Supporting Information

Contents

1. General Information

The ^{1}H NMR and ^{13}C NMR spectra were recorded at Bruker AV 400 MHz. ^{1}H and ^{13}C NMR Chemical shifts were calibrated to tetramethylsilane as an internal reference. Chemical shifts are given in (ppm) and coupling constants (*J*) in Hz. The following abbreviations are used to indicate the multiplicity: s, singlet; d, doublet: t, triplet; q, quartet; m, multiplet; Infrared spectra were recorded on an Bruker Fourier transform spectrometer (FT-IR) and are reported in wave numbers. High resolution mass spectrometric (HRMS) analyses spectrum was determined on the Varian 7.0T FTMS instrument.

2. The procedure for the synthesis of thiazine imides 4

To the Schlenk tube was added homopropargylic amines **1** (0.1 mmol), KSCN (14.6 mg, 0.15 mmol, 1.5 equiv.), acyl chlorides (0.15 mmol, 1.5 equiv.) and PEG-400 (12 mg, 0.3 equiv.) as well as 1 mL CH_2Cl_2 at N_2 atmosphere, the reaction mixture was stirred (for about 1 h) at room temperature and traced by the thin layer

chromatography (TLC) until the homopropargylic amines **1** disappeared. The diiodine (38 mg, 0.15 mmol, 1.5 equiv.) was then added into the above mixture and continued to stirred for another 3 h at room temperature. After completion, the mixture was treated with the saturated sodium thiosulfate solution ($Na_2S_2O_3$) and extracted with ethyl acetate (3×10 mL), the coombined organic phase was dried with anhydrous $MgSO_4$ and then filtered. The filtrate was concentrated under vacuo and purified by the flash silica gel column chromatography with the elution (PE:EA = 10:1) to give the corresponding thiazine imides **4**.

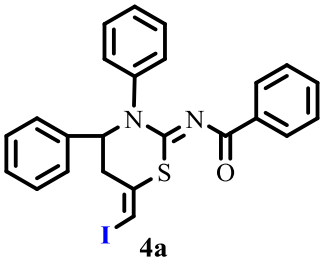
3. The procedure for the synthesis of thiourea 5o

To the Schlenk tube was added homopropargylic amine **1** (23 mg, 0.1 mmol), 4-methoxybenzoyl isothiocyanate **2** (29 mg, 0.15 mmol, 1.5 equiv.) and 1mL CH_2Cl_2 at N_2 atmosphere. The reaction mixture was stirred at room temperature for 1 hour and traced by the thin layer chromatography (TLC) until the homopropargylic amine **1** disappeared. The mixture was concentrated under vacuo and purified by the flash silica gel column chromatography with the elution (PE:EA = 5:1) to give the corresponding thiourea **5o** as a yellow liquid 38 mg, yield 93%.

4. The procedure for the synthesis of 6a

A dried round-bottom flask was charged with thiazine imide **4a** (49 mg 0.1 mmol), phenylboronic acid (20 mg, 0.15 mmol, 1.5 equiv.), $Pd(PPh_3)_4$ (9 mg, 7 mol%) and Cs_2CO_3 (98 mg, 0.3 mmol, 3.0 equiv.) which was dissolved in the mix of toulene : H_2O = 3:1 (1.5 mL : 0.5 mL). The mixture was stirred at 80 ^oC for 5 h. After completion, the reaction mixture was treated with saturated sodium chloride solution and extracted with ethyl acetate (3×20 mL), the organic layer was dried with $MgSO_4$ and then filtered. The filtrate was concentrated under vacuo and purified by the flash silica gel column chromatography with the elution (PE : EA = 10 : 1) to give **6a** as a yellow oil 35 mg, yield 80%.

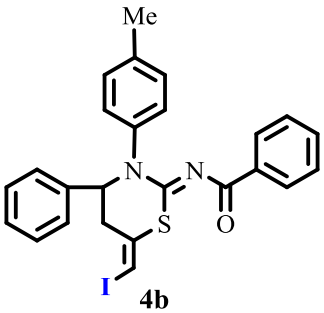
5. The characterization of the thiazine imides 4



4a

***N*-((2*Z*,6*E*)-6-(iodomethylene)-3,4-diphenyl-1,3-thiazinan-2-ylidene)benzamide (4a)**

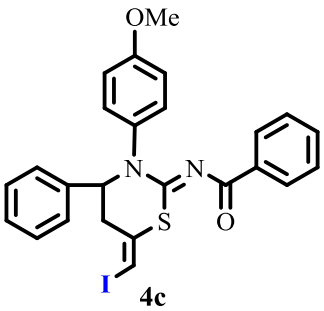
White solid, 41 mg, yield 85%, m.p. 158-160 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 6.9 Hz, 2H), 7.27 (d, *J* = 10.5 Hz, 6H), 7.24 – 7.10 (m, 7H), 6.33 (s, 1H), 5.18 (s, 1H), 3.44 (d, *J* = 14.3 Hz, 1H), 3.13 (d, *J* = 14.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.7, 163.5, 145.9, 137.9, 136.8, 134.8, 131.8, 129.8, 129.4, 129.2, 128.8, 128.6, 128.4, 128.2, 128.0, 127.6, 126.8, 126.6, 76.2, 64.2, 40.7. HRMS (ESI+) calculated for $C_{24}H_{19}IN_2OS$ $(M+H)^+$ 511.0336; found 511.0334.



4b

***N*-((2*Z*,6*E*)-6-(iodomethylene)-4-phenyl-3-(*p*-tolyl)-1,3-thiazinan-2-ylidene)benzamide (4b)**

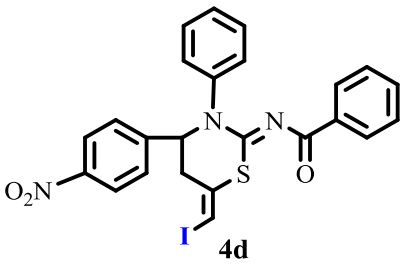
Yellow oil, 44 mg, yield 84% , ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 (t, *J* = 8.3 Hz, 2H), 7.41 – 7.24 (m, 8H), 7.17 – 7.05 (m, 4H), 6.39 (d, *J* = 8.4 Hz, 1H), 5.23 (q, *J* = 4.2 Hz, 1H), 3.57 – 3.47 (m, 1H), 3.27 – 3.12 (m, 1H), 2.35 (d, *J* = 9.0 Hz, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 174.7, 163.3, 143.3, 137.9, 137.3, 136.8, 134.8, 131.7, 129.74, 129.71, 128.7, 128.1, 127.9, 126.5, 126.4, 75.9, 64.4, 40.6, 21.2. HRMS (ESI+) calculated for $C_{25}H_{21}IN_2OS(M+H)^+$ 525.0492; found 525.0497.



4c

(*Z*)-*N*-((*E*)-6-(iodomethylene)-3-(4-methoxyphenyl)-4-phenyl-1,3-thiazinan-2-ylidene)benzamide (4c)

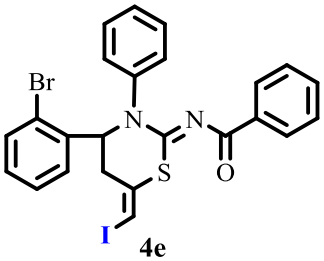
Brown solid, 42 mg, yield 80%, m.p. 187-190 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.4 Hz, 2H), 7.45 – 7.22 (m, 8H), 7.14 (d, *J* = 8.8 Hz, 2H), 6.87 (d, *J* = 8.8 Hz, 2H), 6.41 (s, 1H), 5.22 (t, *J* = 3.8 Hz, 1H), 3.78 (d, *J* = 14.9 Hz, 3H), 3.51 (dd, *J* = 14.3, 3.3 Hz, 1H), 3.21 (dd, *J* = 14.6, 3.9 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.7, 163.6, 158.5, 138.7, 137.9, 136.7, 134.7, 131.8, 129.7, 128.7, 128.2, 127.9, 127.8, 126.5, 114.3, 76.1, 64.5, 55.5, 40.6. HRMS (ESI+) calculated for $C_{25}H_{21}IN_2O_2S(M+H)^+$ 541.0441; found 541.0442.



4d

(*Z*)-*N*-((*E*)-6-(iodomethylene)-4-(4-nitrophenyl)-3-phenyl-1,3-thiazinan-2-ylidene) benzamide (4d)

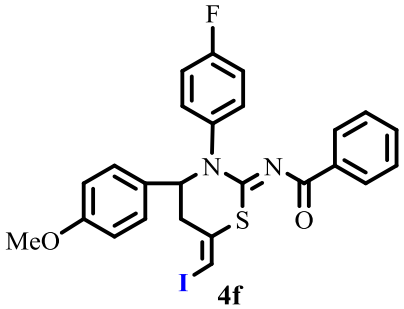
Yellow liquid, 35 mg, yield 66%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.8 Hz, 2H), 7.88 – 7.77 (m, 2H), 7.58 (d, *J* = 8.7 Hz, 2H), 7.48 – 7.18 (m, 9H), 6.51 (d, *J* = 1.3 Hz, 1H), 5.41 (t, *J* = 3.8 Hz, 1H), 3.61 (dd, *J* = 14.4, 3.3 Hz, 1H), 3.33 (ddd, *J* = 14.4, 4.6, 1.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.9, 147.8, 145.5, 145.3, 136.3, 133.7, 132.1, 129.7, 129.5, 128.0, 127.6, 126.7, 124.0, 77.2, 63.8, 40.3. HRMS (ESI+) calculated for $C_{24}H_{18}IN_3O_3S$ $(M+H)^+$ 556.0186; found 556.0198.



4e

(*Z*)-*N*-((*E*)-4-(2-bromophenyl)-6-(iodomethylene)-3-phenyl-1,3-thiazinan-2-yliden e)benzamide (4e)

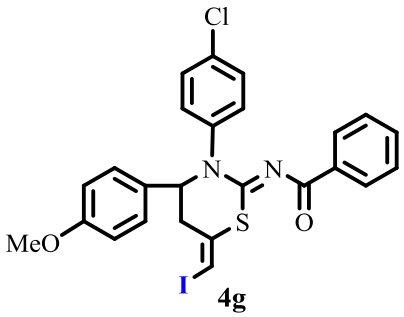
Yellow solid, 45 mg, yield 78%, m.p. 161-163 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.27 – 8.22 (m, 2H), 7.80 (dd, *J* = 8.2, 1.5 Hz, 2H), 7.56 (d, *J* = 8.5 Hz, 2H), 7.45 – 7.34 (m, 4H), 7.30 – 7.20 (m, 4H), 6.49 (d, *J* = 1.4 Hz, 1H), 5.39 (t, *J* = 3.9 Hz, 1H), 3.58 (dd, *J* = 14.4, 3.3 Hz, 1H), 3.37 – 3.22 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.8, 164.1, 145.8, 136.6, 136.4, 134.0, 133.4, 131.9, 129.9, 129.7, 129.3, 128.6, 127.9, 127.8, 127.6, 126.8, 122.1, 77.7, 63.9, 38.1. HRMS (ESI+) calculated for $C_{24}H_{18}BrIN_2OS$ $(M+H)^+$ 588.9441; found 588.9433.



4f

(*Z*)-*N*-((*E*)-3-(4-fluorophenyl)-6-(iodomethylene)-4-(4-methoxyphenyl)-1,3-thiazi nan-2-ylidene)benzamide (4f)

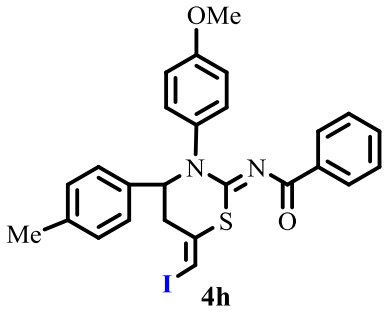
Yellow oil, 43 mg, yield 83%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 7.5 Hz, 2H), 7.40 (t, *J* = 7.3 Hz, 1H), 7.32 – 7.12 (m, 6H), 7.05 (t, *J* = 8.5 Hz, 2H), 6.87 (d, *J* = 8.6 Hz, 2H), 6.47 (s, 1H), 5.14 (t, *J* = 3.9 Hz, 1H), 3.80 (s, 3H), 3.47 (dd, *J* = 14.3, 3.5 Hz, 1H), 3.20 (dd, *J* = 14.3, 3.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.7, 163.7, 162.7, 160.2, 159.8(d, *J* = 272.4 Hz), 141.7(d, *J* = 12.4 Hz), 136.6, 134.6, 131.9, 129.7, 128.7, 128.6(d, *J* = 34 Hz), 128.0, 127.8, 116.0(d, *J* = 90.4 Hz), 115.9, 114.2, 76.5, 64.0, 55.3, 40.6. HRMS (ESI+) calculated for $C_{25}H_{20}FIN_2O_2S$ $(M+H)^+$ 559.0347; found 559.0342.



4g

(*Z*)-*N*-((*E*)-3-(4-chlorophenyl)-6-(iodomethylene)-4-(4-methoxyphenyl)-1,3-thiazinan-2-ylidene)benzamide (4g)

Yellow solid, 41 mg, yield 75%. m.p. 159-163 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.78 (m, 2H), 7.48 – 7.11 (m, 10H), 6.95 – 6.83 (m, 2H), 6.49 (d, *J* = 1.5 Hz, 1H), 5.16 (t, *J* = 4.0 Hz, 1H), 3.83 (s, 3H), 3.50 (dd, *J* = 14.3, 3.6 Hz, 1H), 3.21 (ddd, *J* = 14.3, 4.5, 1.7 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.7, 163.5, 159.5, 144.2, 136.5, 134.5, 133.2, 132.0, 129.7, 129.6, 129.3, 128.3, 128.0, 127.7, 114.2, 76.6, 63.8, 55.3, 40.7. HRMS (ESI+) calculated for $C_{25}H_{20}ClIN_2O_2S$ $(M+H)^+$ 575.0051; found 575.0056.

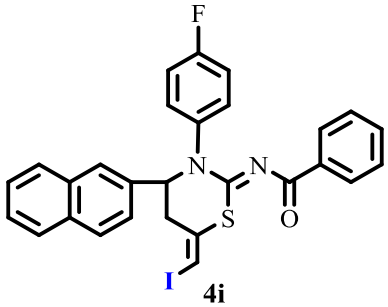


4h

(*Z*)-*N*-((*E*)-6-(iodomethylene)-3-(4-methoxyphenyl)-4-(p-tolyl)-1,3-thiazinan-2-ylidene)benzamide (3h)

Brown solid, 49 mg, yield 88%, m.p. 160-165 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 7.5 Hz, 2H), 7.42 (t, *J* = 7.1 Hz, 2H), 7.34 – 7.11 (m, 9H), 6.90 (d, *J* = 8.7 Hz, 2H), 6.42 (s, 1H), 5.21 (t, *J* = 3.7 Hz, 1H), 3.82 (s, 3H), 3.52 (dd, *J* = 14.3, 3.3 Hz, 1H), 3.21 (dd, *J* = 14.3, 3.3 Hz, 1H), 2.36 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.7, 163.6, 158.5, 138.8, 137.9, 136.8, 134.9, 134.8, 131.8, 129.7, 129.4, 127.9,

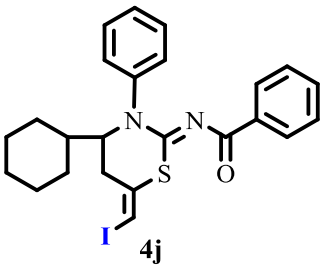
127.8, 126.4, 114.2, 75.9, 64.3, 55.5, 40.7, 21.2. HRMS (ESI+) calculated for $C_{26}H_{23}IN_2O_2S$ $(M+H)^+$ 555.0598; found 555.0601.



4i

(*Z*)-*N*-((*E*)-3-(4-fluorophenyl)-6-(iodomethylene)-4-(naphthalen-2-yl)-1,3-thiazinan-2-ylidene)benzamide (4i)

Yellow solid, 43 mg, yield 78%, m.p. 170-173 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.83 (m, 5H), 7.71 (d, *J* = 7.1 Hz, 1H), 7.64 – 7.49 (m, 3H), 7.49 – 7.41 (m, 1H), 7.39 – 7.24 (m, 5H), 7.12 – 6.98 (m, 2H), 6.41 (d, *J* = 1.0 Hz, 1H), 6.07 (t, *J* = 3.8 Hz, 1H), 3.80 (dd, *J* = 13.9, 3.3 Hz, 1H), 3.37 (ddd, *J* = 13.8, 4.6, 1.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.8, 164.7, 160.2, 142.0(d, J = 13.2 Hz), 136.6, 134.3, 133.9, 132.2, 132.0, 129.7, 129.5, 129.2, 128.6(d, J = 34.4 Hz) 128.0, 126.9, 125.9, 125.0, 124.7, 121.2, 116.1(d, J = 90.4 Hz), 116.0, 76.8, 61.5, 39.3. HRMS (ESI+) calculated for $C_{28}H_{20}FIN_2OS$ $(M+H)^+$ 579.0398; found 579.0396.

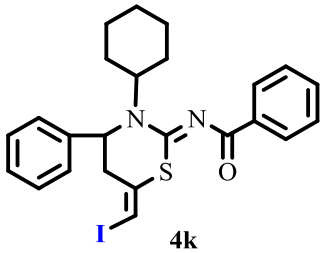


4j

(*Z*)-*N*-((*E*)-4-cyclohexyl-6-(iodomethylene)-3-phenyl-1,3-thiazinan-2-ylidene)benzamide (4j)

Yellow liquid, 42 mg, yield 81%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.85 – 7.77 (m, 2H), 7.52 – 7.46 (m, 2H), 7.37 (ddt, *J* = 8.5, 3.1, 1.8 Hz, 4H), 7.29 – 7.23 (m, 2H), 6.42 (d, *J* = 2.3 Hz, 1H), 3.93 – 3.86 (m, 1H), 3.55 – 3.47 (m, 1H), 2.87 (ddd, *J* = 15.7, 4.3, 2.4 Hz, 1H), 2.10 – 1.96 (m, 2H), 1.84 – 1.68 (m, 4H), 1.20 – 0.94 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.5, 161.9, 146.4, 137.2, 136.6, 131.7, 129.6, 128.9,

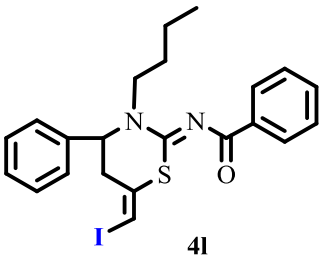
127.9, 127.3, 127.2, 72.4, 66.4, 39.5, 37.0, 31.0, 29.7, 25.99, 25.95, 25.92. HRMS (ESI+) calculated for $C_{24}H_{25}IN_2OS$ $(M+H)^+$ 517.0805; found 517.0812.



4k

(*Z*)-*N*-((*E*)-3-cyclohexyl-6-(iodomethylene)-4-phenyl-1,3-thiazinan-2-ylidene)benzamide 4k

Transparent oil, 51 mg, yield 99%. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.31 – 8.20 (m, 2H), 7.60 – 7.44 (m, 3H), 7.39 – 7.27 (m, 5H), 6.16 (d, J = 1.7 Hz, 1H), 5.30 (td, J = 10.2, 8.6, 5.8 Hz, 1H), 5.17 (t, J = 3.8 Hz, 1H), 3.55 (dd, J = 14.5, 3.4 Hz, 1H), 2.79 (ddd, J = 14.5, 4.1, 1.9 Hz, 1H), 2.11 (d, J = 11.1 Hz, 1H), 1.95 (dq, J = 13.1, 2.8 Hz, 1H), 1.80 – 1.60 (m, 4H), 1.33 – 1.11 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.5, 162.5, 138.5, 137.3, 135.2, 131.7, 129.6, 128.5, 128.0, 127.74, 127.72, 126.1, 73.8, 61.1, 55.5, 41.1, 30.4, 30.1, 26.03, 25.99, 25.5. HRMS (ESI+) calculated for $C_{24}H_{26}IN_2OS$ $(M+H)^+$ 517.0805; found 517.0806

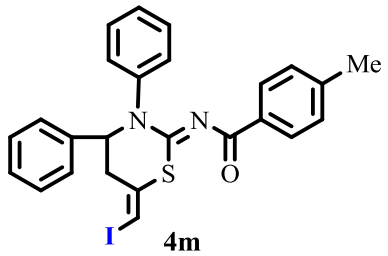


4l

(*Z*)-*N*-((*E*)-3-butyl-6-(iodomethylene)-4-phenyl-1,3-thiazinan-2-ylidene) benzamide 4l

Transparent oil, 47 mg, yield 96%. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.30 – 8.21 (m, 1H), 7.54 – 7.49 (m, 1H), 7.47 – 7.43 (m, 1H), 7.41 – 7.33 (m, 2H), 7.27 – 7.20 (m, 1H), 6.34 (d, J = 1.4 Hz, 0H), 5.01 (dd, J = 4.6, 3.2 Hz, 1H), 4.53 (ddd, J = 13.1, 9.8, 5.5 Hz, 1H), 3.47 (dd, J = 14.1, 3.2 Hz, 1H), 3.19 – 3.11 (m, 0H), 3.00 (ddd, J = 14.1, 4.7, 1.6 Hz, 1H), 1.98 – 1.71 (m, 1H), 1.44 (q, J = 7.4 Hz, 1H), 0.99 (t, J = 7.3 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.7, 162.9, 137.7, 137.3, 134.7, 132.9,

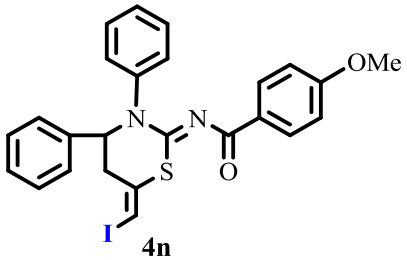
131.7, 129.59, 129.57, 128.9, 128.8, 128.7, 128.39, 128.24, 128.0, 127.9, 126.29, 126.27, 77.4, 77.1, 76.8, 75.8, 61.2, 54.3, 39.9, 29.6, 20.34, 20.31, 13.9, 13.6. HRMS (ESI+) calculated for $C_{22}H_{24}IN_2OS$ $(M+H)^+$ 491.0649; found 491.0649



4m

(*Z*)-*N*-((*E*)-6-(iodomethylene)-3,4-diphenyl-1,3-thiazinan-2-ylidene)-4-methylbenzamide (4m)

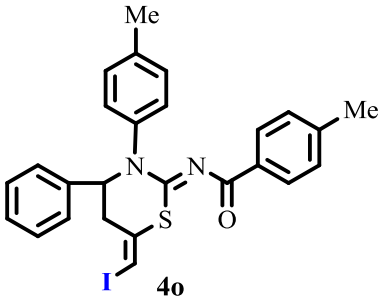
Yellow oil, 50 mg, yield 94%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.78 – 7.70 (m, 2H), 7.48 – 7.26 (m, 10H), 7.10 (d, *J* = 8.0 Hz, 2H), 6.44 (d, *J* = 1.5 Hz, 1H), 5.29 (t, *J* = 4.0 Hz, 1H), 3.56 (dd, *J* = 14.3, 3.4 Hz, 1H), 3.25 (ddd, *J* = 14.3, 4.6, 1.7 Hz, 1H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.7, 163.0, 145.9, 142.3, 137.9, 134.8, 134.1, 129.8, 129.1, 128.7, 128.7, 128.2, 127.5, 126.8, 126.5, 64.1, 40.7, 21.6. HRMS (ESI+) calculated for $C_{25}H_{21}IN_2OS$ $(M+H)^+$ 525.0492; found 525.0494.



