Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Visible-Light-Promoted N-Centered Radical Generation for Remote Heteroaryl Migration

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Table of Contents

1. General Remarks

Reagents: Commercially available reagents and solvents were of reagent grade quality without any further purification. Flash column chromatography was performed using silicycle silica gel (200-300 mesh). Analytical thin-layer chromatography (TLC) was performed on 0.2 mm coated silica gel plates (HSGF 254) and visualized using a UV lamp (254 nm or 365 nm). ^{1}H NMR and ^{13}C NMR were recorded on magnet system 400’54 ascend purchased from Bruker Biospin AG, which were reported in parts per million (ppm) referenced to hydrogen resonances and carbon resonances in the NMR solvent (DMSO-d_6). ESI-MS spectra were recorded on Agilent Q-TOF 6520.

2. Synthesis of the Starting Materials and Catalysts

2.1 Synthesis of the Starting Materials

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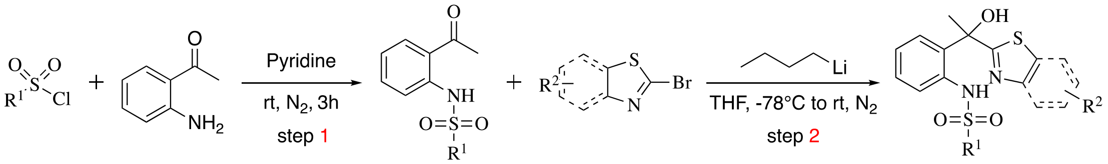

Step 1[1]:

2-Aminoacetophenone (1 eq, 20 mmol, 2.7014 g) and the corresponding sulfonyl chloride (1.05 eq, 21 mmol) were dissolved in anhydrous pyridine (15 mL) under N_2. The reaction mixture was stirred for 3h at ambient temperature. The mixture was diluted with CH_2Cl_2 (150 mL), which was washed with HCl solution (3%, 150 mL × 2) and water (150 mL). The separated organic layer was dried over anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure to give the crude product, which was purified by column chromatographic on silica gel (200-300 mesh, eluent: petroleum ether/ethyl acetate 20:1).

Step 2[2]:

To a stirred solution of the corresponding brominated heterocycle (15 mmol, 1.5 eq) in anhydrous THF (35 mL) was added *n*-butyllithium (15 mmol, 6 mL, 2.5 M, 1.5 eq) dropwise at -78℃ under N_2. After stirred for 0.5 h, the solution of sulfonamide (10 mmol, 1 eq) in anhydrous THF (30 mL) was added dropwise to the mixture. The mixture was stirred for another 2h at 0℃ and quenched with saturated aq. NH_4Cl (100 mL). The aqueous layer was extracted with EA (120 mL) for 2 times. The separated organic layer was dried over anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure to give the crude product, which was purified by column chromatographic on silica gel (200-300 mesh).

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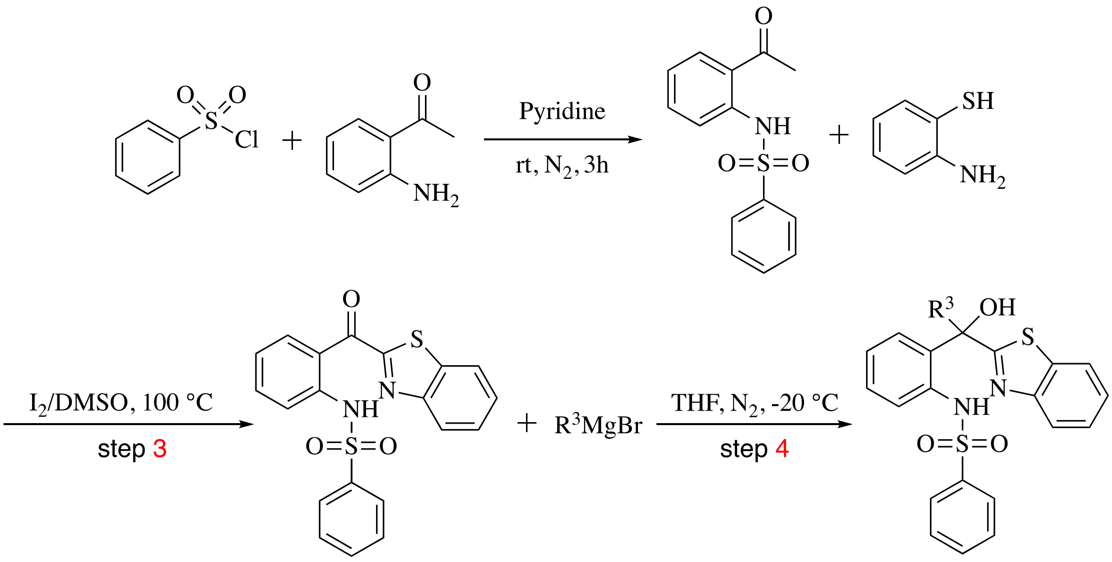


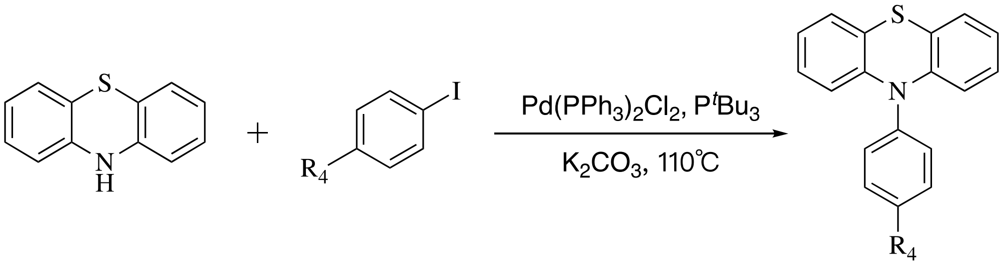
Step 3[3]:

N-(2-acetylphenyl)benzenesulfonamide (10 mmol, 2.7506 g, 1 eq), 2-aminobenzenethiol (12 mmol, 1.5004 g, 1.2 eq) and iodine (15 mmol, 3.8072 g, 1.5 eq) were dissolved in DMSO (15 mL). The mixture was stirred for 1h at 100 ℃ (temperature of the oil bath) and quenched with saturated aq. Na_2SO_3 (150 mL). The aqueous layer was extracted with EA (150 mL) for 2 times. The separated organic layer was dried over anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure to give the crude product, which was purified by column chromatographic on silica gel (200-300 mesh, eluent: petroleum ether/ethyl acetate 18:1).

Step 4[4]:

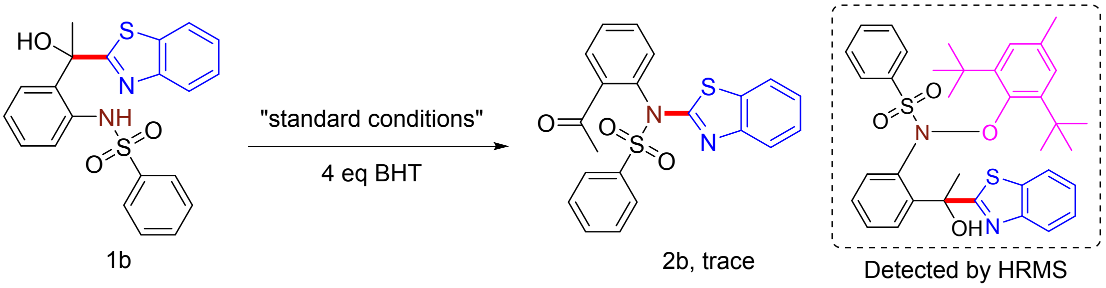
To a stirred solution of the *N*-(2-(benzo[*d*]thiazole-2-carbonyl)phenyl)benzenesulfon amide (3 mmol, 1.1821 g, 1.0 eq) in anhydrous THF (15 mL) was added dropwise the corresponding Grignard reagent (3.3 mmol, 1.1 eq) at -20℃. The mixture was stirred for 2h and quenched with saturated aq. NH_4Cl (100 mL). The aqueous layer was extracted with EA (120 mL) for 2 times. The separated organic layer was dried over anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure to give the crude product, which was purified by column chromatographic on silica gel (200-300 mesh).

2.2 Synthesis of the Catalysts[5]



The corresponding iodine benzene (3 mmol, 1eq), phenothiazine (1.1 eq, 3.3 mmol, 656.9 mg), K_2CO_3 (3 eq, 9 mmol, 1243.9 mg), $Pd(PPh_3)_2Cl_2$ (0.03 eq, 0.09 mmol, 63.2 mg) and P^tBu_3 (0.11 mmol, 66.8 mg) were added to a dry Schlenk tube. The flask was evacuated and backfilled with pure N_2 for 3 times. Then anhydrous toluene (10 mL) was added. The mixture was stirred at 110℃ (temperature of the oil bath) for 24h and quenched with saturated aq. NH_4Cl (150 mL). The aqueous layer was extracted with EA (150 mL). The separated organic layer was dried over anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure to give the crude product, which was purified by column chromatographic on silica gel (200-300 mesh).

3. Radical trapping experiment



An oven-dried 10 mL reaction tube equipped with a magnetic stir bar was charged with substrate 1b (0.3 mmol, 123.0 mg), PC 1 (0.015 mmol, 4.1 mg), Ag_2CO_3 (0.75 mmol, 206.8 mg), KH_2PO_4 (0.9 mmol, 122.5 mg) and BHT (1.2 mmol, 264.4 mg). Then, the tube was evacuated and backfilled with nitrogen (three times). Subsequently, 1,4-dioxane (3 mL) was injected into the tube under a nitrogen atmosphere. The reaction mixture was stirred under the irradiation of a 60 W blue LED at 60 ℃ for 48 h. And, the corresponding radical-trapping intermediate was detected by HRMS-ESI (Calcd for $C_{36}H_{41}N_2O_4S_2$ $[M+H]^+$: 629.2502; found: 629.2522. $C_{36}H_{40}N_2O_4S_2Na$ $[M+Na]^+$: 651.2322; found: 651.2345. Fig. S1).

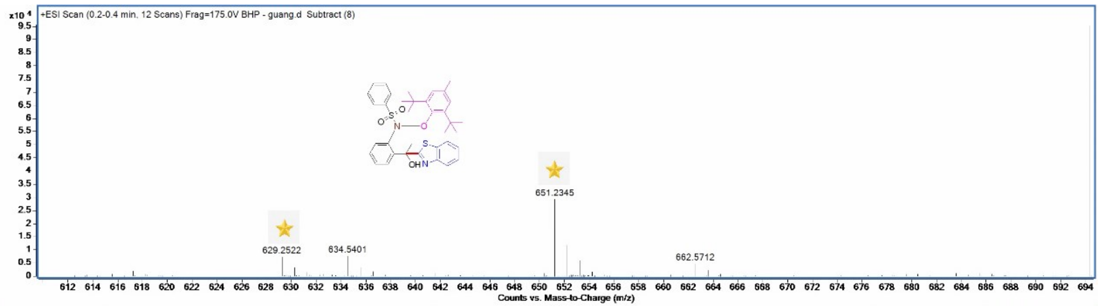


Fig. S1 HRMS (ESI) analysis of BHT trapping intermediate

4. References

[1] Youn, S. W.; Ko, T. Y.; Jang, Y. H. Palladium-catalyzed regioselective synthesis of 3-arylindoles from N-Ts-anilines and styrenes. *Angew. Chem., Int. Ed.,* **2017**, 56, 6636-6640.

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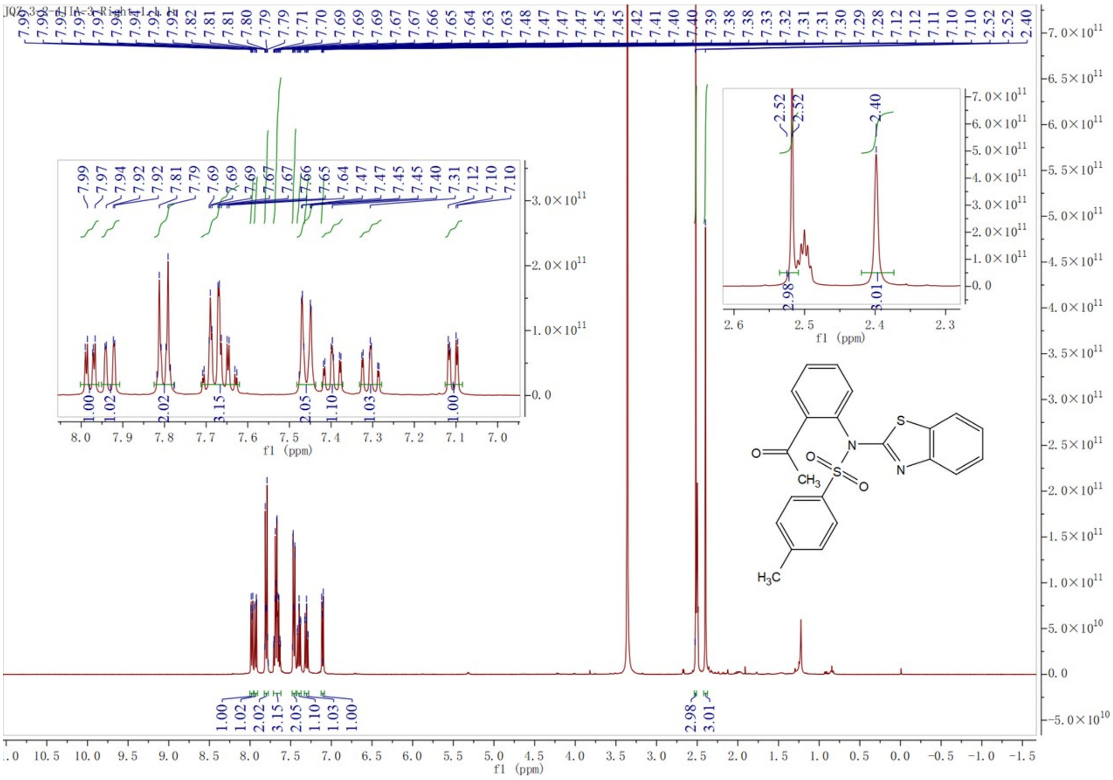
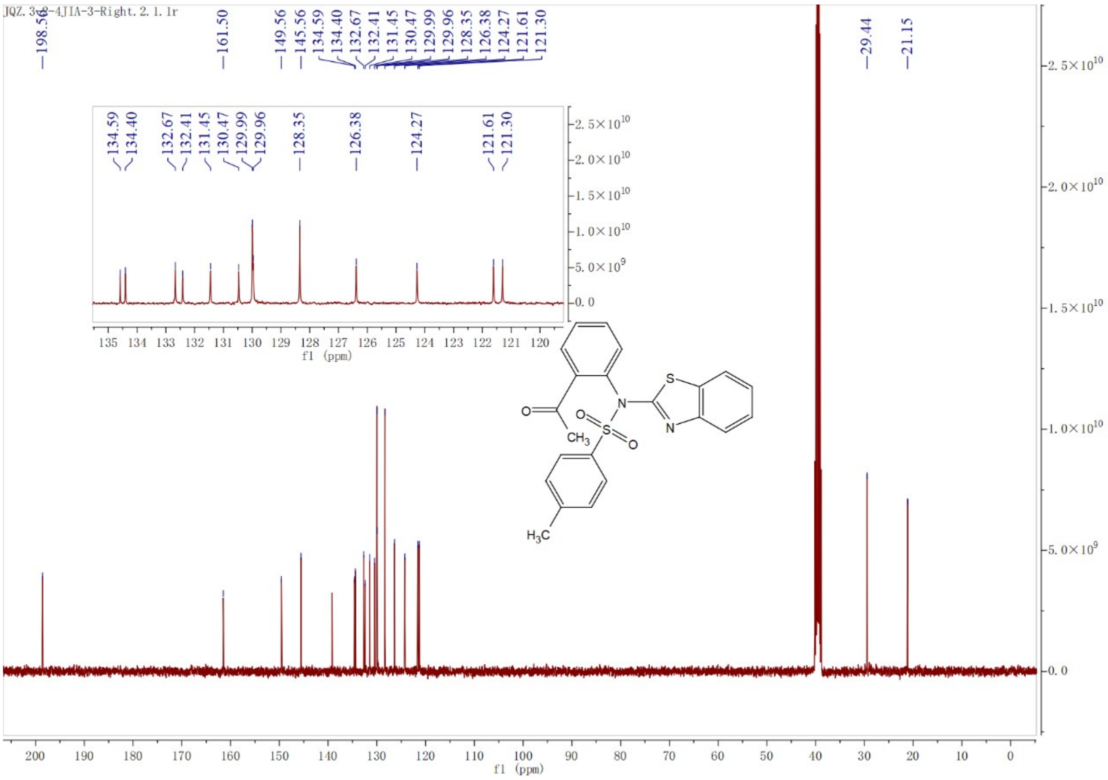
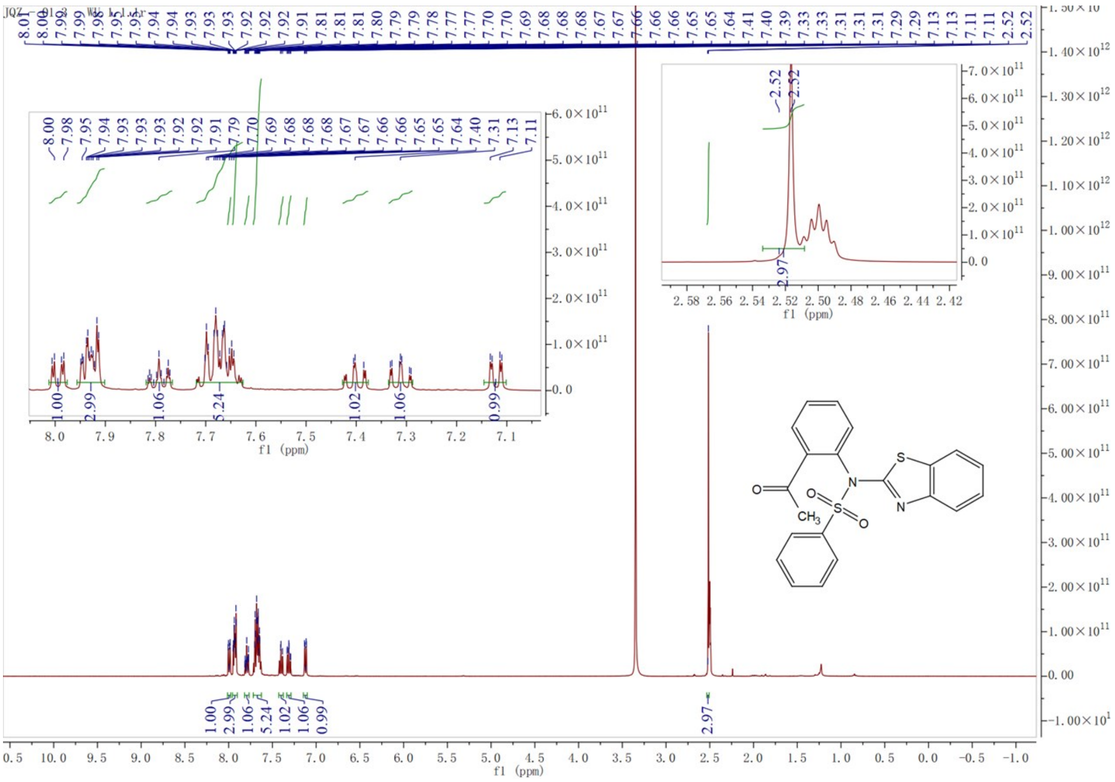
5. NMR-Spectra of 2



