Supporting Information

Selective halocyclization and iodosulfonylation of *N*-benzothiazol-2-yl alkynamides under mild conditions

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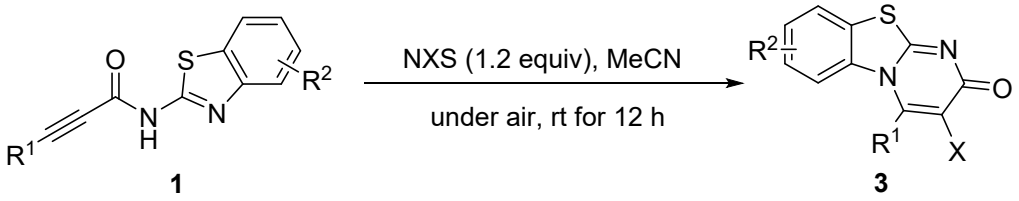
1. General experimental methods.

Unless otherwise noted, all of the reagents were purchased from commercial suppliers and used without purification. Reactions were monitored by thin layer chromatography (TLC) supplied by Yantai Xinnuo New Material Company (China). Purification of products was conducted by flash chromatography on silica gel (200-300 mesh). Melting point were determined using WRX-4 (Shanghai Physico-Optical instrument). Nuclear magnetic resonance (NMR) spectra were measured on a Bruker Avance NEO (400 MHz). Chemical shifts are reported in ppm using tetramethylsilane as internal standard (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, m = multiplet). HRMS data were obtained on a VG ZAB-HS mass spectrometer, Brucker Apex IV FTMS spectrometer. X-Ray single-crystal diffraction data were collected on an Agilent Technologies Gemini single-crystal diffractometer.

2. General experimental procedure

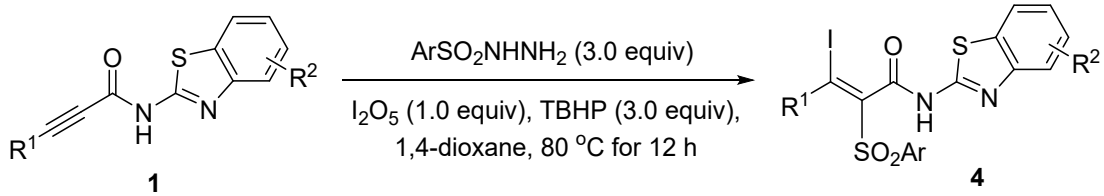
2.1 Synthesis of compound 3



1 **3**

To a mixture of *N*-benzothiazol-2-yl alkynamides **1** (0.2 mmol) and NXS (0.24 mmol) in a 20 mL test tube at room temperature was added the MeCN (2 mL). The reaction vessel was allowed to stir at room temperature for 12 h. After completion of reaction as indicated by TLC, the solvent was evaporated and the residue was purified directly by flash column chromatography using a mixture of dichloromethane and ethyl acetate as eluent to give the desired product **3a-3q**.

2.2 Synthesis of compound 4

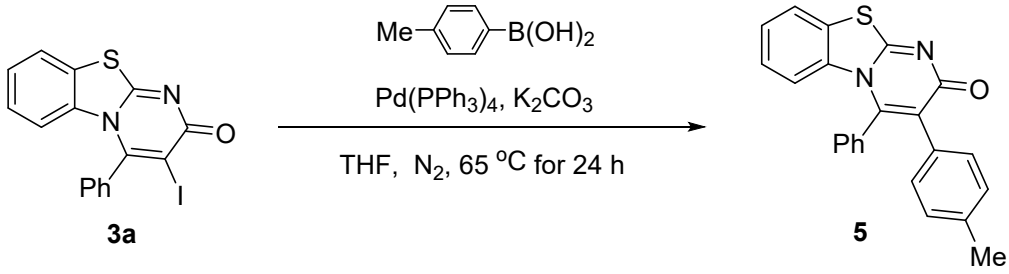


1 **4**

N-benzothiazol-2-yl alkynamides **1** (0.2 mmol), sulfonylhydrazides (0.6 mmol), I_2O_5 (0.2 mmol), TBHP (0.6 mmol) were mixed with 1,4-dioxane (2 mL). The reaction was then heated in an oil bath at 80 ℃ for 12 h. After completion of reaction as indicated by TLC, the reaction was cooled to room temperature, extracted with

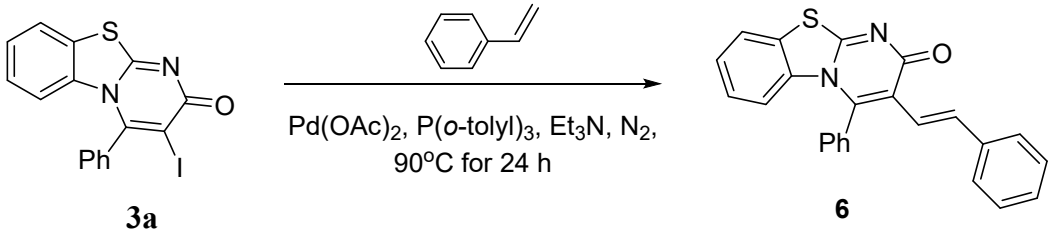
ethyl acetate (10 mL), the organic phase was separated, dried over Na_2SO_4 and concentrated under vacuum. The residue was purified by flash column chromatography using petroleum ether/ethyl acetate solution as eluent to give the desired product **4a-4f**.

2.3 Synthesis of compound 5 and 6



3a **5**

To a mixture of 3-iodo-4-phenyl-2H-benzo[4,5]thiazolo[3,2-a]pyrimidin-2-one **3a** (0.2 mmol), $Pd(PPh_3)_4$ (0.08 mmol) and *p*-tolylboronic acid (0.6 mmol) in THF (2 mL) at room temperature in N_2 atmosphere. The reaction was then heated in an oil bath at 65 °C for 24 h. After that, the reaction was cooled to room temperature, diluted with ethyl acetate (2 mL), and then washed with sat. NH_4Cl (5 mL). The organic phase was separated, dried over Na_2SO_4 and concentrated under vacuum. The residue was purified by flash column chromatography using petroleum ether/ethyl acetate solution as eluent to give the desired product **5** in 85% yield.

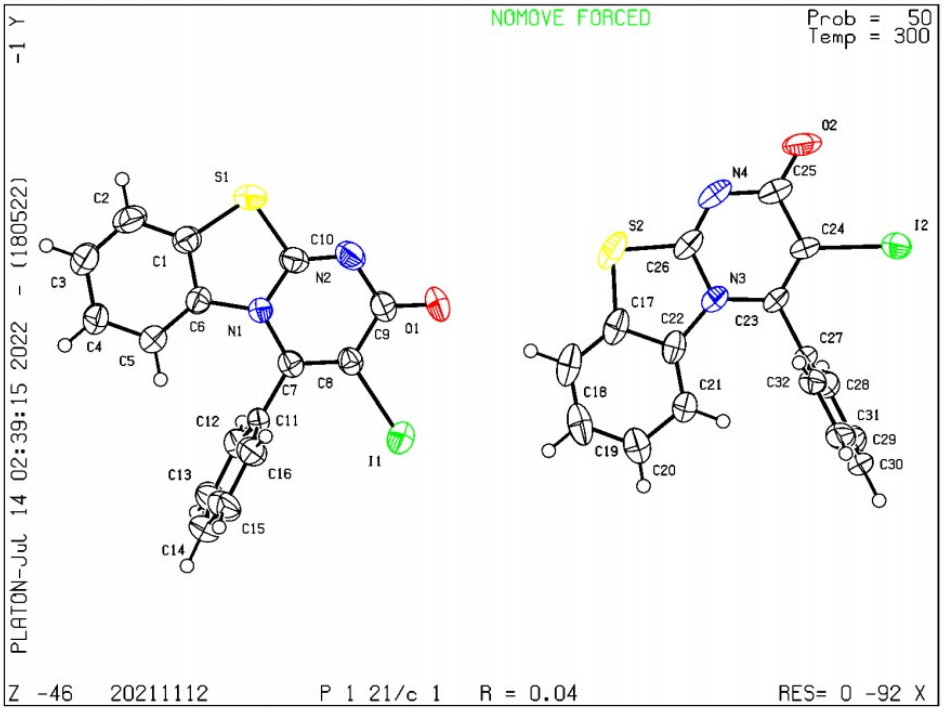


3a **6**

A 10-mL Schlenk tube was charged with 3-iodo-4-phenyl-2H-benzo[4,5]thiazolo[3,2-a]pyrimidin-2-one **3a** (0.2 mmol), $Pd(OAc)_2$ (0.004 mmol), P(*o*-tolyl)$_3$ (0.012 mmol), styrene (0.3 mmol) and triethylamine (0.8 mmol). The reaction was heated at 90 °C under N_2 for 24 h. After that, the reaction was concentrated under vacuum and directly purified by flash column chromatography using methanol/dichloromethane solution as eluent to give the desired product **6** in 71% yield.

3. X-ray Crystal structure and crystal data of compound 3a

Datablock 20211112 - ellipsoid plot



Datablock: 20211112

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Bond precision:   C-C = 0.0070 A          Wavelength=0.71073