4n

(*Z*)-*N*-((E)-6-(iodomethylene)-3,4-diphenyl-1,3-thiazinan-2-ylidene)-4-methoxybenzamide (4n)

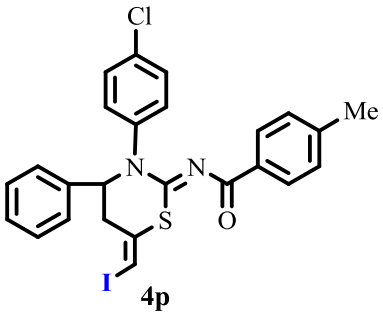
Yellow liquid, 47 mg, yield 87%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 – 7.75 (m, 2H), 7.41 – 7.27 (m, 8H), 6.85 – 6.73 (m, 2H), 6.42 (d, *J* = 1.6 Hz, 1H), 5.38 – 5.21 (m, 1H), 3.80 (s, 3H), 3.55 (dd, *J* = 14.4, 3.4 Hz, 1H), 3.24 (ddd, *J* = 14.3, 4.5, 1.8 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.3, 162.8, 162.6, 146.0, 138.0, 134.9, 131.8, 129.5, 129.2, 128.7, 128.2, 127.5, 126.8, 126.5, 113.2, 76.0, 64.1, 55.3, 40.7. HRMS (ESI+) calculated for $C_{25}H_{21}IN_2O_2S$ $(M+H)^+$ 541.0441; found 541.0443.



4o

(*Z*)-*N*-((*E*)-6-(iodomethylene)-4-phenyl-3-(p-tolyl)-1,3-thiazinan-2-ylidene)-4-methylbenzamide (4o)

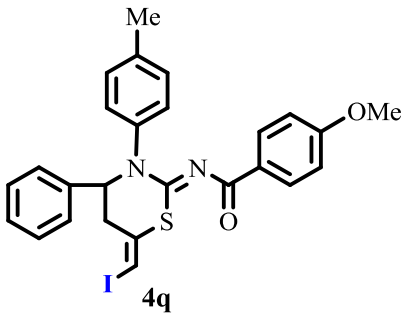
Brown liquid, 48 mg, yield 90%. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.77 (d, J = 7.7 Hz, 2H), 7.36 (d, J = 6.2 Hz, 5H), 7.20 – 7.01 (m, 6H), 6.42 (s, 1H), 5.26 (s, 1H), 3.53 (s, 1H), 3.33 – 3.17 (m, 1H), 2.37 (d, J = 12.7 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.8, 162.8, 143.4, 142.2, 138.0, 137.2, 134.9, 134.2, 129.8, 129.7, 128.7, 128.1, 126.5, 126.4, 75.6, 64.3, 40.7, 21.6, 21.1. HRMS (ESI+) calculated for $C_{26}H_{23}IN_2OS$ $(M+H)^+$ 539.0649; found 539.0650.



4p

(*Z*)-*N*-((*E*)-3-(4-chlorophenyl)-6-(iodomethylene)-4-phenyl-1,3-thiazinan-2-ylidene)-4-methylbenzamide (4p)

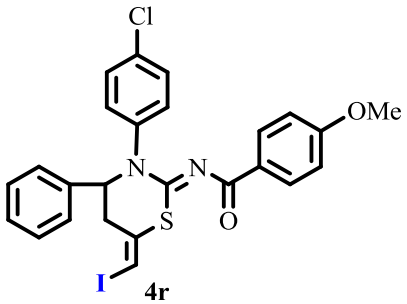
Yellow oil, 49 mg, yield 88%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.75 (d, *J* = 7.9 Hz, 2H), 7.44 – 7.30 (m, 7H), 7.16 (dd, *J* = 23.3, 8.1 Hz, 4H), 6.46 (s, 1H), 5.22 (t, *J* = 4.0 Hz, 1H), 3.54 (dd, *J* = 14.3, 3.4 Hz, 1H), 3.24 (dd, *J* = 14.4, 4.4 Hz, 1H), 2.36 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.8, 163.1, 144.2, 142.5, 137.8, 134.5, 133.9, 133.1, 129.8, 129.3, 128.82, 128.78, 128.4, 128.3, 126.5, 76.4, 64.2, 40.6, 21.6. HRMS (ESI+) calculated for $C_{25}H_{20}ClIN_2OS$ $(M+H)^+$ 559.0810; found 559.0815.



4q

(*Z*)-*N*-((*E*)-6-(iodomethylene)-4-phenyl-3-(p-tolyl)-1,3-thiazinan-2-ylidene)-4-methoxybenzamide (4q)

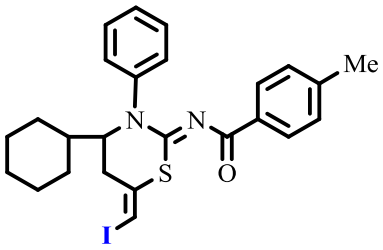
Yellow liquid, 50 mg, yield 90%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 – 7.79 (m, 2H), 7.51 – 7.34 (m, 5H), 7.23 – 7.06 (m, 4H), 6.91 – 6.71 (m, 2H), 6.40 (d, *J* = 1.5 Hz, 1H), 5.33 – 5.21 (m, 1H), 3.81 (s, 3H), 3.54 (dd, *J* = 14.4, 3.4 Hz, 1H), 3.25 (dd, *J* = 4.5, 1.8 Hz, 1H), 2.39 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.3, 162.62, 162.60, 143.4, 138.0, 137.2, 135.0, 131.8, 129.7, 129.59, 129.56, 128.7, 128.4, 128.1, 126.5, 126.4, 113.9, 113.2, 75.7, 64.3, 55.5, 55.3, 40.7, 21.2. HRMS (ESI+) calculated for $C_{26}H_{23}IN_2O_2S$ $(M+H)^+$ 555.0598; found 555.0602.



4r

(*Z*)-*N*-((*E*)-3-(4-chlorophenyl)-6-(iodomethylene)-4-phenyl-1,3-thiazinan-2-ylidene)-4-methoxybenzamide (4r)

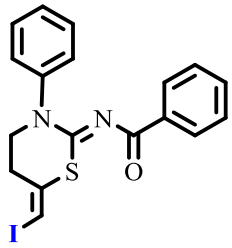
Brown solid, 48 mg, yield 84%. m.p. 170-175 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.85 – 7.68 (m, 2H), 7.40 – 7.29 (m, 7H), 7.19 – 7.13 (m, 2H), 6.87 – 6.74 (m, 2H), 6.42 (t, *J* = 1.4 Hz, 1H), 5.18 (t, *J* = 4.0 Hz, 1H), 3.79 (d, *J* = 1.3 Hz, 3H), 3.50 (dd, *J* = 14.3, 3.4 Hz, 1H), 3.25 – 3.13 (m, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.3, 162.8, 144.3, 137.8, 134.5, 133.1, 131.7, 129.3, 129.2, 128.8, 128.33, 128.28, 126.5, 113.3, 76.4, 64.1, 55.4, 40.6. HRMS (ESI+) calculated for $C_{25}H_{20}ClIN_2O_2S$ $(M+H)^+$ 575.0051; found 557.0052.



4s

(*Z*)-*N*-((*E*)-4-cyclohexyl-6-(iodomethylene)-3-phenyl-1,3-thiazinan-2-ylidene)-4-methylbenzamide (4s)

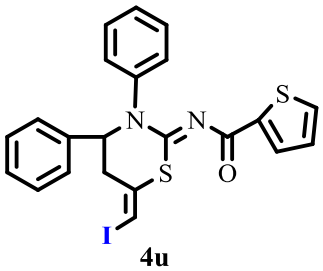
Yellow liquid, 45 mg, yield 85%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.78 – 7.71 (m, 2H), 7.47 (dd, *J* = 8.4, 7.1 Hz, 2H), 7.38 – 7.35 (m, 2H), 7.08 (d, *J* = 7.9 Hz, 2H), 6.40 (d, *J* = 2.3 Hz, 1H), 3.86 (ddd, *J* = 9.2, 4.3, 3.1 Hz, 1H), 3.47 (dd, *J* = 15.7, 3.1 Hz, 1H), 2.86 (ddd, *J* = 15.7, 4.4, 2.4 Hz, 1H), 2.33 (s, 3H), 2.13 – 1.94 (m, 2H), 1.76 (t, *J* = 3.4 Hz, 4H), 0.99 (s, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.5, 161.4, 146.5, 142.1, 137.4, 134.0, 129.7, 128.9, 128.6, 127.3, 127.2, 72.3, 66.3, 39.5, 37.0, 31.0, 29.7, 26.00, 25.96, 25.93, 21.6. HRMS (ESI+) calculated for $C_{25}H_{27}IN_2OS$ $(M+H)^+$ 531.0962; found 531.0967.



4t

***N*-((2*Z*,6*E*)-6-(iodomethylene)-3-phenyl-1,3-thiazinan-2-ylidene)benzamide (4t)**

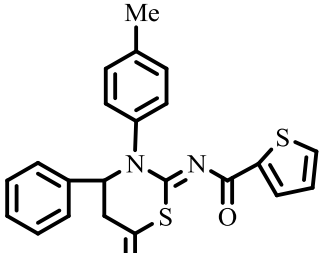
Yellow oil, 33 mg, yield 77%. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.92 – 7.80 (m, 2H), 7.51 – 7.26 (m, 8H), 6.50 (t, *J* = 2.1 Hz, 1H), 4.01 (dd, *J* = 6.5, 5.3 Hz, 2H), 3.04 – 2.82 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-d) δ 174.7, 163.6, 144.9, 137.4, 136.1, 131.9, 129.7, 129.3, 127.9, 127.5, 126.3, 73.7, 51.1, 36.9, 29.7. HRMS (ESI+) calculated for $C_{18}H_{15}IN_2OS$ $(M+H)^+$ 435.0023; found 435.0025.



4u

(*Z*)-*N*-((*E*)-6-(iodomethylene)-3,4-diphenyl-1,3-thiazinan-2-ylidene)thiophene-2-carboxamide (4u)

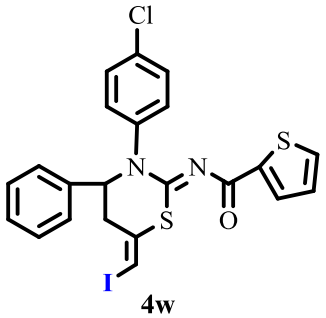
Yellow oil, 45 mg, yield 87%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.54 (dd, *J* = 3.7, 1.2 Hz, 1H), 7.46 – 7.30 (m, 9H), 7.25 (dd, *J* = 7.4, 1.8 Hz, 2H), 6.98 (dd, *J* = 4.9, 3.7 Hz, 1H), 6.46 (d, *J* = 1.5 Hz, 1H), 5.29 (t, *J* = 3.9 Hz, 1H), 3.56 (dd, *J* = 14.3, 3.4 Hz, 1H), 3.26 (dd, *J* = 4.5, 1.7 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 145.6, 137.8, 134.4, 131.9, 131.8, 129.1, 128.7, 128.3, 127.7, 127.6, 126.8, 126.5, 64.2, 40.5. HRMS (ESI+) calculated for $C_{22}H_{17}IN_2OS_2$ $(M+H)^+$ 516.9900; found 516.9899.



4v

(*Z*)-*N*-((*E*)-6-(iodomethylene)-4-phenyl-3-(p-tolyl)-1,3-thiazinan-2-ylidene)thiophene-2-carboxamide (4v)

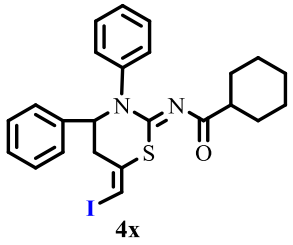
Brown oil, 38 mg, yield 75%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.55 (dd, *J* = 3.7, 1.3 Hz, 1H), 7.40 – 7.32 (m, 6H), 7.22 – 7.10 (m, 4H), 7.01 – 6.98 (m, 1H), 6.44 (d, *J* = 1.5 Hz, 1H), 5.26 (t, *J* = 3.9 Hz, 1H), 3.54 (dd, *J* = 14.3, 3.3 Hz, 1H), 3.26 – 3.14 (m, 1H), 2.38 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 169.5, 163.2, 143.1, 137.8, 137.3, 134.4, 131.9, 131.8, 129.7, 128.7, 128.2, 127.7, 126.5, 126.4, 64.3, 40.5, 21.2. HRMS (ESI+) calculated for $C_{23}H_{19}IN_2OS_2$$(M+H)^+$ 531.0056; found 531.0060.



4w

(*Z*)-*N*-((*E*)-3-(4-chlorophenyl)-6-(iodomethylene)-4-phenyl-1,3-thiazinan-2-yliden e)thiophene-2-carboxamide (4w)

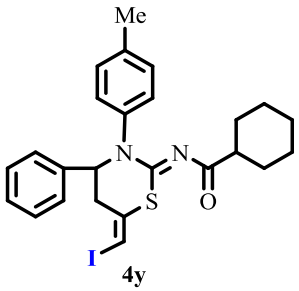
Yellow solid, 40 mg, yield 73%, m.p. 160-163 ^{o}C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.56 (d, *J* = 3.7 Hz, 1H), 7.45 – 7.28 (m, 8H), 7.17 (d, *J* = 8.4 Hz, 2H), 7.01 (t, *J* = 4.4 Hz, 1H), 6.49 (s, 1H), 5.22 (t, *J* = 4.0 Hz, 1H), 3.54 (dd, *J* = 14.3, 3.4 Hz, 1H), 3.22 (dt, *J* = 14.2, 2.9 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 169.4, 163.2, 144.0, 142.9, 137.6, 134.0, 133.2, 132.1, 131.9, 129.3, 128.8, 128.4, 128.3, 127.8, 126.4, 100.0, 64.2, 40.5. HRMS (ESI+) calculated for $C_{22}H_{16}ClIN_2OS_2$ $(M+H)^+$ 550.9510; found 550.9509.



4x

(*Z*)-*N*-((*E*)-6-(iodomethylene)-3,4-diphenyl-1,3-thiazinan-2-ylidene)cyclohexaneca rboxamide (4x)

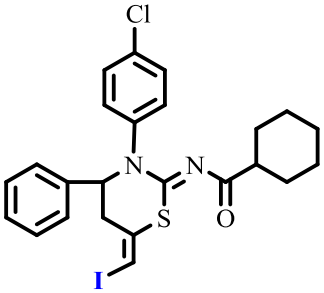
Brown oil, 40 mg, yield 78%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.43 – 7.23 (m, 8H), 7.14 (d, *J* = 7.6 Hz, 2H), 6.31 (d, *J* = 1.5 Hz, 1H), 5.19 (t, *J* = 4.0 Hz, 1H), 3.50 (dd, *J* = 14.4, 3.5 Hz, 1H), 3.17 (ddd, *J* = 14.5, 4.5, 1.7 Hz, 1H), 2.14 (d, *J* = 3.7 Hz, 1H), 1.73 (d, *J* = 13.7 Hz, 2H), 1.66 – 1.59 (m, 2H), 1.58 – 1.47 (m, 1H), 1.27 – 1.10 (m, 5H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 145.6, 138.0, 134.9, 129.0, 128.7, 128.1, 127.2, 126.6, 126.5, 75.1, 64.0, 47.8, 40.7, 29.13, 29.10, 26.1, 25.72, 25.67. HRMS (ESI+) calculated for $C_{24}H_{25}IN_2OS$ $(M+H)^+$ 517.0810; found 517.0815.



4y

(*Z*)-*N*-((*E*)-6-(iodomethylene)-4-phenyl-3-(*p*-tolyl)-1,3-thiazinan-2-ylidene)cyclohexanecarboxamide (4y)

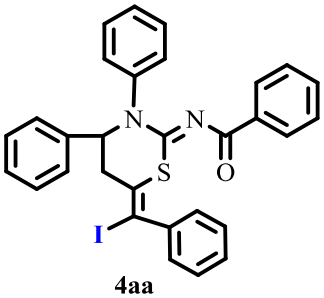
Yellow oil, 37 mg, yield 70%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.39 – 7.25 (m, 5H), 7.16 – 7.03 (m, 4H), 6.31 (d, *J* = 1.6 Hz, 1H), 5.20 (t, *J* = 4.0 Hz, 1H), 3.52 (dd, *J* = 14.5, 3.5 Hz, 1H), 3.18 (ddd, *J* = 14.4, 4.5, 1.8 Hz, 1H), 2.34 (s, 3H), 2.19 (d, *J* = 3.6 Hz, 1H), 1.82 – 1.56 (m, 5H), 1.31 – 1.14 (m, 5H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 187.2, 160.6, 143.1, 138.1, 137.0, 135.0, 129.6, 128.6, 128.0, 126.4, 126.2, 74.9, 64.1, 47.7, 40.7, 29.1, 26.1, 25.74, 25.70, 21.1. HRMS (ESI+) calculated for $C_{25}H_{27}IN_2OS$ $(M+H)^+$ 531.0962; found 531.0972.



4z

(*Z*)-*N*-((*E*)-3-(4-chlorophenyl)-6-(iodomethylene)-4-phenyl-1,3-thiazinan-2-ylidene)cyclohexanecarboxamide (4z)

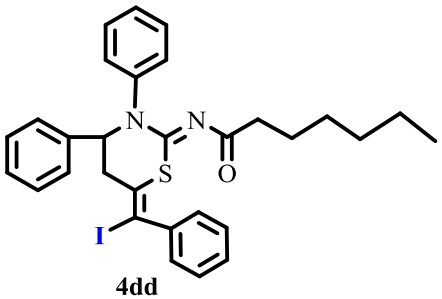
Brown solid, 32 mg, yield 58%, m.p. 148-150 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.27 – 7.14 (m, 7H), 7.00 (dd, *J* = 8.7, 3.3 Hz, 2H), 6.26 (d, *J* = 3.4 Hz, 1H), 5.06 (t, *J* = 4.0 Hz, 1H), 3.49 – 3.36 (m, 1H), 3.10 (s, 1H), 2.09 (d, *J* = 3.7 Hz, 1H), 1.67 – 1.47 (m, 5H), 1.19 – 1.05 (m, 5H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 187.2, 160.7, 143.9, 137.8, 134.5, 132.8, 129.1, 128.8, 128.2, 128.0, 126.4, 75.6, 64.0, 47.8, 40.7, 29.13, 29.10, 26.1, 25.69 , 25.65. HRMS (ESI+) calculated for $C_{24}H_{24}ClIN_2OS$ $(M+H)^+$ 551.0415; found 551.0412.



4aa

(*Z*)-*N*-((*E*)-6-(iodo(phenyl)methylene)-3,4-diphenyl-1,3-thiazinan-2-ylidene)benzamide (4aa)

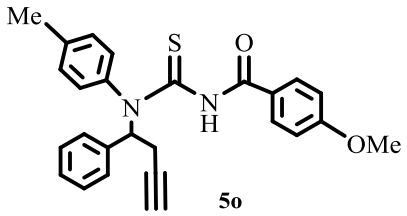
Brown oil, 33 mg, yield 72%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.77 (d, *J* = 7.7 Hz, 2H), 7.45 – 7.25 (m, 16H), 7.09 (d, *J* = 7.4 Hz, 2H), 5.34 (d, *J* = 3.9 Hz, 1H), 3.80 (dd, *J* = 14.1, 3.6 Hz, 1H), 3.50 (dd, *J* = 14.1, 4.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.1, 145.9, 141.5, 137.9, 136.8, 131.6, 130.3, 129.7, 129.6, 129.2, 129.0, 128.8, 128.7, 128.4, 128.3, 128.1, 127.8, 127.5, 126.9, 126.8, 95.9, 64.5, 44.8, 29.7. HRMS (ESI+) calculated for $C_{30}H_{23}INO_2S$ $(M+H)^+$ 587.0649; found 587.0653.



4dd

***N*-((2*Z*,6*E*)-6-(iodomethylene)-3,4-diphenyl-1,3-thiazinan-2-ylidene)heptanamide (4dd)**

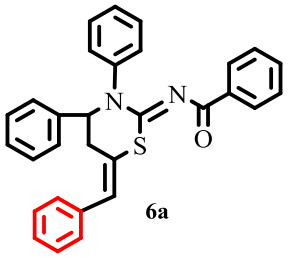
Yellow oil, 39 mg, yield 75%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.53 – 7.07 (m, 1H), 6.35 (d, *J* = 1.6 Hz, 10H), 5.21 (t, *J* = 4.0 Hz, 1H), 3.83 – 3.60 (m, 1H), 3.53 (dd, *J* = 14.4, 3.5 Hz, 2H), 3.19 (ddd, *J* = 14.4, 4.5, 1.8 Hz, 1H), 2.26 (t, *J* = 7.4 Hz, 1H), 1.46 (t, *J* = 7.2 Hz, 2H), 1.32 – 1.12 (m, 4H), 0.88 (d, *J* = 6.7 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 185.4, 161.1, 146.2, 138.6, 135.4, 130.2, 129.7, 129.4, 129.2, 129.1, 129.0, 128.8, 128.0, 127.3, 127.2, 77.9, 75.9, 73.2, 72.1, 71.4, 64.8, 62.5, 41.4, 40.9, 32.3, 32.2, 29.6, 25.9, 25.5, 23.2, 14.8. HRMS (ESI+) calculated for $C_{24}H_{27}IN_2OS$ $(M+H)^+$ 519.0962; found 519.0946.