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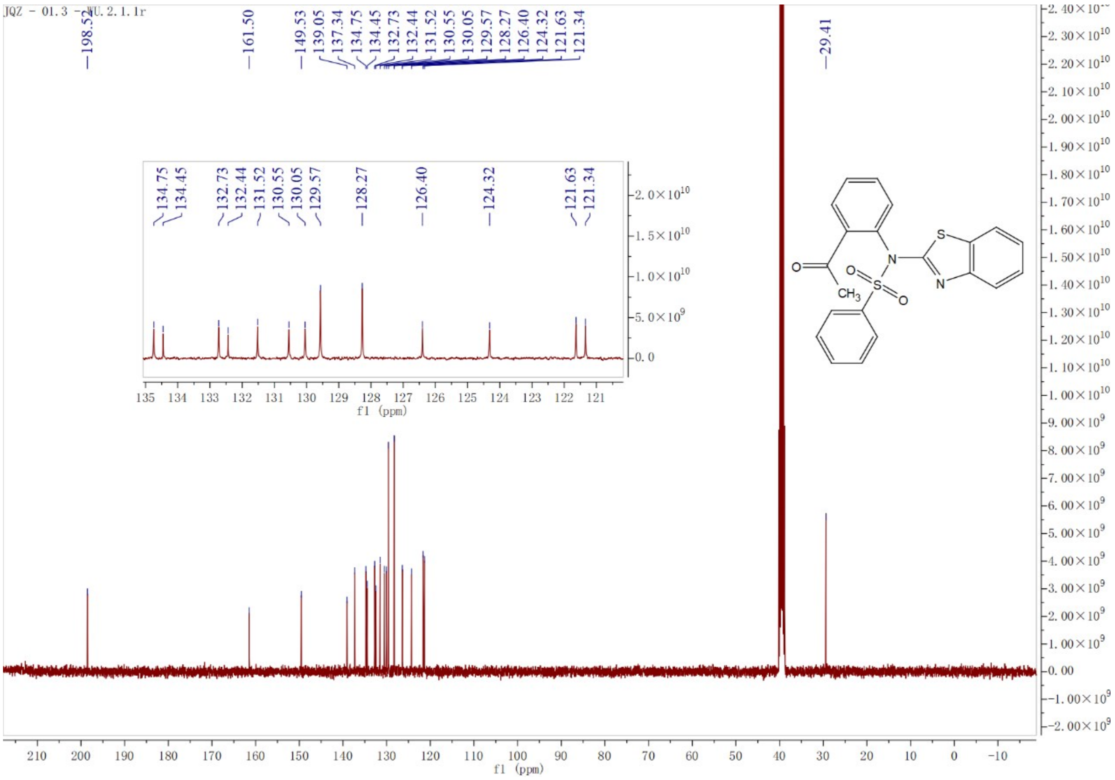
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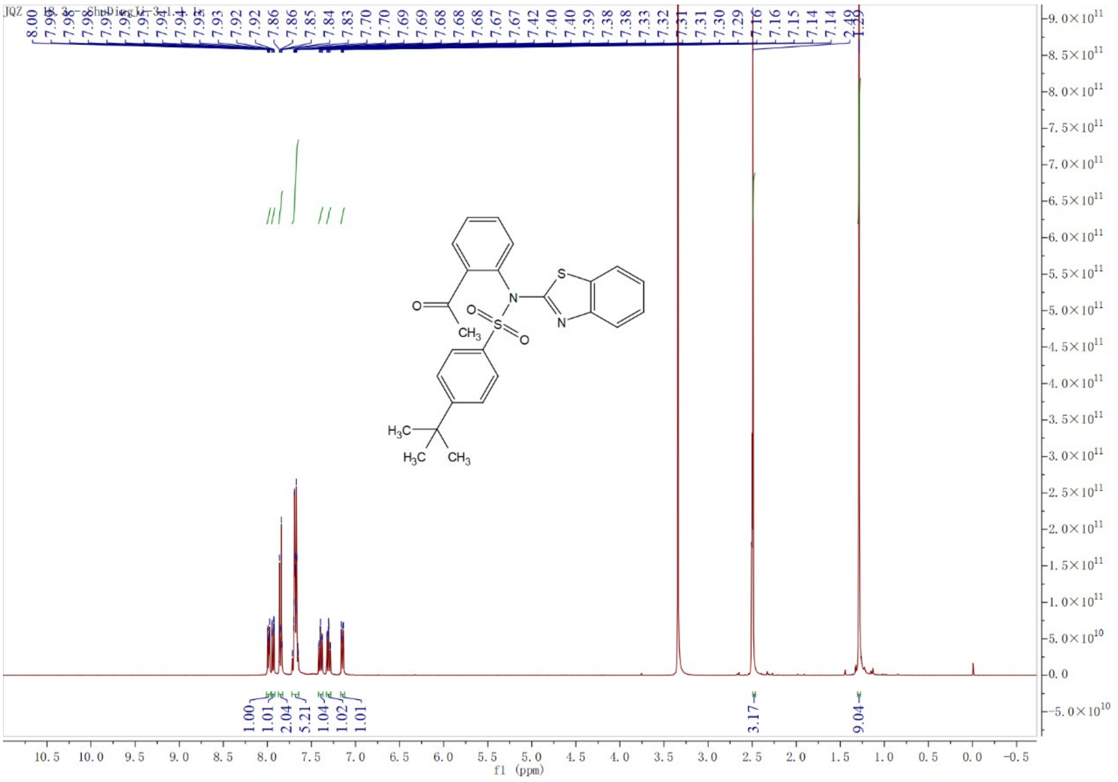
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H3C
CH3
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1.02
1.01
3.17
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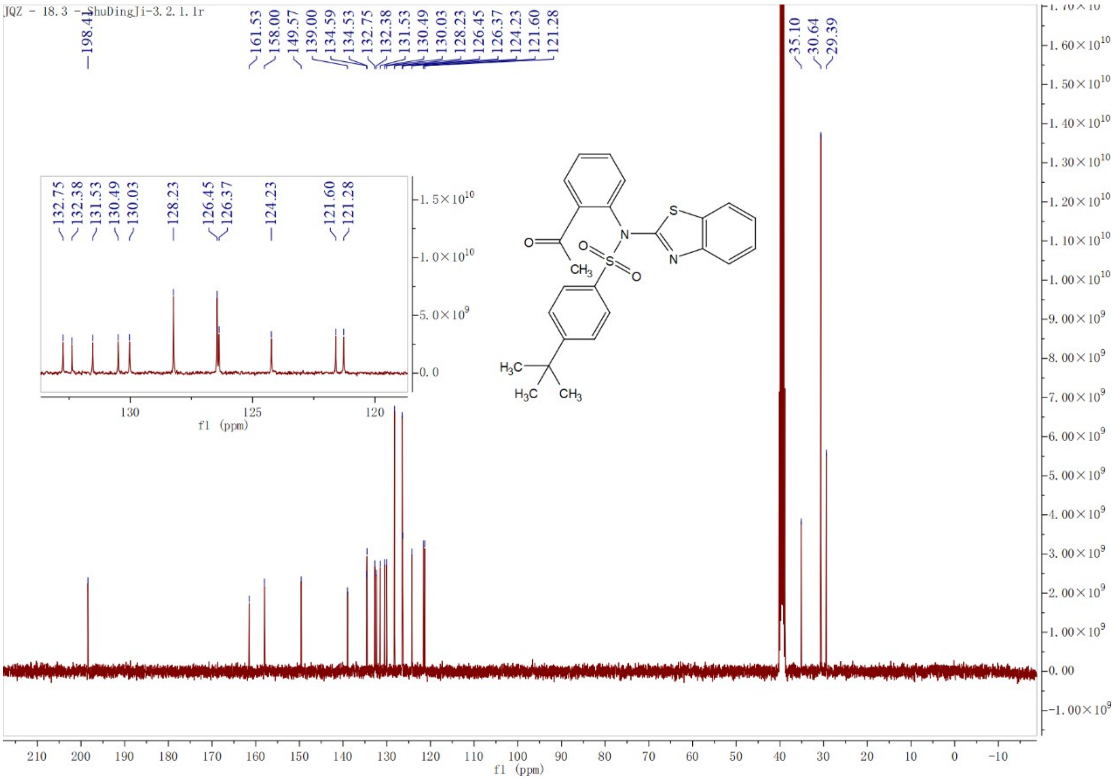
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H3C
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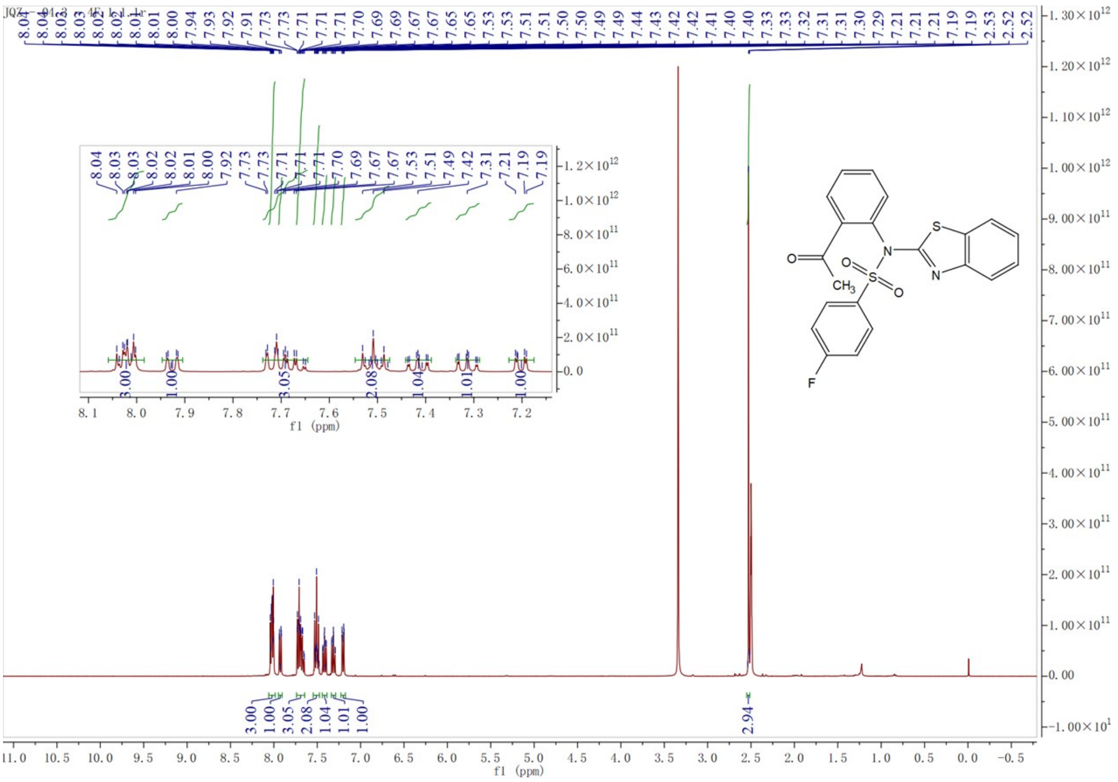
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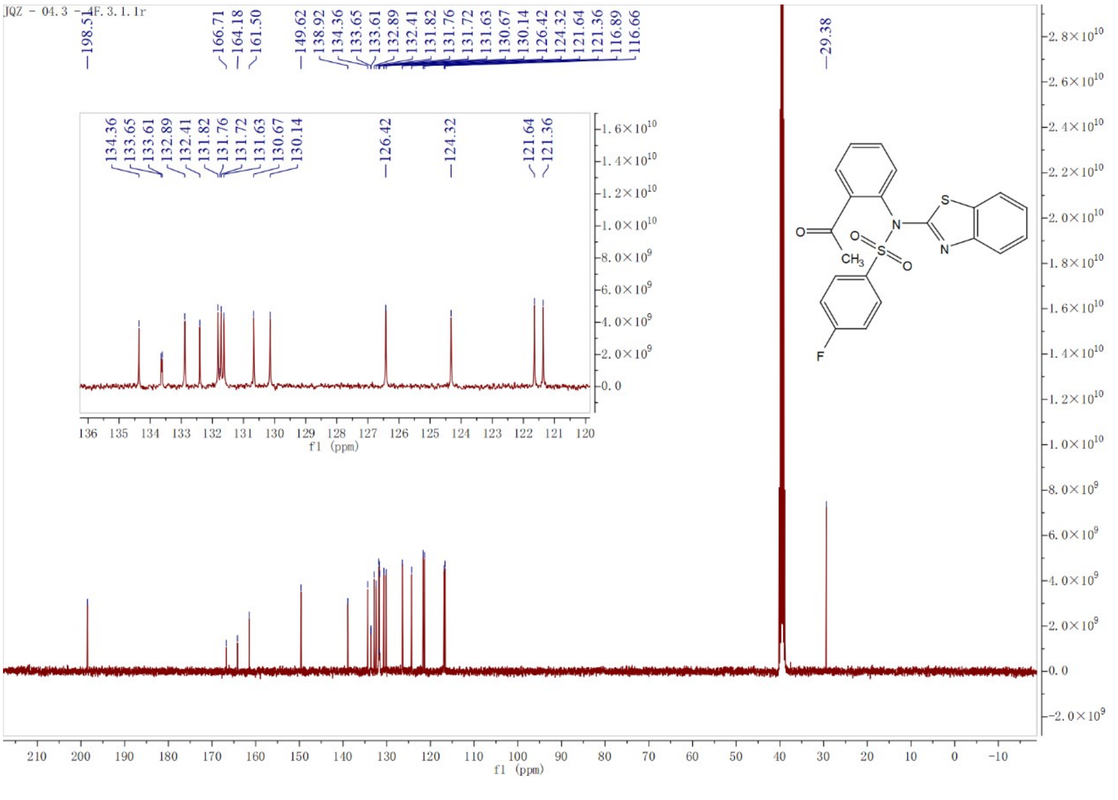
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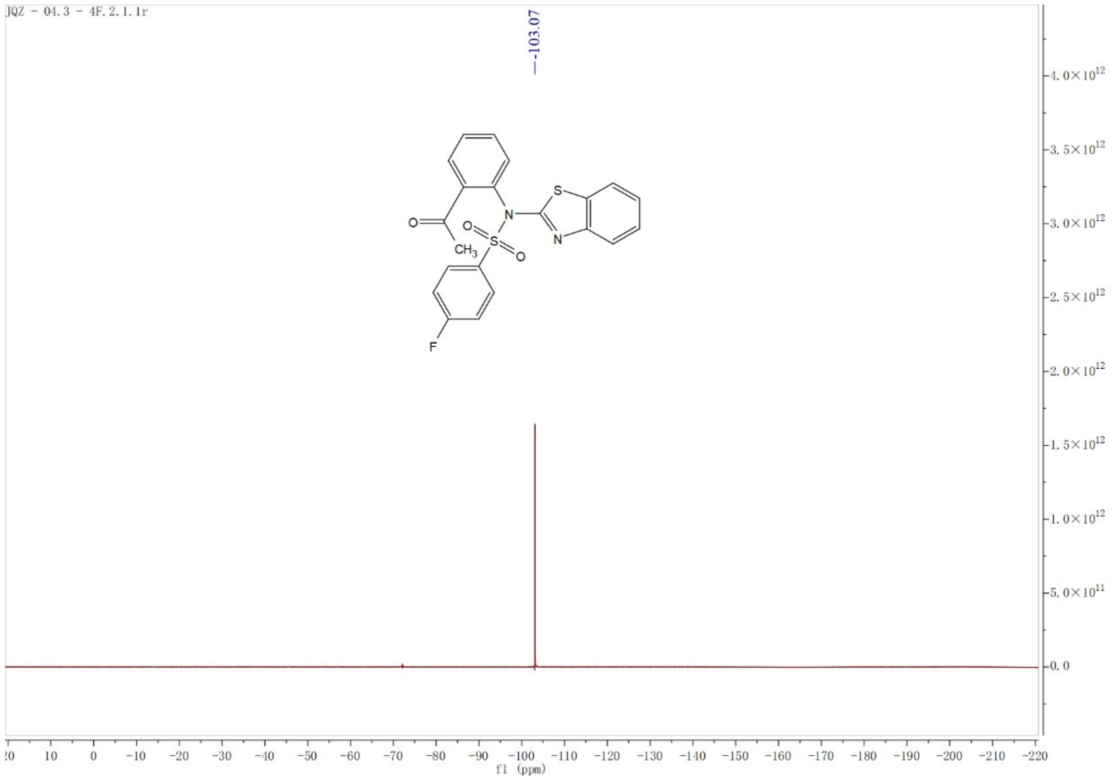
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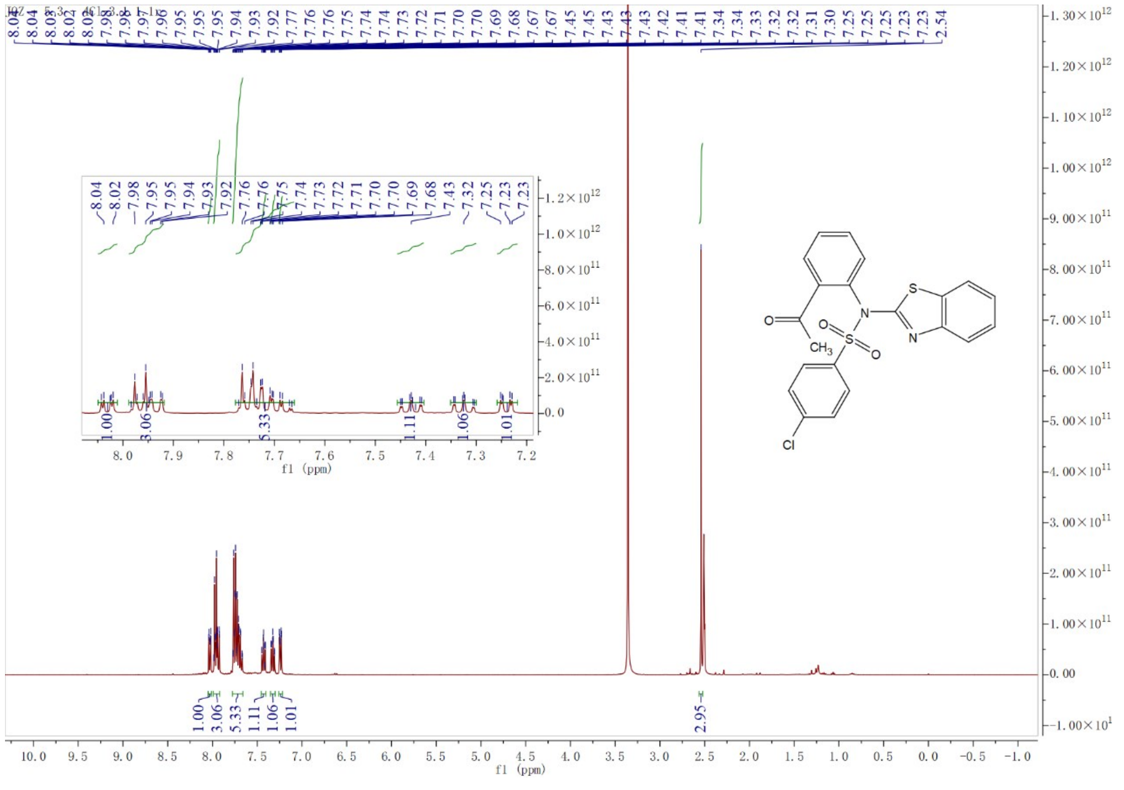
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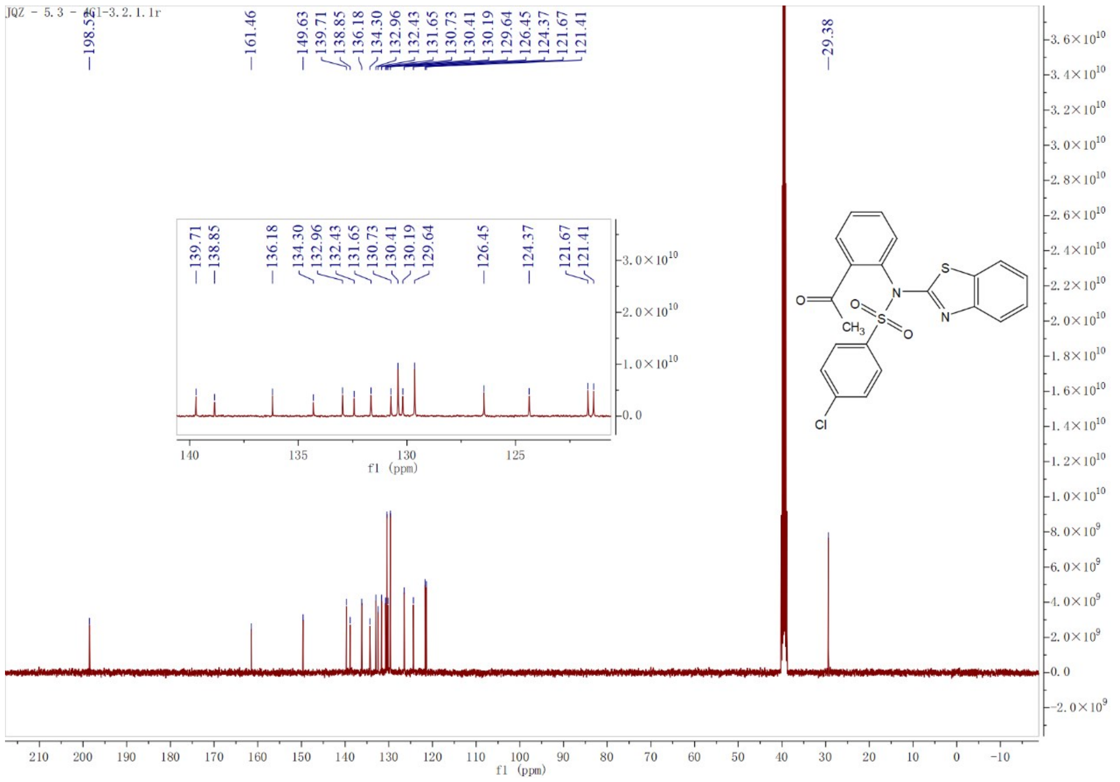
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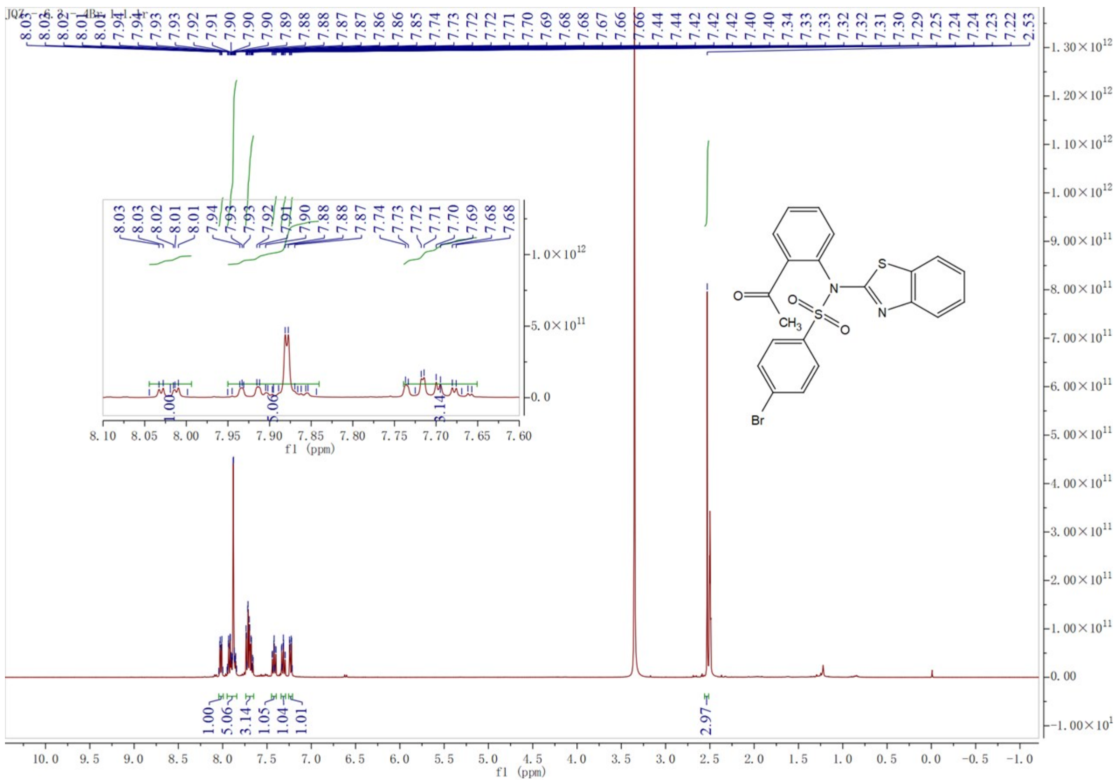