Cell:             a=19.9343(14)    b=7.2169(5)        c=20.7700(14)
                  alpha=90         beta=104.434(7)    gamma=90
Temperature:      300 K
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	Calculated	Reported
Volume	2893.7(4)	2893.7(4)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C16 H9 I N2 O S	C16 H9 I N2 O S
Sum formula	C16 H9 I N2 O S	C16 H9 I N2 O S
Mr	404.21	404.21
Dx,g cm-3	1.856	1.856
Z	8	8
Mu (mm-1)	2.356	2.356
F000	1568.0	1568.0
F000'	1565.69	
h,k,lmax	27,10,28	27,9,28
Nref	8098	6791
Tmin,Tmax	0.661,0.736	0.496,1.000
Tmin'	0.633	

```
Correction method= # Reported T Limits: Tmin=0.496 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.839          Theta(max)= 29.577

R(reflections)= 0.0432( 4708)                wR2(reflections)=
                                             0.0940( 6791)
S = 1.022                 Npar= 380
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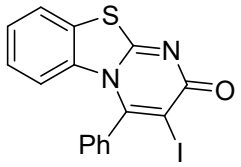
4. Characterization data

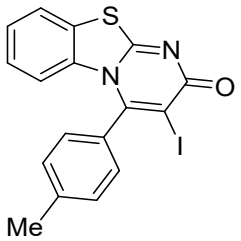


3-iodo-4-phenyl-2H-benzo[4,5]thiazolo[3,2-a]pyrimidin-2-one **(3a)**

white solid, m.p. 232-237 ℃

77.4 mg, 96%; ethyl acetate/dichloromethane = 1/8, R_f = 0.5

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.88 (d, J = 7.8 Hz, 1H), 7.61 (d, J = 5.6 Hz, 3H), 7.48 (d, J = 5.7 Hz, 2H), 7.24 (t, J = 7.6 Hz, 1H), 6.96 (t, J = 8.0 Hz, 1H), 5.54 (d, J = 8.7 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.1, 164.3, 151.2, 136.6, 136.3, 131.4, 130.1, 129.5, 126.7, 126.6, 124.4, 124.3, 116.4, 96.1. HRMS (ESI) m/z: calcd for $C_{16}H_9IN_2NaOS$ $[M+Na]^+$426.9372, found: 426.9369.

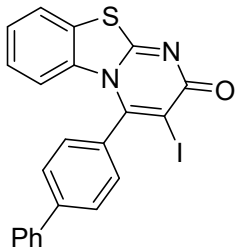


3-iodo-4-(p-tolyl)-2H-benzo[4,5]thiazolo[3,2-a]pyrimidin-2-one **(3b)**

white solid, m.p. 242-243 ℃

70.0 mg, 85%; methanol/dichloromethane = 1/50, R_f = 0.5

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (dd, J = 7.9, 1.4 Hz, 1H), 7.49-7.43 (m, 2H), 7.31-7.26 (m, 3H), 7.01 (ddd, J = 8.8, 7.4, 1.4 Hz, 1H), 5.89-5.83 (m, 1H), 2.56 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.6, 141.7, 135.7, 133.0, 130.7, 128.7, 126.6, 126.4, 124.5, 123.0, 116.8, 96.0, 21.8. HRMS (ESI) m/z: calcd for $C_{17}H_{12}IN_2OS$ $[M+H]^+$ 418.9710, found: 418.9709.

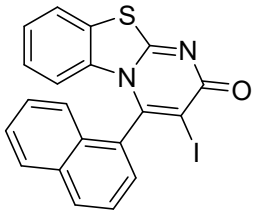


4-([1,1'-biphenyl]-4-yl)-3-iodo-2H-benzo[4,5]thiazolo[3,2-a]pyrimidin-2-one **(3c)**

White solid, m.p. 285-288 ℃

83.4 mg, 88%; ethyl acetate/dichloromethane = 1/8, R_f = 0.6

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.94 (d, J = 8.0 Hz, 2H), 7.89 (d, J = 7.9 Hz, 1H), 7.79 (d, J = 7.7 Hz, 2H), 7.57 (d, J = 8.0 Hz, 2H), 7.47 (t, J = 7.5 Hz, 2H), 7.38 (t, J = 7.3 Hz, 1H), 7.25 (t, J = 7.6 Hz, 1H), 7.00 (t, J = 8.1 Hz, 1H), 5.77 (d, J = 8.8 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.2, 164.3, 151.0, 142.5, 139.2, 136.4, 135.6, 130.2, 129.6, 128.8, 128.1, 127.4, 126.8, 126.6, 124.4, 124.3, 116.5, 96.3. HRMS (ESI) m/z: calcd for $C_{20}H_{11}IN_2NaOS$ $[M+Na]^+$ 502.9685, found : 502.9679.

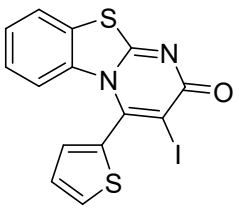


3-iodo-4-(naphthalen-1-yl)-2H-benzo[4,5]thiazolo[3,2-a]pyrimidin-2-one (**3d**)

white solid, m.p. 261-263 ℃

71.1 mg, 79%; ethyl acetate/dichloromethane = 1/8, R_f = 0.4

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.31-8.29 (m, 1H), 8.15 (d, J = 8.2 Hz, 1H), 7.94 (d, J = 7.9 Hz, 1H), 7.84 (d, J = 8.4 Hz, 1H), 7.80-7.75 (m, 2H), 7.64 (t, J = 7.5 Hz, 1H), 7.55-7.51 (m, 1H), 7.24 (t, J = 7.6 Hz, 1H), 6.86-6.80 (m, 1H), 5.76 (s, 1H), 5.37 (d, J = 8.7 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.5, 164.3, 149.7, 136.0, 133.8, 133.6, 131.7, 130.1, 129.3, 128.5, 128.4, 127.7, 126.8, 126.6, 126.5, 125.0, 124.5, 124.3, 115.8, 98.0. HRMS (ESI) m/z: calcd for $C_{20}H_{11}IN_2NaOS$ $[M+Na]^+$ 476.9529, found : 476.9519.



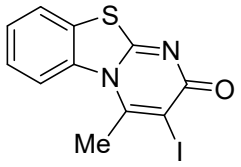
3-iodo-4-(thiophen-2-yl)-2H-benzo[4,5]thiazolo[3,2-a]pyrimidin-2-one **(3e)**

white solid, m.p. 231-233 ℃

41.8 mg, 51%; ethyl acetate/dichloromethane = 1/8, R_f = 0.5

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.05 (d, J = 5.0 Hz, 1H), 7.98 (d, J = 7.9 Hz, 1H), 7.45-7.44 (m, 1H), 7.39-7.35 (m, 2H), 7.20-7.15 (m, 1H), 5.80 (d, J = 8.7 Hz, 1H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 165.3 164.1, 145.2, 136.3, 131.6, 131.4, 128.8, 126.9, 126.7, 124.2, 116.2, 100.1. HRMS (ESI) m/z: calcd for $C_{14}H_7IN_2NaOS_2$ $[M+Na]^+$ 432.8937, found : 432.8933.