5o

4-methoxy-*N*-((1-phenylbut-3-yn-1-yl)(*p*-tolyl)carbamothioyl)benzamide (5o)

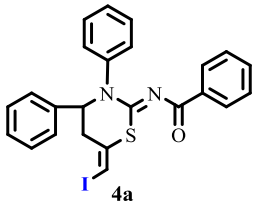
Yellow liquid, 38 mg, yield 93%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.19 (s, 1H), 7.55 (s, 1H), 7.32 (s, 8H), 6.97 (s, 1H), 6.78 (d, *J* = 8.4 Hz, 2H), 6.13 (s, 1H), 3.80 (s, 3H), 2.84 (t, *J* = 11.0 Hz, 2H), 2.33 (s, 3H), 2.10 (d, *J* = 2.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.2, 163.0, 139.6, 137.4, 132.9, 130.1, 129.6, 129.3, 128.6, 128.42, 128.37, 126.4, 125.9, 114.3, 113.9, 80.2, 71.6, 60.8, 55.5, 21.6, 20.7. HRMS (ESI+) calculated for $C_{26}H_{24}N_2O_2S$ $(M+H)^+$ 429.1637; found 429.1635.



6a

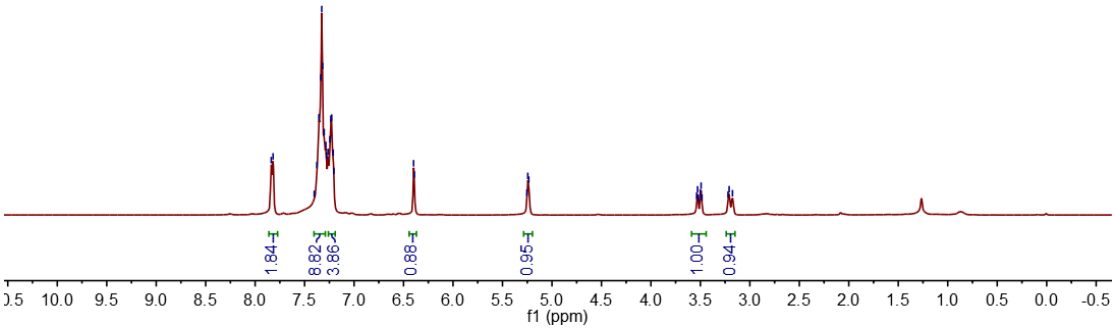
***N*-((*Z*)-6-((*Z*)-benzylidene)-3,4-diphenyl-1,3-thiazinan-2-ylidene)benzamide (6a)**

Yellow oil, 35 mg, yield 80%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 (d, *J* = 7.6 Hz, 2H), 7.34 (dddd, *J* = 29.9, 25.1, 13.5, 8.0 Hz, 15H), 6.83 – 6.60 (m, 3H), 5.22 (t, *J* = 3.9 Hz, 1H), 3.53 (dd, *J* = 14.3, 3.2 Hz, 1H), 3.32 (d, *J* = 4.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.6, 164.4, 146.1, 139.0, 137.1, 135.1, 131.5, 129.7, 129.1, 128.7, 128.4, 128.3, 128.2, 128.1, 127.8, 127.4, 127.2, 126.9, 126.7, 64.6, 34.6, 29.7. HRMS (ESI+) calculated for $C_{30}H_{24}N_2OS$ $(M+H)^+$ 461.1688; found 461.1684.

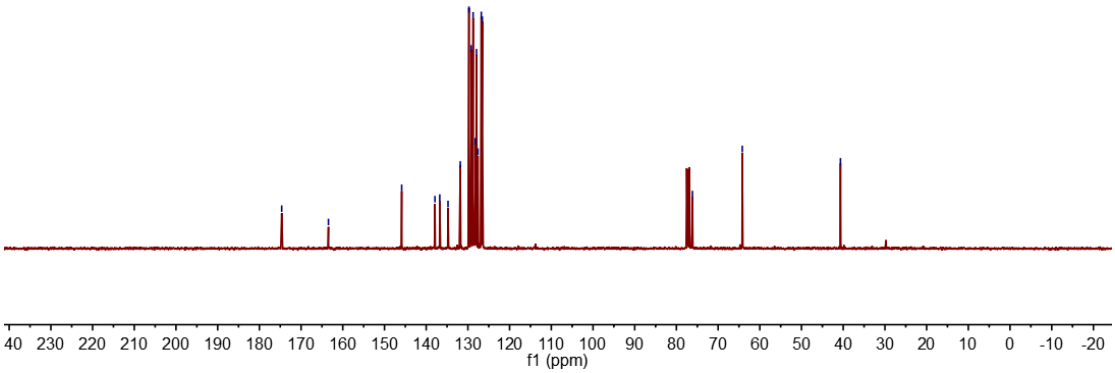


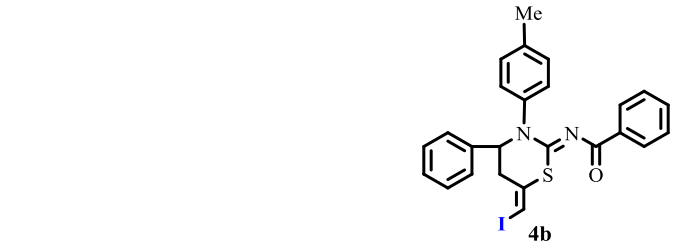
4a


3a/1
H1
7.84
7.82
7.40
7.38
7.36
7.34
7.33
7.32
7.30
7.29
7.28
7.26
7.25
7.23
7.23
7.21
7.20
6.40
6.39
5.25
5.24
5.23
3.54
3.53
3.52
3.50
3.49
3.48
3.22
3.21
3.18

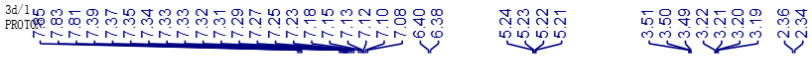

1.84
8.82
3.86
0.88
0.95
1.00
0.94
f1 (ppm)

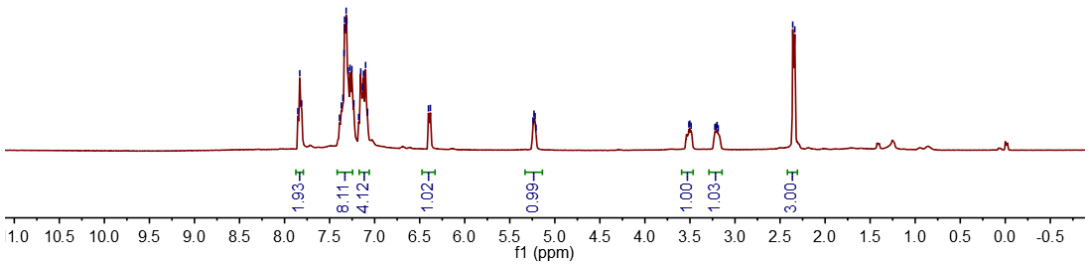

wj-125a.2.fid
C13CPD
174.65
163.44
145.87
137.90
136.75
134.77
131.82
129.74
129.21
128.75
128.23
127.95
127.60
126.79
126.54
76.16
64.20
40.66

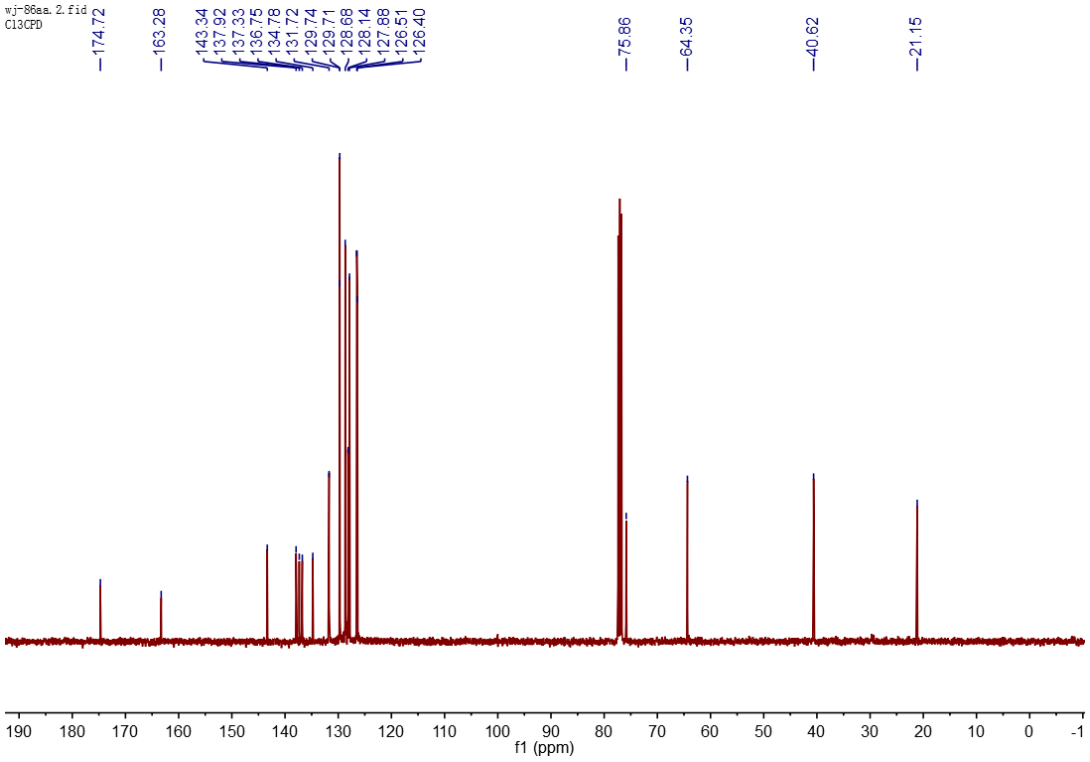

f1 (ppm)

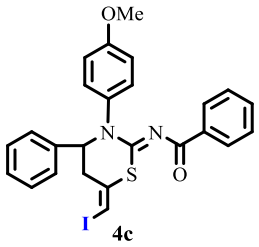

Me
N
N
S
O
I

4b


3d/1
PROTON
7.85
7.83
7.81
7.39
7.37
7.35
7.34
7.33
7.33
7.32
7.31
7.29
7.27
7.25
7.23
7.18
7.15
7.13
7.12
7.10
7.08
6.40
6.38
5.24
5.23
5.22
5.21
3.51
3.50
3.49
3.22
3.21
3.20
3.19
2.36
2.34

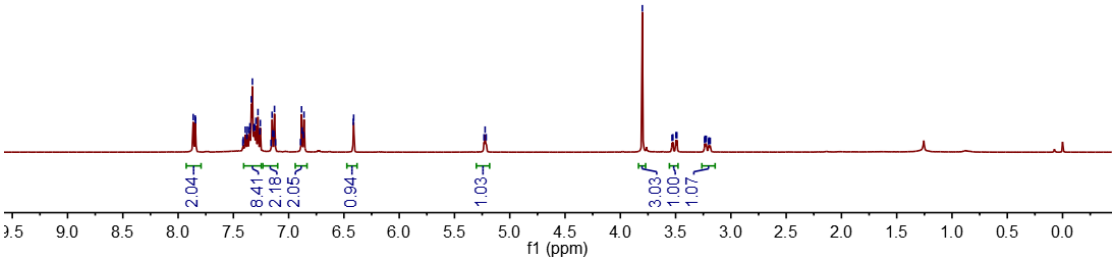

1.93
8.11
4.12
1.02
0.99
1.00
1.03
3.00
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

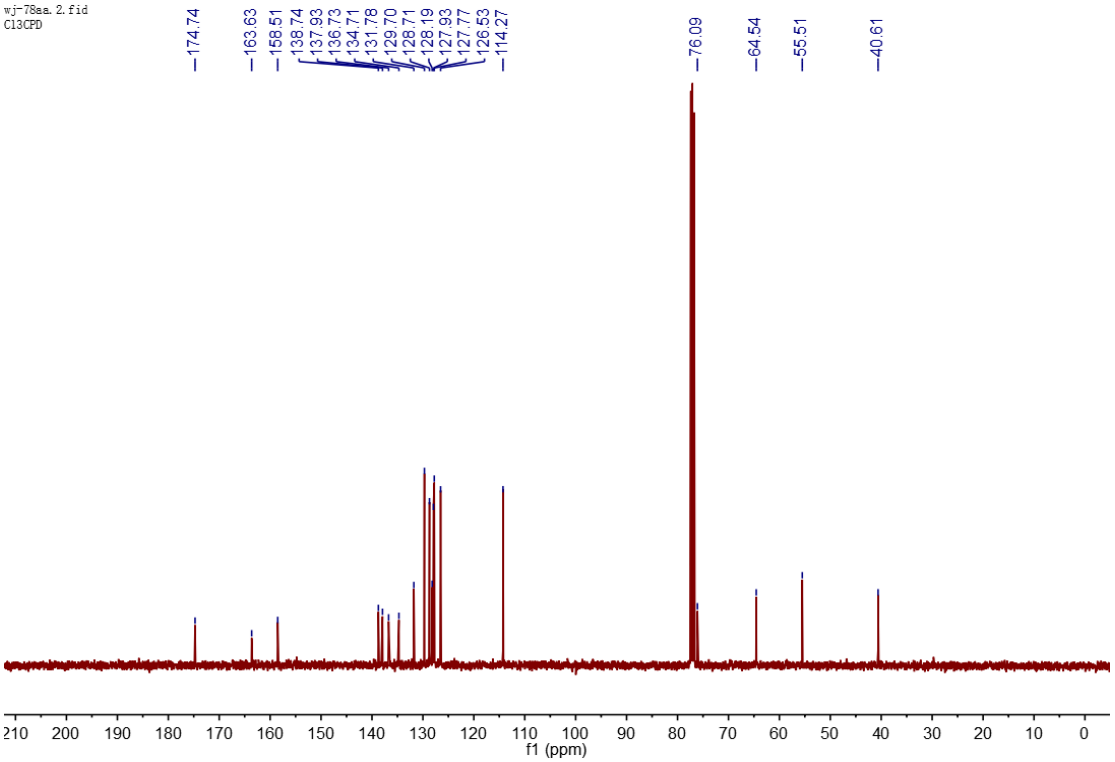

wj-86aa.2.fid
C13CPD
174.72
163.28
143.34
137.92
137.33
136.75
134.78
131.72
129.74
129.71
128.68
128.14
127.88
126.51
126.40
75.86
64.35
40.62
21.15
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

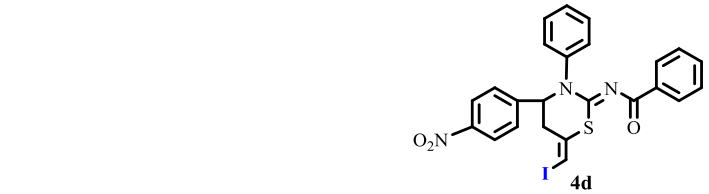

OMe
N
N
S
O
I

4c

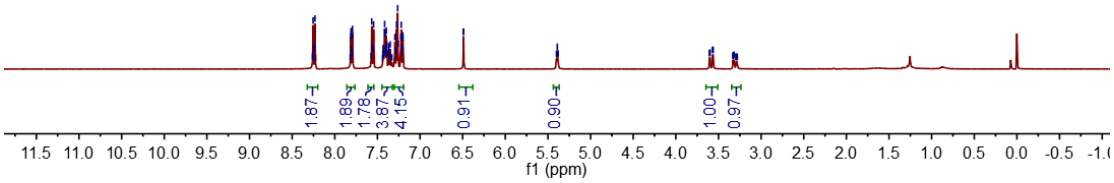

wj-78aa.1.fid
PROTON
7.86
7.85
7.84
7.41
7.41
7.39
7.38
7.37
7.36
7.35
7.34
7.33
7.32
7.31
7.31
7.30
7.28
7.26
7.26
7.16
7.15
7.15
7.13
7.13
7.12
6.89
6.88
6.88
6.87
6.86
6.42
6.41
5.23
5.22
5.21
3.80
3.53
3.52
3.50
3.49
3.24
3.23
3.23
3.22
3.20
3.20
3.19
3.19

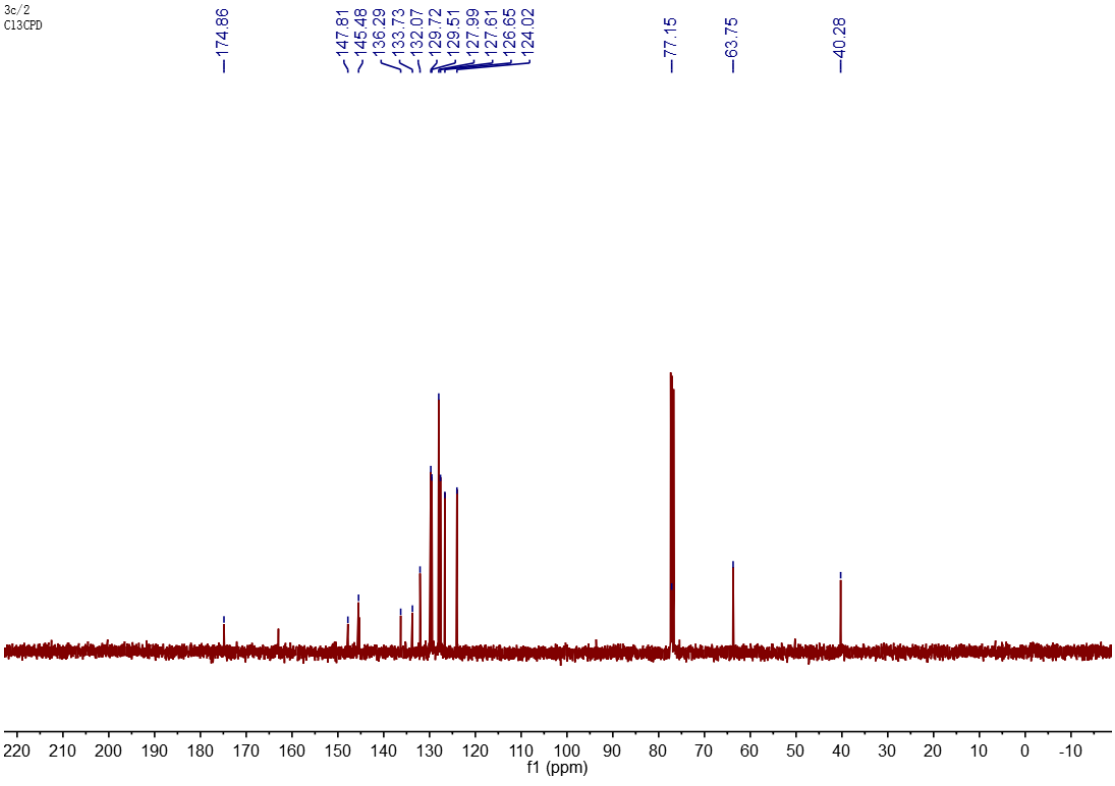

2.04
8.41
2.18
2.05
0.94
1.03
3.03
1.00
1.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

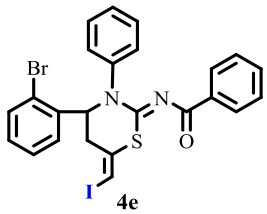

wj-78aa.2.fid
C13CPD
174.74
163.63
158.51
138.74
137.93
136.73
134.71
131.78
129.70
128.71
128.19
127.93
127.77
126.53
114.27
76.09
64.54
55.51
40.61
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O2N
N
N
S
O
I

4d

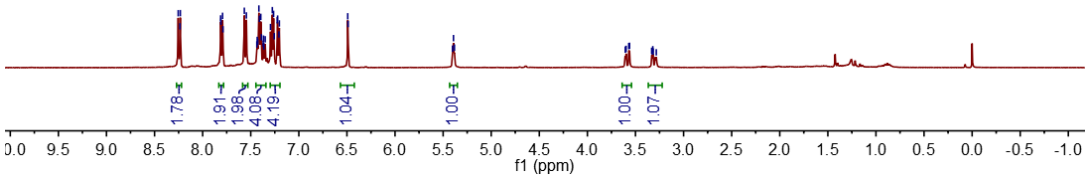

1.87
1.89
1.78
3.87
4.15
0.91
0.90
1.00
0.97
f1 (ppm)


174.86
147.81
145.48
136.29
133.73
132.07
129.72
129.51
127.99
127.61
126.65
124.02
77.15
63.75
40.28
f1 (ppm)

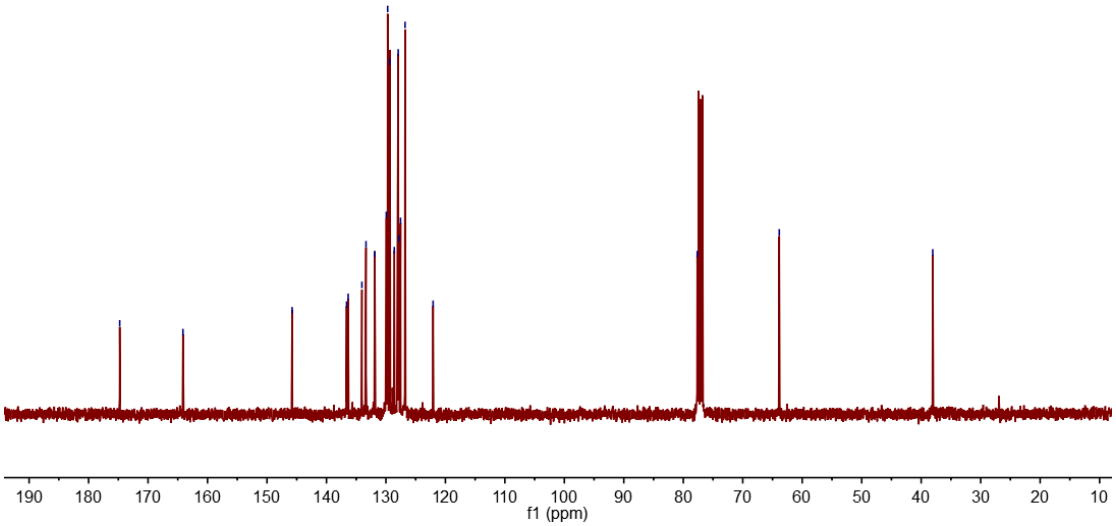

Br
N
N
S
O
I

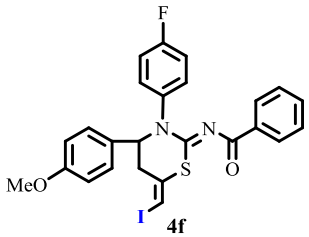
4e


Desktop/1 下午2.53.22
PROTON
8.25
8.24
8.23
7.81
7.81
7.79
7.79
7.79
7.57
7.55
7.44
7.43
7.43
7.42
7.41
7.40
7.39
7.37
7.37
7.36
7.35
7.29
7.28
7.26
7.26
7.22
7.22
7.21
7.20
6.49
6.49
5.40
5.39
5.38
3.61
3.60
3.57
3.56
3.33
3.33
3.32
3.32
3.28