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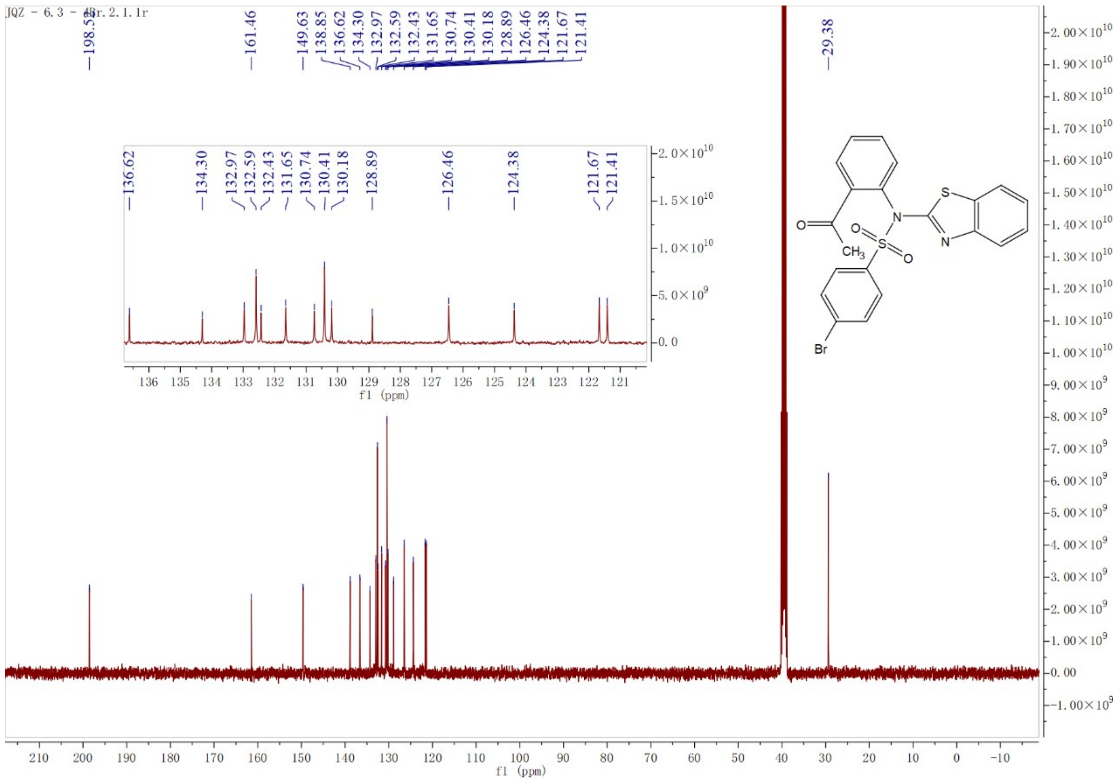
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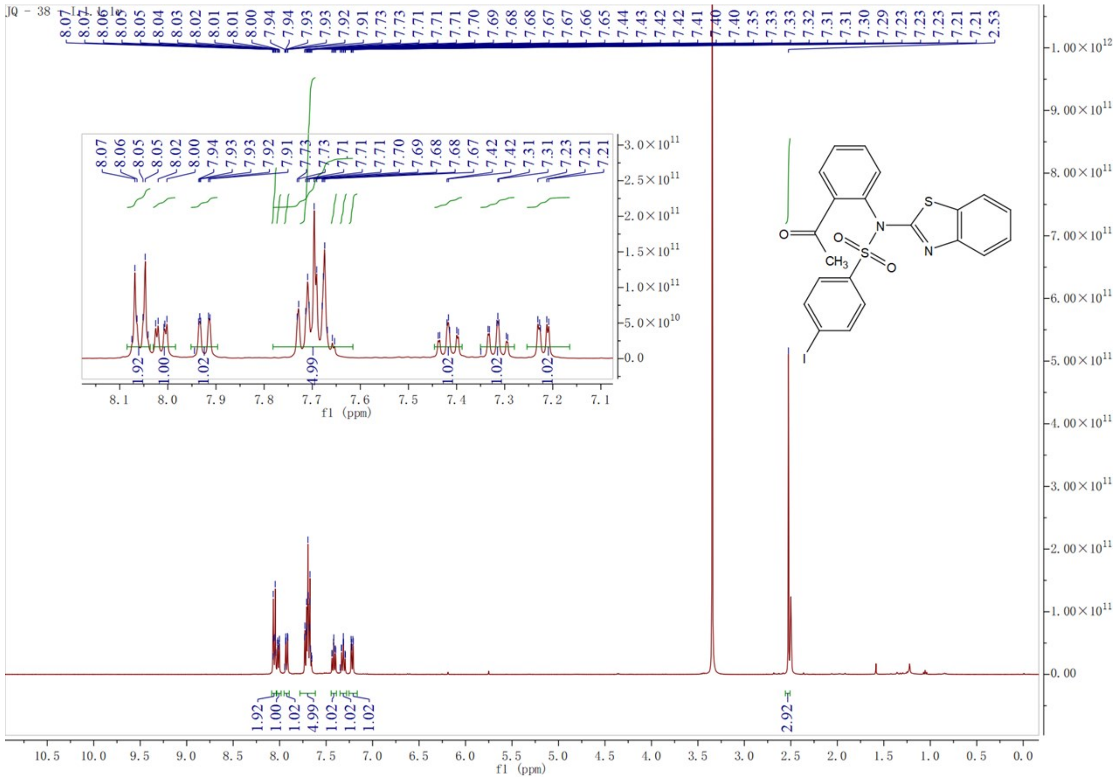
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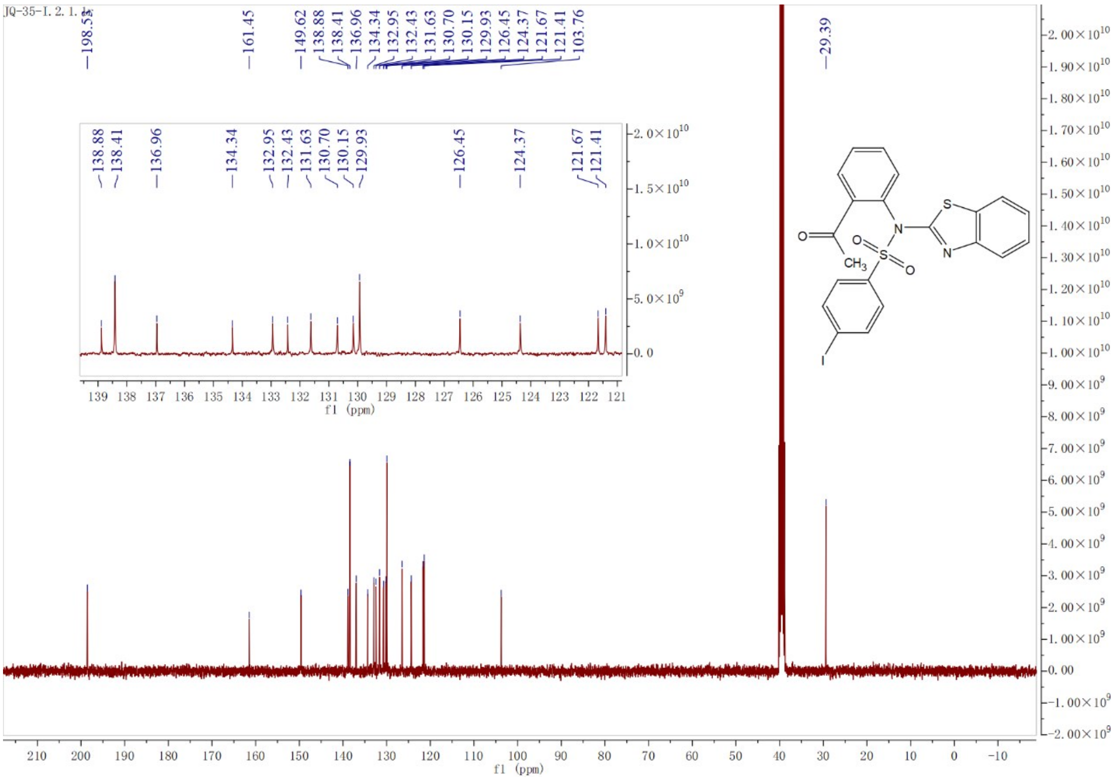
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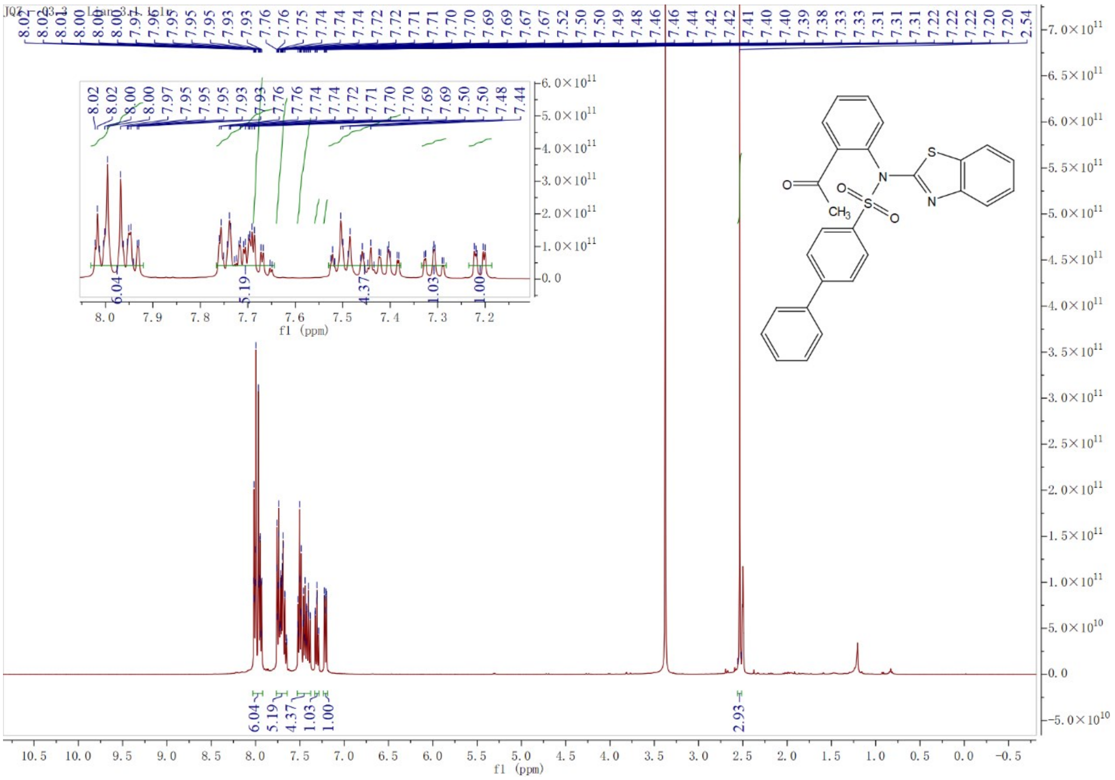
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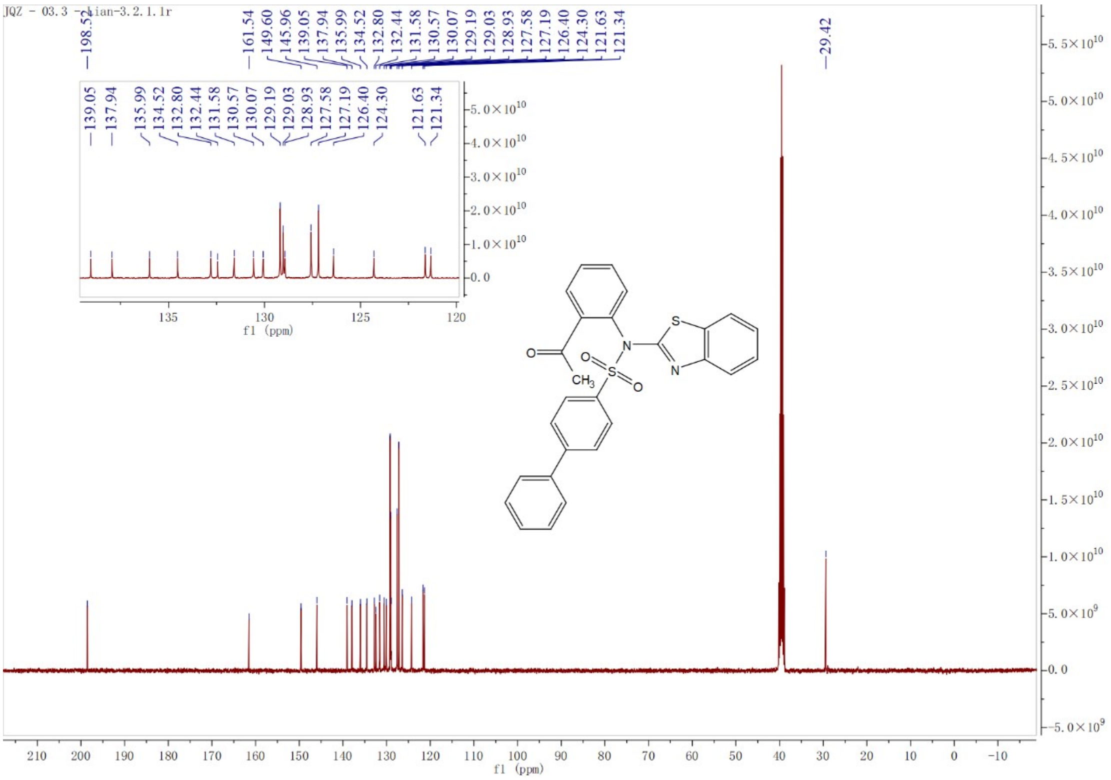
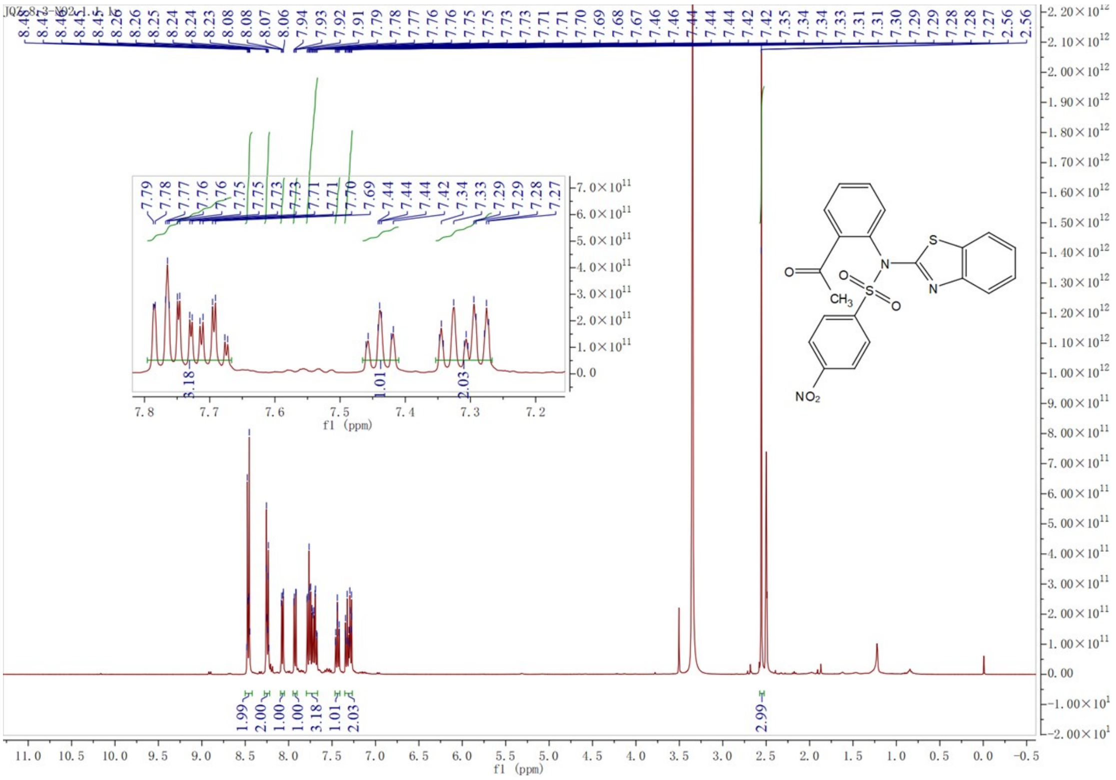
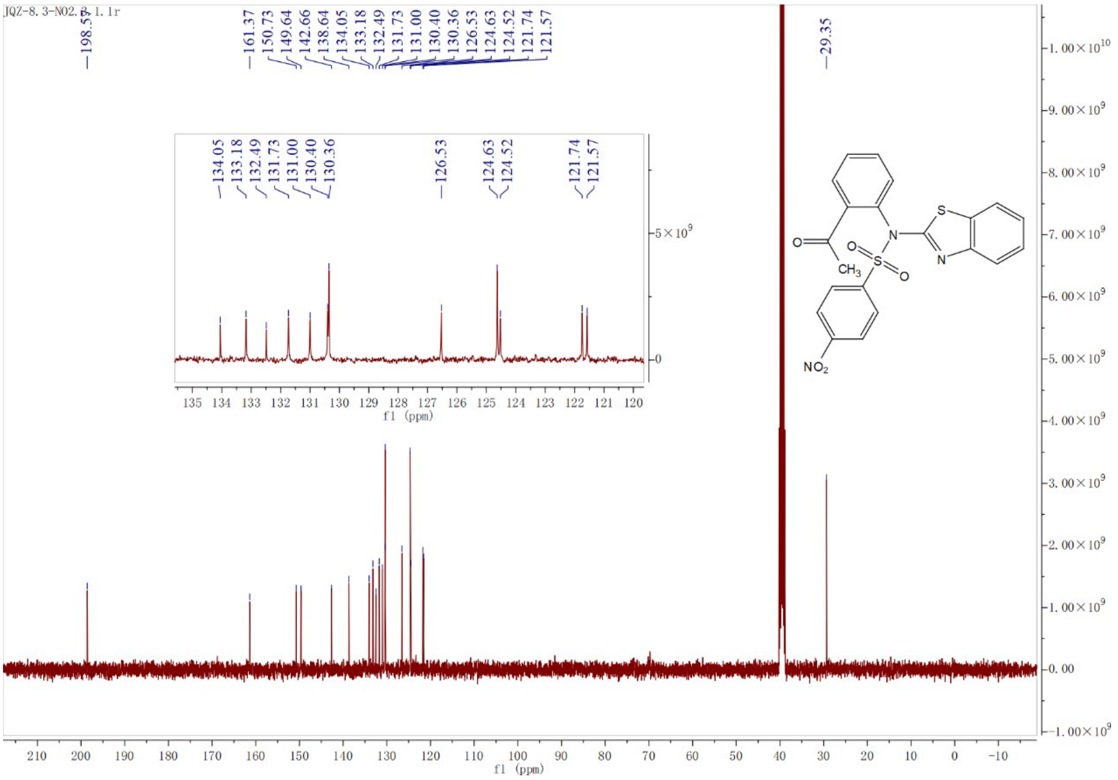
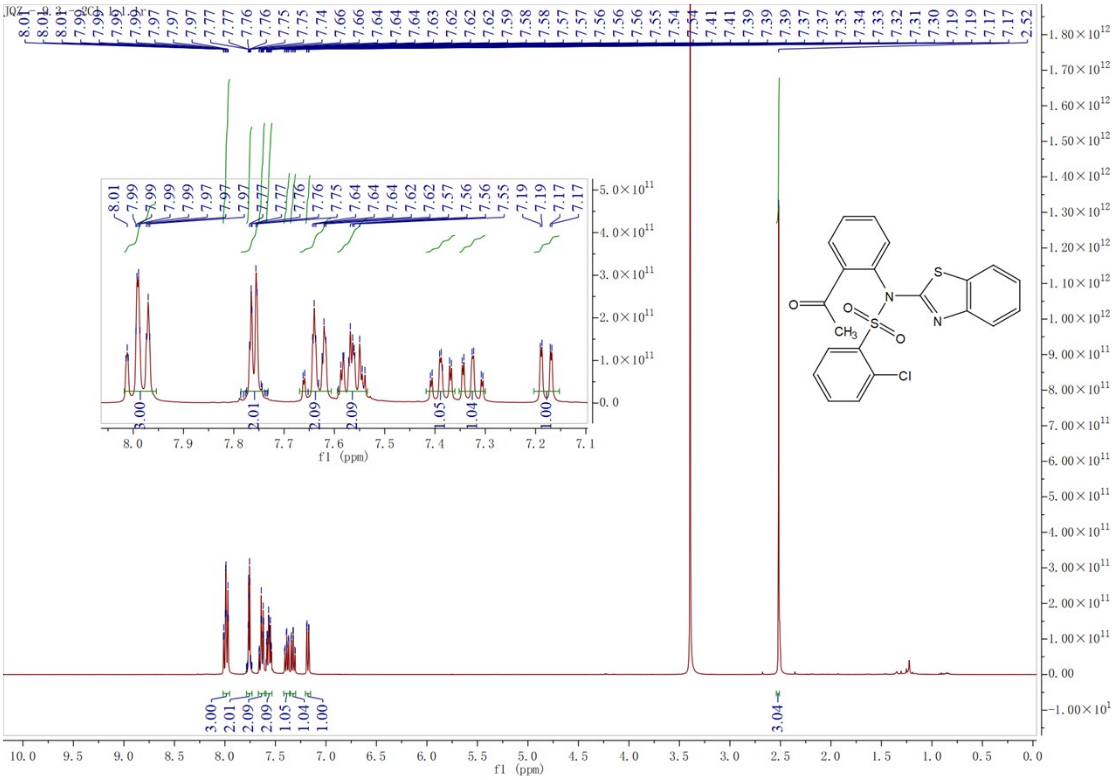
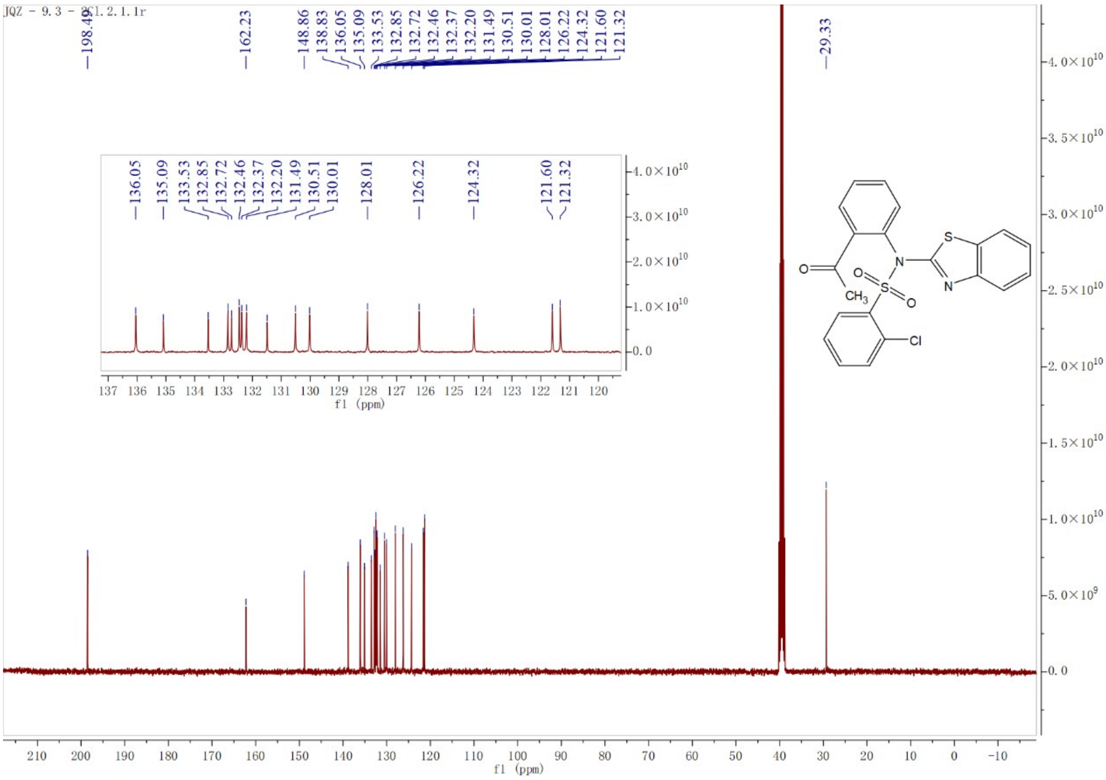
8.02 8.02 8.01 8.00 8.00 8.00 7.97 7.96 7.95 7.95 7.95 7.93 7.93 7.76 7.76 7.75 7.74 7.74 7.72 7.72 7.71 7.71 7.70 7.69 7.69 7.67 7.67 7.52 7.50 7.50 7.49 7.48 7.46 7.46 7.44 7.42 7.42 7.41 7.40 7.40 7.39 7.38 7.33 7.33 7.31 7.31 7.31 7.22 7.22 7.22 7.20 2.54
6.04
5.19
4.37
1.03
1.00
2.93
O
CH3
N
S
O
O
S
N
f1 (ppm)

