Supporting Information

For

Copper(I)-Catalyzed Tandem C−N Coupling/Condensation Cyclization for the Synthesis of Benzothiadiazine 1‑Oxides

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Contents

1. General information

Unless otherwise specified, all tandem C−N coupling/condensation cyclization reactions were carried out under nitrogen atmosphere. The glass tubes were dried in an electric oven at 120 ºC. Chemicals were purchased from Kelong, Tansoole, Bidepharm and Aladdin chemical companies, and used as received. ^{1}H NMR (400 MHz) and ^{13}C NMR (101 MHz) spectra were determined on a Bruker Avance III 400 MHz instrument or on an Agilent Technologies 400 MHz instrument. The chemical shifts (δ) and coupling constants (J) were expressed in ppm and Hz, respectively. Coupling constants are reported in hertz with multiplicities denoted as s (singlet), d (doublet), t (triplet), dd (doublet of doublets), q (quartet), p (pentet), h (hextet), ddd (doublet of doublets of doublets), tt (triplet of triplets), td (triplet of doublets), dt (doublet of triplets), dq (doublet of quartets), ddp (doublet of doublets of pentets), m (multiplet), High-resolution mass spectra were recorded on a Shimadzu LCMS-IT-TOF instrument or on a Vion UPLC instrument.

2. Optimization process of reaction conditions of the model substrates

Table 1. Optimization of reaction temperature

Entry[a]	Catalyst	Base	Solvent	Temp(°C)	Yield[b] (%)
1	CuI	KOH	^{t}BuOH	80	85
2	CuI	KOH	^{t}BuOH	70	40
3	CuI	KOH	^{t}BuOH	60	Trace
4	CuI	KOH	^{t}BuOH	r.t	NR

[a] Conditions: **1a** (0.30 mmol), base (0.90 mmol), **2a** (0.90 mmol), CuI (0.03 mmol), ^{t}BuOH (3 mL), N_2, 16 h. [b] Yield of isolated product.

Table 2. Optimization of ratios of reactants

Entry[a]	Catalyst	Base	Solvent	1a(0.3mmol)/2a	Yield[b] (%)
1	CuI	KOH	^{t}BuOH	1:1	Trace
2	CuI	KOH	^{t}BuOH	1:1.5	Trace
3	CuI	KOH	^{t}BuOH	1:2	65
4	CuI	KOH	^{t}BuOH	1:2.5	84

[a] Conditions: **1a**/**2a**, KOH (3.0 equiv), CuI (0.1 equiv), ^{t}BuOH (3 mL), N_2, at 90 °C for 16 h. [b] Yield of isolated product.

Table 3. Optimization of reaction time

Entry[a]	Catalyst	Base	Solvent	Time(h)	Yield[b] (%)
1	CuI	KOH	^{t}BuOH	14	88
2	CuI	KOH	^{t}BuOH	12	78
3	CuI	KOH	^{t}BuOH	6	30

[a] Conditions: **1a** (0.3 mmol), **2a** (0.9 mmol), KOH (3.0 equiv), CuI (0.1 equiv), ^{t}BuOH (3 mL), N_2, 90 °C. [b] Yield of isolated product.

Table 4. Optimization of catalyst and amount of base KOH

Entry	Catalyst dosage	Base dosage	Yield[d](%)
1[a]	2.5 equiv	3.0equiv	78
2[a]	2.0 equiv	3.0 equiv	74
3[a]	1.5 equiv	3.0 equiv	65
4[a]	1.0 equiv	3.0 equiv	Trace
5[a]	0 equiv	3.0 equiv	NR
6[b]	3.0 equiv	2.5 equiv	84
7[b]	3.0 equiv	2.0 equiv	37
8[b]	3.0 equiv	1.5 equiv	Trace
9[b]	3.0 equiv	1.0 equiv	Trace
10[b]	3.0 equiv	0 equiv	NR
11[c]	0 equiv	0 equiv	NR

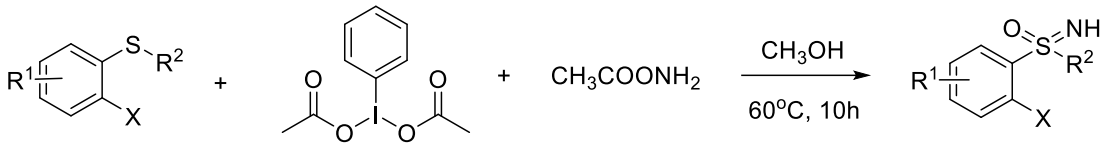
[a] Conditions: **1a** (0.3 mmol), **2a** (0.9 mmol), KOH (3.0 equiv), CuI, ^{t}BuOH (3 mL), N_2, at 90 °C for 16 h. [b] Conditions: **1a** (0.3 mmol), **2a** (0.9 mmol), KOH, CuI (3.0 equiv), ^{t}BuOH (3 mL), N_2, 90 °C, 16 h. [c] Conditions: **1a** (0.3 mmol), **2a** (0.9 mmol), ^{t}BuOH (3 mL), N_2, 90 °C, 16 h. [d] Yield of isolated product.

Based on the above results, the optimized conditions for this reaction: 90 ℃, **1a**:**2a** = 1.0 : 3.0, 16 h, 3.0 equiv. base KOH, 0.1 equiv. (10 mol%) CuI.

3. General procedure for the synthesis of sulfoximines 1

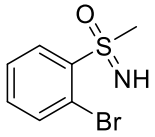
To a 50 mL round bottom flask was added *ortho*-bromoaryl organyl thioethers (1.0 equiv), (diacetoxyiodo)benzene (2.1 equiv), and ammonium acetate (3.0 equiv), and 15 mL anhydrous methanol. The mixture was stirred at 60 °C for 10 h. The progress of the reaction was monitored by TLC. After 10 h the reaction was stopped and then solvent was removed under reduced pressure. Saturated aqueous salt solution was added and the mixture was extracted with 15 mL ethyl acetate for three times. The combined organic solution was dried over anhydrous magnesium sulfate, filtered, and condensed on a rotary evaporator under reduced pressure to give the crude product. The crude product was purified by silica gel column chromatography by gradient elution with n-

hexane:ethyl acetate = 3:1 to afford the corresponding sulfoximines. All the physical data of the known compounds were in agreement with those reported in the literatures.



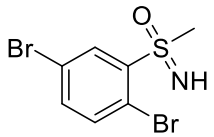
4. Characterization data of sulfoximines 1

(2-bromophenyl)(imino)(methyl)-λ⁶-sulfanone (1a)[1].



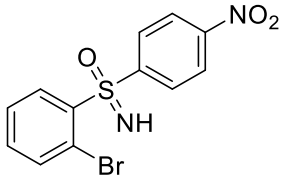
Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving yellow solid. CAS: 833459-47-5. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.23 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.75 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.50 (td, *J* = 7.6, 1.3 Hz, 1H), 7.42 (td, *J* = 7.6, 1.8 Hz, 1H), 3.32 (s, 3H), 2.70 (s, 1H).

(2,5-dibromophenyl)(imino)(methyl)-λ⁶-sulfanone (1b).



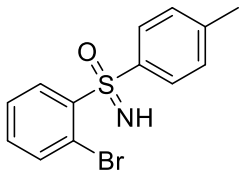
Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.35 (q, *J* = 2.0 Hz, 1H), 7.63 – 7.49 (m, 2H), 3.31 (t, *J* = 1.7 Hz, 3H).

(2-bromophenyl)(imino)(4-nitrophenyl)-λ⁶-sulfanone (1c)[2].



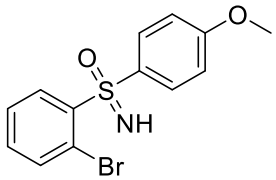
Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving yellow solid. CAS: 2909528-85-2. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.48 (dd, *J* = 8.0, 1.7 Hz, 1H), 8.36 – 8.17 (m, 4H), 7.66 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.57 (td, *J* = 7.7, 1.2 Hz, 1H), 7.44 (td, *J* = 7.7, 1.6 Hz, 1H).

(2-bromophenyl)(imino)(p-tolyl)-λ⁶-sulfanone (1d)[2].



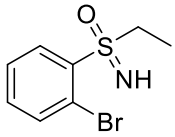
Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving yellow solid. CAS: 2909528-79-4. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.33 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.93 – 7.78 (m, 3H), 7.63 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.47 (d, *J* = 1.2 Hz, 1H), 7.39 – 7.27 (m, 4H), 2.41 (d, *J* = 2.8 Hz, 4H).

(2-bromophenyl)(imino)(4-methoxyphenyl)-λ^6-sulfanone (1e)[2].



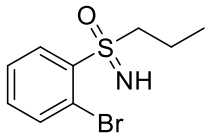
Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving yellow solid. CAS: 2909528-81-8. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.30 (dd, *J* = 8.0, 1.7 Hz, 1H), 8.01 – 7.93 (m, 2H), 7.63 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.45 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.34 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.02 – 6.92 (m, 2H), 3.85 (s, 3H).

(2-bromophenyl)(ethyl)(imino)-λ^6-sulfanone (1f)[3].



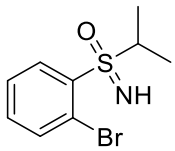
Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving yellow oil. CAS: 2059937-30-1. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.25 – 7.38 (m, 1H), 3.69 – 3.34 (m, 0H), 1.25 (t, *J* = 7.4 Hz, 1H).

(2-bromophenyl)(imino)(propyl)-λ^6-sulfanone (1g)[3].



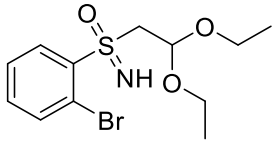
Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving yellow oil. CAS: 2827021-07-6. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.22 – 7.39 (m, 1H), 3.44 (ddd, *J* = 25.6, 10.4, 5.7 Hz, 0H), 0.98 (t, *J* = 7.5 Hz, 1H).

(2-bromophenyl)(imino)(isopropyl)-λ^6-sulfanone (1h)[3].



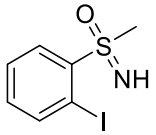
Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving white solid. CAS: 2092067-06-4. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.54 (s, 1H), 7.33 (d, *J* = 1.6 Hz, 2H), 7.25 (d, *J* = 1.3 Hz, 2H), 3.49 (s, 1H), 1.34 (d, *J* = 6.7 Hz, 21H).

(2-bromophenyl)(2,2-diethoxyethyl)(imino)-λ^6-sulfanone (1i)[4].



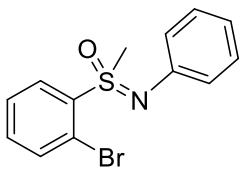
Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving yellow oil. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.17 (dt, *J* = 7.9, 1.8 Hz, 1H), 7.72 (dq, *J* = 7.8, 1.4 Hz, 1H), 7.50 – 7.36 (m, 2H), 4.98 (ddt, *J* = 6.6, 5.0, 1.4 Hz, 1H), 3.92 (ddt, *J* = 14.3, 6.0, 1.4 Hz, 1H), 3.73 (ddt, *J* = 14.3, 4.9, 1.4 Hz, 1H), 3.51 (ddddd, *J* = 28.8, 14.5, 9.1, 7.2, 1.4 Hz, 3H), 3.40 – 3.30 (m, 1H), 0.98 (dtt, *J* = 61.2, 7.1, 1.4 Hz, 6H).

imino(2-iodophenyl)(methyl)-λ^6-sulfanone (1j)[5].



Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving yellow oil. CAS: 1374991-59-9. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.20 (ddt, *J* = 72.0, 7.8, 1.5 Hz, 1H), 7.53 (tq, *J* = 7.8, 1.1 Hz, 1H), 7.24 – 7.16 (m, 1H), 3.44 – 3.08 (m, 1H).

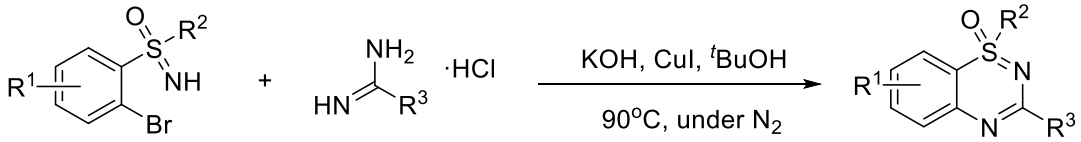
(2-bromophenyl)(methyl)(phenylimino)-λ^6-sulfanone (1k)[10]



According to literature reports,[10] the crude product was purified using n-hexane and ethyl acetate on a silica gel column to obtain a white solid. CAS: 1622220-25-0. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.30 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.68 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.53 – 7.44 (m, 1H), 7.43 – 7.34 (m, 1H), 7.16 – 7.06 (m, 2H), 7.04 – 6.99 (m, 2H), 6.92 – 6.86 (m, 1H), 3.47 (s, 3H).

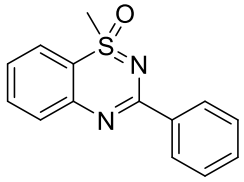
5. General procedure for the synthesis of Benzothiadiazine 1-Oxides 3.

To a 25 mL dry testing tube were added *ortho*-haloaryl organyl NH-sulfoximine (**1**, 0.3 mmol), amidinium chlorides (**2**, 0.9 mmol), CuI (0.03 mmol), KOH (0.6 mmol), and ^{t}BuOH (3 mL). The testing tube was sealed with a sleeve rubber stopper and then it is excavated and refilled with nitrogen for three cycles. The testing tube was then put on a 90 ^{o}C preheated oil bath pot and stirred at 90 ℃, and the reaction progress was monitored by TLC. After the reaction is complete, the reaction mixture was cooled to room temperature, and the solvent was removed under reduced pressure. The residual mixture was added saturated NaCl solution and extracted by ethyl acetate (15 mL) for three times. The combined organic solution was dried over anhydrous magnesium sulfate and filtered and condensed on a rotary evaporator under reduced pressure. The resulting crude product was subjected to column chromatography on silica gel (200-300 mesh) using a gradient elution with n-hexane: ethyl acetate as the eluent to afford the desired product **3**.



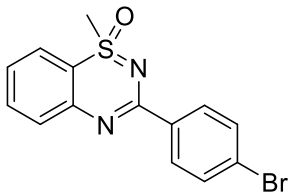
6. Characterization data of Benzothiadiazine 1-Oxides 3.

1-methyl-3-phenyl-λ^{6}-benzo[*e*][1,2,4]thiadiazine 1-oxide (3aa)[6].



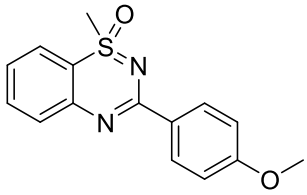
Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving white solid (75.3 mg, 98% yield). CAS: 1956357-52-0. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.43 – 8.33 (m, 1H), 7.86 – 7.77 (m, 1H), 7.74 – 7.61 (m, 1H), 7.46 – 7.40 (m, 1H), 3.55 (s, 1H).^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.99, 147.46, 137.36, 135.11, 131.18, 128.99, 128.61, 128.29, 126.35, 123.65, 113.04, 47.21.

3-(4-bromophenyl)-1-methyl-λ^{4}-benzo[*e*][1,2,4]thiadiazine-1-oxide (3ab)[6].



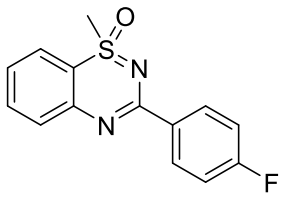
Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving white solid (45.3 mg, 45% yield). CAS: 1956357-54-2. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.25 (dq, *J* = 7.7, 1.0 Hz, 2H), 7.81 (dq, *J* = 8.0, 1.0 Hz, 1H), 7.75 – 7.67 (m, 1H), 7.63 – 7.54 (m, 3H), 7.46 – 7.38 (m, 1H), 3.55 (t, *J* = 0.9 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.96, 147.31, 136.38, 135.20, 131.43, 130.22, 129.01, 126.56, 125.91, 123.69, 113.09, 47.22.

3-(4-methoxyphenyl)-1-methyl-λ^{4}-benzo[*e*][1,2,4]thiadiazine-1-oxide (3ac)[6].



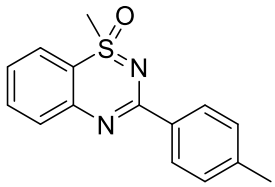
Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving white solid (74.6 mg, 87% yield). CAS: 2404654-43-7. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.37 – 8.31 (m, 1H), 7.79 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.70 – 7.64 (m, 0H), 7.58 (dd, *J* = 8.4, 1.3 Hz, 0H), 7.40 – 7.33 (m, 0H), 6.98 – 6.92 (m, 1H), 3.86 (d, *J* = 1.1 Hz, 1H), 3.52 (d, *J* = 0.9 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.07, 157.50, 147.55, 134.85, 130.22, 129.77, 128.60, 125.68, 123.47, 113.39, 112.68, 55.32, 46.99.

3-(4-fluorophenyl)-1-methyl-λ^{4}-benzo[*e*][1,2,4]thiadiazine-1-oxide (3ad).



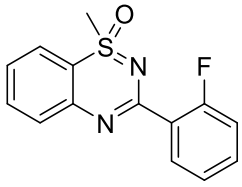
Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving white solid (46.0 mg, 56% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.43 – 8.36 (m, 1H), 7.82 (dd, *J* = 7.9, 1.4 Hz, 0H), 7.71 (ddd, *J* = 8.5, 7.1, 1.5 Hz, 1H), 7.61 (dd, *J* = 8.2, 1.2 Hz, 0H), 7.45 – 7.38 (m, 0H), 7.12 (t, *J* = 8.7 Hz, 1H), 3.55 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.22, 163.72, 156.96, 147.24, 135.23, 130.81, 128.84, 126.43, 123.67, 115.13, 112.89, 47.19. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -109.63. IR (thin film) ν_{max} (cm^{-1}): 3433, 2958, 2829, 2717, 2342, 1609, 1363, 1146, 856, 774, 549, 519. HRMS (ESI): [M+H]$^{+}$calculated for $C_{14}H_{12}FN_2OS^{+}$: 275.0649; found: 275.0649.

1-methyl-3-(p-tolyl)-λ^{4}-benzo[*e*][1,2,4]thiadiazine-1-oxide (3ae)[6].



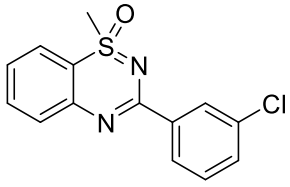
Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving white solid (72.1 mg, 88% yield). CAS: 1956357-53-1. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.29 – 8.24 (m, 1H), 7.81 (dd, *J* = 8.0, 1.4 Hz, 0H), 7.69 (ddd, *J* = 8.5, 7.1, 1.5 Hz, 1H), 7.61 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.39 (ddd, *J* = 8.1, 7.1, 1.3 Hz, 1H), 7.28 – 7.22 (m, 1H), 3.53 (s, 2H), 2.41 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.89, 146.45, 141.42, 135.35, 134.93, 129.37, 128.53, 128.33, 126.69, 124.88, 114.38, 45.55, 21.51.

3-(2-fluorophenyl)-1-methyl-λ^{4}-benzo[*e*][1,2,4]thiadiazine-1-oxide (3af).



Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving white solid (69.1 mg, 84% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.95 (d, *J* = 1.9 Hz, 1H), 7.81 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.64 (ddd, *J* = 33.1, 7.8, 1.4 Hz, 2H), 7.50 – 7.35 (m, 2H), 7.23 – 7.07 (m, 2H), 3.55 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 161.13, 158.62, 155.29, 145.86, 134.07, 130.33, 127.86, 125.79, 122.85, 122.45, 115.81, 111.69, 45.97. IR (thin film) ν_{max} (cm^{-1}): 3446, 2959, 2830, 2717, 2371, 1611, 1362, 1141, 851, 774, 547, 511. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -112.99. HRMS (ESI): [M+H]$^{+}$calculated for $C_{14}H_{12}FN_2OS^{+}$: 275.0649; found: 275.0649.

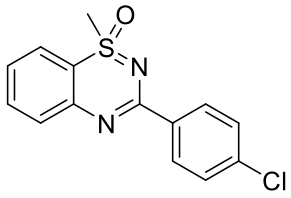
3-(3-chlorophenyl)-1-methyl-λ^{4}-benzo[*e*][1,2,4]thiadiazine-1-oxide (3ag).



Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving yellow solid (57.6 mg, 66% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.38 (t, J = 1.9 Hz, 1H), 8.27 (dt, *J* = 7.7, 1.4 Hz, 1H), 7.83 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.72 (ddd, *J* = 8.5, 7.1, 1.5 Hz, 1H), 7.62 (dd, *J* = 8.4, 1.3 Hz, 1H), 7.47 – 7.35 (m, 3H), 3.56 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.53, 147.20, 139.27, 135.20, 134.34, 131.01, 129.47, 128.68, 126.68, 123.64, 113.18, 47.19. IR (thin film) ν_{max} (cm^{-1}): 3432, 2959, 2826, 2781, 2718, 2367, 1621,

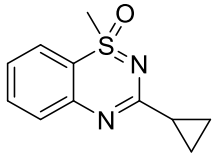
1362, 1138, 854, 774, 518, 549. HRMS (ESI): $[M+H]^+$calculated for $C_{14}H_{12}ClN_2OS^+$: 291.0353; found: 291.0353.

3-(4-chlorophenyl)-1-methyl-λ⁴-benzo[*e*][1,2,4]thiadiazine-1-oxide (3ah)[6].



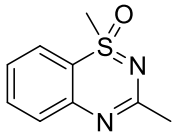
Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving white solid (58.4 mg, 67% yield). CAS: 2404654-48-2. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.36 – 8.28 (m, 1H), 7.81 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.71 (ddd, *J* = 8.6, 7.1, 1.5 Hz, 1H), 7.60 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.46 – 7.36 (m, 2H), 3.55 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.77, 147.23, 137.20, 135.83, 135.11, 129.90, 128.91, 128.38, 126.44, 123.59, 112.98, 47.13.

3-cyclopropyl-1-methyl-λ⁴-benzo[*e*][1,2,4]thiadiazine-1-oxide (3ai)[6].



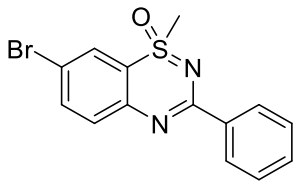
Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving white solid (58.1 mg, 88% yield). CAS: 2404654-98-2. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.71 (s, 1H), 7.63 (s, 1H), 7.44 (d, *J* = 1.1 Hz, 2H), 7.32 (s, 1H), 3.40 (s, 11H), 1.24 (s, 3H), 1.14 (d, *J* = 12.1 Hz, 1H), 0.91 (d, *J* = 8.1 Hz, 4H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.27, 147.18, 135.12, 127.68, 125.48, 123.60, 112.87, 46.97, 19.28, 9.44, 8.54.

1,3-dimethyl-λ⁴-benzo[*e*][1,2,4]thiadiazine-1-oxide (3aj)[7].



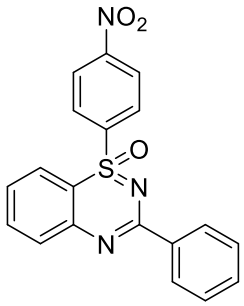
Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving yellow solid (43.7 mg, 75% yield). CAS: 501359-05-3. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.76 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.69 – 7.64 (m, 1H), 7.45 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.41 – 7.35 (m, 1H), 3.46 (d, *J* = 0.8 Hz, 3H), 2.38 (d, *J* = 0.8 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.02, 146.86, 135.26, 127.84, 126.21, 123.61, 112.17, 46.98, 27.61.

7-bromo-1-methyl-3-phenyl-λ⁴-benzo[*e*][1,2,4]thiadiazine-1-oxide (3ba).



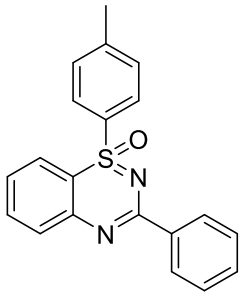
Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving white solid (96.4 mg, 96% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.40 – 8.34 (m, 1H), 7.93 (d, *J* = 2.2 Hz, 0H), 7.52 (s, 0H), 3.57 (s, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.26, 145.49, 137.37, 136.08, 130.53, 129.94, 127.73, 127.44, 125.09, 117.24, 113.12, 46.33. IR (thin film) ν_{max} (cm^{-1}): 3432, 2952, 2833, 2781, 2714, 2682, 2363, 1619, 1359, 1149, 833, 777, 620, 543, 515. HRMS (ESI): [M+H]$^{+}$calculated for $C_{14}H_{12}BrN_2OS^{+}$: 334.9848; found: 334.9859.

1-(4-nitrophenyl)-3-phenylbenzo[*e*][1,2,4]thiadiazine-1-oxide (3ca).



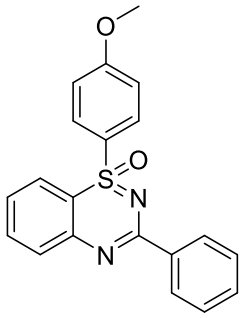
Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving yellow solid (59.9 mg, 55% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.45 – 8.38 (m, 1H), 8.10 – 8.04 (m, 1H), 7.72 – 7.68 (m, 0H), 7.54 – 7.44 (m, 1H), 7.34 (d, *J* = 4.0 Hz, 0H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.01, 149.79, 146.93, 145.69, 136.12, 134.51, 130.63, 128.98, 128.35, 127.84, 127.50, 126.01, 123.92, 123.68, 111.48. IR (thin film) ν_{max} (cm^{-1}): 3435, 2973, 2830, 2781, 2718, 2367, 1614, 1359, 1149, 861, 777, 539, 518. HRMS (ESI): [M+H]$^{+}$calculated for $C_{19}H_{14}N_3O_3S^{+}$: 364.0750; found: 364.0750.

3-phenyl-1-(p-tolyl)benzo[*e*][1,2,4]thiadiazine-1-oxide (3da)[8].



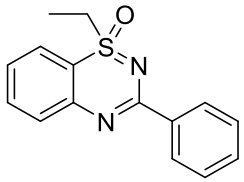
Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving white solid (74.7 mg, 75% yield). CAS:77198-20-0. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.46 – 8.38 (m, 1H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.62 (d, *J* = 16.2 Hz, 0H), 7.50 – 7.39 (m, 2H), 7.38 – 7.32 (m, 1H), 7.24 (d, *J* = 1.0 Hz, 0H), 2.43 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.16, 147.14, 145.23, 137.66, 134.36, 131.09, 130.06, 128.81, 128.72, 128.65, 128.27, 126.28, 124.85, 21.75.

1-(4-methoxyphenyl)-3-phenylbenzo[*e*][1,2,4]thiadiazine-1-oxide (3ea).



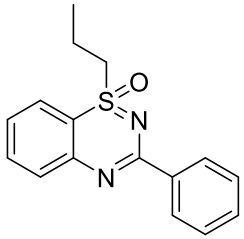
Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving yellow solid (57.4 mg, 55% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.49 – 8.41 (m, 1H), 7.88 – 7.80 (m, 1H), 7.68 (s, 0H), 7.52 – 7.43 (m, 2H), 7.32 – 7.28 (m, 1H), 7.12 – 7.03 (m, 1H), 4.06 – 3.66 (m, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.34, 157.46, 146.35, 137.07, 133.48, 131.13, 130.32 (d, *J* = 2.7 Hz), 127.99, 127.93, 127.54, 125.50, 124.03, 113.89 (d, *J* = 3.7 Hz), 55.21. IR (thin film) ν_{max} (cm^{-1}): 3435, 2963, 2826, 2784, 2718, 2371, 1611, 1362, 1145, 858, 770, 542, 518. HRMS (ESI): $[M+H]^{+}$calculated for $C_{20}H_{17}N_2O_2S^{+}$: 349.1005; found: 349.1005.

1-ethyl-3-phenyl-λ^{4}-benzo[*e*][1,2,4]thiadiazine-1-oxide (3fa)[6].



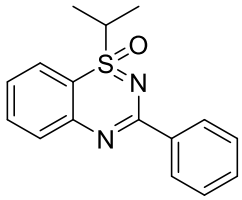
Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving white solid (48.6 mg, 60% yield). CAS:2404655-11-2. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.44 – 8.34 (m, 1H), 7.79 – 7.63 (m, 1H), 7.49 – 7.37 (m, 2H), 3.73 – 3.51 (m, 1H), 1.19 (t, *J* = 7.3 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.68, 148.64, 137.42, 135.19, 131.15, 128.89 (d, *J* = 3.8 Hz), 128.58, 128.26, 126.55, 126.31, 123.79, 52.65, 8.29.

3-phenyl-1-propyl-λ^{4}-benzo[*e*][1,2,4]thiadiazine-1-oxide (3ga).



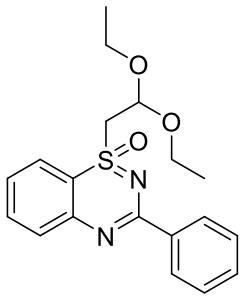
Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving yellow solid (73.2 mg, 86% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.43 – 8.35 (m, 1H), 7.79 – 7.61 (m, 2H), 7.52 – 7.36 (m, 2H), 3.58 (dddd, *J* = 41.4, 14.5, 10.6, 5.4 Hz, 1H), 1.39 – 1.20 (m, 1H), 0.97 (t, *J* = 7.4 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.46, 148.40, 137.44, 135.11, 131.12, 128.86, 128.57, 128.25, 126.25, 123.83, 110.71, 59.82, 17.32, 12.64. IR (thin film) ν_{max} (cm^{-1}): 3442, 2784, 2956, 2837, 2721, 2364, 1618, 1359, 1148, 861, 770, 546, 515. HRMS (ESI): $[M+H]^+$calculated for $C_{16}H_{17}N_2OS^+$: 285.1056; found: 285.1055.

1-isopropyl-3-phenyl-λ^4-benzo[*e*][1,2,4]thiadiazine-1-oxide (3ha)[9].



Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving yellow oil (45.2 mg, 53% yield). CAS:2412713-25-6. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.46 – 8.35 (m, 1H), 7.80 – 7.60 (m, 2H), 7.52 – 7.34 (m, 2H), 3.84 – 3.71 (m, 0H), 1.59 – 1.15 (m, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.95, 149.05, 137.40, 135.22, 131.15, 128.57, 128.55, 128.24, 126.14, 124.20, 109.08, 59.04, 16.96, 13.64.

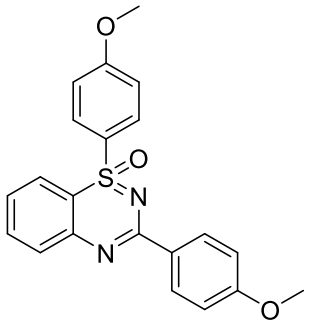
1-(2,2-diethoxyethyl)-3-phenyl-λ^4-benzo[*e*][1,2,4]thiadiazine-1-oxide (3ia).



Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving yellow oil (80.6 mg, 75% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.45 – 8.31 (m, 1H), 7.84 (dd, *J* = 8.0, 1.4 Hz, 0H),

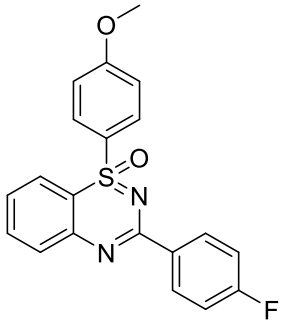
7.73 – 7.61 (m, 1H), 7.53 – 7.37 (m, 2H), 4.68 (dd, *J* = 6.8, 3.7 Hz, 0H), 4.03 (dd, *J* = 14.8, 6.8 Hz, 0H), 3.81 (dd, *J* = 14.9, 3.7 Hz, 0H), 3.61 – 3.36 (m, 1H), 3.02 (dd, *J* = 9.1, 7.0 Hz, 0H), 1.16 (td, *J* = 7.0, 0.8 Hz, 1H), 0.73 (td, *J* = 7.1, 0.9 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.94, 147.01, 136.52, 134.03, 130.19, 127.68, 127.36, 125.23, 123.93, 111.33, 97.27, 62.65, 61.66, 60.51, 14.32. IR (thin film) ν_{max} (cm^{-1}): 3421, 2952, 2833, 2784, 2718, 2367, 1607, 1366, 1142, 1065, 854, 777, 546, 518. HRMS (ESI): [M+H]$^+$calculated for $C_{19}H_{23}N_2O_3S^+$: 359.1424; found: 359.1425.

1,3-bis(4-methoxyphenyl)benzo[*e*][1,2,4]thiadiazine-1-oxide (3ec).



Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving white solid (85.1 mg, 75% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.46 – 8.34 (m, 1H), 7.84 – 7.78 (m, 1H), 7.65 – 7.57 (m, 1H), 7.42 (ddd, *J* = 7.9, 1.3, 0.7 Hz, 1H), 7.27 – 7.18 (m, 1H), 6.99 (ddq, *J* = 26.5, 8.0, 0.9 Hz, 2H), 3.87 (dt, *J* = 3.2, 1.0 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.28, 161.45, 157.21, 146.54, 133.44, 131.30, 130.31, 129.77, 129.60, 127.70, 125.06, 124.03, 113.89, 113.67, 112.83, 55.21, 54.79. IR (thin film) ν_{max} (cm^{-1}): 3435, 2956, 2837, 2788, 2721, 2367, 1614, 1366, 1145, 851, 774, 620, 536, 511. HRMS (ESI): [M+H]$^+$ calculated for $C_{21}H_{19}N_2O_3S^+$: 379.1111; found: 379.1119.

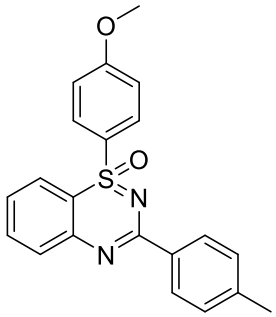
3-(4-fluorophenyl)-1-(4-methoxyphenyl)benzo[*e*][1,2,4]thiadiazine-1-oxide (3ed.)



Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving white solid (50.0 mg, 46% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.49 – 8.40 (m, 1H), 7.85 – 7.77 (m, 1H), 7.68 – 7.58 (m, 1H), 7.47 – 7.39 (m, 0H), 7.30 – 7.23 (m, 0H), 7.15 – 6.99 (m, 2H), 3.87 (dt, *J* = 3.9, 1.5 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 165.41, 163.40, 162.92,

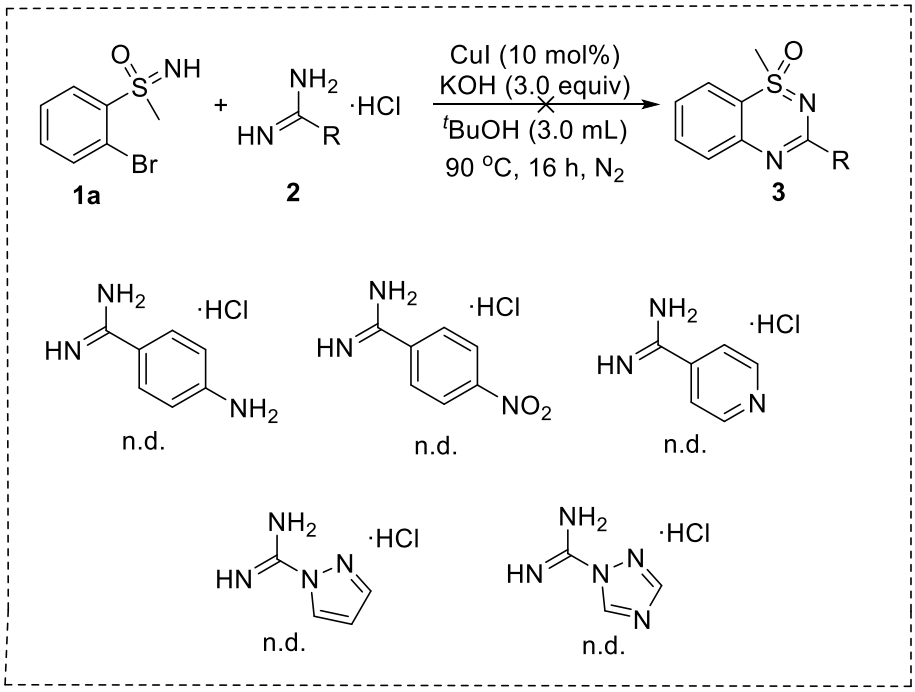
156.43, 146.26, 133.56, 130.34, 130.22, 130.13, 127.83, 114.56, 114.34, 113.95, 55.22. IR (thin film) ν_{max} (cm^{-1}): 3442, 2923, 2826, 2781, 2718, 2367, 1614, 1362, 1152, 840, 770, 546, 525. HRMS (ESI): $[M+H]^+$ calculated for $C_{20}H_{16}FN_2O_2S^+$: 367.0911; found: 367.0913.

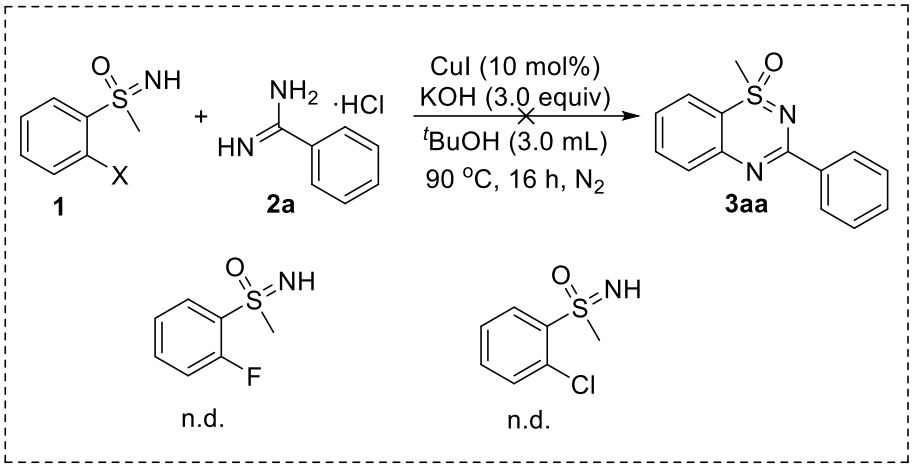
1-(4-methoxyphenyl)-3-(p-tolyl)benzo[*e*][1,2,4]thiadiazine-1-oxide (3ee).



Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving white solid (40.2 mg, 37% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.41 – 8.33 (m, 1H), 7.89 – 7.80 (m, 1H), 7.72 – 7.61 (m, 1H), 7.46 (s, 0H), 7.33 – 7.28 (m, 2H), 7.06 (dd, *J* = 9.1, 1.0 Hz, 1H), 3.91 (d, *J* = 1.0 Hz, 1H), 2.45 (s, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.30, 157.55, 146.48, 140.65, 134.33, 133.43, 131.29, 130.32, 128.30, 128.00, 127.85, 125.28, 124.03, 113.89, 113.83, 55.21, 20.94. IR (thin film) ν_{max} (cm^{-1}): 3442, 2952, 2883, 2781, 2718, 2367, 1607, 1362, 1142, 854, 770, 627, 529. HRMS (ESI): $[M+H]^+$ calculated for $C_{21}H_{19}N_2O_2S^+$: 363.1162; found: 363.1166.

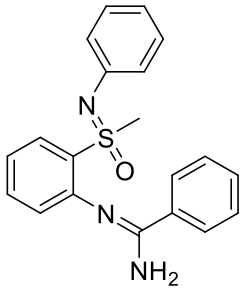
7.Unsuccessful substrates screened





8. Characterization data of compound 4

N'-(2-(S-methyl-N-phenylsulfonimidoyl)phenyl)benzimidamide 4



Following the general procedure, the crude product was purified over a silica gel column using n-hexane and ethyl acetate giving white solid (60.2 mg, 57% yield). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.29 – 8.23 (m, 1H), 7.87 (s, 2H), 7.57 – 7.46 (m, 4H), 7.25 (d, *J* = 9.9 Hz, 1H), 6.98 (t, *J* = 7.8 Hz, 2H), 6.83 – 6.72 (m, 3H), 4.35 (s, 2H), 3.53 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 146.05, 134.45, 132.34, 131.07, 128.80, 128.74, 127.05, 123.25, 122.65, 120.93, 42.36. IR (thin film) ν_{max} (cm^{-1}): 3442, 2959, 2830, 2780, 2714, 1611, 1355, 1145, 865, 777, 623, 543, 518.
HRMS (ESI): $[M+H]^+$calculated for $C_{20}H_{20}N_3OS^+$: 350.1322; found: 350.1321.

9. References

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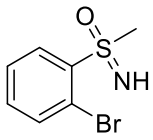
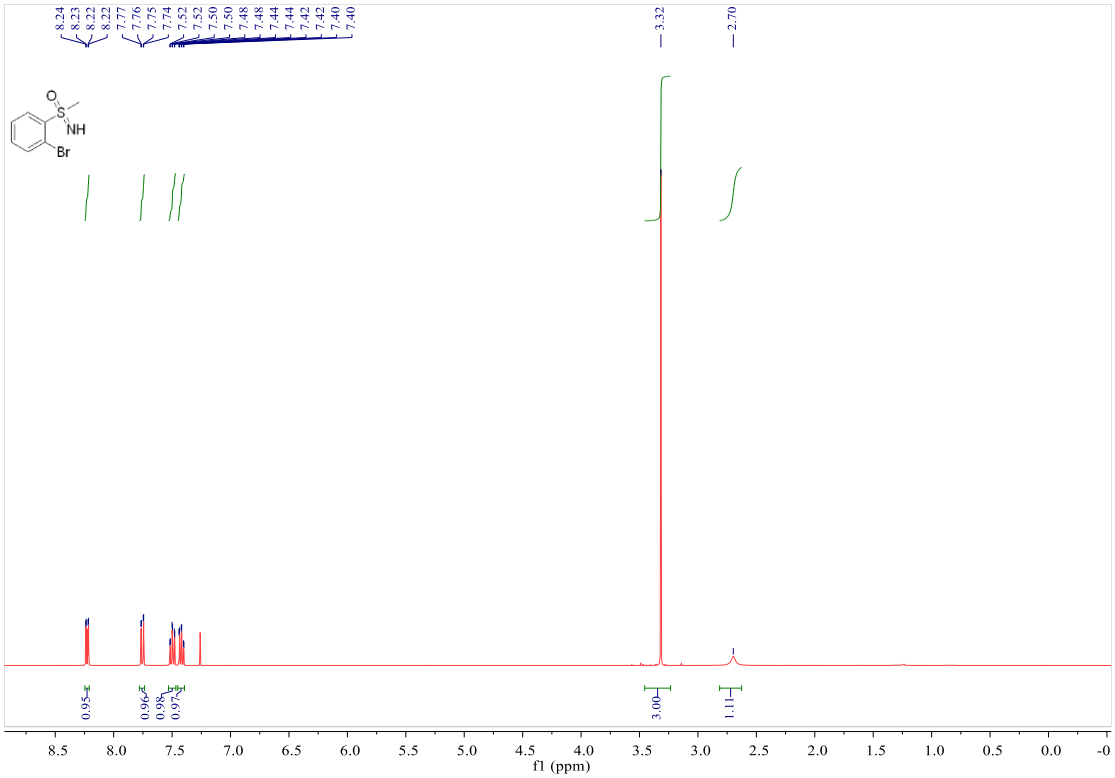
10. Electronic copies of ^{1}H and ^{13}C NMR, and HRMS Spectra of 1, 3 and 4

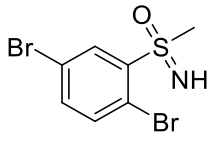
(2-bromophenyl)(imino)(methyl)-λ^{6}-sulfanone (1a)



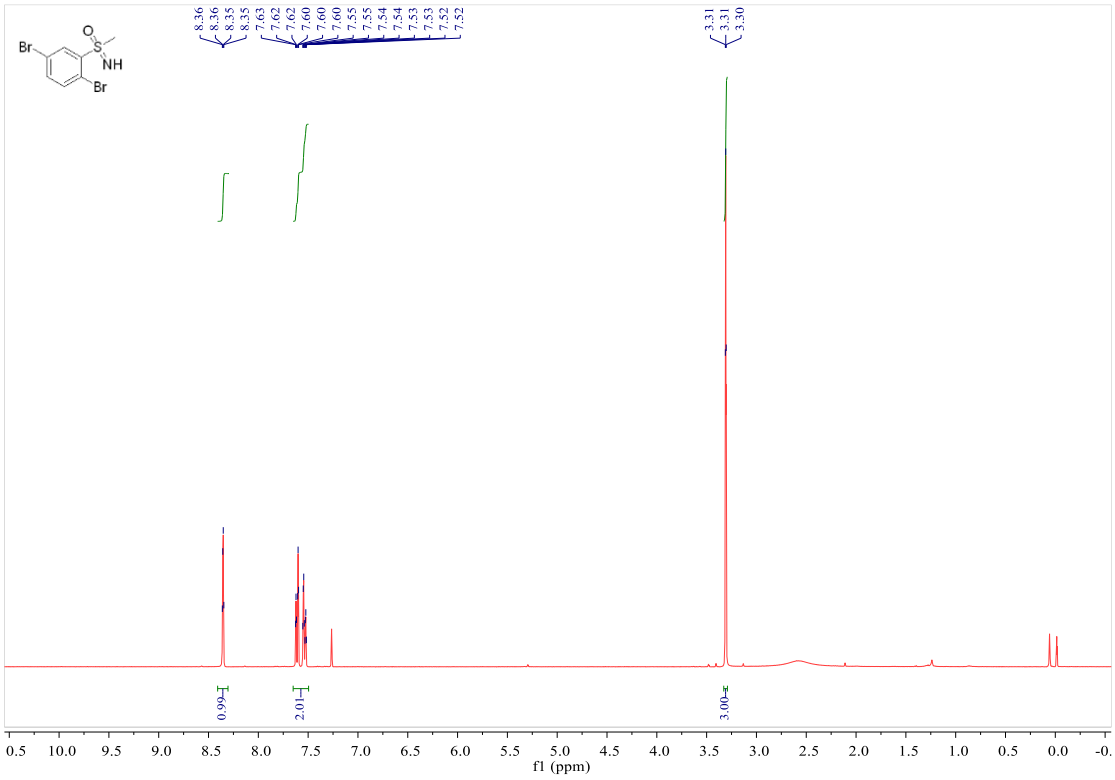
^{1}H NMR (400 MHz, $CDCl_3$)



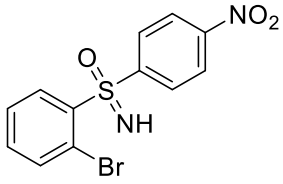
(2,5-dibromophenyl)(imino)(methyl)-λ^{6}-sulfanone (1b)



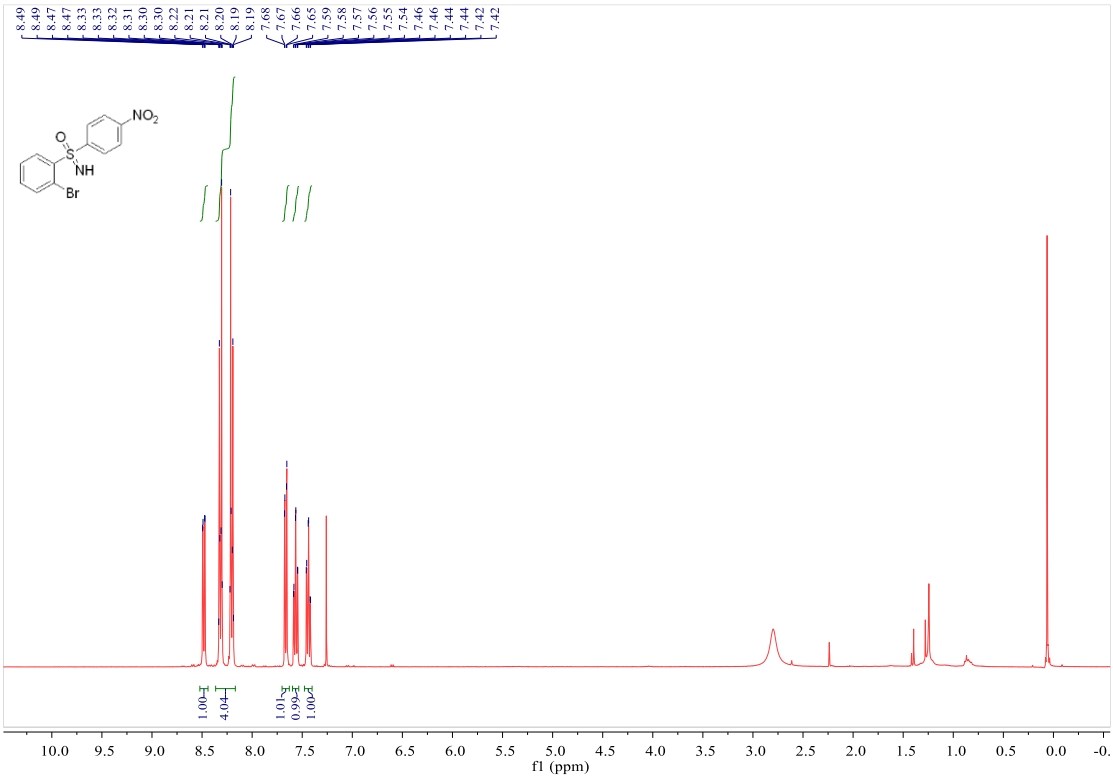
^{1}H NMR (400 MHz, $CDCl_3$)



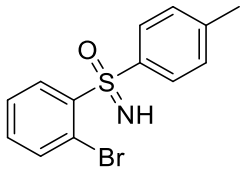
(2-bromophenyl)(imino)(4-nitrophenyl)-λ⁶-sulfanone (1c)



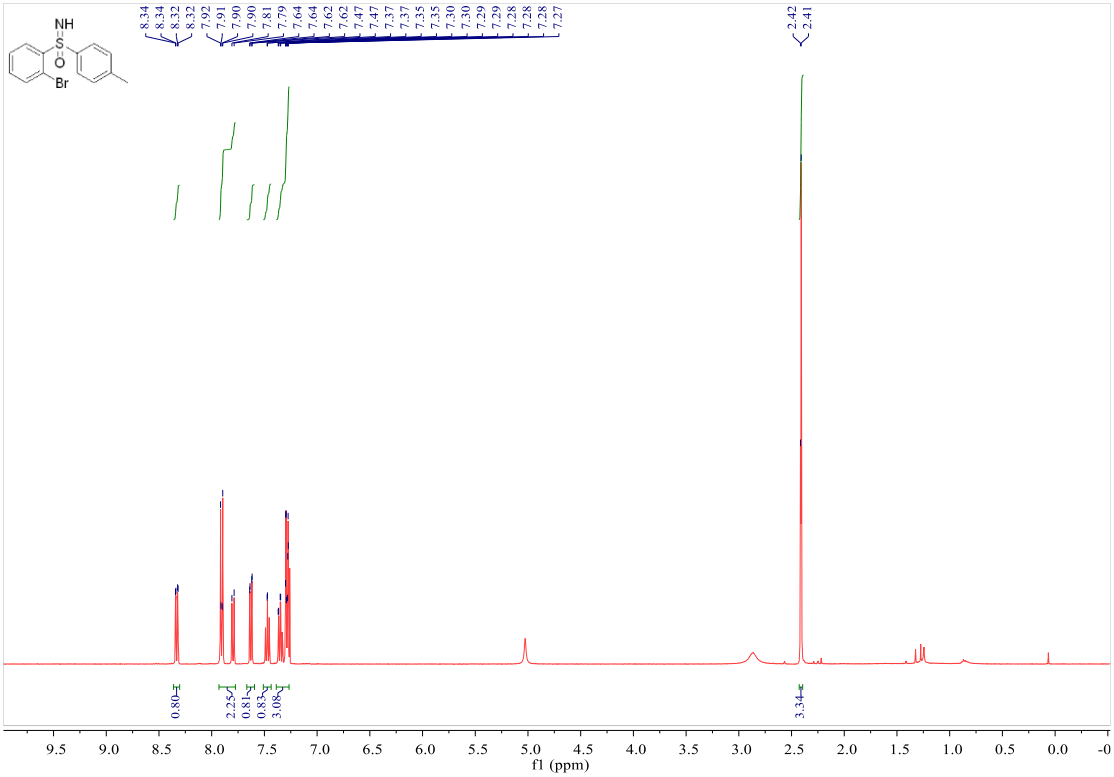
^{1}H NMR (400 MHz, $CDCl_3$)



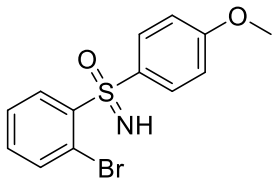
(2-bromophenyl)(imino)(p-tolyl)-λ^6-sulfanone (1d)



^{1}H NMR (400 MHz, $CDCl_3$)



(2-bromophenyl)(imino)(4-methoxyphenyl)-λ^6-sulfanone (1e)



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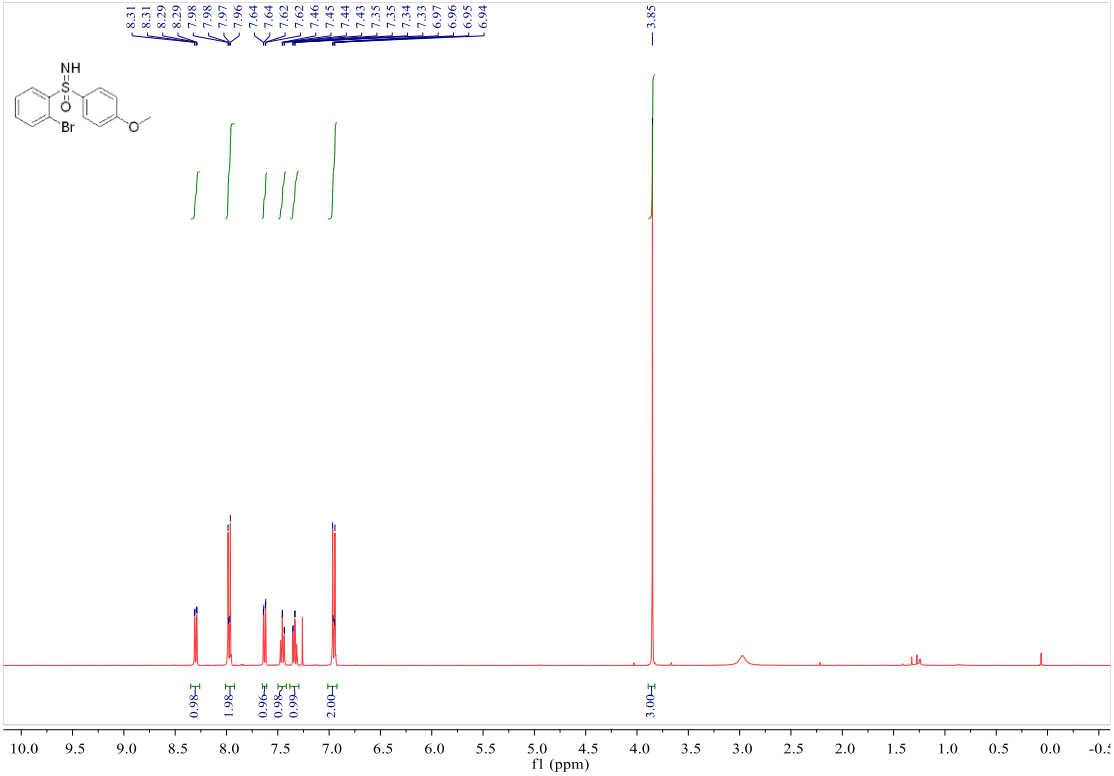
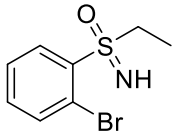


(2-bromophenyl)(ethyl)(imino)-λ^6-sulfanone (1f)



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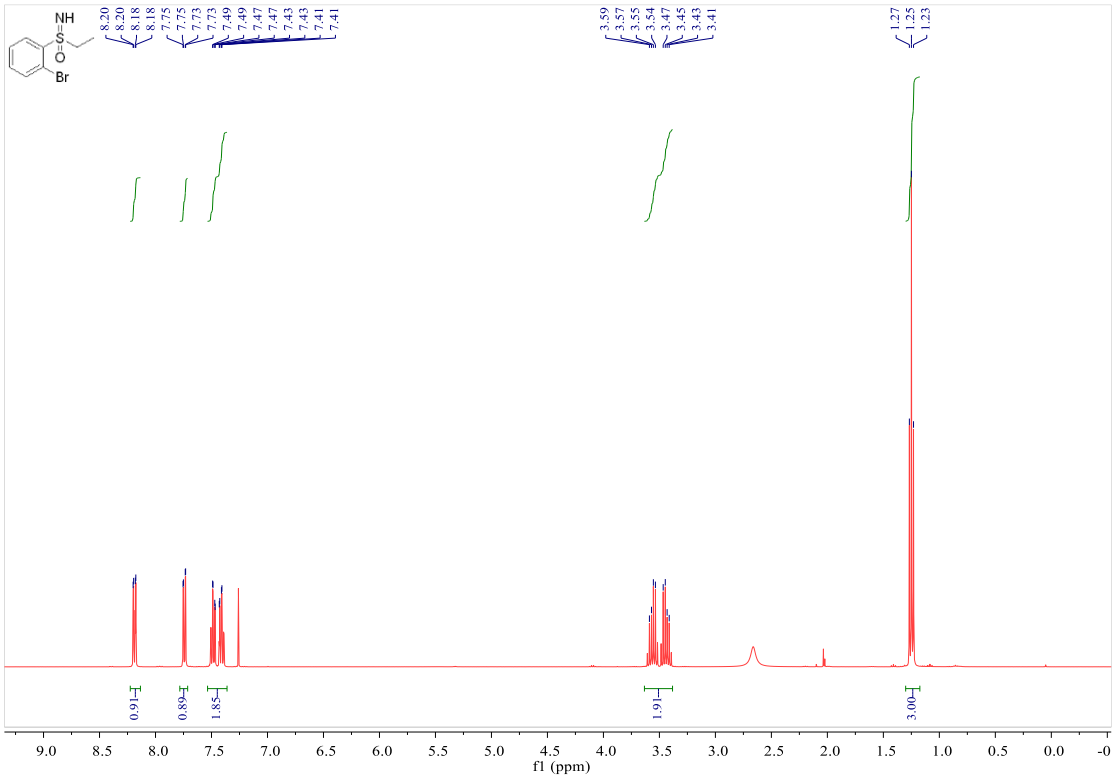
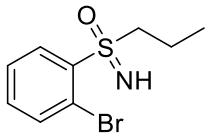


(2-bromophenyl)(imino)(propyl)-λ⁶-sulfanone (1g)