1.78
1.91
1.98
4.08
4.19
1.04
1.00
1.00
1.07
f1 (ppm)

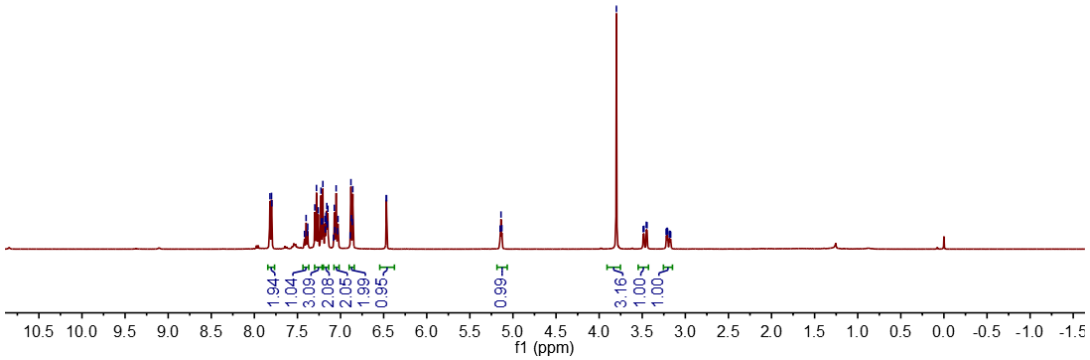

3i/2
test
174.77
164.13
145.77
136.61
136.35
134.04
133.35
131.88
129.94
129.71
129.33
128.60
127.94
127.78
127.54
126.78
122.07
77.65
63.86
38.05

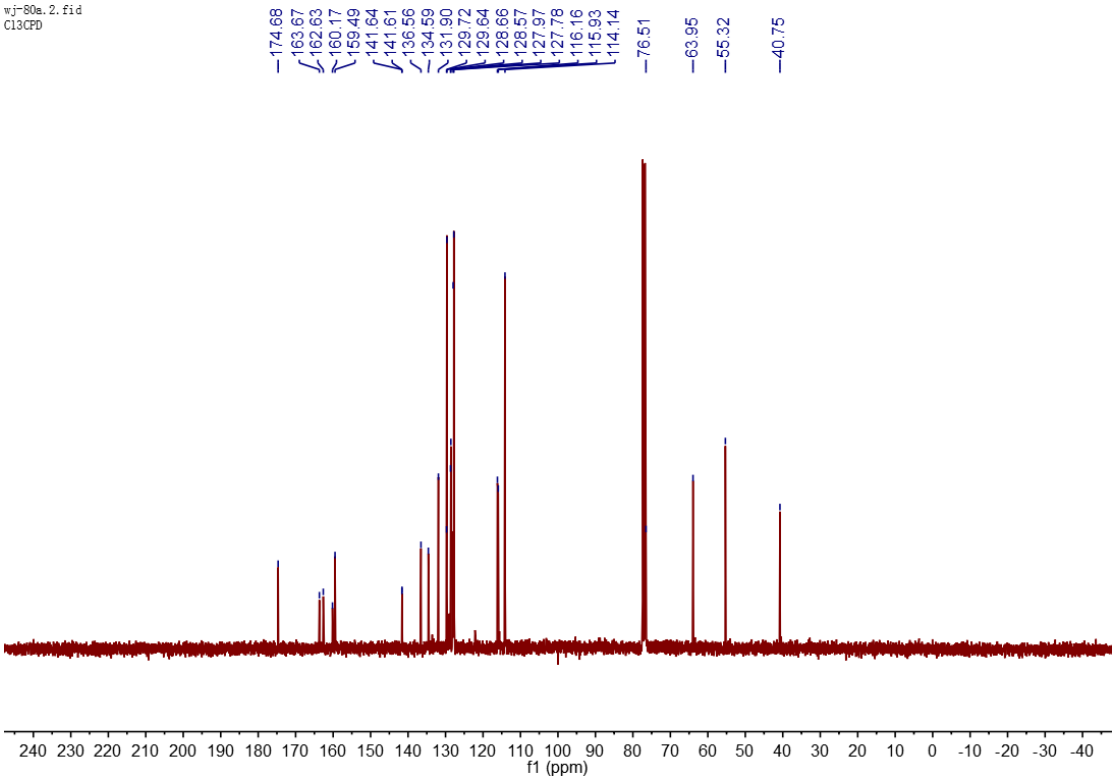

f1 (ppm)

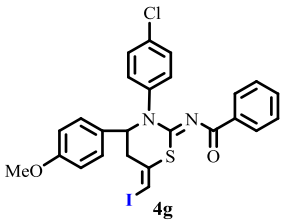

F
N
N
S
O
MeO
I

4f

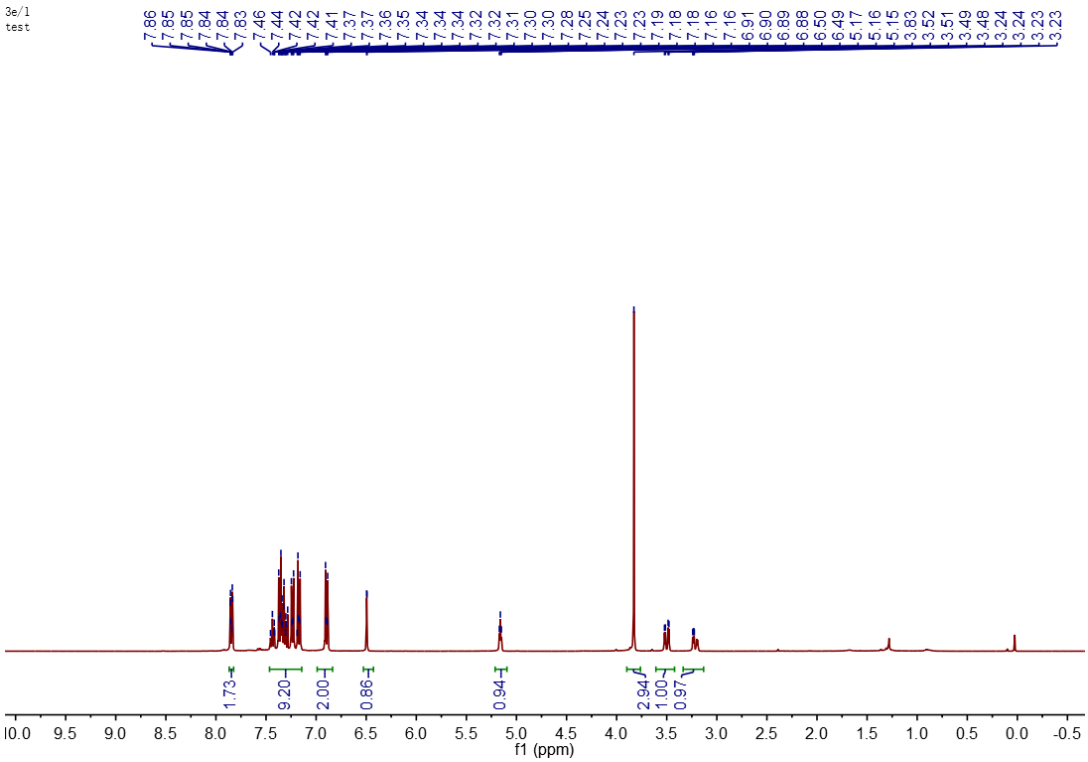

wj-80a.1.fid
PROTON
7.87
7.85
7.40
7.30
7.28
7.26
7.23
7.22
7.21
7.21
7.18
7.17
7.16
7.16
7.15
7.07
7.05
7.03
6.88
6.87
6.86
6.86
6.47
6.47
5.15
5.14
5.13
3.80
3.49
3.48
3.45
3.44
3.22
3.22
3.21
3.21
3.19
3.18
3.17
3.17

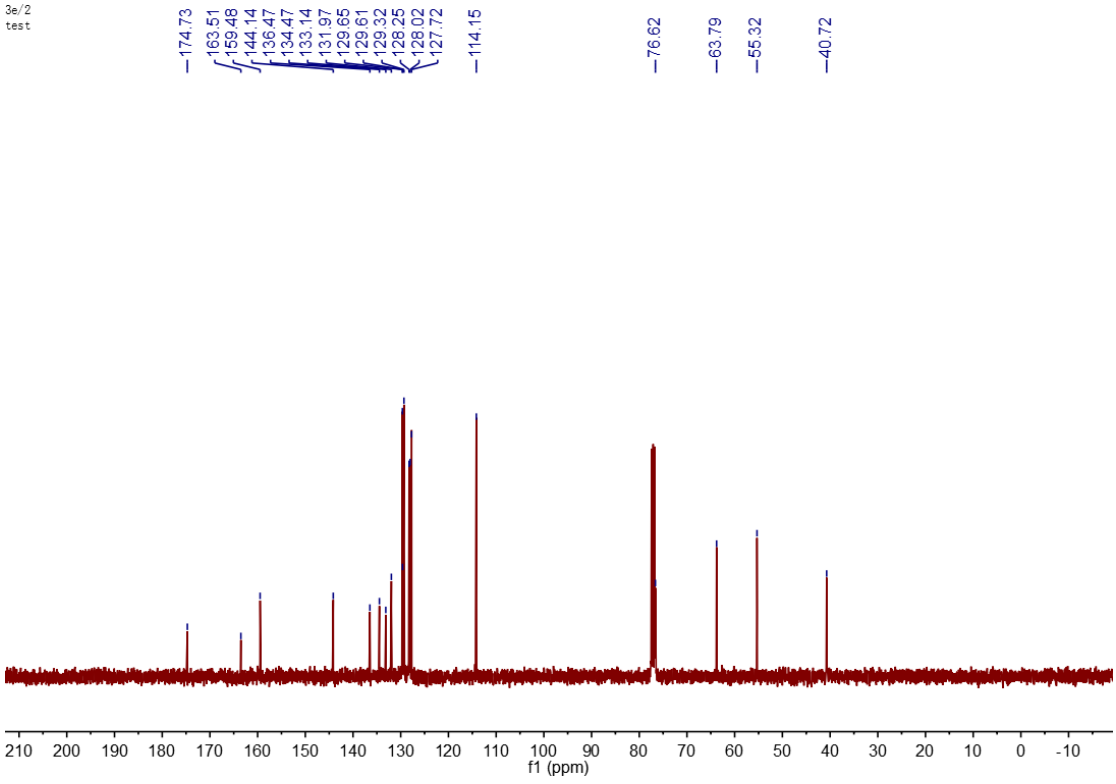

1.94
1.04
3.09
2.08
2.05
1.99
0.95
0.99
3.16
1.00
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

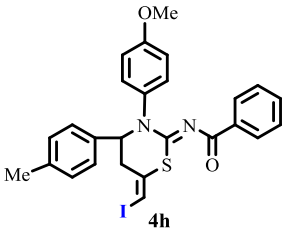

wj-80a.2.fid
C13CPD
174.68
163.67
162.63
160.17
159.49
141.64
141.61
136.56
134.59
131.90
129.72
129.64
128.66
128.57
127.97
127.78
116.16
115.93
114.14
76.51
63.95
55.32
40.75
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40
f1 (ppm)


Cl
N
N
S
O
MeO
I

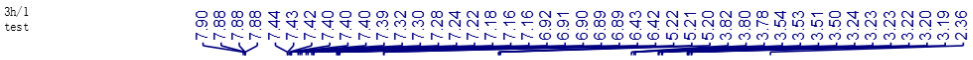
4g

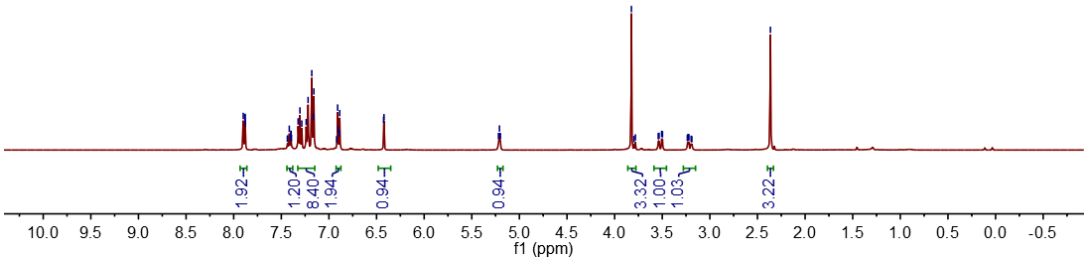

3e/1
test
7.86 7.85 7.85 7.84 7.84 7.83 7.46 7.44 7.42 7.42 7.41 7.37 7.37 7.36 7.35 7.34 7.34 7.34 7.32 7.32 7.31 7.30 7.30 7.28 7.25 7.24 7.23 7.23 7.19 7.18 7.18 7.16 7.16 6.91 6.90 6.89 6.88 6.50 6.49 5.17 5.16 5.15 3.83 3.52 3.51 3.49 3.48 3.24 3.24 3.23 3.23
1.73
9.20
2.00
0.86
0.94
2.94
1.00
0.97
f1 (ppm)


3e/2
test
174.73 163.51 159.48 144.14 136.47 134.47 133.14 131.97 129.65 129.61 129.32 128.25 128.02 127.72 114.15 76.62 63.79 55.32 40.72
f1 (ppm)


OMe
N
N
S
O
Me
I

4h


3h/1
test
7.90
7.88
7.88
7.88
7.44
7.43
7.42
7.40
7.40
7.40
7.39
7.32
7.30
7.28
7.24
7.22
7.18
7.16
7.16
6.92
6.91
6.90
6.89
6.89
6.43
6.42
5.22
5.21
5.20
3.82
3.80
3.78
3.54
3.53
3.51
3.50
3.24
3.23
3.23
3.22
3.20
3.19
2.36


1.92
1.20
8.40
1.94
0.94
0.84
3.32
1.00
1.03
3.22
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)


3h/2
test
174.70
163.62
158.45
138.77
137.87
136.77
134.93
134.83
131.76
129.70
129.38
127.93
127.74
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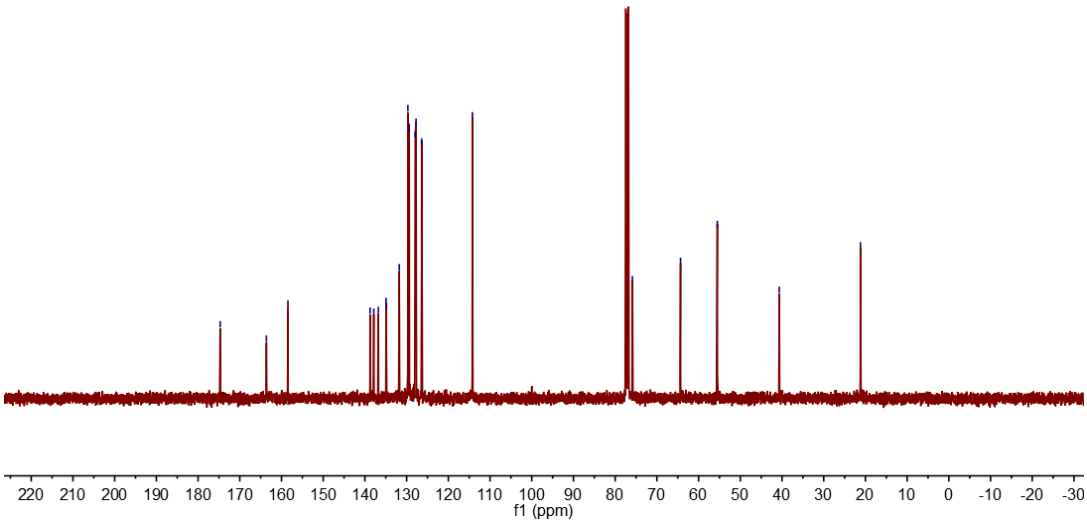
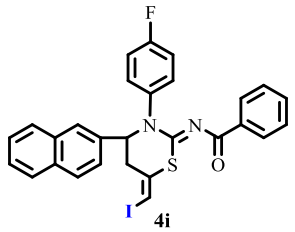
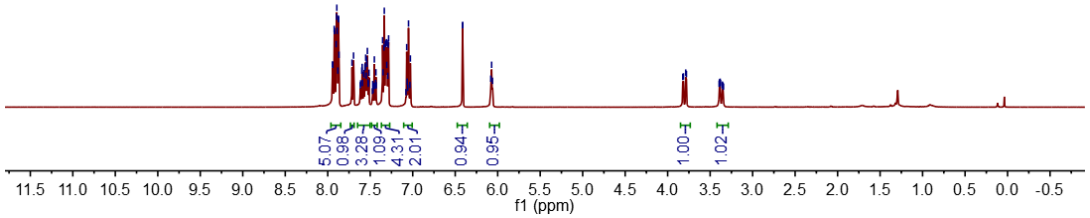
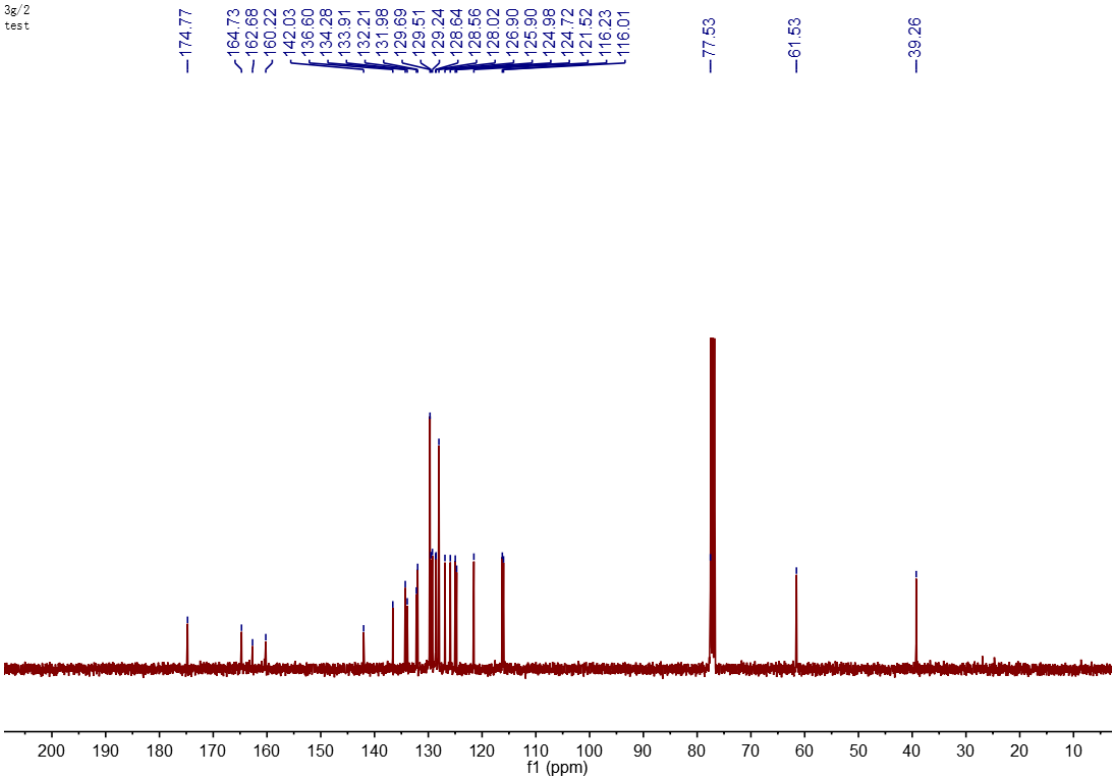
114.23
75.86
64.33
55.51
40.65
21.20

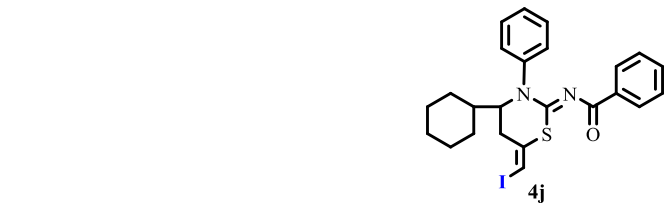

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30
f1 (ppm)


F
N
N
S
O
I

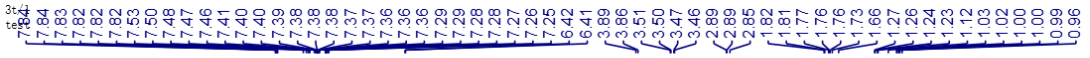
4i

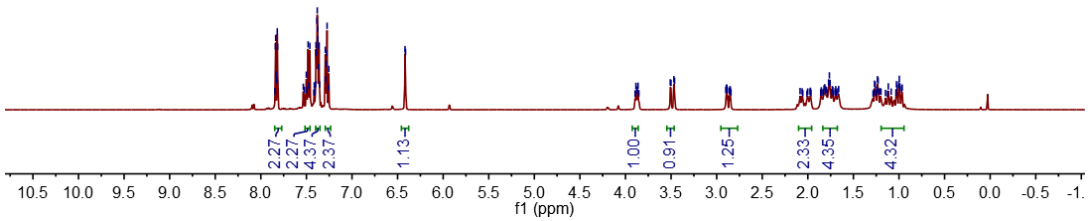

5.07
0.98
3.28
1.09
4.31
2.01
0.94
0.95
1.00
1.02
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