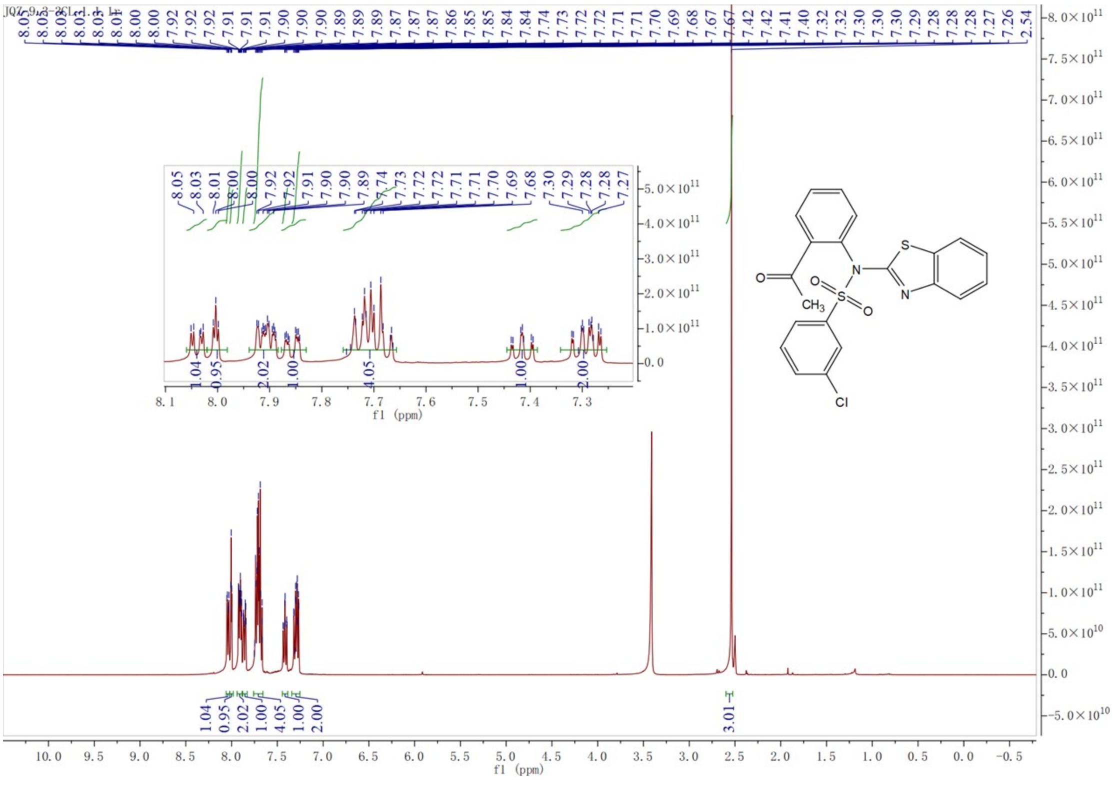

JQZ - 03.3 -lian-3.2.1.1r
198.52
161.54
149.60
145.96
139.05
137.94
135.99
134.52
132.80
132.44
131.58
130.57
130.07
129.19
129.03
128.93
127.58
127.19
126.40
124.30
121.63
121.34
29.42
O
CH3
N
S
N
S
O
O
f1 (ppm)

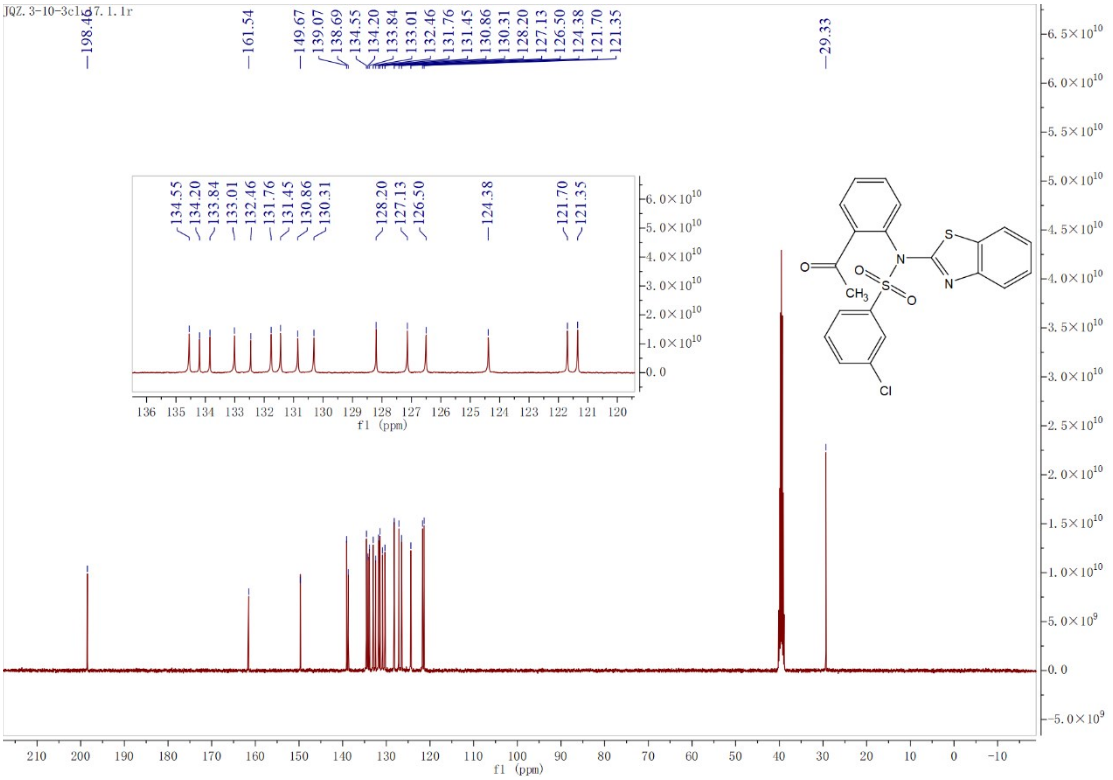

JQZ-8-3-NO2.1.1.1r
8.48
8.47
8.46
8.45
8.45
8.26
8.26
8.25
8.24
8.24
8.23
8.08
8.08
8.07
8.06
7.94
7.93
7.92
7.91
7.79
7.78
7.77
7.76
7.76
7.75
7.75
7.73
7.73
7.71
7.71
7.70
7.69
7.68
7.67
7.46
7.46
7.44
7.44
7.44
7.42
7.42
7.35
7.34
7.34
7.33
7.31
7.31
7.30
7.29
7.29
7.28
7.28
7.27
2.56
2.56
1.99
2.00
1.00
1.00
3.18
1.01
2.03
2.99
O
CH3
N
S
N
S
O
O
NO2
f1 (ppm)

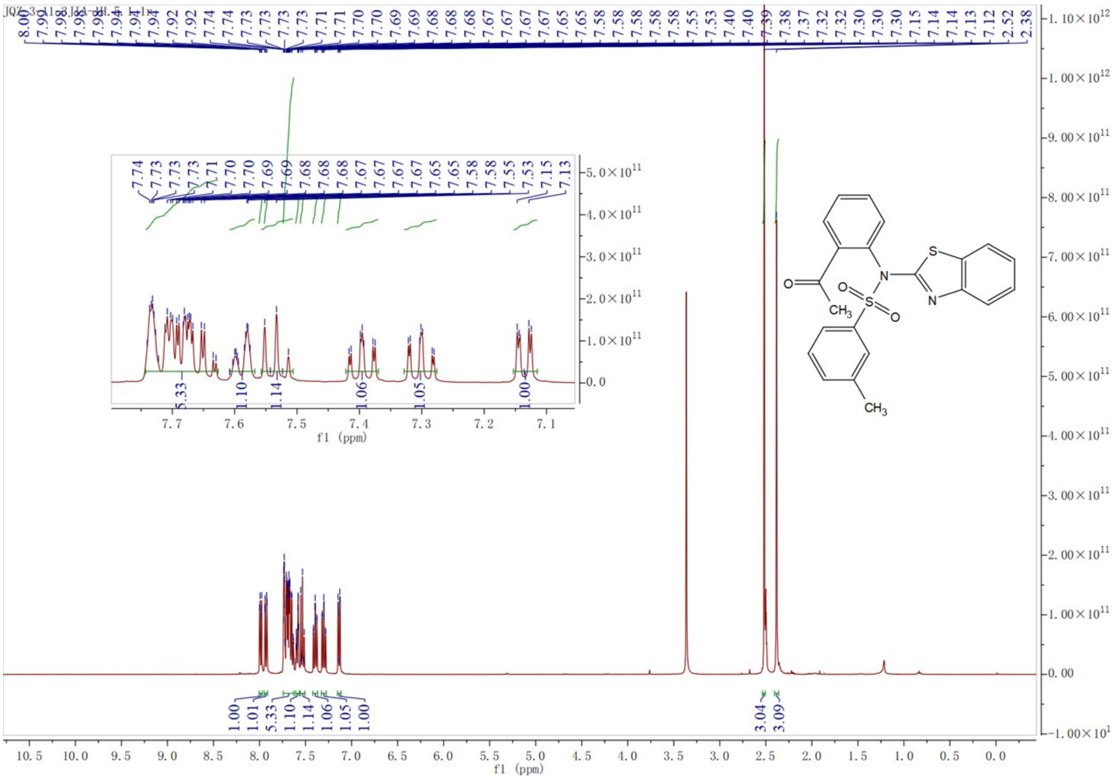

JQZ-8.3-NO2.3.1.1r
198.57
161.37
150.73
149.64
142.66
138.64
134.05
133.18
132.49
131.73
131.00
130.40
130.36
126.53
124.63
124.52
121.74
121.57
29.35
5×10⁹
0
135 134 133 132 131 130 129 128 127 126 125 124 123 122 121 120
f1 (ppm)
O
CH3
N
S
N
O
S
O
NO2
1.00×10¹⁰
9.00×10⁹
8.00×10⁹
7.00×10⁹
6.00×10⁹
5.00×10⁹
4.00×10⁹
3.00×10⁹
2.00×10⁹
1.00×10⁹
0.00
−1.00×10⁹
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

