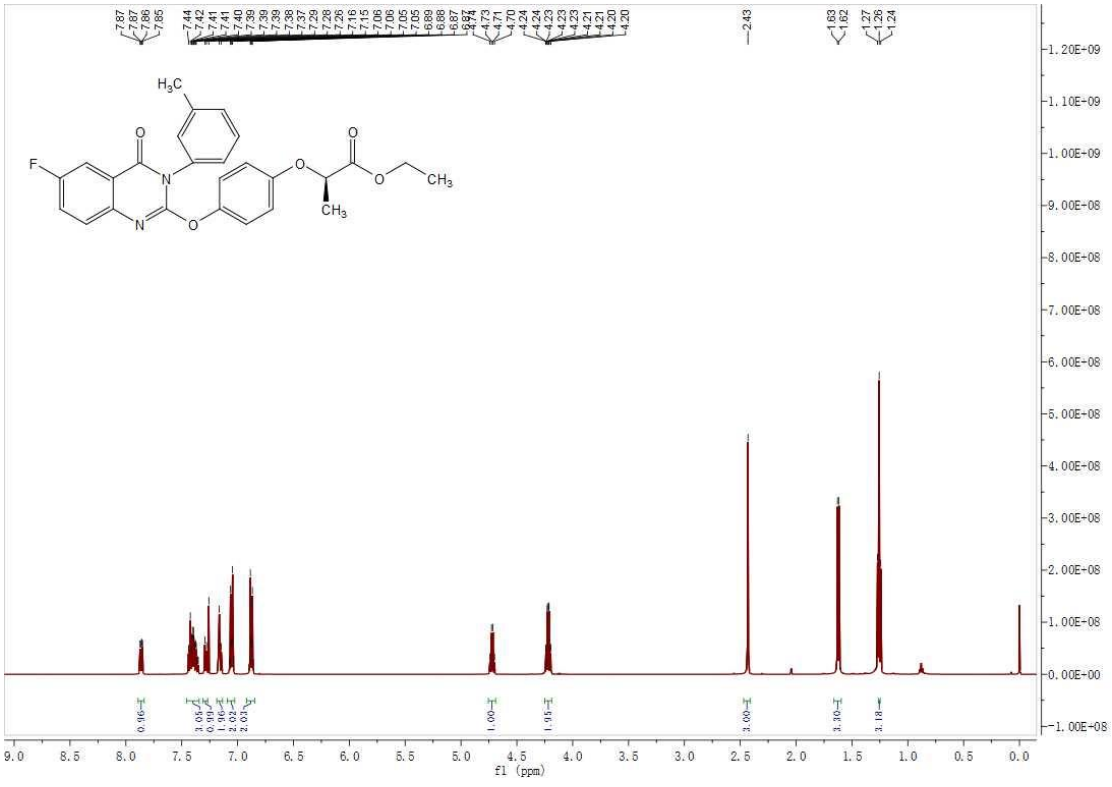

172.00
162.19
162.16
158.94
155.36
151.59
145.83
143.32
134.96
129.53
129.11
123.04
122.48
120.57
120.50
116.02
115.79
112.43
112.24
77.32
77.26
77.06
76.81
73.12
61.36
18.56
14.14
F
O
N
O
O
O
CH3
CH3
f1 (ppm)

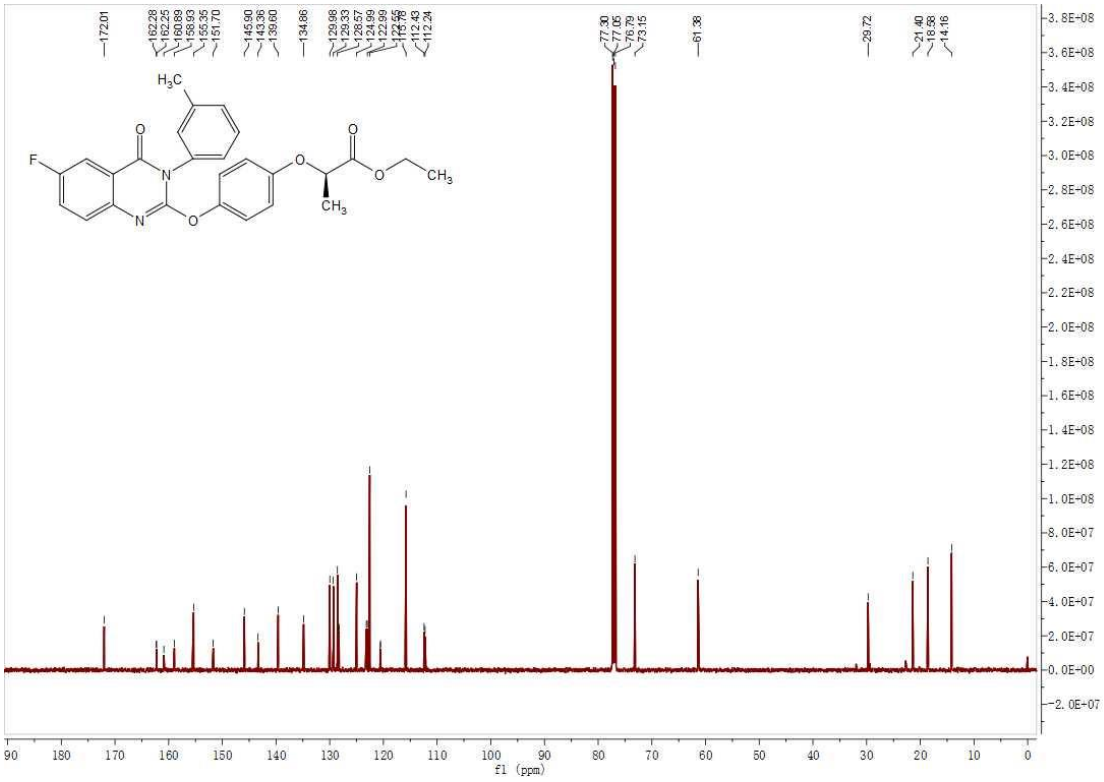

6
0301-1-B-17 244 (1.368)
1: TOF MS ES+
2.91e6
100
%
0
449.1516
450.1551
139.9910
165.9931
185.1152
239.0757
301.1426
338.3406
383.2043
449.0931
471.1327
487.1031
539.1212
610.1743
684.1874
746.8851
763.1793
m/z

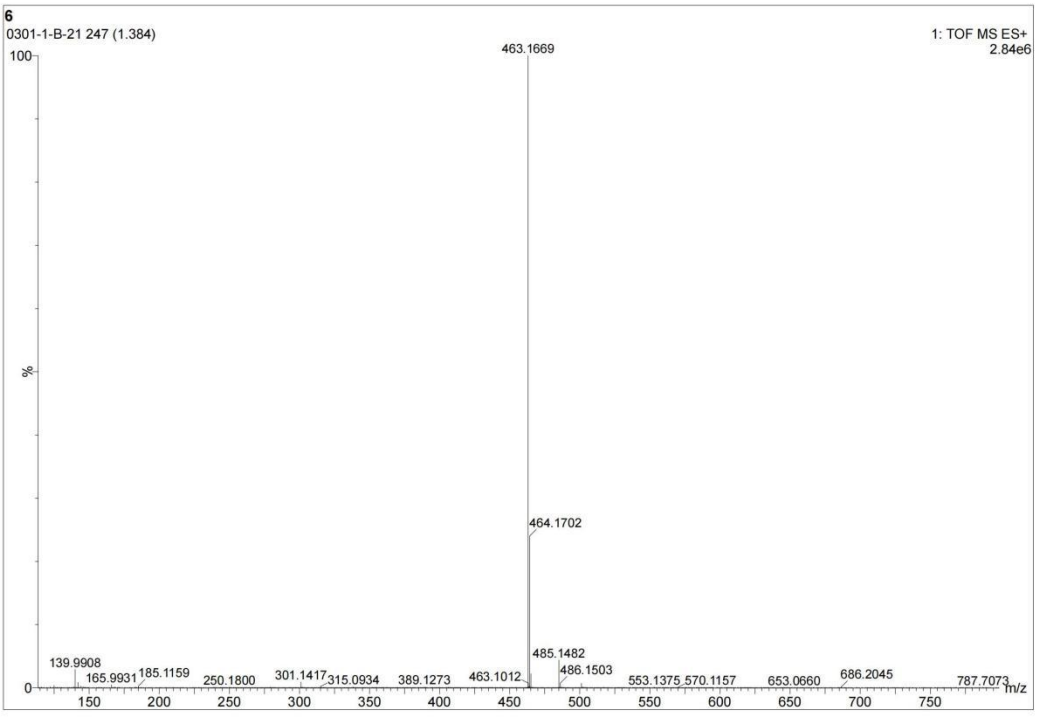

7.89
7.88
7.87
7.87
7.44
7.43
7.42
7.41
7.40
7.40
7.39
7.39
7.38
7.37
7.37
7.36
7.35
7.34
7.26
7.25
7.04
7.02
7.02
6.89
6.88
6.87
6.86
4.74
4.73
4.71
4.70
4.24
4.22
4.21
4.19
2.23
1.63
1.61
1.27
1.27
1.25
1.25
1.24
1.24
H3C
O
N
O
F
O
O
O
CH3
CH3
1.02
5.26
1.24
2.01
2.08
1.02
2.05
3.00
3.16
3.20
f1 (ppm)