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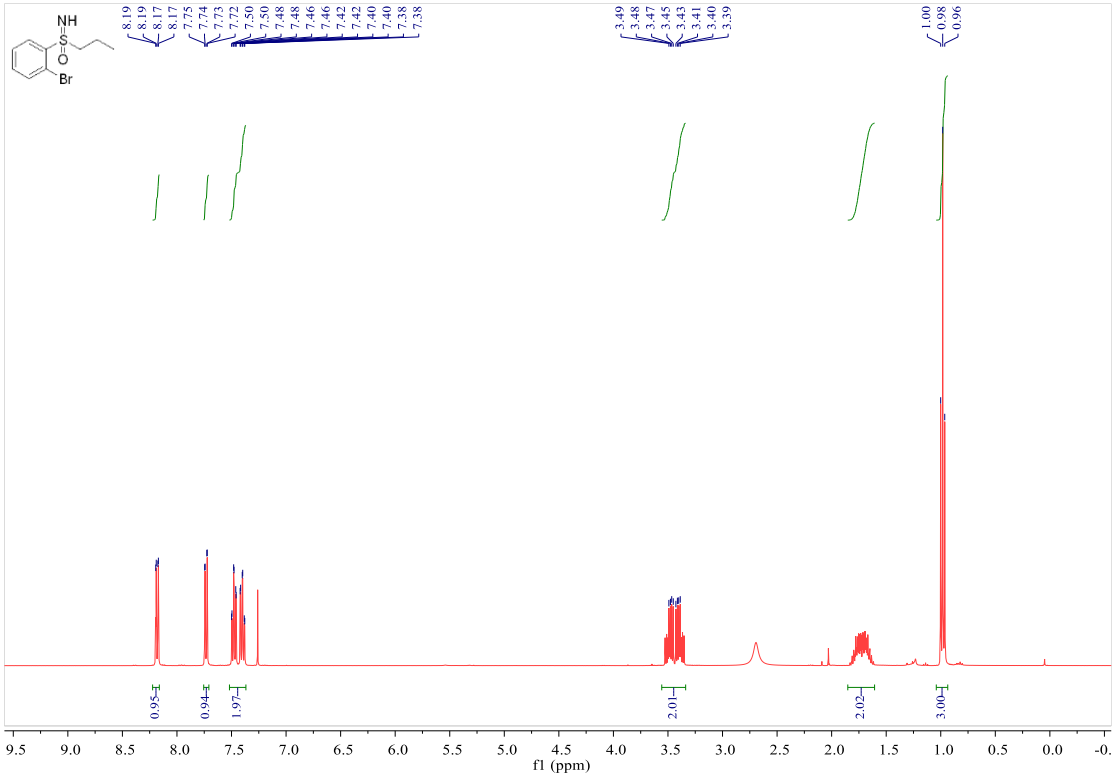
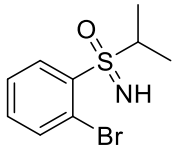
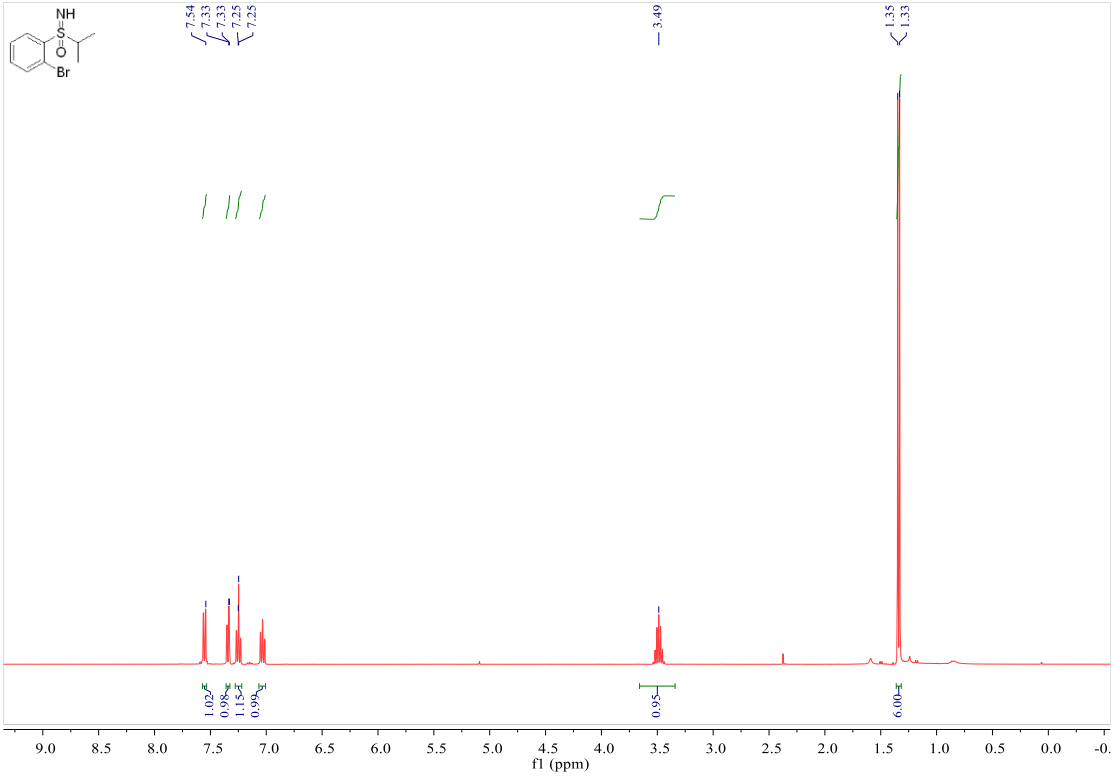


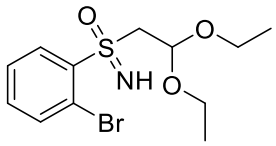
(2-bromophenyl)(imino)(isopropyl)-λ⁶-sulfanone (1h)



^{1}H NMR (400 MHz, $CDCl_3$)



(2-bromophenyl)(2,2-diethoxyethyl)(imino)-λ^6-sulfanone (1i)



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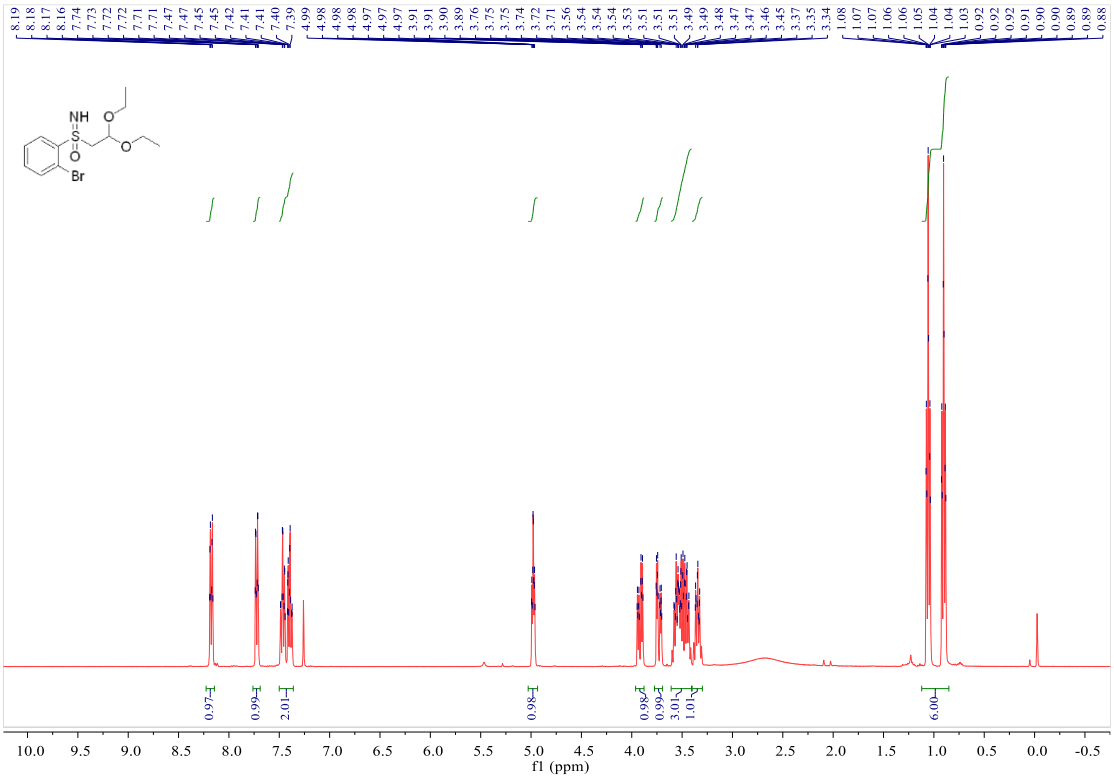
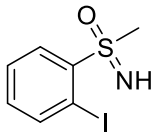


imino(2-iodophenyl)(methyl)-λ^6-sulfanone (1j)



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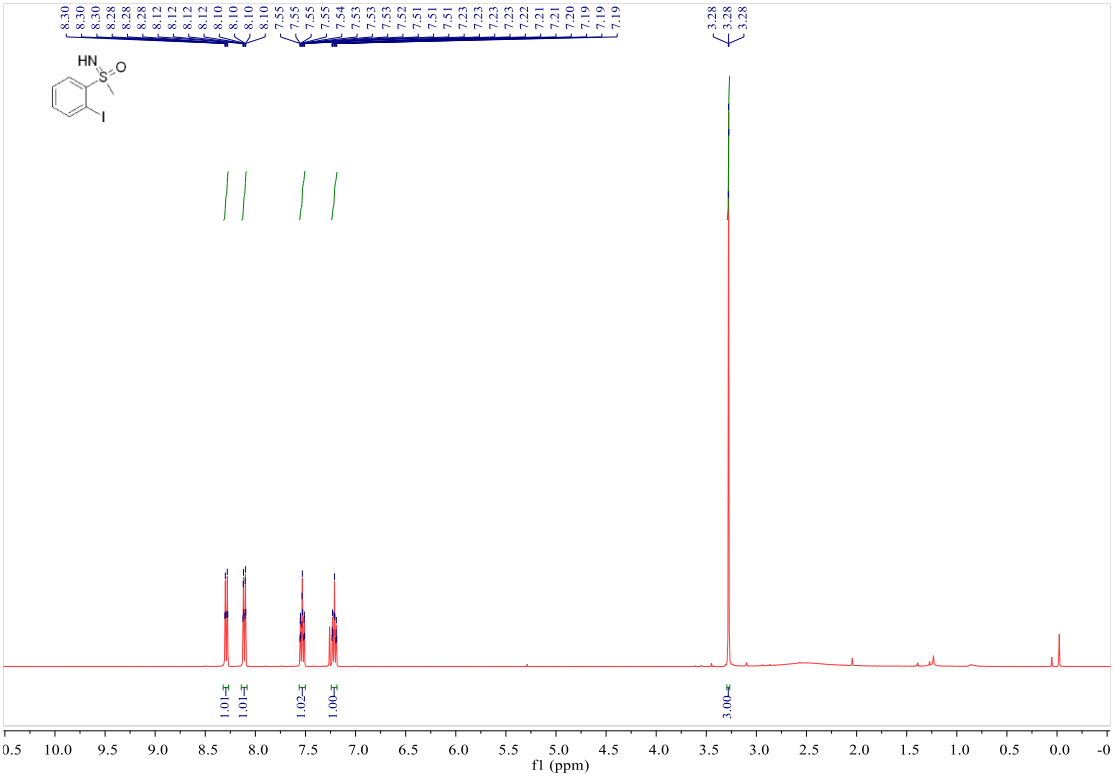
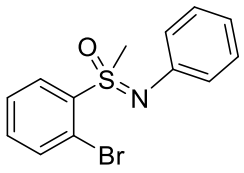


(2-bromophenyl)(methyl)(phenylimino)-λ^6-sulfanone(1k).



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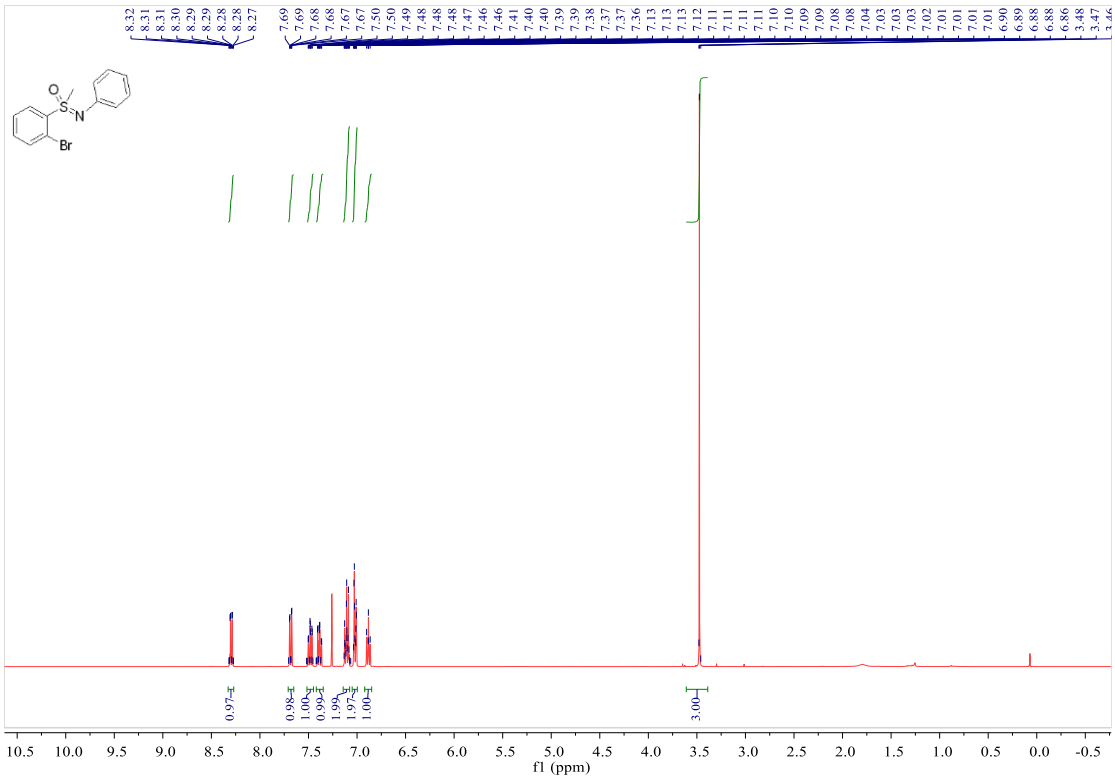
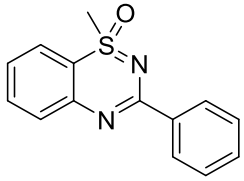


1-methyl-3-phenyl-λ^6-benzo[*e*][1,2,4]thiadiazine 1-oxide (3aa)



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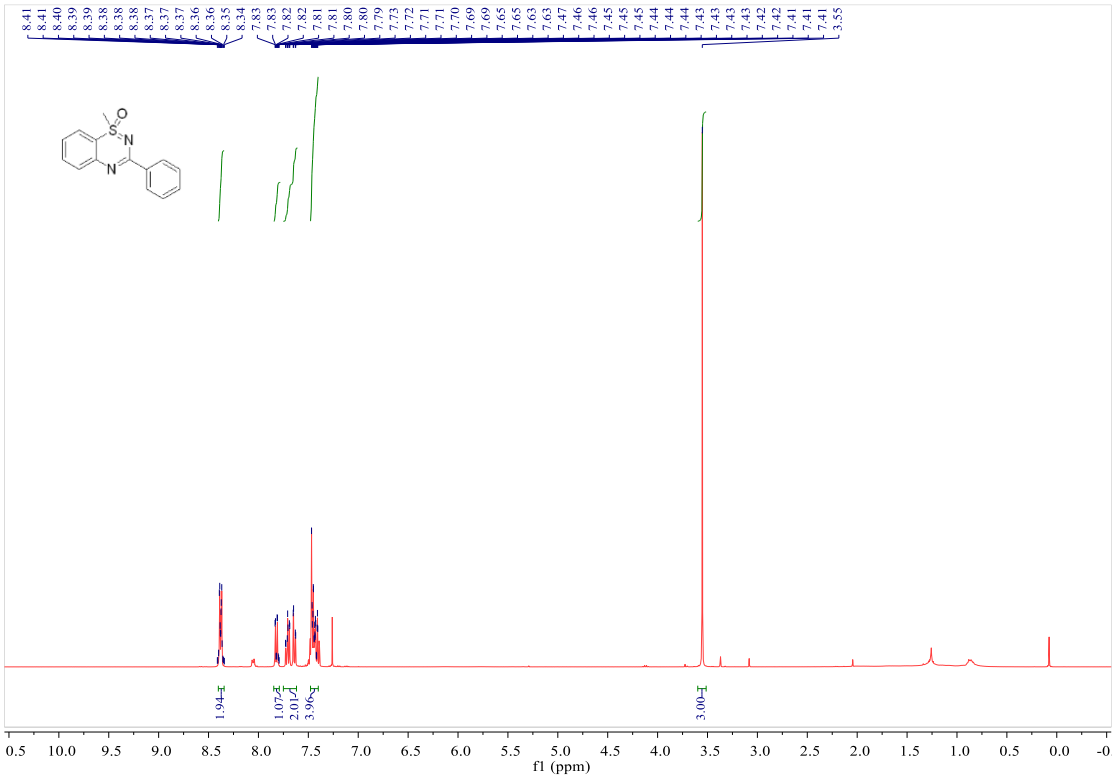
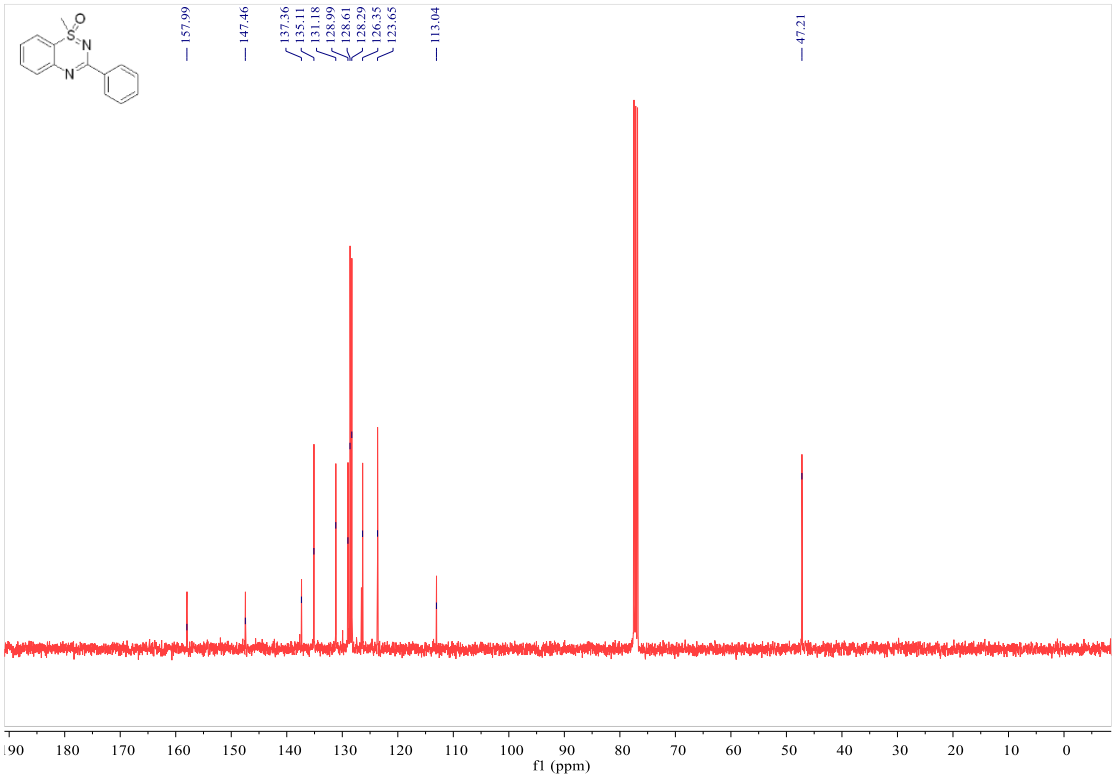
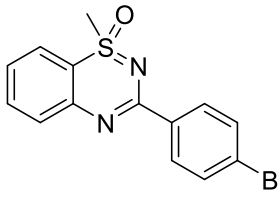


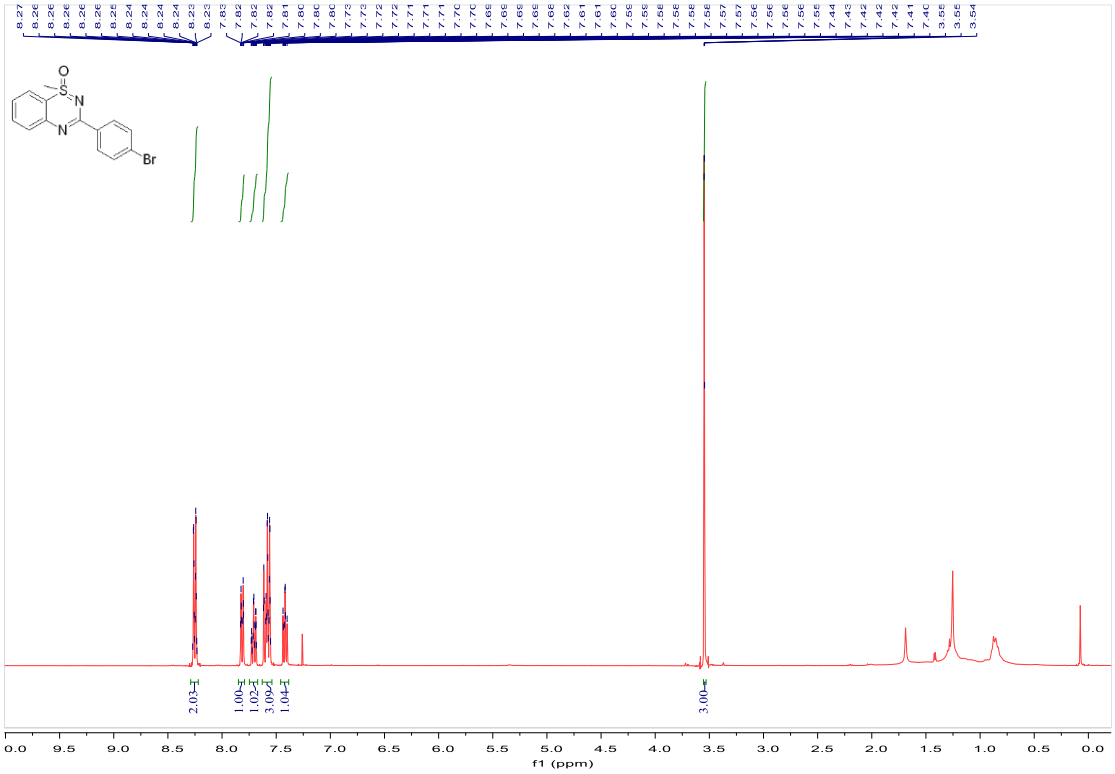
^{13}C NMR (101 MHz, $CDCl_3$)



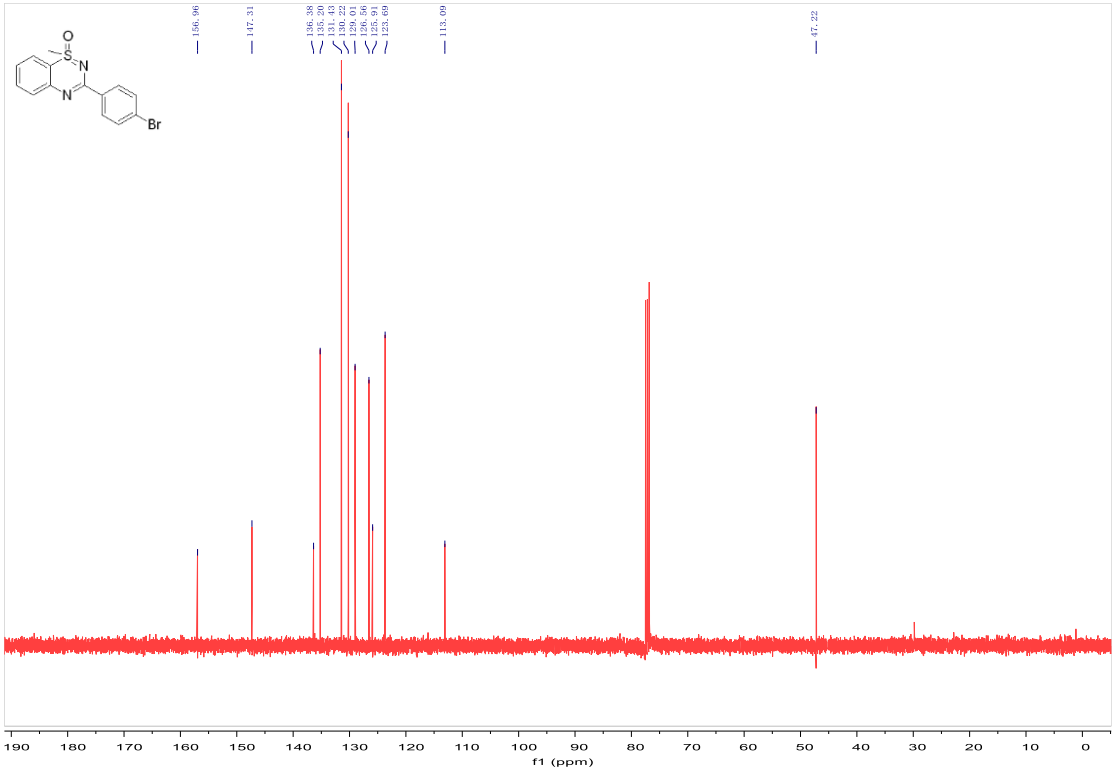
3-(4-bromophenyl)-1-methyl-λ^4-benzo[*e*][1,2,4]thiadiazine-1-oxide (3ab)



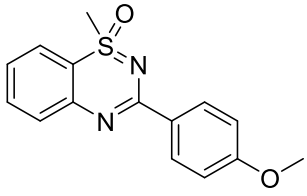
^{1}H NMR (400 MHz, $CDCl_3$)



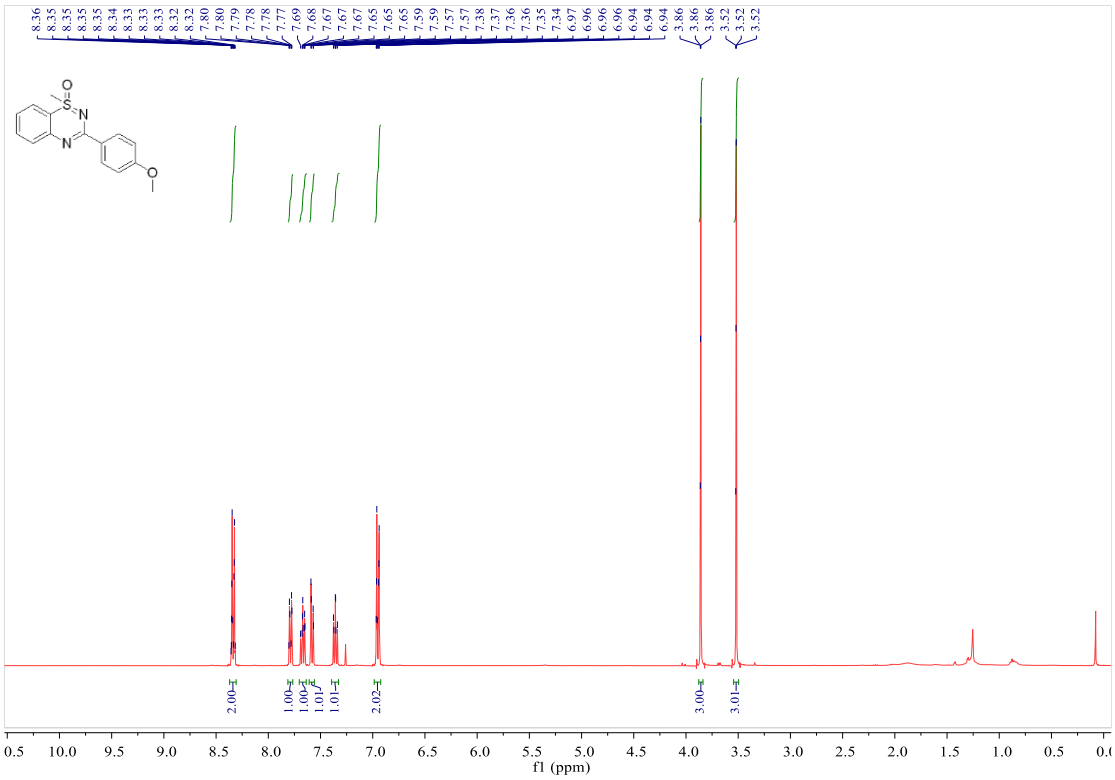
^{13}C NMR (101 MHz, $CDCl_3$)



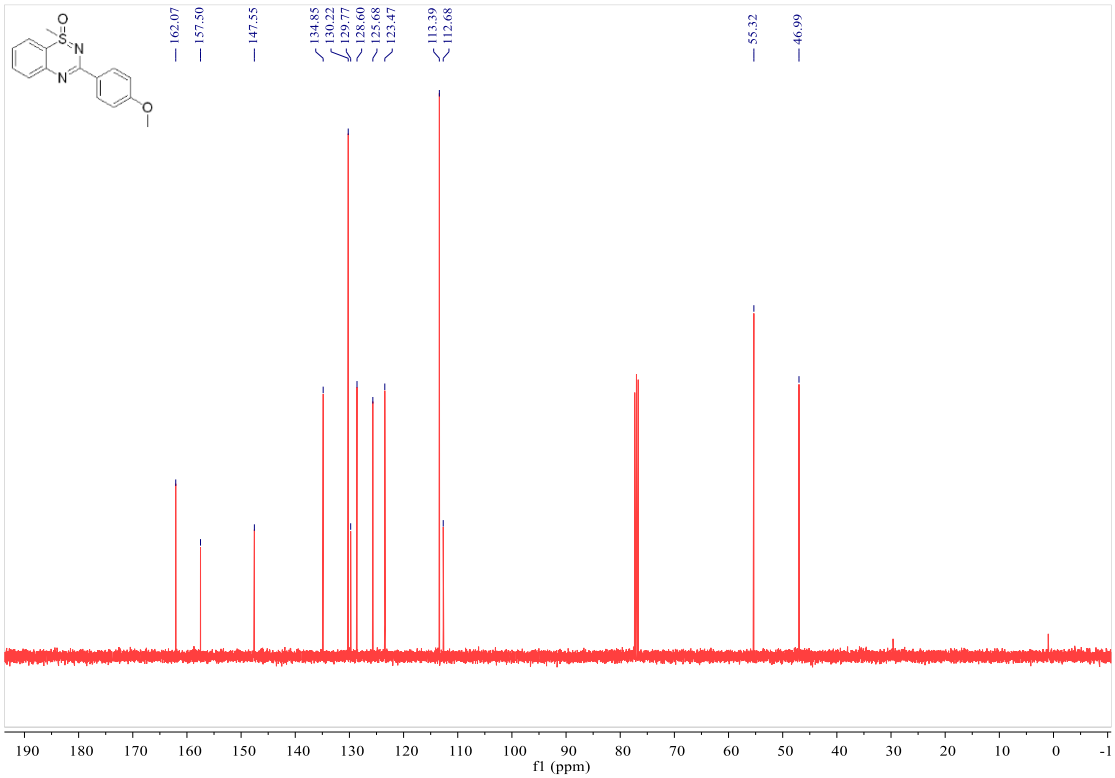
3-(4-methoxyphenyl)-1-methyl-λ⁴-benzo[*e*][1,2,4]thiadiazine-1-oxide (3ac)



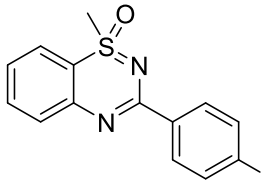
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)



3-(4-fluorophenyl)-1-methyl-λ⁴-benzo[*e*][1,2,4]thiadiazine-1-oxide (3ad).