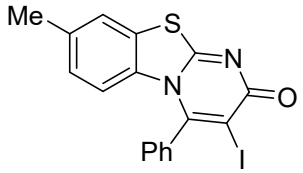


3-iodo-4-methyl-2H-benzo[4,5]thiazolo[3,2-a]pyrimidin-2-one **(3f)**

white solid, m.p. 219-220 ℃

62.7 mg, 92%; ethyl acetate/dichloromethane = 1/8, R_f = 0.5

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.00 (d, J = 8.2 Hz, 1H), 7.93 (d, J = 7.1 Hz, 1H), 7.46-7.35 (m, 2H), 3.07 (s, 3H). ^{13}C NMR (101 MHz, DMSO) δ 164.8, 163.9, 150.6, 136.9, 127.4, 126.7, 124.3, 124.2, 118.4, 95.7, 40.6, 40.4, 40.2, 40.0, 39.8, 39.6, 39.4, 28.5. HRMS (ESI) m/z: calcd for $C_{11}H_7IN_2NaOS$ $[M+Na]^+$ 364.9216, found : 364.9215.

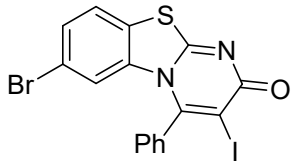


3-iodo-8-methyl-4-phenyl-2H-benzo[4,5]thiazolo[3,2-a]pyrimidin-2-one **(3g)**

white solid, m.p. 284-286 ℃

36.5 mg, 44%; ethyl acetate/dichloromethane = 1/8, R_f = 0.5

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.75 (s, 1H), 7.70-7.68 (m, 3H), 7.55-7.53 (m, 2H), 6.87-6.84 (m, 1H), 5.48 (d, J = 8.8 Hz, 1H), 2.27 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 164.9, 164.4, 151.1, 136.5, 136.5, 134.2, 131.4, 130.1, 129.5, 127.6, 124.3, 124.0, 116.1, 95.7, 20.8. HRMS (ESI) m/z: calcd for $C_{17}H_{12}IN_2OS$ $[M+H]^+$ 418.9710, found : 418.9709

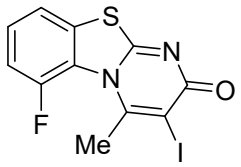


7-bromo-3-iodo-4-phenyl-2H-benzo[4,5]thiazolo[3,2-a]pyrimidin-2-one **(3h)**

white solid, m.p. 237-240 ℃

49.1 mg, 51%; ethyl acetate/dichloromethane = 1/8, R_f = 0.6

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.83 (d, J = 8.5 Hz, 1H), 7.68-7.61 (m, 3H), 7.43-7.47 (m, 3H), 5.51 (s, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.4, 164.2, 150.9, 137.2, 136.2, 131.5, 130.2, 129.5, 129.0, 125.8, 123.8, 119.5, 119.2, 95.9. HRMS (ESI) m/z: calcd for $C_{16}H_8BrIN_2NaOS$ $[M+Na]^+$ 504.8478, found : 504.8469.

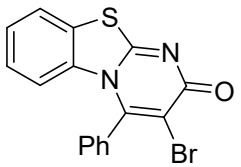


6-fluoro-3-iodo-4-methyl-2H-benzo[4,5]thiazolo[3,2-a]pyrimidin-2-one **(3i)**

white solid, m.p. 220-222 ℃

14.4 mg, 20%; ethyl acetate/dichloromethane = 1/8, R_f = 0.5

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51-7.43 (m, 2H), 7.29-7.24 (m, 1H), 2.87 (d, J = 10.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.9 (d, J = 3.3 Hz), 151.1, 149.4, 148.5, 128.1 (d, J = 8.5 Hz), 127.6, 123.2, 119.2 (d, J = 3.7 Hz), 115.3 (d, J = 22.6 Hz), 92.9, 28.4 (d, J = 20.8 Hz). ^{19}F NMR (377 MHz, $CDCl_3$) δ -109.4. HRMS (ESI) m/z: calcd for $C_{11}H_7FIN_2OS$ $[M+H]^+$ 360.9302, found : 360.9287.

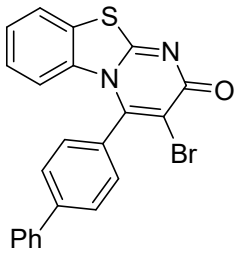


3-bromo-4-phenyl-2H-benzo[4,5]thiazolo[3,2-a]pyrimidin-2-one **(3j)**

white solid, m.p. 239-240 ℃

62.5 mg, 88%; ethyl acetate/dichloromethane = 1/8, R_f = 0.5

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.90 (d, J = 7.4 Hz, 1H), 7.64-7.58 (m, 3H), 7.54-7.52 (m, 2H), 7.26 (t, J = 7.6 Hz, 1H), 7.01-6.95 (m, 1H), 5.60 (d, J = 8.7 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 164.3, 162.4, 148.3, 136.4, 133.2, 131.5, 130.2, 129.4, 126.8, 126.6, 124.7, 124.4, 116.1, 113.8. HRMS (ESI) m/z: calcd for $C_{16}H_9BrN_2NaOS$ $[M+Na]^+$ 378.9511; found : 378.9501.

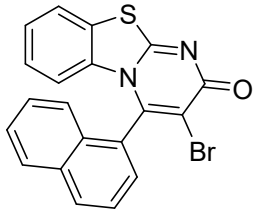


4-([1,1'-biphenyl]-4-yl)-3-bromo-2H-benzo[4,5]thiazolo[3,2-a]pyrimidin-2-one **(3k)**

white solid, m.p. 270-272 ℃

69.8 mg, 81%; ethyl acetate/dichloromethane = 1/8, R_f = 0.4

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91-7.89 (m, 2H), 7.76-7.74 (m, 2H), 7.63-7.61 (m, 1H), 7.56-7.44 (m, 5H), 7.30 (t, J = 7.7 Hz, 1H), 7.04-6.99 (m, 1H), 6.05 (d, J = 8.7 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.8, 162.6, 147.1, 143.9, 139.3, 135.7, 131.1, 129.3, 129.2, 128.5, 128.4, 127.2, 126.7, 126.5, 124.7, 123.2, 116.4, 114.9. HRMS (ESI) m/z: calcd for $C_{22}H_{13}BrN_2NaOS$ $[M+Na]^+$ 454.9824, found : 454.9816.

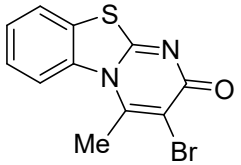


3-bromo-4-(naphthalen-1-yl)-2H-benzo[4,5]thiazolo[3,2-a]pyrimidin-2-one **(3l)**

white solid, m.p. 240-245 ℃

59.5 mg, 74%; ethyl acetate/dichloromethane = 1/8, R_f = 0.4