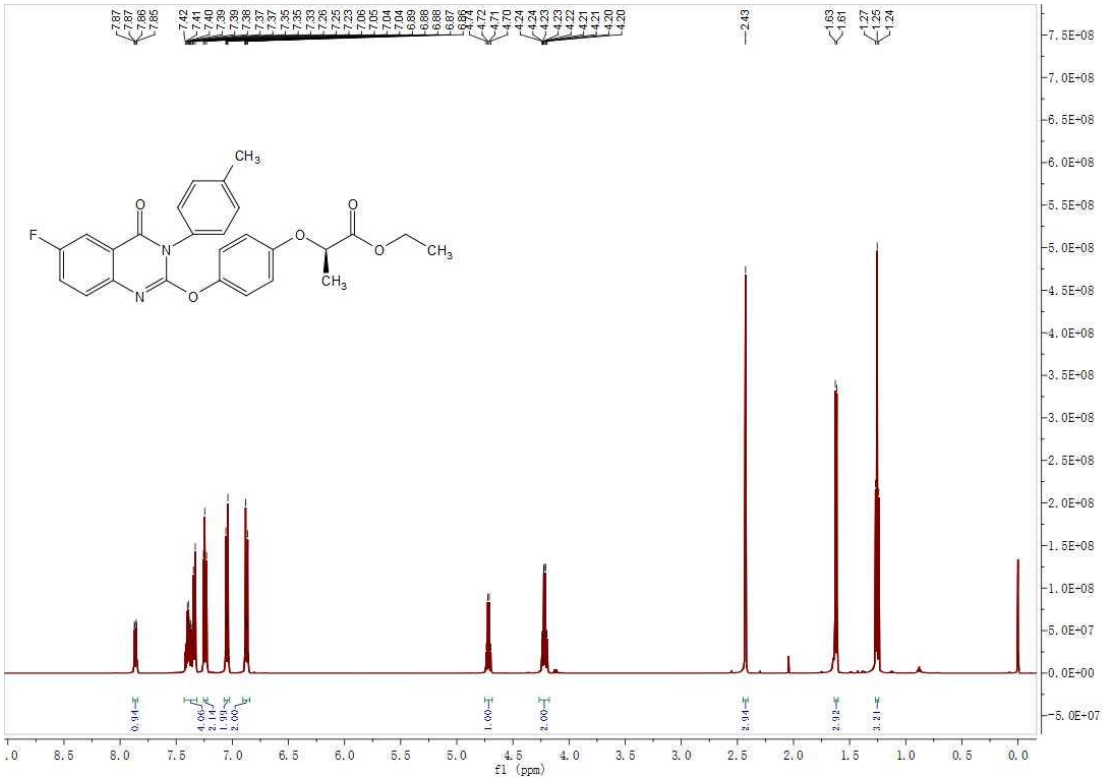

171.99
161.76
161.73
160.89
158.94
155.37
151.08
145.80
143.66
135.45
134.24
131.19
129.47
128.37
128.31
128.08
127.27
123.23
123.04
122.53
120.53
120.46
115.81
112.49
112.30
77.32
77.06
76.81
73.14
61.39
18.68
17.39
14.17
H3C
O
N
O
F
O
O
O
CH3
CH3
f1 (ppm)

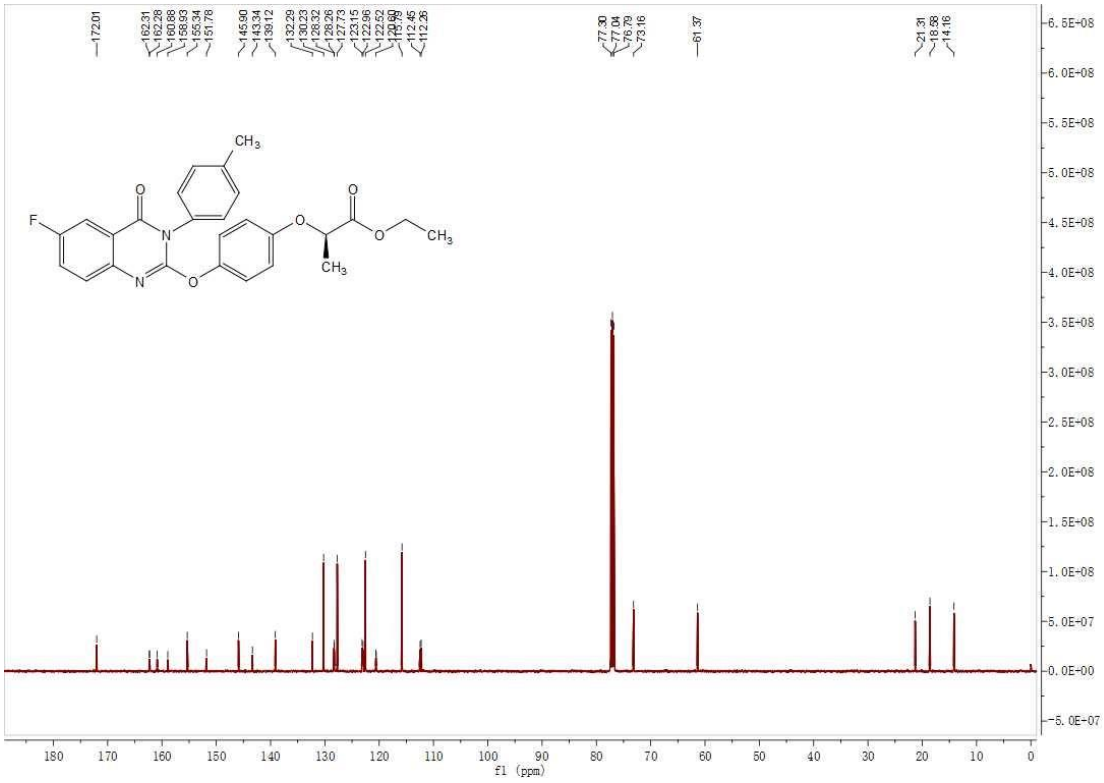

6
0301-1-B-20 252 (1.410)
1: TOF MS ES+
3.17e6
100
%
0
463.1672
464.1705
485.1483
139.9908
165.9928
250.1812
301.1420
338.3456
463.1035
501.1212
585.1147
611.1758
667.0418
713.6608
803.3885
829.6854
849.6556
m/z
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850

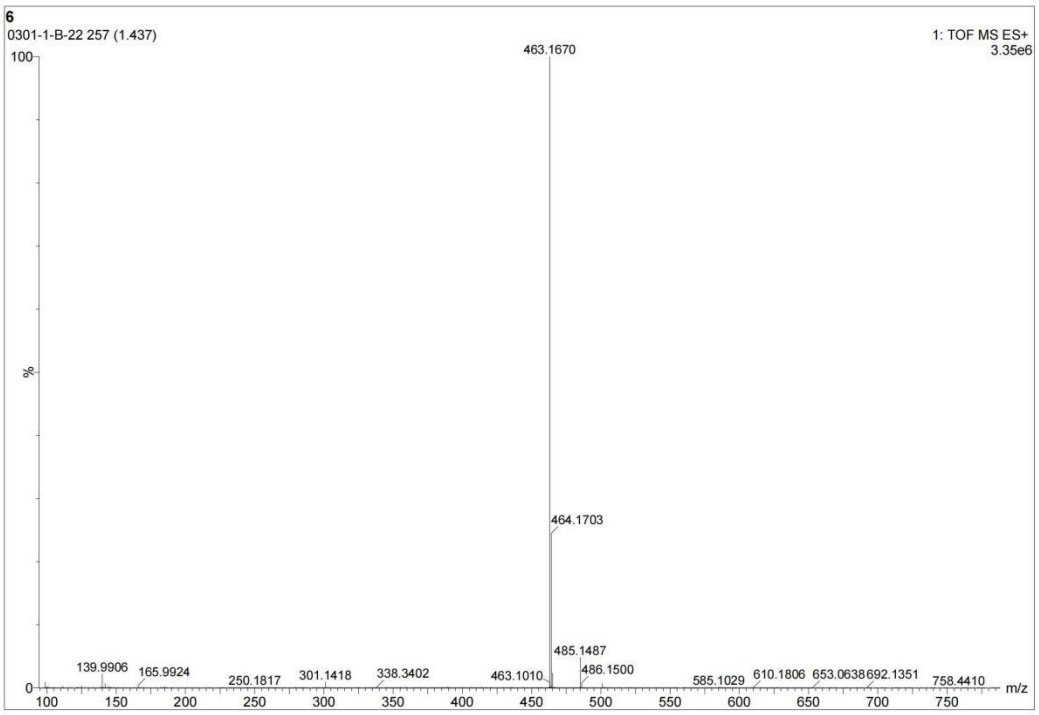

7.87
7.87
7.86
7.85
7.44
7.42
7.41
7.41
7.40
7.39
7.39
7.38
7.37
7.29
7.28
7.26
7.16
7.15
7.06
7.06
7.05
7.05
6.89
6.88
6.87
6.87
4.73
4.71
4.70
4.24
4.24
4.23
4.23
4.23
4.21
4.21
4.20
4.20
2.43
1.63
1.62
1.27
1.26
1.24
H3C
O
O
F
N
N
O
O
O
CH3
CH3
1.20E-09
1.10E-09
1.00E-09
9.00E-08
8.00E-08
7.00E-08
6.00E-08
5.00E-08
4.00E-08
3.00E-08
2.00E-08
1.00E-08
0.00E-00
-1.00E-08
0.96
3.05
0.91
1.06
2.02
2.03
1.00
1.05
3.00
3.30
3.18
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)