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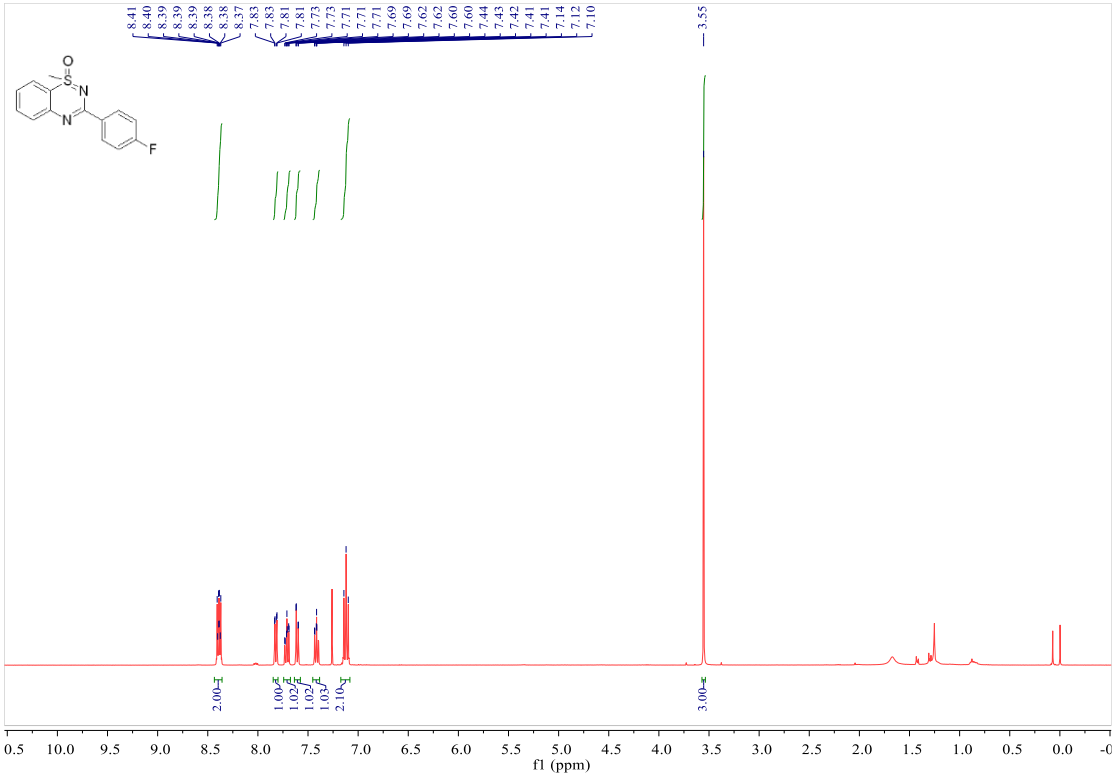
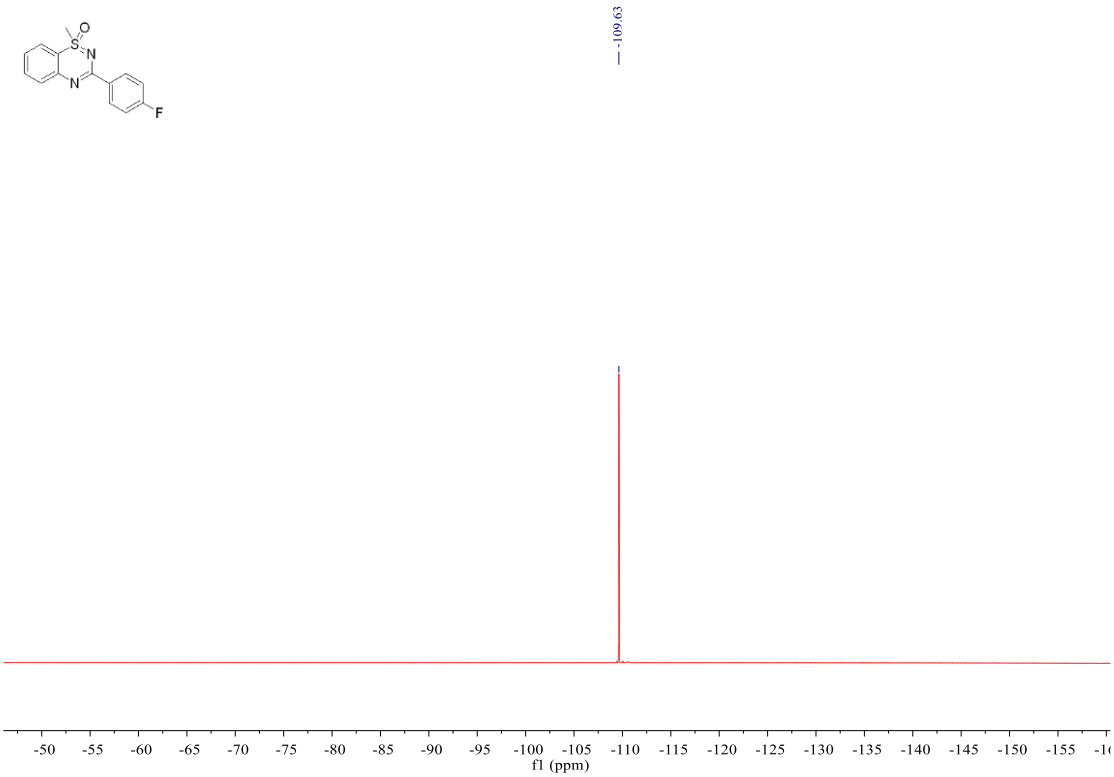


^{19}F NMR (376 MHz, $CDCl_3$)



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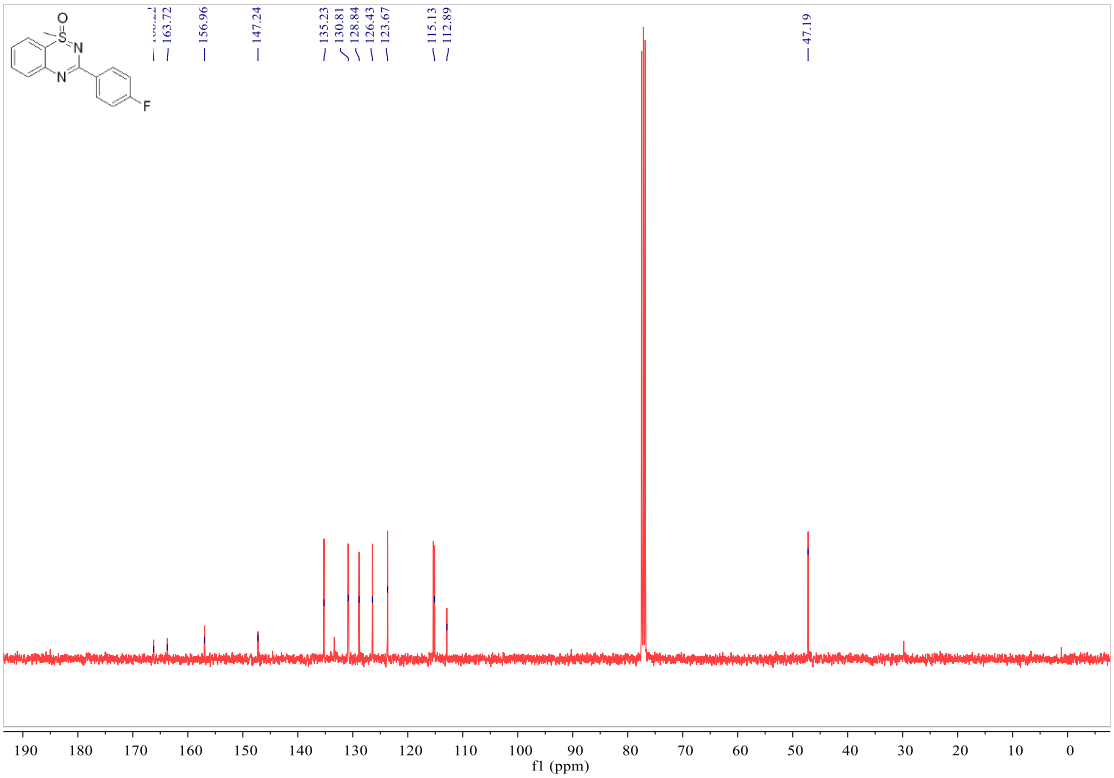
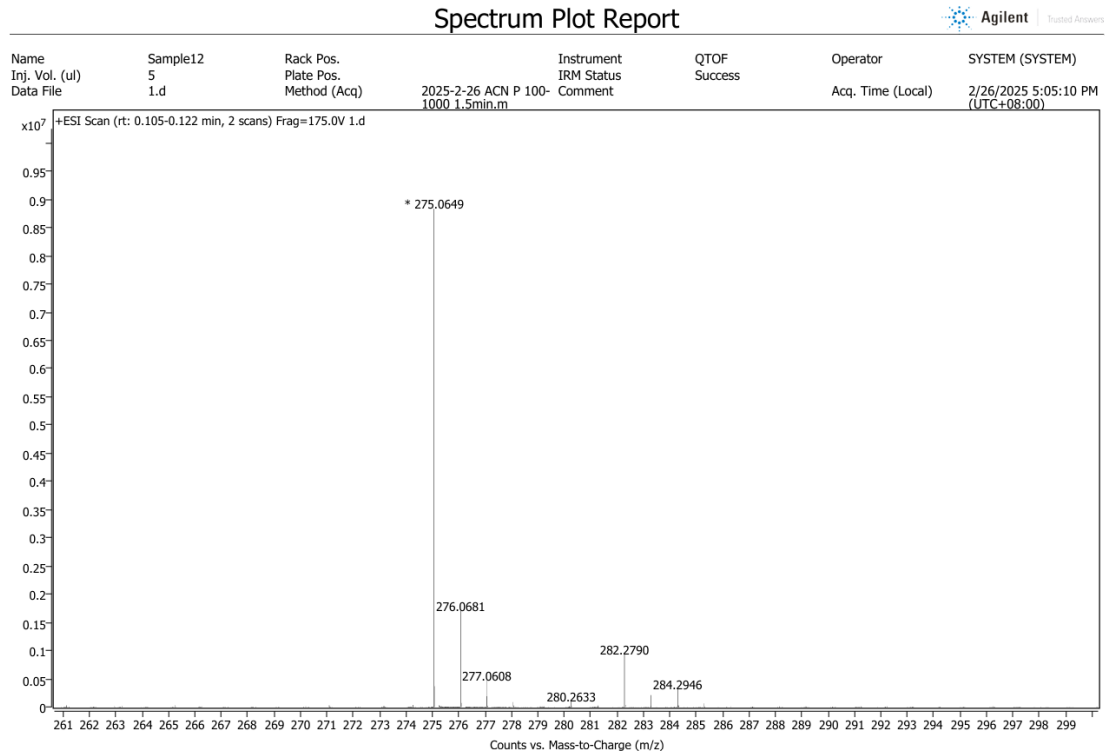


HRMS



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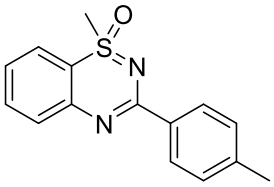
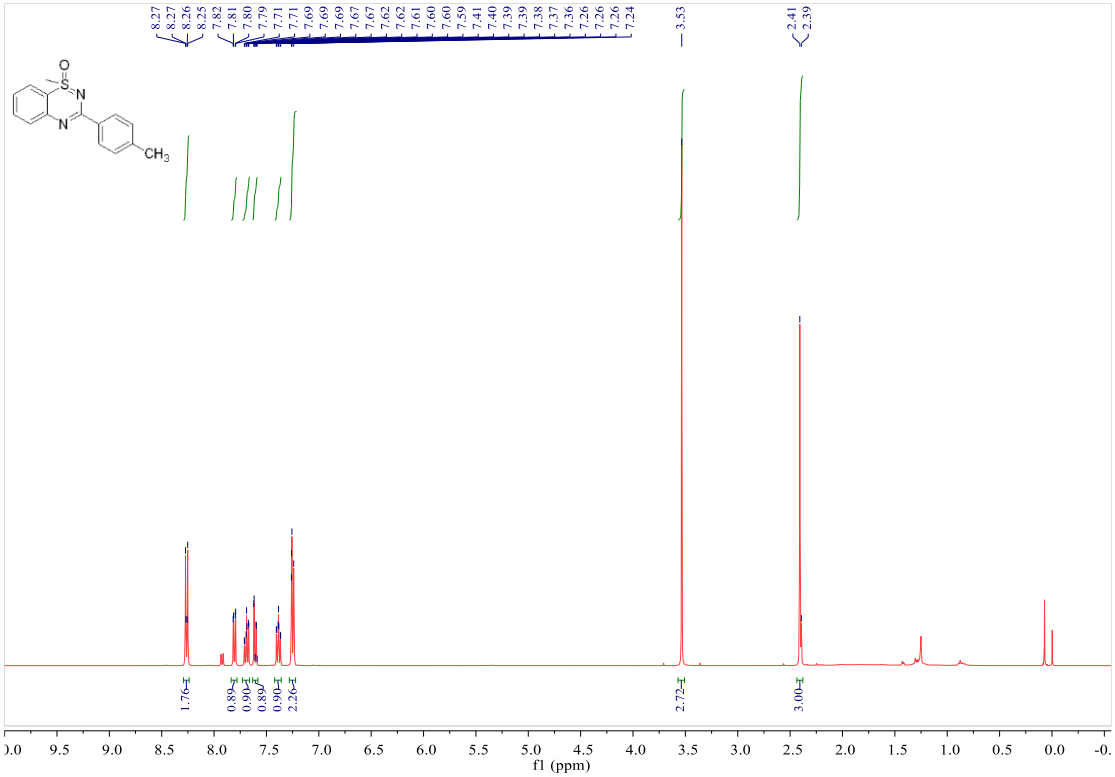


^{1}H NMR (400 MHz, $CDCl_3$)



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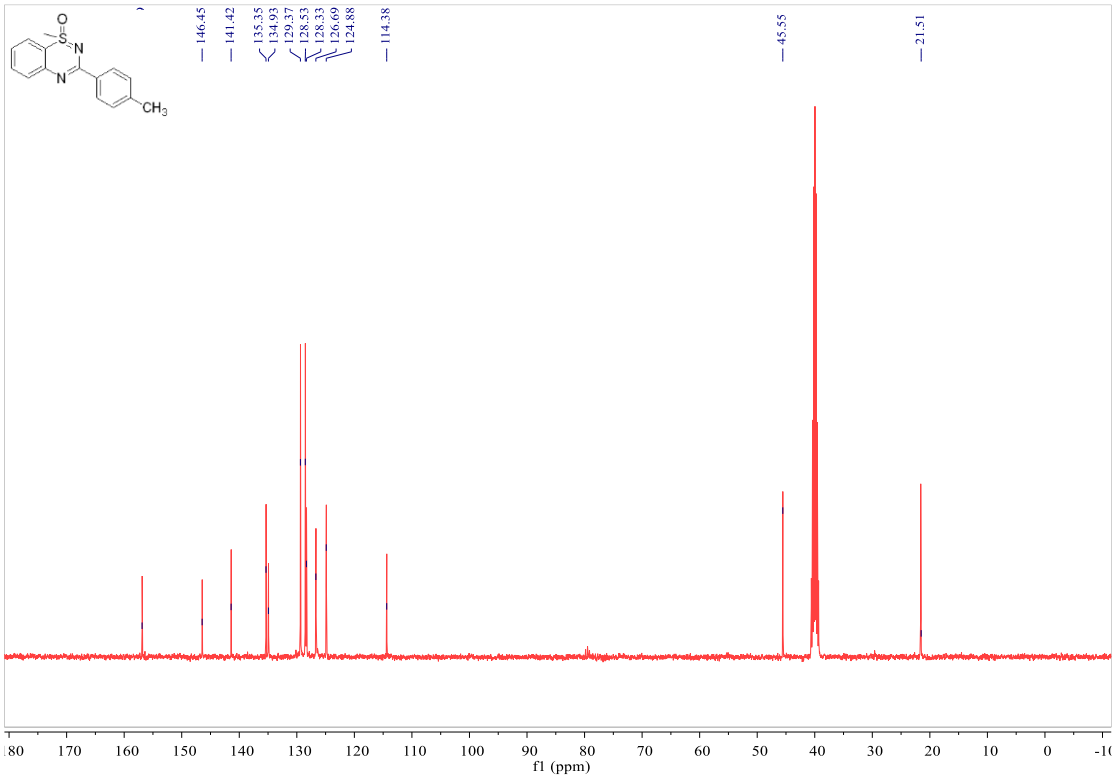
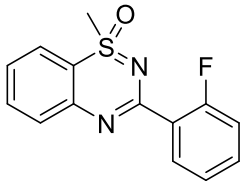
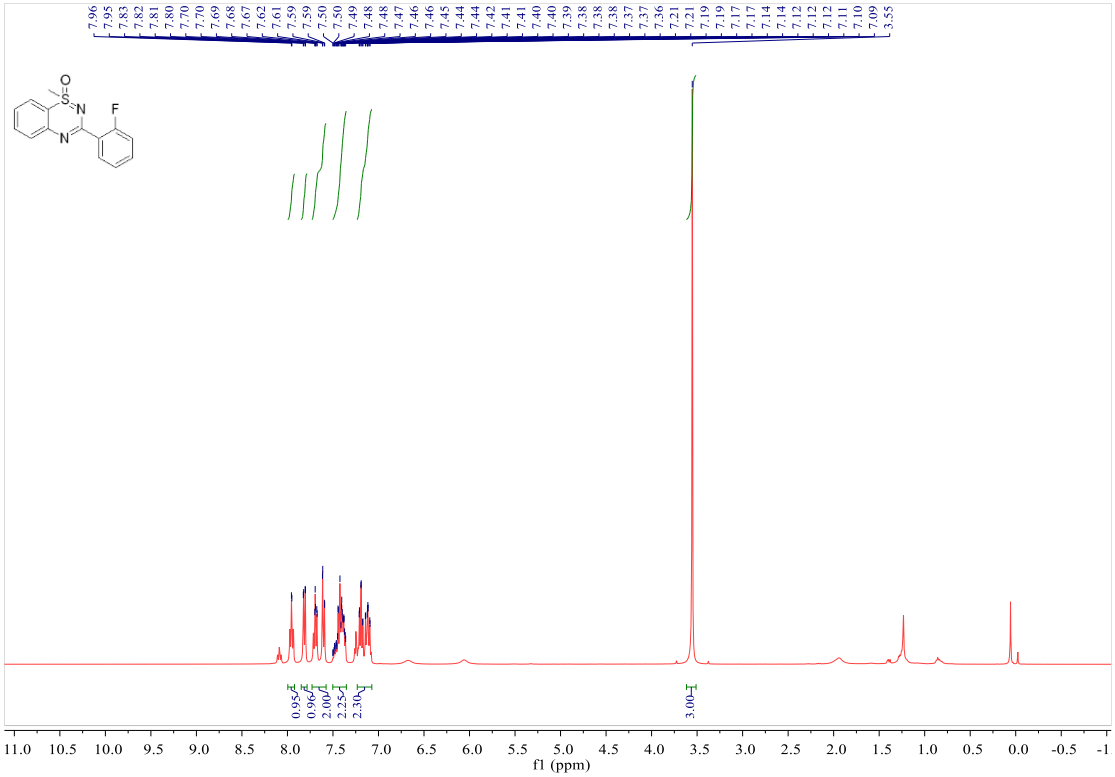


3-(2-fluorophenyl)-1-methyl-λ^4-benzo[*e*][1,2,4]thiadiazine-1-oxide (3af).



^{1}H NMR (400 MHz, $CDCl_3$)



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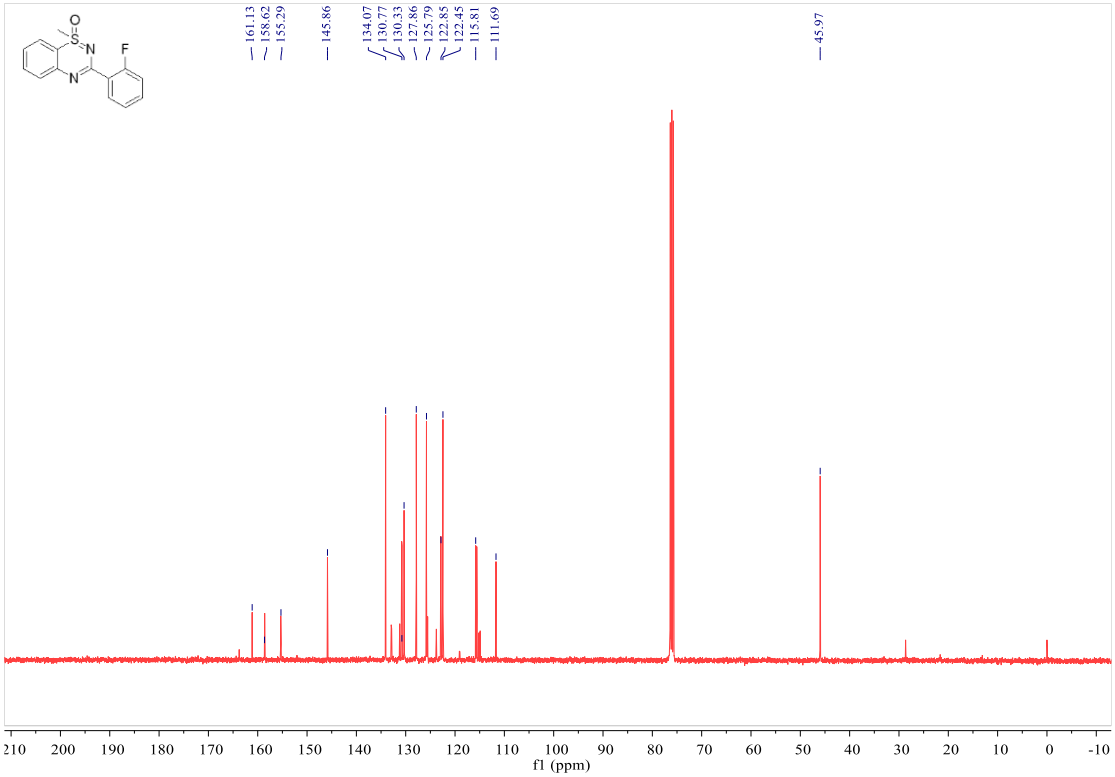
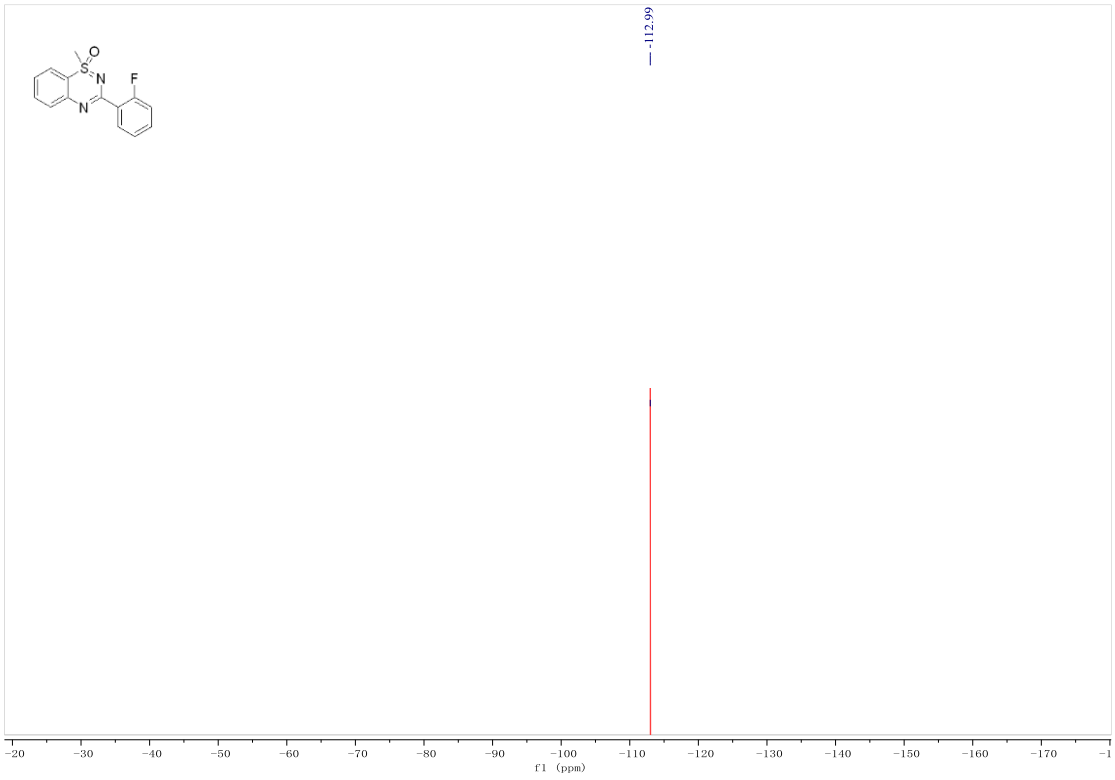
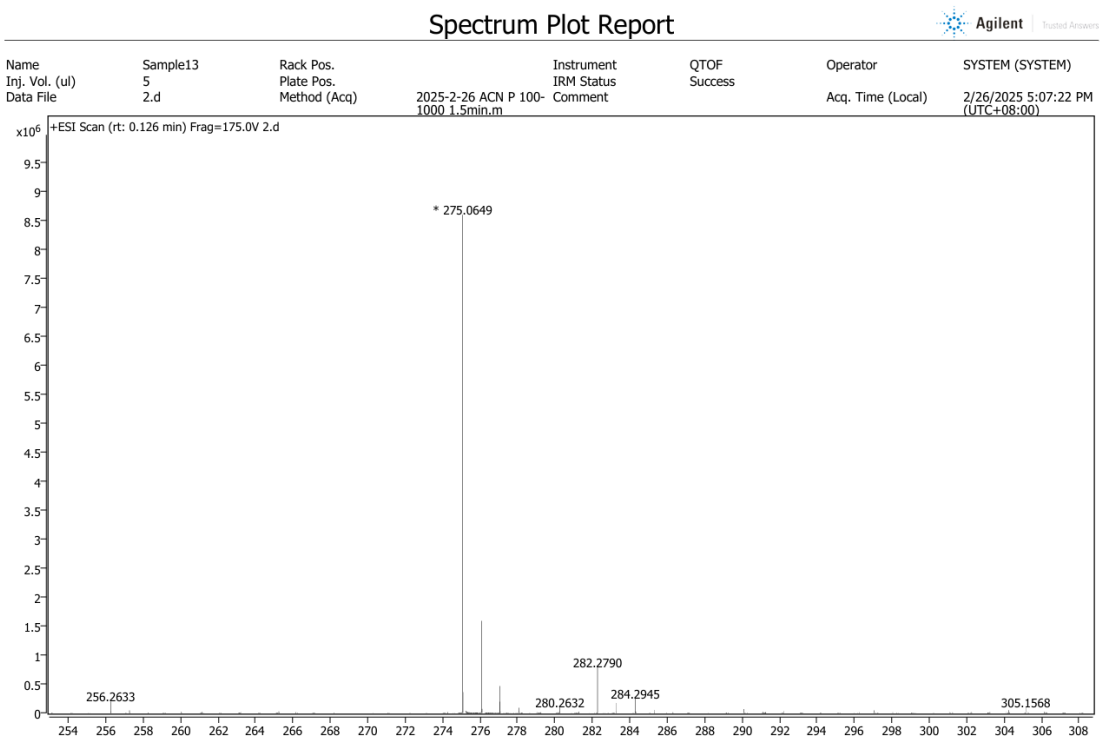


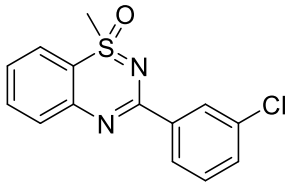
^{19}F NMR (376 MHz, $CDCl_3$)