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.30 (d, J = 6.7 Hz, 1H), 8.15 (d, J = 7.0 Hz, 1H), 7.98-7.86 (m, 2H), 7.82-7.74 (m, 2H), 7.66-7.50 (m, 2H), 7.27-7.19 (m, 1H), 6.88-6.80 (m, 1H), 5.42 (s, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 164.8, 162.3, 146.7, 136.0, 133.6, 131.8, 130.3, 130.1, 129.3, 128.5, 128.3, 127.7, 126.9, 126.6, 126.5, 125.0, 124.8, 124.4, 115.4. HRMS (ESI) m/z: calcd for $C_{20}H_{11}BrN_2NaOS$ $[M+Na]^+$ 428.9668, found : 428.9661.

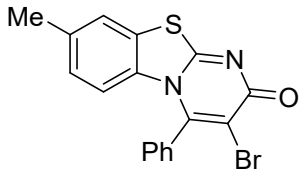


3-bromo-4-methyl-2H-benzo[4,5]thiazolo[3,2-a]pyrimidin-2-one **(3m)**

white solid, m.p. 239-240 ℃

41.02 mg, 70%; ethyl acetate/dichloromethane = 1/8, R_f = 0.5

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97-7.92 (m, 1H), 7.73-7.67 (m, 1H), 7.53-7.45 (m, 2H), 3.15 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.5, 162.2, 145.8, 136.4, 127.1, 126.7, 125.1, 123.7, 116.5, 114.9, 22.7. HRMS (ESI) m/z: calcd for $C_{11}H_7BrN_2NaOS$ $[M+Na]^+$ 316.9355, found : 316.9358.

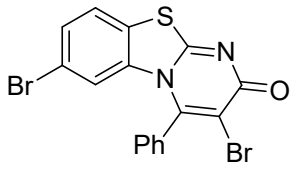


3-bromo-8-methyl-4-phenyl-2H-benzo[4,5]thiazolo[3,2-a]pyrimidin-2-one (**3n**)

white solid, m.p. 265-266 ℃

25.8 mg, 35%; ethyl acetate/dichloromethane = 1/8, R_f = 0.5

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.78 (s, 1H), 7.69 (d, J = 7.5 Hz, 3H), 7.63-7.56 (m, 2H), 6.88 (d, J = 8.8 Hz, 1H), 5.53 (d, J = 8.8 Hz, 1H), 2.27 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 164.1, 162.4, 148.2, 136.5, 134.3, 133.1, 131.5, 130.1, 129.3, 127.7, 124.6, 124.1, 115.8, 113.5, 20.9. HRMS (ESI) m/z: calcd for $C_{17}H_{12}BrN_2OS$ $[M+H]^+$ 370.9848, found : 370.9848.

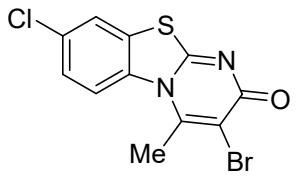


3,7-dibromo-4-phenyl-2H-benzo[4,5]thiazolo[3,2-a]pyrimidin-2-one **(3o)**

white solid, m.p. 236-237 ℃

34.6 mg, 40%; ethyl acetate/dichloromethane = 1/8, R_f = 0.5

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.86 (d, J = 8.4 Hz, 1H), 7.65 (d, J = 7.4 Hz, 3H), 7.54 (d, J = 6.6 Hz, 2H), 7.47 (d, J = 8.4 Hz, 1H), 5.58 (s, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 164.7, 162.2, 148.0, 137.3, 132.8, 131.6, 130.2, 129.4, 129.1, 125.9, 124.1, 119.3, 119.2, 113.7. HRMS (ESI) m/z: calcd for $C_{16}H_8Br_2N_2NaOS$ $[M+Na]^+$ 456.8616, found : 456.8607.

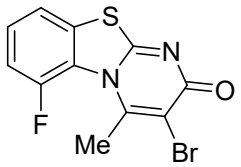


4-bromo-8-chloro-4-methyl-2H-benzo[4,5]thiazolo[3,2-a]pyrimidin-2-one (**3p**)

white solid, m.p. 267-268 ℃

45.8 mg, 70%; ethyl acetate/dichloromethane = 1/8, R_f = 0.5

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.22 (d, J = 2.4 Hz, 1H), 8.14 (d, J = 9.2 Hz, 1H), 7.59-7.56 (m, 1H), 3.05 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 163.9, 161.8, 148.2, 136.0, 130.8, 127.4, 126.6, 123.8, 119.4, 113.5, 22.8. HRMS (ESI) m/z: calcd for $C_{11}H_6BrClN_2NaOS$ $[M+Na]^+$ 350.8965, found : 350.8961.

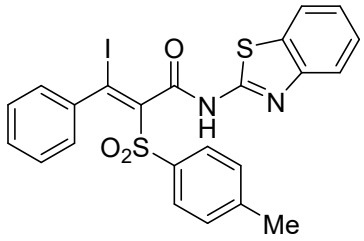


4-bromo-6-fluoro-4-methyl-2H-benzo[4,5]thiazolo[3,2-a]pyrimidin-2-one **(3q)**

white solid, m.p. 250-251 ℃

40.3 mg, 65%; ethyl acetate/dichloromethane = 1/8, R_f = 0.5

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54-7.41 (m, 2H), 7.30-7.23 (m, 1H), 2.79 (d, J = 10.9 Hz, 3H).. ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.0, 162.2, 150.9, 148.4, 146.7, 128.2 (d, J = 8.3 Hz), 127.8 (d, J = 1.8 Hz), 123.2 (d, J = 11.5 Hz), 119.3 (d, J = 3.7 Hz), 115.4 (d, J = 22.9 Hz), 113.4, 23.2 (d, J = 21.4 Hz). ^{19}F NMR (377 MHz, $CDCl_3$) δ -109.1. HRMS (ESI) m/z: calcd for $C_{11}H_6BrFN_2NaOS$ $[M+Na]^+$ 334.9260, found : 334.9273.



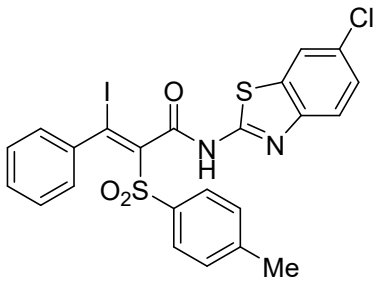
(E)-*N*-(benzo[d]thiazol-2-yl)-3-iodo-3-phenyl-2-tosylacrylamide **(4a)**

white solid, m.p. 215-216 ℃

100.6 mg, 90%; ethyl acetate/petroleum ether = 1/5, R_f = 0.5

^{1}H NMR (400 MHz, DMSO-d_6) δ 13.48 (s, 1H), 7.97 (d, J = 7.z, 1H), 7.76 (d, J = 7.6 Hz, 1H), 7.44-7.40 (m, 1H), 7.35-7.13 (m, 10H), 6.99 (d, J = 2.4 Hz, 2H), 2.27 (s,

3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 163.5, 158.0, 149.1, 145.5, 145.3, 140.7, 137.5, 132.1, 130.0, 129.6, 128.3, 128.2, 127.0, 126.9, 124.6, 122.4, 121.4, 118.8, 21.6. HRMS (ESI) m/z: calcd for $C_{23}H_{17}IN_2NaO_3S_2$ $[M+Na]^+$ 582.9617, found : 582.9610.

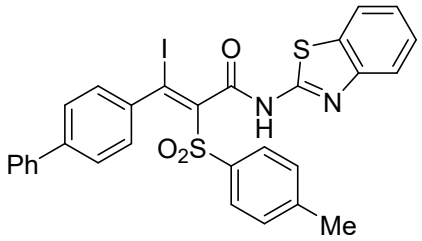


(E)-*N*-(6-chlorobenzo[d]thiazol-2-yl)-3-iodo-3-phenyl-2-tosylacrylamide **(4b)**

white solid, m.p. 215-218 ℃

85.6 mg, 75%; methanol/dichloromethane = 1/50, R_f = 0.5