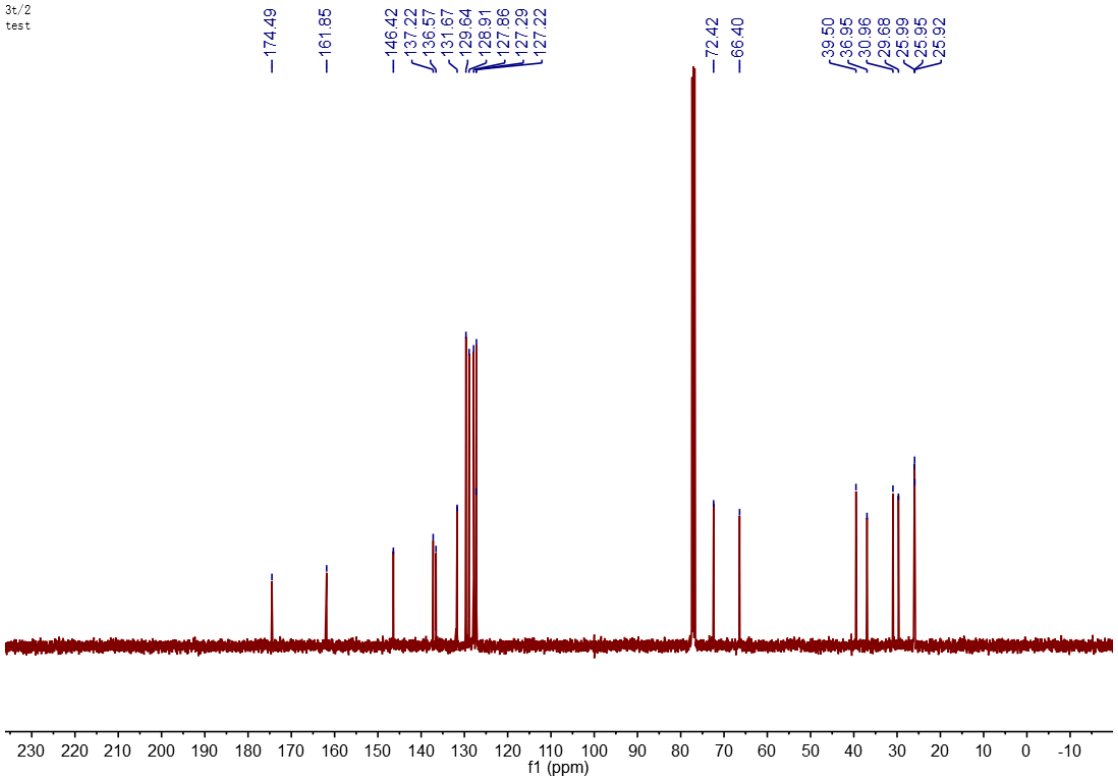

174.77
164.73
162.68
160.22
142.03
136.60
134.28
133.91
132.21
131.98
129.69
129.51
129.24
128.64
128.56
128.02
126.90
125.90
124.98
124.72
121.52
116.23
116.01
77.53
61.53
39.26
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

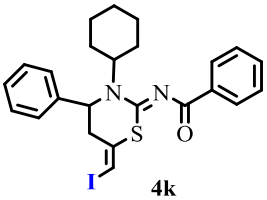


4j

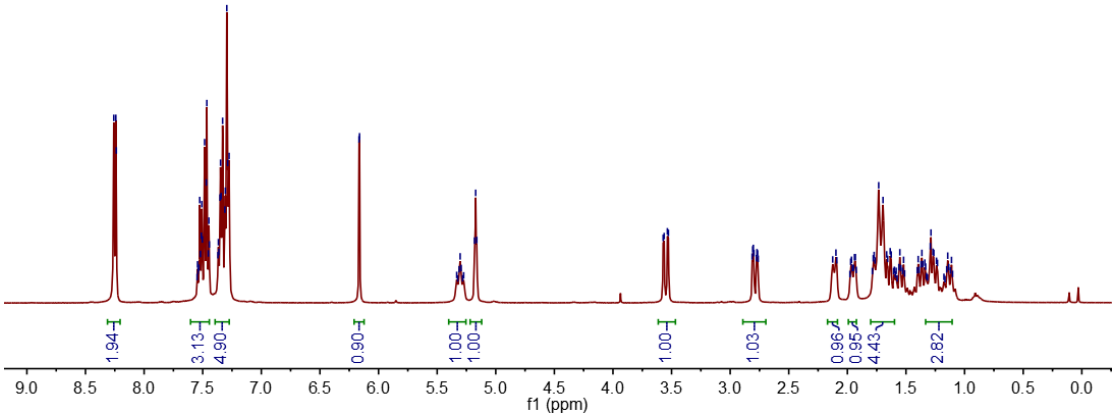


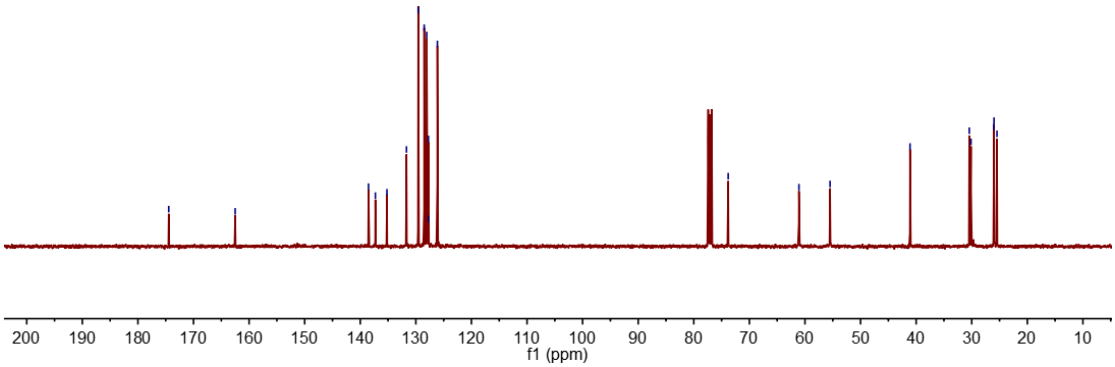


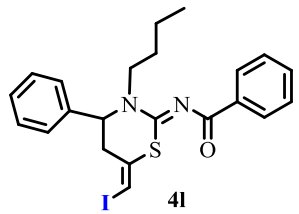




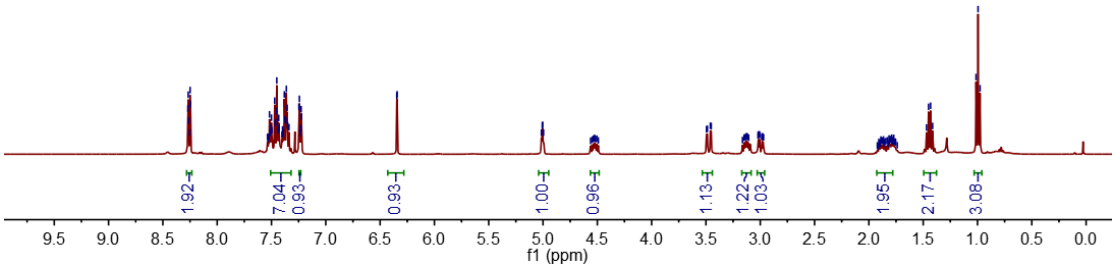
4k

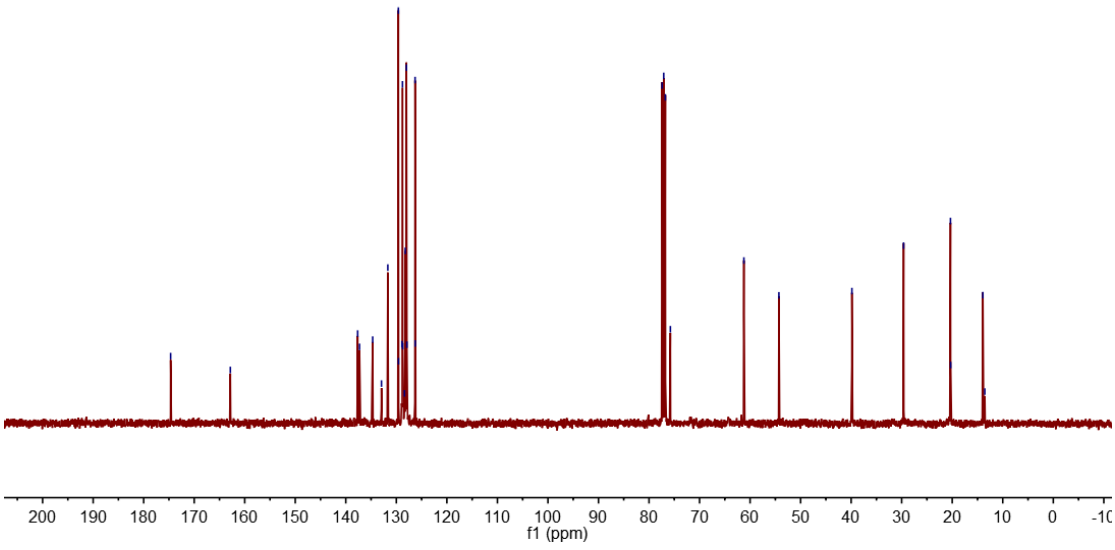


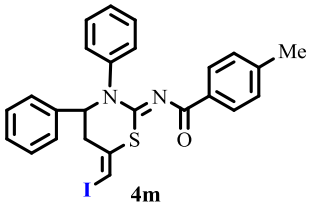




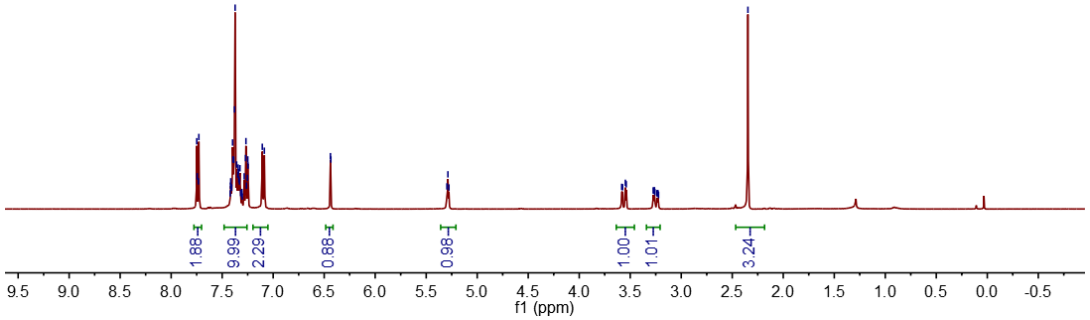
4l

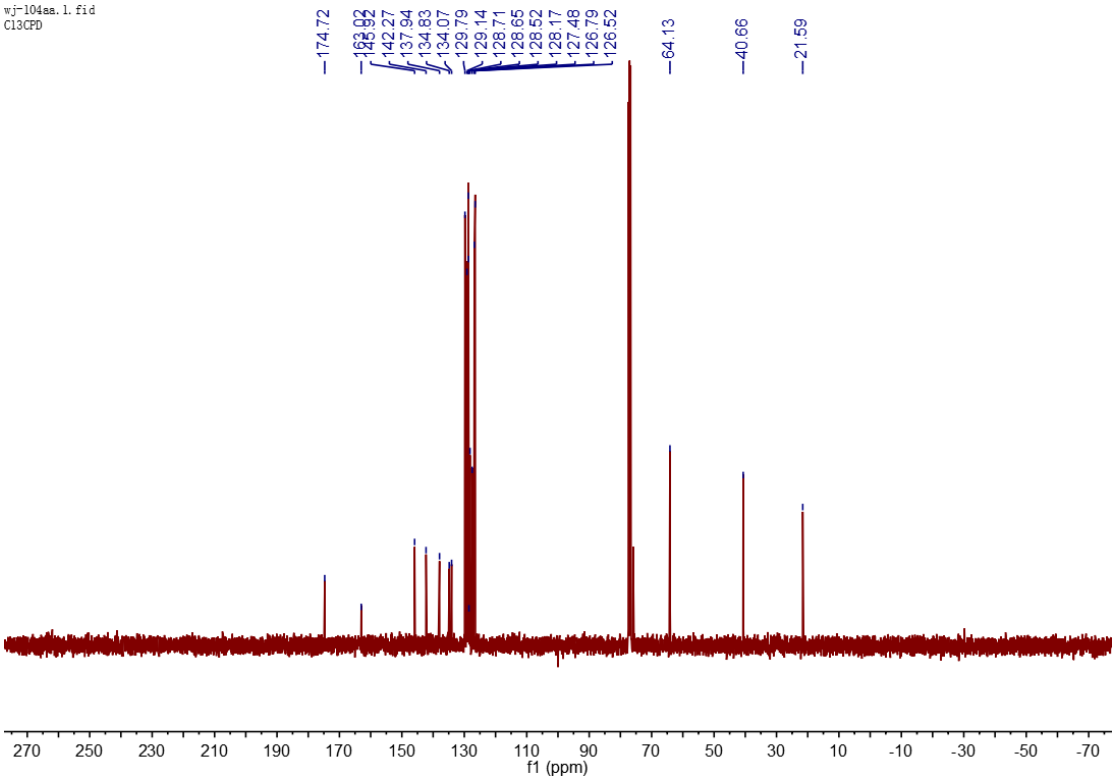


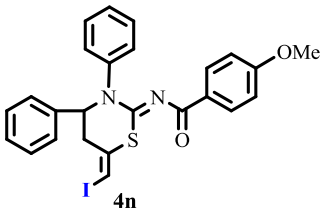



Me
N
N
S
O
I

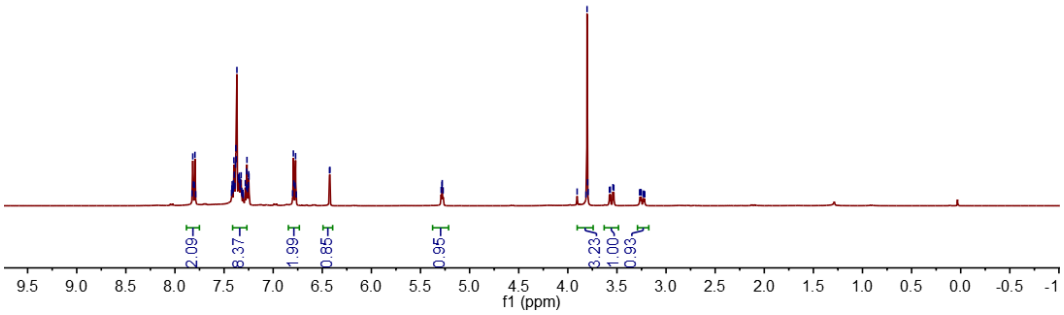
4m

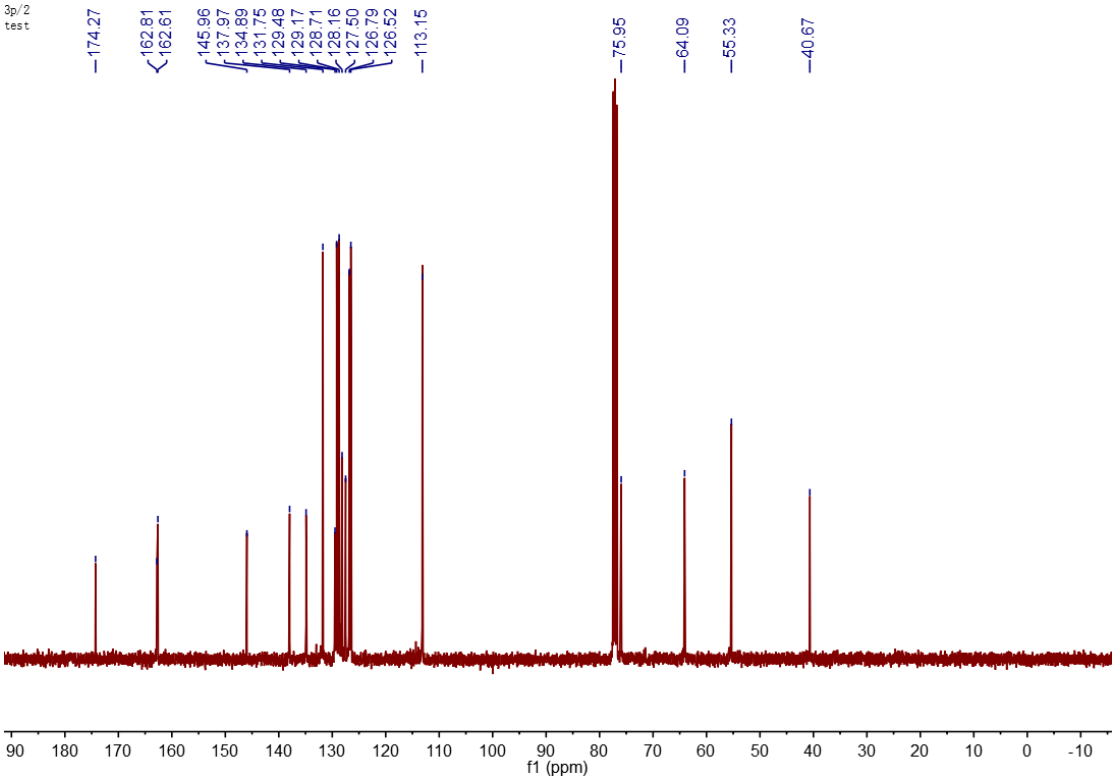

1.88
9.99
2.29
0.88
0.98
1.00
1.01
3.24
f1 (ppm)

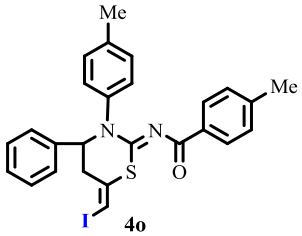

wj-104aa.1.fid
C13CPD
174.72
142.27
137.94
134.83
134.07
129.79
129.14
128.71
128.65
128.52
128.17
127.48
126.79
126.52
64.13
40.66
21.59
f1 (ppm)


OMe
N
N
S
O
I

4n

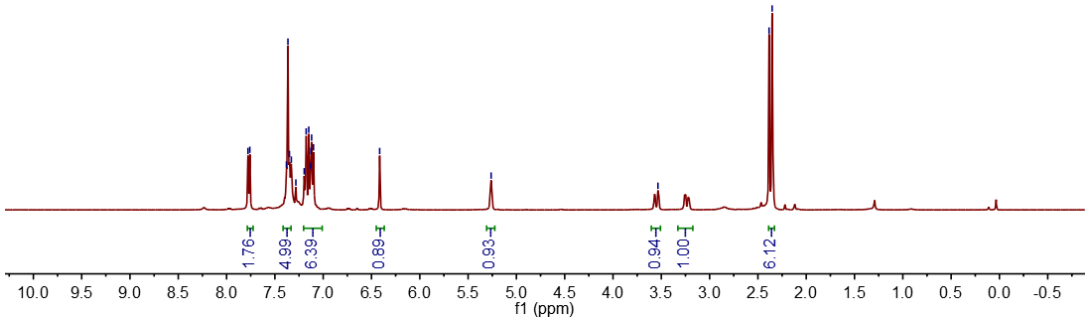

2.09
8.37
1.99
0.85
0.95
3.23
1.00
0.93
f1 (ppm)

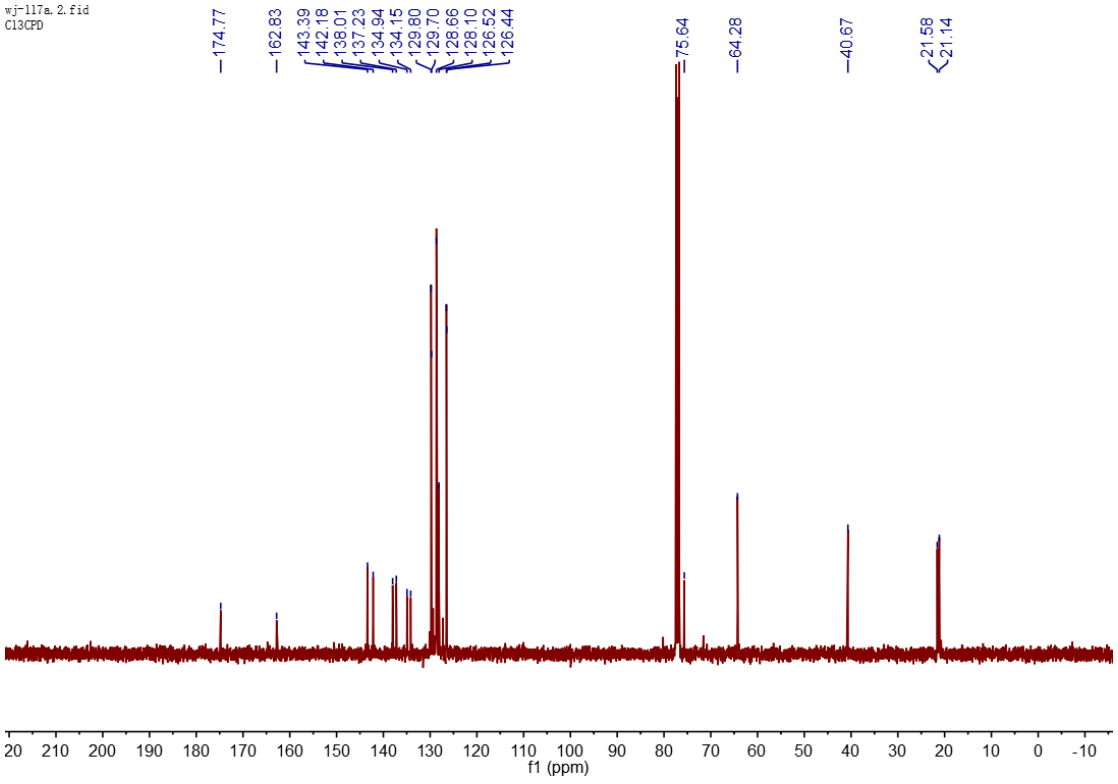

3p/2
test
174.27
162.81
162.61
145.96
137.97
134.89
131.75
129.48
129.17
128.71
128.16
127.50
126.79
126.52
113.15
75.95
64.09
55.33
40.67
f1 (ppm)

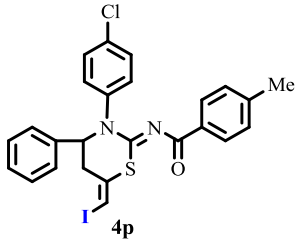

Me
Me
N
N
S
O
I

4o


wj-117a.1.fid
PROTON
7.78
7.76
7.38
7.36
7.35
7.33
7.28
7.20
7.18
7.15
7.13
7.13
7.12
7.10
6.42
5.26
3.53
2.38
2.35

