

Electronic Supplementary Information

Rhodium-Catalyzed Cascade C-H Activation/Annulation Strategy for Expedient Assembly of Pyrrolidinedione-Fused 1,2- Benzothiazines

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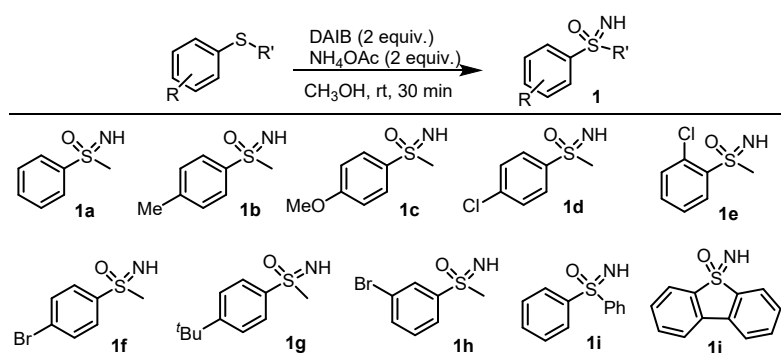
1. General information

Experimental: Unless otherwise noted, all the reactions were set up under air atmosphere. Reactions were monitored using thin-layer chromatography (TLC) on Silica Gel plates. Visualization of the developed plates was performed under UV light (245 or 365 nm) stain. Silica-gel flash column chromatography was performed using 200–300 mesh silica gel.

Materials: Unless otherwise indicated, starting catalysts and materials were obtained from Energy Chemicals, Bidepharm. Moreover, commercially available reagents were used without additional purification

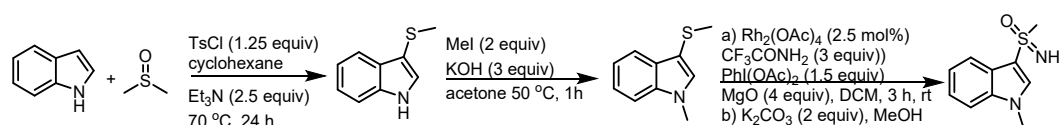
Instrumentation: Melting points were recorded on an uncorrected Melting Point instrument. The ^1H and ^{13}C NMR spectra were recorded on a 400 MHz and 100 MHz NMR spectrometers, unless otherwise specified. Chemical shifts (δ) in parts per million were reported relative to the residual signals of chloroform (7.26 ppm for ^1H and 77.0 ppm for ^{13}C) or DMSO- d_6 (2.54 ppm for ^1H and 40.5 ppm for ^{13}C), and all ^{13}C NMR were recorded with proton broadband decoupling and indicated as $^{13}\text{C}\{^1\text{H}\}$ NMR. Multiplicities are described as s (singlet), d (doublet), t (triplet), q (quartet), or m (multiplet), and the coupling constants (J) are reported in Hertz (Hz). HRMS analysis with a quadrupole time-of-flight mass spectrometer yielded ion mass/charge (m/z) ratios in atomic mass units.

2. General procedure for the synthesis of sulfoximines 1



According to the reported literature,^[1] a mixture of aryl sulfide (5 mol), ammonium acetate (10 mol, 0.77 g), iodobenzene acetate (10 mol, 3.22 g) were added to a 50 mL round-bottomed flask equipped with a stirring bar. Methanol was then added. The resulting mixture was stirred at room temperature for 30 minutes. Upon completion of the reaction, the reaction mixture was cooled to room temperature, evaporation under vacuum to remove the solvent, then extracted with CH_2Cl_2 (3 \times 15 mL), and washed with brine. The organic layer was combined, dried over Na_2SO_4 , filtered, and then evaporated under a vacuum. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:1, v/v) as the elution solvent to give desired white solid or colorless oily liquid.

3. General procedure for the synthesis of indolyl sulfoximine 4



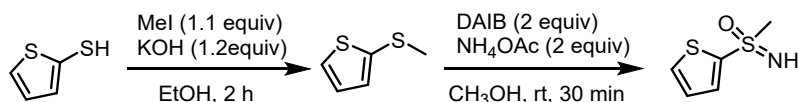
Step 1: According to the reported literature,^[2] a mixture of indole (5 mmol, 0.59 g), DMSO (3 equiv,

15 mmol, 1.1 mL), *p*-toluenesulfonyl chloride (1.25 equiv, 1.19 g) were added to a 50 mL round-bottomed flask equipped with a stirring bar. Cyclohexane (20 mL) was then added. The resulting mixture was stirred in an oil bath preheated to 70 °C for 24 hours. Upon completion of the reaction, the reaction mixture was cooled to room temperature, extracted with EtOAc (3×15 mL), and washed with brine. The organic layer was combined, dried over Na₂SO₄, filtered, and then evaporated under a vacuum. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:10 v/v) as the elution solvent to give red liquid 3-(methylthio)-1*H*-indole in 80% yield.