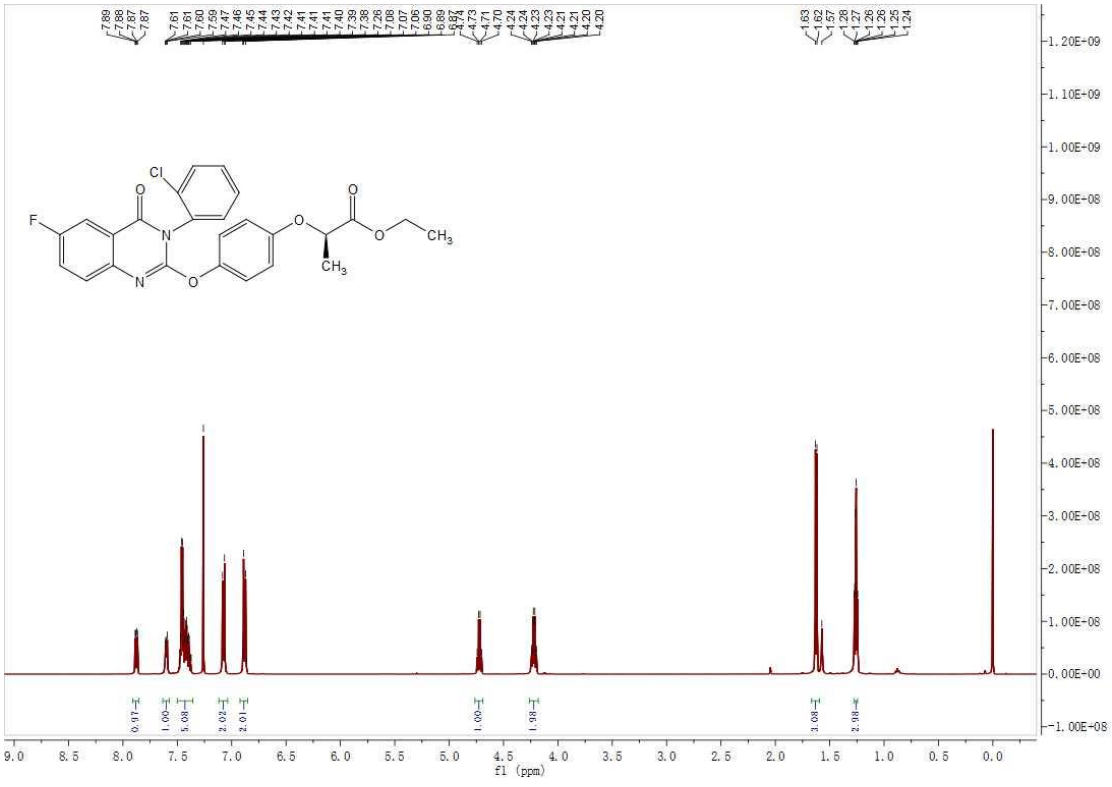

172.01
162.28
162.25
160.89
158.93
155.35
151.70
145.90
143.36
139.60
134.86
129.98
129.33
128.57
124.99
122.99
112.43
112.24
77.90
77.05
76.79
73.15
61.38
29.72
21.40
18.58
14.16
H3C
F
O
N
O
O
O
CH3
CH3
f1 (ppm)

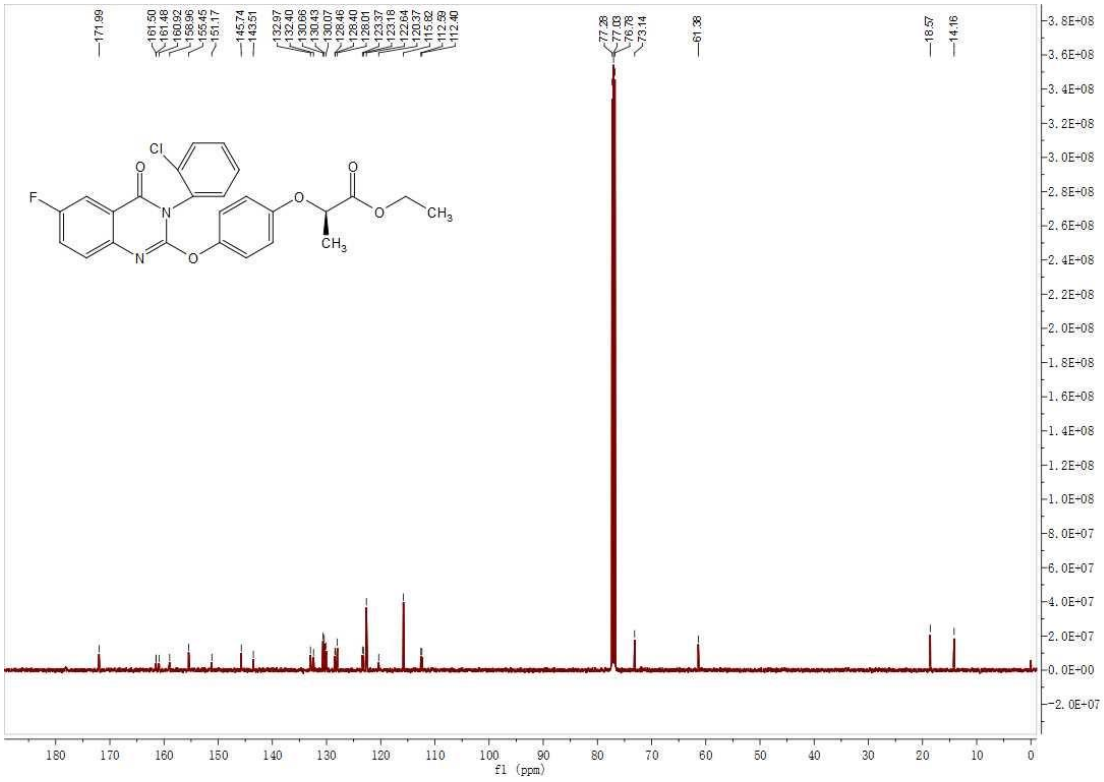

6
0301-1-B-21 247 (1.384)
1: TOF MS ES+
2.84e6
100
%
0
463.1669
464.1702
485.1482
486.1503
139.9908
165.9931
185.1159
250.1800
301.1417
315.0934
389.1273
463.1012
553.1375
570.1157
653.0660
686.2045
787.7073
m/z

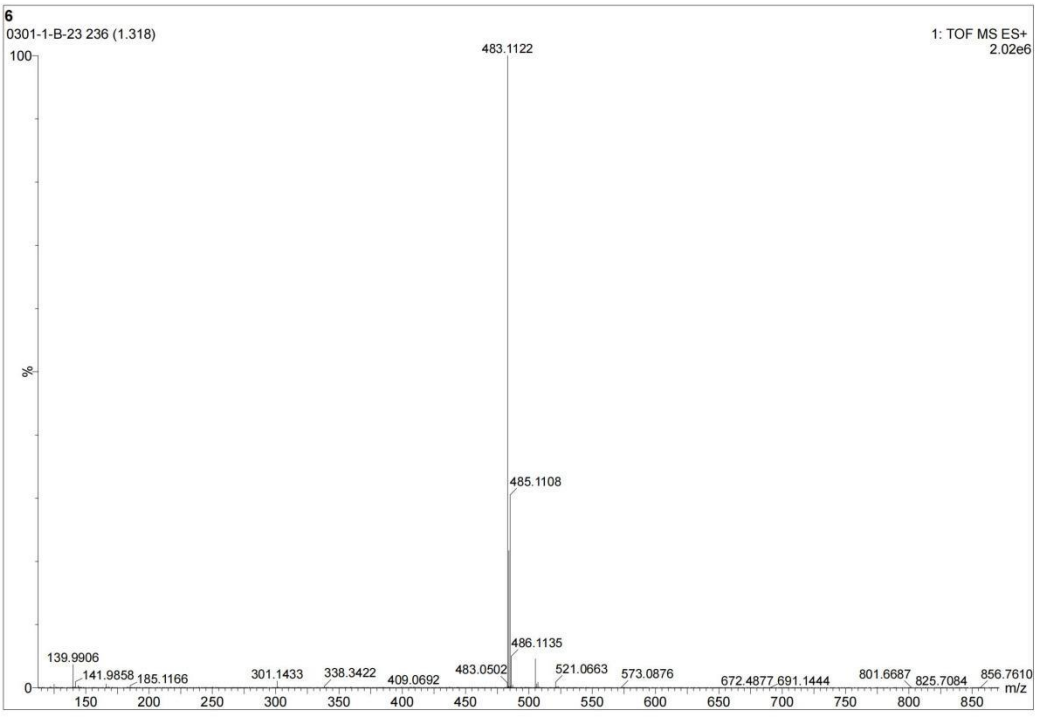

7.87
7.87
7.86
7.85
7.42
7.41
7.40
7.39
7.39
7.38
7.37
7.37
7.35
7.35
7.33
7.26
7.25
7.23
7.06
7.05
7.04
7.04
6.89
6.88
6.88
6.87
6.87
4.74
4.72
4.71
4.70
4.24
4.24
4.23
4.23
4.22
4.21
4.21
4.20
4.20
2.43
1.63
1.61
1.27
1.25
1.24
CH3
O
O
F
N
O
O
O
CH3
CH3
0.94
4.00
1.91
2.00
1.00
2.00
2.94
2.92
3.21
f1 (ppm)