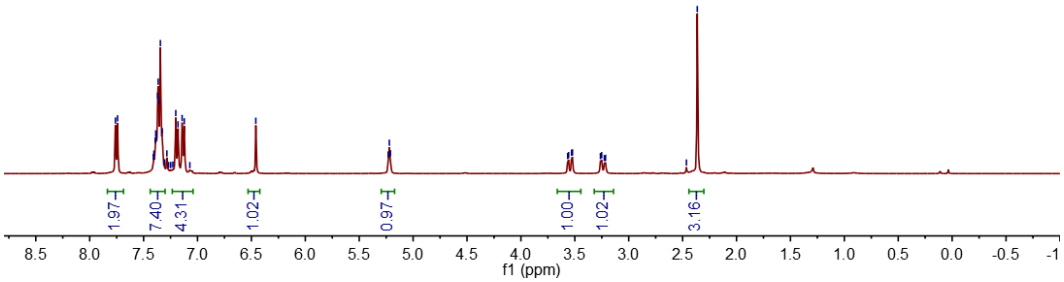

1.76
4.99
6.39
0.89
0.93
0.94
1.00
6.12
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

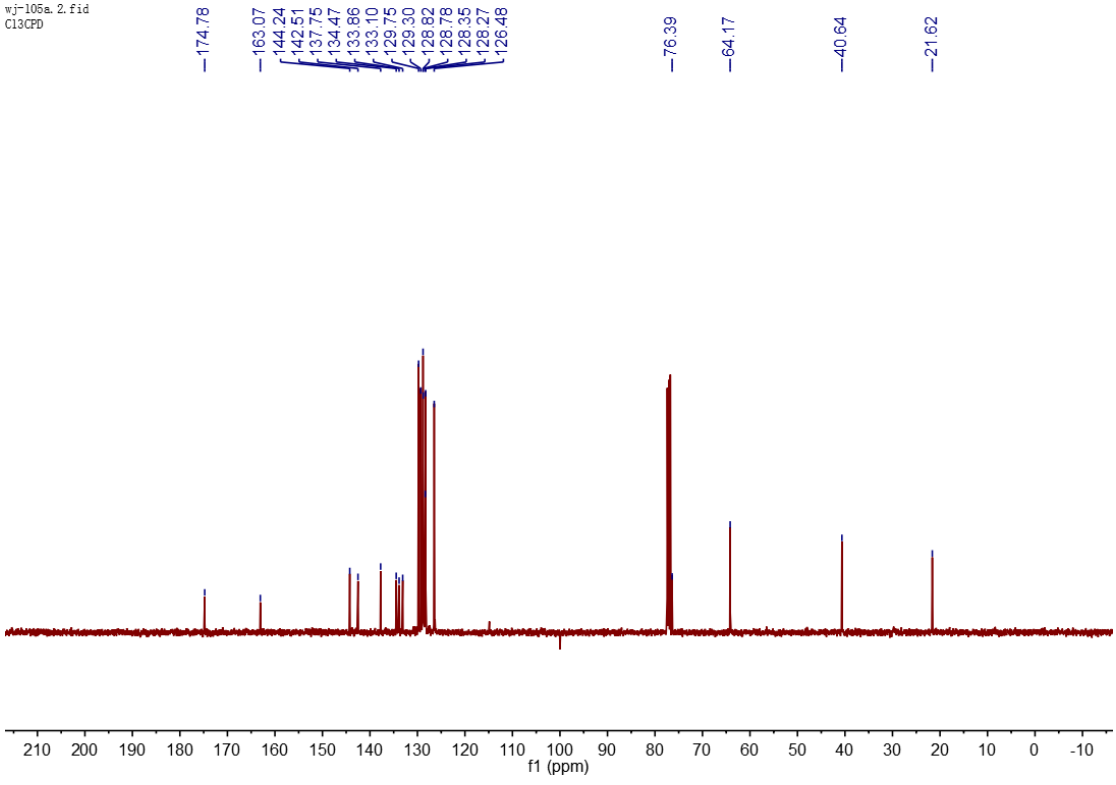

wj-117a.2.fid
C13CPD
174.77
162.83
143.39
142.18
138.01
137.23
134.94
134.15
129.80
129.70
128.66
128.10
126.52
126.44
75.64
64.28
40.67
21.58
21.14
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

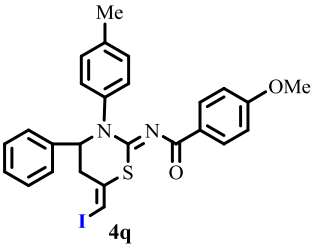

Cl
Me
N
N
S
O
I

4p


wj-105a. 1. fid
PROTON
7.76
7.74
7.41
7.40
7.39
7.39
7.38
7.37
7.36
7.36
7.34
7.33
7.31
7.28
7.27
7.25
7.23
7.20
7.18
7.14
7.12
7.07
6.46
5.23
5.22
5.21
3.57
3.56
3.53
3.52
3.26
3.25
3.23
3.22
2.46
2.36

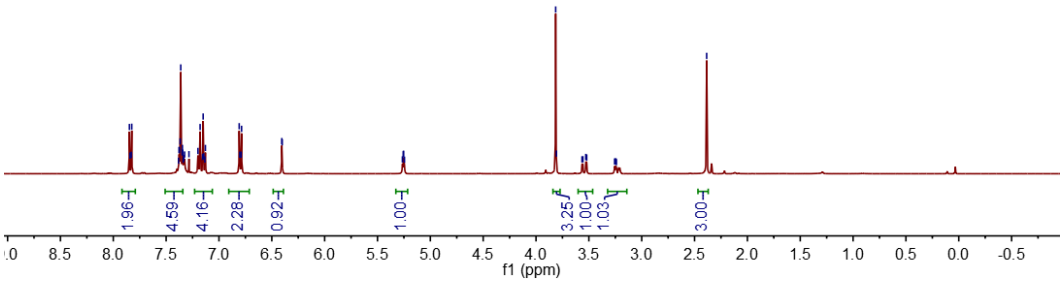

1.97
7.40
4.31
1.02
0.97
1.00
1.02
3.16
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

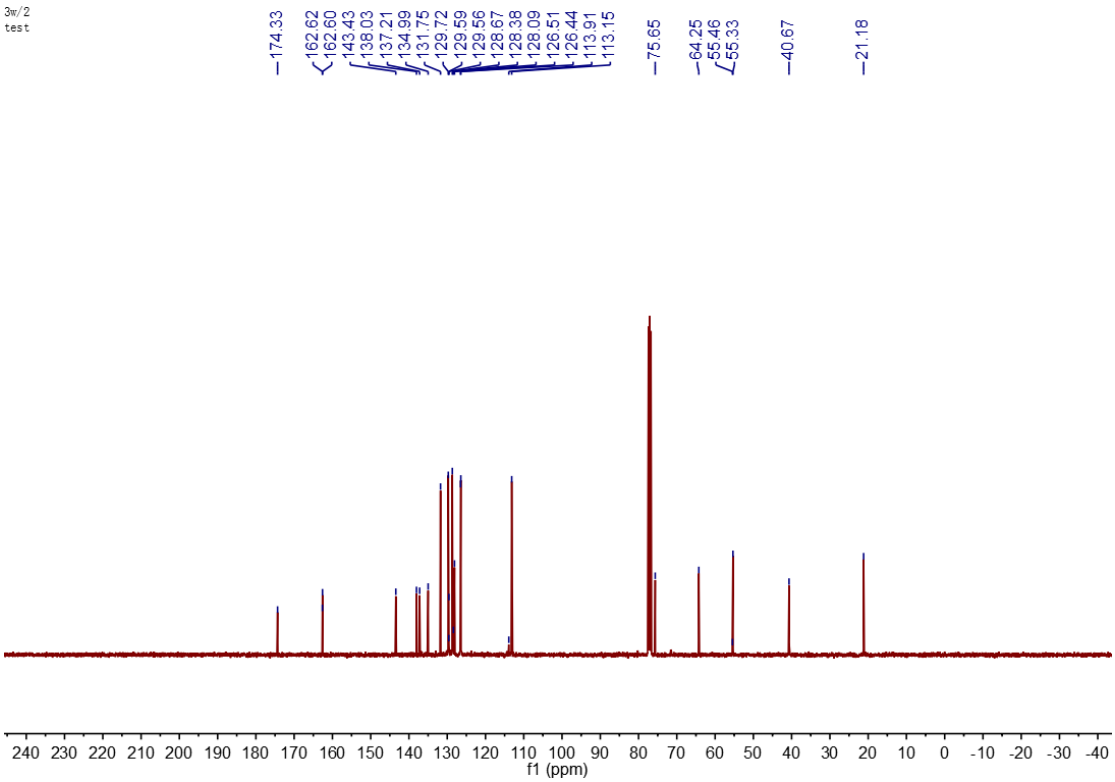

wj-105a. 2. fid
C13CPD
174.78
163.07
144.24
142.51
137.75
134.47
133.86
133.10
129.75
129.30
128.82
128.78
128.35
128.27
126.48
76.39
64.17
40.64
21.62
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

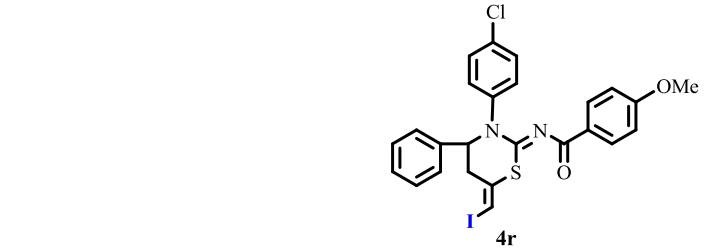

Me
OMe
N
N
S
O
I

4q


3w/1
test
7.85
7.84
7.83
7.83
7.38
7.38
7.37
7.37
7.36
7.35
7.35
7.35
7.34
7.34
7.33
7.33
7.28
7.20
7.18
7.15
7.15
7.14
7.13
7.13
6.81
6.80
6.79
6.79
6.41
6.40
5.26
5.26
5.25
5.24
3.81
3.81
3.56
3.56
3.53
3.52
3.26
3.25
3.24
3.24
2.39

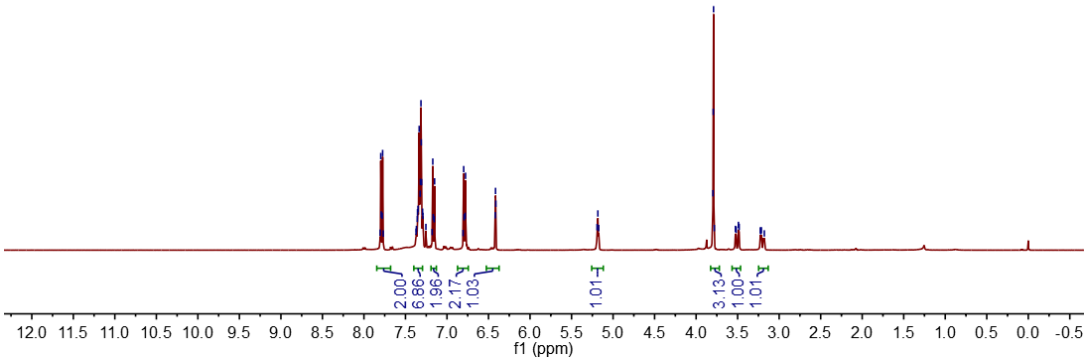

1.96
4.59
4.16
2.28
0.92
1.00
3.25
1.00
1.03
3.00
f1 (ppm)

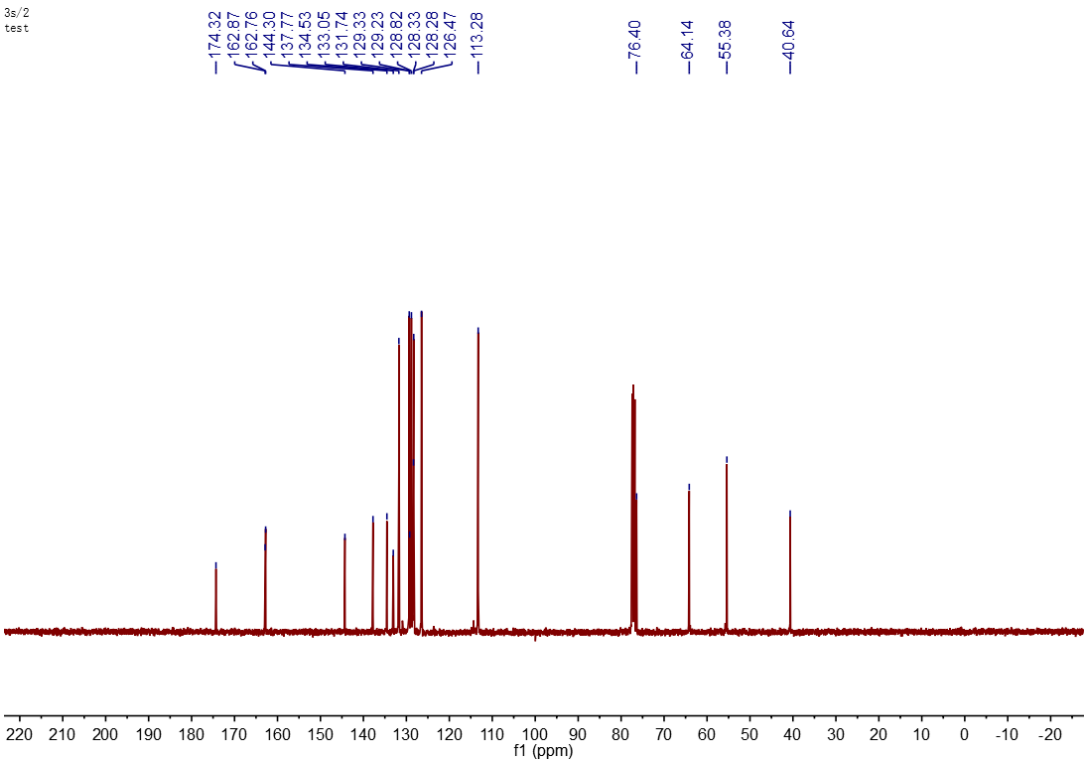

3w/2
test
174.33
162.62
162.60
143.43
138.03
137.21
134.99
131.75
129.72
129.59
129.56
128.67
128.38
128.09
126.51
126.44
113.91
113.15
75.65
64.25
55.46
55.33
40.67
21.18
f1 (ppm)

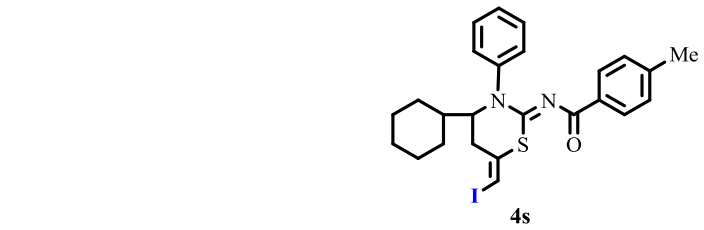

Cl
OMe
N
N
S
O
I

4r

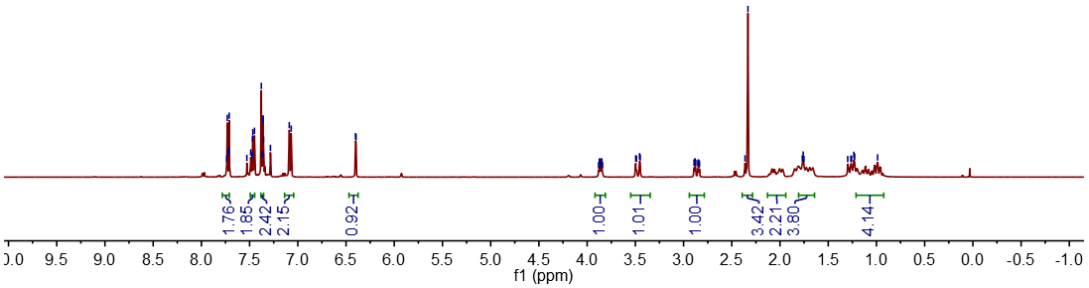

3s/1
test
7.80
7.80
7.79
7.78
7.77
7.37
7.37
7.36
7.35
7.35
7.33
7.32
7.32
7.31
7.31
7.31
7.29
7.29
7.25
7.18
7.17
7.17
7.15
6.80
6.79
6.78
6.78
6.42
6.42
6.41
5.19
5.18
5.17
3.80
3.79
3.79
3.78
3.53
3.52
3.49
3.48
3.23
3.22
3.21
3.18

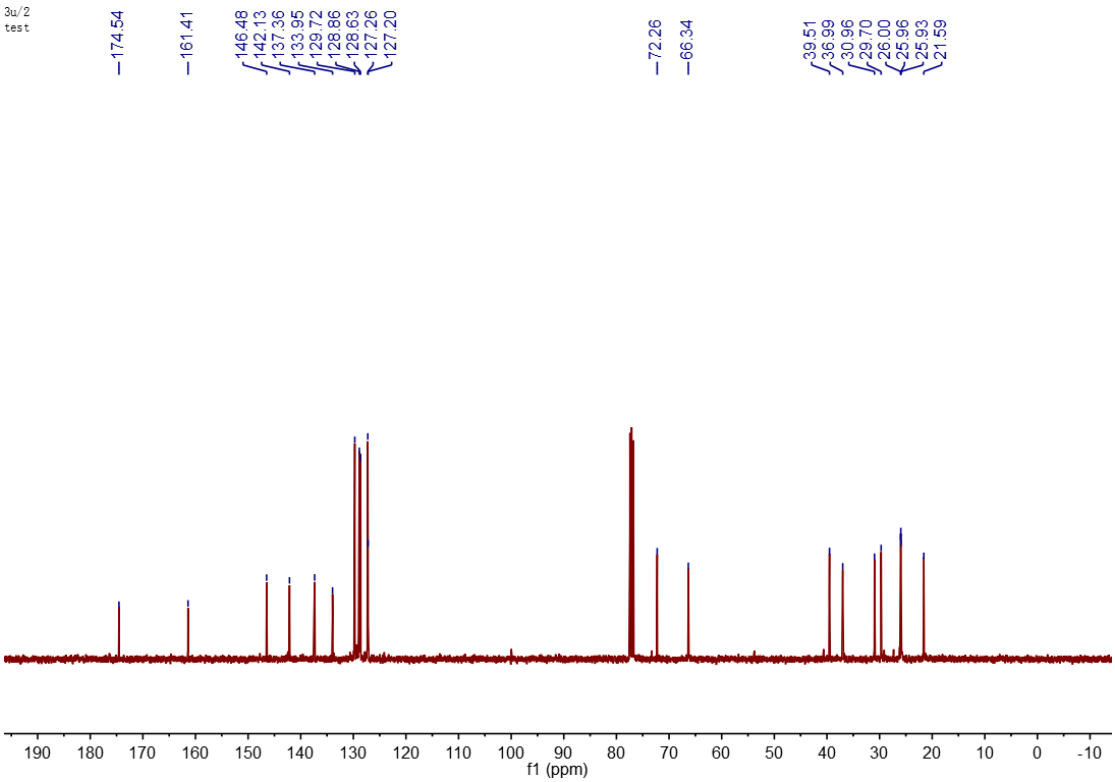

2.00
6.86
1.96
2.17
1.03
1.01
3.13
1.00
1.01
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

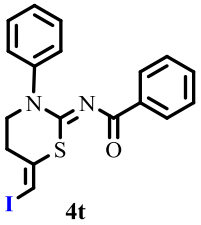

3s/2
test
174.32
162.87
162.76
144.30
137.77
134.53
133.05
131.74
129.33
129.23
128.82
128.33
128.28
126.47
113.28
76.40
64.14
55.38
40.64
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


Me
N
N
S
O
I

4s

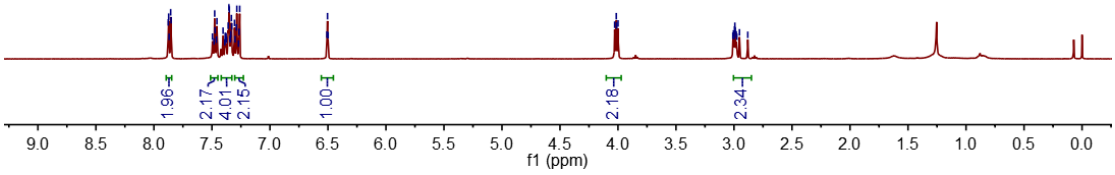

1.76
1.85
2.42
2.15
0.92
1.00
1.01
1.00
3.42
2.21
3.80
4.14
f1 (ppm)

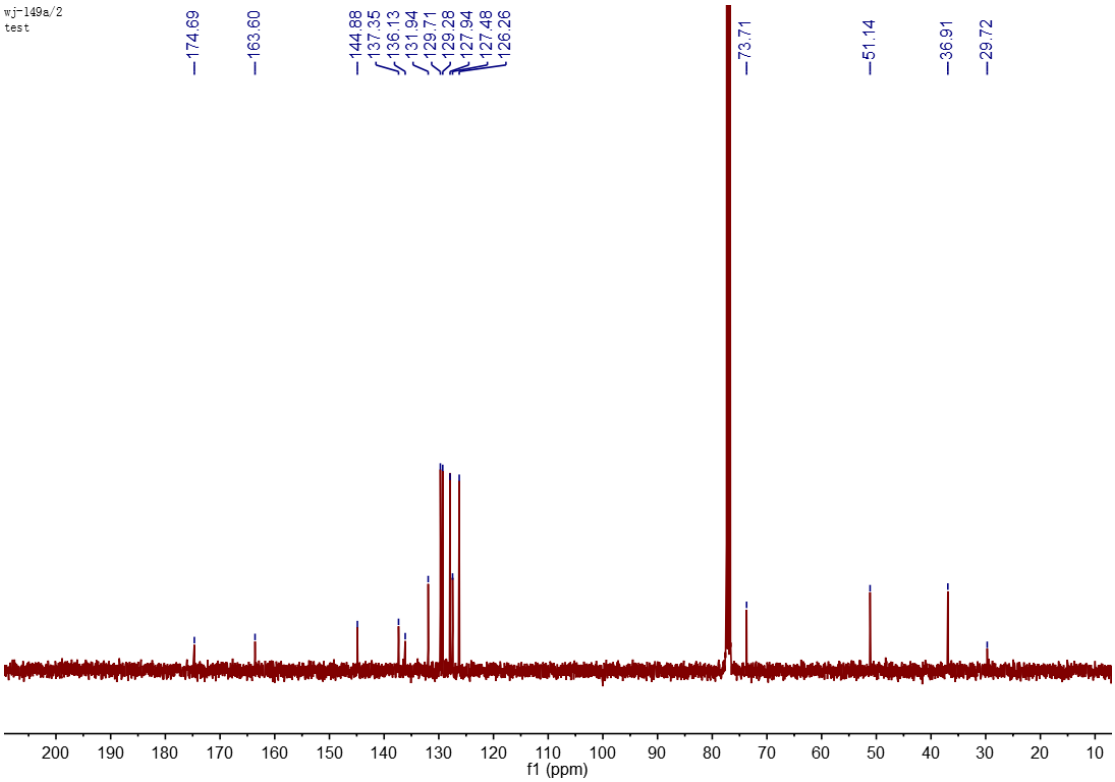

174.54
161.41
146.48
142.13
137.36
133.95
129.72
128.86
128.63
127.26
127.20
72.26
66.34
39.51
36.99
30.96
29.70
26.00
25.96
25.93
21.59
f1 (ppm)