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95-7.89 (m, 2H), 7.49-7.43 (m, 3H), 7.28-7.26 (m, 1H), 7.23-7.16 (m, 4H), 6.77 (d, J = 7.0 Hz, 2H), 2.39 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.6, 159.4, 146.6, 146.0, 145.4, 139.7, 136.7, 133.4, 130.2, 129.9, 129.6, 128.6, 127.8, 127.6, 126.9, 122.6, 121.2, 117.6, 21.8. HRMS (ESI) m/z: calcd for $C_{23}H_{17}ClIN_2O_3S_2$ $[M+H]^+$ 594.9408, found : 594.9405.

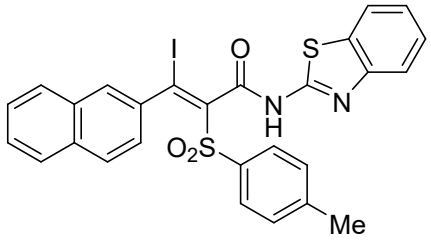


(E)-3-([1,1'-biphenyl]-4-yl)-*N*-(benzo[d]thiazol-2-yl)-3-iodo-2-tosylacrylamide **(4c)**

white solid, m.p. 206-209 ℃

69.9 mg, 55%; ethyl acetate/petroleum ether = 1/5, R_f = 0.6

^{1}H NMR (400 MHz, DMSO-d_6) δ 13.50 (s, 1H), 7.98 (d, J = 7.9 Hz, 1H), 7.77 (d, J = 7.9 Hz, 1H), 7.62 (d, J = 7.7 Hz, 2H), 7.52 (d, J = 8.0 Hz, 2H), 7.43 (t, J = 7.5 Hz, 3H), 7.37-7.28 (m, 4H), 7.18 (d, J = 8.1 Hz, 2H), 7.08 (d, J = 8.0 Hz, 2H), 2.27 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 163.5, 158.0, 149.1, 145.7, 145.3, 141.4, 139.7, 139.7, 137.5, 132.2, 130.0, 129.5, 128.47, 128.4, 127.8, 127.3, 126.9, 126.5, 124.6, 122.4, 121.5, 118.3, 21.7. HRMS (ESI) m/z: calcd for $C_{29}H_{20}IN_2O_3S_2$ $[M-H]^-$ 634.9967, found : 634.9966.

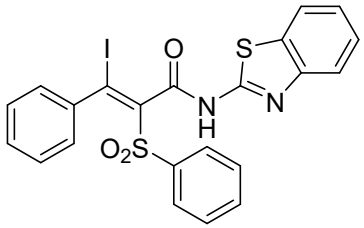


(E)-*N*-(benzo[d]thiazol-2-yl)-3-iodo-3-(naphthalen-2-yl)-2-tosylacrylamide **(4d)**

white solid, m.p. 250-251 ℃

69.8 mg, 53%; petroleum ether/ethyl acetate = 1/5, R_f = 0.5

^{1}H NMR (400 MHz, DMSO-d_6) δ 13.77 (s, 1H), 8.01 (d, J = 7.9 Hz, 1H), 7.84-7.78 (m, 3H), 7.67 (s, 1H), 7.46-7.40 (m, 3H), 7.36-7.30 (m, 2H), 7.17 (d, J = 5.7 Hz, 1H), 7.05 (d, J = 7.8 Hz, 2H), 6.82 (d, J = 8.0 Hz, 2H), 2.04 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 163.4, 158.1, 149.1, 147.8, 144.9, 136.7, 136.3, 133.4, 132.1, 130.2, 129.5, 128.5, 128.3, 128.1, 127.0, 126.8, 126.3, 125.3, 124.7, 124.6, 122.5, 121.5, 116.1, 21.4. HRMS (ESI) m/z: calcd for $C_{27}H_{19}IN_2NaO_3S_2$ $[M+Na]^+$ 632.9774, found : 632.9767.

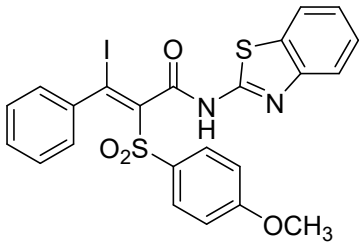


(E)-*N*-(benzo[d]thiazol-2-yl)-3-iodo-3-phenyl-2-(phenylsulfonyl)acrylamide **(4e)**

white solid, m.p. 188-189 ℃

80.6 mg, 74%; petroleum ether/ethyl acetate = 1/5, R_f = 0.5

^{1}H NMR (400 MHz, DMSO-d_6) δ 13.53 (s, 1H), 8.00 (d, J = 7.8 Hz, 1H), 7.78 (d, J = 7.9 Hz, 1H), 7.61-7.58 (m, 1H), 7.46-7.39 (m, 5H), 7.34-7.30 (m, 1H), 7.25-7.20 (m, 3H), 6.99-697 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 163.4, 157.9, 151.4, 149.0, 145.3, 140.6, 140.3, 1346, 132.1, 129.7, 129.7, 129.6, 129.6, 128.3, 128.3, 128.2, 128.2, 127.0, 127.0, 124.6, 124.6, 122.5, 122.5, 121.5, 121.5, 119.3. HRMS (ESI) m/z: calcd for $C_{22}H_{16}IN_2O_3S_2$ $[M+H]^+$ 546.9642, found: 546.9647.

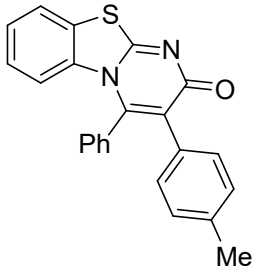


(E)-*N*-(benzo[d]thiazol-2-yl)-3-iodo-2-((4-methoxyphenyl)sulfonyl)-3-phenylacrylamide **(4f)**

white solid, m.p. 203-205 ℃

86.2 mg, 75%; methanol/dichloromethane = 1/50, R_f= 0.5

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04-8.01 (m, 1H), 7.93-7.91 (m, 1H), 7.55-7.40 (m, 4H), 7.29-7.25 (m, 3H), 7.21 (t, J = 7.5 Hz, 2H), 6.83-6.80 (m, 4H), 3.84 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.09, 158.5, 146.5, 139.9, 131.1, 130.9, 129.7, 127.8, 126.9, 126.9, 124.6, 121.5, 114.2, 55.7. HRMS (ESI) m/z: calcd for $C_{23}H_{18}IN_2O_4S_2$ $[M+H]^+$ 576.9747, found: 576.9742.

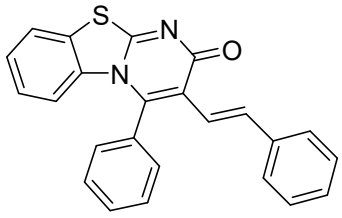


4-phenyl-3-(p-tolyl)-2H-benzo[4,5]thiazolo[3,2-a]pyrimidin-2-one **(5)**

white solid, m.p. 250-253 ℃

62.5 mg, 85%; petroleum ether/ethyl acetate = 1/1, R_f= 0.4

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (dd, J = 7.9, 1.3 Hz, 1H), 7.48-7.37 (m, 3H), 7.28-7.24 (m, 3H), 7.01-6.93 (m, 5H), 5.83 (d, J = 8.5 Hz, 1H), 2.23 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.6, 163.8, 145.8, 137.0, 136.2, 131.4, 130.5, 130.2, 129.8, 129.4, 129.2, 128.5, 126.2, 125.8, 124.5, 124.5, 122.9, 116.6, 21.3. HRMS (ESI) m/z: calcd for $C_{23}H_{16}N_2NaOS$ $[M+Na]^+$ 391.0876, found: 391.0875.



(E)-4-phenyl-3-styryl-2H-benzo[4,5]thiazolo[3,2-a]pyrimidin-2-one **(6)**

white solid, m.p. 236-238 ℃

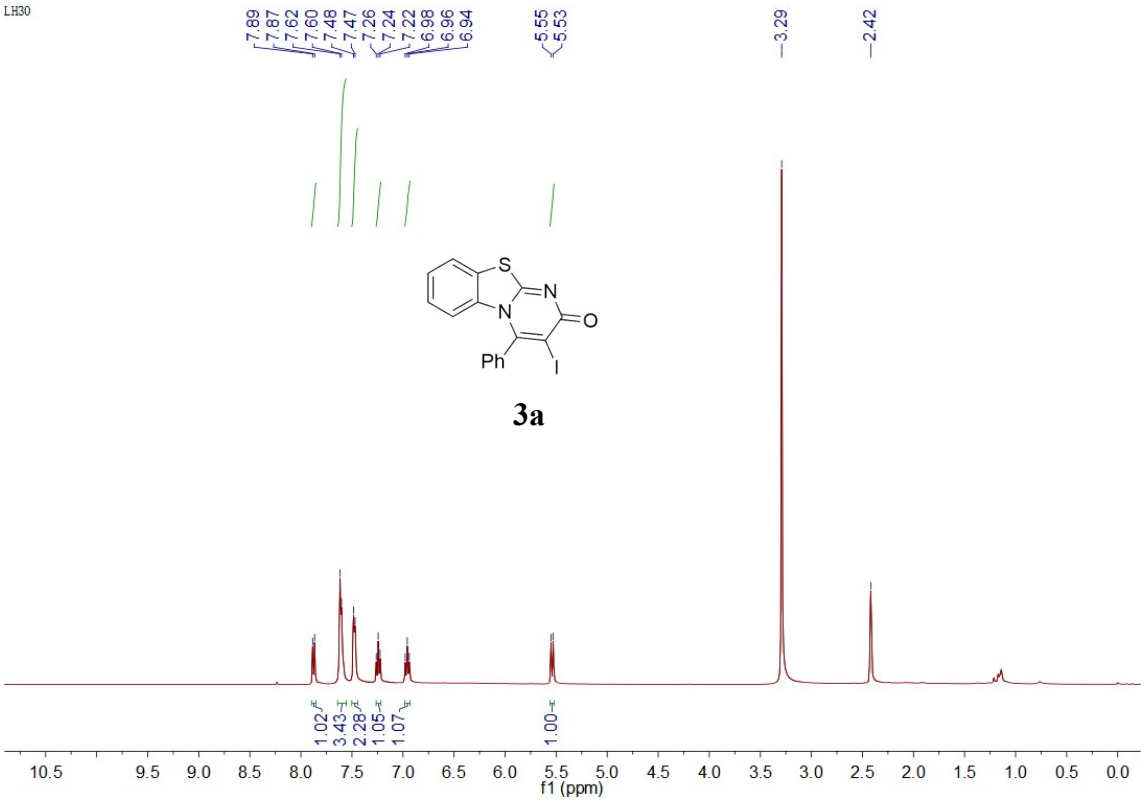
54.0 mg, 71%; methanol/dichloromethane = 1/50, R_f= 0.45

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, J = 16.1 Hz, 1H), 7.79-7.69 (m, 3H), 7.63 (dd, J = 7.9, 1.5 Hz, 1H), 7.53-7.50 (m, 2H), 7.31-7.29 (m, 1H), 7.28-7.25 (m, 4H), 7.23-7.19 (m, 1H), 7.03-6.98 (m, 1H), 6.55 (d, J = 16.1 Hz, 1H), 5.86 (d, J = 8.7 Hz, 1H).