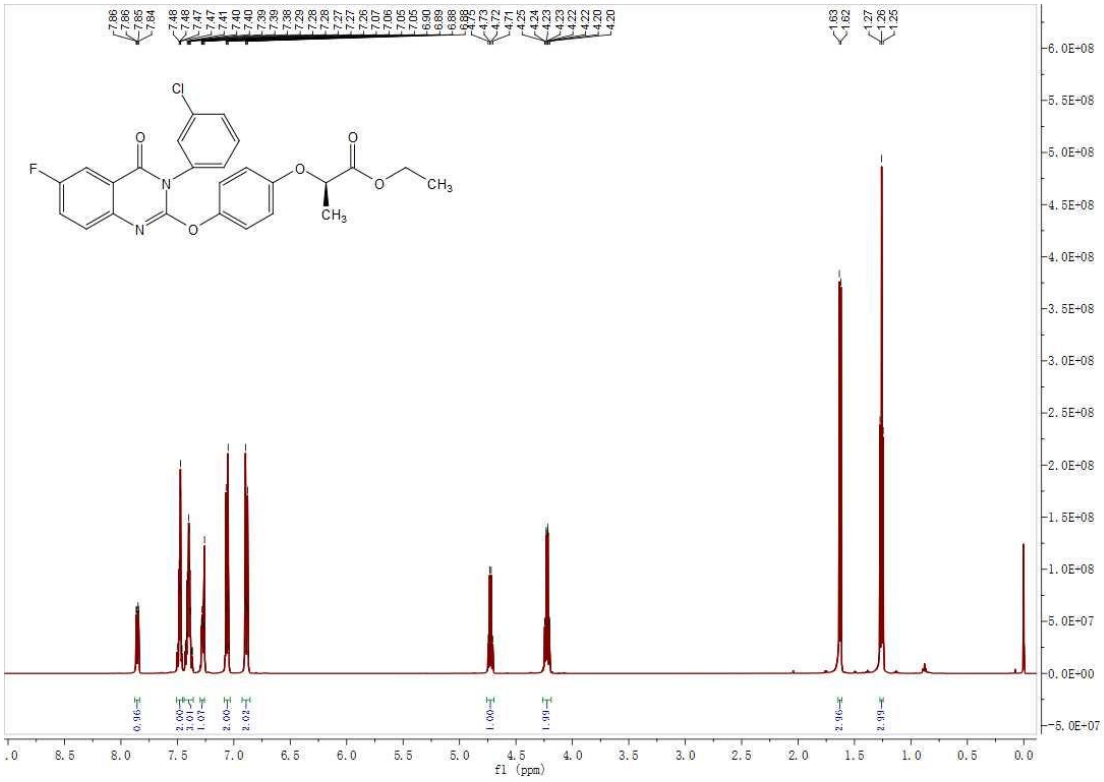

172.01
162.31
162.26
160.88
160.83
155.34
151.78
145.90
143.34
139.12
132.29
130.23
128.32
128.26
127.73
123.15
122.96
122.82
120.60
119.79
112.45
112.26
77.30
77.04
76.79
73.16
61.37
21.31
18.38
14.16
CH3
O
O
F
N
O
O
O
CH3
CH3
f1 (ppm)

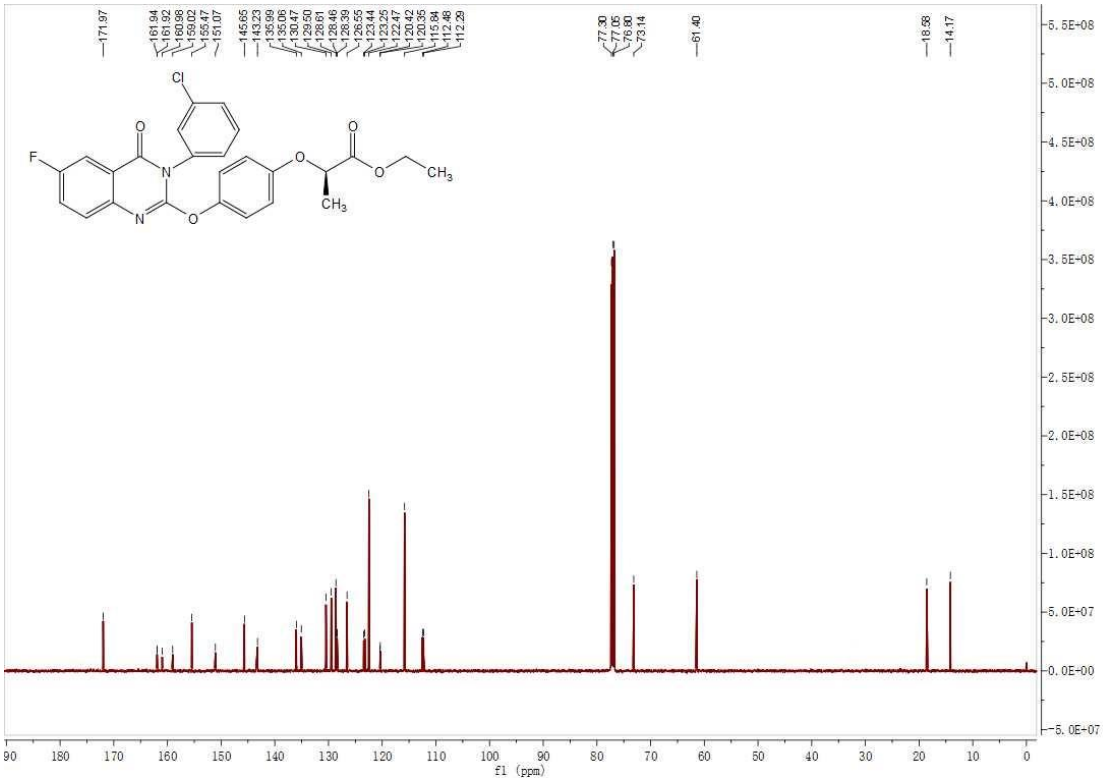

6
0301-1-B-22 257 (1.437)
1: TOF MS ES+
3.35e6
100
%
0
463.1670
464.1703
485.1487
486.1500
139.9906
165.9924
250.1817
301.1418
338.3402
463.1010
585.1029
610.1806
653.0638
692.1351
758.4410
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750

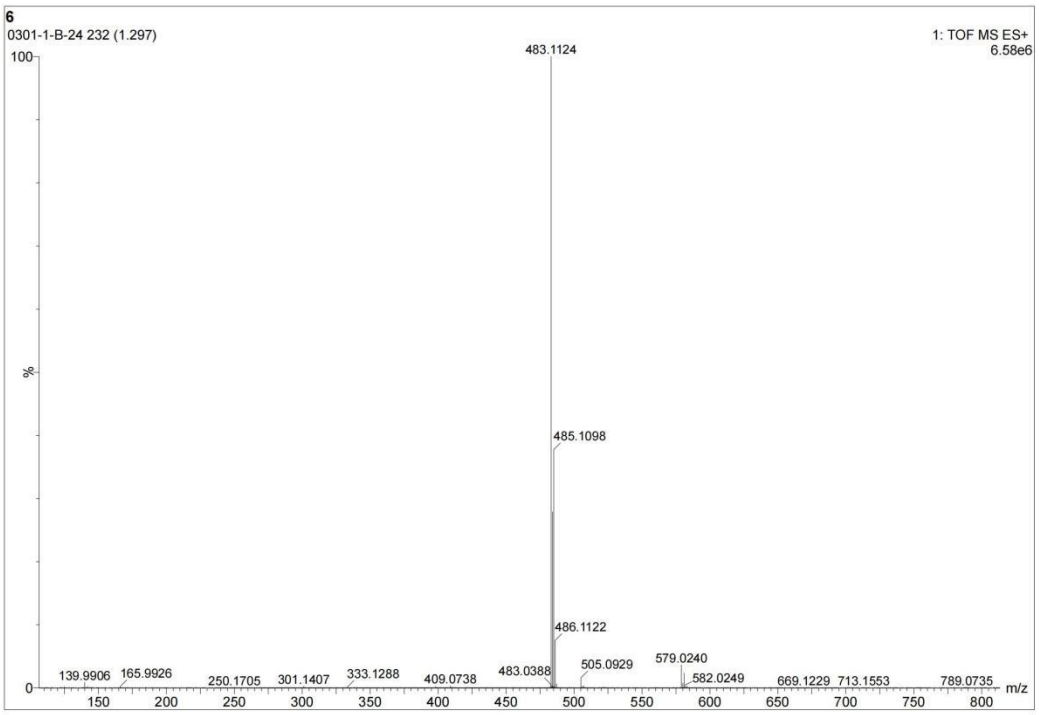

Cl
O
F
N
O
O
O
O
CH3
CH3
N
1.20E-09
1.10E-09
1.00E-09
9.00E-08
8.00E-08
7.00E-08
6.00E-08
5.00E-08
4.00E-08
3.00E-08
2.00E-08
1.00E-08
0.00E-00
-1.00E-08
0.97
1.00
5.08
2.02
2.01
1.00
1.98
3.08
2.98
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