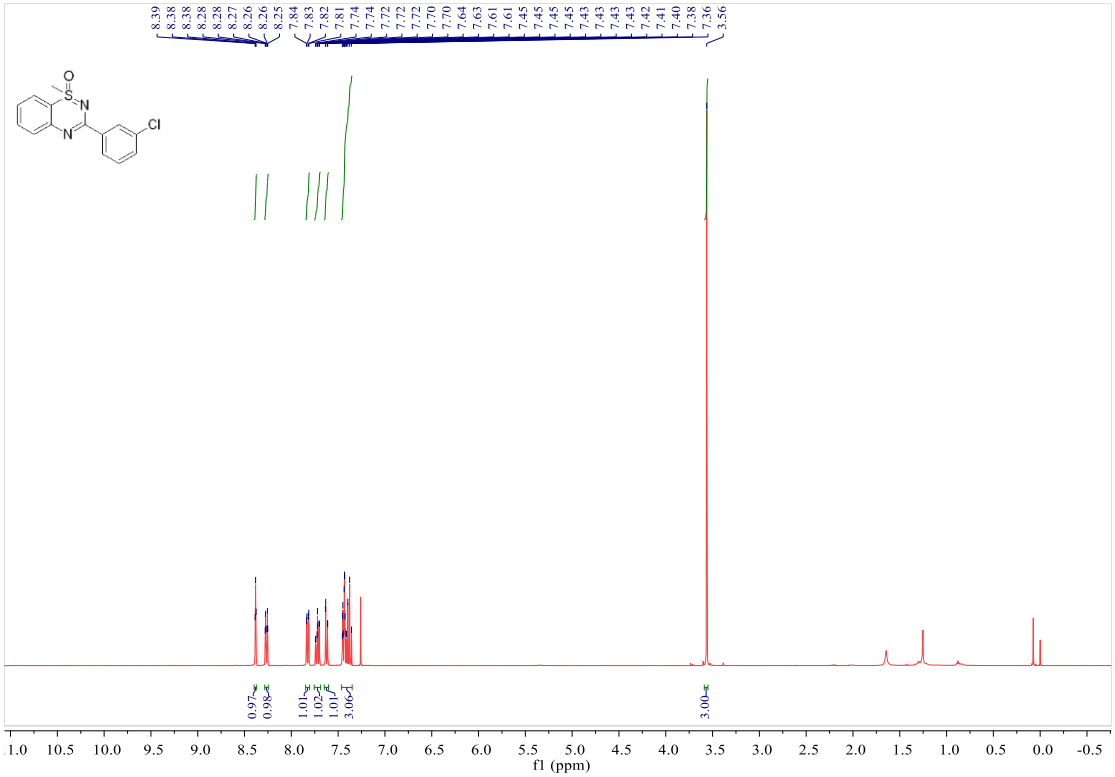
HRMS



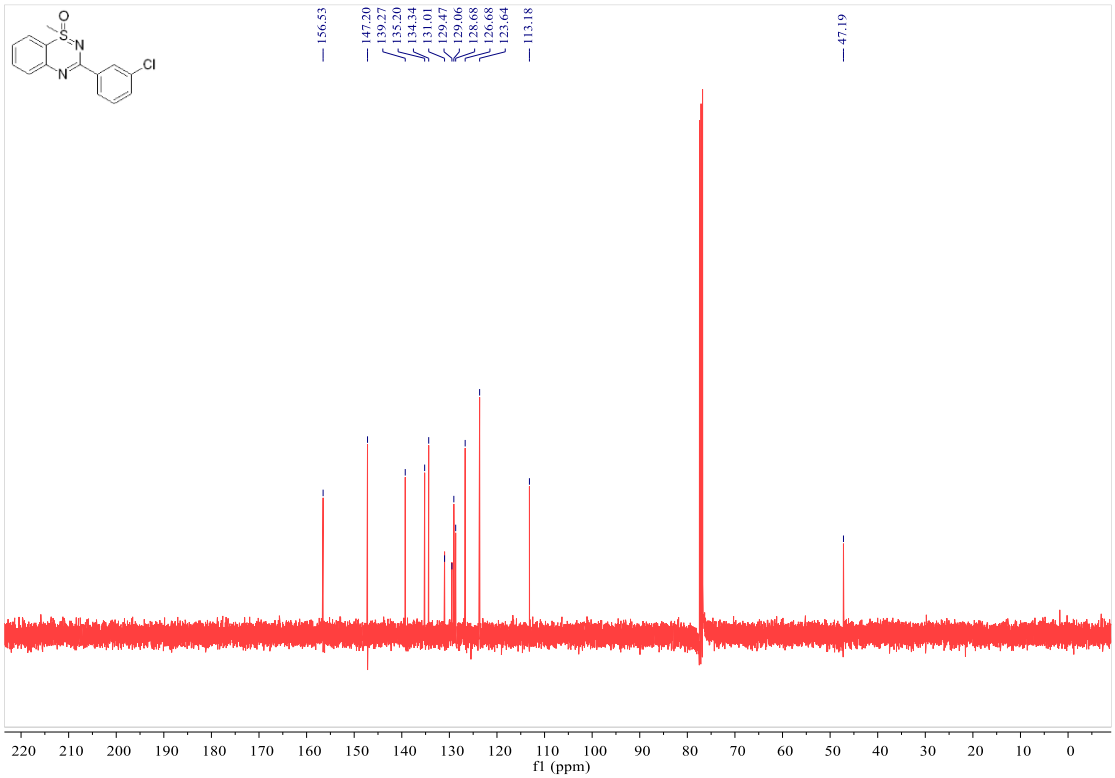
3-(3-chlorophenyl)-1-methyl-λ^4-benzo[*e*][1,2,4]thiadiazine-1-oxide (3ag).



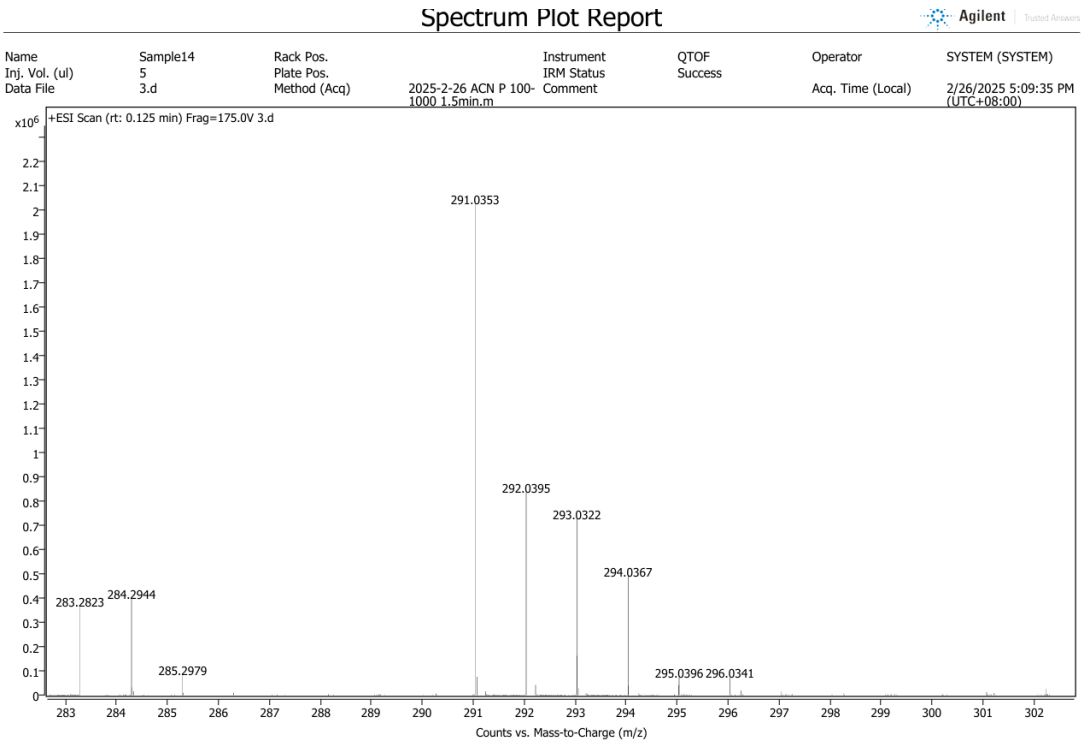
^{1}H NMR (400 MHz, $CDCl_3$)



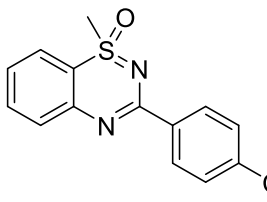
^{13}C NMR (101 MHz, $CDCl_3$)



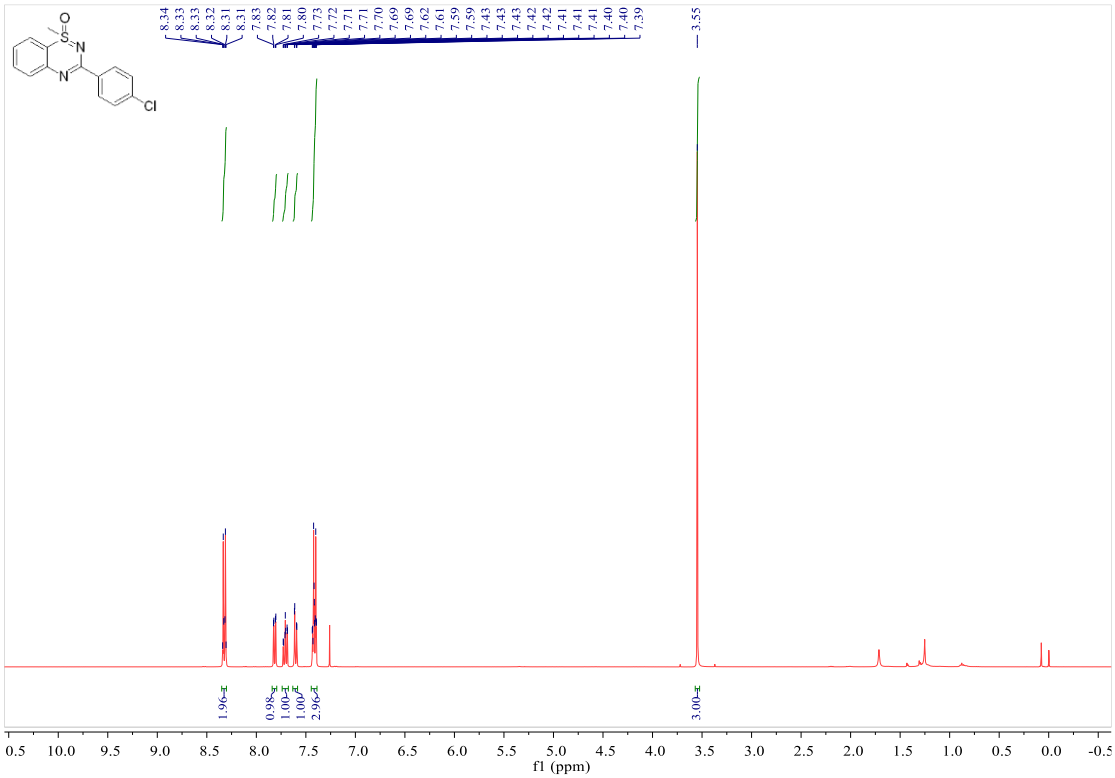
HRMS



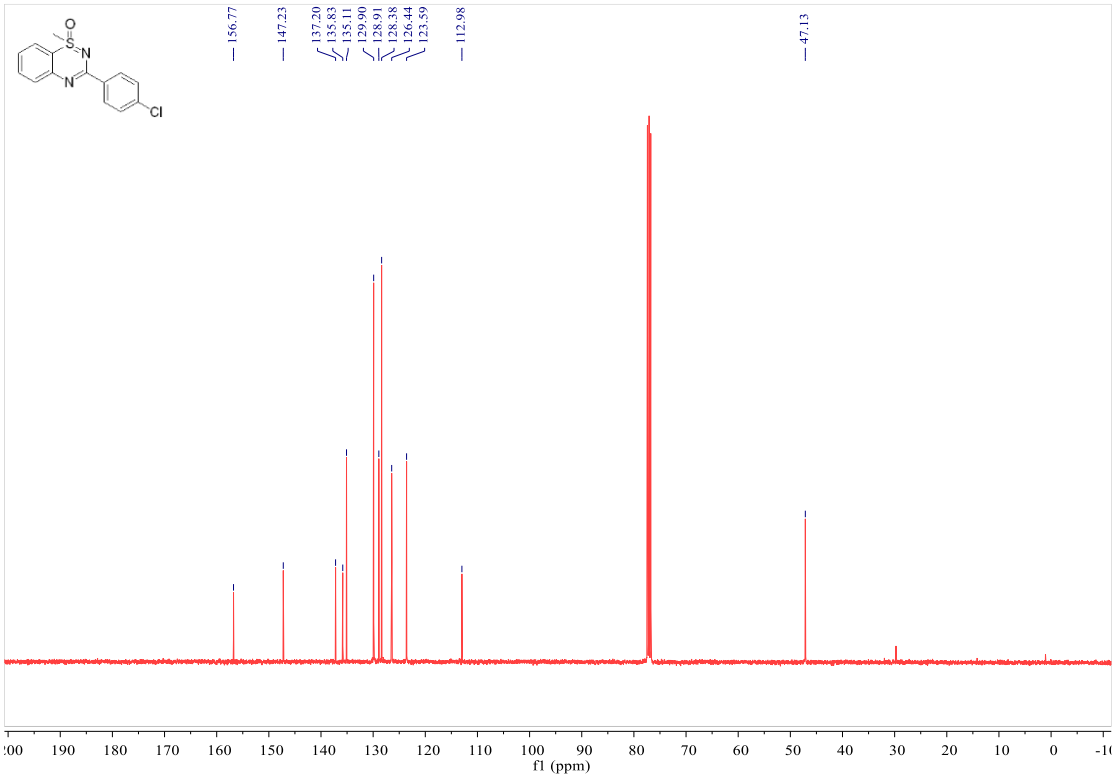
3-(4-chlorophenyl)-1-methyl-λ⁴-benzo[*e*][1,2,4]thiadiazine-1-oxide (3ah)



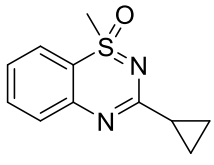
^{1}H NMR (400 MHz, $CDCl_3$)



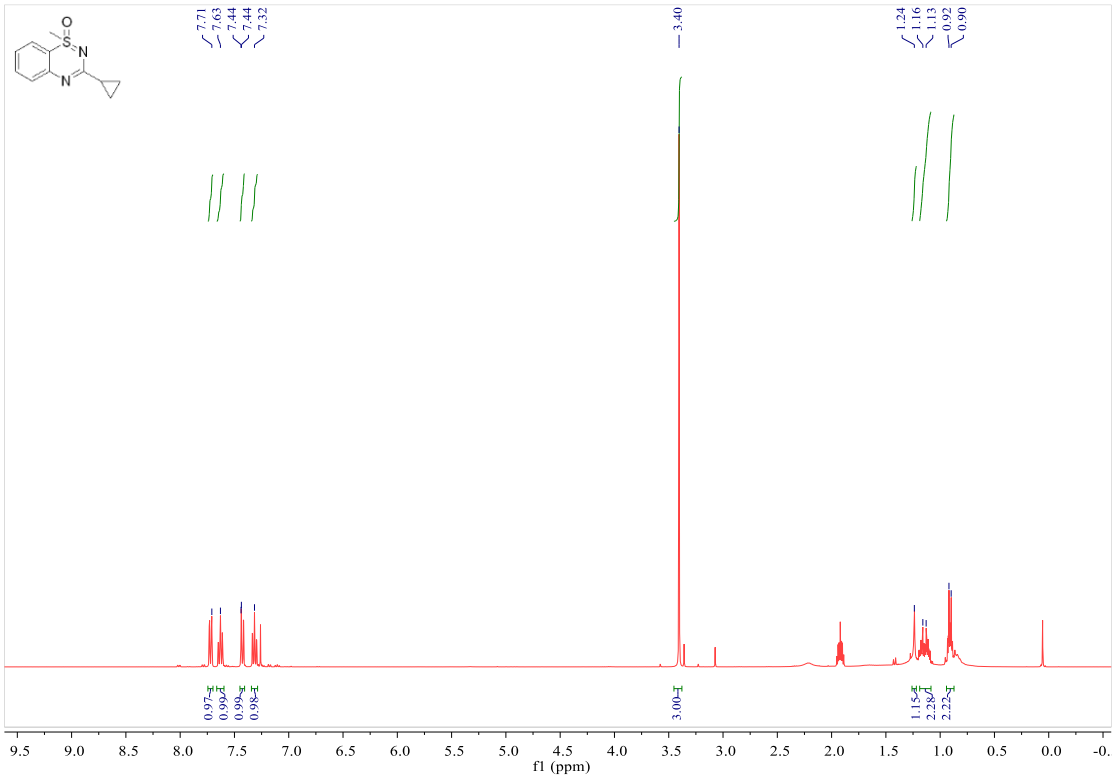
^{13}C NMR (101 MHz, $CDCl_3$)



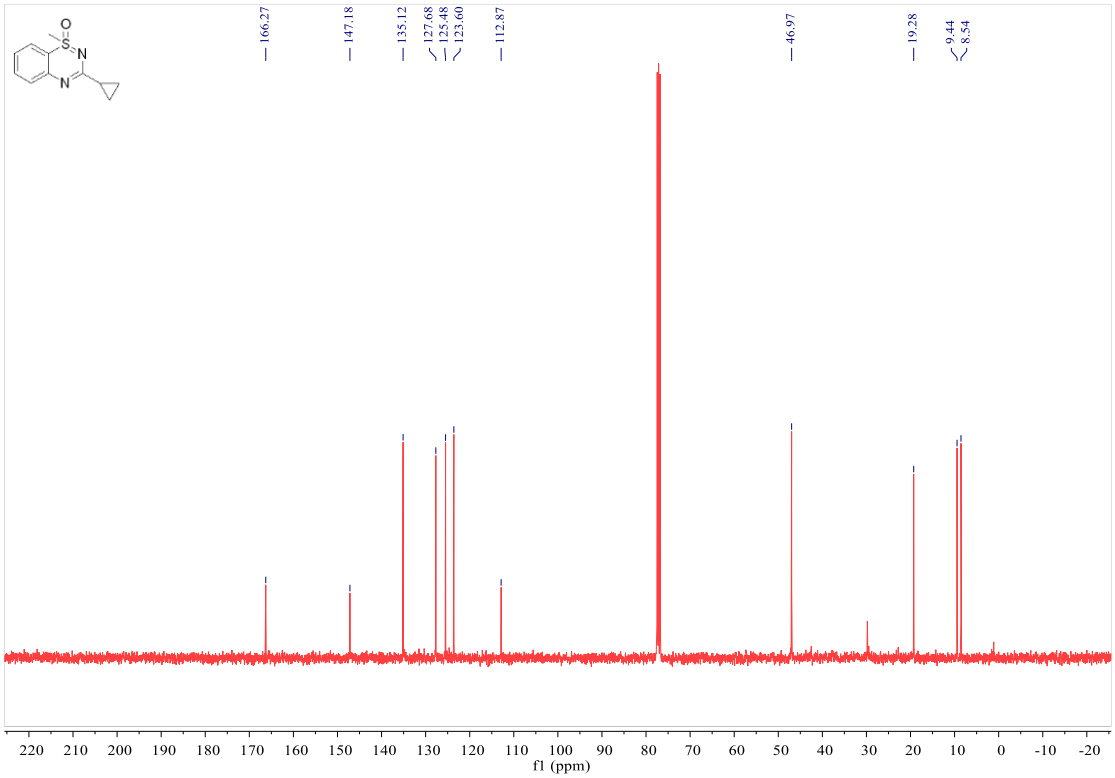
3-cyclopropyl-1-methyl-λ⁴-benzo[*e*][1,2,4]thiadiazine-1-oxide (3ai)



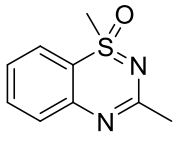
^{1}H NMR (400 MHz, $CDCl_3$)



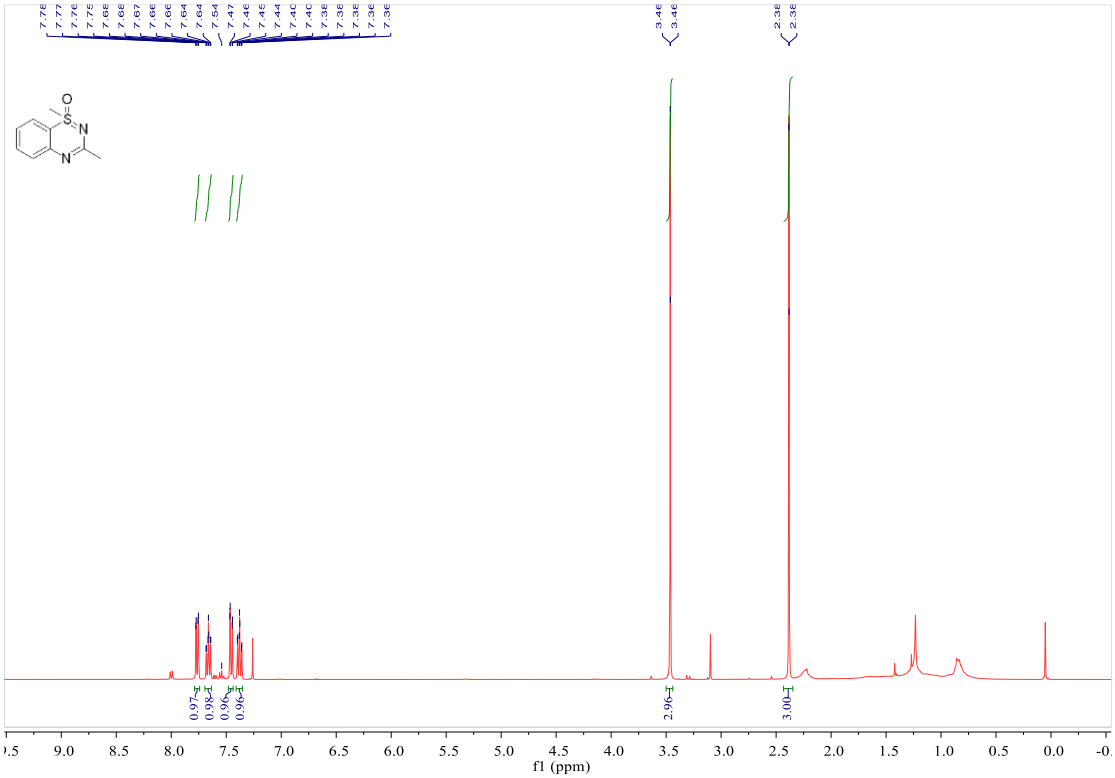
^{13}C NMR (101 MHz, $CDCl_3$)



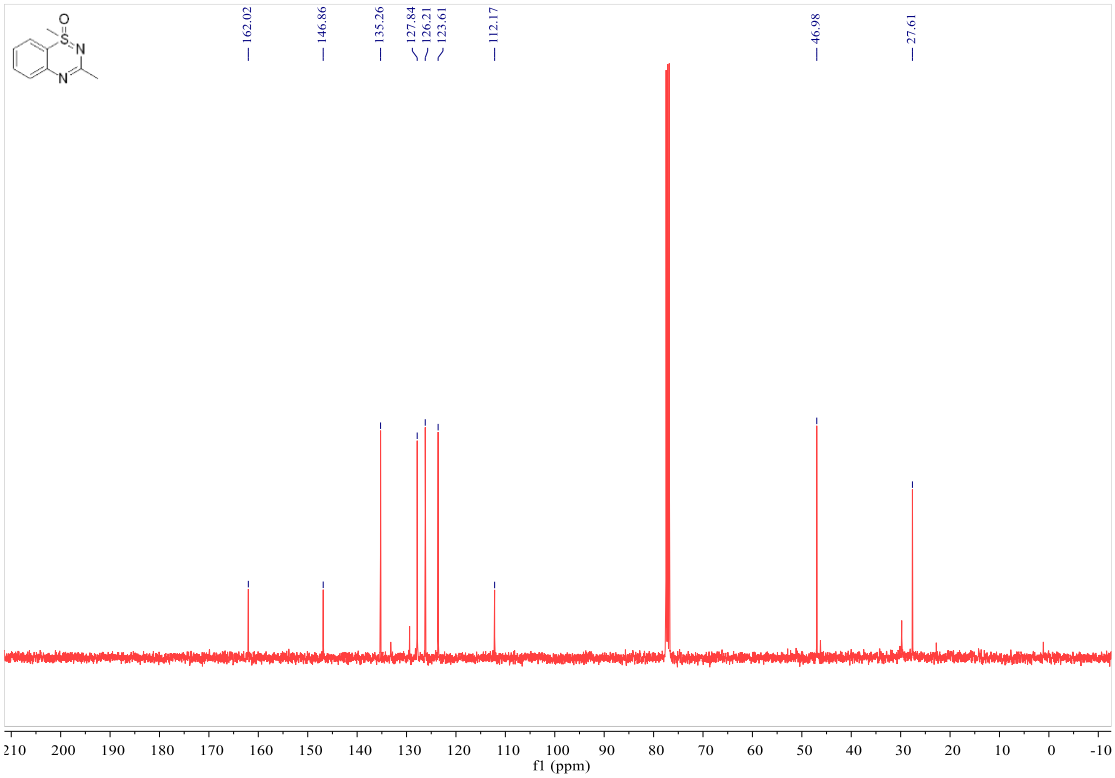
1,3-dimethyl-λ^4-benzo[*e*][1,2,4]thiadiazine-1-oxide (3aj)



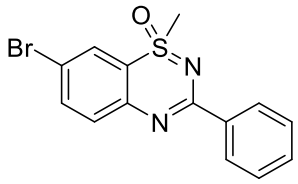
^1H NMR (400 MHz, $CDCl_3$)



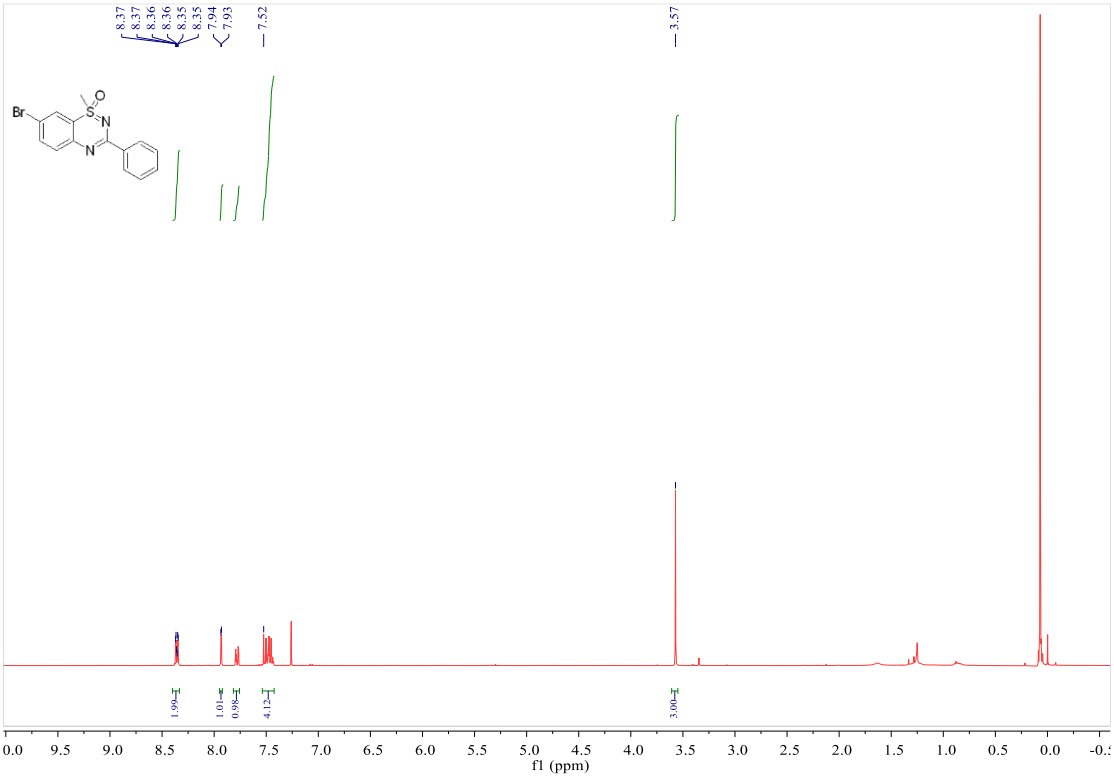
^{13}C NMR (101 MHz, $CDCl_3$)



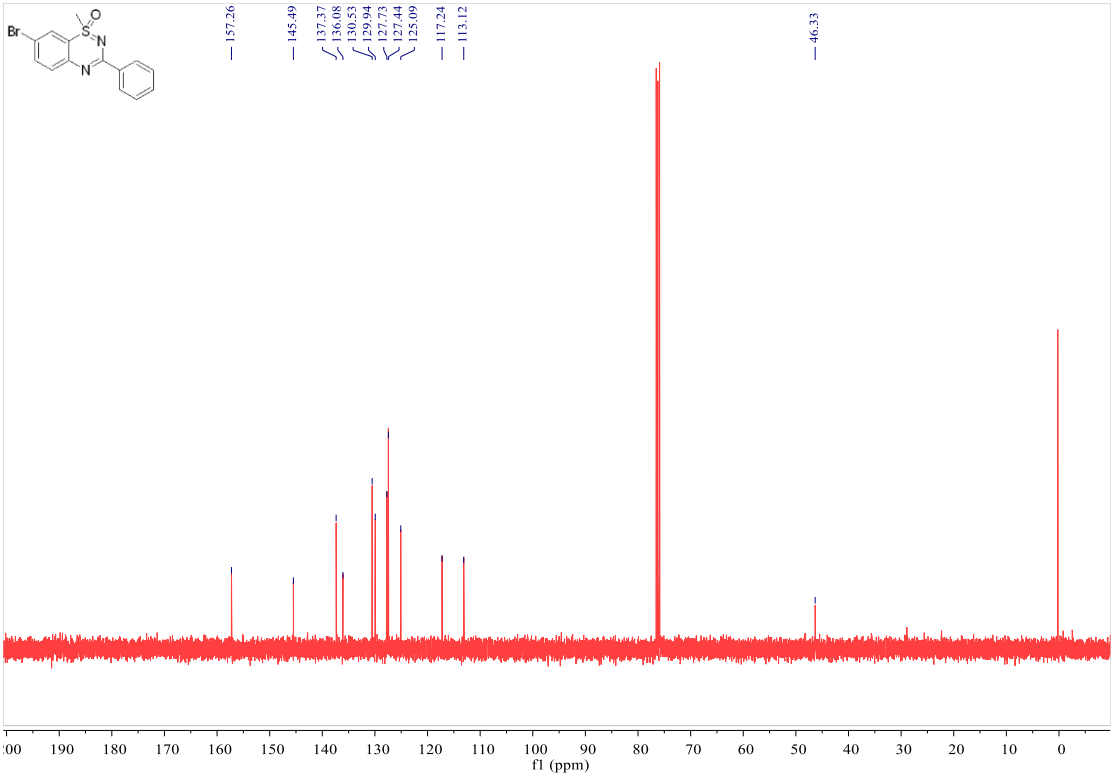
7-bromo-1-methyl-3-phenyl-λ^4-benzo[*e*][1,2,4]thiadiazine-1-oxide (3ba).