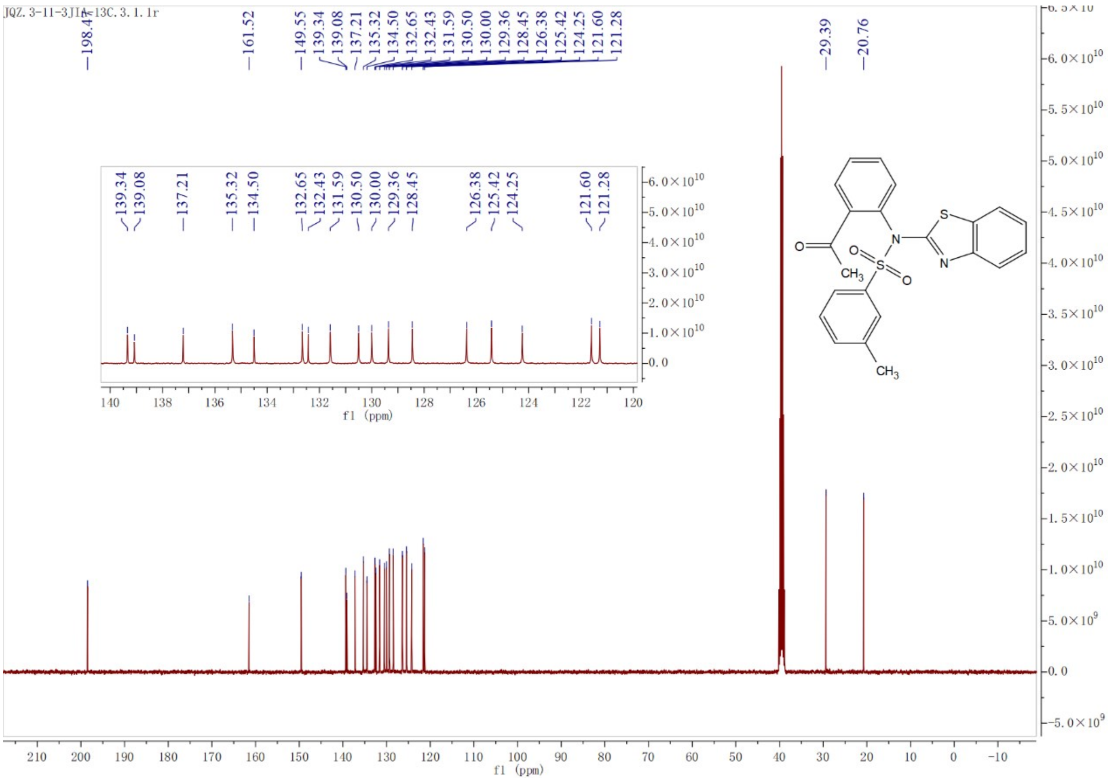

JQZ-9.3-2Cl.1.1.1r
8.01
8.01
8.01
7.99
7.99
7.99
7.99
7.97
7.97
7.97
7.77
7.77
7.76
7.76
7.75
7.75
7.74
7.66
7.64
7.64
7.63
7.62
7.62
7.59
7.58
7.58
7.57
7.56
7.56
7.56
7.55
7.54
7.54
7.41
7.39
7.39
7.37
7.35
7.34
7.33
7.32
7.31
7.30
7.19
7.19
7.17
7.17
2.52
3.00
2.01
2.09
2.09
1.05
1.04
1.00
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1
f1 (ppm)
5.0×10¹¹
4.0×10¹¹
3.0×10¹¹
2.0×10¹¹
1.0×10¹¹
0.0
O
CH3
N
S
N
O
S
O
Cl
3.04
1.80×10¹²
1.70×10¹²
1.60×10¹²
1.50×10¹²
1.40×10¹²
1.30×10¹²
1.20×10¹²
1.10×10¹²
1.00×10¹²
9.00×10¹¹
8.00×10¹¹
7.00×10¹¹
6.00×10¹¹
5.00×10¹¹
4.00×10¹¹
3.00×10¹¹
2.00×10¹¹
1.00×10¹¹
0.00
−1.00×10¹
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

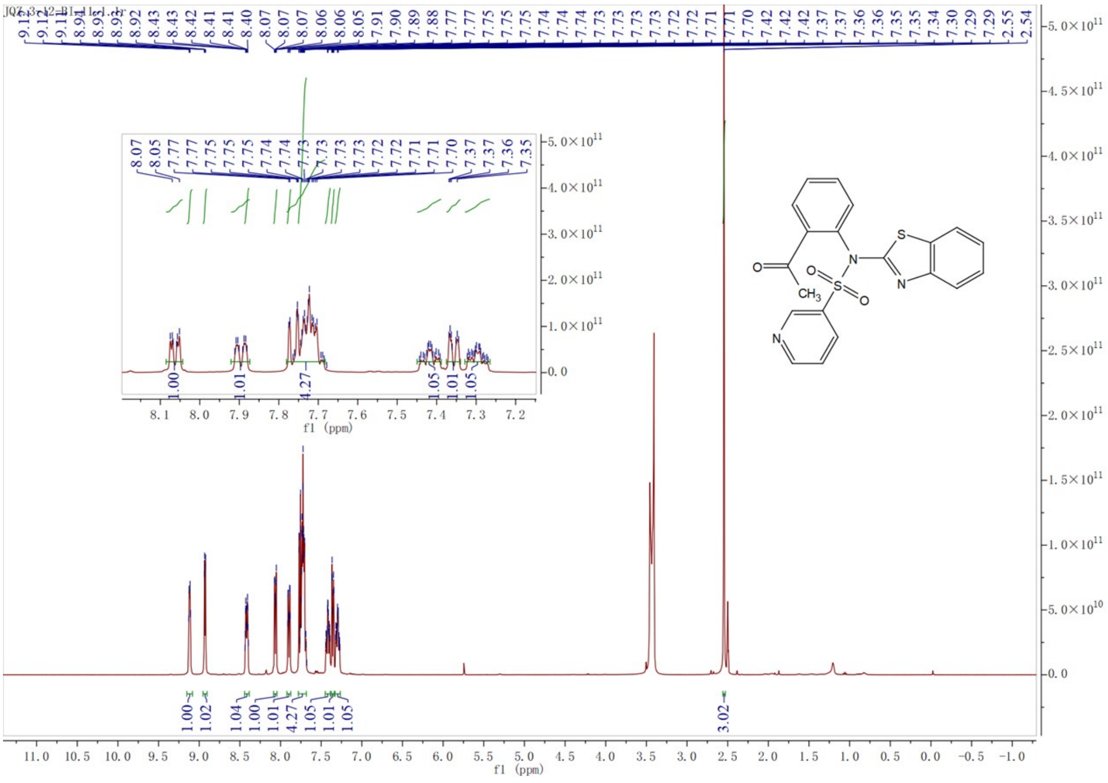

JQZ - 9.3 - 2Cl.2.1.1r
198.49
162.23
148.86
138.83
136.05
135.09
133.53
132.85
132.72
132.46
132.37
132.20
131.49
130.51
130.01
128.01
126.22
124.32
121.60
121.32
29.33
f1 (ppm)
O
N
S
CH3
Cl

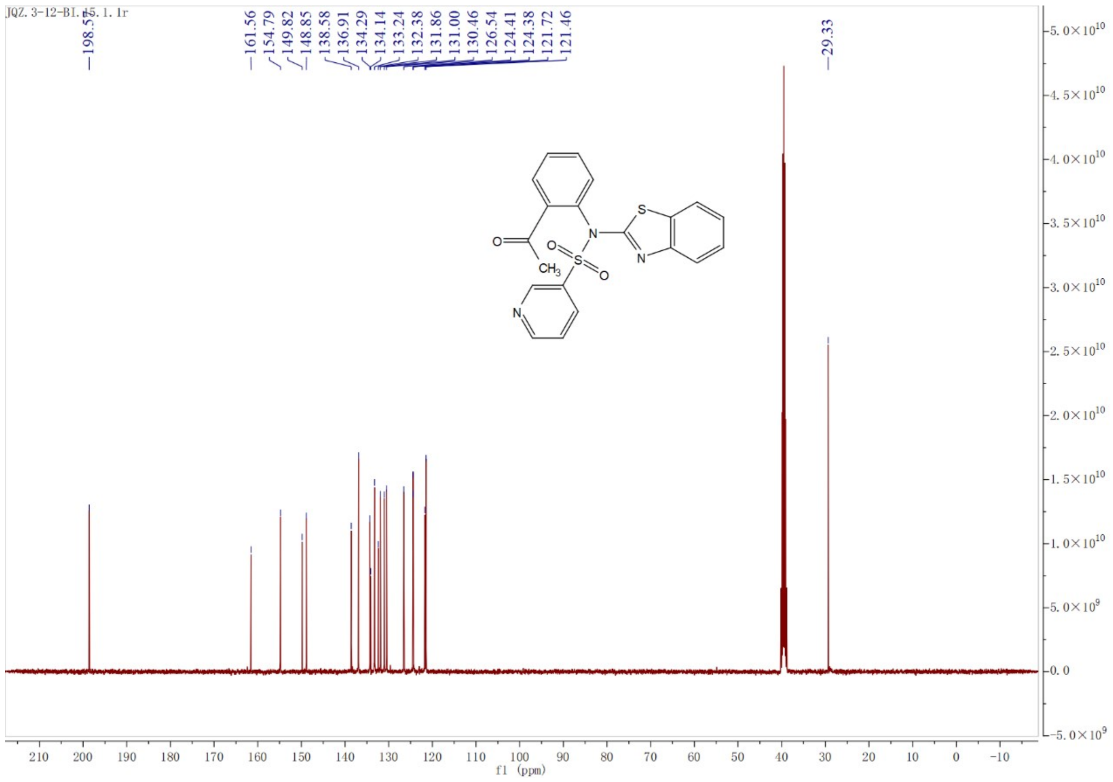

8.05
8.03
8.01
8.00
7.92
7.91
7.90
7.89
7.87
7.86
7.85
7.84
7.74
7.73
7.72
7.71
7.70
7.69
7.68
7.67
7.42
7.41
7.40
7.32
7.30
7.29
7.28
7.27
7.26
2.54
1.04
0.95
2.02
1.00
4.05
1.00
2.00
3.01
f1 (ppm)
O
N
S
CH3
Cl

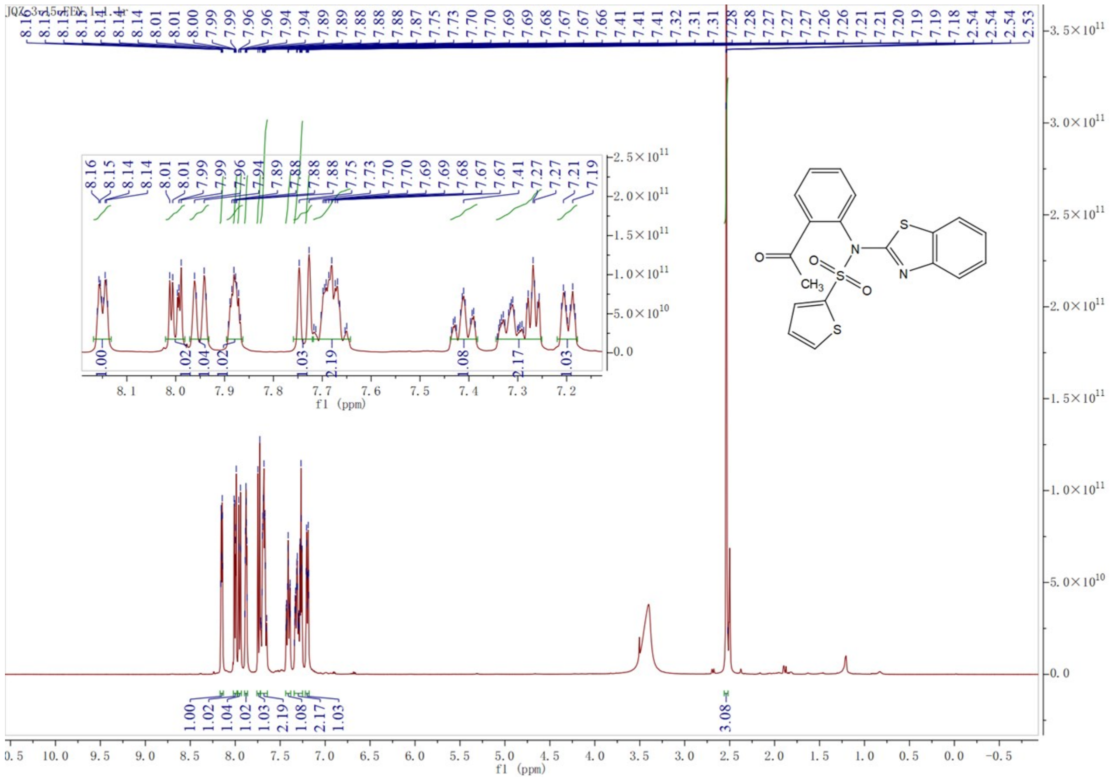

JQZ.3-10-3cl.17.1.1r
198.46
161.54
149.67
139.07
138.69
134.55
134.20
133.84
133.01
132.46
131.76
131.45
130.86
130.31
128.20
127.13
126.50
124.38
121.70
121.35
29.33
f1 (ppm)
S
N
N
O
CH3
O
S
O
Cl

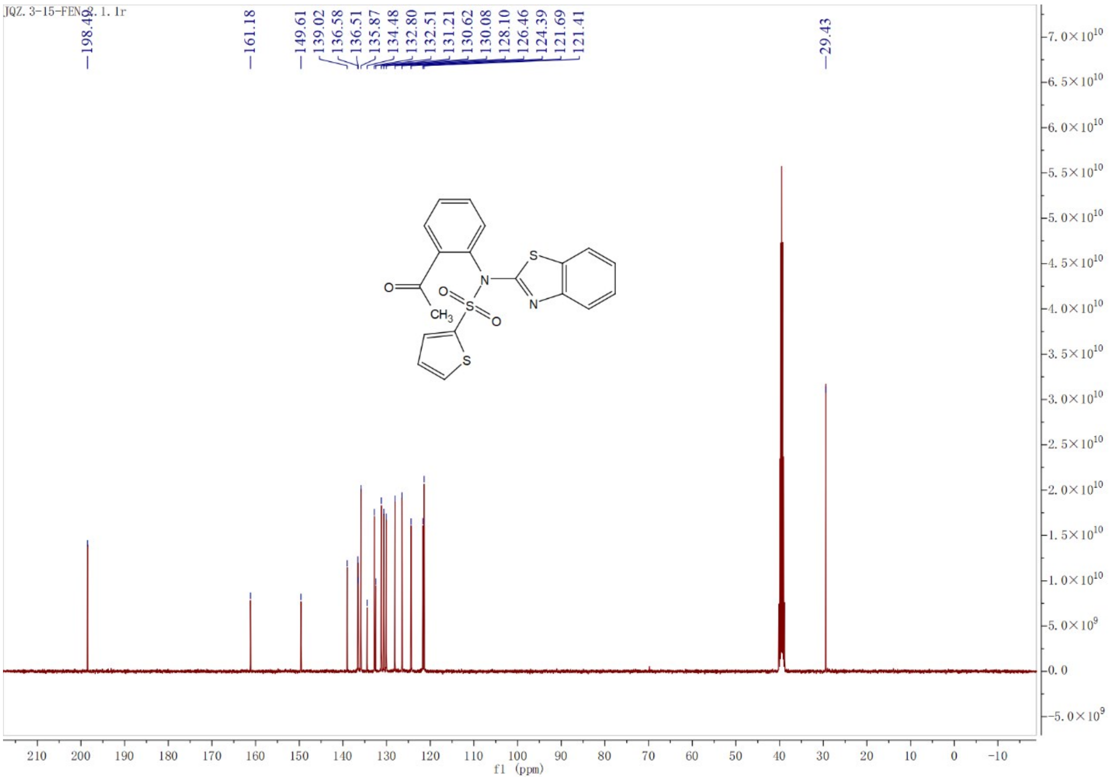

JQZ-3-11-3JJA-1H.5.1.1r
8.00
7.99
7.98
7.98
7.98
7.94
7.94
7.94
7.92
7.92
7.74
7.74
7.73
7.73
7.73
7.73
7.71
7.71
7.70
7.70
7.69
7.69
7.68
7.68
7.68
7.67
7.67
7.67
7.67
7.65
7.58
7.58
7.58
7.58
7.58
7.55
7.53
7.40
7.40
7.39
7.38
7.37
7.32
7.32
7.30
7.30
7.30
7.15
7.14
7.14
7.13
7.12
2.52
2.38
1.00
1.01
5.33
1.10
1.14
1.06
1.05
1.00
3.04
3.09
f1 (ppm)
S
N
N
O
CH3
O
S
O
CH3

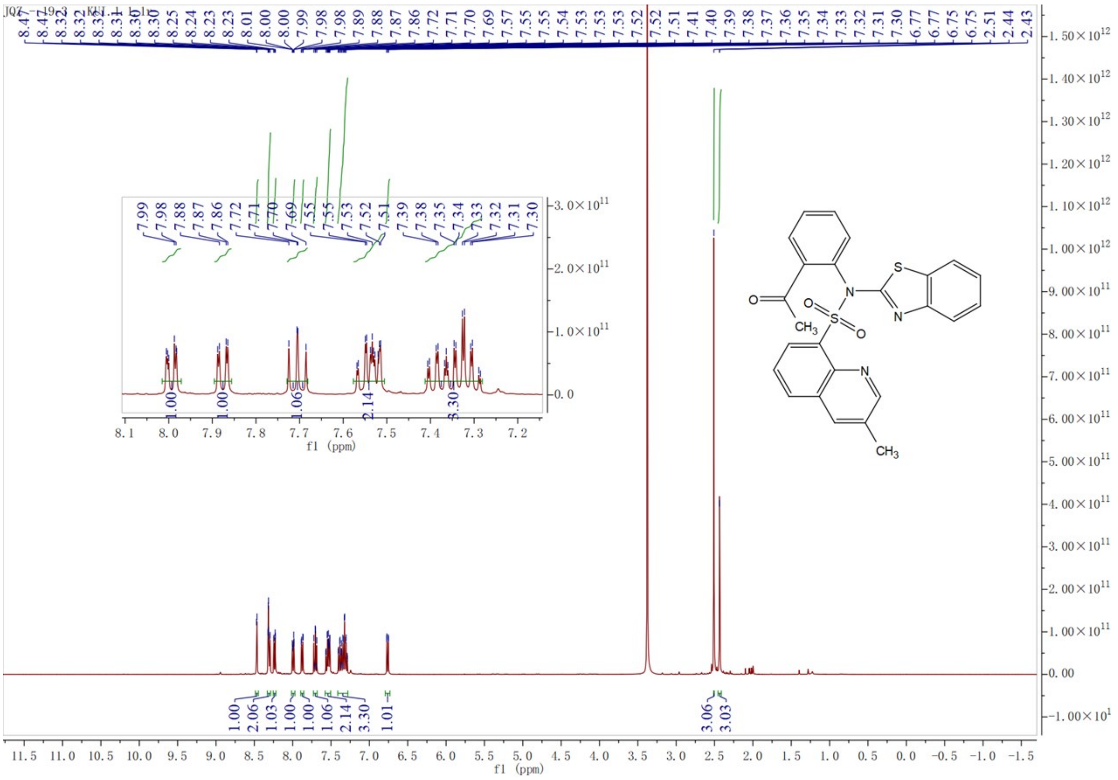

JQZ.3-11-3JIA-13C.3.1.1r
198.47
161.52
149.55
139.34
139.08
137.21
135.32
134.50
132.65
132.43
131.59
130.50
130.00
129.36
128.45
126.38
125.42
124.25
121.60
121.28
29.39
20.76
O
CH3
N
S
N
O
S
O
CH3
f1 (ppm)