171.99
161.50
161.48
160.92
158.96
155.45
151.17
145.74
143.51
132.97
132.40
130.66
130.43
130.07
128.46
128.40
128.01
123.37
123.18
122.64
120.37
115.82
112.59
112.40
77.26
77.00
76.78
73.14
61.38
18.57
14.16
Cl
F
O
N
O
O
O
CH3
CH3
f1 (ppm)

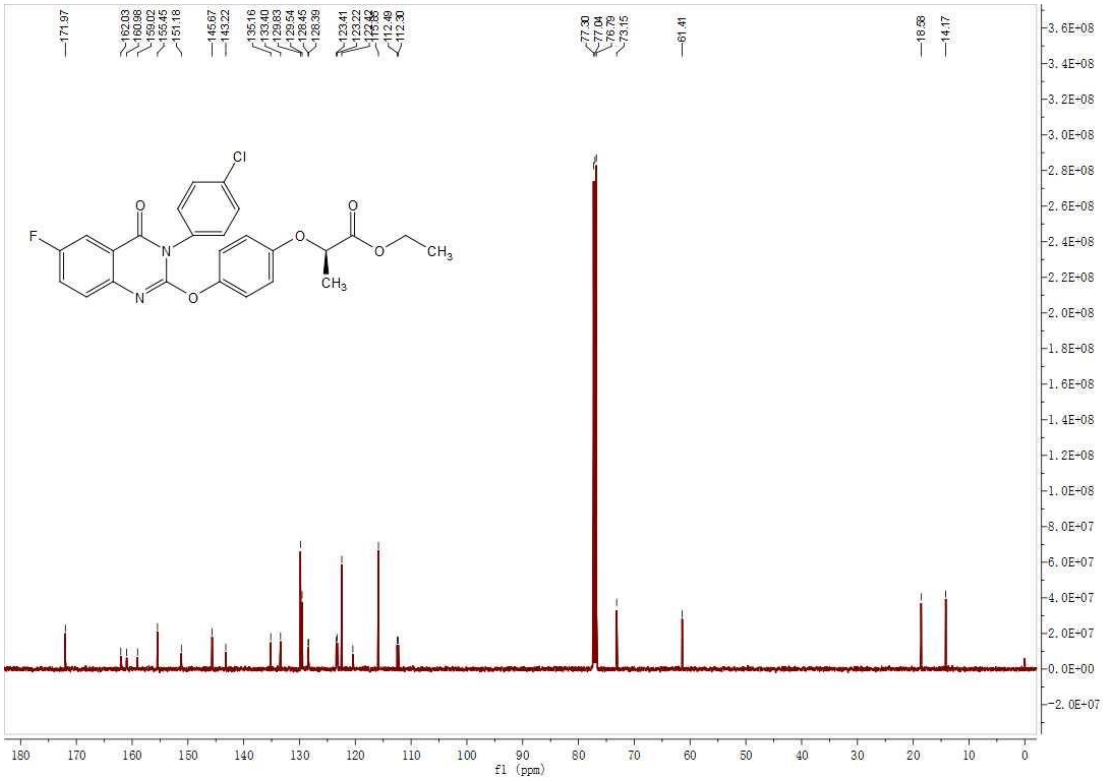

6
0301-1-B-23 236 (1.318)
1: TOF MS ES+
2.02e6
100
%
0
483.1122
485.1108
486.1135
139.9906
141.9858
185.1166
301.1433
338.3422
409.0692
483.0502
521.0663
573.0876
672.4877
691.1444
801.6687
825.7084
856.7610
m/z

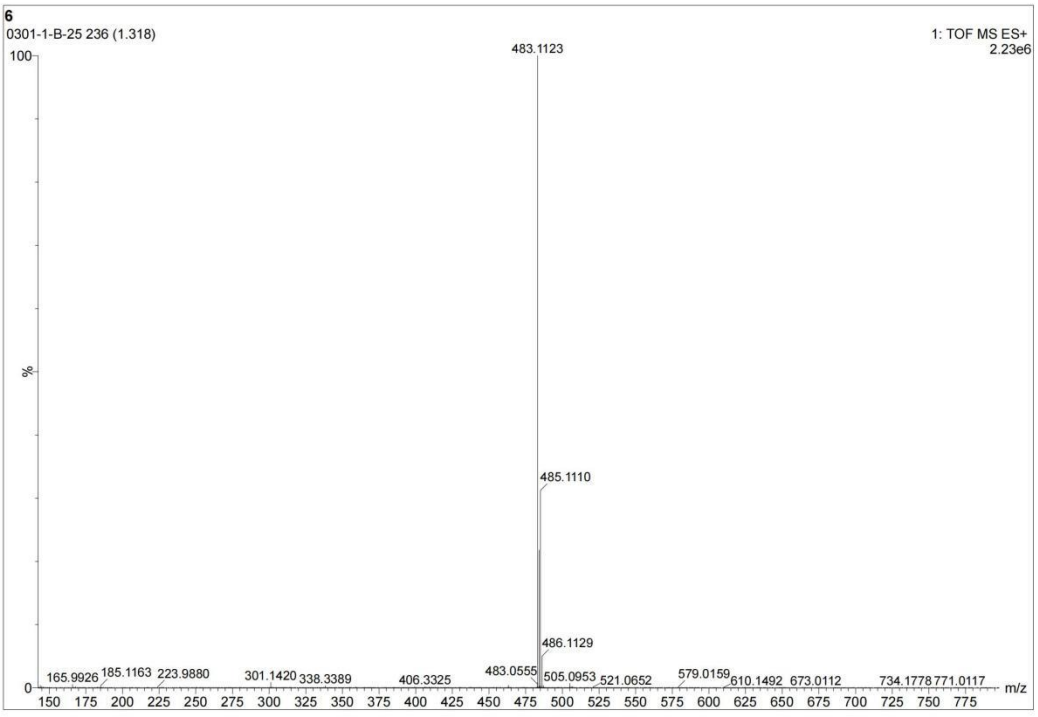

7.86
7.86
7.85
7.84
7.48
7.48
7.47
7.47
7.47
7.41
7.40
7.40
7.39
7.39
7.38
7.29
7.28
7.28
7.27
7.27
7.26
7.07
7.06
7.05
7.05
6.90
6.89
6.88
6.88
4.73
4.72
4.71
4.25
4.24
4.23
4.23
4.22
4.22
4.20
4.20
1.63
1.62
1.27
1.26
1.25
Cl
O
F
N
O
O
O
O
CH3
CH3
6.0E-08
5.5E-08
5.0E-08
4.5E-08
4.0E-08
3.5E-08
3.0E-08
2.5E-08
2.0E-08
1.5E-08
1.0E-08
5.0E-07
0.0E+00
-5.0E-07
0.96
2.00
3.01
1.07
2.00
2.02
1.00
1.99
2.96
2.99
.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)

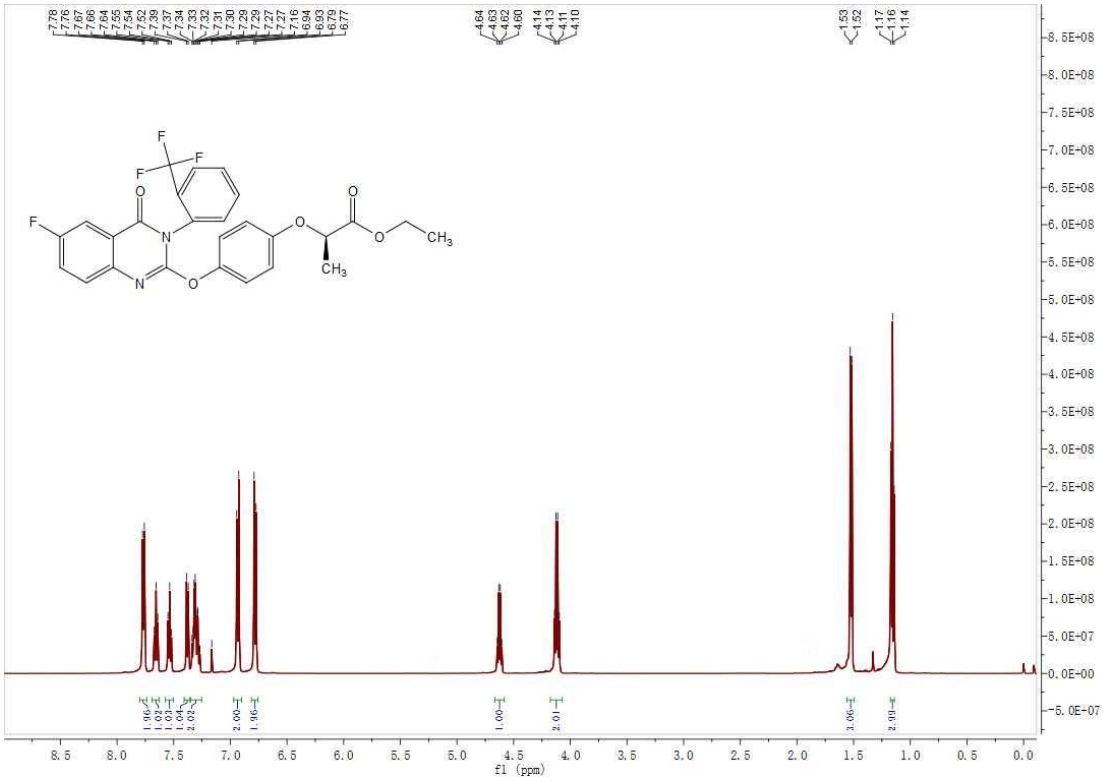

171.97
161.94
161.92
160.98
159.02
155.47
151.07
145.65
143.23
135.99
135.86
130.47
129.50
128.61
128.46
128.39
126.55
123.44
123.25
122.47
120.42
120.35
115.94
112.48
112.29
77.30
77.05
76.80
73.14
61.40
18.68
14.17
Cl
O
F
N
O
O
O
O
CH3
CH3
5.5E-08
5.0E-08
4.5E-08
4.0E-08
3.5E-08
3.0E-08
2.5E-08
2.0E-08
1.5E-08
1.0E-08
5.0E-07
0.0E+00
-5.0E-07
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