^{1}H NMR (400 MHz, $CDCl_3$)



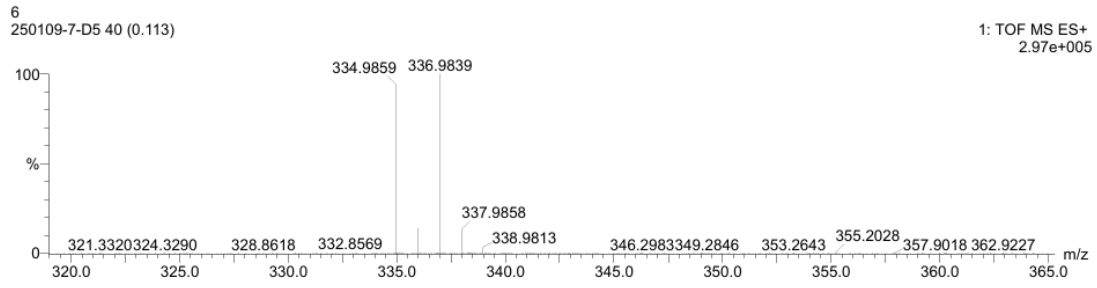
^{13}C NMR (101 MHz, $CDCl_3$)



HRMS

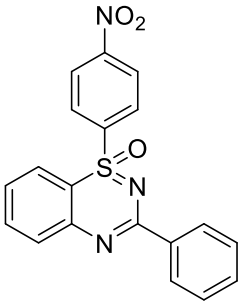
Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
678 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 14-14 H: 0-50 N: 0-200 O: 0-10 Si: 0-5 S: 1-2 Br: 1-1

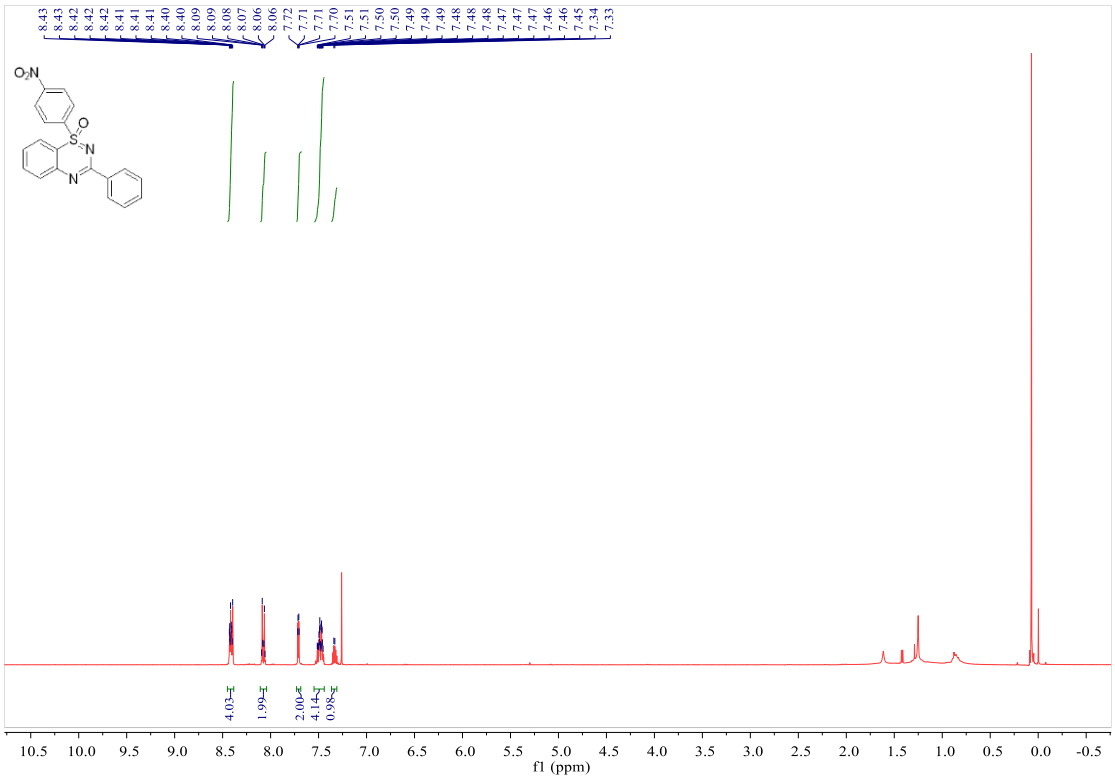


Minimum:				-1.5				
Maximum:		5.0	20.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
334.9859	334.9854	0.5	1.5	9.5	532.0	n/a	n/a	C14 H12 N2 O S Br

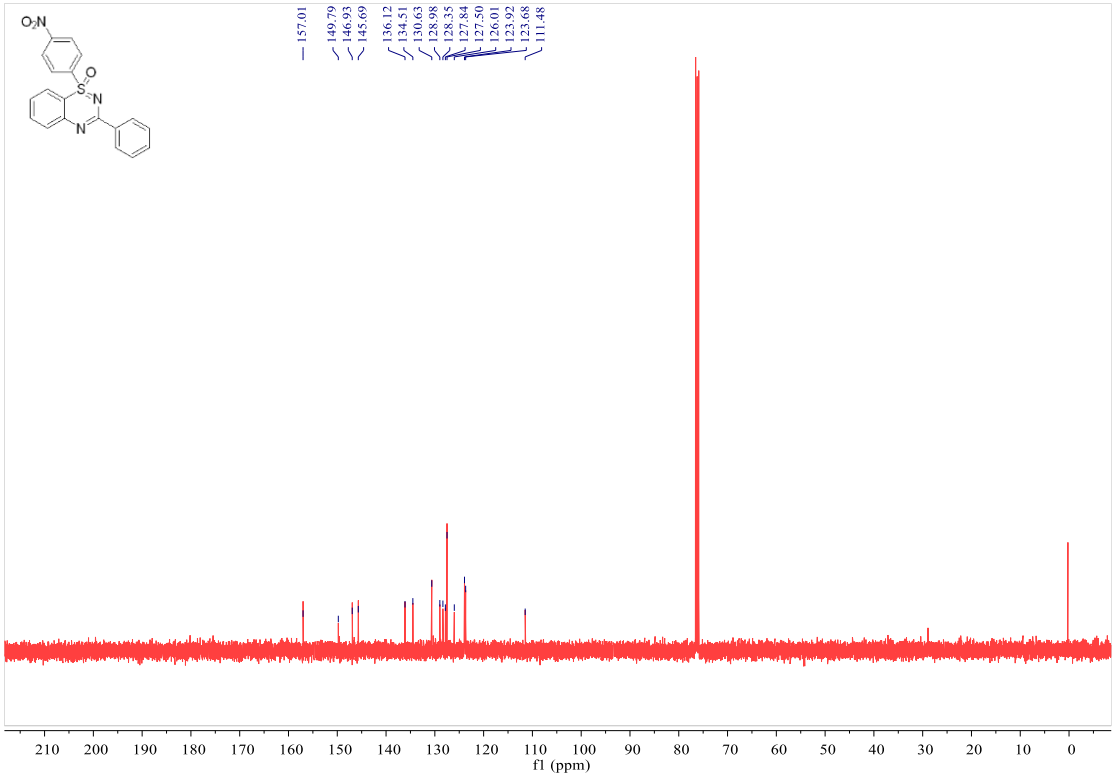
1-(4-nitrophenyl)-3-phenylbenzo[*e*][1,2,4]thiadiazine-1-oxide (3ca).



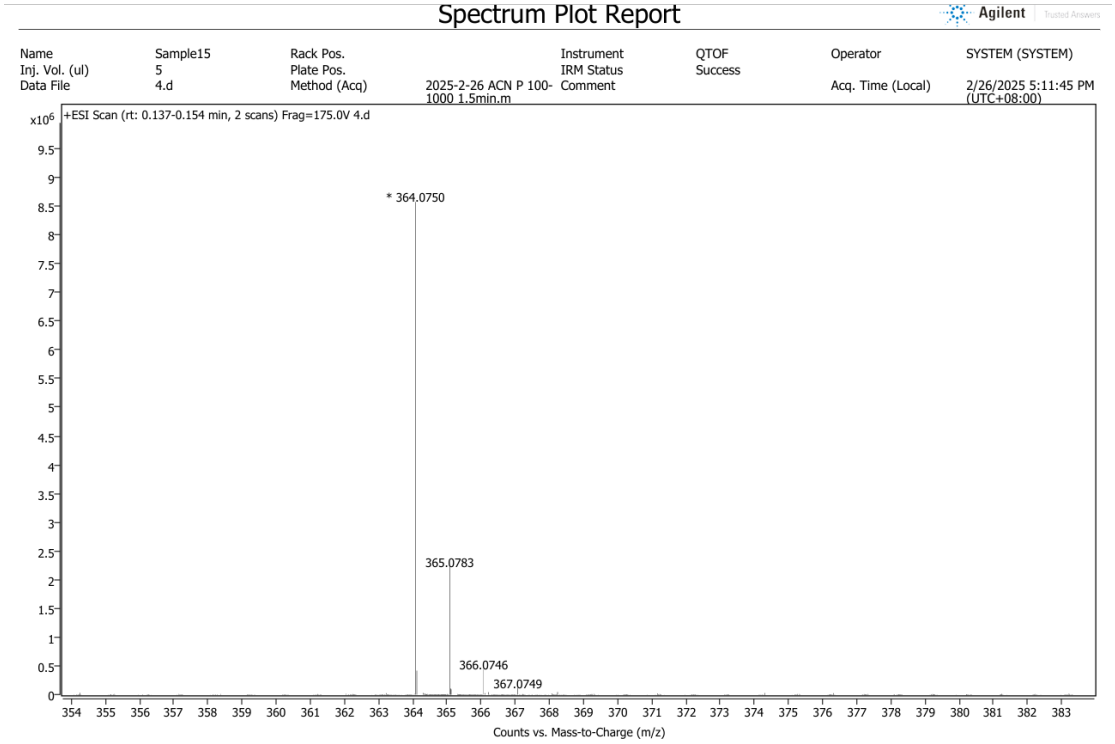
^{1}H NMR (400 MHz, $CDCl_3$)



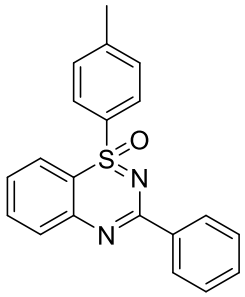
^{13}C NMR (101 MHz, $CDCl_3$)



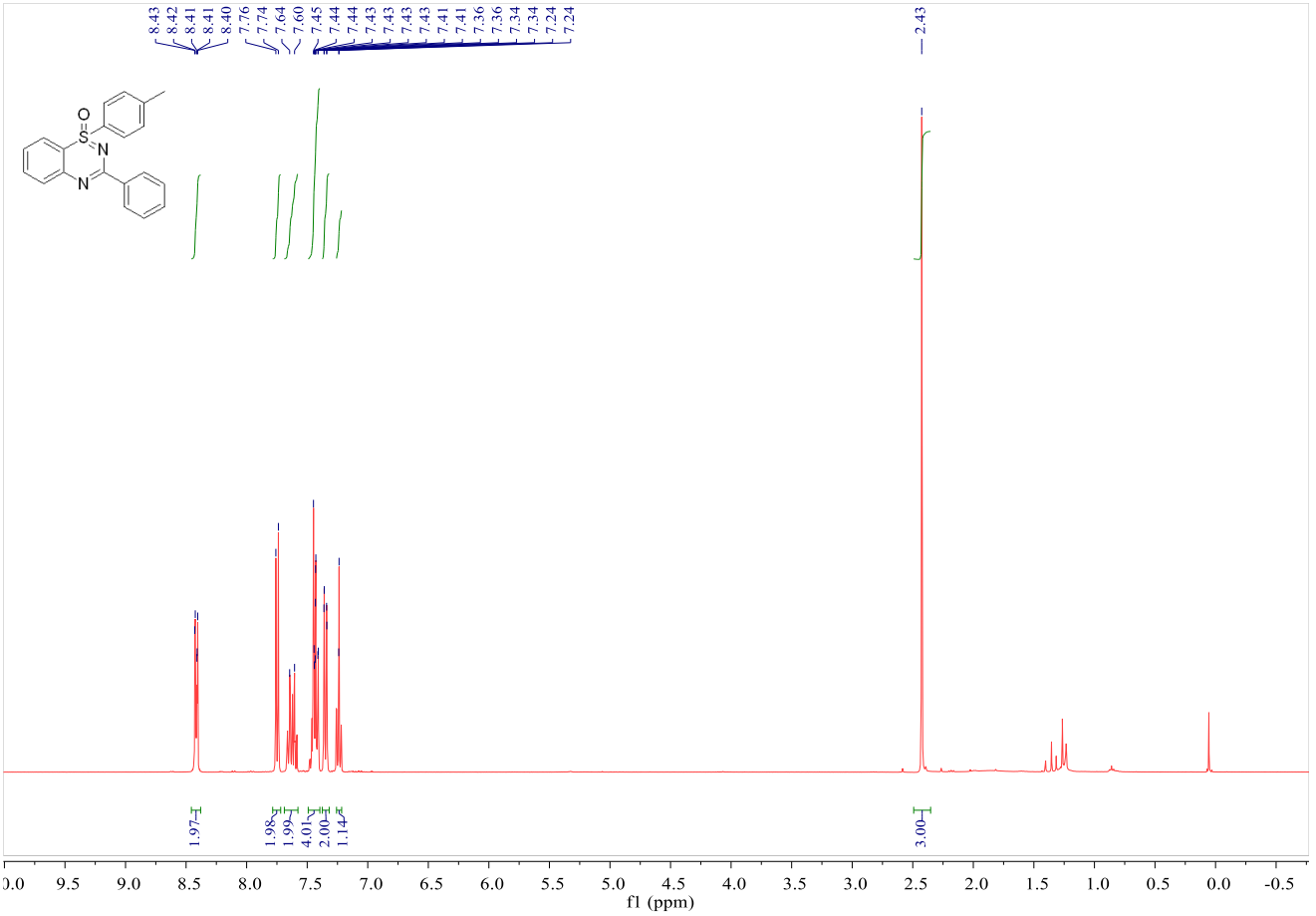
HRMS



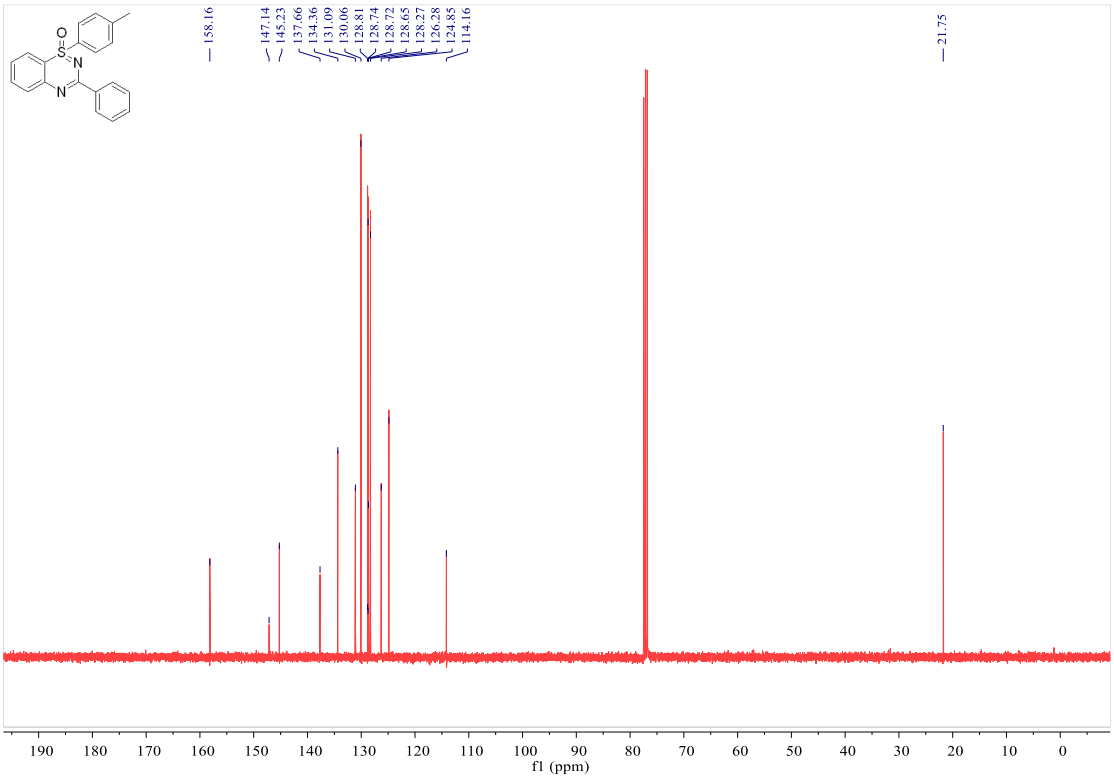
3-phenyl-1-(p-tolyl)benzo[*e*][1,2,4]thiadiazine-1-oxide (3da)



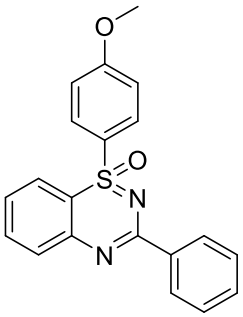
^{1}H NMR (400 MHz, $CDCl_3$)



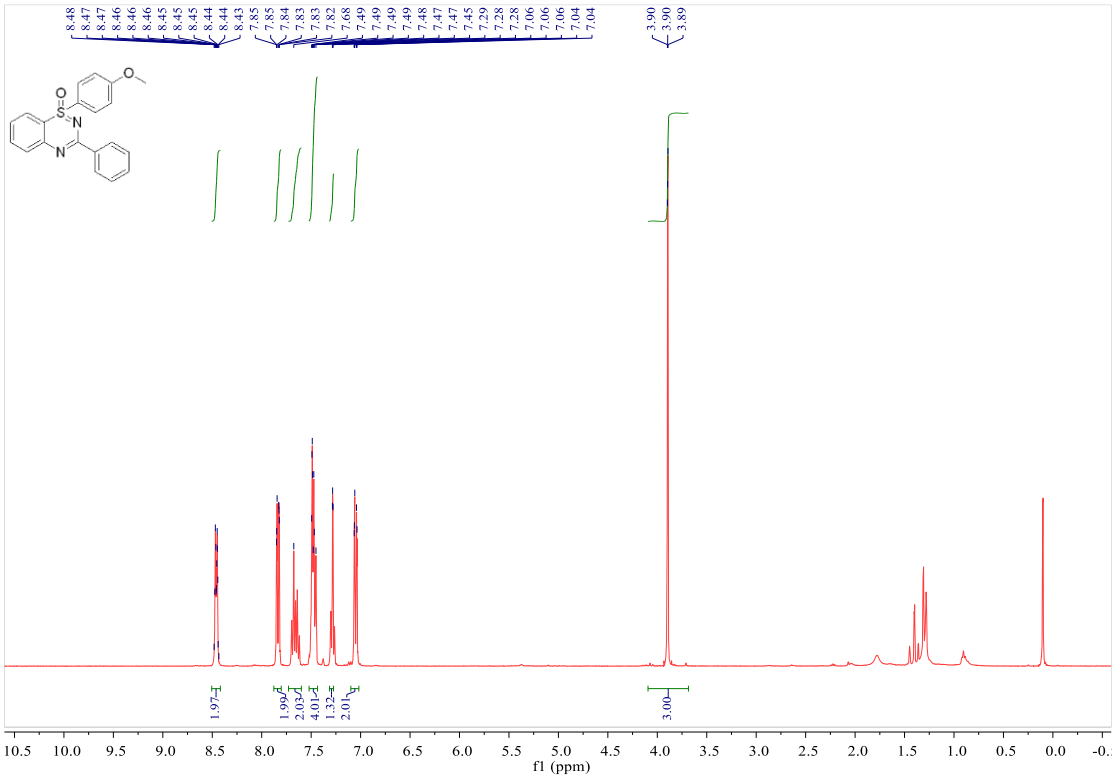
^{13}C NMR (101 MHz, $CDCl_3$)



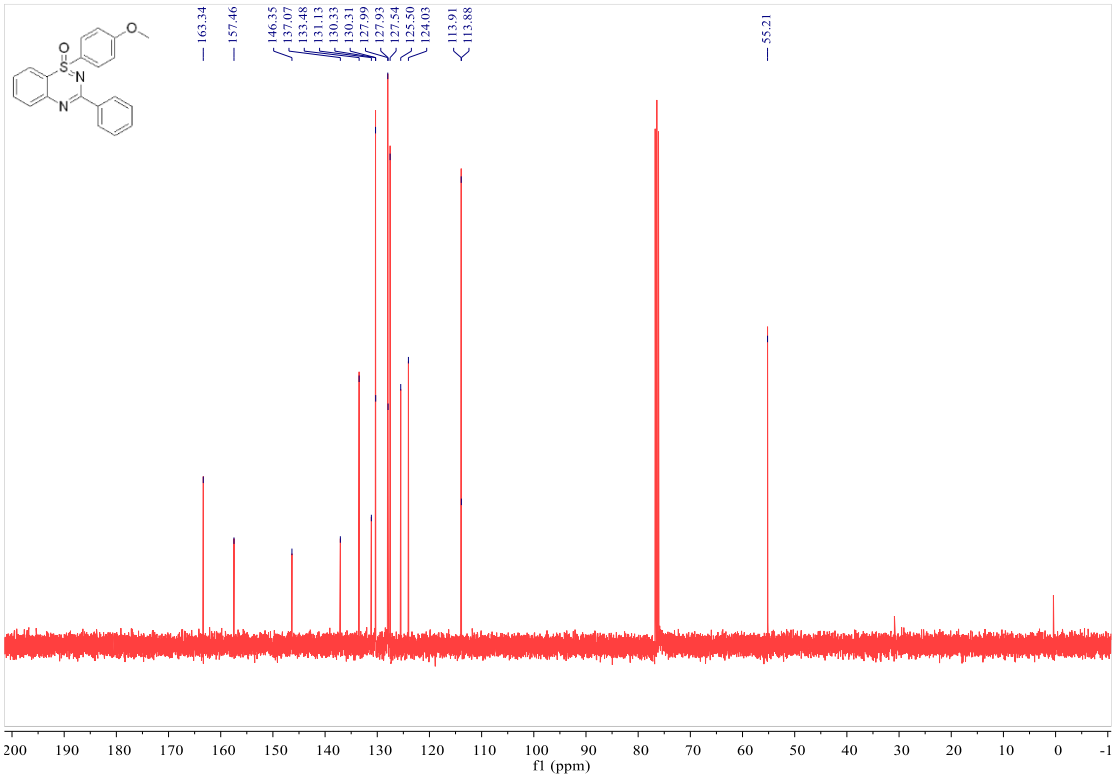
1-(4-methoxyphenyl)-3-phenylbenzo[*e*][1,2,4]thiadiazine-1-oxide (3ea).



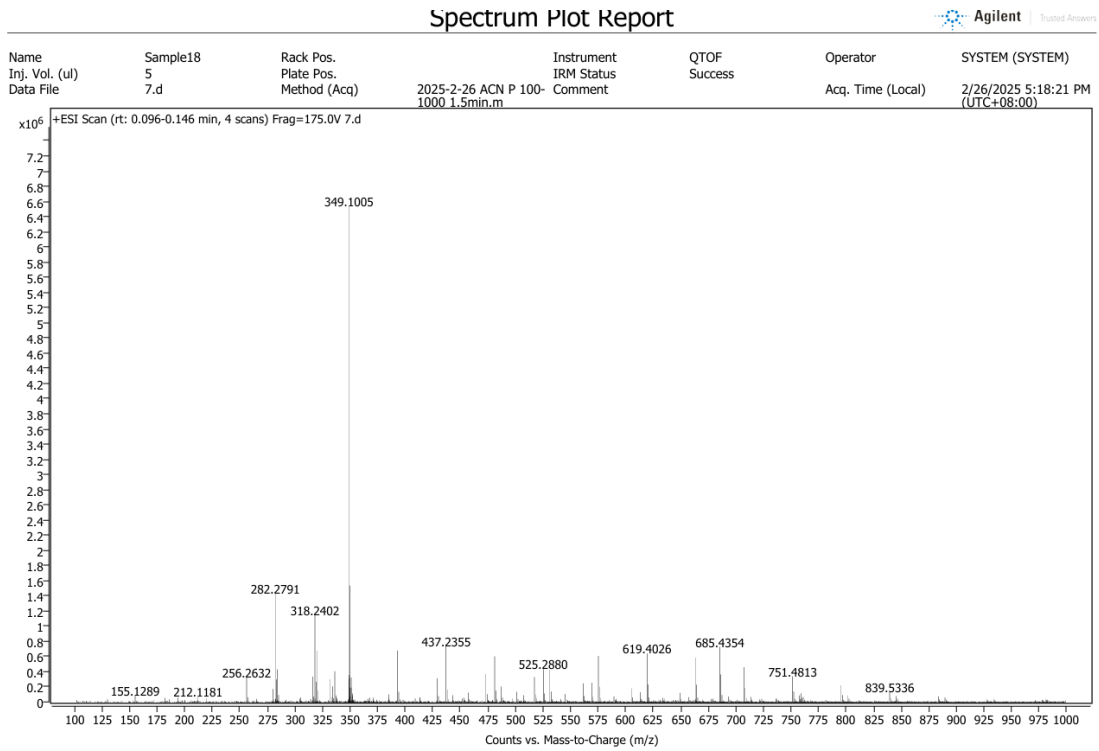
^{1}H NMR (400 MHz, $CDCl_3$)



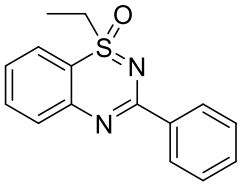
^{13}C NMR (101 MHz, $CDCl_3$)



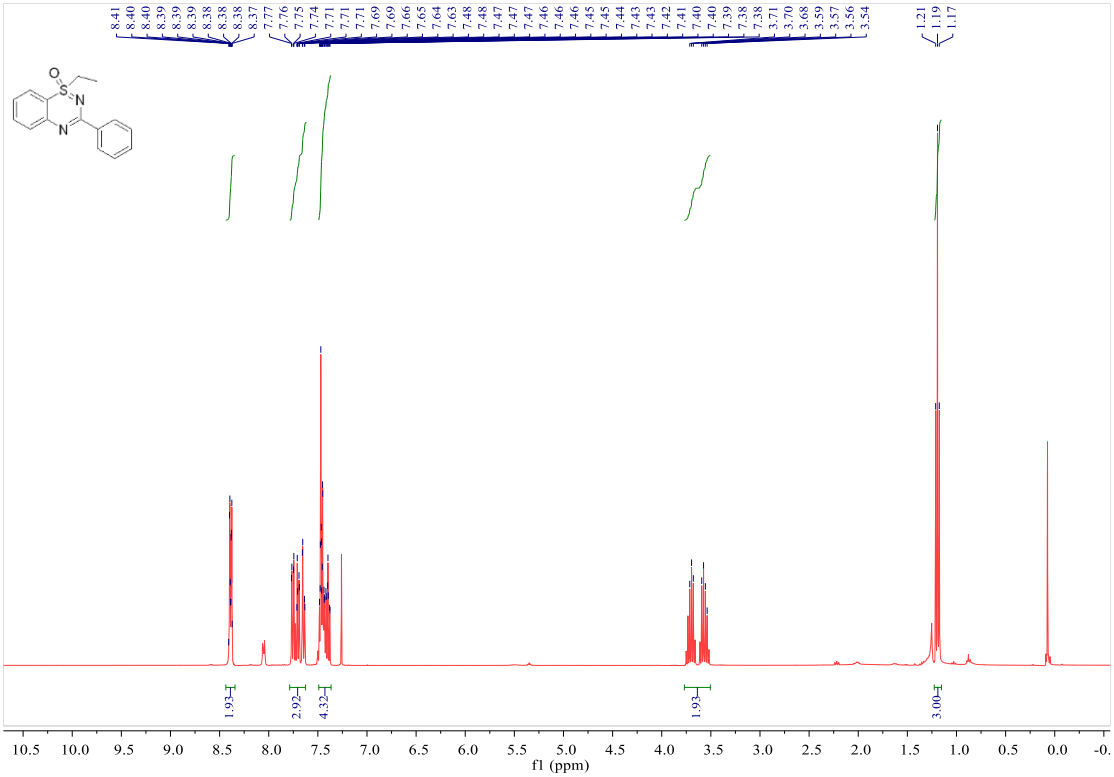
HRMS



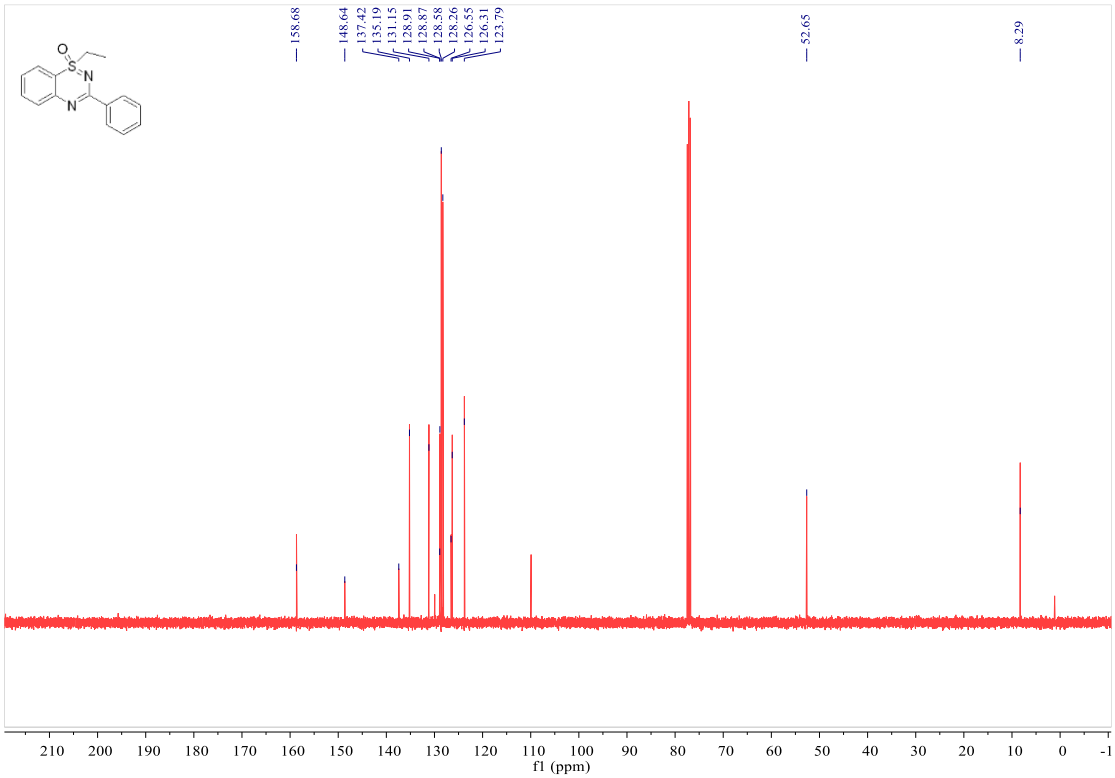
1-ethyl-3-phenyl-λ^4-benzo[*e*][1,2,4]thiadiazine-1-oxide (3fa)