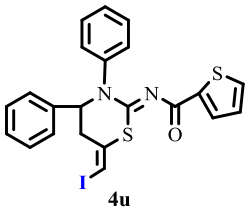


4t

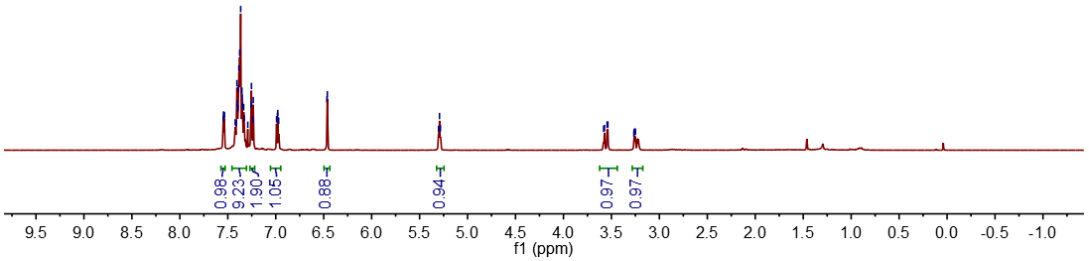

wj-149a/1
test
7.88 7.87 7.87 7.86 7.85 7.50 7.48 7.48 7.47 7.46 7.46 7.40 7.39 7.39 7.38 7.38 7.37 7.36 7.35 7.35 7.34 7.34 7.34 7.33 7.31 7.30 7.29 7.29 7.27 7.27 7.26 6.51 6.50 6.50 4.03 4.01 4.01 4.00 4.00 3.01 3.00 3.00 3.00 2.99 2.99 2.98 2.98 2.95 2.88

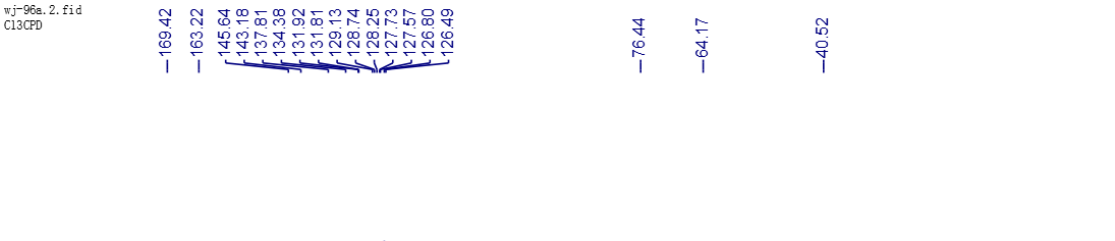

1.96
2.17
4.01
2.15
1.00
2.18
2.34
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

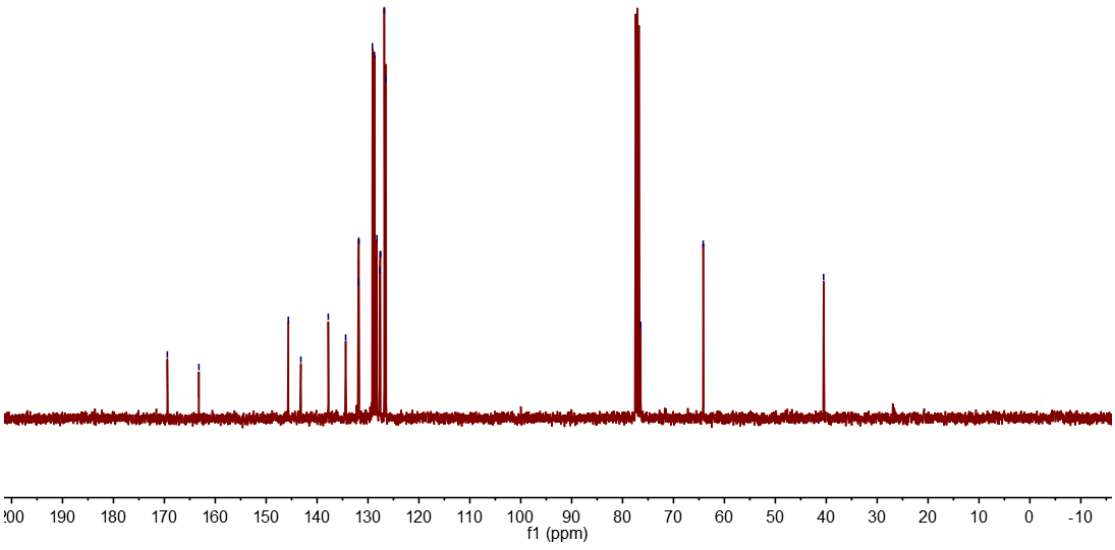

wj-149a/2
test
174.69
163.60
144.88
137.35
136.13
131.94
129.71
129.28
127.94
127.48
126.26
73.71
51.14
36.91
29.72
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

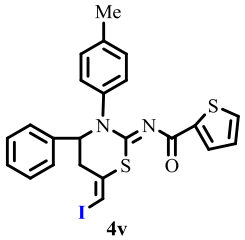


4u



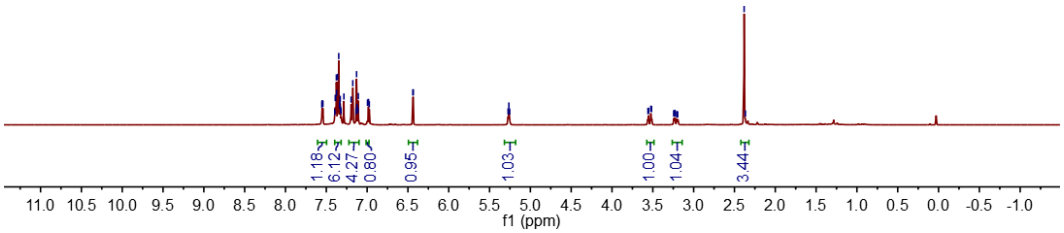


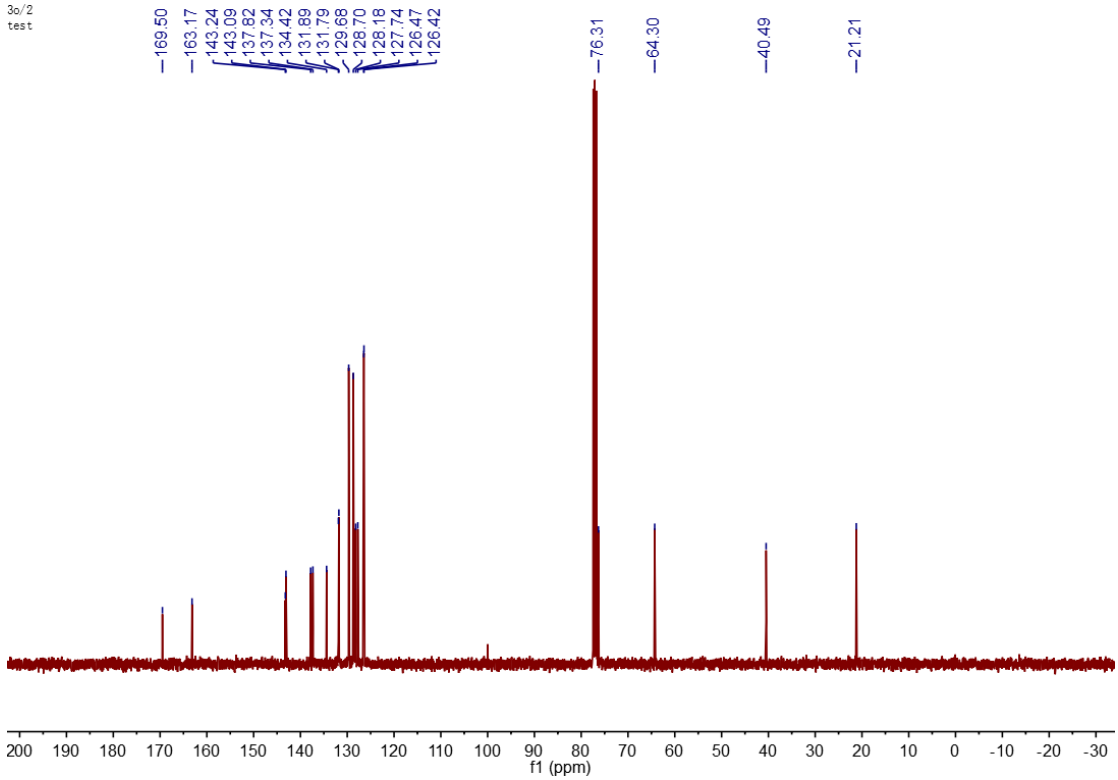


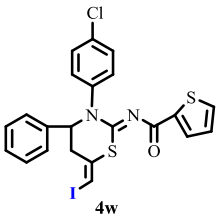

Me
N
N
S
S
O
I

4v


7.55
7.55
7.55
7.54
7.39
7.39
7.38
7.37
7.36
7.35
7.34
7.33
7.33
7.28
7.20
7.18
7.13
7.11
7.00
6.99
6.98
6.97
6.44
5.27
5.26
5.25
3.56
3.55
3.52
3.52
3.24
3.24
3.23
3.23
3.21
3.20
3.20
2.38
2.37

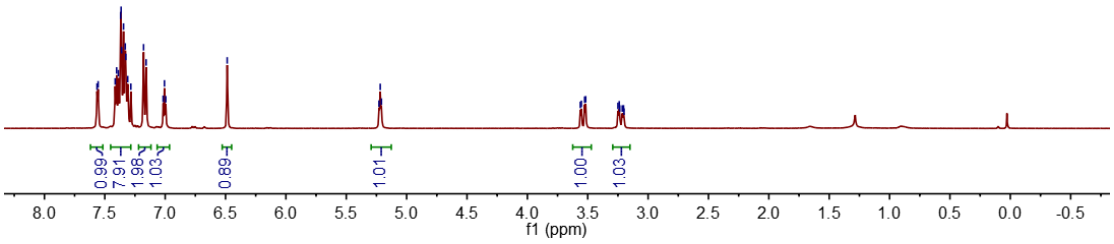

1.18
6.12
4.27
0.80
0.95
1.03
1.00
1.04
3.44
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

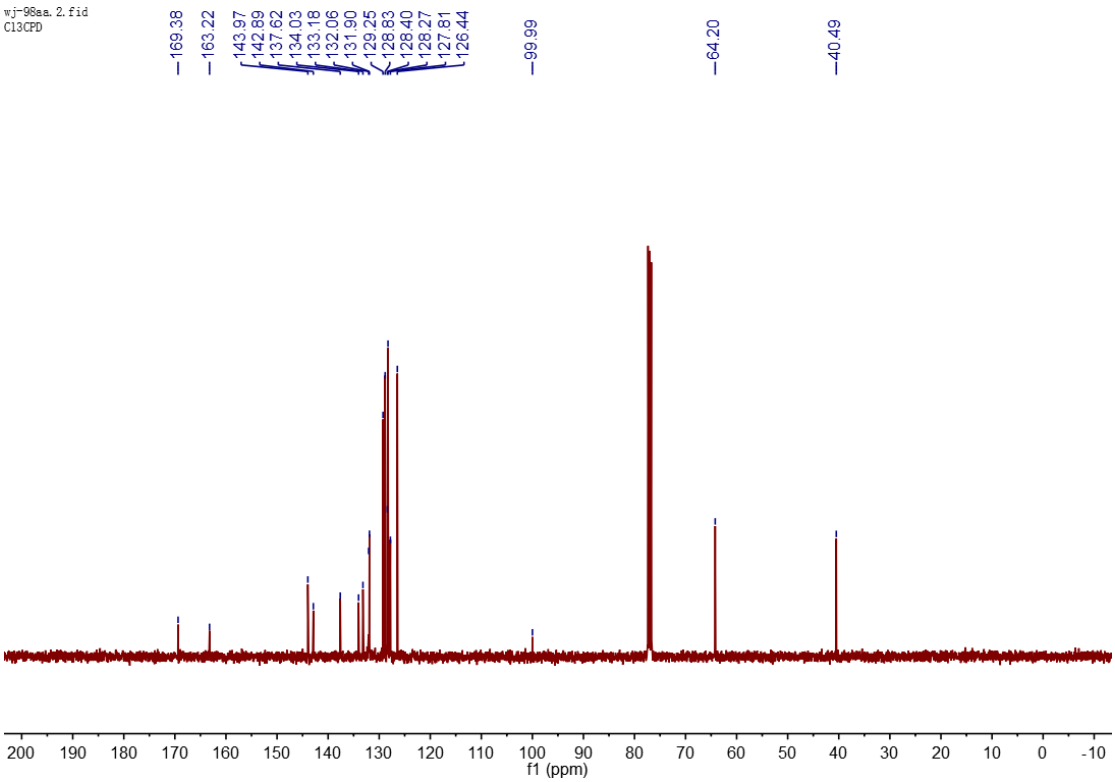

3o/2
test
169.50
163.17
143.24
143.09
137.82
137.34
134.42
131.89
131.79
129.68
128.70
128.18
127.74
126.47
126.42
76.31
64.30
40.49
21.21
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30
f1 (ppm)

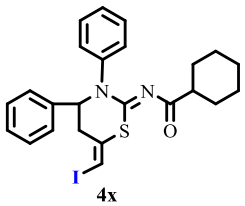

Cl
N
N
S
S
O
I

4w

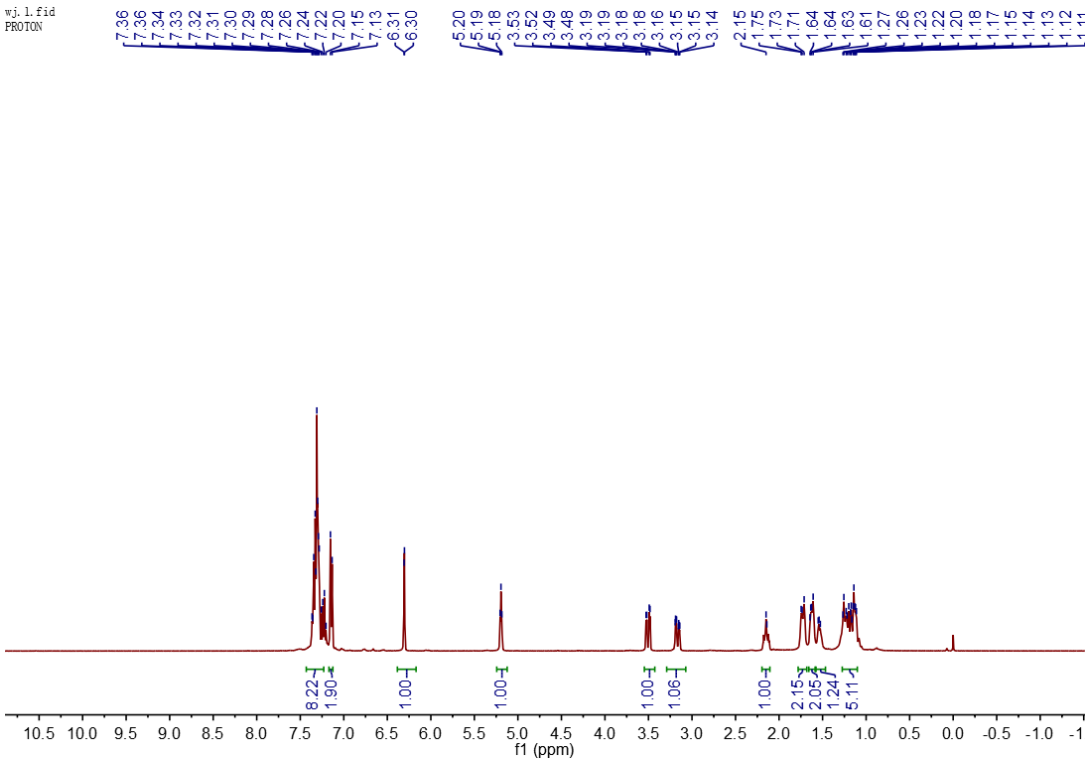

wj-98aa.1.fid
PROTON
7.56
7.41
7.40
7.39
7.37
7.36
7.36
7.34
7.33
7.33
7.31
7.28
7.18
7.16
7.02
7.01
6.99
6.49
5.23
5.22
5.21
3.56
3.55
3.53
3.52
3.25
3.24
3.24
3.21
3.20
3.20

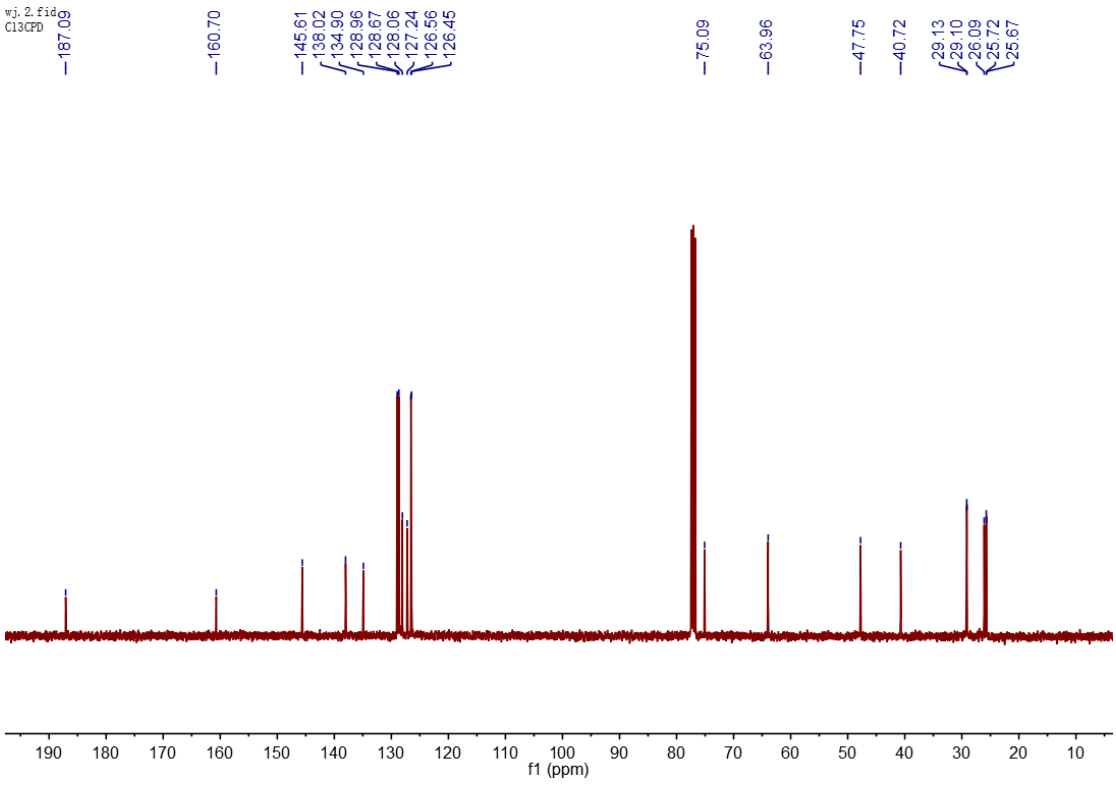

0.99
7.91
1.98
1.03
0.89
1.01
1.00
1.03
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

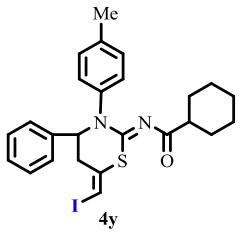

wj-98aa.2.fid
C13CPD
169.38
163.22
143.97
142.89
137.62
134.03
133.18
132.06
131.90
129.25
128.83
128.40
128.27
127.81
126.44
99.99
64.20
40.49
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