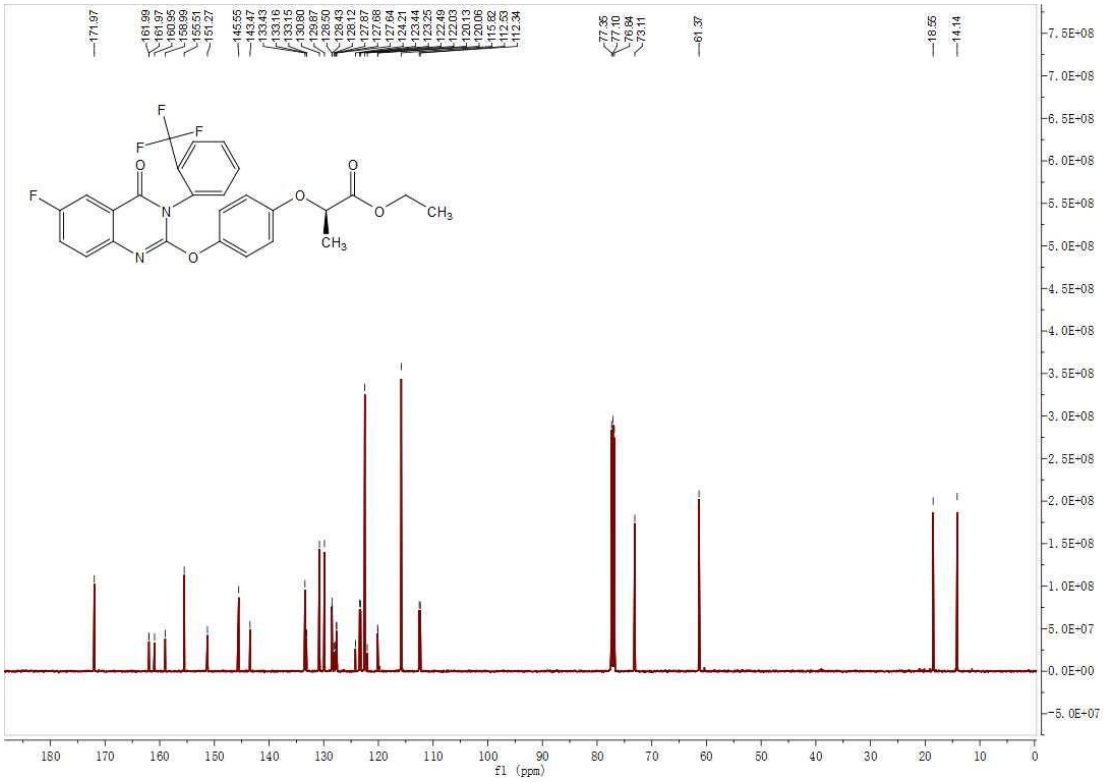

6
0301-1-B-24 232 (1.297)
1: TOF MS ES+
6.58e6
100
%
0
483.1124
485.1098
486.1122
139.9906
165.9926
250.1705
301.1407
333.1288
409.0738
483.0388
505.0929
579.0240
582.0249
669.1229
713.1553
789.0735
150
200
250
300
350
400
450
500
550
600
650
700
750
800
m/z

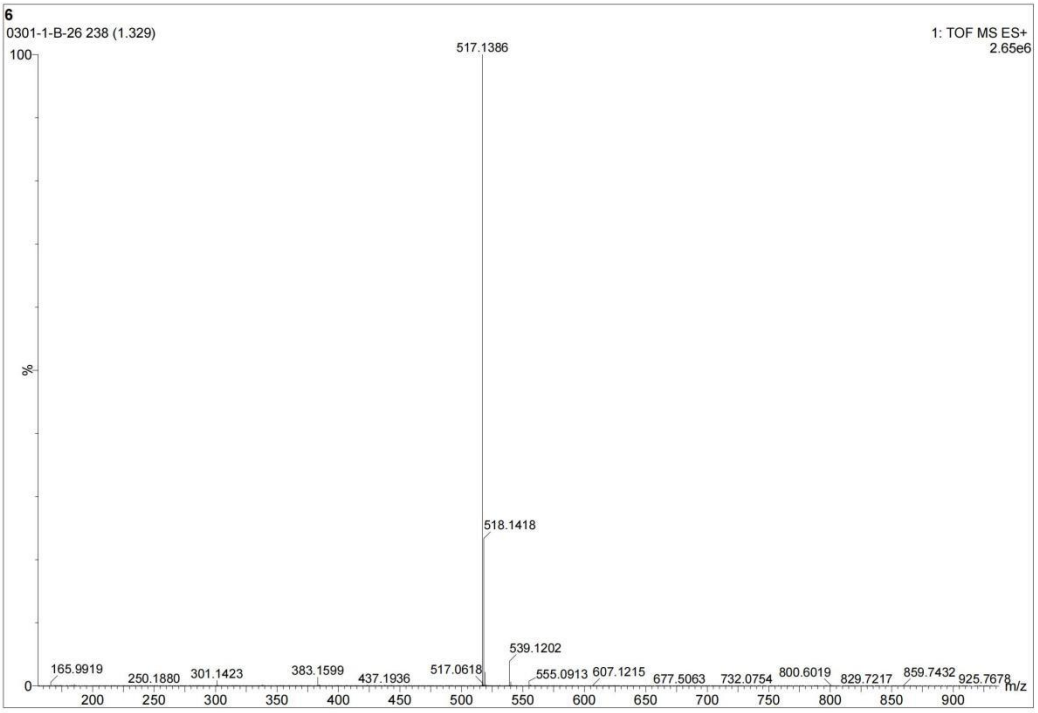

Cl
F
O
N
O
O
O
N
O
CH3
CH3
f1 (ppm)

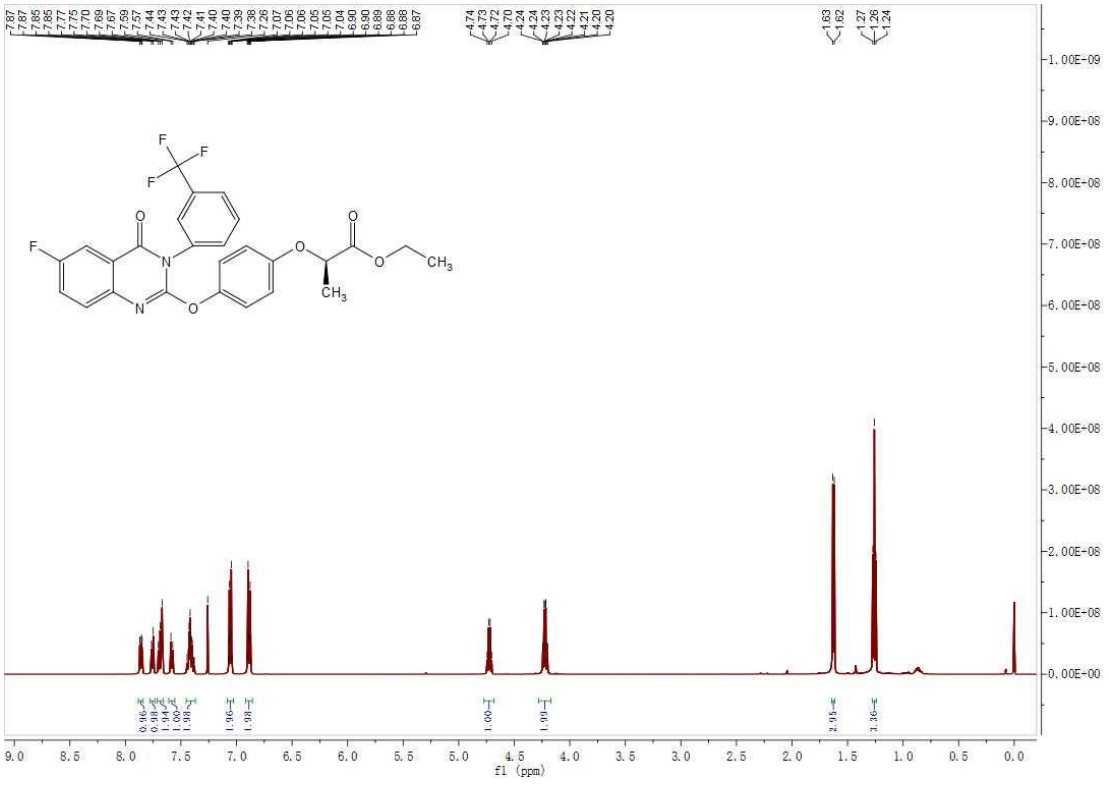

171.97
162.03
160.98
159.02
155.45
151.18
145.67
143.22
135.16
133.40
129.83
129.54
128.45
128.39
123.41
123.22
112.49
112.30
77.30
77.04
76.79
73.15
61.41
18.59
14.17
Cl
F
O
N
O
O
O
CH3
CH3
f1 (ppm)