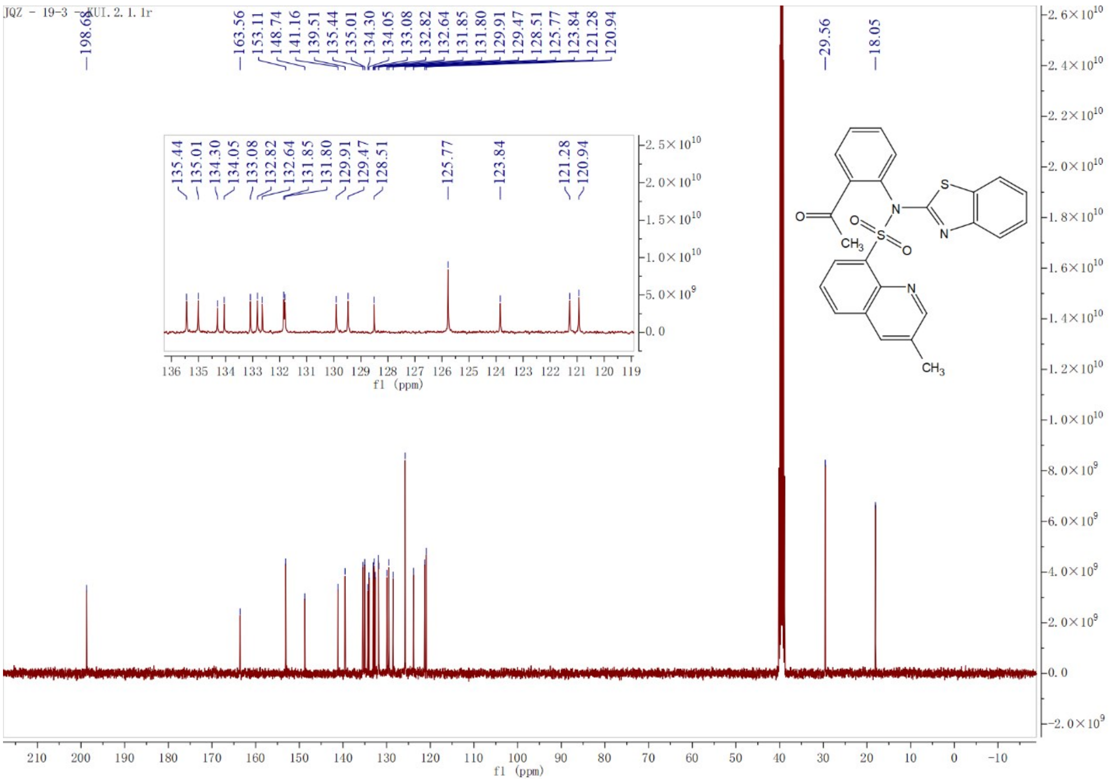

9.12
9.12
9.11
8.94
8.93
8.93
8.92
8.43
8.43
8.42
8.41
8.41
8.40
8.07
8.07
8.07
8.06
8.06
8.05
7.91
7.90
7.89
7.88
7.77
7.77
7.75
7.75
7.75
7.74
7.74
7.74
7.73
7.73
7.73
7.73
7.72
7.72
7.71
7.71
7.71
7.70
7.42
7.42
7.37
7.37
7.36
7.35
7.35
7.34
7.30
7.29
2.55
2.54
1.00
1.02
1.04
1.00
1.01
4.27
1.05
1.01
1.05
3.02
O
CH3
N
S
N
O
S
O
N
f1 (ppm)

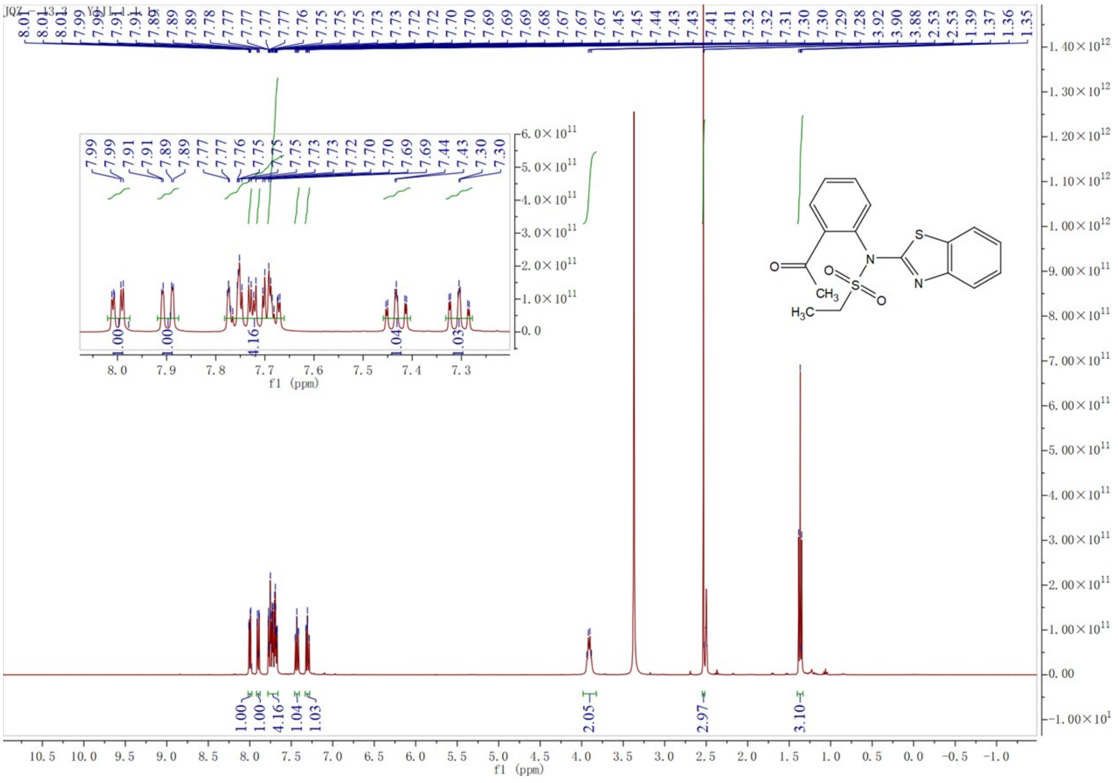

JQZ.3-12-B1.15.1.1r
198.5
161.56
154.79
149.82
148.85
138.58
136.91
134.29
134.14
133.24
132.38
131.86
131.00
130.46
126.54
124.41
124.38
121.72
121.46
29.33
O
CH3
N
S
N
O
S
O
N
5.0×10^10
4.5×10^10
4.0×10^10
3.5×10^10
3.0×10^10
2.5×10^10
2.0×10^10
1.5×10^10
1.0×10^10
5.0×10^9
0.0
−5.0×10^9
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

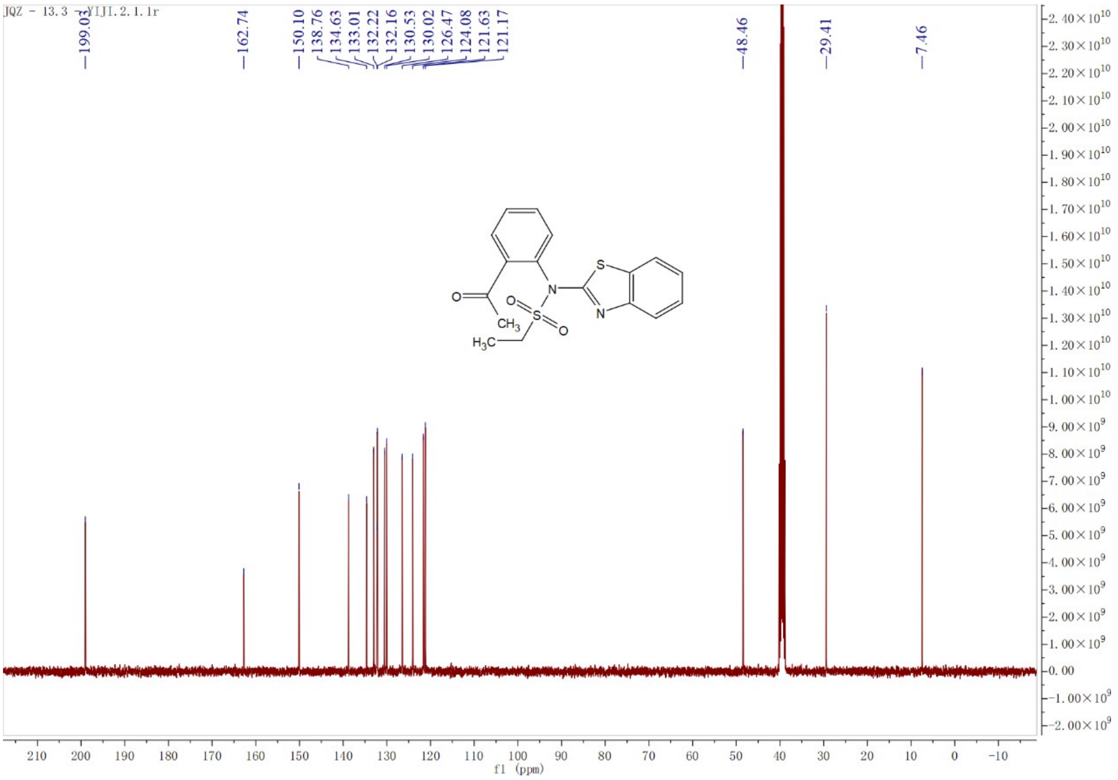

JQZ.3-15-FEN.1.1.1r
8.15
8.14
8.14
8.01
8.00
7.99
7.99
7.96
7.96
7.94
7.94
7.89
7.89
7.88
7.88
7.87
7.75
7.73
7.70
7.70
7.69
7.69
7.68
7.67
7.67
7.66
7.41
7.41
7.41
7.32
7.31
7.31
7.28
7.28
7.27
7.27
7.27
7.26
7.21
7.21
7.20
7.19
7.19
7.18
2.54
2.54
2.54
2.53
8.16 8.15 8.14 8.14 8.01 8.01 7.99 7.99 7.96 7.94 7.89 7.88 7.88 7.75 7.73 7.70 7.70 7.69 7.68 7.67 7.41 7.27 7.27 7.21 7.19
2.5×10^11
2.0×10^11
1.5×10^11
1.0×10^11
5.0×10^10
0.0
1.00 1.02 1.04 1.02 1.03 2.19 1.08 2.17 1.03
8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2
f1 (ppm)
O
CH3
N
S
N
O
S
O
S
3.5×10^11
3.0×10^11
2.5×10^11
2.0×10^11
1.5×10^11
1.0×10^11
5.0×10^10
0.0
1.00 1.02 1.04 1.02 1.03 2.19 1.08 2.17 1.03
3.08
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
f1 (ppm)

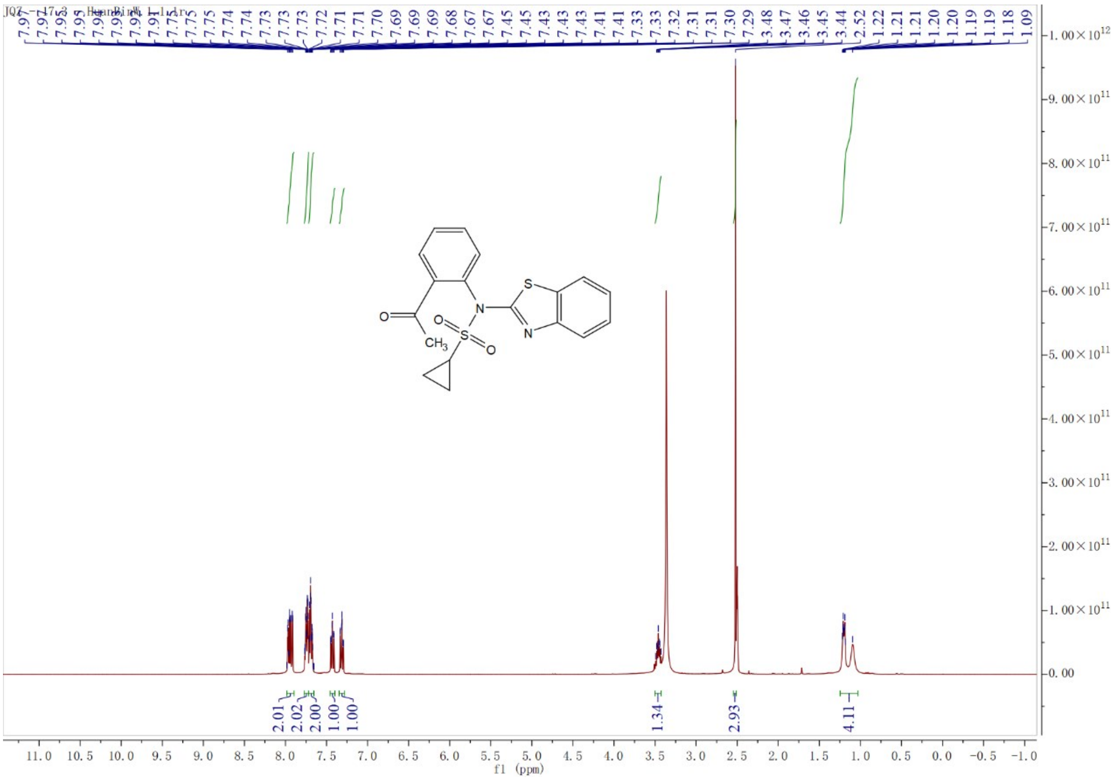

JQZ.3-15-FEN.2.1.1r
198.49
161.18
149.61
139.02
136.58
136.51
135.87
134.48
132.80
132.51
131.21
130.62
130.08
128.10
126.46
124.39
121.69
121.41
29.43
O
CH3
N
S
O
O
S
N
S
f1 (ppm)

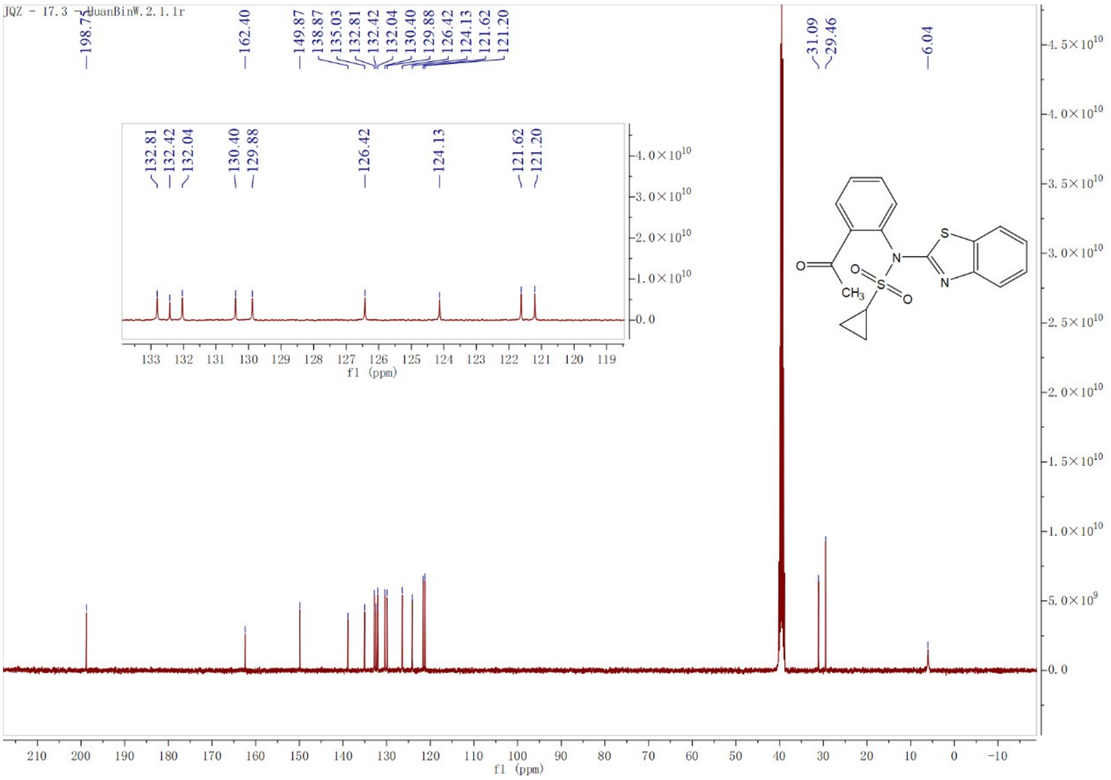

8.47
8.47
8.32
8.32
8.32
8.31
8.30
8.25
8.24
8.23
8.23
8.01
8.00
8.00
7.99
7.98
7.98
7.89
7.88
7.87
7.86
7.72
7.71
7.70
7.69
7.57
7.55
7.55
7.54
7.53
7.53
7.53
7.52
7.52
7.52
7.51
7.41
7.40
7.39
7.38
7.37
7.36
7.35
7.34
7.33
7.32
7.31
7.30
6.77
6.77
6.75
6.75
2.51
2.44
2.43
1.00
2.06
1.03
1.00
1.00
1.06
2.14
3.30
1.01
3.06
3.03
O
CH3
N
S
O
O
S
N
N
CH3
f1 (ppm)

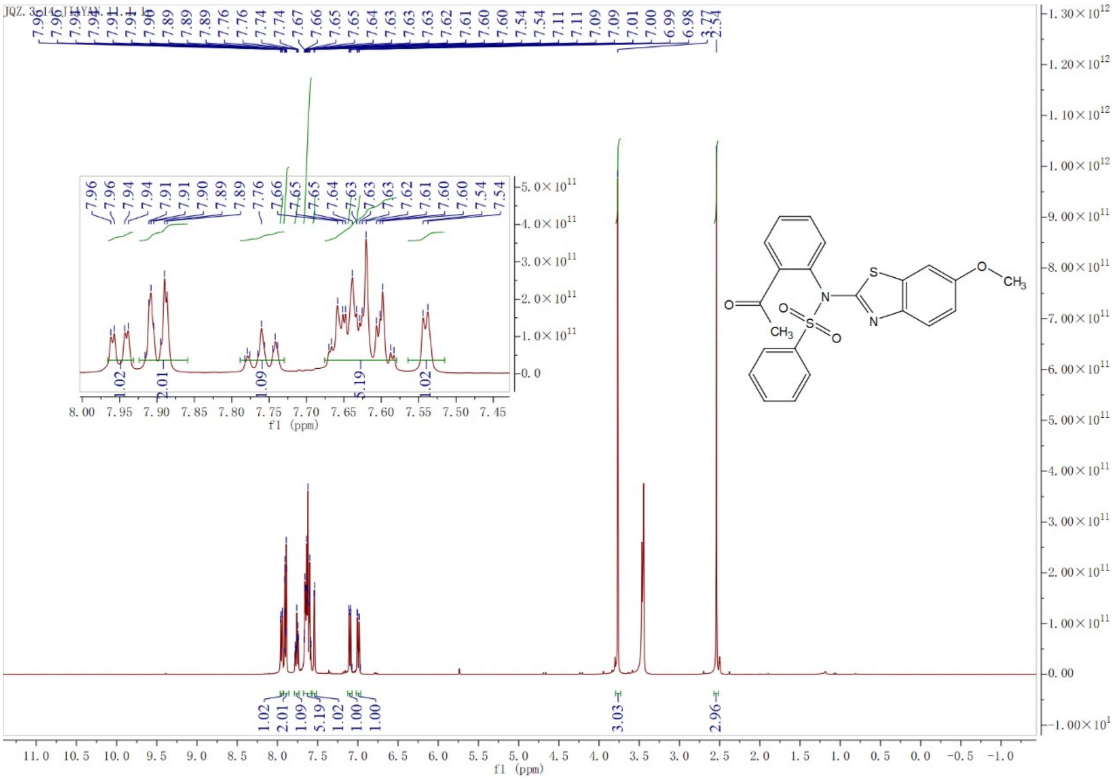

JQZ - 19-3 -XUI.2.1.1r
198.68
163.56
153.11
148.74
141.16
139.51
135.44
135.01
134.30
134.05
133.08
132.82
132.64
131.85
131.80
129.91
129.47
128.51
125.77
123.84
121.28
120.94
29.56
18.05
f1 (ppm)
O
N
S
CH3
N
CH3