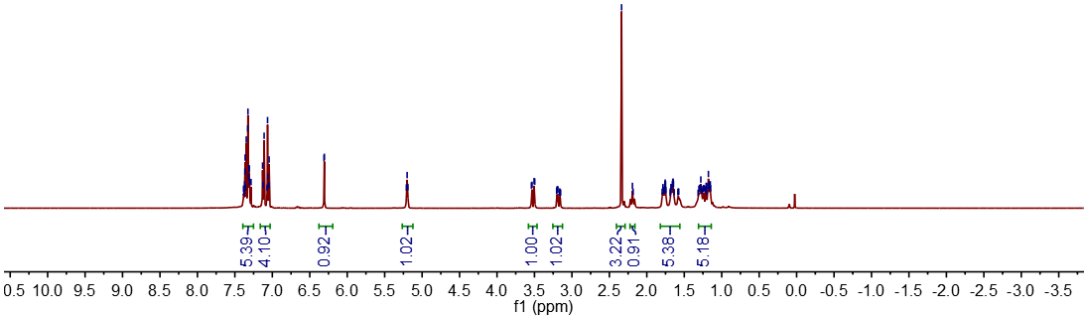
4x

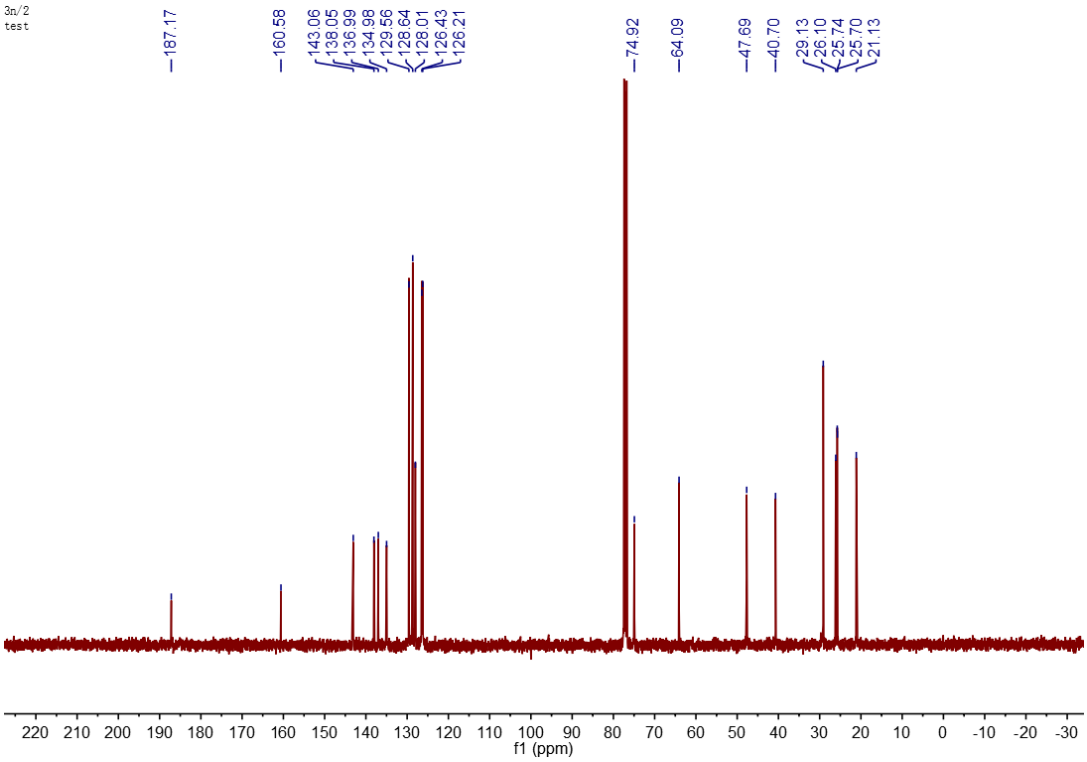


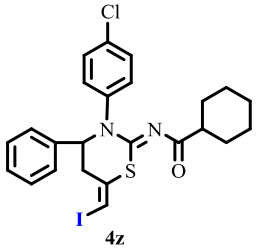



Me
N
N
S
O
I

4y

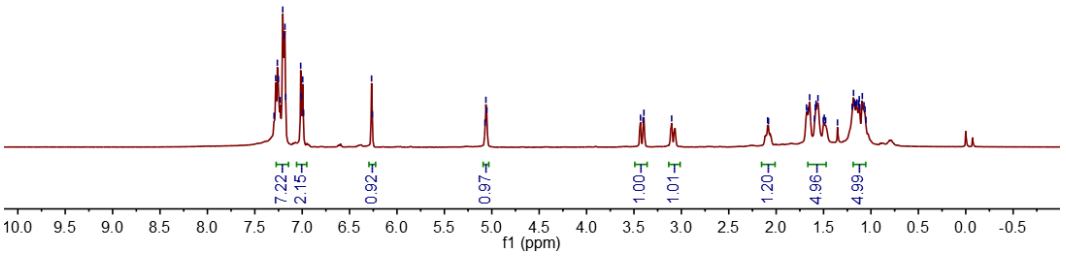

5.39
4.10
0.92
1.02
1.00
1.02
3.22
0.91
5.38
5.18
f1 (ppm)

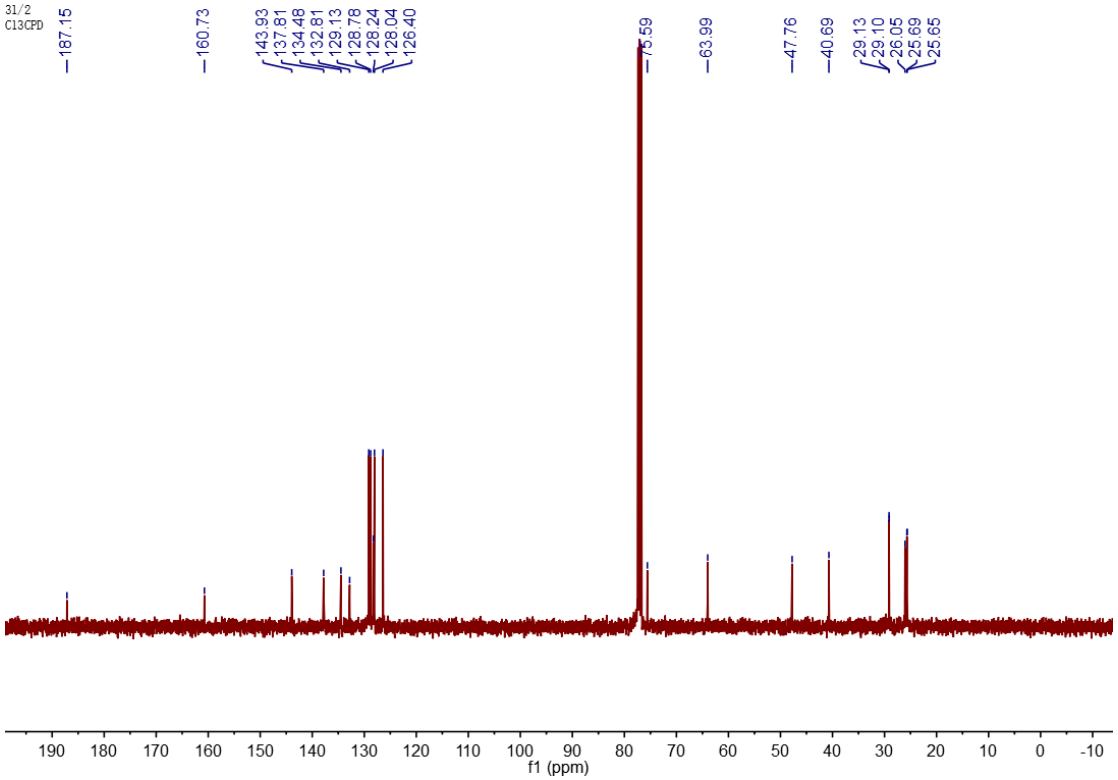

187.17
160.58
143.06
138.05
136.99
134.98
129.56
128.64
128.01
126.43
126.21
74.92
64.09
47.69
40.70
29.13
26.10
25.74
25.70
21.13
f1 (ppm)

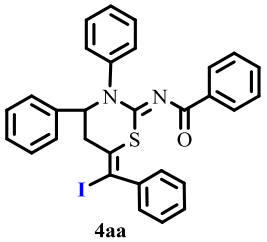

Cl
N
N
S
O
I

4z


31/1
PROTON
7.30
7.28
7.26
7.25
7.23
7.21
7.19
7.18
7.17
7.02
7.01
6.99
6.99
6.27
6.26
5.07
5.06
5.05
3.43
3.40
3.40
3.10
2.09
2.08
1.68
1.65
1.59
1.58
1.56
1.20
1.18
1.17
1.16
1.15
1.13
1.12
1.12
1.09

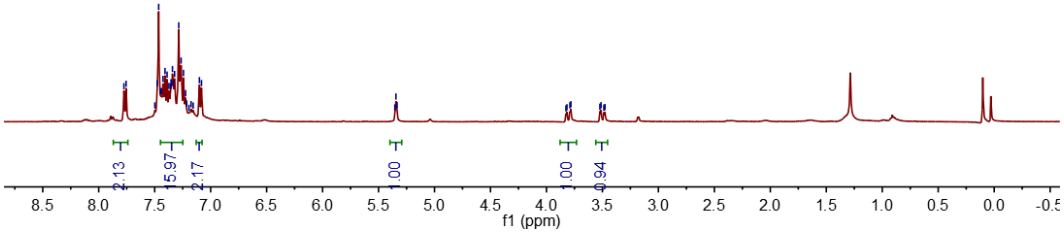

7.22
2.15
0.92
0.97
1.00
1.01
1.20
4.96
4.99
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

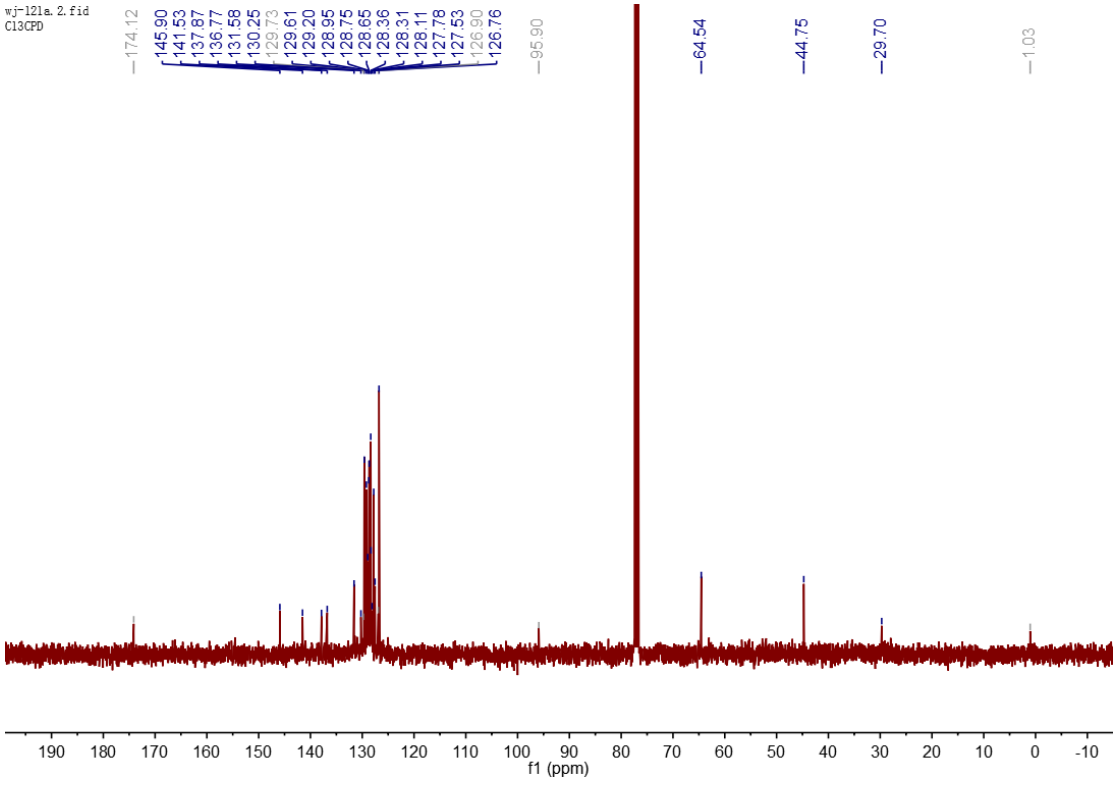

31/2
C13CPD
187.15
160.73
143.93
137.81
134.48
132.81
129.13
128.78
128.24
128.04
126.40
75.59
63.99
47.76
40.69
29.13
29.10
26.05
25.69
25.65
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

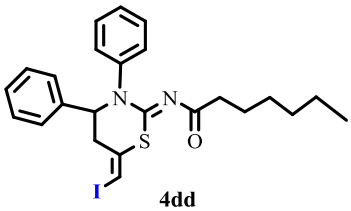


4aa

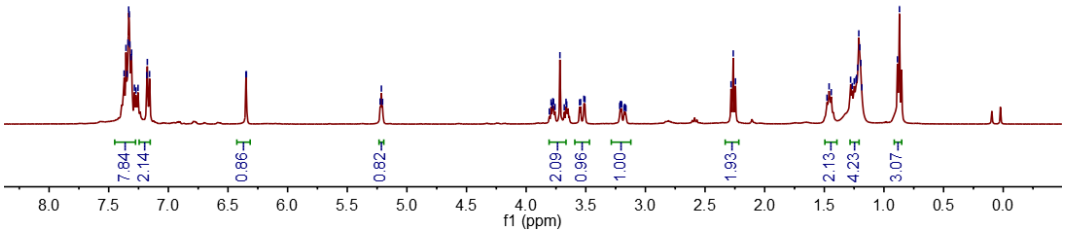

wj-121a.1.fid
PROTON
7.77
7.76
7.50
7.48
7.46
7.45
7.44
7.43
7.41
7.39
7.37
7.36
7.35
7.34
7.33
7.32
7.28
7.26
7.24
7.22
7.22
7.19
7.17
7.16
7.10
7.08
5.35
5.34
5.34
3.83
3.82
3.79
3.78
3.52
3.51
3.49
3.48

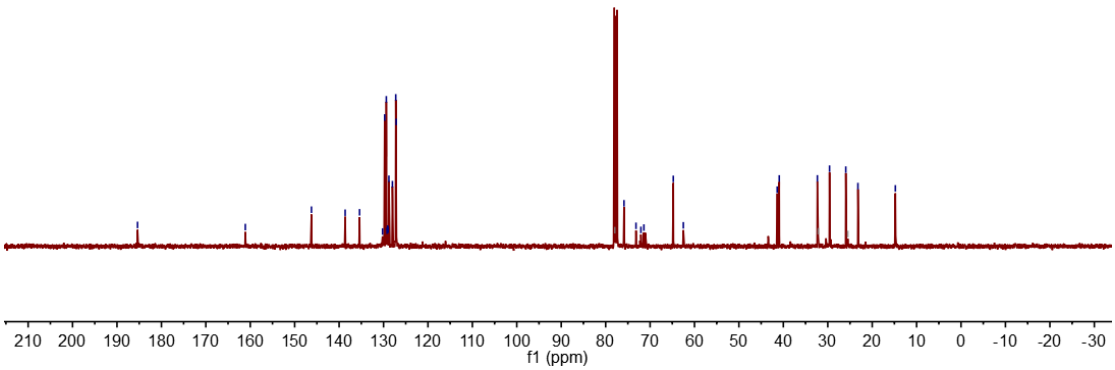

2.13
5.97
2.17
1.00
1.00
0.94
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

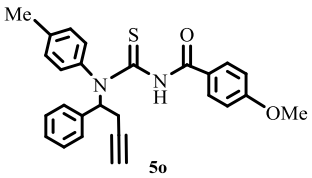

wj-121a.2.fid
C13CPD
174.12
145.90
141.53
137.87
136.77
131.58
130.25
129.73
129.61
129.20
128.95
128.75
128.65
128.36
128.31
128.11
127.78
127.53
126.90
126.76
95.90
64.54
44.75
29.70
1.03
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



4dd

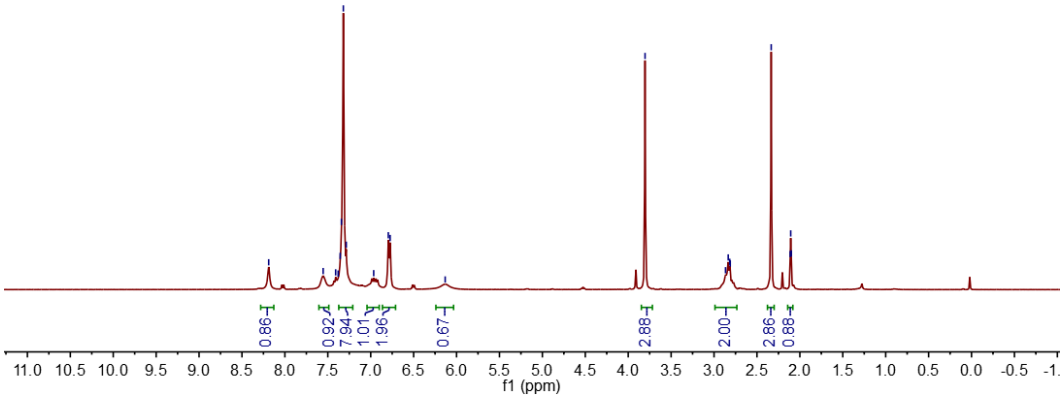


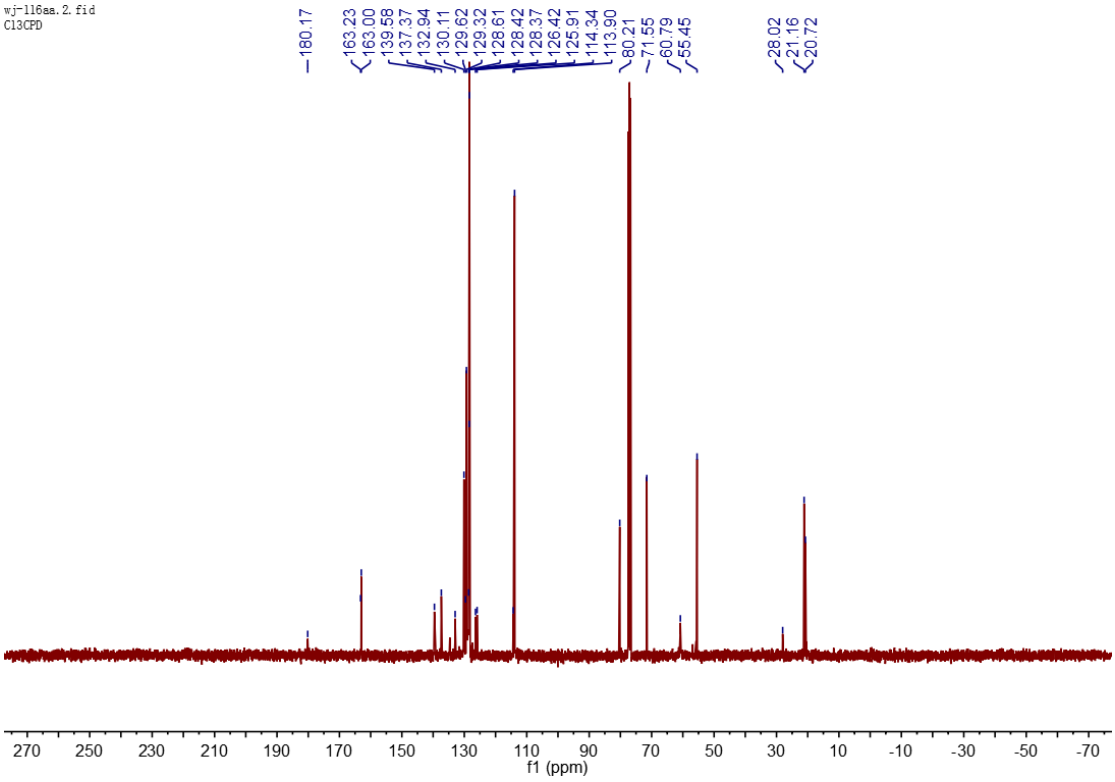


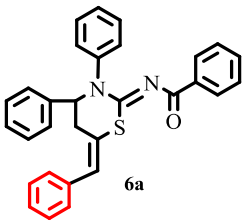

Me
S
O
N
N
H
OMe

5o


wj-116aa.1.fid
PROTON
8.19
7.55
7.41
7.38
7.36
7.34
7.32
7.28
6.97
6.80
6.77
6.13
3.80
2.87
2.83
2.82
2.81
2.33
2.11
2.11
2.10

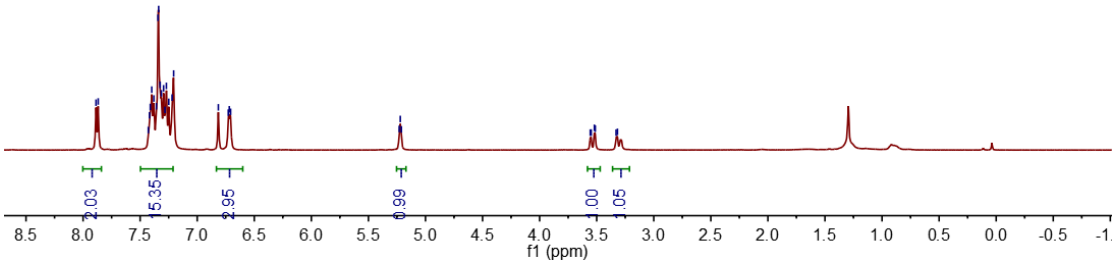

0.86
0.92
7.94
1.01
1.96
0.67
2.88
2.00
2.86
0.88
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)


wj-116aa.2.fid
C13CPD
180.17
163.23
163.00
139.58
137.37
132.94
130.11
129.62
129.32
128.61
128.42
128.37
126.42
125.91
114.34
113.90
80.21
71.55
60.79
55.45
28.02
21.16
20.72
270 250 230 210 190 170 150 130 110 90 70 50 30 10 -10 -30 -50 -70
f1 (ppm)

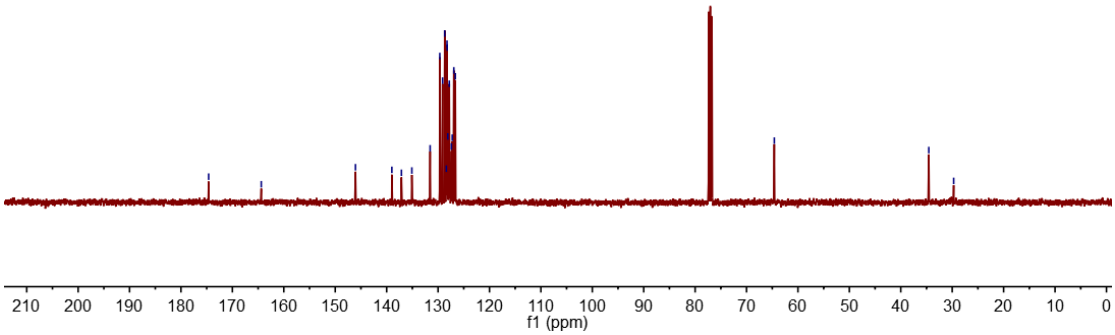

N
N
S
O

6a


wj-124a.1.fid
PROTON
7.89
7.87
7.43
7.42
7.41
7.40
7.38
7.36
7.34
7.34
7.32
7.31
7.29
7.28
7.27
7.25
7.22
7.21
6.81
6.73
6.72
6.71
5.23
5.22
5.21
3.56
3.55
3.52
3.51
3.33
3.32


2.03
15.35
2.95
0.99
1.00
1.05
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)


wj-124a.2.fid
C13CPD
174.62
164.39
146.06
138.98
137.12
135.09
131.54
129.66
129.12
128.71
128.39
128.26
128.23
128.11
127.82
127.40
127.24
126.93
126.65
64.60
34.55
29.71


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