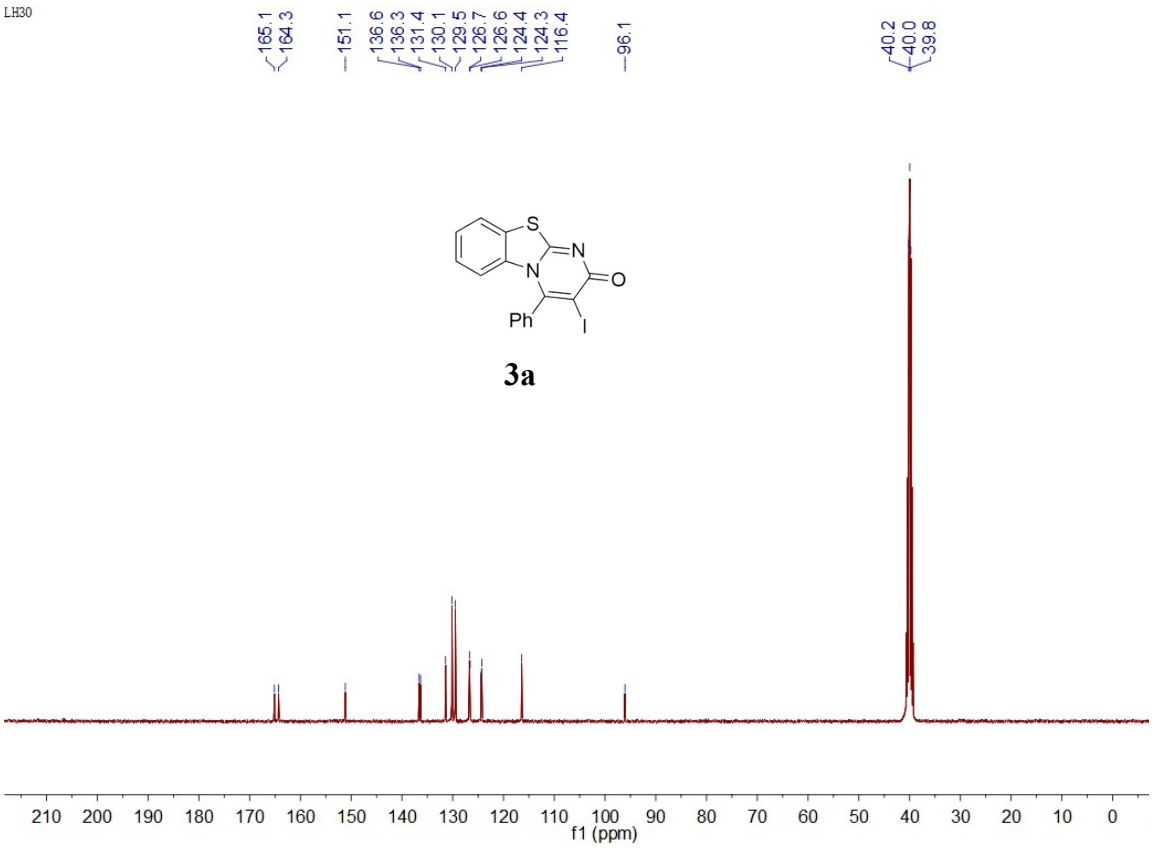
^{13}C NMR (101 MHz, $CDCl_3$) δ 165.8, 161.9, 145.4, 137.9, 136.1, 135.9, 131.4, 131.0, 130.0, 129.8, 128.5, 127.9, 126.8, 126.3, 125.9, 124.5, 123.0, 119.9, 118.2, 116.5.

HRMS (ESI) m/z: calcd for $C_{24}H_{17}N_2OS$ $[M+H]^+$ 381.1062, found: 381.1069.

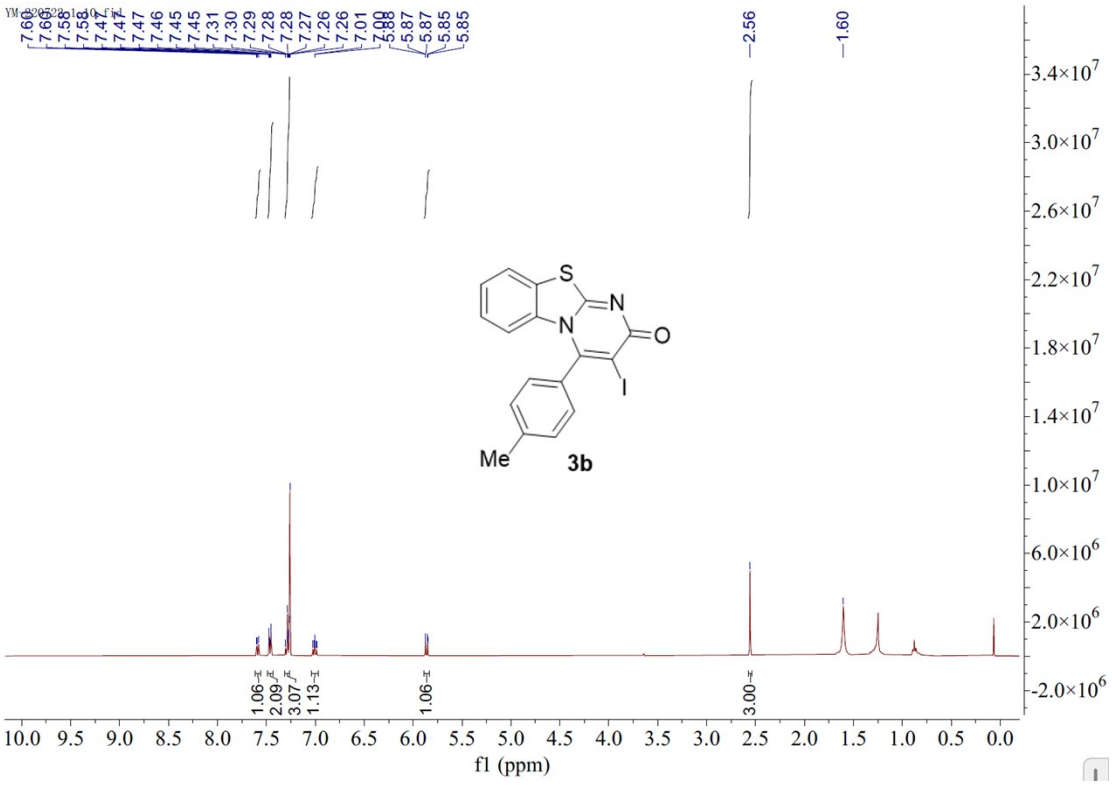
5. ^{1}H, ^{13}C and ^{19}F NMR of Compounds 3, 4, 5, 6.



3a



3a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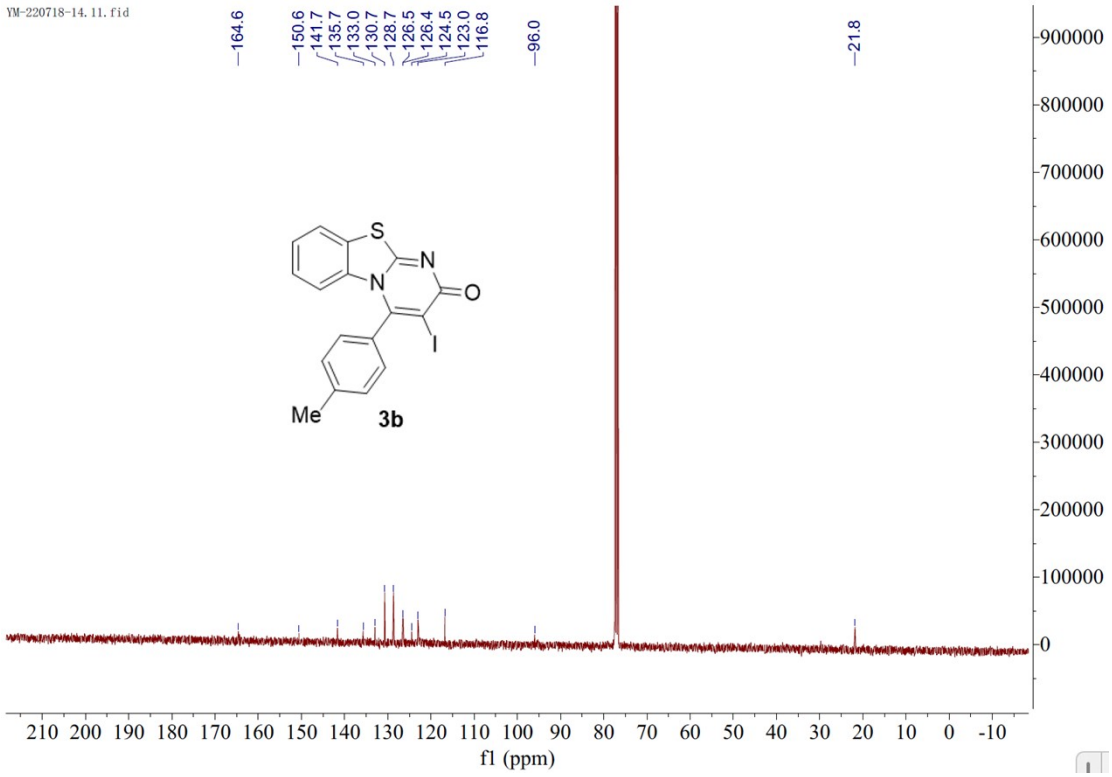
7.68
7.58
7.55
7.47
7.47
7.47
7.46
7.45
7.45
7.31
7.30
7.29
7.28
7.28
7.27
7.26
7.26
7.01
5.88
5.87
5.87
5.85
5.85
2.56
1.60
S
N
N
O
I
Me
3b
1.06
2.09
3.07
1.13
1.06
3.00
fl (ppm)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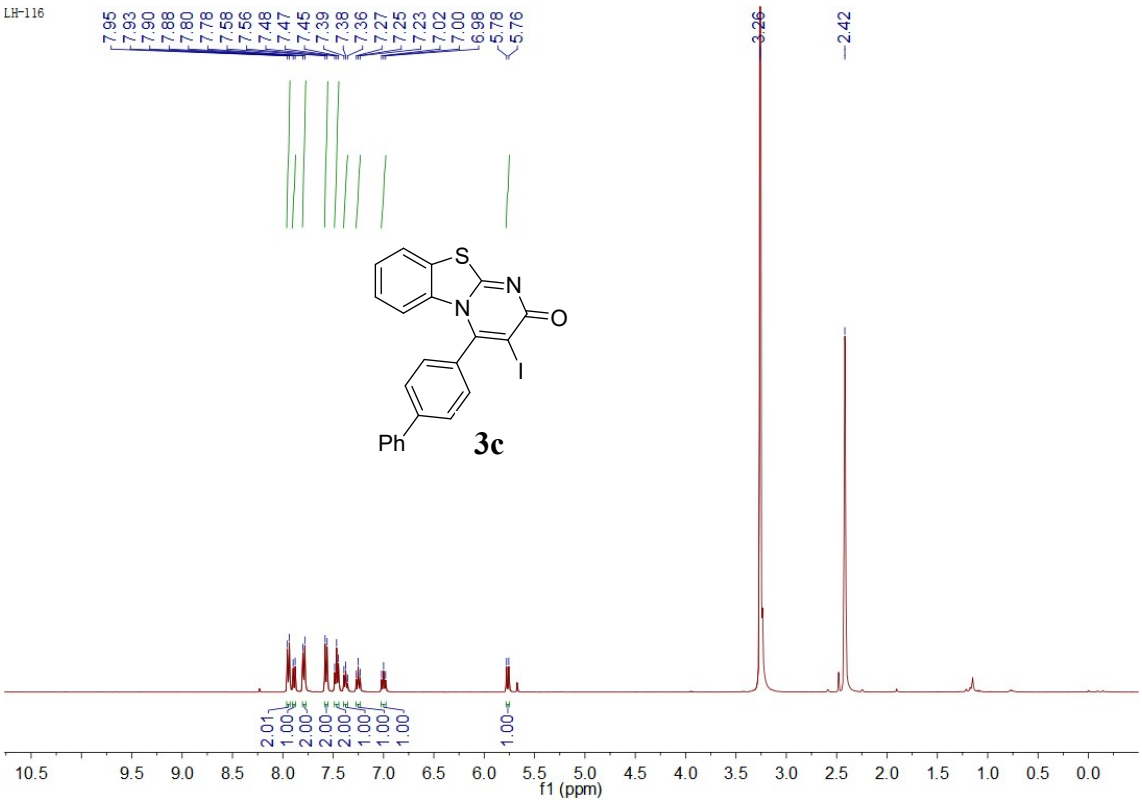
150.6
141.7
135.7
133.0
130.7
128.7
126.5
126.4
124.5
123.0
116.8
96.0
21.8
S
N
N
O
I
Me
3b
fl (ppm)


LH-116
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7.93
7.90
7.88
7.80
7.78
7.58
7.56
7.48
7.47
7.45
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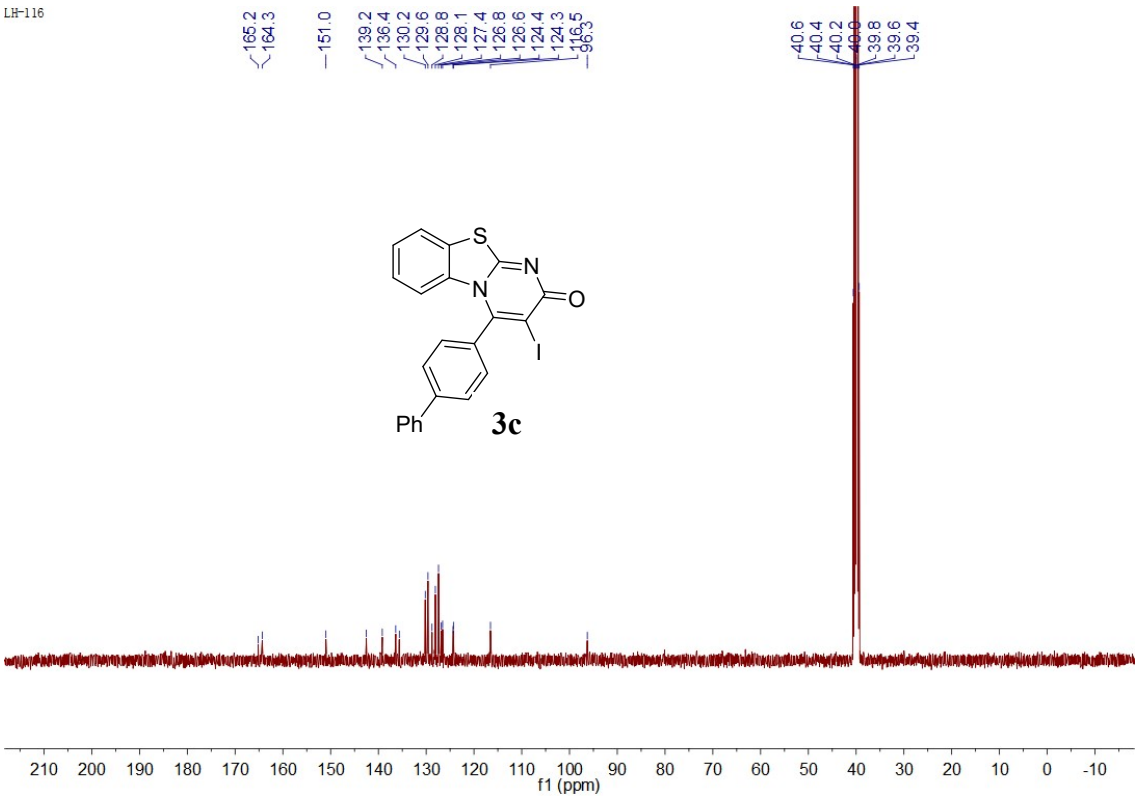
7.38
7.36
7.27
7.25
7.23
7.02
7.00
6.98
5.78
5.76
3.26
2.42
S
N
N
O
I
Ph
3c
2.01
1.00
2.00
2.00
2.00
1.00
1.00
1.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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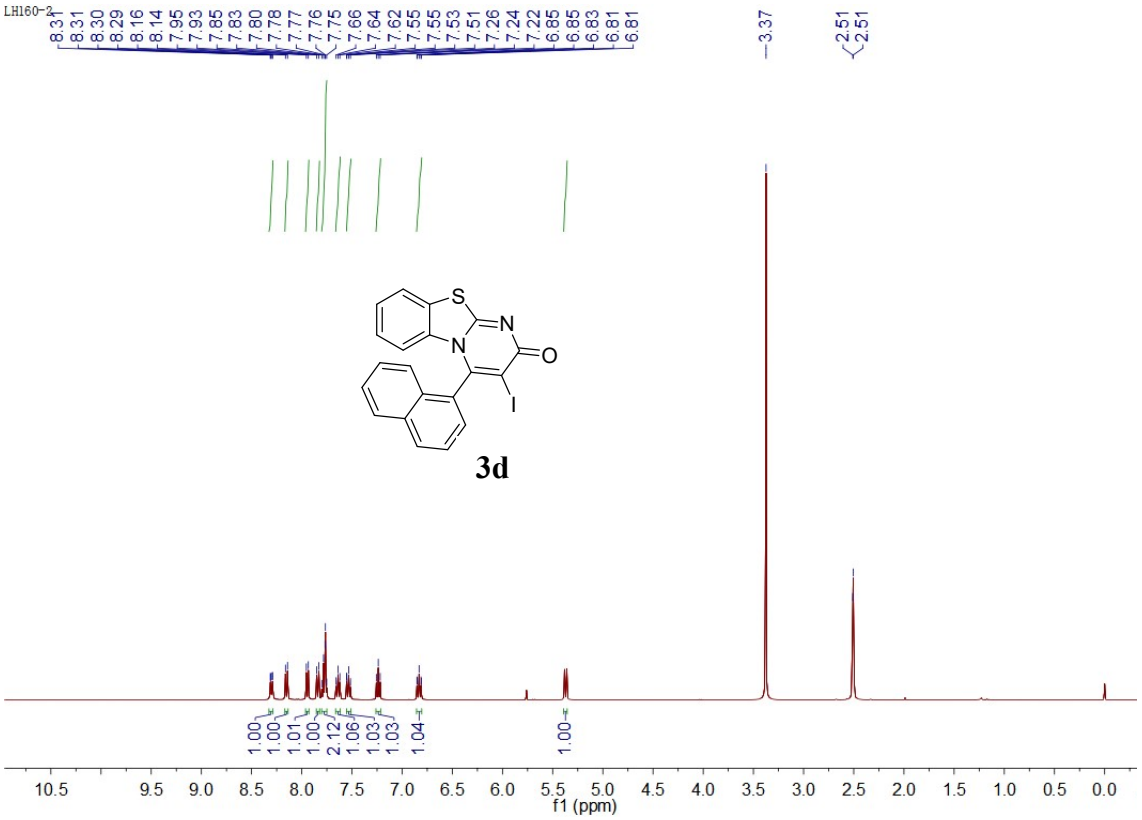
164.3
151.0
139.2
136.4
130.2
129.6
128.8
128.1
127.4
126.8
126.6
124.4
124.3
116.5
96.3
40.6
40.4
40.2
40.0
39.8
39.6
39.4
S
N
N
O
I
Ph
3c
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


LH160-2
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8.31
8.30
8.29
8.16
8.14
7.95
7.93
7.85
7.83
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7.77
7.76
7.75
7.66
7.64
7.62
7.55
7.55
7.53
7.51
7.26
7.24
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6.85
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6.81
6.81
3.37
2.51
2.51
S
N
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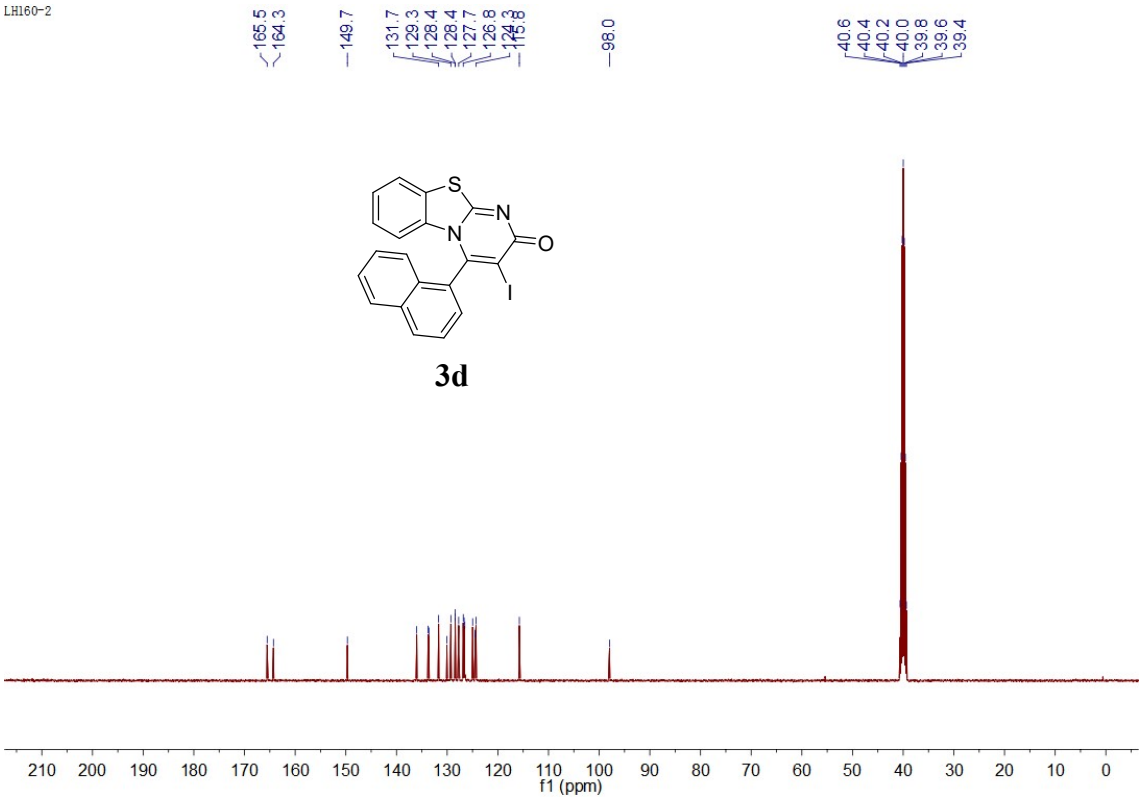
O
I
1.00
1.00
1.01
1.00
2.12
1.06
1.03
1.03
1.04
1.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

3d


LH160-2
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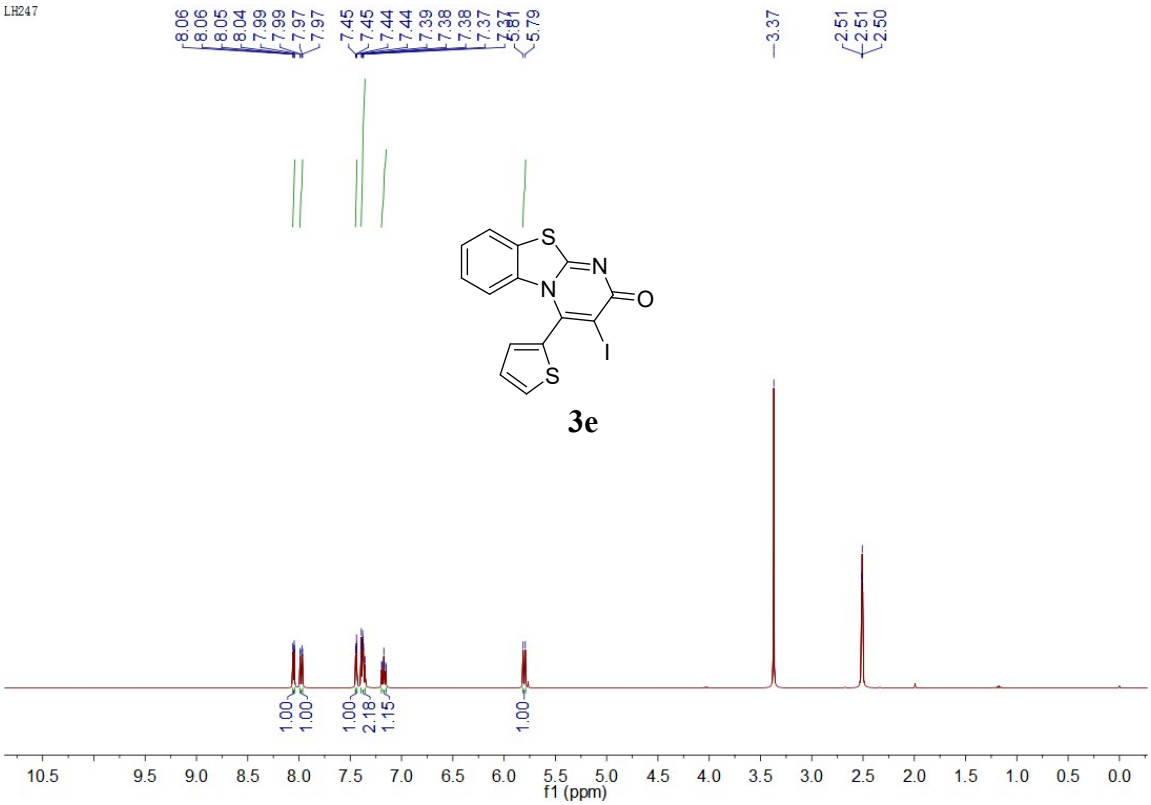
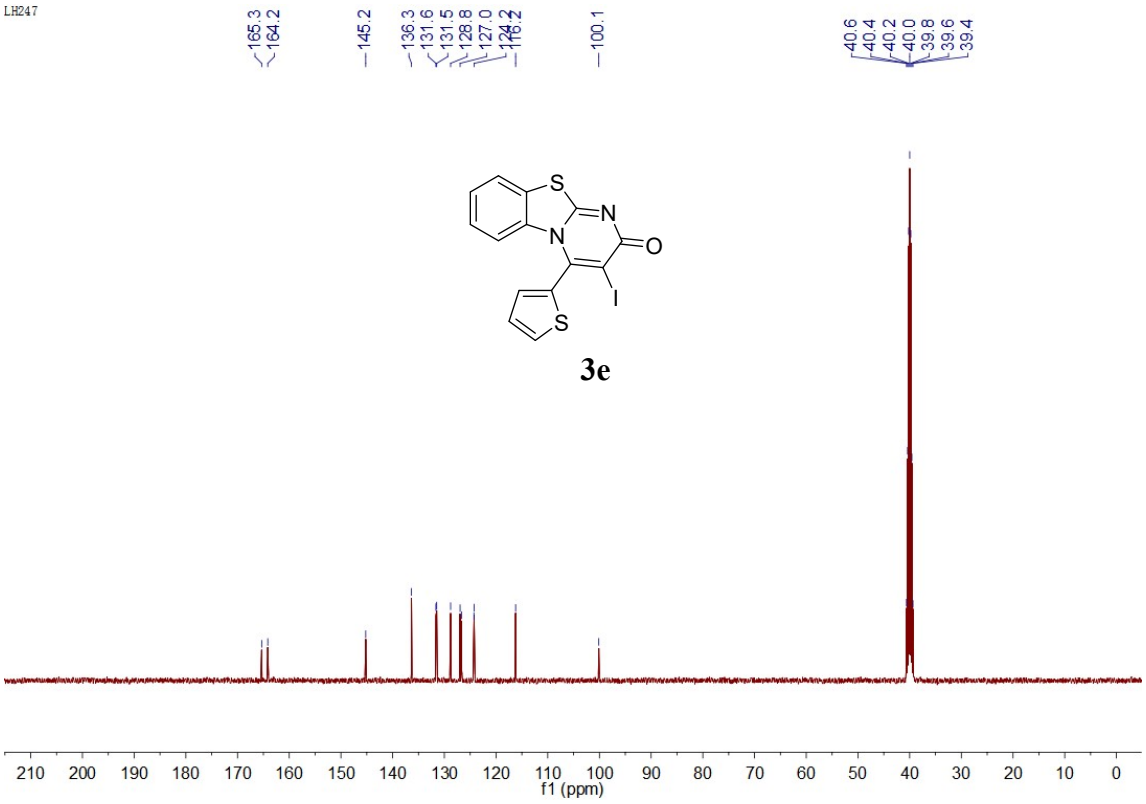
164.3
149.7
131.7
129.3
128.4
128.4
127.7
126.8
124.3
115.8
98.0
40.6
40.4
40.2
40.0
39.8
39.6
39.4
S
N
N
O
I
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

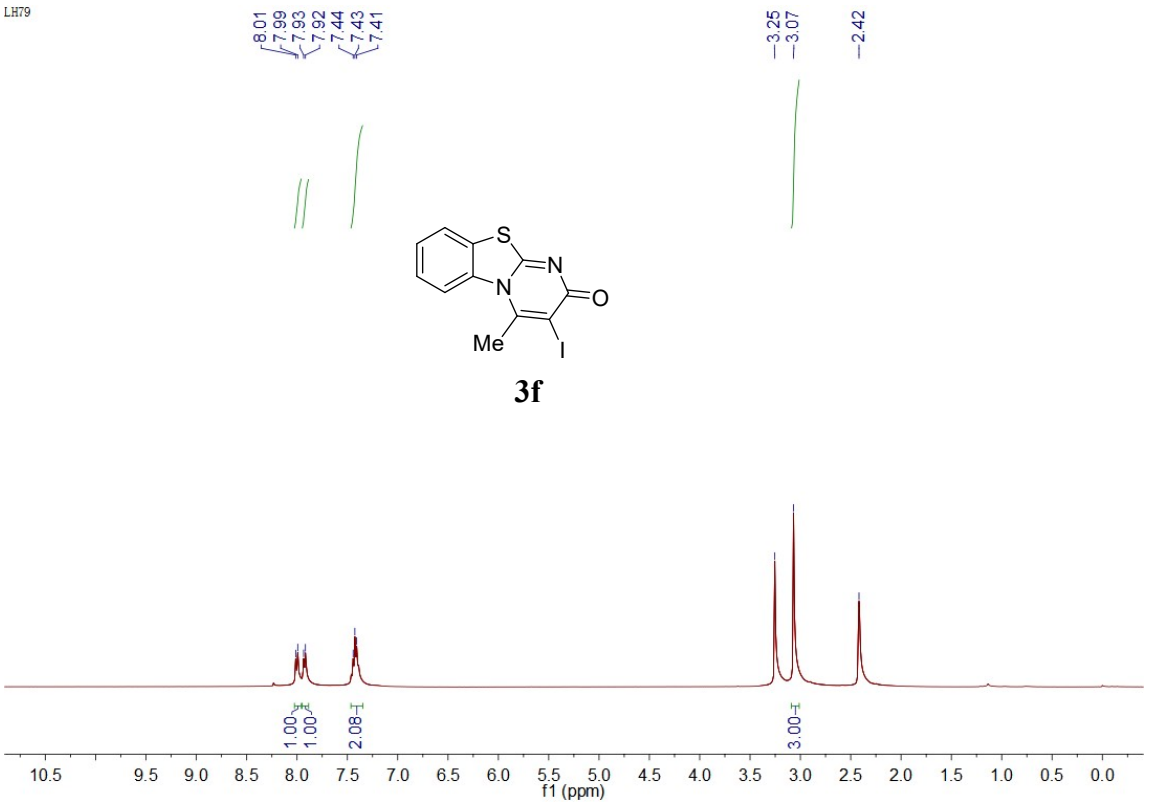
3d


LH247
8.06
8.06
8.05
8.04
7.99
7.99
7.97
7.97
7.45
7.45
7.44
7.44
7.39
7.38
7.37
7.37
5.81
5.79
3.37
2.51
2.51
2.50
S
N
N
O
I
S
1.00
1.00
1.00
2.18
1.15
1.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

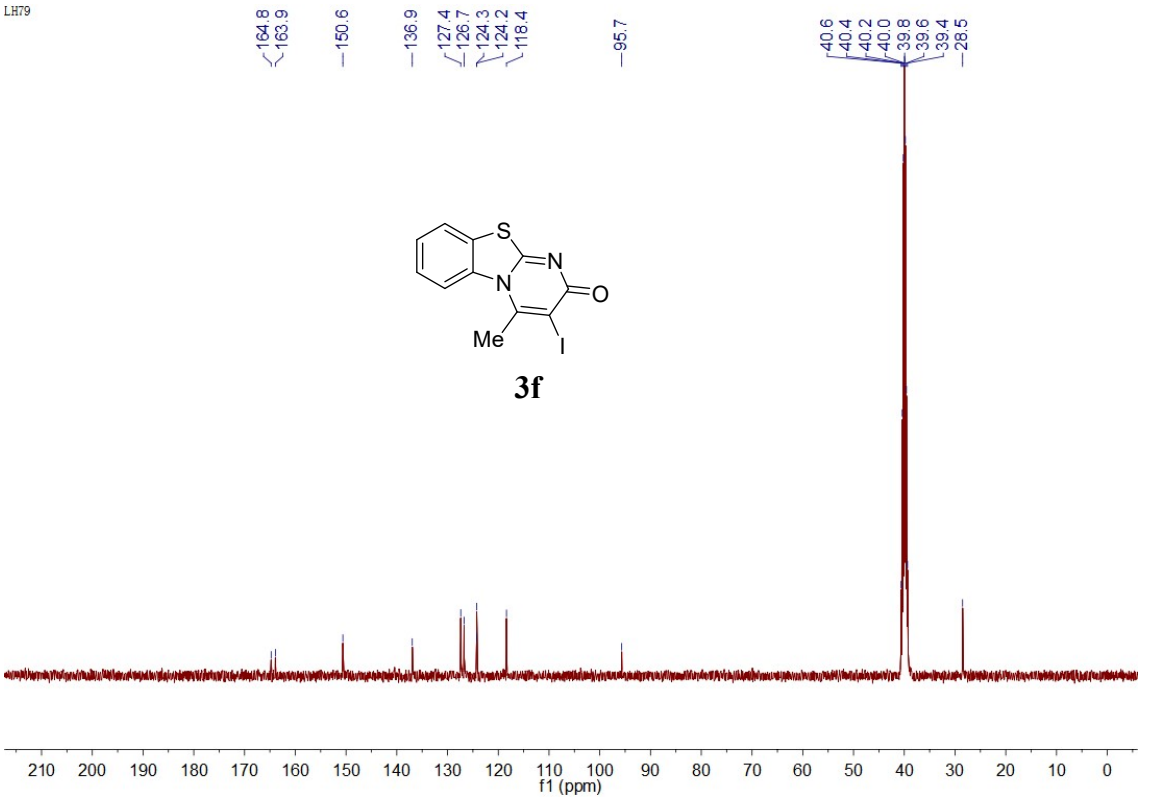
3e


LH247
165.3
164.2
145.2
136.3
131.6
131.5
128.8
127.0
124.2
116.2
100.1
40.6
40.4
40.2
40.0
39.8
39.6
39.4
S
N
N
O
I
S
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

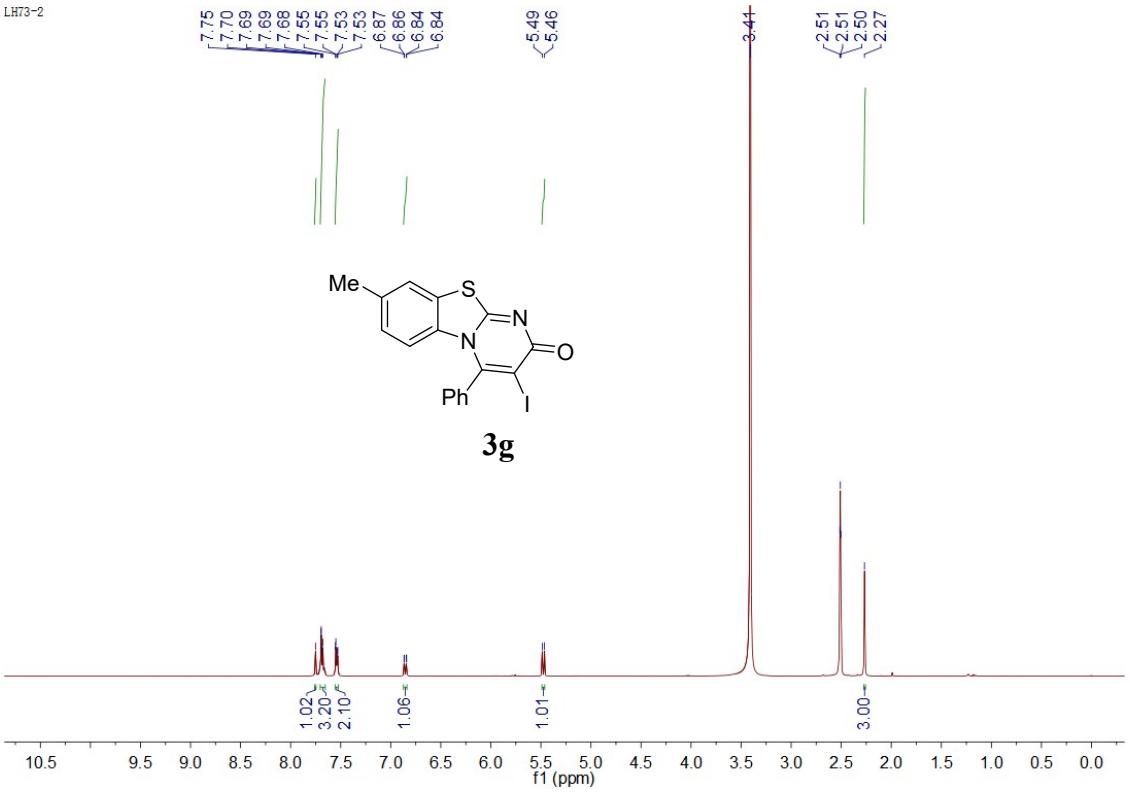
3e


LH79
8.01
7.99
7.93
7.92
7.44
7.43
7.41
3.25
3.07
2.42
S
N
N
O
Me
I
1.00
1.00
2.08
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

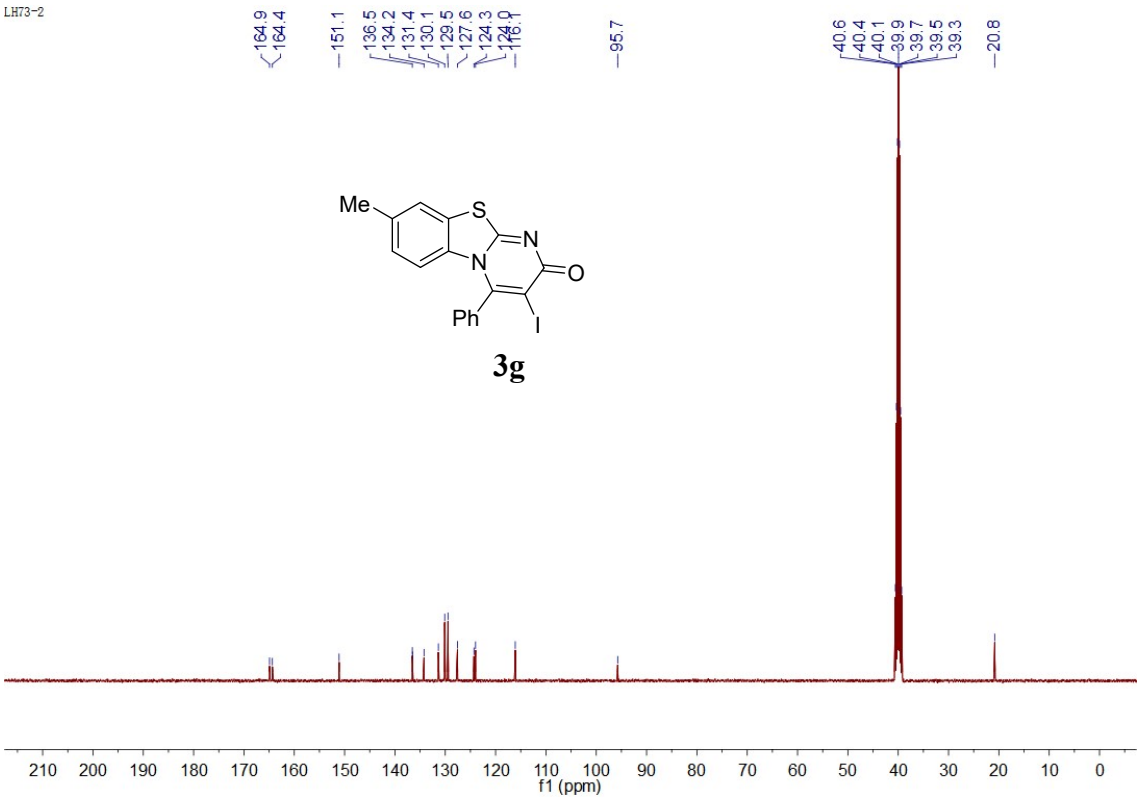
3f


LH79
164.8
163.9
150.6
136.9
127.4
126.7
124.3
124.2
118.4
95.7
40.6
40.4
40.2
40.0
39.8
39.6
39.4
28.5
S
N
N
O
Me
I
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

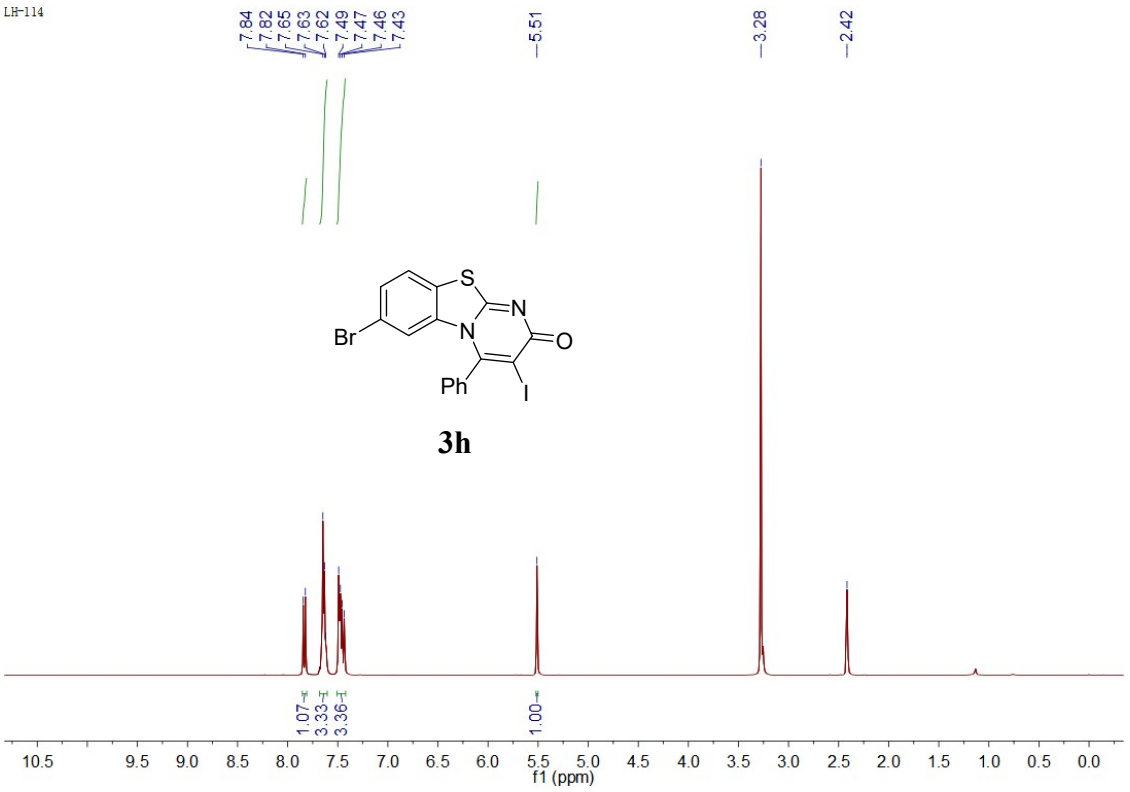
3f


LH73-2
7.75
7.70
7.69
7.69
7.68
7.55
7.55
7.53
7.53
6.87
6.86
6.84
6.84
5.49
5.46
3.41
2.51
2.51
2.50
2.27
Me
S
N
N
O
Ph
I
1.02
3.20
2.10
1.06
1.01
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

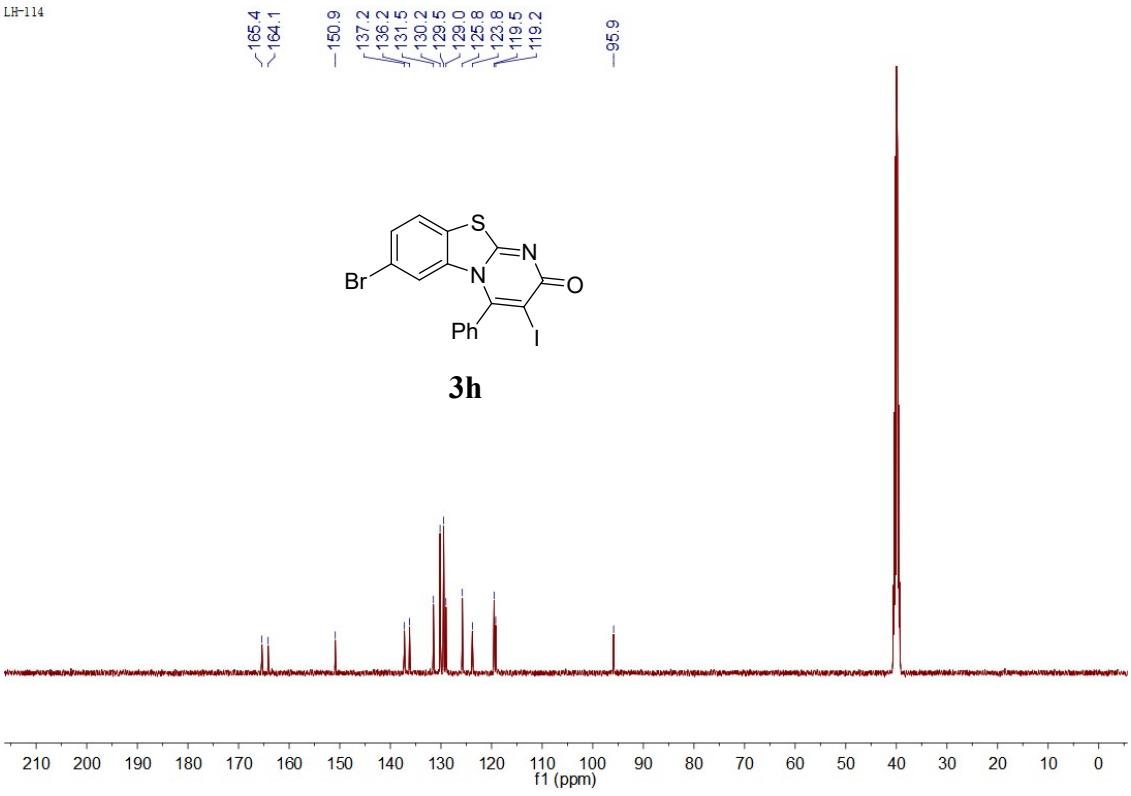
3g


LH73-2
164.9
164.4
151.1
136.5
134.2
131.4
130.1
129.5
127.6
124.3
124.0
116.1
95.7
40.6
40.4
40.1
39.9
39.7
39.5
39.3
20.8
Me
S
N
N
O
Ph
I
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

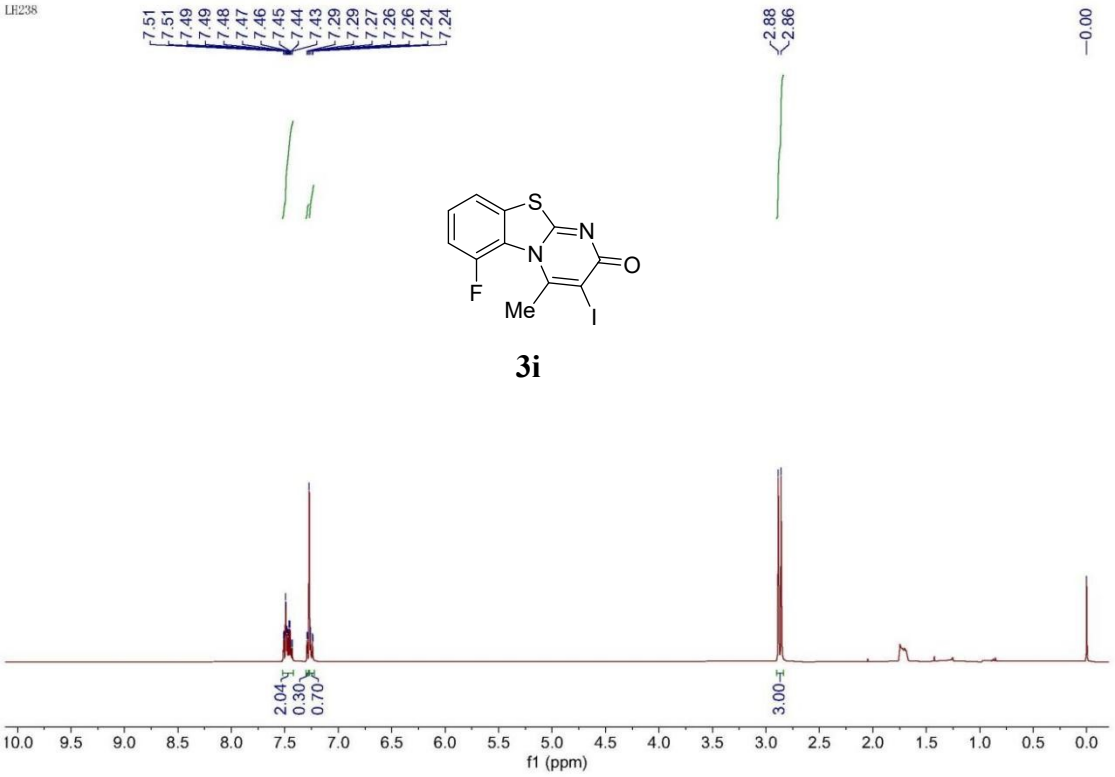
3g


LH-114
7.84
7.82
7.65
7.63
7.62
7.49
7.47
7.46
7.43
5.51
3.28
2.42
S
N
N
O
Br
Ph
I
1.07
3.33
3.36
1.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

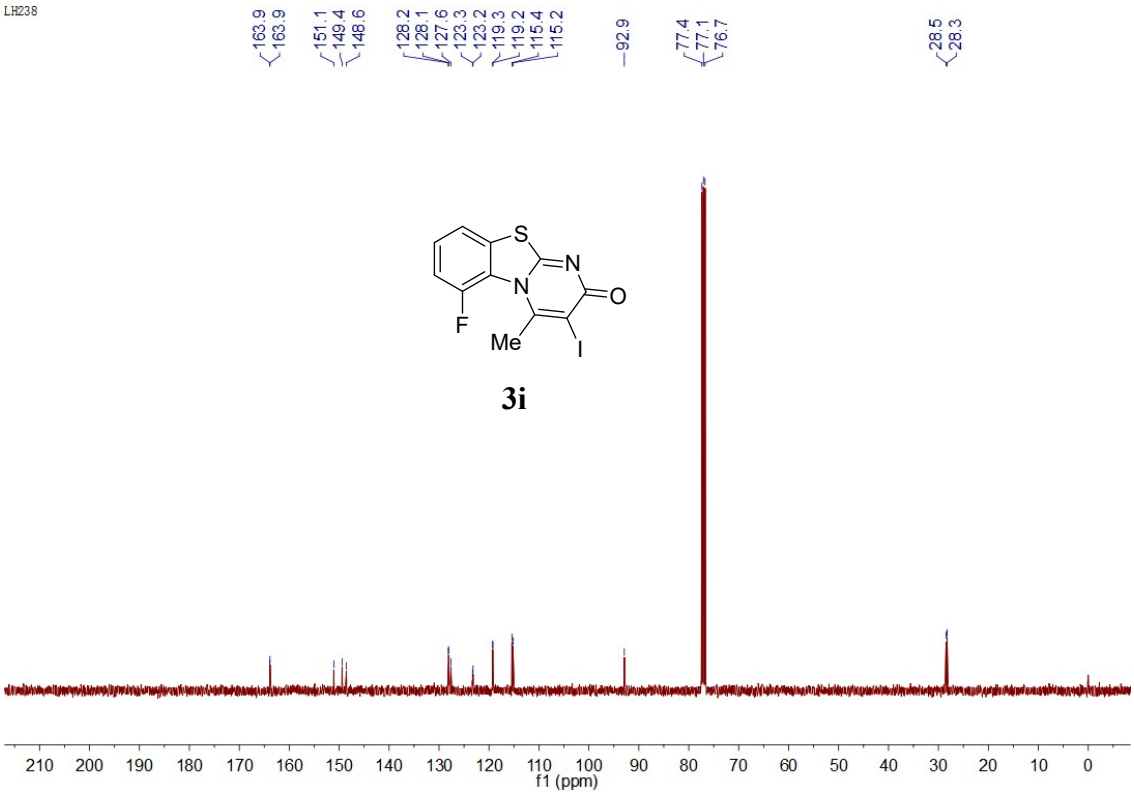
3h


LH-114
165.4
164.1
150.9
137.2
136.2
131.5
130.2
129.5
129.0
125.8
123.8
119.5
119.2
95.9
S
N
N
O
Br
Ph
I
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