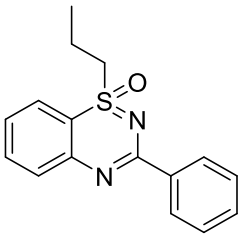
^{1}H NMR (400 MHz, $CDCl_3$)



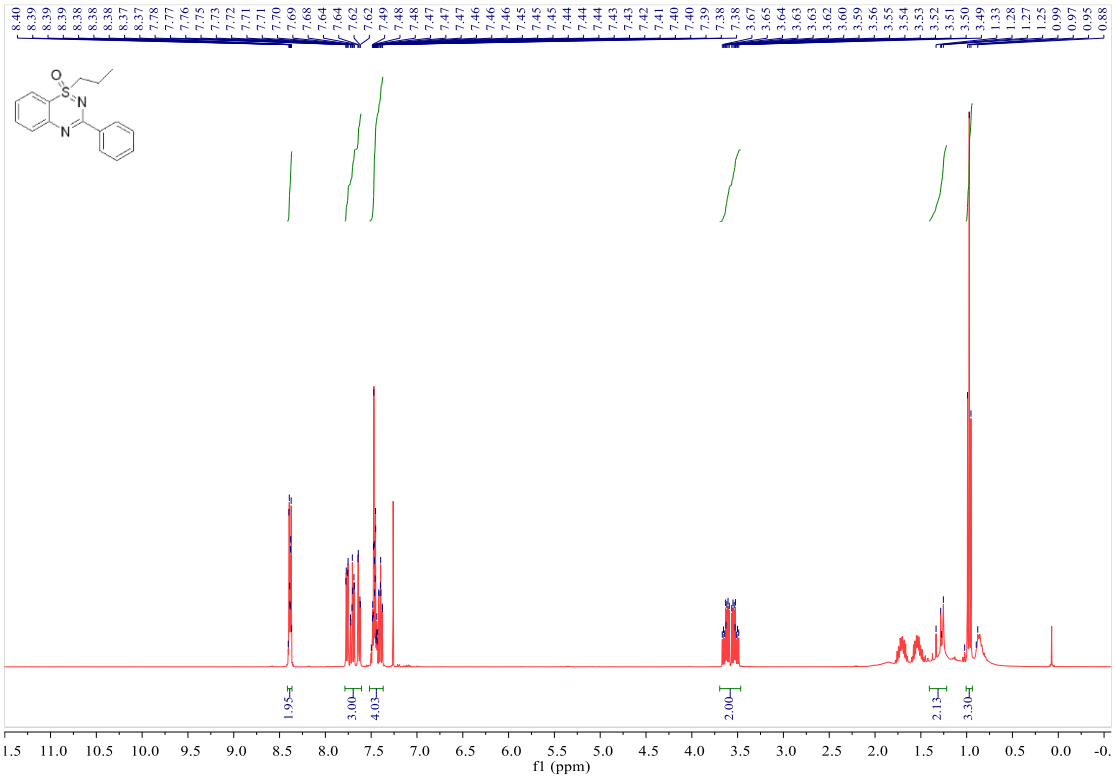
^{13}C NMR (101 MHz, $CDCl_3$)



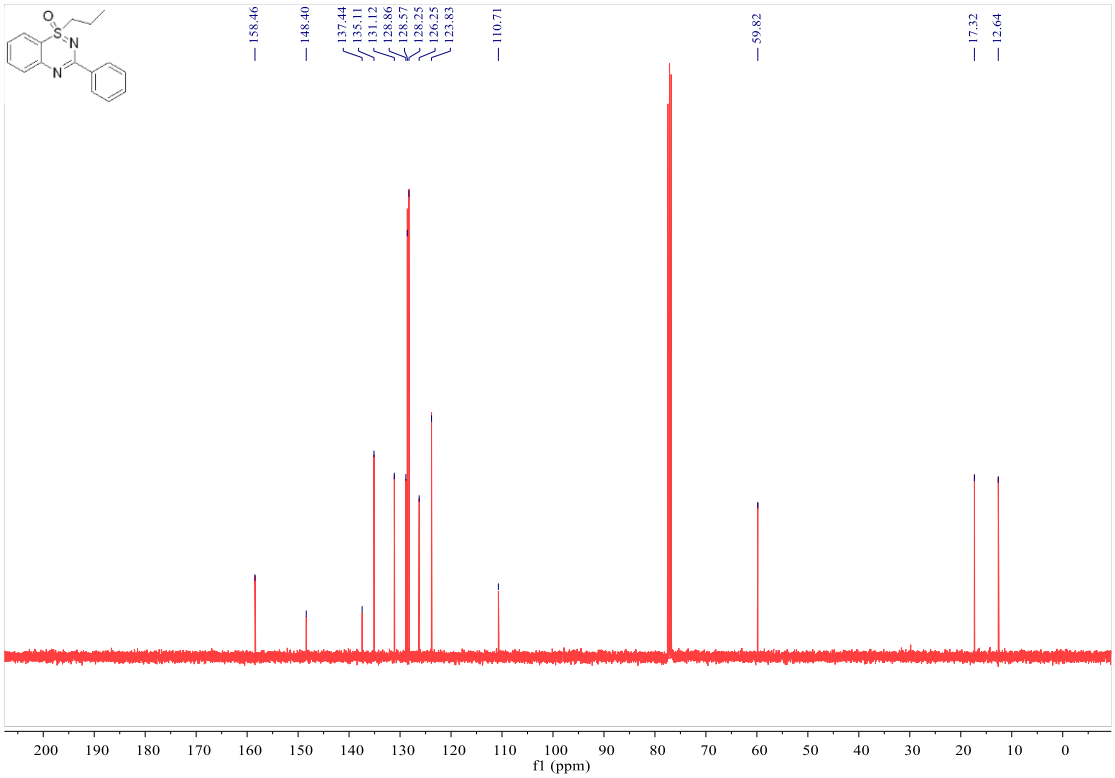
3-phenyl-1-propyl-λ⁴-benzo[*e*][1,2,4]thiadiazine-1-oxide (3ga).



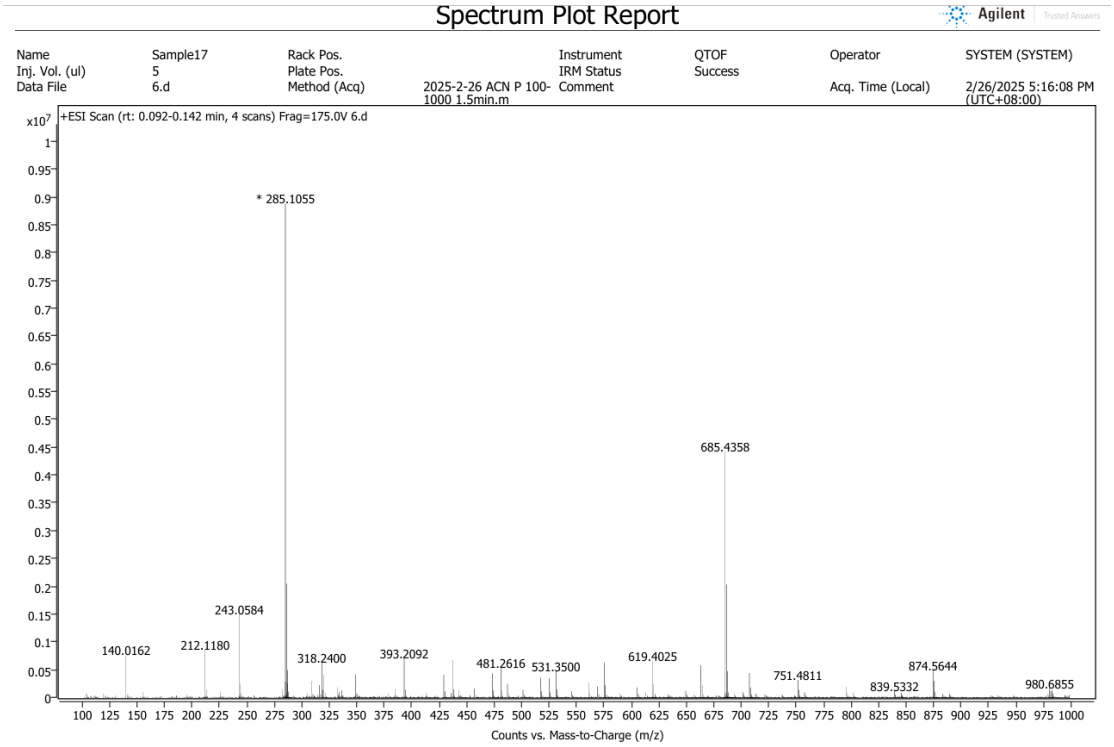
^{1}H NMR (400 MHz, $CDCl_3$)



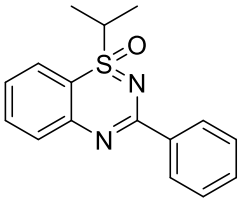
^{13}C NMR (101 MHz, $CDCl_3$)



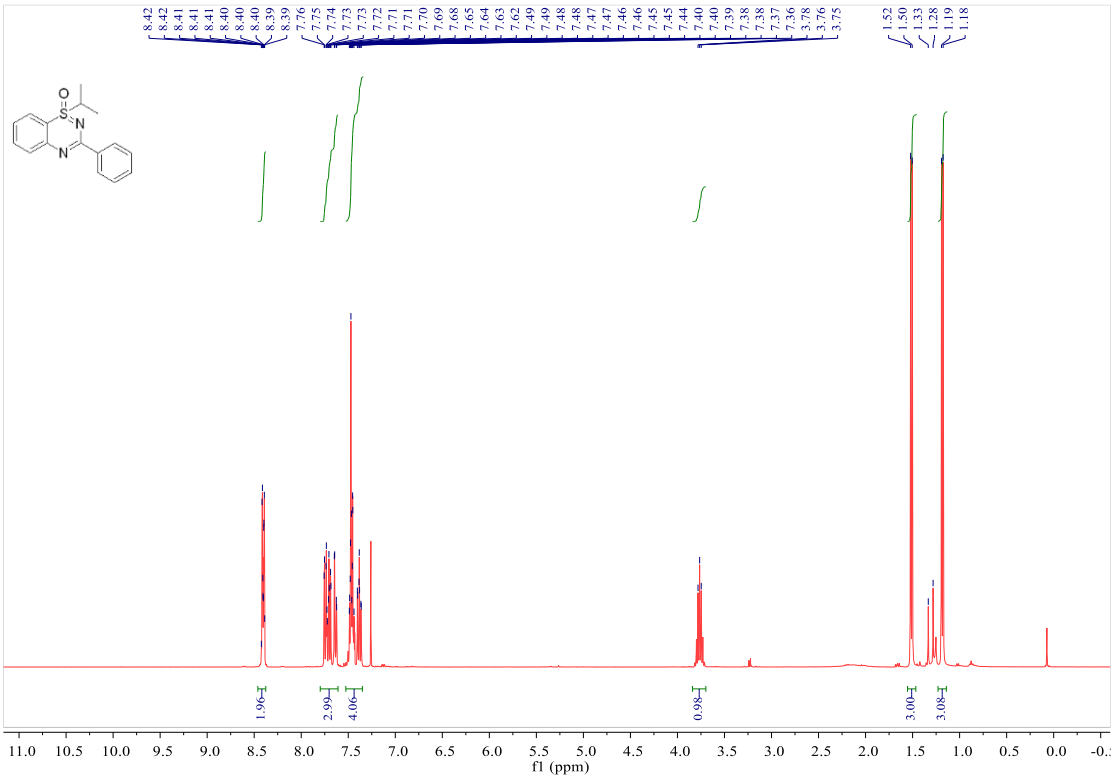
HRMS



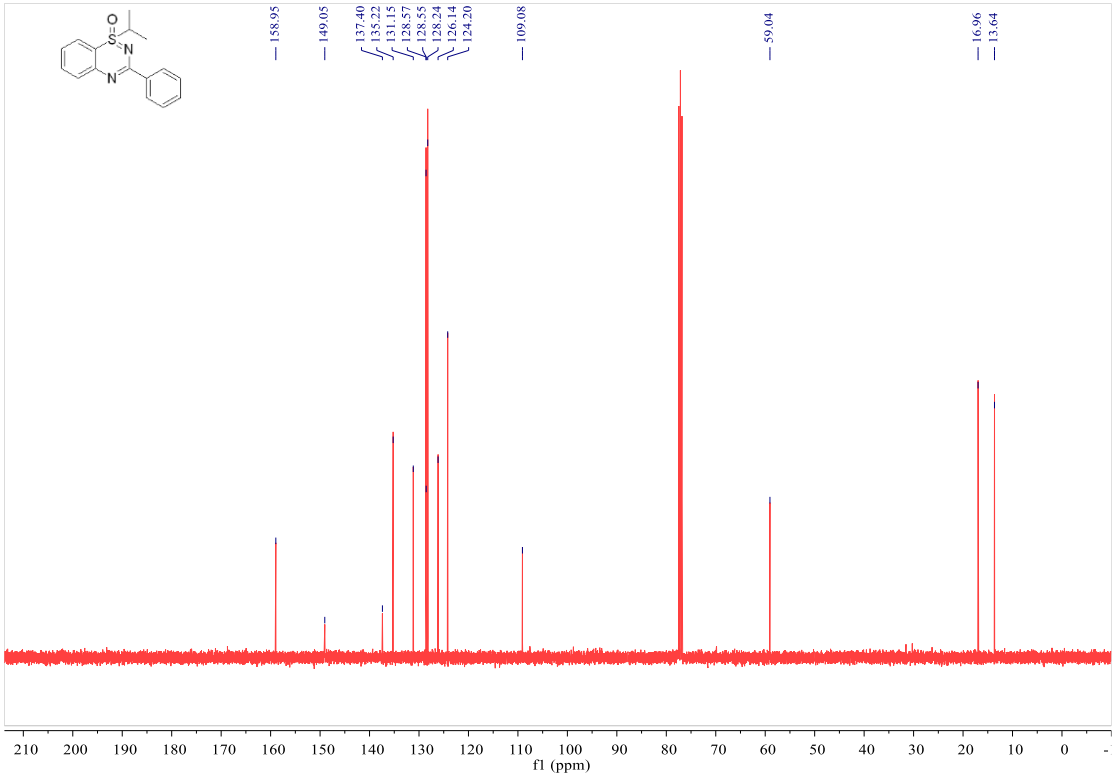
1-isopropyl-3-phenyl-λ⁴-benzo[*e*][1,2,4]thiadiazine-1-oxide (3ha)



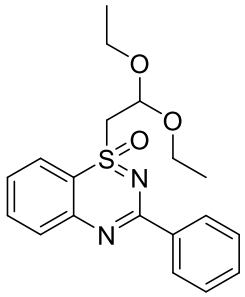
^{1}H NMR (400 MHz, $CDCl_3$)



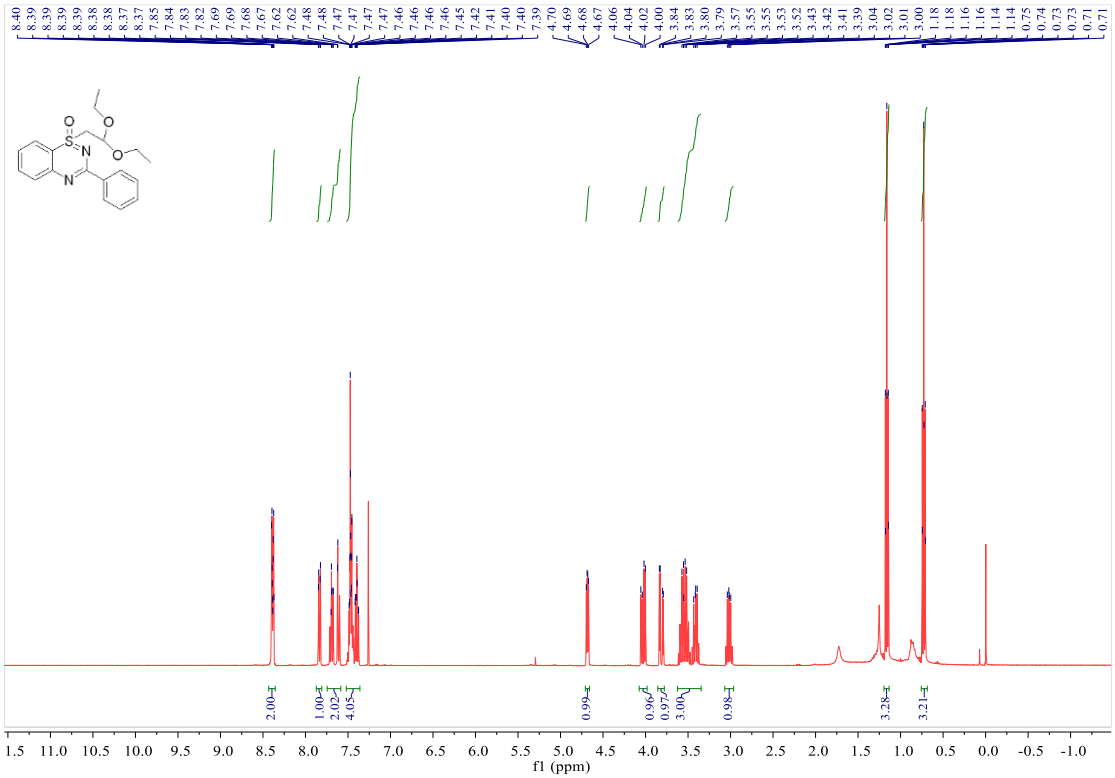
^{13}C NMR (101 MHz, $CDCl_3$)



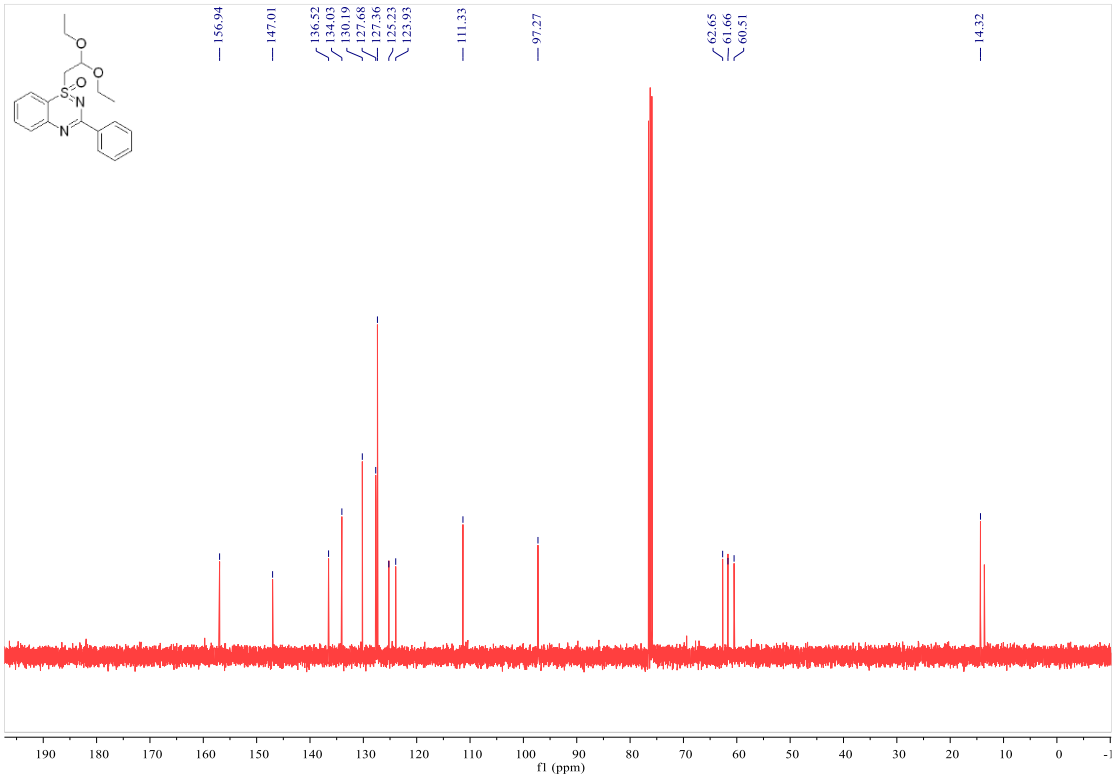
1-(2,2-diethoxyethyl)-3-phenyl-λ^4-benzo[*e*][1,2,4]thiadiazine-1-oxide (3ia).



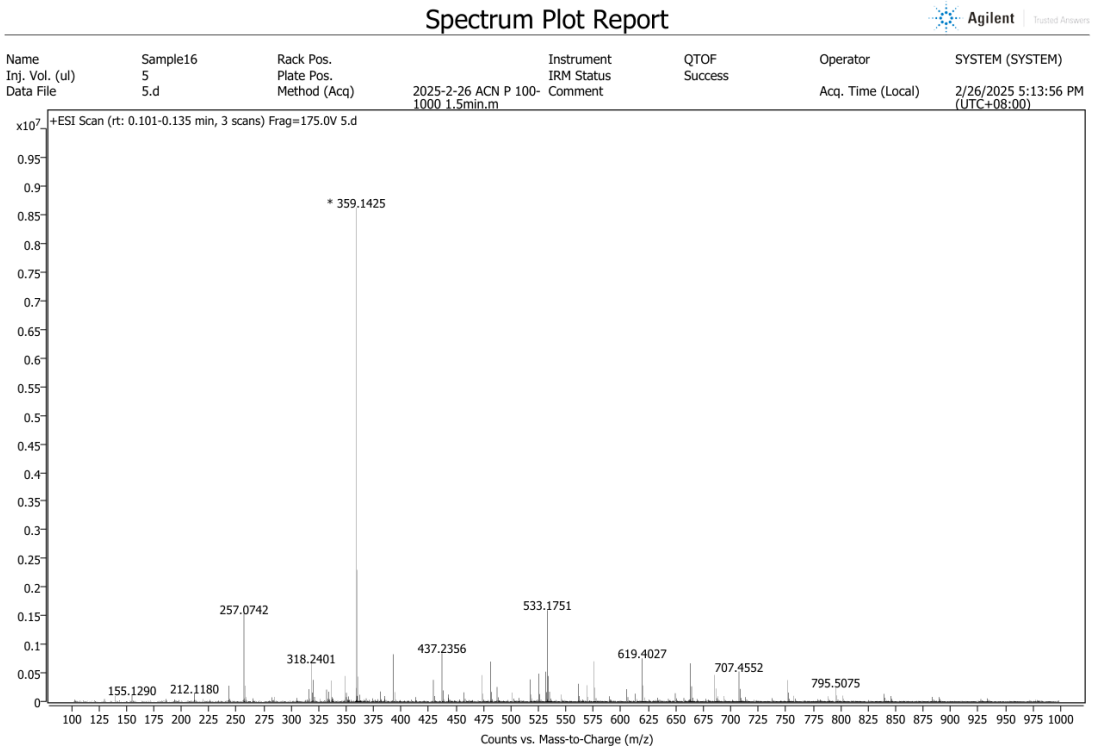
^1H NMR (400 MHz, $CDCl_3$)



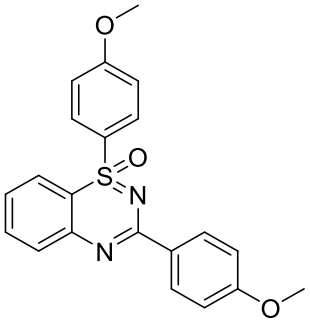
^{13}C NMR (101 MHz, $CDCl_3$)



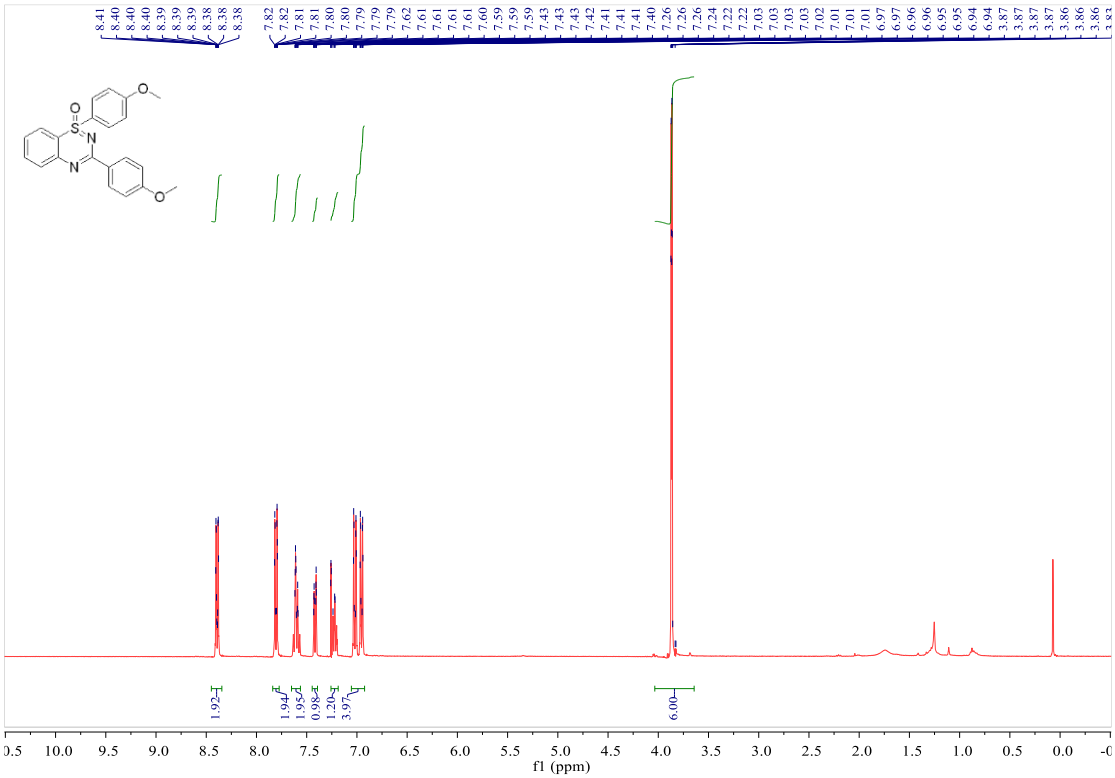
HRMS



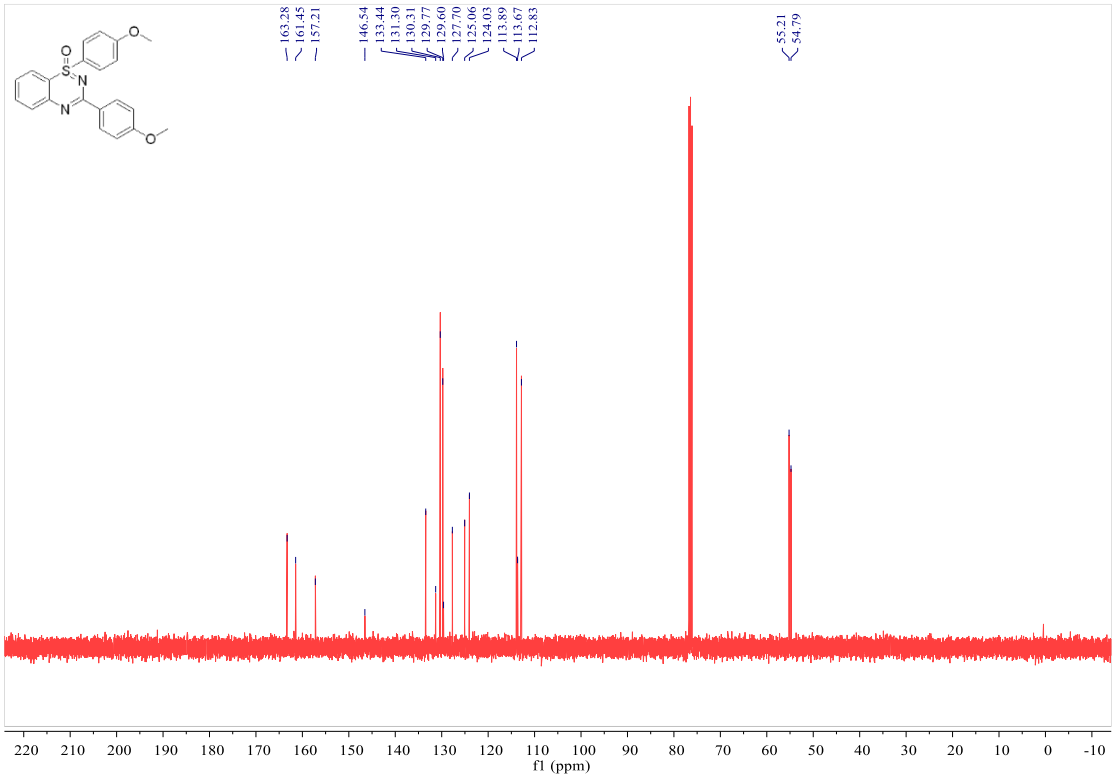
1,3-bis(4-methoxyphenyl)benzo[*e*][1,2,4]thiadiazine-1-oxide (3ec).