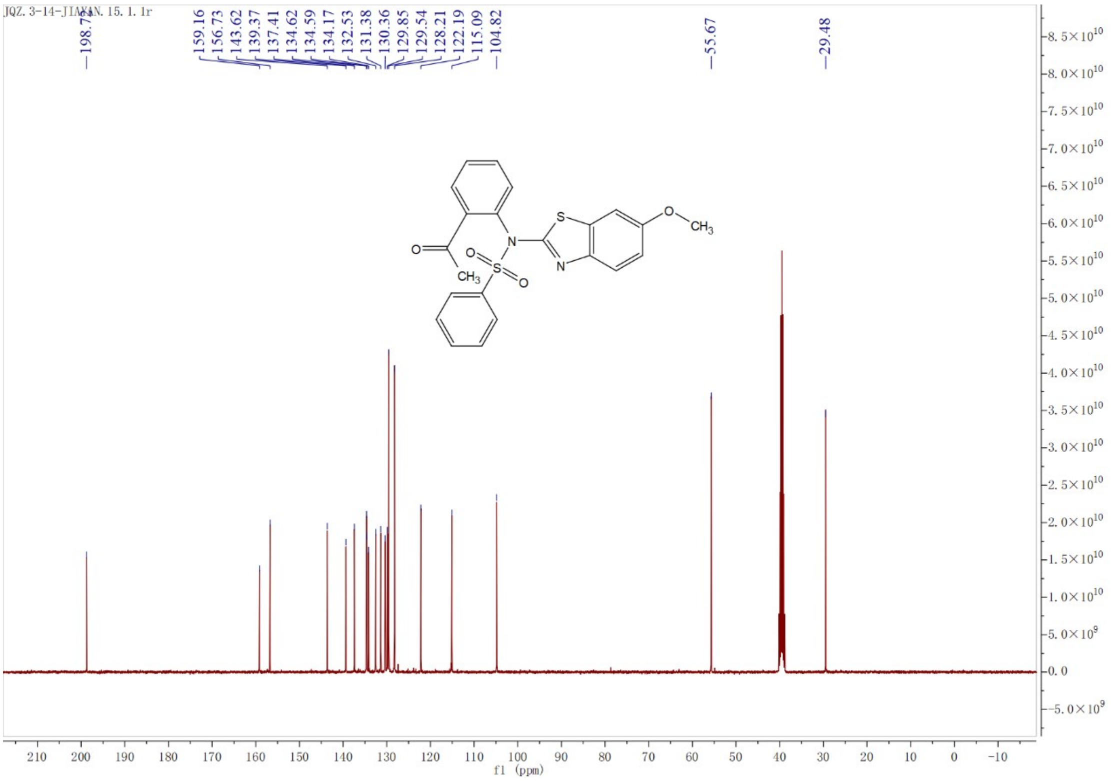

8.01
7.99
7.91
7.89
7.77
7.75
7.73
7.70
7.69
7.67
7.45
7.43
7.41
7.32
7.30
7.28
3.92
3.90
3.88
2.53
1.39
1.37
1.35
1.00
1.00
4.16
1.04
1.03
2.05
2.97
3.10
f1 (ppm)
O
N
S
CH3
H3C

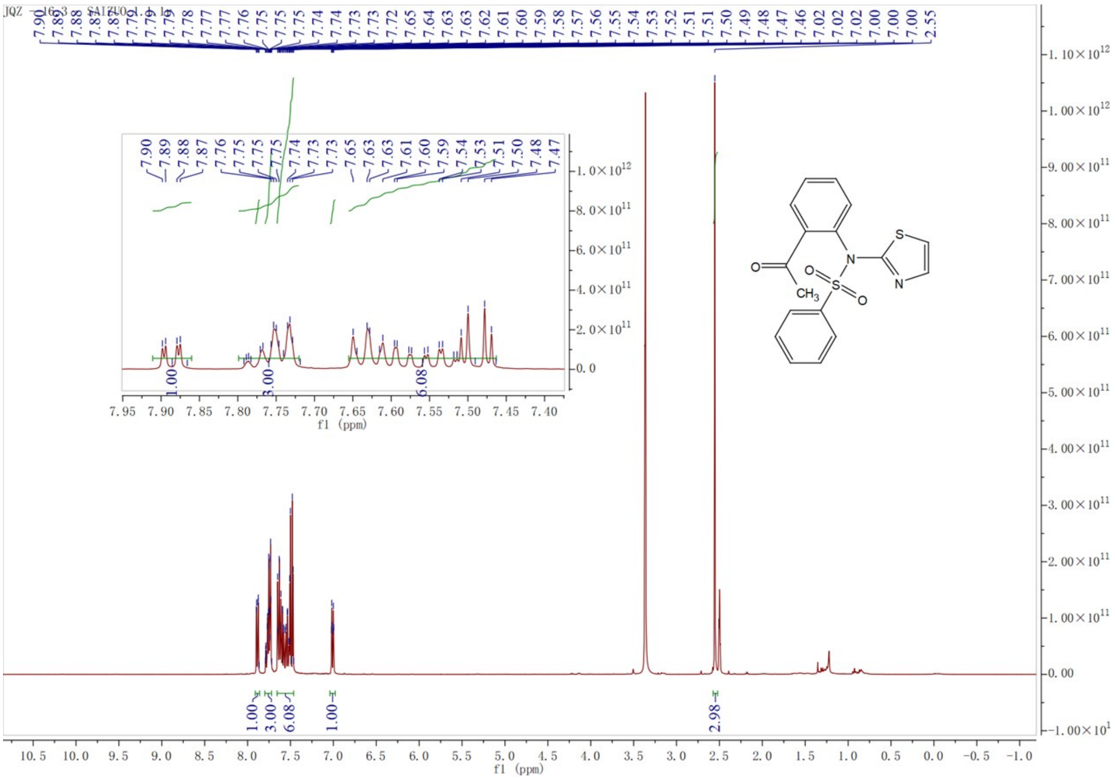

JQZ - 13.3 - YIJI.2.1.1r
199.03
162.74
150.10
138.76
134.63
133.01
132.22
132.16
130.53
130.02
126.47
124.08
121.63
121.17
48.46
29.41
7.46
S
N
N
O
O
S
O
CH3
H3C
2.40×10^10
2.30×10^10
2.20×10^10
2.10×10^10
2.00×10^10
1.90×10^10
1.80×10^10
1.70×10^10
1.60×10^10
1.50×10^10
1.40×10^10
1.30×10^10
1.20×10^10
1.10×10^10
1.00×10^10
9.00×10^9
8.00×10^9
7.00×10^9
6.00×10^9
5.00×10^9
4.00×10^9
3.00×10^9
2.00×10^9
1.00×10^9
0.00
−1.00×10^9
−2.00×10^9
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

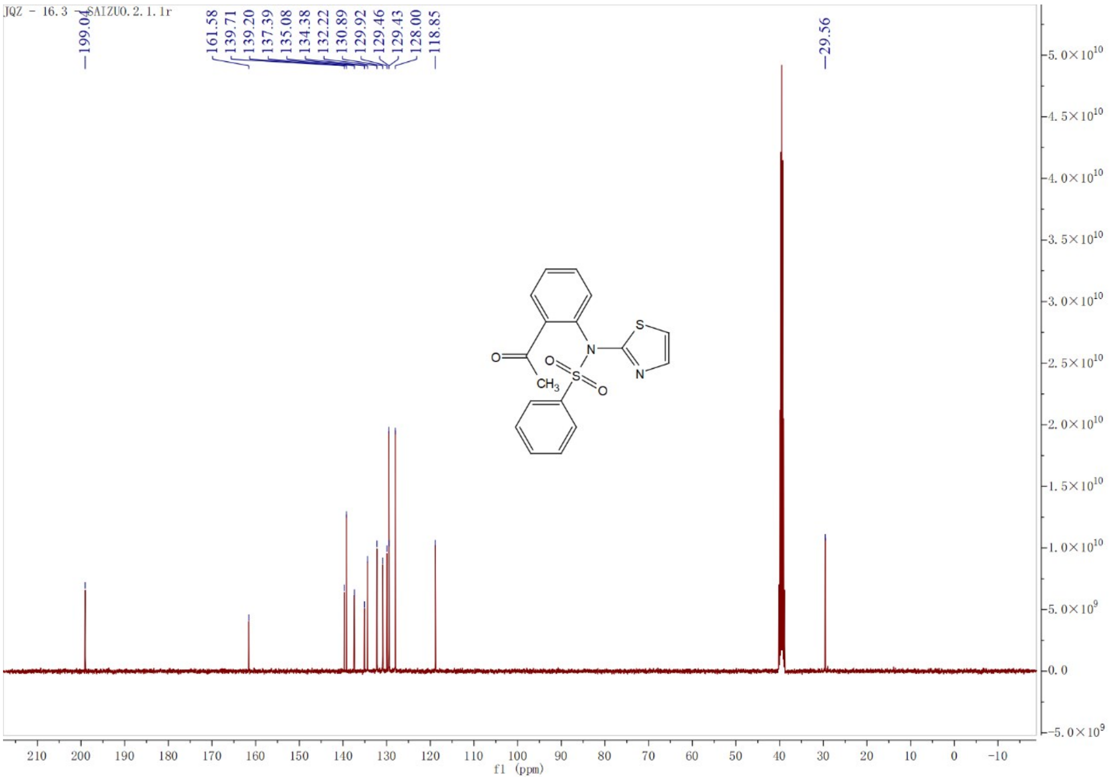

JQZ - 17.3 - HuanBinW.1.1.1r
7.97
7.97
7.95
7.95
7.93
7.93
7.91
7.91
7.75
7.75
7.74
7.73
7.73
7.73
7.72
7.71
7.71
7.70
7.69
7.69
7.69
7.68
7.67
7.67
7.45
7.45
7.43
7.43
7.43
7.41
7.41
7.33
7.33
7.32
7.31
7.31
7.30
7.29
3.48
3.47
3.46
3.45
3.44
2.52
1.22
1.21
1.21
1.20
1.20
1.19
1.19
1.18
1.09
S
N
N
O
O
S
O
CH3
2.01
2.02
2.00
1.00
1.00
1.34
2.93
4.11
1.00×10^12
9.00×10^11
8.00×10^11
7.00×10^11
6.00×10^11
5.00×10^11
4.00×10^11
3.00×10^11
2.00×10^11
1.00×10^11
0.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0
f1 (ppm)

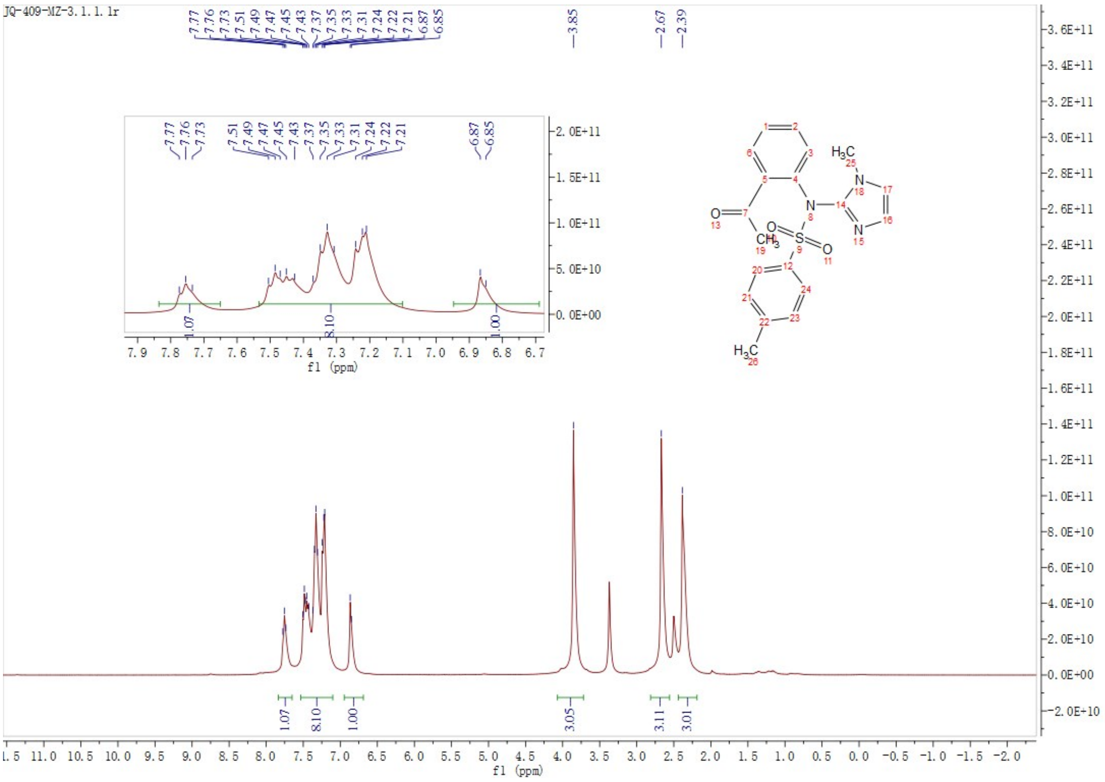

JQZ - 17.3 - HuanBinW.2.1.1r
198.7
162.40
149.87
138.87
135.03
132.81
132.42
132.04
130.40
129.88
126.42
124.13
121.62
121.20
31.09
29.46
6.04
f1 (ppm)
S
N
O
CH3
O
S
O

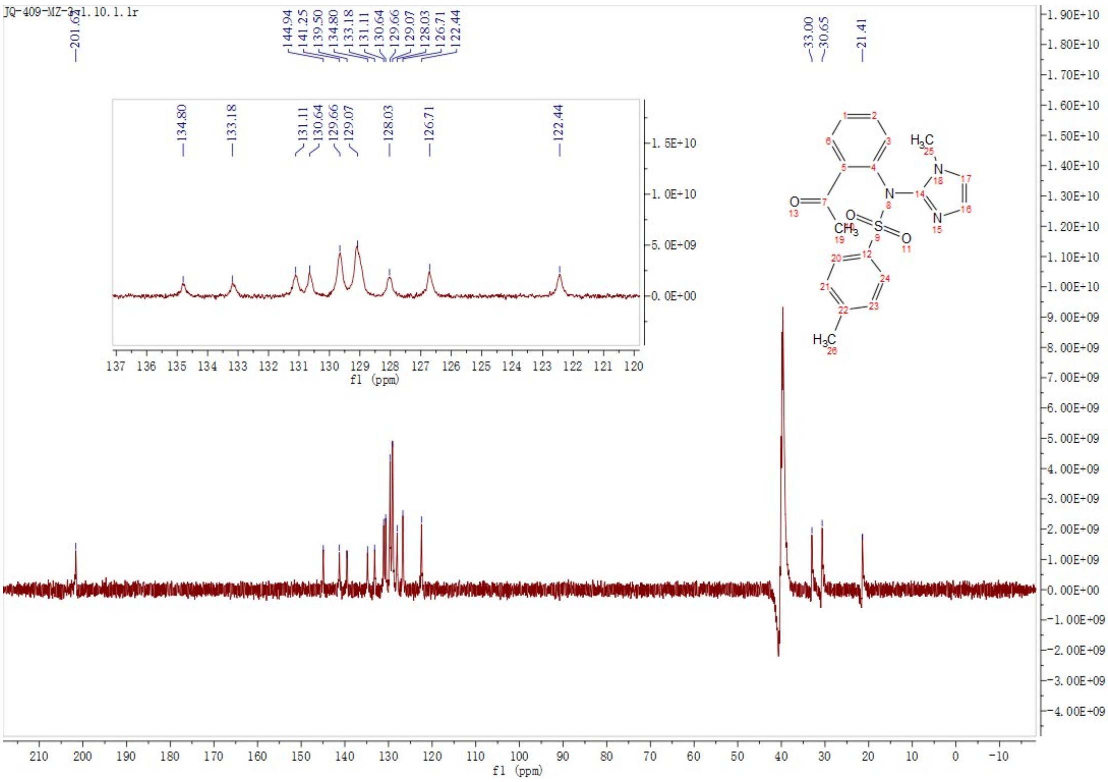

7.96
7.96
7.94
7.94
7.91
7.91
7.90
7.89
7.89
7.76
7.76
7.74
7.74
7.67
7.66
7.65
7.65
7.64
7.63
7.63
7.63
7.62
7.61
7.60
7.60
7.54
7.54
7.11
7.11
7.09
7.09
7.01
7.00
6.99
6.98
3.77
2.54
1.02
2.01
1.09
5.19
1.02
1.00
1.00
3.03
2.96
f1 (ppm)
S
N
O
CH3
O
S
O
O
CH3

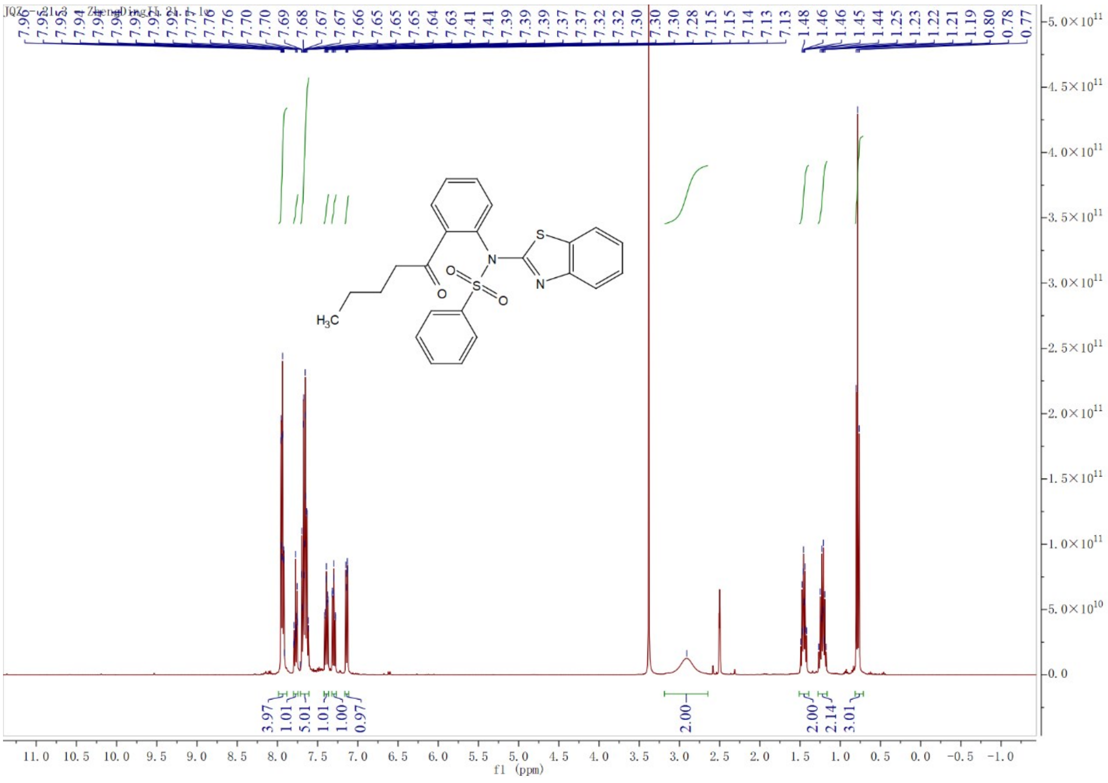

JQZ.3-14-JIAJIAN.15.1.1r
198.7
159.16
156.73
143.62
139.37
137.41
134.62
134.59
134.17
132.53
131.38
130.36
129.85
129.54
128.21
122.19
115.09
104.82
55.67
29.48
S
N
N
O
CH3
O
S
O
CH3
O
8.5×10^10
8.0×10^10
7.5×10^10
7.0×10^10
6.5×10^10
6.0×10^10
5.5×10^10
5.0×10^10
4.5×10^10
4.0×10^10
3.5×10^10
3.0×10^10
2.5×10^10
2.0×10^10
1.5×10^10
1.0×10^10
5.0×10^9
0.0
−5.0×10^9
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