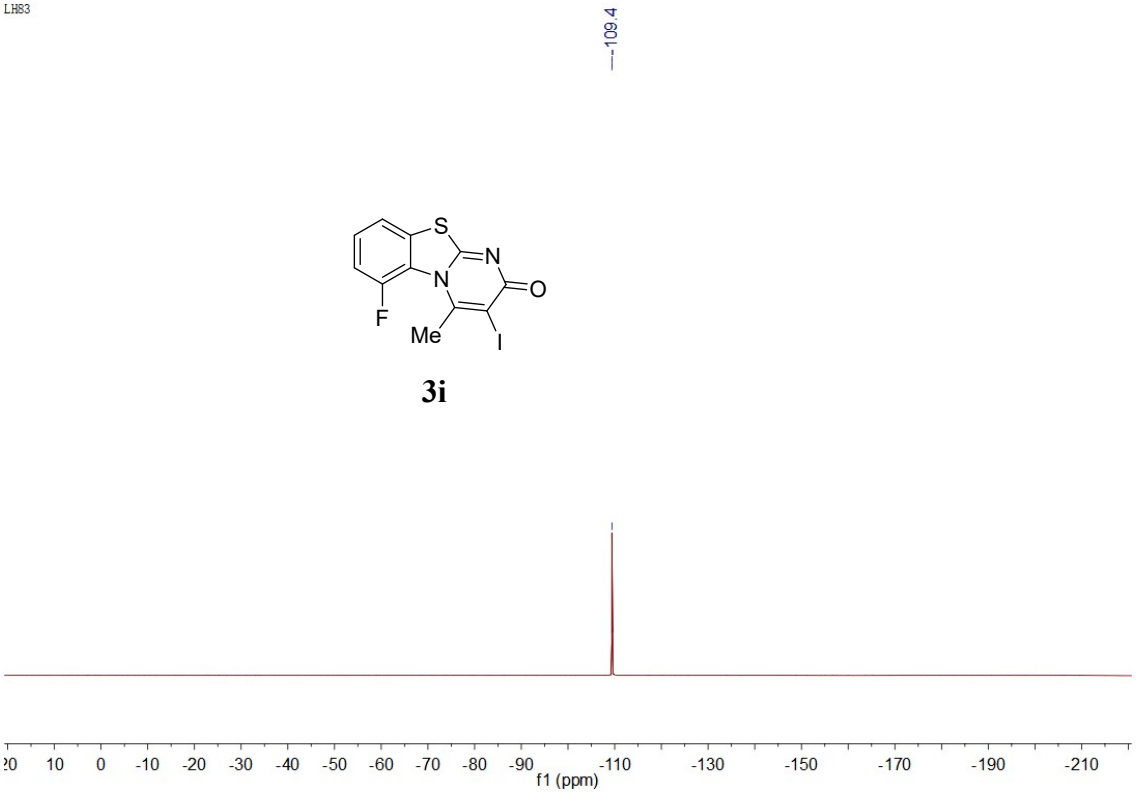
3h


LH238
7.51
7.51
7.49
7.49
7.48
7.47
7.46
7.45
7.44
7.43
7.29
7.29
7.27
7.26
7.26
7.24
7.24
2.88
2.86
0.00
S
N
N
O
F
Me
I
2.04
0.30
0.70
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

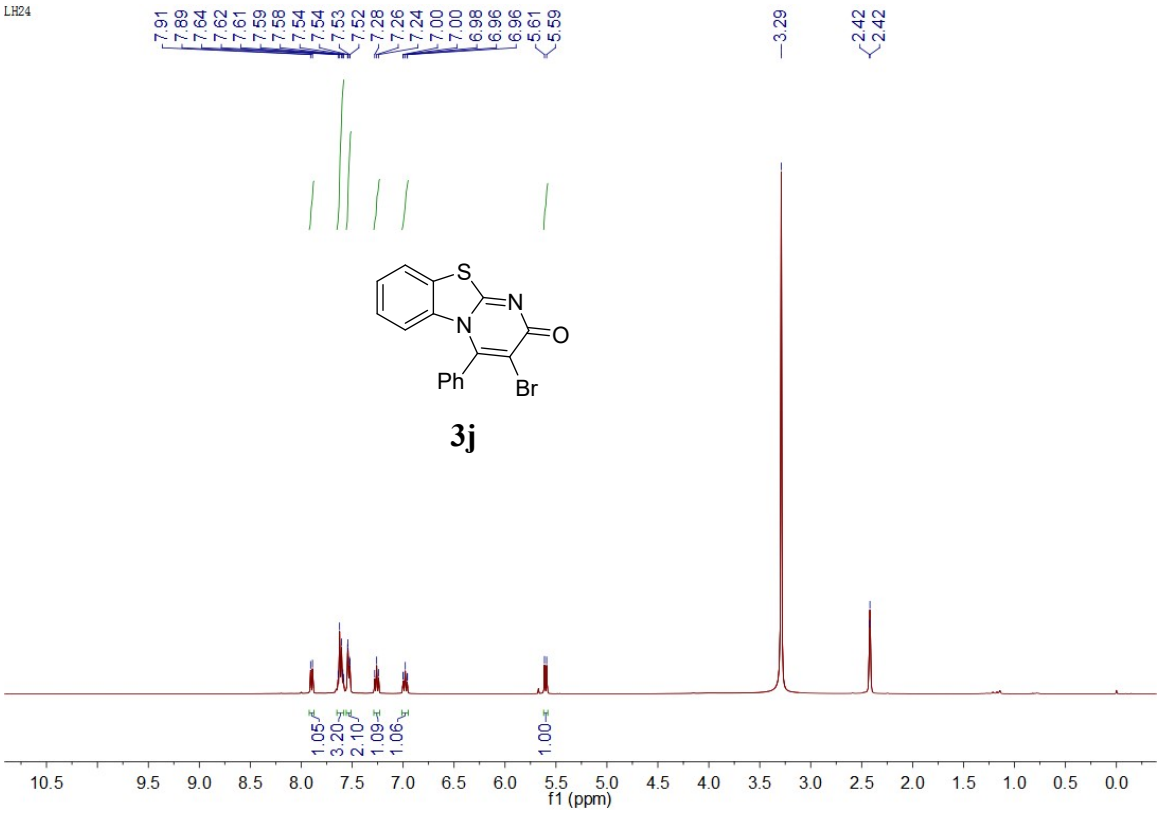
3i


LH238
163.9
163.9
151.1
149.4
148.6
128.2
128.1
127.6
123.3
123.2
119.3
119.2
115.4
115.2
92.9
77.4
77.1
76.7
28.5
28.3
S
N
N
O
F
Me
I
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

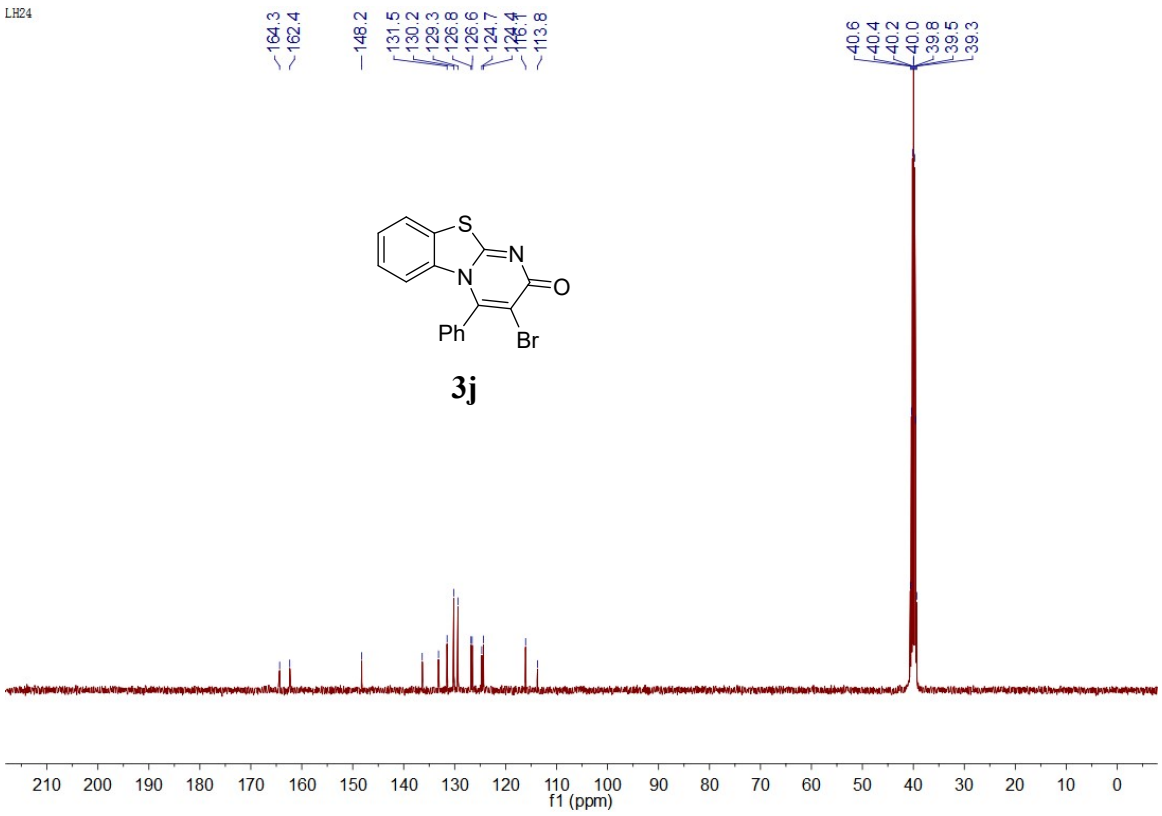
3i

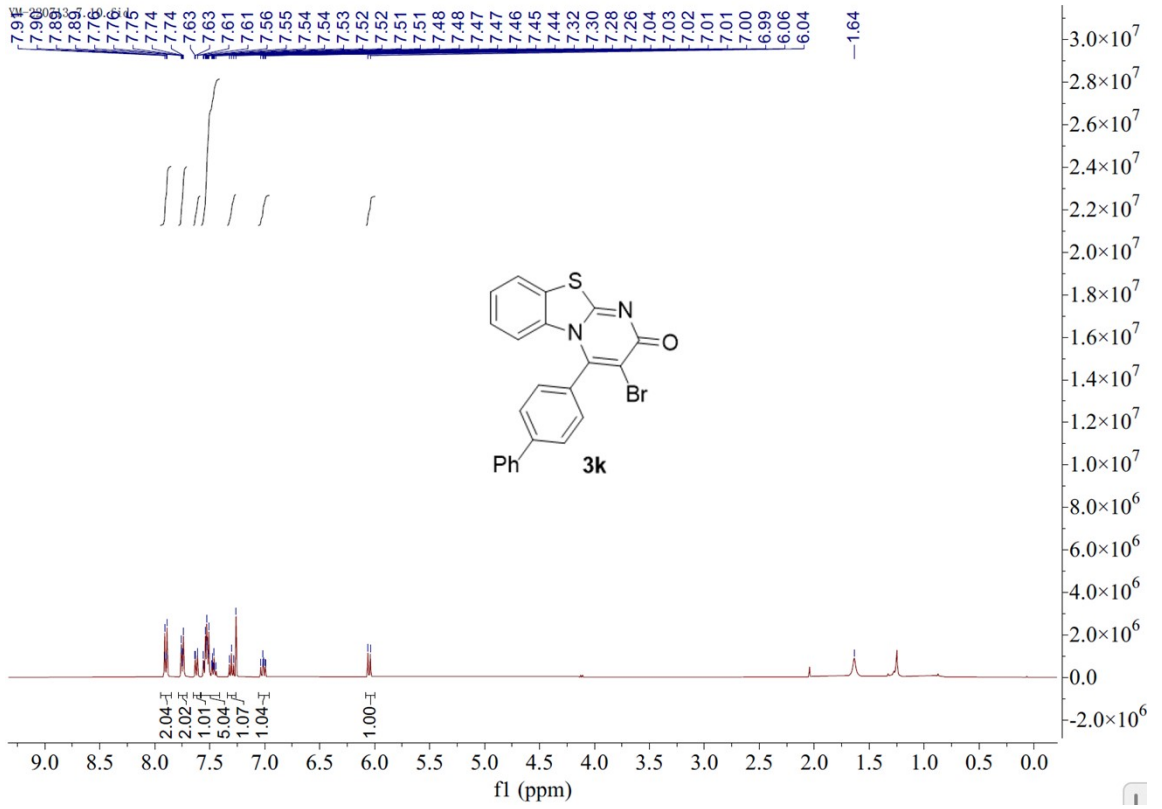

LH83
-109.4
S
N
N
O
F
Me
I
f1 (ppm)

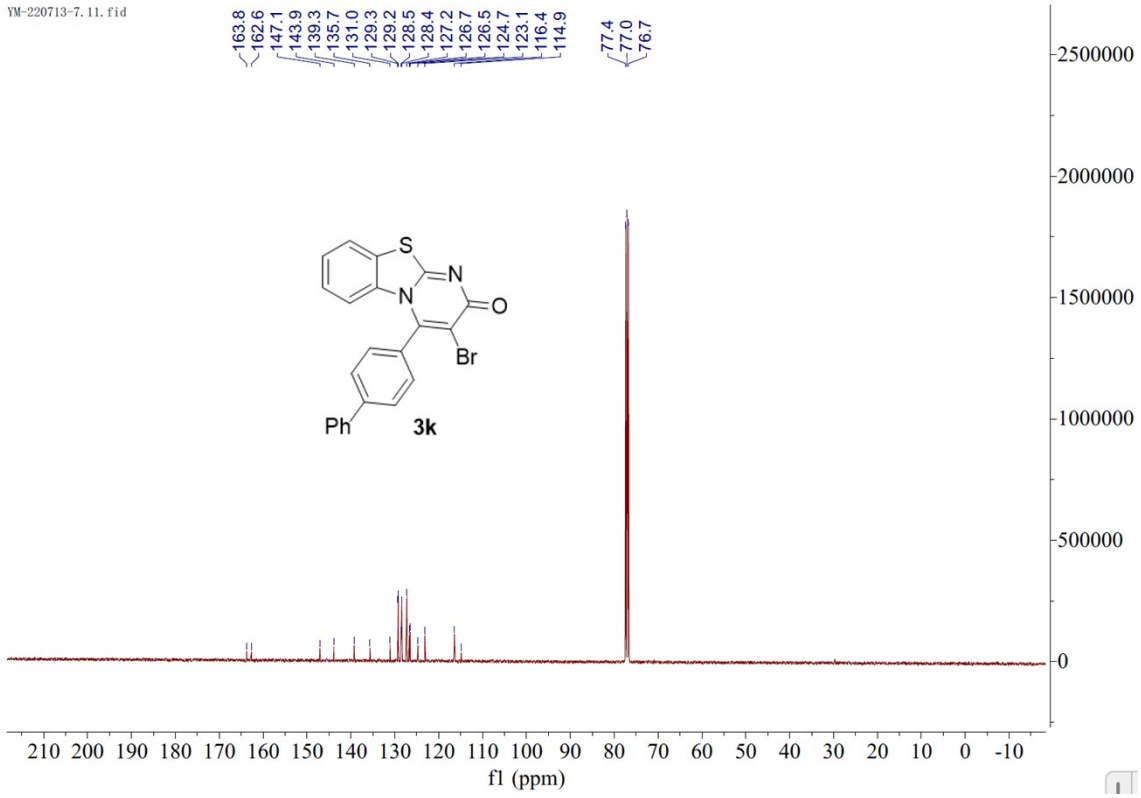
3i

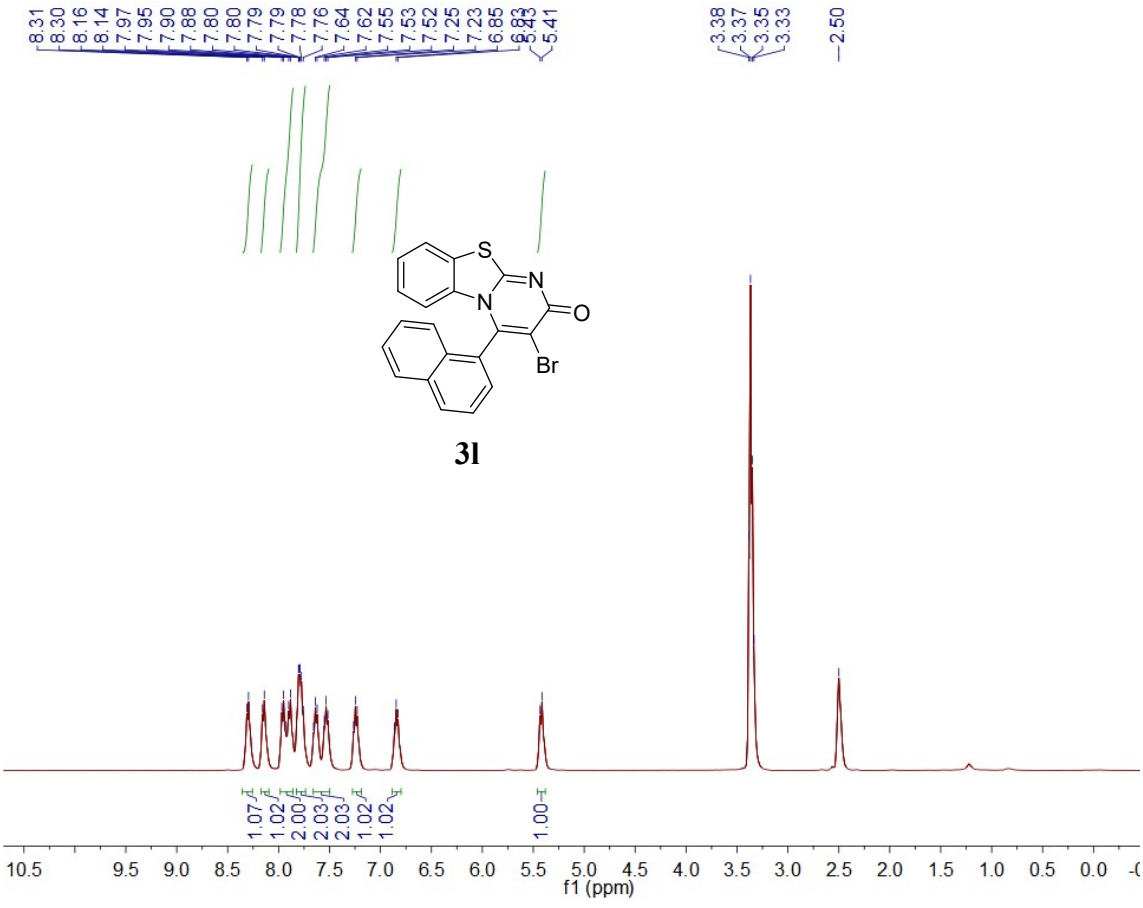

LH24
7.91
7.89
7.64
7.62
7.61
7.59
7.58
7.54
7.54
7.53
7.52
7.28
7.26
7.24
7.00
7.00
6.98
6.96
6.96
5.61
5.59
3.29
2.42
2.42
S
N
N
O
Ph
Br
1.05
3.20
2.10
1.09
1.06
1.00
f1 (ppm)

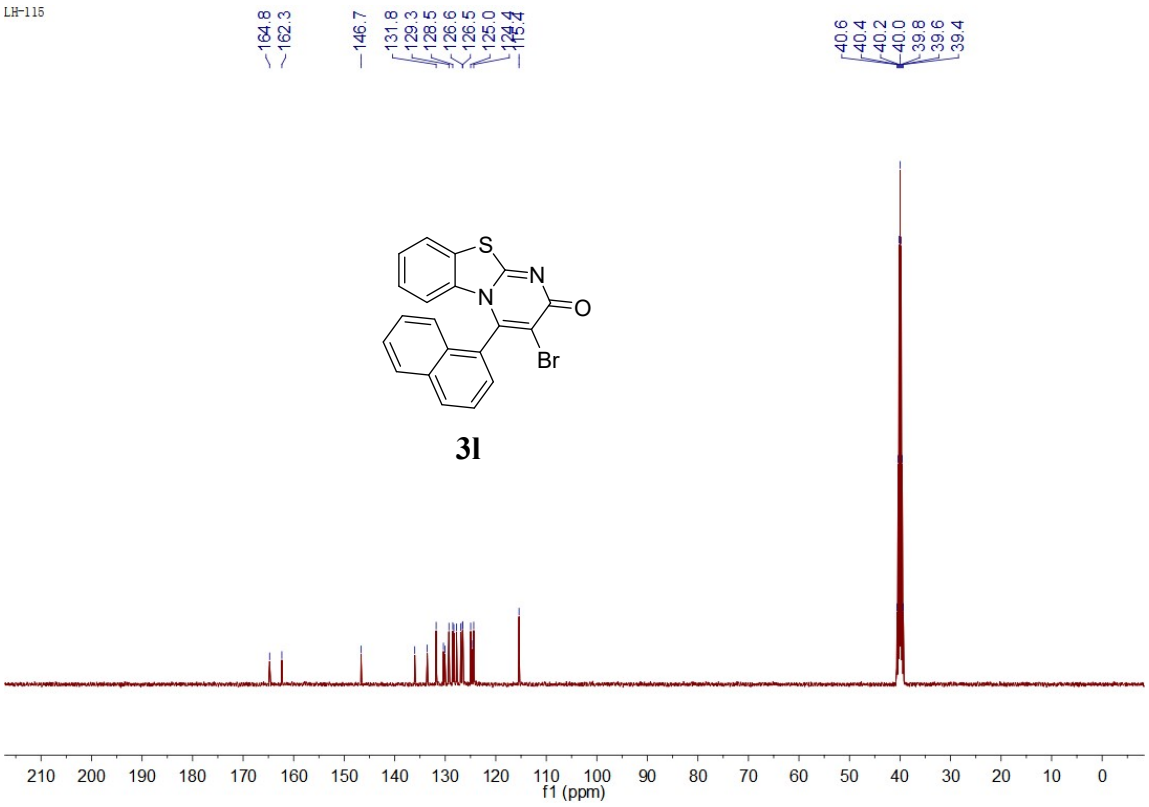
3j


LH24
164.3
162.4
148.2
131.5
130.2
129.3
126.8
126.6
124.7
40.6
40.4
40.2
40.0
39.8
39.5
39.3
S
N
N
O
Ph
Br
3j
f1 (ppm)

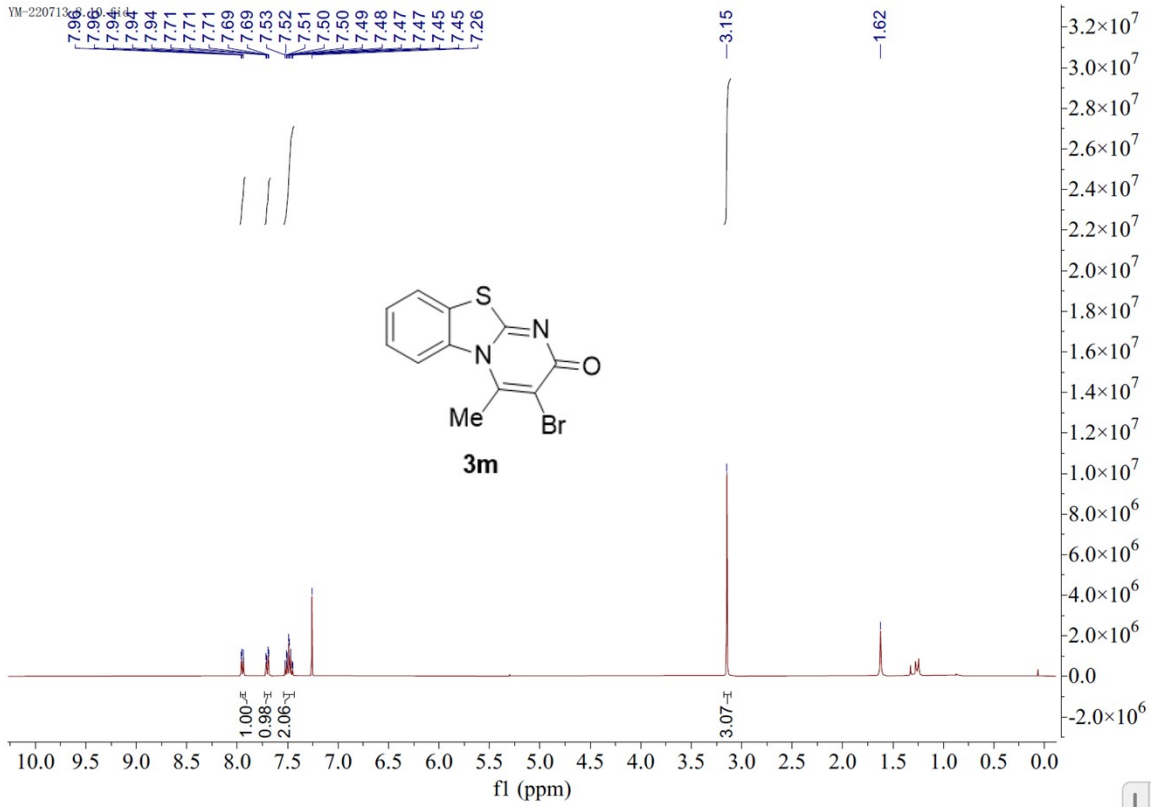

1.64
S
N
N
O
Br
Ph
3k
2.04
2.02
1.01
5.04
1.07
1.04
1.00
f1 (ppm)


YM-220713-7.11.fid
163.8
162.6
147.1
143.9
139.3
135.7
131.0
129.3
129.2
128.5
128.4
127.2
126.7
126.5
124.7
123.1
116.4
114.9
77.4
77.0
76.7
2500000
2000000
1500000
1000000
500000
0
S
N
N
O
Br
Ph
3k
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)

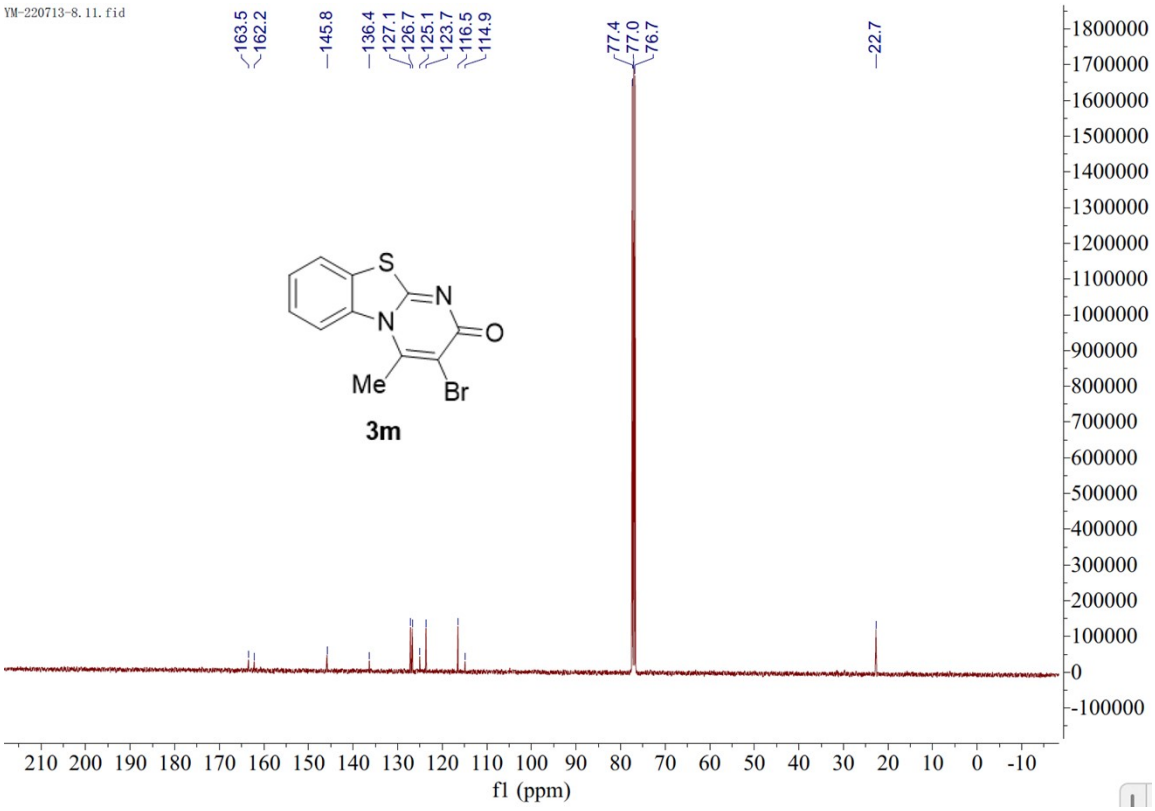

8.31
8.30
8.16
8.14
7.97
7.95
7.90
7.88
7.80
7.80
7.79
7.79
7.78
7.76
7.64
7.62
7.55
7.53
7.52
7.25
7.23
6.85
5.43
5.41
3.38
3.37
3.35
3.33
2.50
S
N
N
O
Br
3l
1.07
1.02
2.00
2.03
2.03
1.02
1.02
1.00
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


LH-115
164.8
162.3
146.7
131.8
129.3
128.5
126.6
126.5
125.0
124.4
115.4
40.6
40.4
40.2
40.0
39.8
39.6
39.4
S
N
N
O
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

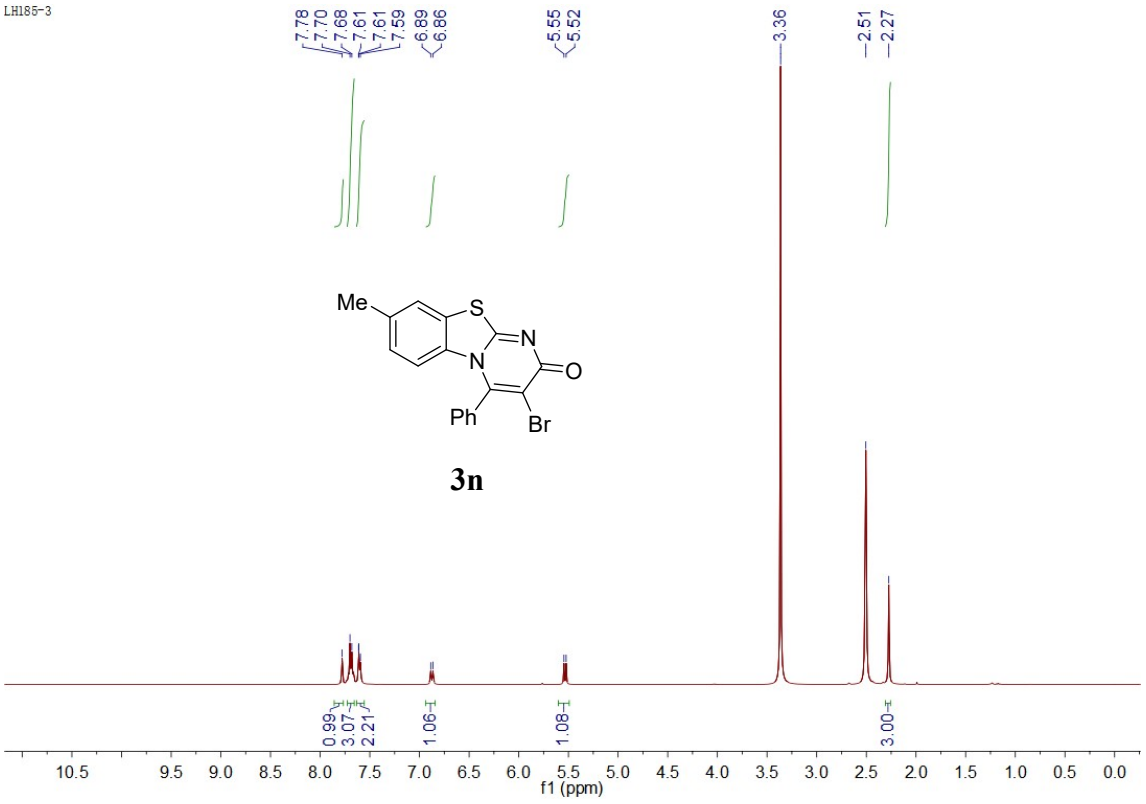
3l


7.96
7.96
7.94
7.94
7.94
7.71
7.71
7.71
7.69
7.69
7.53
7.52
7.51
7.50
7.50
7.49
7.48
7.47
7.47
7.45
7.45
7.26
3.15
1.62
S
N
N
O
Me
Br
1.00
0.98
2.06
3.07
3.2×10^7
3.0×10^7
2.8×10^7
2.6×10^7
2.4×10^7
2.2×10^7
2.0×10^7
1.8×10^7
1.6×10^7
1.4×10^7
1.2×10^7
1.0×10^7
8.0×10^6
6.0×10^6
4.0×10^6
2.0×10^6
0.0
-2.0×10^6
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)

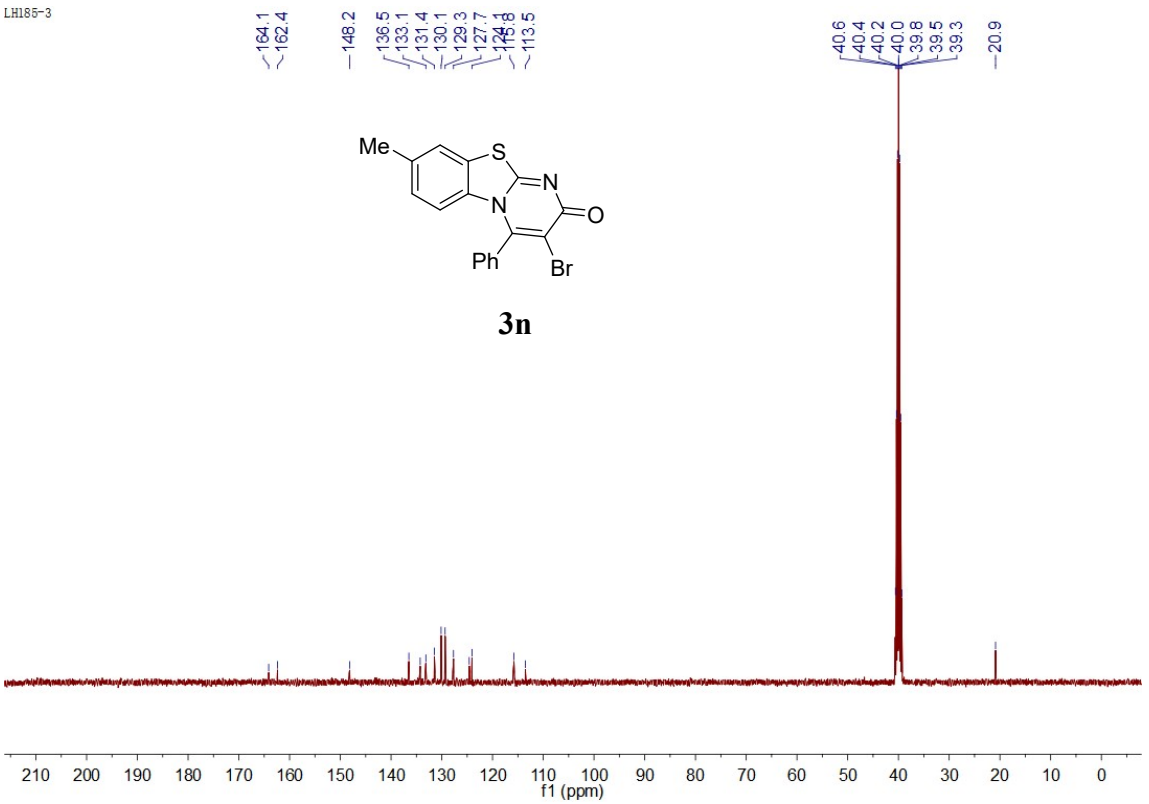
3m


YM-220713-8.11.fid
163.5
162.2
145.8
136.4
127.1
126.7
125.1
123.7
116.5
114.9
77.4
77.0
76.7
22.7
S
N
N
O
Me
Br
f1 (ppm)

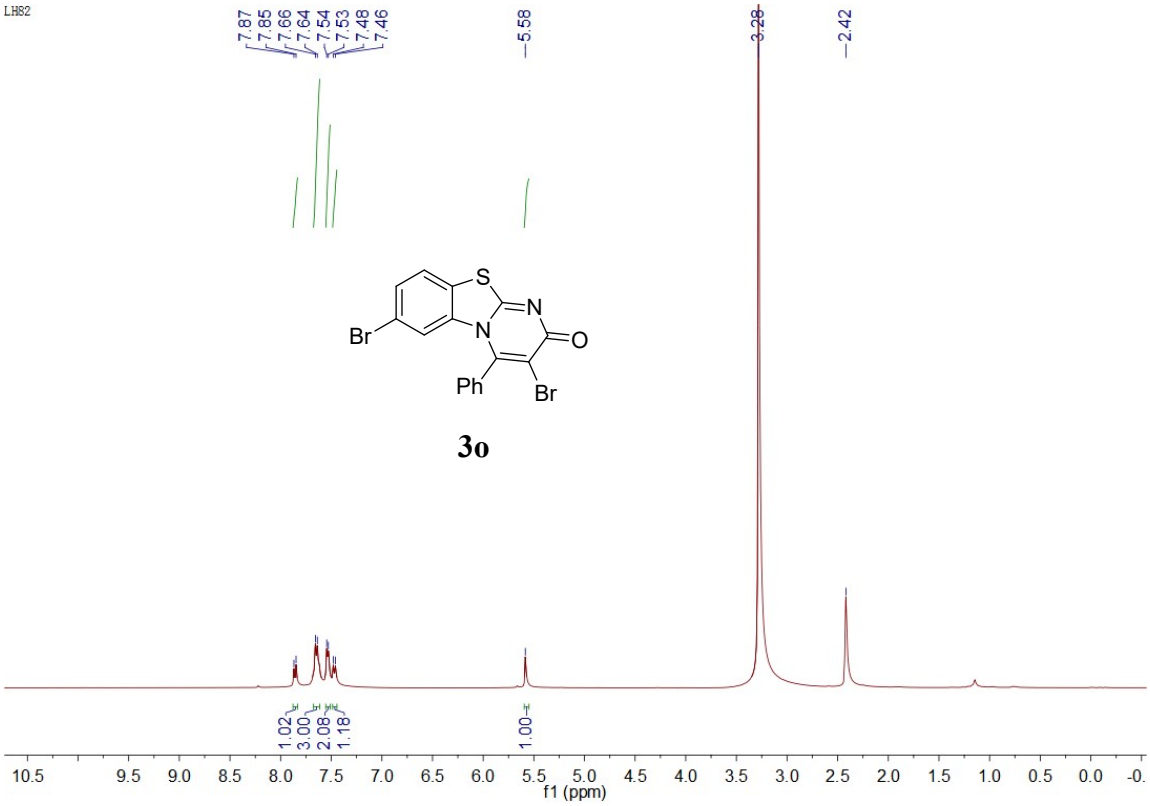
3m


LH185-3
7.78
7.70
7.68
7.61
7.61
7.59
6.89
6.86
5.55
5.52
3.36
2.51
2.27
Me
S
N
N
O
Ph
Br
0.99
3.07
2.21
1.06
1.08
3.00
f1 (ppm)

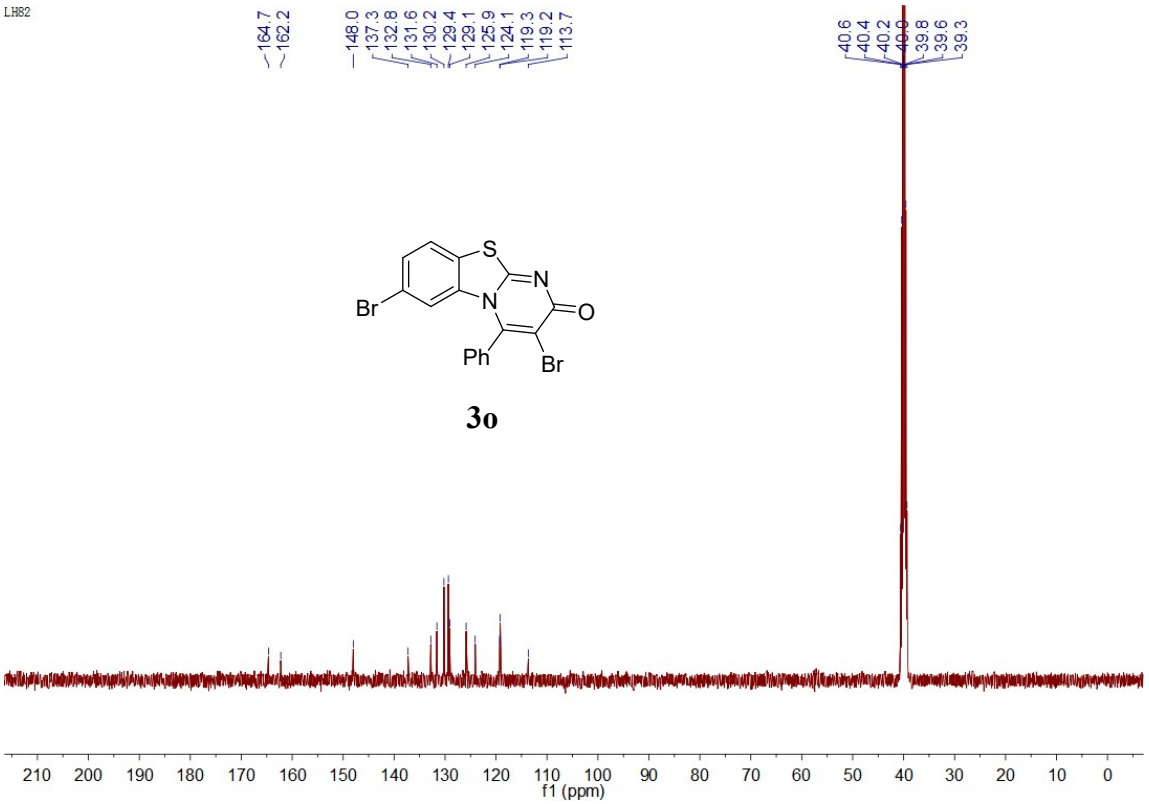
3n


LH185-3
164.1
162.4
148.2
136.5
133.1
131.4
130.1
129.3
127.7
124.1
115.8
113.5
40.6
40.4
40.2
40.0
39.8
39.5
39.3
20.9
Me
S
N
N
O
Ph
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

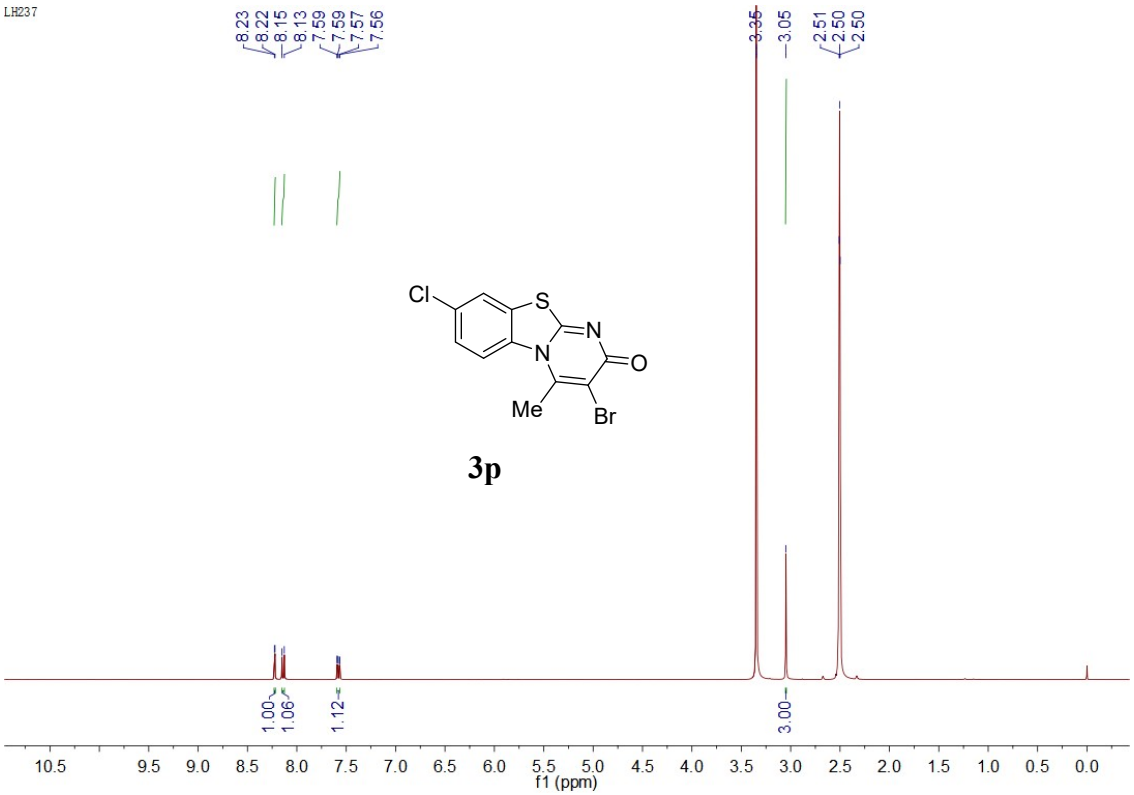
3n


LH82
7.87
7.85
7.66
7.64
7.54
7.53
7.48
7.46
5.58
3.28
2.42
Br
S
N
N
O
Ph
Br
1.02
3.00
2.08
1.18
1.00
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)

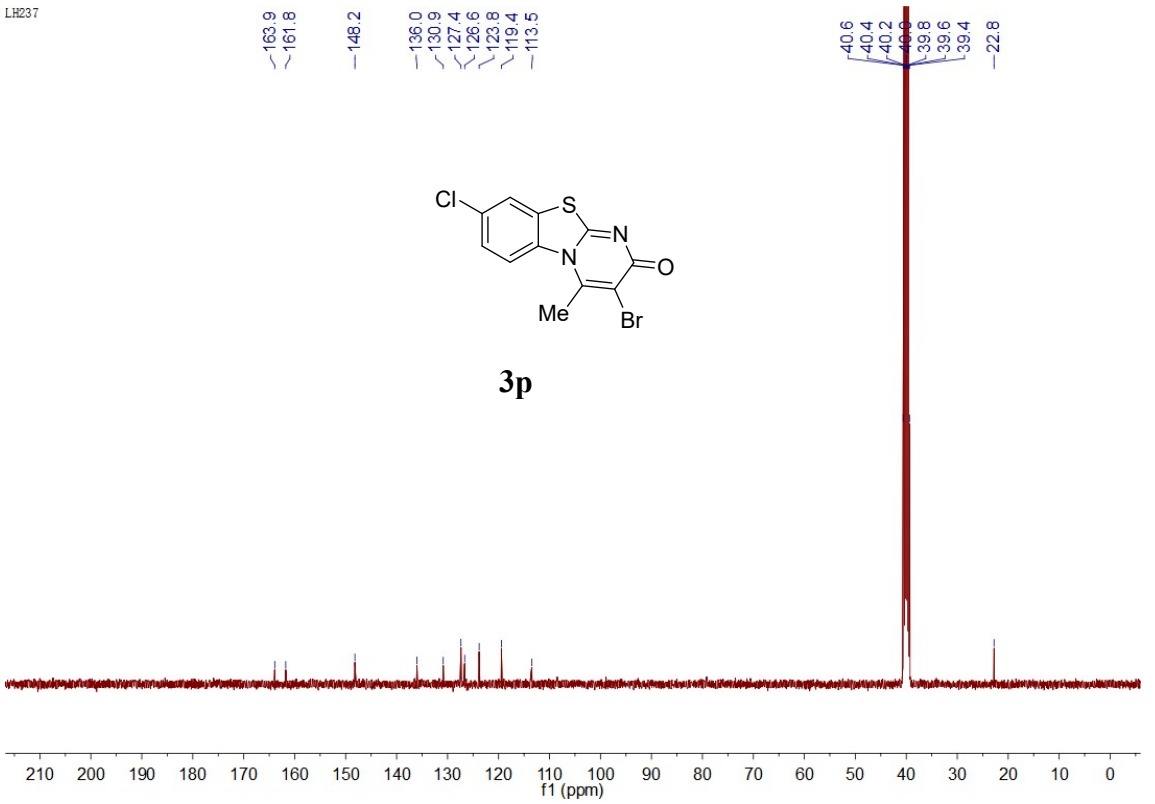
3o


LH82
164.7
162.2
148.0
137.3
132.8
131.6
130.2
129.4
129.1
125.9
124.1
119.3
119.2
113.7
40.6
40.4
40.2
40.0
39.8
39.6
39.3
S
N
N
O
Br
Ph
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

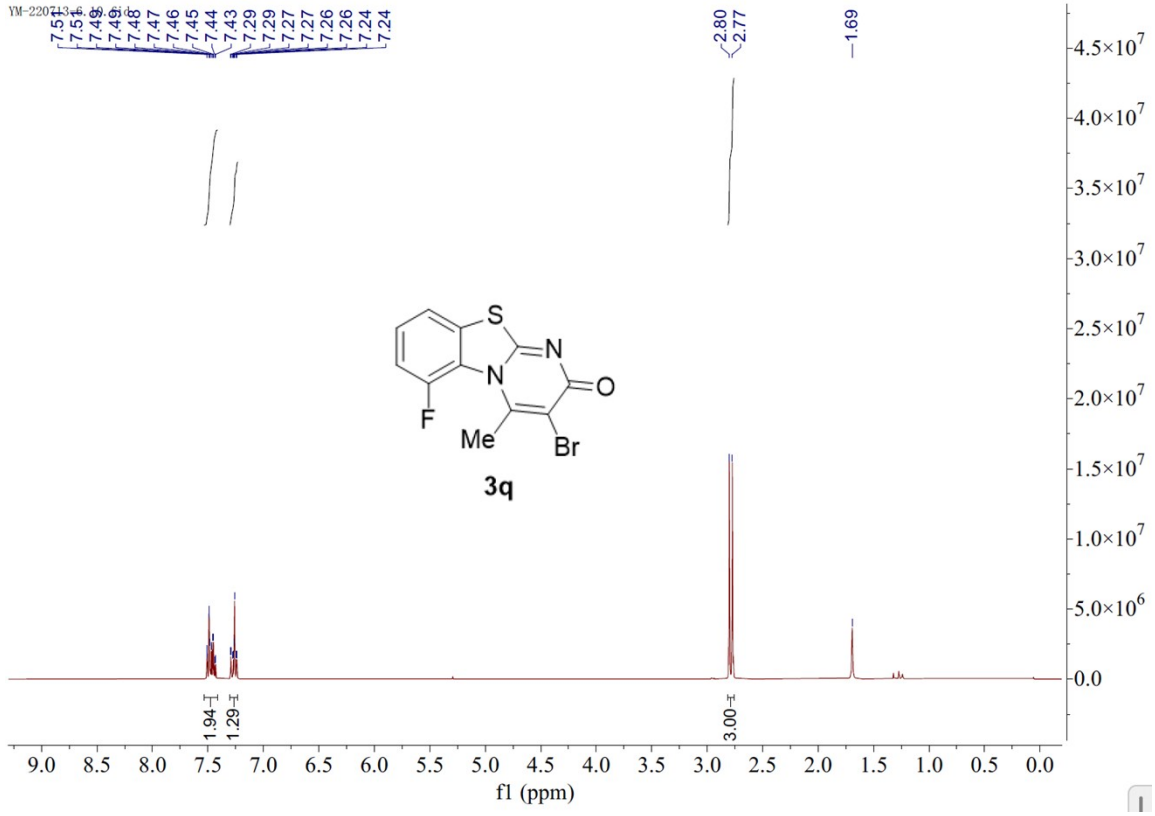
3o


LH237
8.23
8.22
8.15
8.13
7.59
7.59
7.57
7.56
3.35
3.05
2.51
2.50
2.50
Cl
S
N
N
O
Me
Br
1.00
1.06
1.12
3.00
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

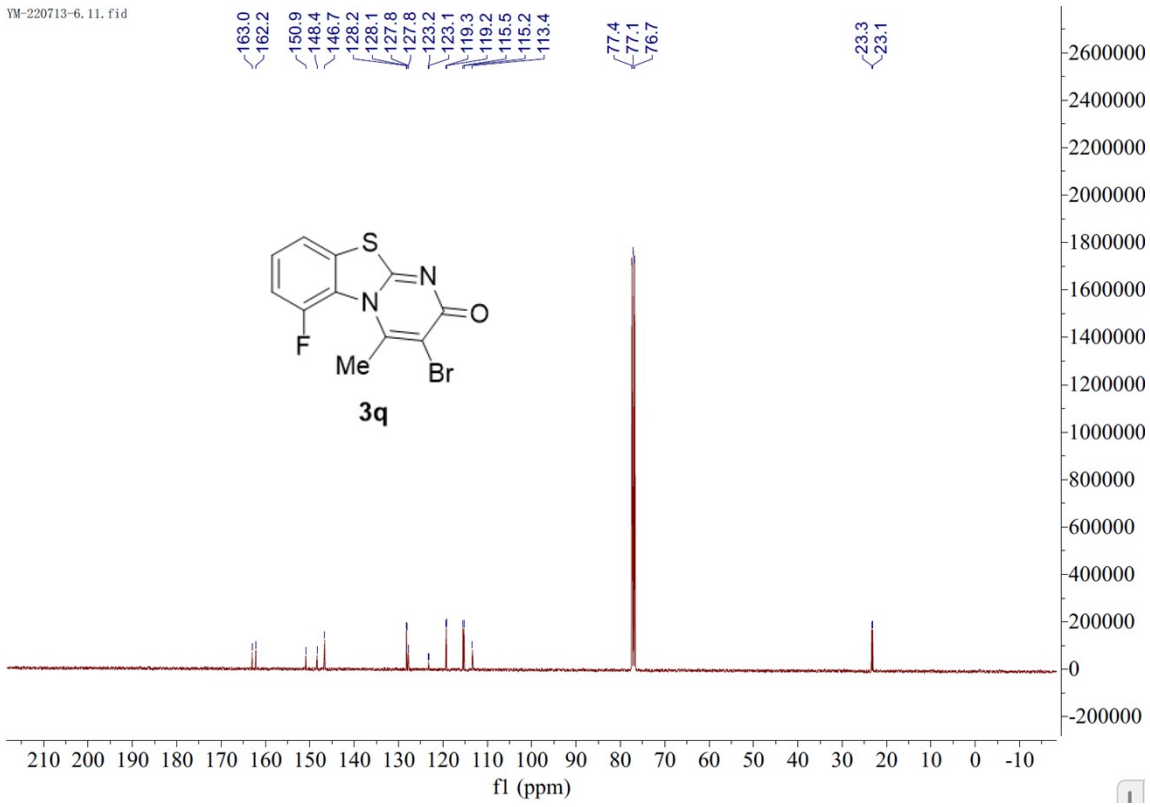
3p

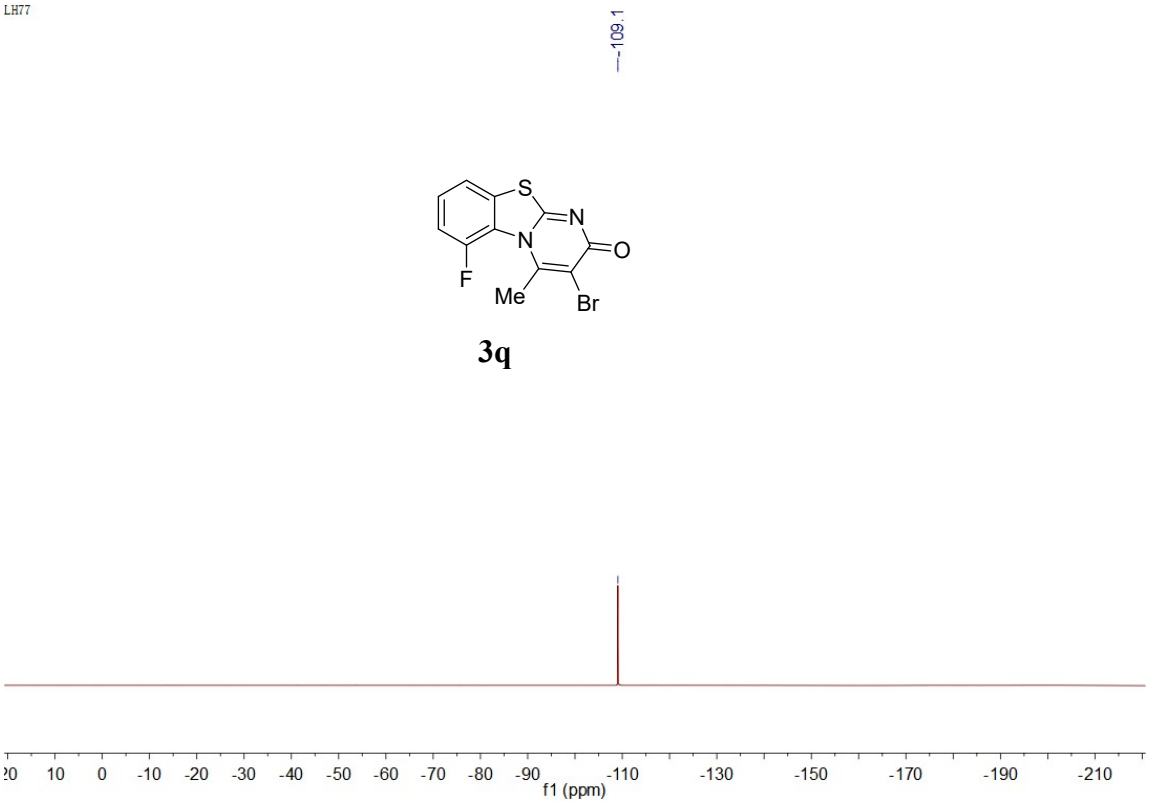

LH237
163.9
161.8
148.2
136.0
130.9
127.4
126.6
123.8
119.4
113.5
40.6
40.4
40.2
40.0
39.8
39.6
39.4
22.8
Cl
S
N
N
O
Me
Br
f1 (ppm)

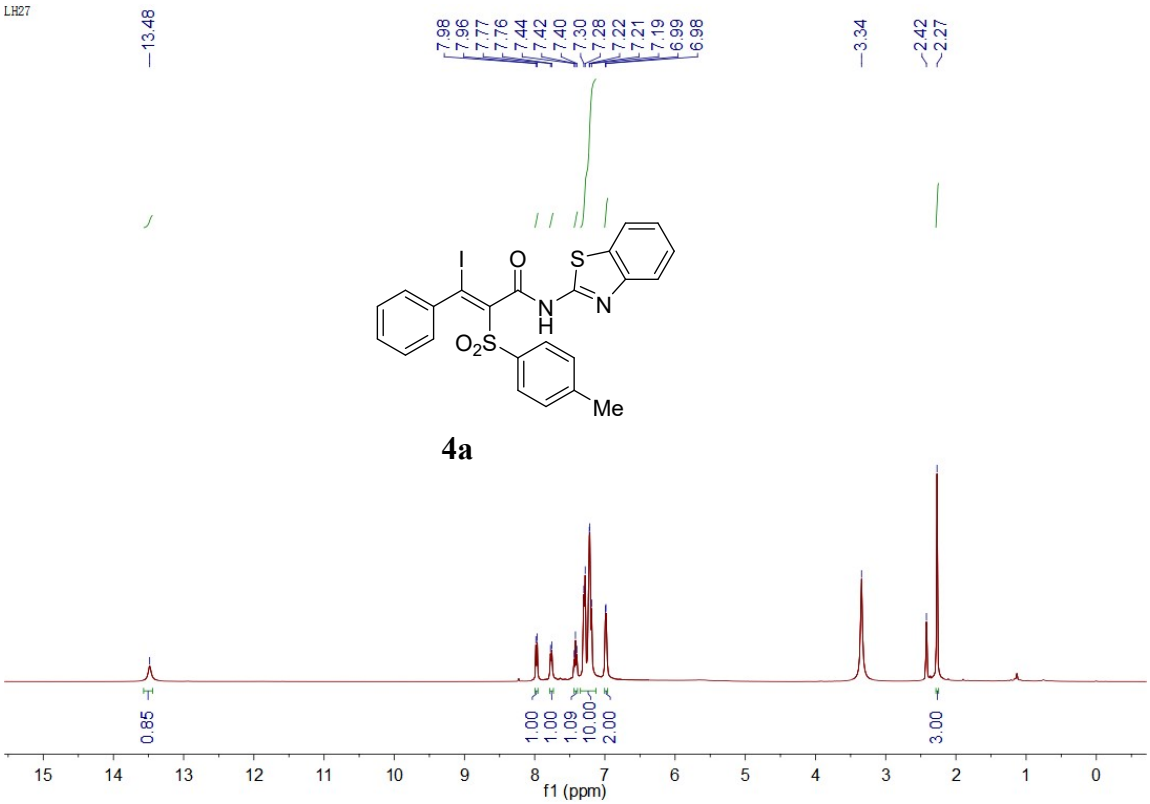
3p


7.51
7.49
7.48
7.47
7.46
7.45
7.44
7.43
7.29
7.29
7.27
7.27
7.26
7.26
7.24
7.24
2.80
2.77
1.69
S
N
N
O
F
Me
Br
1.94
1.29
3.00
f1 (ppm)

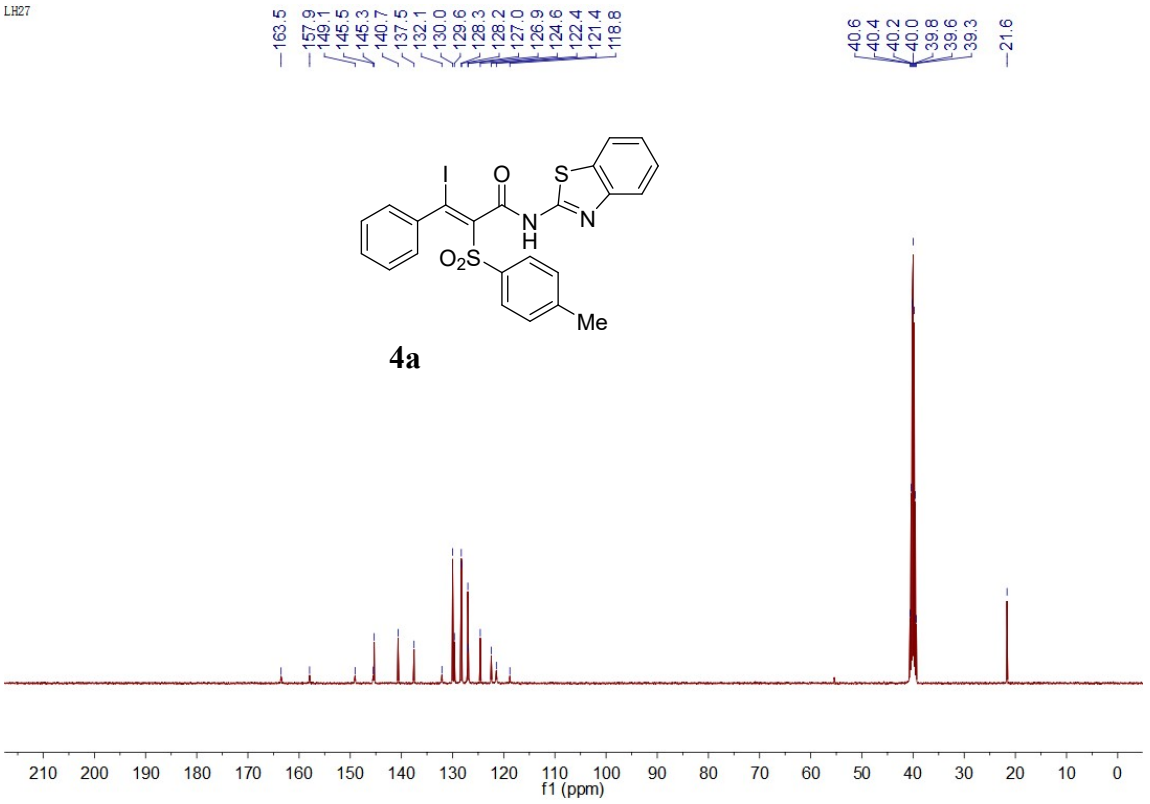
3q


YM-220713-6.11.fid
163.0
162.2
150.9
148.4
146.7
128.2
128.1
127.8
127.8
123.2
123.1
119.3
119.2
115.5
115.2
113.4
77.4
77.1
76.7
23.3
23.1
S
N
N
O
F
Me
Br
3q
f1 (ppm)

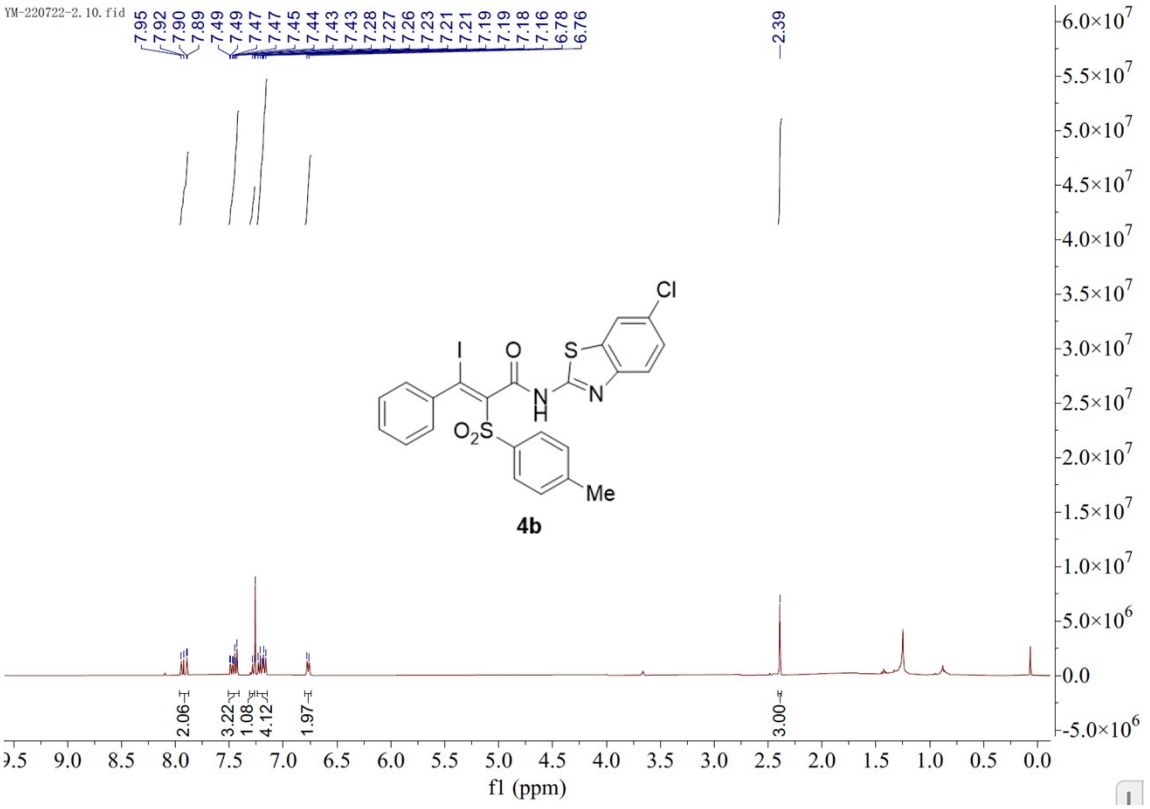

LH77
109.1
S
N
N
O
F
Me
Br
3q
f1 (ppm)

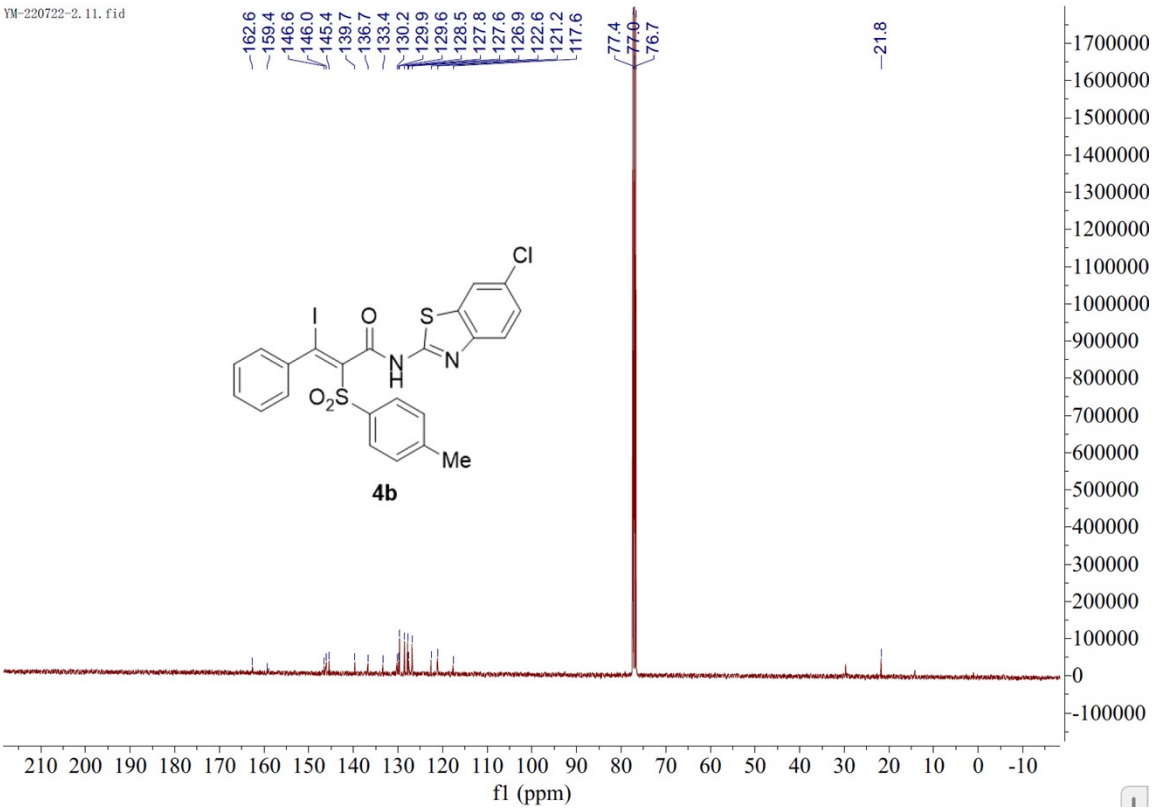

LH27
13.48
7.98
7.96
7.77
7.76
7.44
7.42