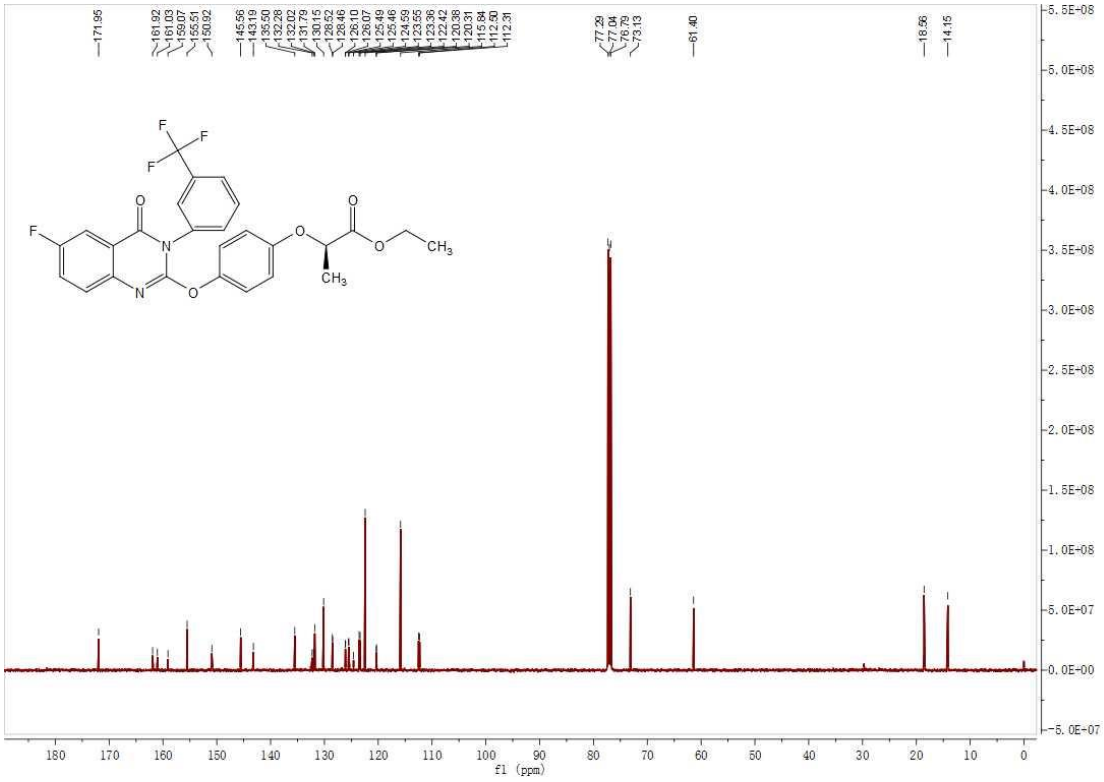

6
0301-1-B-25 236 (1.318)
1: TOF MS ES+
2.23e6
100
%
0
483.1123
485.1110
486.1129
165.9926
185.1163
223.9880
301.1420
338.3389
406.3325
483.0555
505.0953
521.0652
579.0159
610.1492
673.0112
734.1778
771.0117
m/z

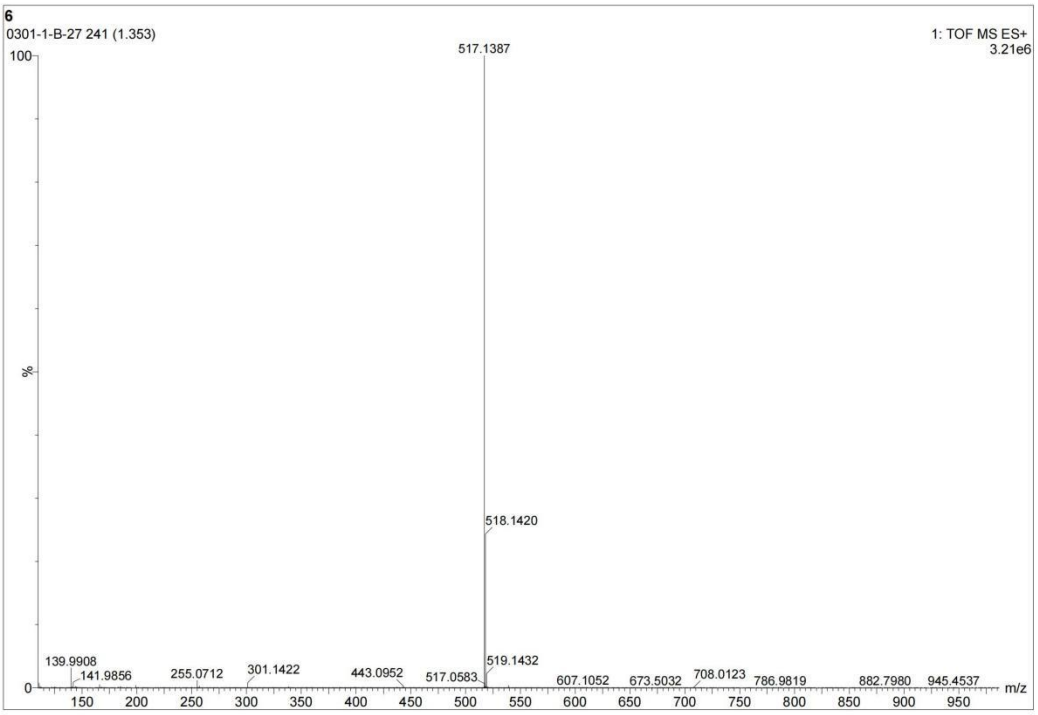

7.78
7.76
7.67
7.66
7.64
7.55
7.54
7.52
7.39
7.37
7.34
7.33
7.32
7.31
7.30
7.29
7.29
7.27
7.27
7.16
6.94
6.93
6.79
6.77
4.64
4.63
4.62
4.60
4.14
4.13
4.11
4.10
1.53
1.52
1.17
1.16
1.14
F
F
F
O
N
O
F
O
O
O
CH3
CH3
1.00
1.03
1.04
2.02
2.00
1.96
1.00
2.01
3.06
2.99
f1 (ppm)

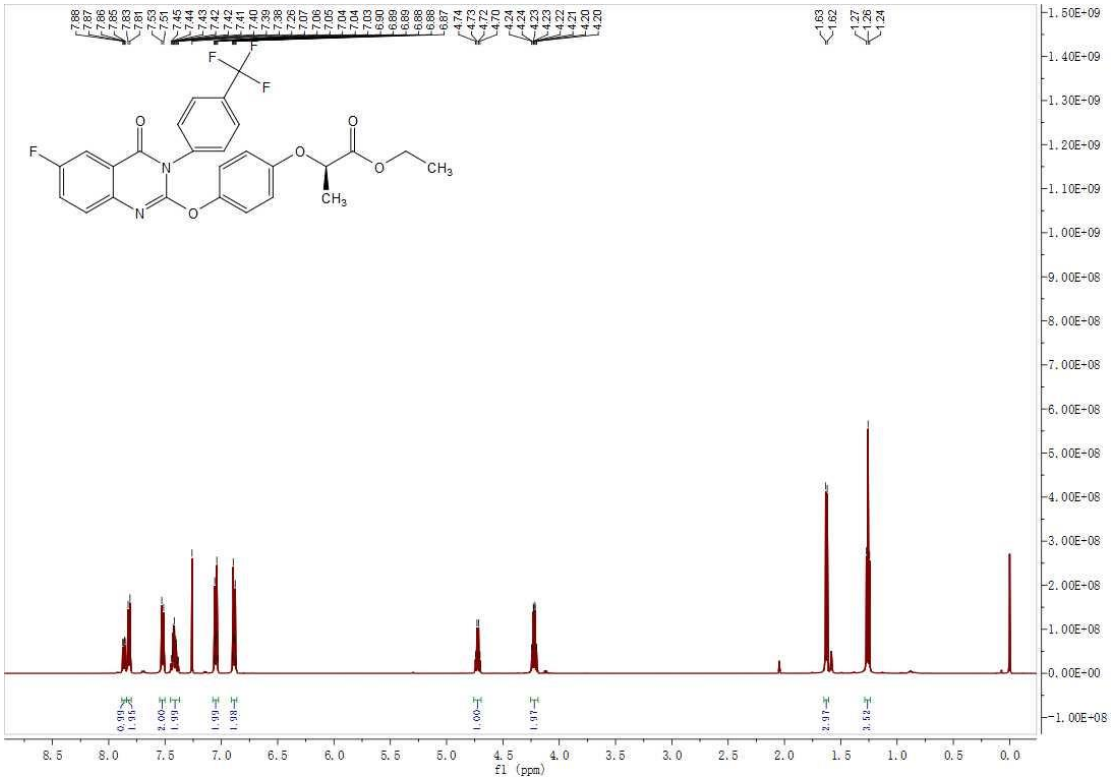

171.97
161.99
161.97
160.96
160.89
155.51
151.27
145.55
143.47
133.43
133.16
133.15
130.80
129.87
128.50
128.43
128.12
127.87
127.68
127.64
124.21
123.44
123.25
122.49
122.03
120.13
120.06
115.82
112.53
112.34
77.36
77.10
76.84
73.11
61.37
18.55
14.14
F
F
F
O
N
O
F
O
O
O
CH3
CH3
f1 (ppm)