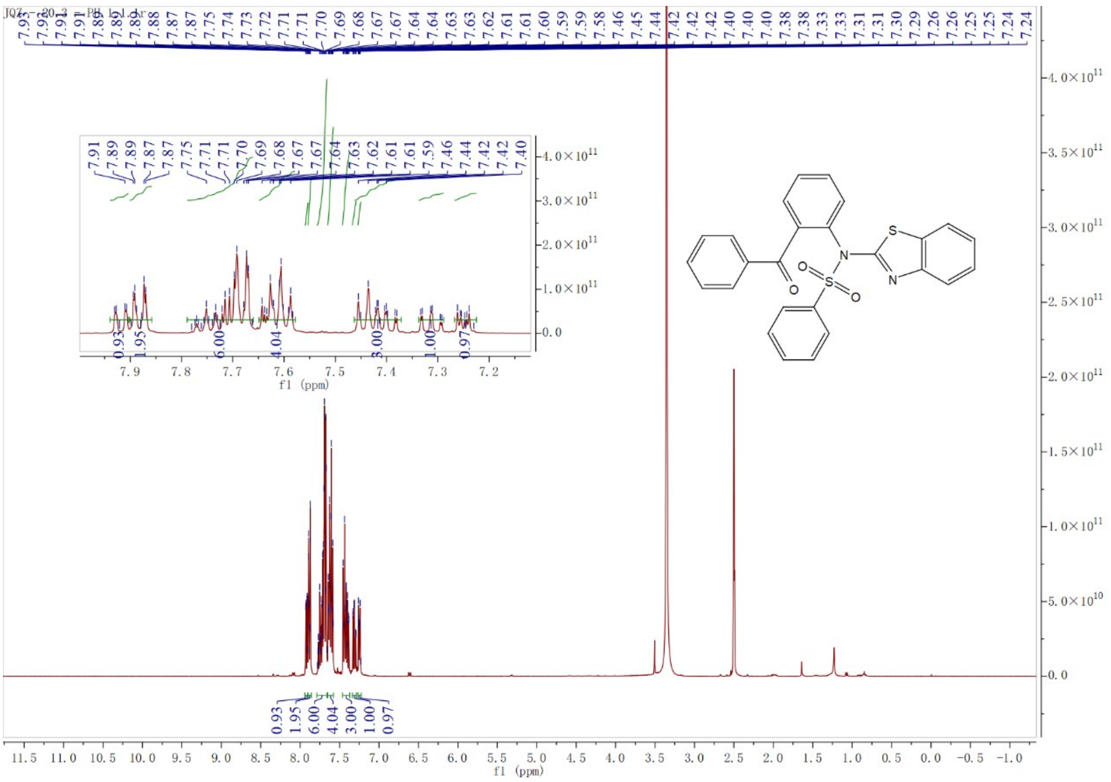

JQZ -16-3 - SAIZUO.1.1.1r
7.90 7.89 7.88 7.87 7.79 7.79 7.79 7.78 7.77 7.77 7.76 7.75 7.75 7.75 7.74 7.74 7.73 7.73 7.72 7.65 7.64 7.63 7.63 7.62 7.61 7.60 7.59 7.58 7.57 7.56 7.55 7.54 7.53 7.52 7.51 7.51 7.50 7.49 7.48 7.47 7.46 7.02 7.02 7.02 7.00 7.00 7.00 2.55
7.90 7.89 7.88 7.87 7.76 7.75 7.75 7.75 7.74 7.73 7.73 7.65 7.63 7.63 7.61 7.60 7.59 7.54 7.53 7.51 7.50 7.48 7.47
1.0×10^12
8.0×10^11
6.0×10^11
4.0×10^11
2.0×10^11
0.0
1.00
3.00
6.08
7.95 7.90 7.85 7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40
f1 (ppm)
S
N
N
O
CH3
O
S
O
1.10×10^12
1.00×10^12
9.00×10^11
8.00×10^11
7.00×10^11
6.00×10^11
5.00×10^11
4.00×10^11
3.00×10^11
2.00×10^11
1.00×10^11
0.00
−1.00×10^1
1.00
3.00
6.08
1.00
2.98
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0
f1 (ppm)

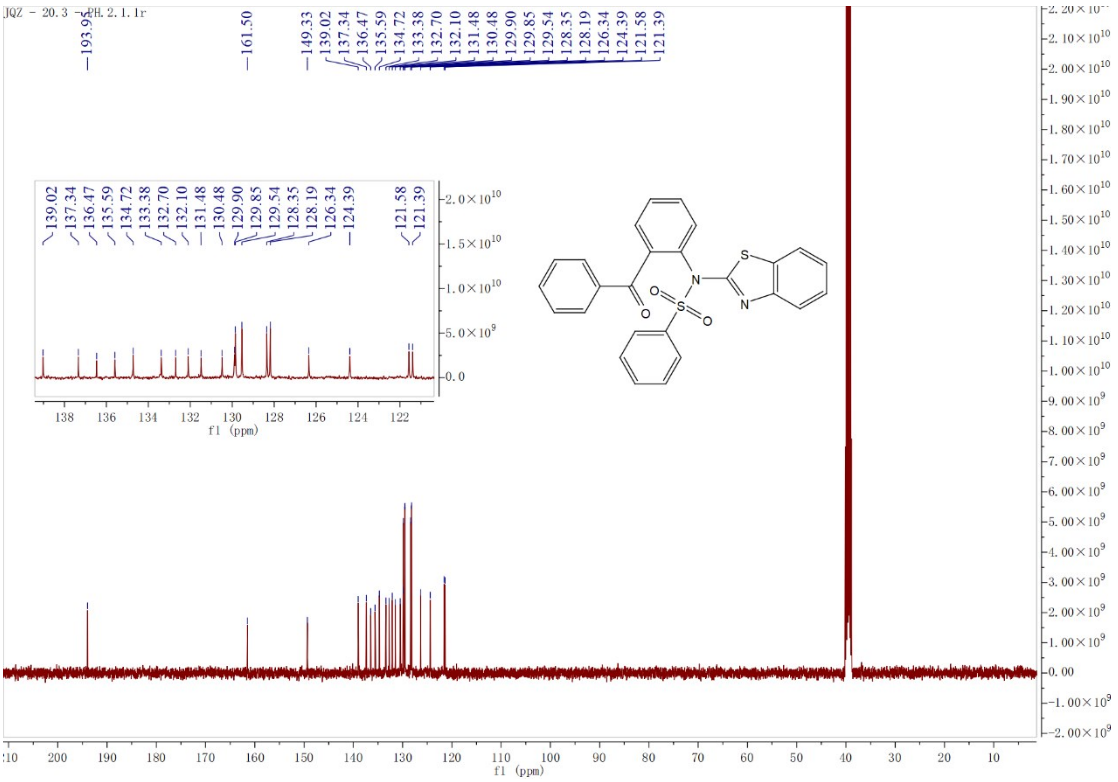

JQZ - 16.3 - SAIZUO.2.1.1r
199.04
161.58
139.71
139.20
137.39
135.08
134.38
132.22
130.89
129.92
129.46
129.43
128.00
118.85
29.56
O
CH3
N
S
N
O
S
O
5.0×10^10
4.5×10^10
4.0×10^10
3.5×10^10
3.0×10^10
2.5×10^10
2.0×10^10
1.5×10^10
1.0×10^10
5.0×10^9
0.0
−5.0×10^9
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

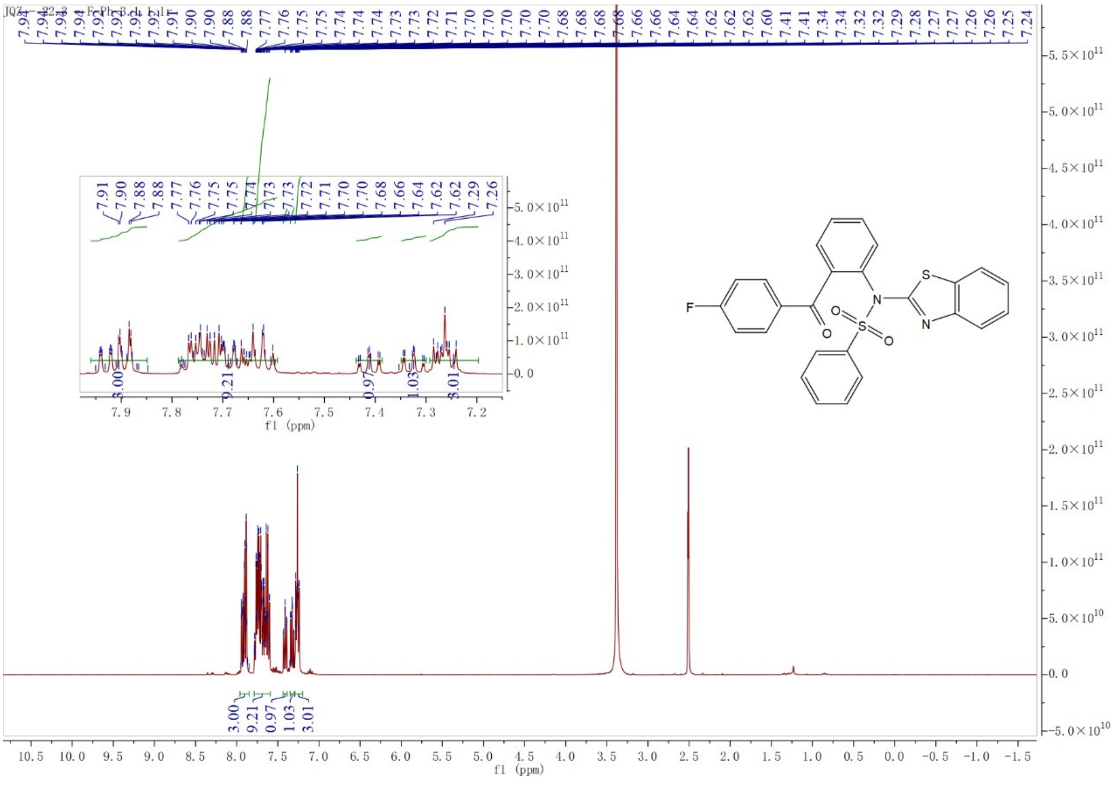

JQ-409-MZ-3.1.1.1r
7.77
7.76
7.73
7.51
7.49
7.47
7.45
7.43
7.37
7.35
7.33
7.31
7.24
7.22
7.21
6.87
6.85
3.85
2.67
2.39
1.07
8.10
1.00
3.05
3.11
3.01
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7
f1 (ppm)
2.0E+11
1.5E+11
1.0E+11
5.0E+10
0.0E+00
H3C 25
N 18
17
16
N 15
N 8
14
1
2
3
4
5
6
O 13
7
CH3 19
O
S 9
O 11
12
20
21
22
23
24
H3C 26
3.6E+11
3.4E+11
3.2E+11
3.0E+11
2.8E+11
2.6E+11
2.4E+11
2.2E+11
2.0E+11
1.8E+11
1.6E+11
1.4E+11
1.2E+11
1.0E+11
8.0E+10
6.0E+10
4.0E+10
2.0E+10
0.0E+00
−2.0E+10
1.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0 −1.5 −2.0
f1 (ppm)

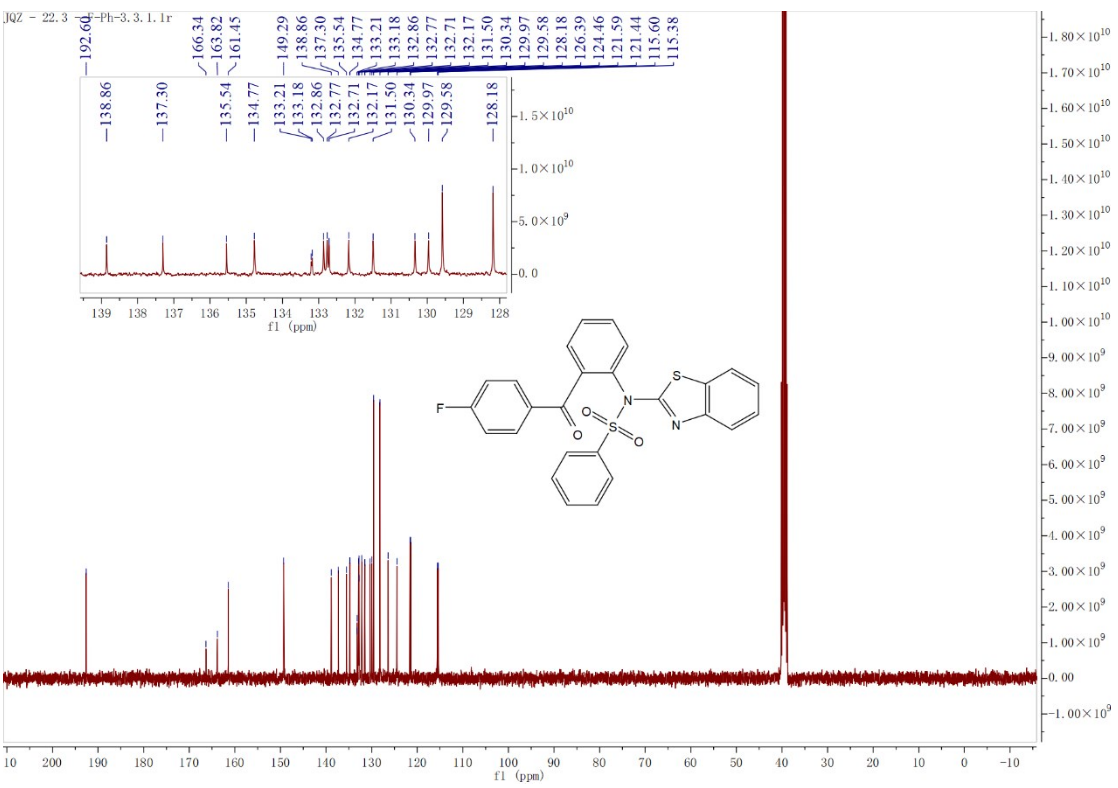

JQ-409-MZ-3.1.10.1.1r
201.62
144.94
141.25
139.50
134.80
133.18
131.11
130.64
129.66
129.07
128.03
126.71
122.44
33.00
30.65
21.41
134.80
133.18
131.11
130.64
129.66
129.07
128.03
126.71
122.44
1.5E+10
1.0E+10
5.0E+09
0.0E+00
137 136 135 134 133 132 131 130 129 128 127 126 125 124 123 122 121 120
f1 (ppm)
H3C
N
O
CH3
S
O
O
N
N
H3C
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26
1.90E+10
1.80E+10
1.70E+10
1.60E+10
1.50E+10
1.40E+10
1.30E+10
1.20E+10
1.10E+10
1.00E+10
9.00E+09
8.00E+09
7.00E+09
6.00E+09
5.00E+09
4.00E+09
3.00E+09
2.00E+09
1.00E+09
0.00E+00
-1.00E+09
-2.00E+09
-3.00E+09
-4.00E+09
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

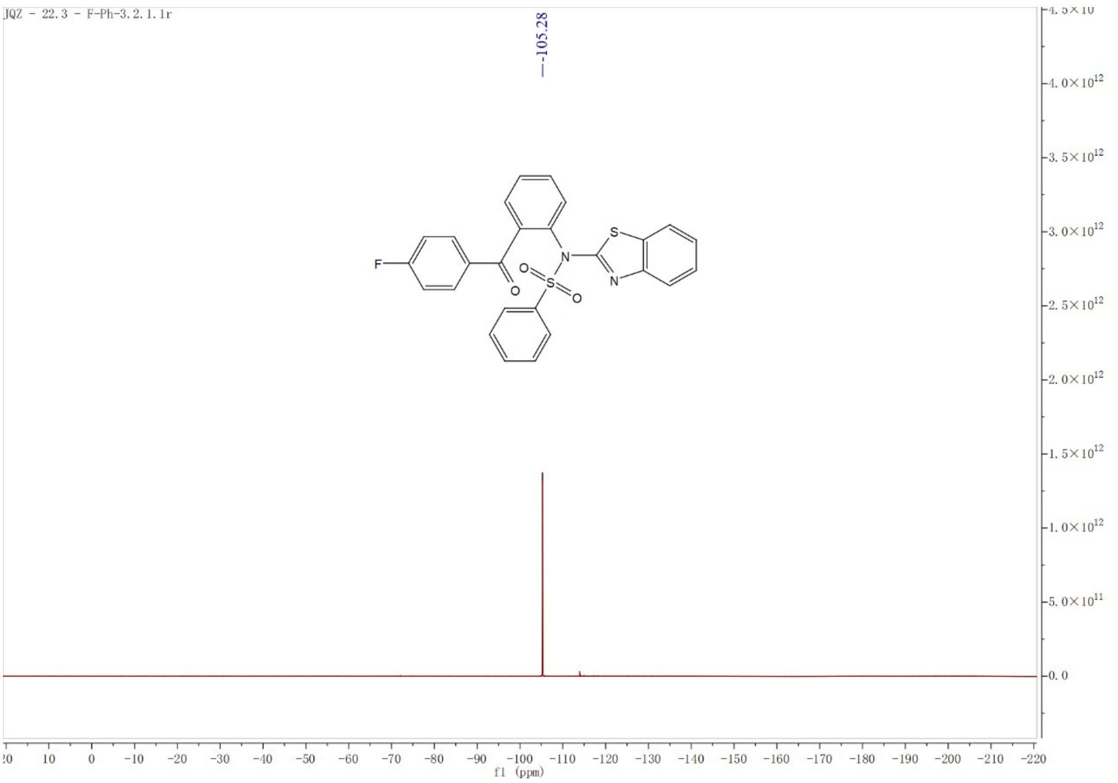

JQZ-21.3-ZhengDing11.21.1.1r
7.96
7.95
7.95
7.94
7.94
7.93
7.93
7.92
7.92
7.77
7.76
7.76
7.70
7.70
7.69
7.68
7.67
7.67
7.66
7.65
7.65
7.65
7.64
7.63
7.41
7.41
7.39
7.39
7.39
7.37
7.37
7.32
7.32
7.30
7.30
7.30
7.28
7.15
7.15
7.14
7.13
7.13
1.48
1.46
1.46
1.45
1.44
1.25
1.23
1.22
1.21
1.19
0.80
0.78
0.77
S
N
N
O
O
S
O
H3C
3.97
1.01
5.01
1.01
1.00
0.97
2.00
2.00
2.14
3.01
5.0×10^11
4.5×10^11
4.0×10^11
3.5×10^11
3.0×10^11
2.5×10^11
2.0×10^11
1.5×10^11
1.0×10^11
5.0×10^10
0.0
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


JQZ-20-3-PH 1.1.1r
7.93
7.93
7.91
7.91
7.89
7.89
7.89
7.88
7.87
7.87
7.75
7.74
7.73
7.72
7.71
7.71
7.70
7.69
7.68
7.67
7.67
7.64
7.64
7.63
7.63
7.62
7.61
7.61
7.60
7.59
7.59
7.58
7.46
7.45
7.44
7.42
7.42
7.42
7.40
7.40
7.40
7.38
7.38
7.33
7.33
7.31
7.31
7.30
7.29
7.26
7.26
7.25
7.24
7.24
0.93
1.95
6.00
4.04
3.00
1.00
0.97
f1 (ppm)
O
N
S
O
O
S
N


JQZ - 20.3 - PH.2.1.1r
193.95
161.50
149.33
139.02
137.34
136.47
135.59
134.72
133.38
132.70
132.10
131.48
130.48
129.90
129.85
129.54
128.35
128.19
126.34
124.39
121.58
121.39
S
N
N
O
O
S
O
f1 (ppm)


7.94
7.91
7.90
7.88
7.77
7.76
7.75
7.74
7.73
7.72
7.71
7.70
7.68
7.66
7.64
7.62
7.60
7.41
7.34
7.32
7.29
7.28
7.27
7.26
7.25
7.24
3.00
9.21
0.97
1.03
3.01
F
S
N
N
O
O
S
O
f1 (ppm)


JQZ - 22.3 - F-Ph-3.3.1.1r
192.60
166.34
163.82
161.45
149.29
138.86
137.30
135.54
134.77
133.21
133.18
132.86
132.77
132.71
132.17
131.50
130.34
129.97
129.58
128.18
126.39
124.46
121.59
121.44
115.60
115.38
F
O
N
S
N
O
S
O
f1 (ppm)
1.80×10^10
1.70×10^10
1.60×10^10
1.50×10^10
1.40×10^10
1.30×10^10
1.20×10^10
1.10×10^10
1.00×10^10
9.00×10^9
8.00×10^9
7.00×10^9
6.00×10^9
5.00×10^9
4.00×10^9
3.00×10^9
2.00×10^9
1.00×10^9
0.00
−1.00×10^9
1.5×10^10
1.0×10^10
5.0×10^9
0.0


JQZ - 22.3 - F-Ph-3.2.1.1r
-105.28
F
O
N
S
N
O
S
O
f1 (ppm)
4.0×10^12
3.5×10^12
3.0×10^12
2.5×10^12
2.0×10^12
1.5×10^12
1.0×10^12
5.0×10^11
0.0