7.40
7.30
7.28
7.22
7.21
7.19
6.99
6.98
3.34
2.42
2.27
I
O
S
N
H
N
O2S
Me
0.85
1.00
1.00
1.09
10.00
2.00
3.00
f1 (ppm)

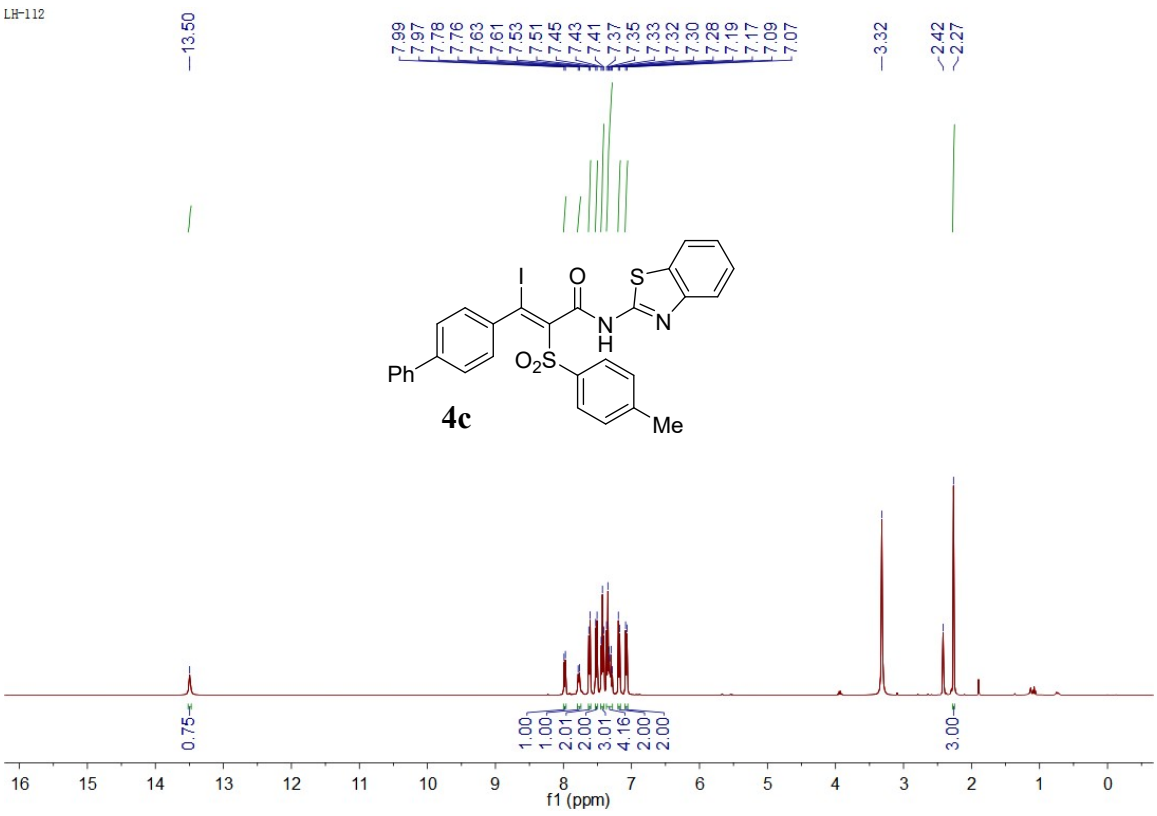
4a

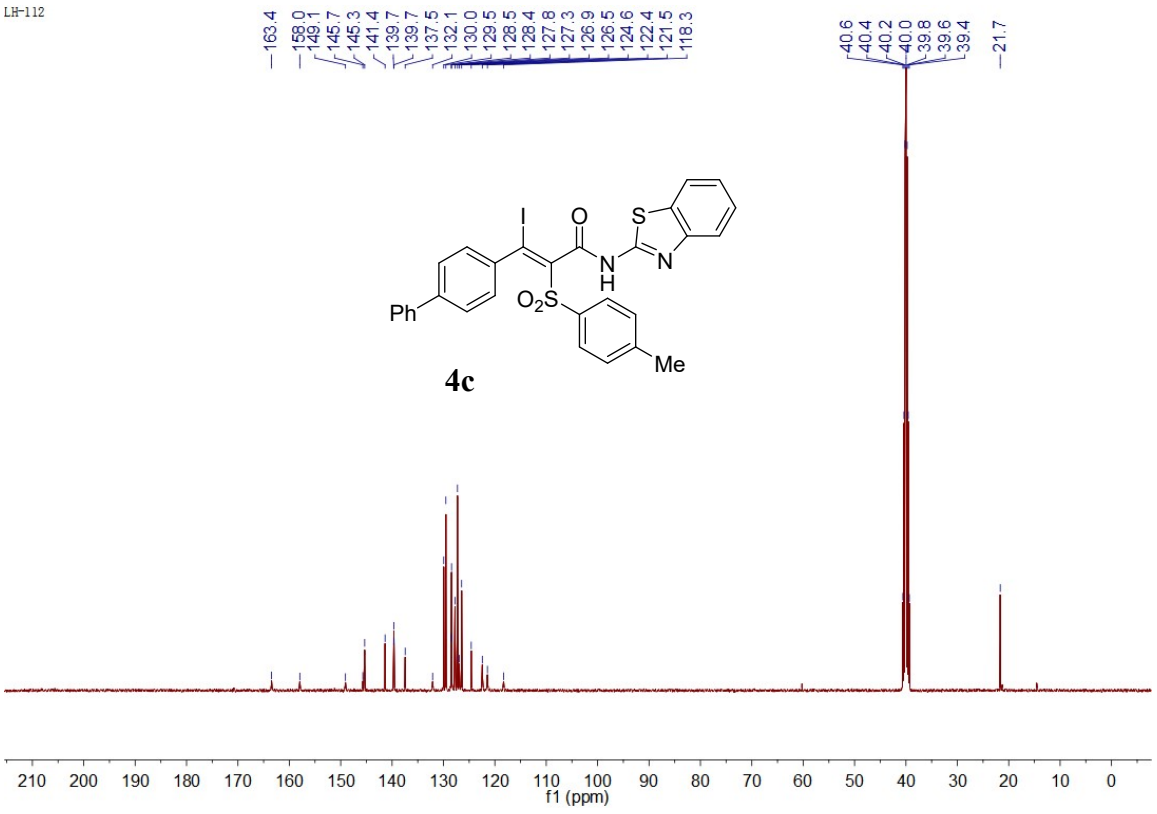

LH27
163.5
157.9
149.1
145.5
145.3
140.7
137.5
132.1
130.0
129.6
128.3
128.2
127.0
126.9
124.6
122.4
121.4
118.8
40.6
40.4
40.2
40.0
39.8
39.6
39.3
21.6
I
O
S
N
H
N
O2S
Me
f1 (ppm)

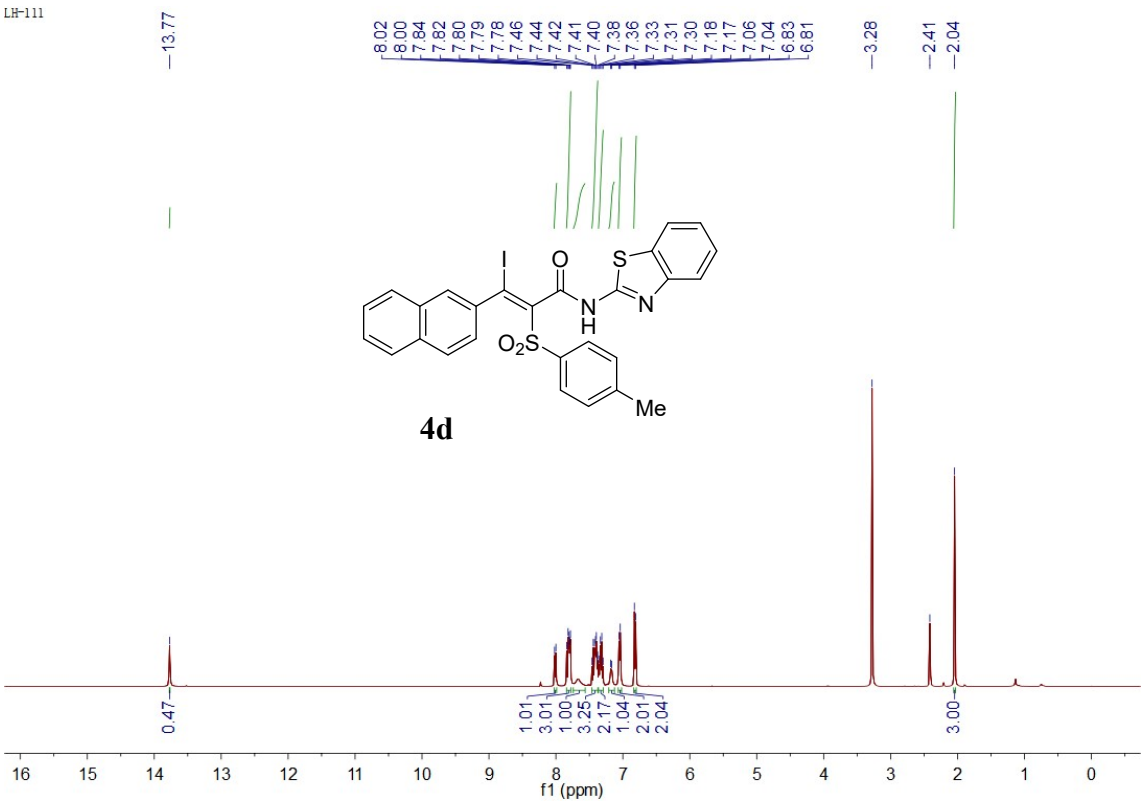
4a

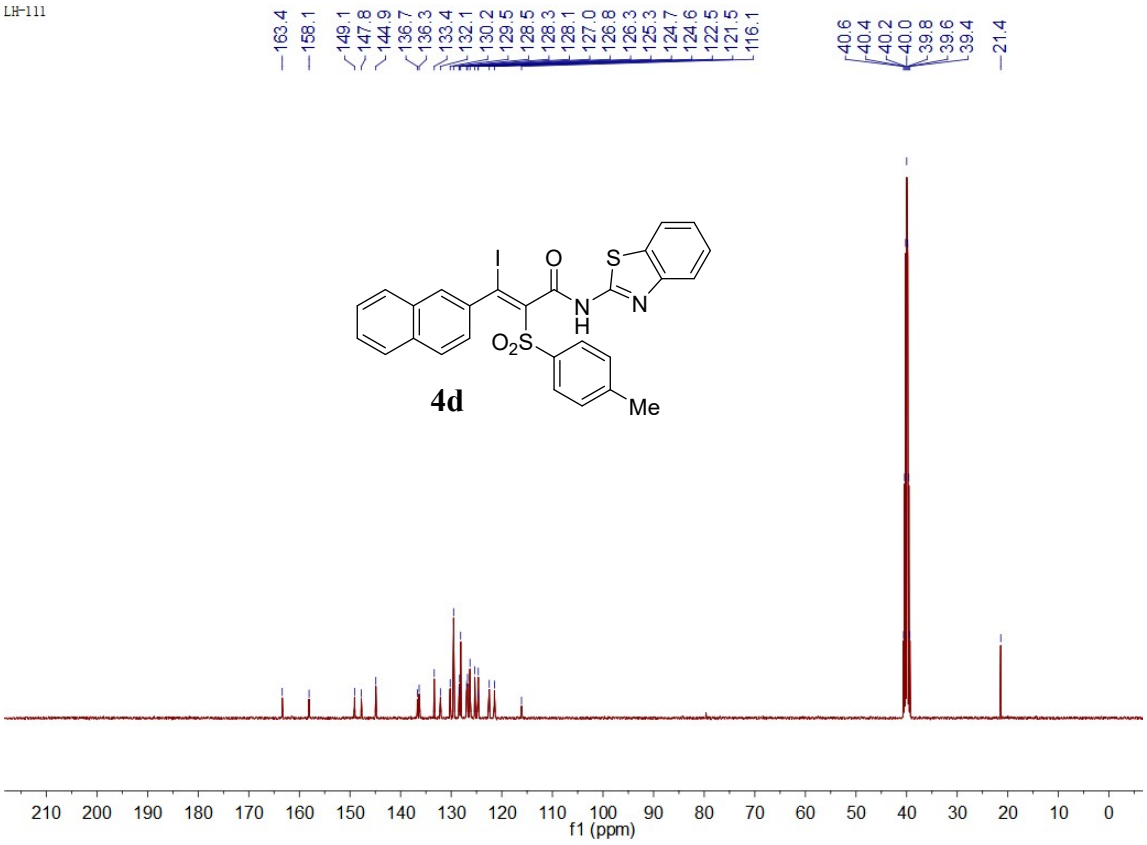

YM-220722-2.10.fid
7.95
7.92
7.90
7.89
7.49
7.49
7.47
7.47
7.45
7.44
7.43
7.43
7.28
7.27
7.26
7.23
7.21
7.21
7.19
7.19
7.18
7.16
6.78
6.76
2.39
Cl
I
O
S
N
H
N
O2S
Me
4b
2.06
3.22
1.08
4.12
1.97
3.00
fl (ppm)

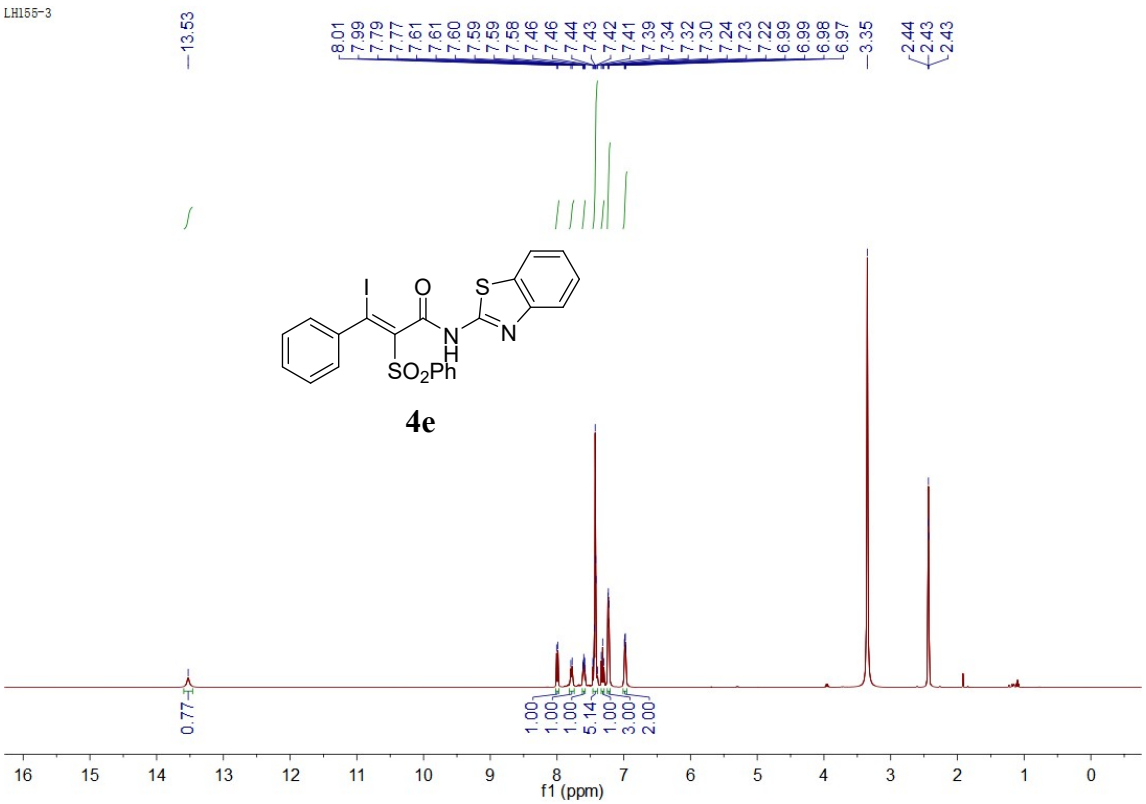

YM-220722-2.11.fid
162.6
159.4
146.6
146.0
145.4
139.7
136.7
133.4
130.2
129.9
129.6
128.5
127.8
127.6
126.9
122.6
121.2
117.6
77.4
77.0
76.7
21.8
Cl
I
O
S
N
H
N
O2S
Me
4b
fl (ppm)

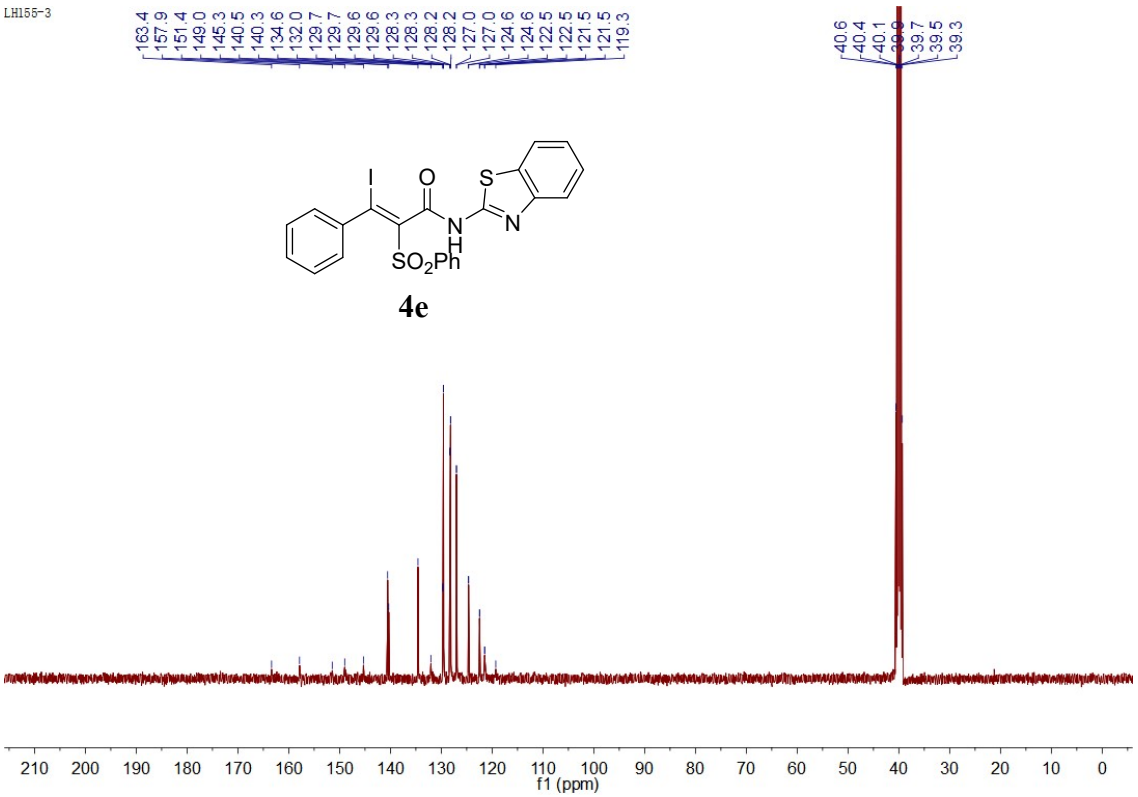

LH-112
13.50
7.99
7.97
7.78
7.76
7.63
7.61
7.53
7.51
7.45
7.43
7.41
7.37
7.35
7.33
7.32
7.30
7.28
7.19
7.17
7.09
7.07
3.32
2.42
2.27
I
O
S
N
H
N
Ph
O2S
Me
4c
0.75
1.00
1.00
2.01
2.00
3.01
4.16
2.00
2.00
3.00
f1 (ppm)

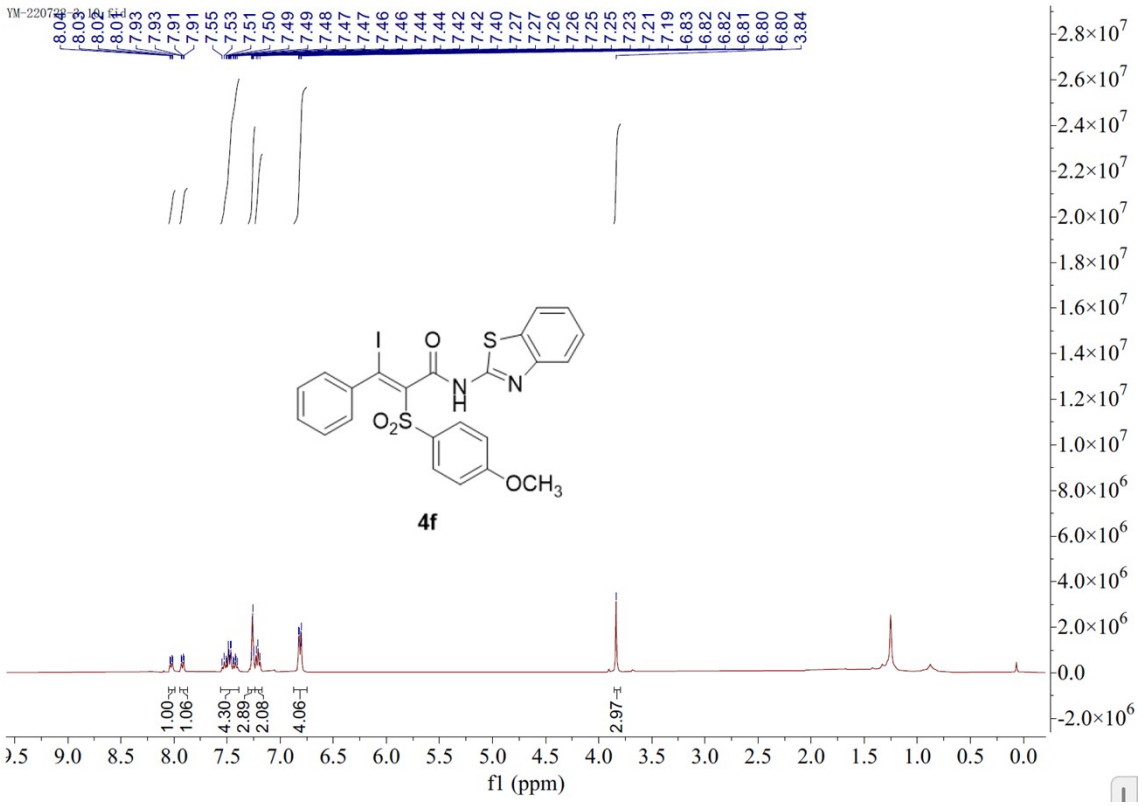

LH-112
163.4
158.0
149.1
145.7
145.3
141.4
139.7
139.7
137.5
132.1
130.0
129.5
128.5
128.4
127.8
127.3
126.9
126.5
124.6
122.4
121.5
118.3
40.6
40.4
40.2
40.0
39.8
39.6
39.4
21.7
I
O
S
N
H
N
Ph
O2S
Me
4c
f1 (ppm)

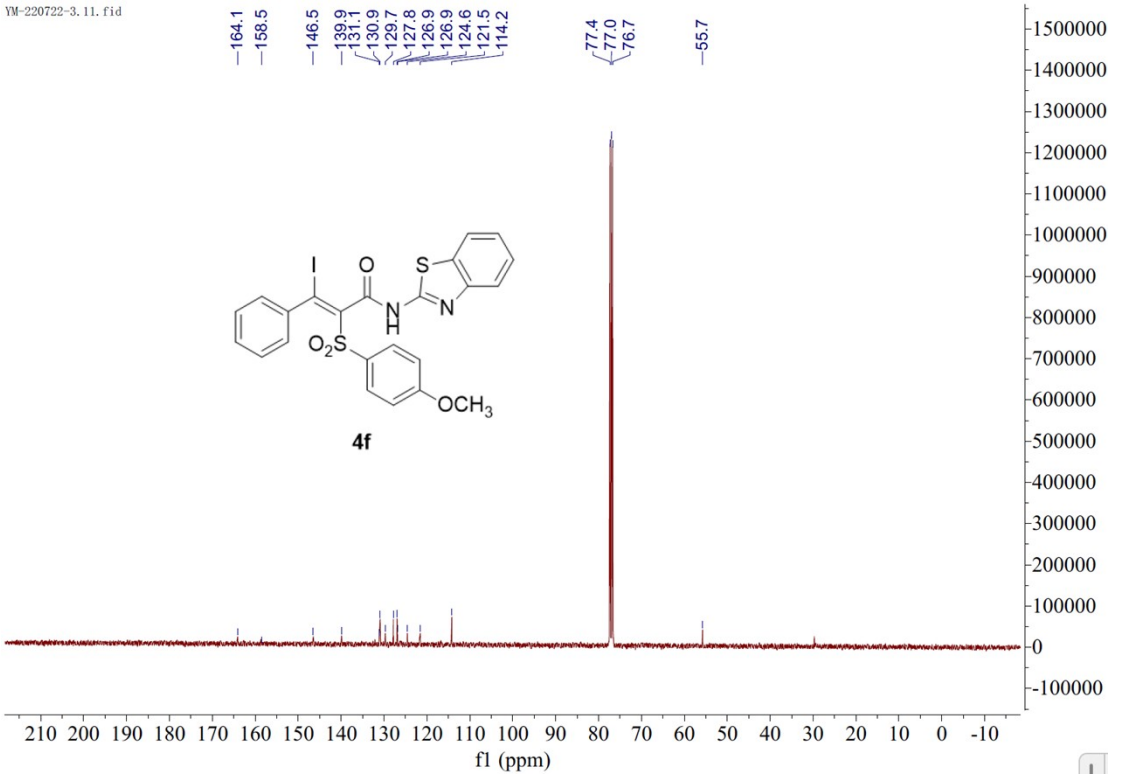

LH-111
13.77
8.02
8.00
7.84
7.82
7.80
7.79
7.78
7.46
7.44
7.42
7.41
7.40
7.38
7.36
7.33
7.31
7.30
7.18
7.17
7.06
7.04
6.83
6.81
3.28
2.41
2.04
I
O
S
N
H
N
O2S
Me
4d
0.47
1.01
3.01
1.00
3.25
2.17
1.04
2.01
2.04
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

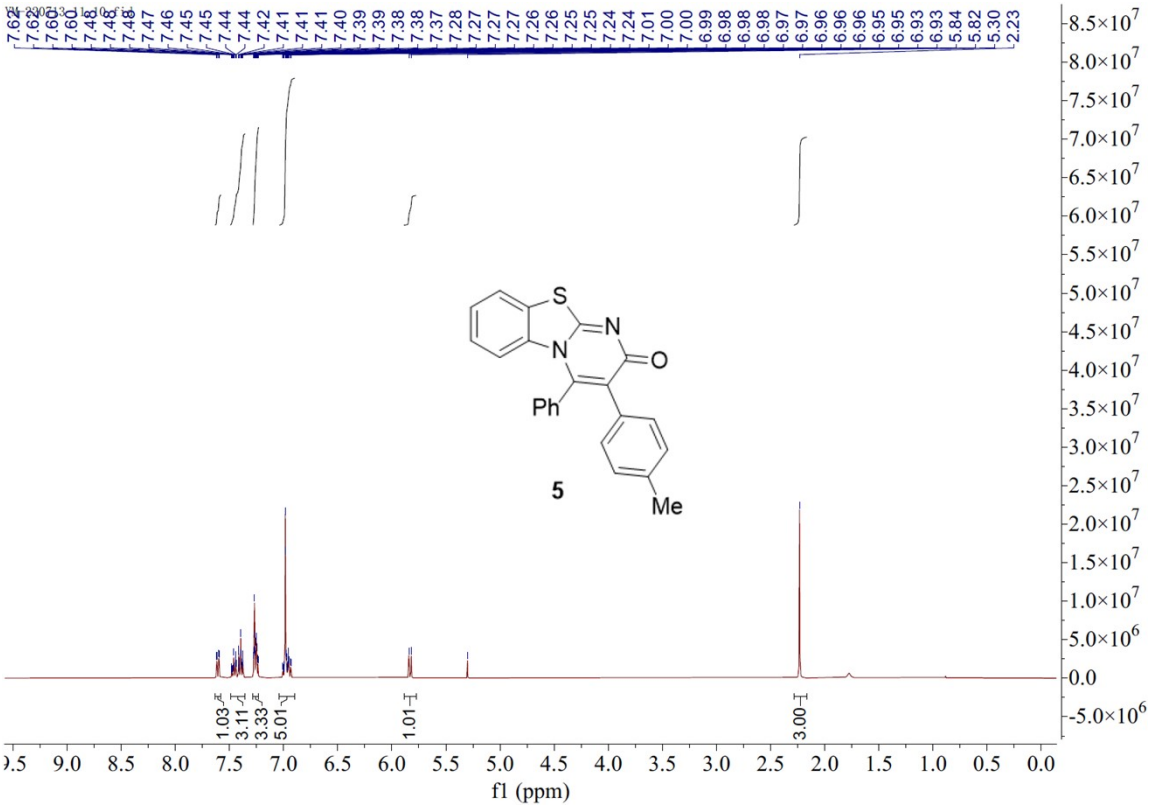

LH-111
163.4
158.1
149.1
147.8
144.9
136.7
136.3
133.4
132.1
130.2
129.5
128.5
128.3
128.1
127.0
126.8
126.3
125.3
124.7
124.6
122.5
121.5
116.1
40.6
40.4
40.2
40.0
39.8
39.6
39.4
21.4
I
O
S
N
H
N
O2S
Me
4d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

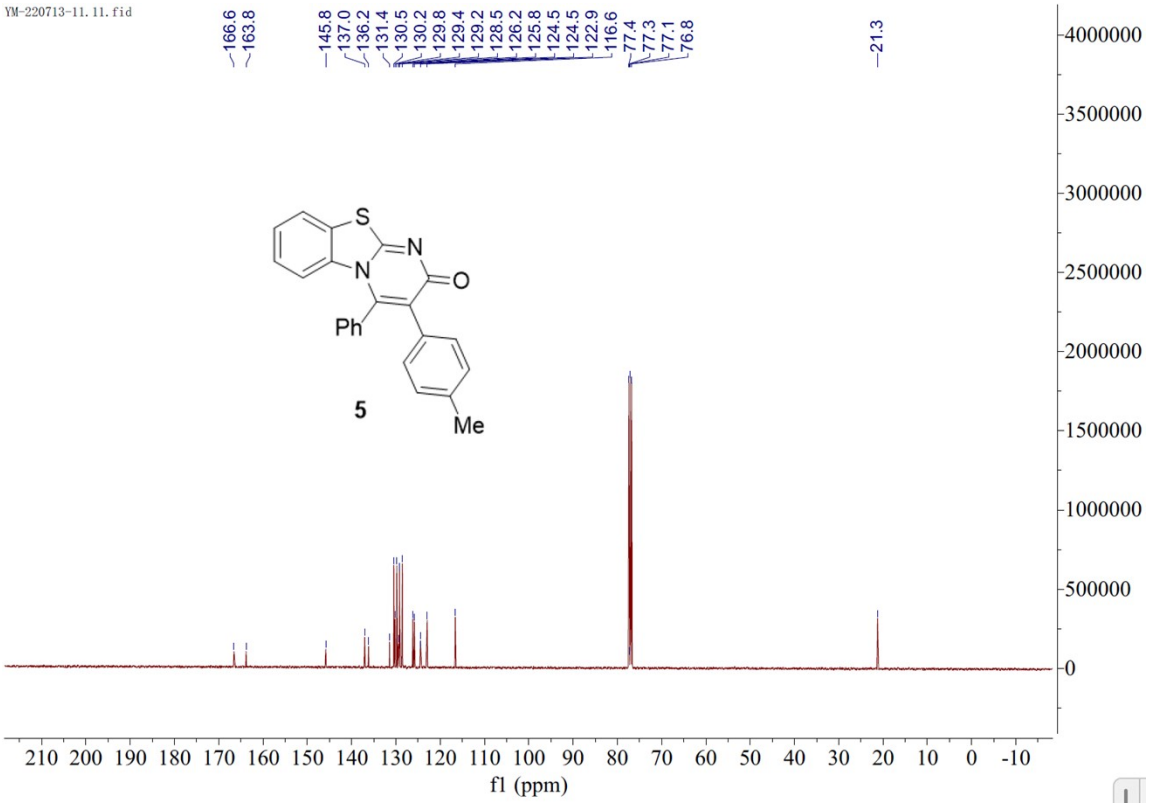

LH155-3
13.53
8.01
7.99
7.79
7.77
7.61
7.61
7.60
7.59
7.59
7.58
7.46
7.44
7.43
7.42
7.41
7.39
7.34
7.32
7.30
7.24
7.23
7.22
6.99
6.98
6.97
3.35
2.44
2.43
2.43
I
O
S
N
H
N
SO2Ph
4e
0.77
1.00
1.00
1.00
5.14
1.00
3.00
2.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

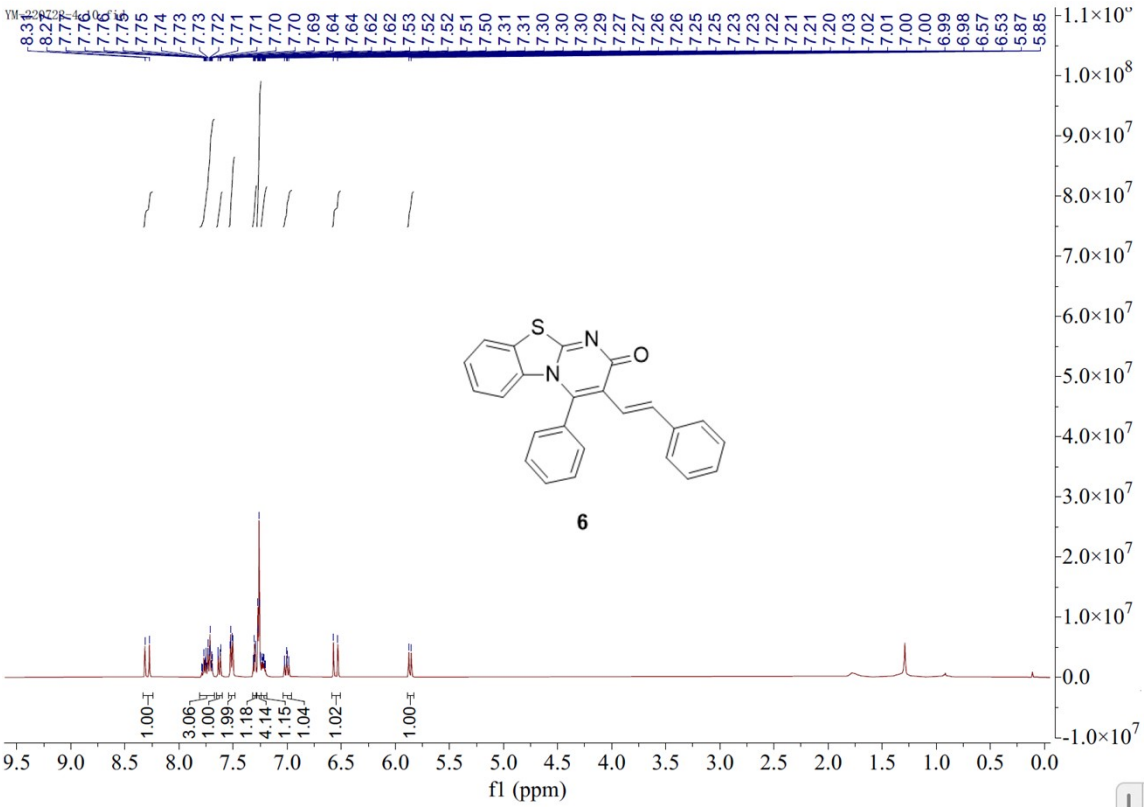

LH155-3
163.4
157.9
151.4
149.0
145.3
140.5
140.3
134.6
132.0
129.7
129.7
129.6
129.6
128.3
128.3
128.2
128.2
127.0
127.0
124.6
124.6
122.5
122.5
121.5
121.5
119.3
40.6
40.4
40.1
39.7
39.5
39.3
I
O
S
N
H
N
SO2Ph
4e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

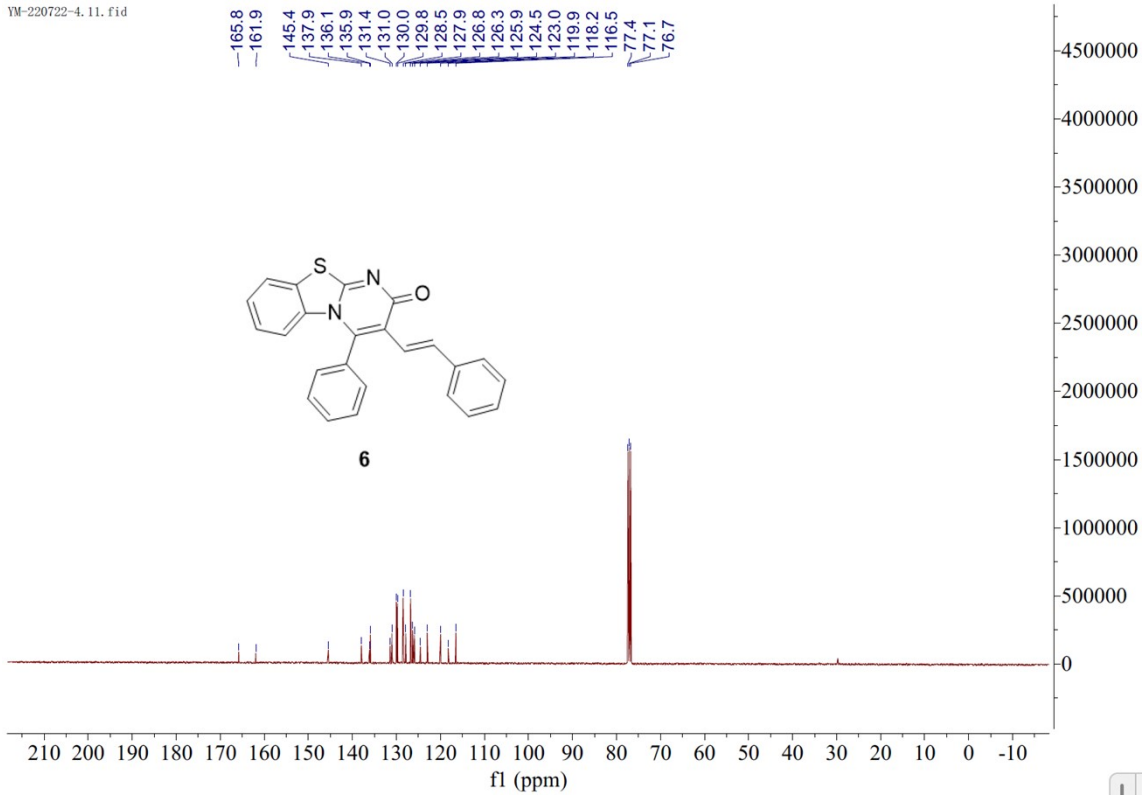

8.04
8.03
8.02
8.01
7.93
7.93
7.91
7.91
7.55
7.53
7.51
7.50
7.49
7.49
7.48
7.47
7.47
7.46
7.46
7.44
7.42
7.42
7.40
7.27
7.27
7.26
7.26
7.25
7.25
7.23
7.21
7.19
6.83
6.82
6.82
6.81
6.80
6.80
3.84
I
O
S
N
H
N
O2S
OCH3
4f
1.00
1.06
4.30
2.89
2.08
4.06
2.97
fl (ppm)


YM-220722-3.11.fid
164.1
158.5
146.5
139.9
131.1
130.9
129.7
127.8
126.9
126.9
124.6
121.5
114.2
77.4
77.0
76.7
55.7
I
O
S
N
H
N
O2S
OCH3
4f
fl (ppm)


7.62 7.60 7.48 7.47 7.46 7.45 7.44 7.42 7.41 7.40 7.39 7.38 7.37 7.28 7.27 7.26 7.25 7.24 7.01 7.00 6.99 6.98 6.97 6.96 6.95 6.93 5.84 5.82 5.30 2.23
S
N
N
O
Ph
Me
5
1.03
3.11
3.33
5.01
1.01
3.00
fl (ppm)


YM-220713-11.11.fid
166.6 163.8 145.8 137.0 136.2 131.4 130.5 130.2 129.8 129.4 129.2 128.5 126.2 125.8 124.5 124.5 122.9 116.6 77.4 77.3 77.1 76.8 21.3
S
N
N
O
Ph
Me
5
fl (ppm)


8.31 8.27 7.77 7.76 7.76 7.75 7.75 7.74 7.73 7.73 7.72 7.71 7.71 7.70 7.70 7.69 7.64 7.64 7.62 7.62 7.53 7.52 7.52 7.51 7.50 7.31 7.30 7.30 7.30 7.29 7.27 7.27 7.26 7.26 7.25 7.25 7.23 7.23 7.22 7.21 7.21 7.20 7.03 7.02 7.01 7.00 7.00 6.99 6.98 6.57 6.53 5.87 5.85
1.1×10^9
1.0×10^8
9.0×10^7
8.0×10^7
7.0×10^7
6.0×10^7
5.0×10^7
4.0×10^7
3.0×10^7
2.0×10^7
1.0×10^7
0.0
-1.0×10^7
S
N
N
O
6
1.00 3.06 1.00 1.99 1.18 4.14 1.15 1.04 1.02 1.00
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)


YM-220722-4.11.fid
165.8 161.9 145.4 137.9 136.1 135.9 131.4 131.0 130.0 129.8 128.5 127.9 126.8 126.3 125.9 124.5 123.0 119.9 118.2 116.5 77.4 77.1 76.7
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
S
N
N
O
6
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)