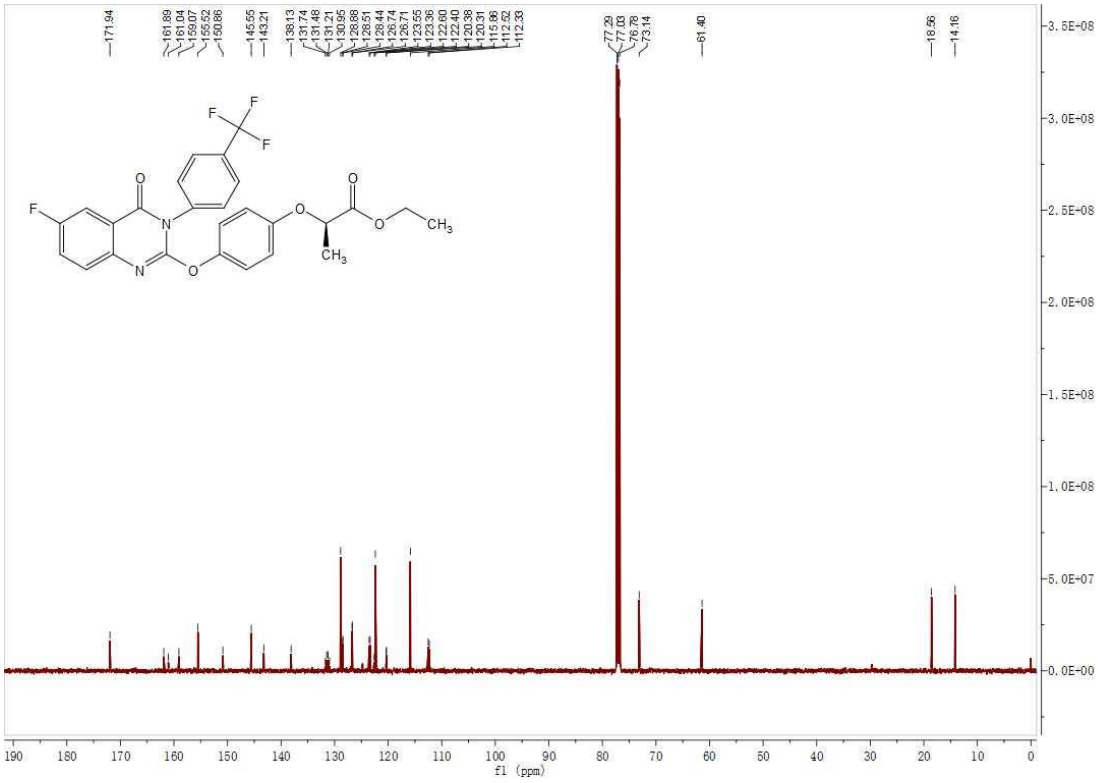

6
0301-1-B-26 238 (1.329)
1: TOF MS ES+
2.65e6
100
%
0
517.1386
518.1418
539.1202
165.9919
250.1880
301.1423
383.1599
437.1936
517.0618
555.0913
607.1215
677.5063
732.0754
800.6019
829.7217
859.7432
925.7678
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
m/z

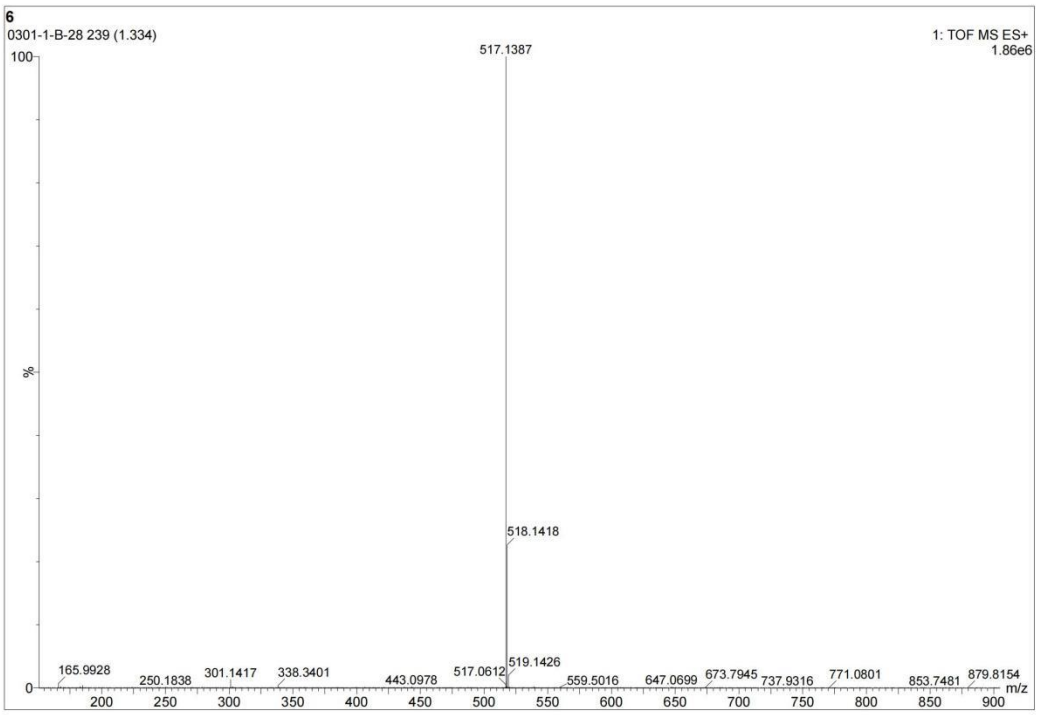

F
F
F
O
N
O
F
O
O
O
CH3
CH3
N
O
f1 (ppm)


171.95
161.92
161.03
159.07
155.51
150.92
145.56
143.19
135.50
132.28
132.02
131.79
130.15
128.52
128.46
126.10
126.07
125.48
125.46
124.59
123.55
123.36
122.42
120.38
120.31
115.84
112.50
112.31
77.29
77.04
76.79
73.13
61.40
18.56
14.15
F
F
F
O
N
O
F
N
O
O
O
CH3
CH3
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


6
0301-1-B-27 241 (1.353)
1: TOF MS ES+
3.21e6
100
%
0
517.1387
518.1420
519.1432
139.9908
141.9856
255.0712
301.1422
443.0952
517.0583
607.1052
673.5032
708.0123
786.9819
882.7980
945.4537
m/z
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950


7.88
7.87
7.86
7.85
7.83
7.81
7.53
7.51
7.45
7.44
7.43
7.42
7.42
7.41
7.41
7.40
7.39
7.38
7.26
7.07
7.06
7.05
7.04
7.04
7.03
6.90
6.89
6.89
6.88
6.88
6.87
4.74
4.73
4.72
4.70
4.24
4.24
4.23
4.23
4.22
4.21
4.20
4.20
1.63
1.62
1.27
1.26
1.24
F
F
F
O
N
O
O
O
O
CH3
CH3
0.93
1.95
2.00
1.99
1.99
1.98
1.00
1.97
2.97
3.52
1.50E-09
1.40E-09
1.30E-09
1.20E-09
1.10E-09
1.00E-09
9.00E-08
8.00E-08
7.00E-08
6.00E-08
5.00E-08
4.00E-08
3.00E-08
2.00E-08
1.00E-08
0.00E-00
-1.00E-08
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)


171.94
161.89
161.04
159.07
155.52
150.86
145.55
143.21
138.13
131.74
131.48
131.21
130.95
128.88
128.51
128.44
126.74
126.71
123.55
123.36
122.60
122.40
120.38
120.31
115.66
115.62
112.33
77.29
77.03
76.78
73.14
61.40
18.56
14.16
F
F
F
O
N
O
O
O
O
CH3
CH3
3.5E-08
3.0E-08
2.5E-08
2.0E-08
1.5E-08
1.0E-08
5.0E-07
0.0E-00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


6
0301-1-B-28 239 (1.334)
1: TOF MS ES+
1.86e6
100
%
0
517.1387
518.1418
519.1426
165.9928
250.1838
301.1417
338.3401
443.0978
517.0612
559.5016
647.0699
673.7945
737.9316
771.0801
853.7481
879.8154
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
m/z