^{1}H NMR (400 MHz, $CDCl_3$)



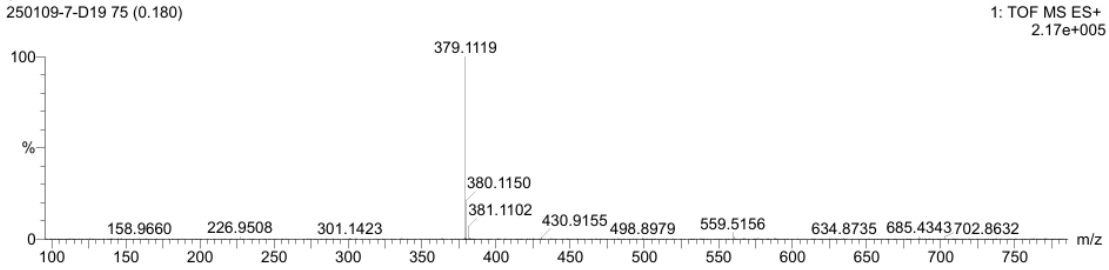
^{13}C NMR (101 MHz, $CDCl_3$)



HRMS

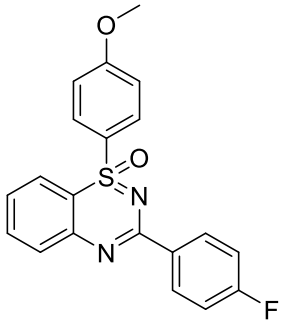
Single Mass Analysis
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1764 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 21-21 H: 0-50 N: 0-200 O: 0-10 Si: 0-5 S: 1-2
6
250109-7-D19 75 (0.180)

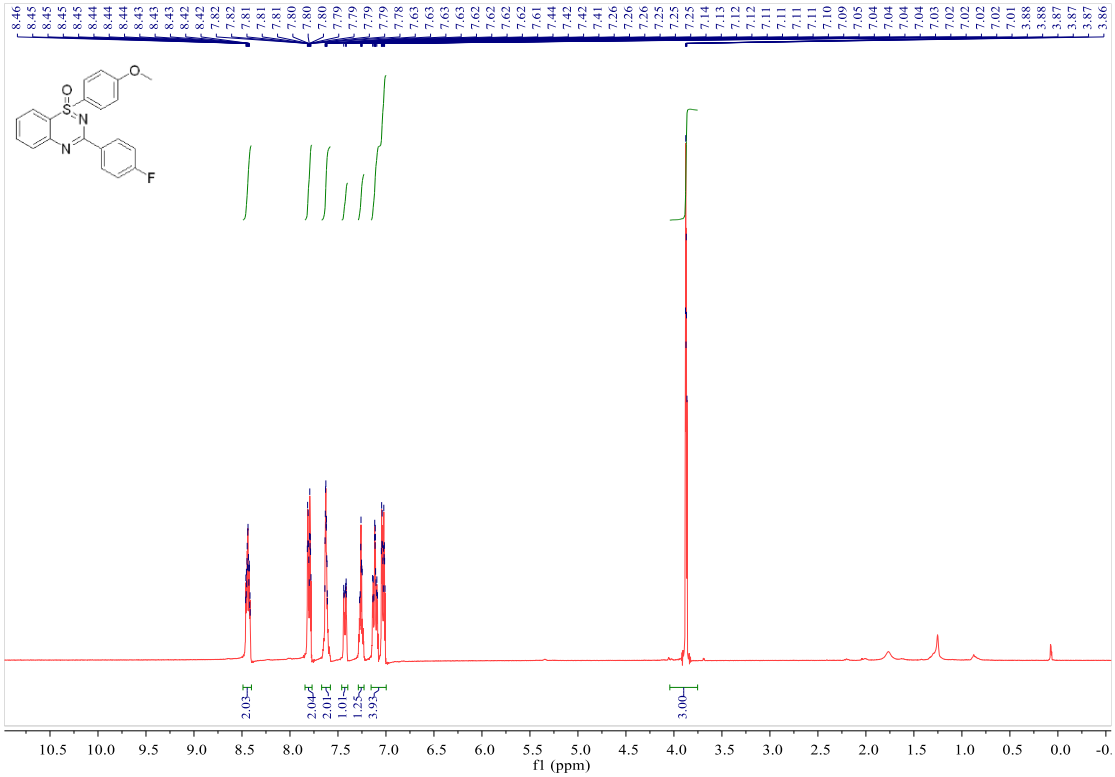


Minimum:				-1.5				
Maximum:		5.0	20.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
379.1119	379.1116	0.3	0.8	13.5	419.8	n/a	n/a	C21 H19 N2 O3 S

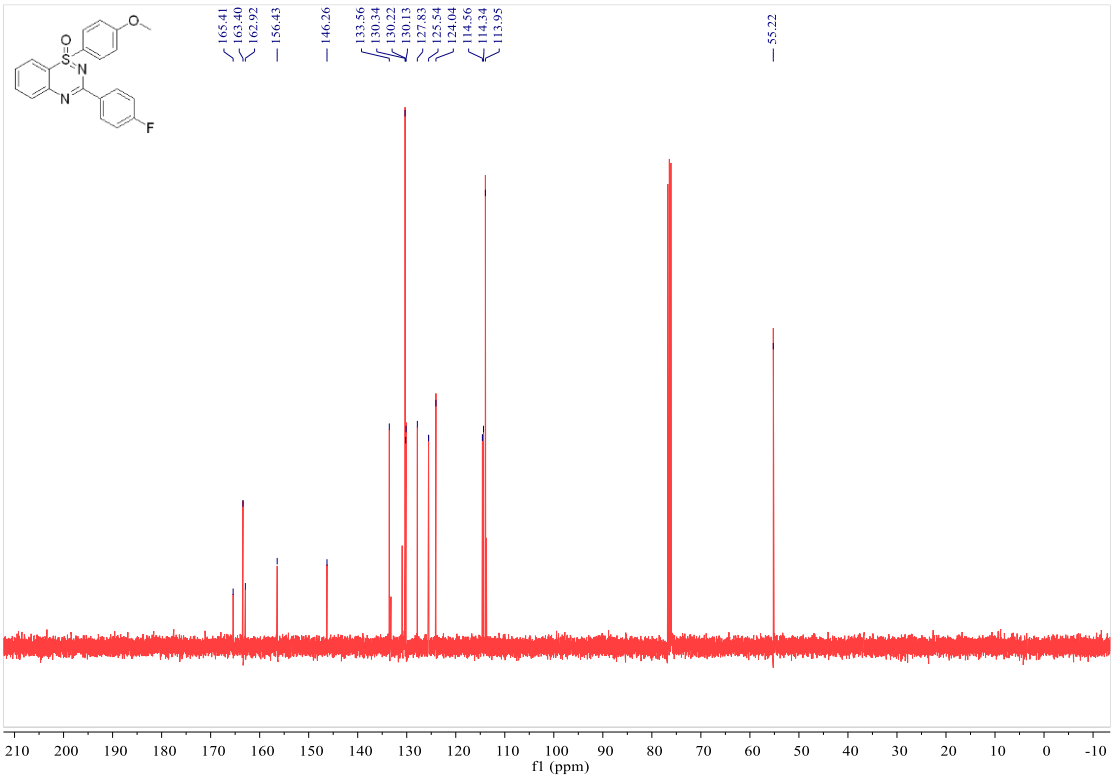
3-(4-fluorophenyl)-1-(4-methoxyphenyl)benzo[*e*][1,2,4]thiadiazine-1-oxide (3ed.)



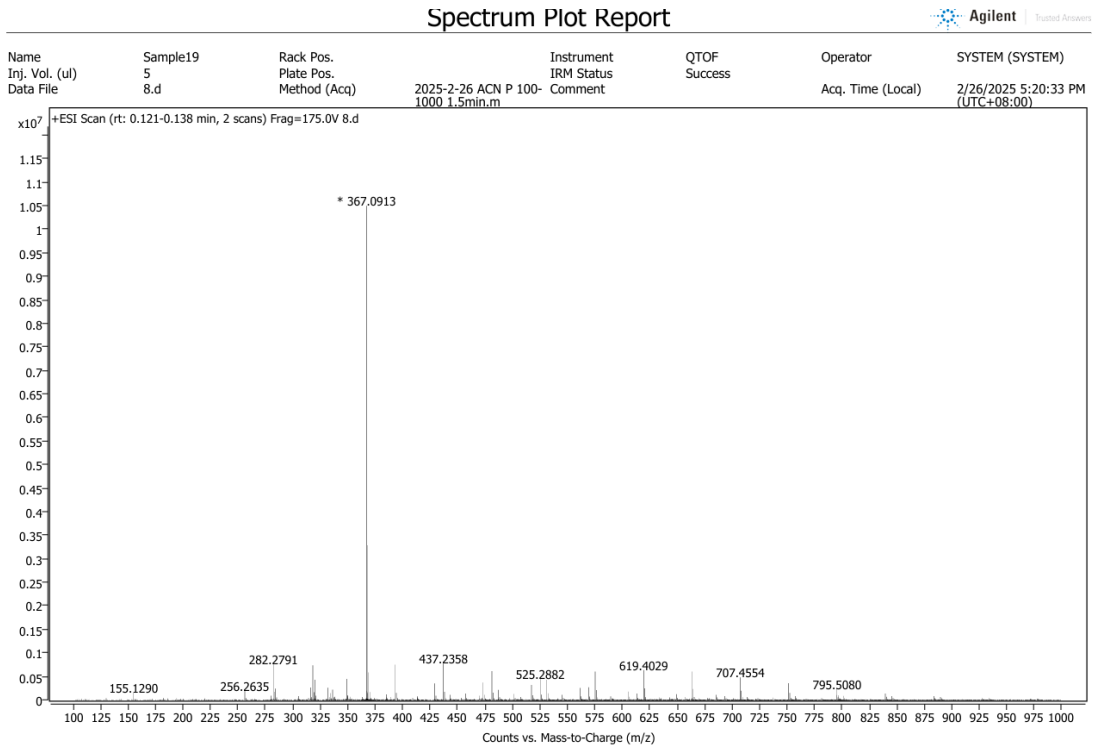
^{1}H NMR (400 MHz, $CDCl_3$)



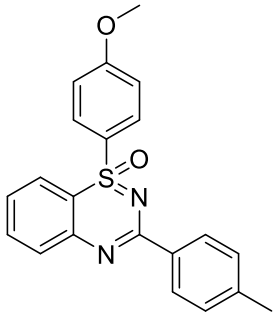
^{13}C NMR (101 MHz, $CDCl_3$)



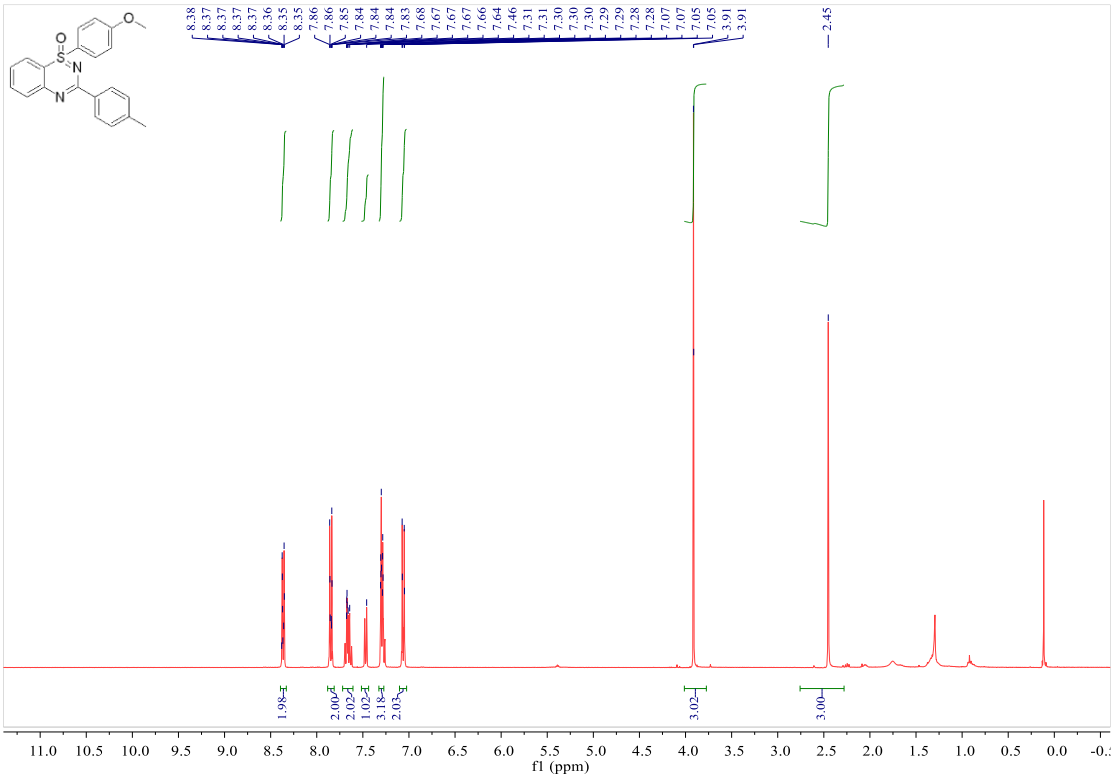
HRMS



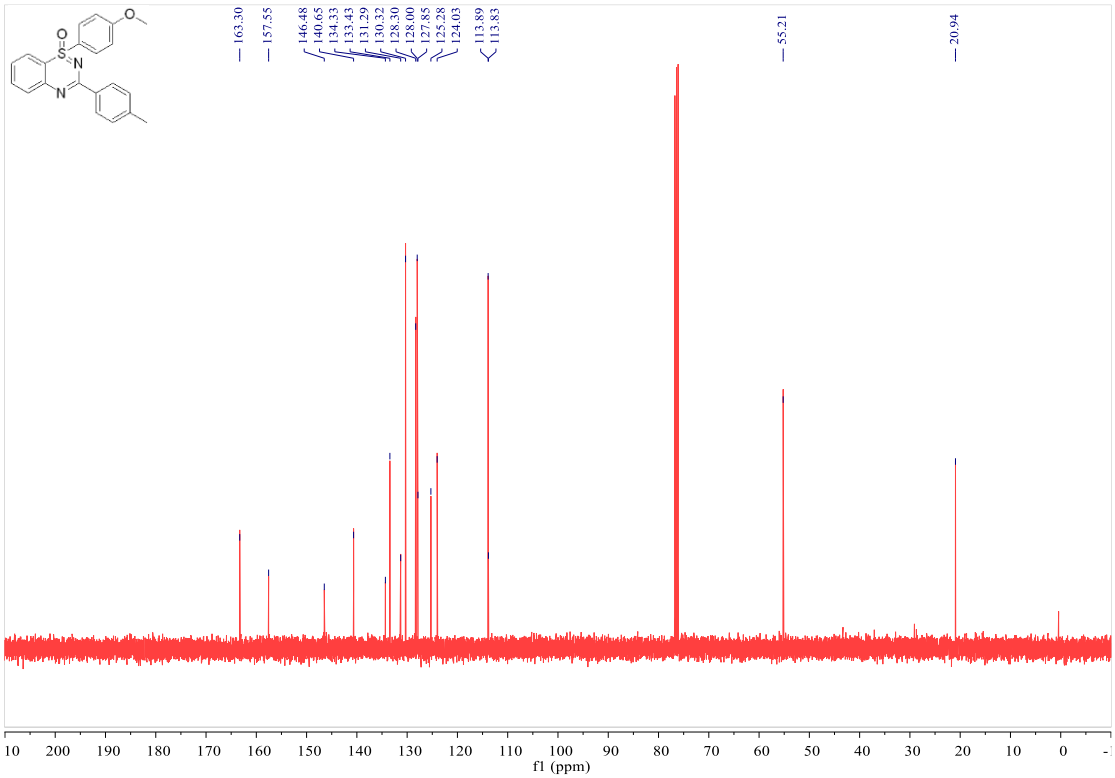
1-(4-methoxyphenyl)-3-(p-tolyl)benzo[*e*][1,2,4]thiadiazine-1-oxide (3ee).



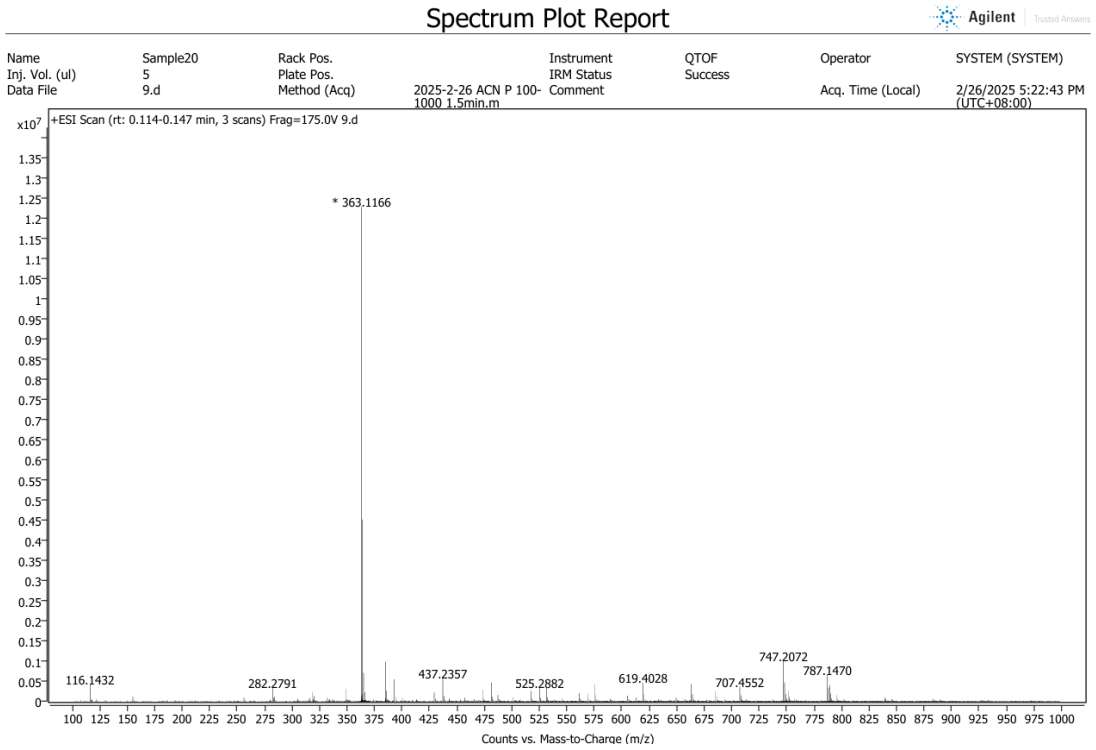
^{1}H NMR (400 MHz, $CDCl_3$)



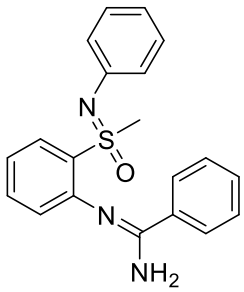
^{13}C NMR (101 MHz, $CDCl_3$)



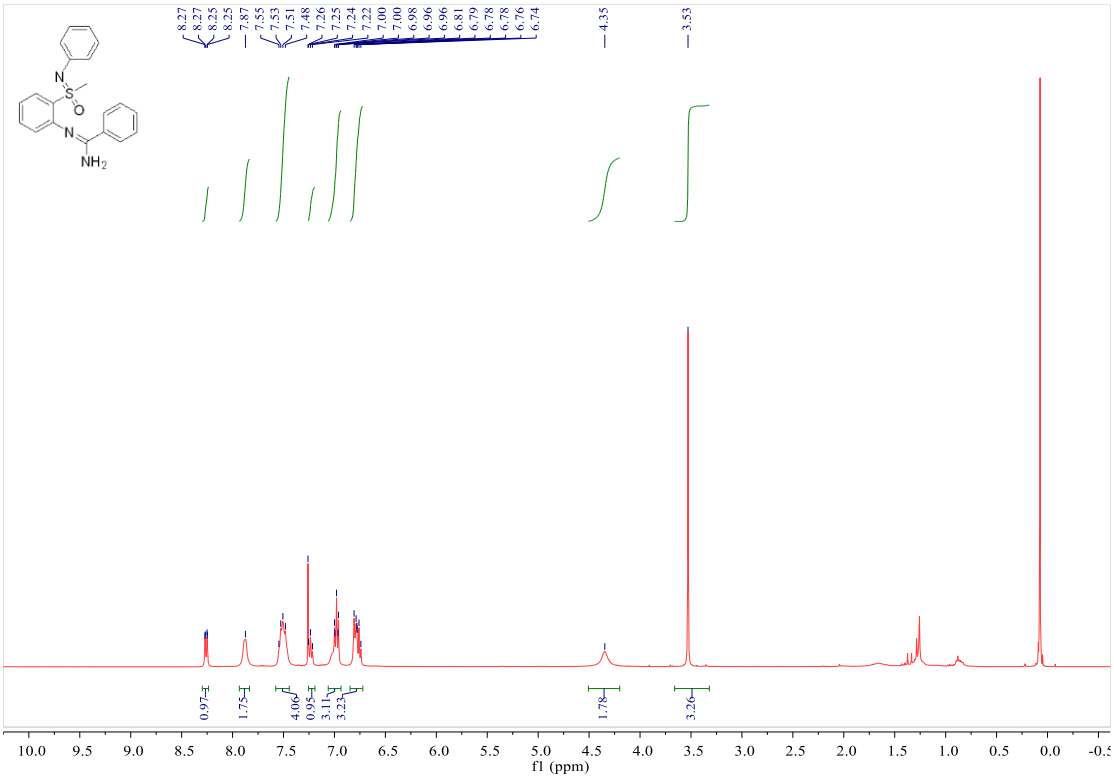
HRMS



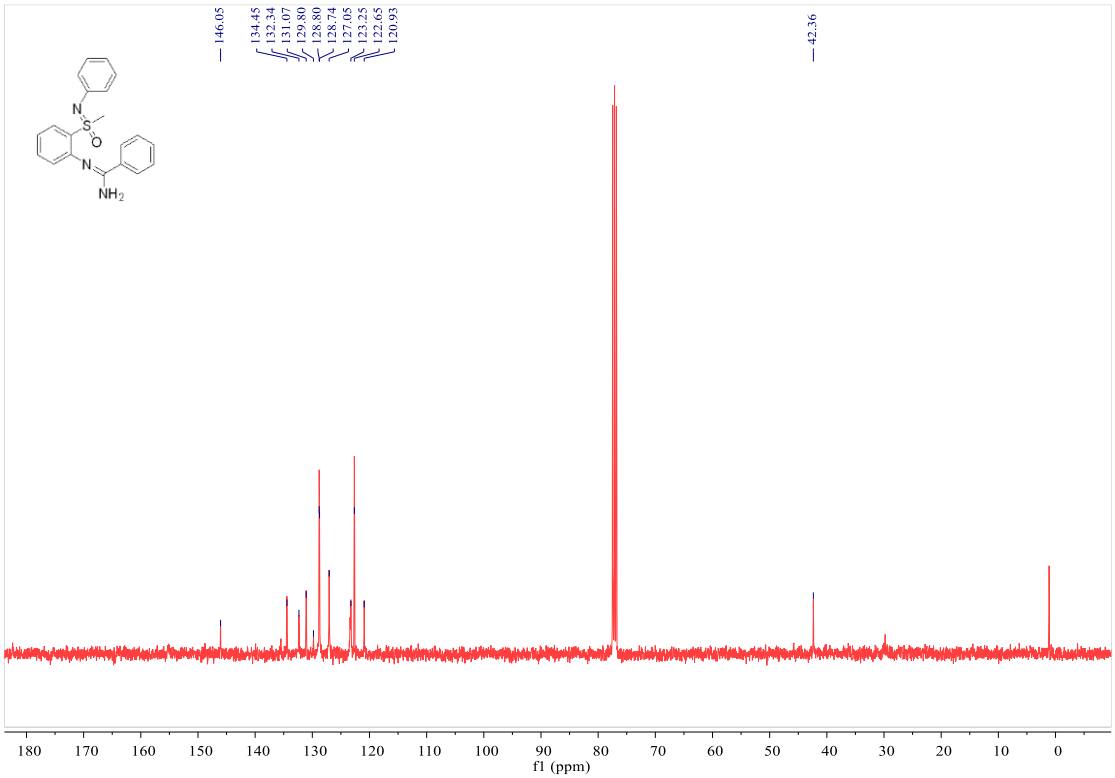
N′-(2-(*S*-methyl-*N*-phenylsulfonimidoyl)phenyl)benzimidamide 4



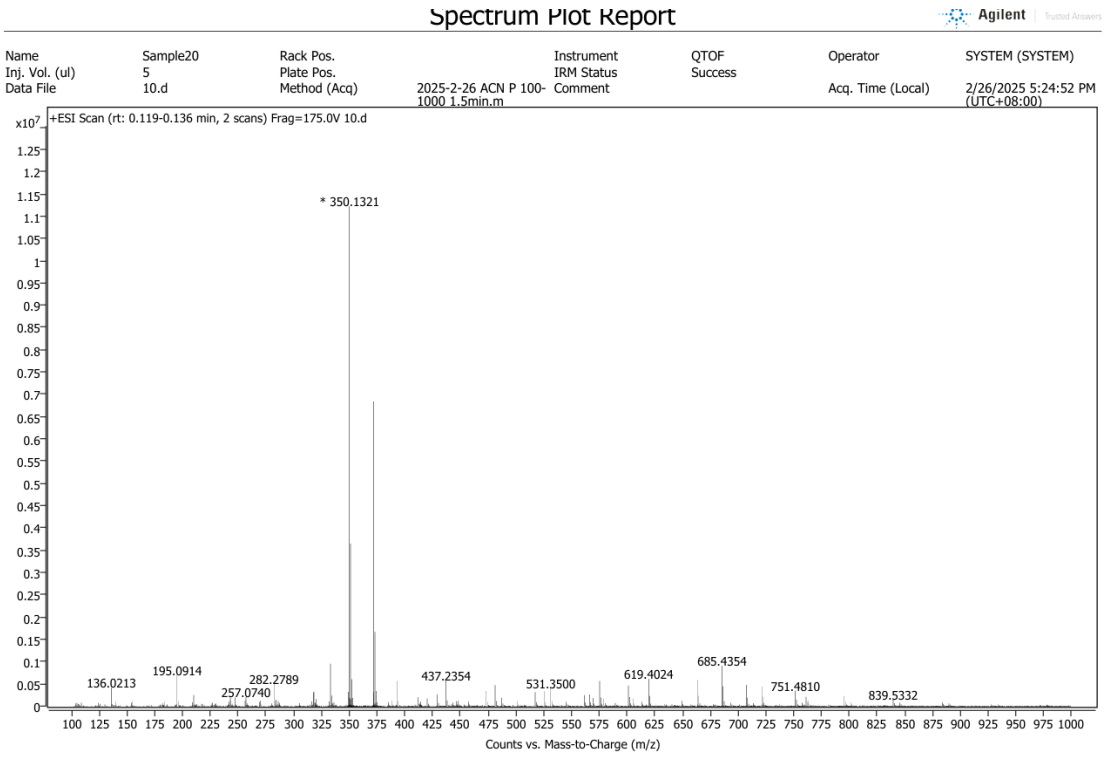
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)


146.05
134.45
132.34
131.07
129.80
128.80
128.74
127.05
123.25
122.65
120.93
42.36
NH2
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

HRMS


Spectrum Plot Report
Agilent
Name Sample20
Inj. Vol. (ul) 5
Data File 10.d
Rack Pos.
Plate Pos.
Method (Acq) 2025-2-26 ACN P 100-1000 1.5min.m
Instrument
IRM Status
Comment
QTOF
Success
Operator
Acq. Time (Local) SYSTEM (SYSTEM)
2/26/2025 5:24:52 PM (UTC+08:00)
+ESI Scan (rt: 0.119-0.136 min, 2 scans) Frag=175.0V 10.d
x10^7
* 350.1321
136.0213
195.0914
257.0740
282.2789
437.2354
531.3500
619.4024
685.4354
751.4810
839.5332
100 125 150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 625 650 675 700 725 750 775 800 825 850 875 900 925 950 975 1000
Counts vs. Mass-to-Charge (m/z)