Step 2: A mixture of 3-(methylthio)-1*H*-indole (5 mmol, 0.82g), iodomethane (2 equiv, 10 mmol, 0.62 mL), KOH (3 equiv, 1.2 g) were added to a 50 mL round-bottomed flask equipped with a stirring bar. Acetone (20 ml) was then added. The resulting mixture was stirred in an oil bath preheated to 50 °C for 1 hours. Upon completion of the reaction, the reaction mixture was cooled to room temperature, evaporation under vacuum to remove the solvent, then extracted with EtOAc (3×15 mL), and washed with brine. The organic layer was combined, dried over Na₂SO₄, filtered, and then evaporated under a vacuum. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:10 v/v) as the elution solvent to give red liquid 1-methyl-3-(methylthio)-1*H*-indole in 90% yield.

Step 3: According to the reported literature,^[3] a mixture of 1-methyl-3-(methylthio)-1*H*-indole (5 mmol, 0.89g), trifluoroacetamide (3 equiv, 1.7 g), Rh₂(OAc)₄ (2.5 mol%, 55 mg), PIDA (1.5 equiv, 2.4 g), MgO (4 equiv, 20 mmol, 0.8 g) were added to a 50 mL round-bottomed flask equipped with a stirring bar. The resulting mixture was stirred at room temperature for 3 hours. Upon completion of the reaction, vacuum pumping removes most of the solids. extracted with CH₂Cl₂ (3×15 mL), and washed with brine. The organic layer was combined, dried over Na₂SO₄, filtered, and then evaporated under a vacuum. Purification is not required, then K₂CO₃ (2 equiv, 10 mmol, 1.38 g) and methanol (20 mL) was added, the resulting mixture was stirred at room temperature for 2 hours. Upon completion of the reaction, evaporation under vacuum to remove the solvent, then extracted with CH₂Cl₂ (3×15 mL), and washed with brine. The organic layer was combined, dried over Na₂SO₄, filtered, and then evaporated under a vacuum. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:3 v/v) to give white solid imino(methyl)(1-methyl-1*H*-indol-3-yl)-λ⁶-sulfanone in 87% yield. mp 134-135 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.97 (d, *J* = 8.0 Hz, 1H), 7.64 (s, 1H), 7.34 (t, *J* = 8.0 Hz, 1H), 7.31 (t, *J* = 6.8 Hz, 1H), 7.27 (t, *J* = 7.6 Hz, 1H), 3.15 (s, 3H), 3.17 (s, 3H), 2.95 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 137.3, 133.8, 124.4, 123.3, 122.0, 119.6, 116.3, 110.3, 46.7, 33.4; HRMS (ESI-TOF) *m/z*: [M+H]⁺ calcd for C₁₀H₁₃N₂OS 209.0743; found 209.0736.

4. General procedure for the synthesis of thienyl sulfoximine 6

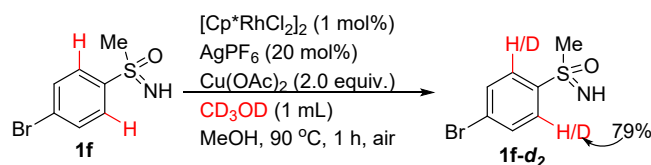


Step 1: According to the reported literature,^[4] a mixture of thiophene-2-thiol (1.0 equiv, 5 mmol, 0.58 g), iodomethane (1.1 equiv., 5.5 mmol, 0.34 mL), NaOH (1.2 equiv., 6 mmol, 0.24 g) were added to a 50 mL round-bottomed flask equipped with a stirring bar. Ethanol (20 mL) was then added. The resulting mixture was stirred at room temperature for 2 hours. Upon completion of the reaction, evaporation under vacuum to remove the solvent, then extracted with EtOAc (3×15 mL).

The organic layer was combined, dried over Na₂SO₄, filtered, and then evaporated under a vacuum. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:100 v/v), to obtain red solid 2-(methylthio)thiophene in 79% yield.

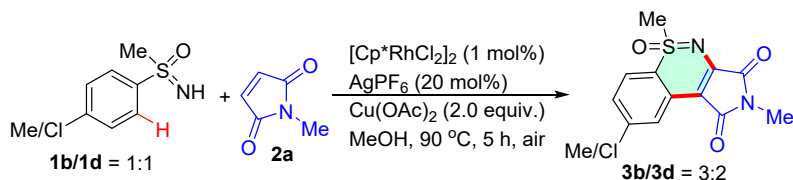
Step 2: According to the reported literature,^[5] a mixture of 2-(methylthio)thiophene (5 mol, 0.65 g), ammonium acetate (10 mol, 0.77 g), iodobenzene acetate (10 mol, 3.22 g) were added to a 50 mL round-bottomed flask equipped with a stirring bar. Methanol (20 mL) was then added. The resulting mixture was stirred at room temperature for 30 minute. Upon completion of the reaction, evaporation under vacuum to remove the solvent, then extracted with EtOAc (3×15 mL). The organic layer was combined, dried over Na₂SO₄, filtered, and then evaporated under a vacuum. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:1 v/v) to obtain colorless oily liquid imino(methyl)(thiophen-2-yl)-λ⁶-sulfanone in 69% yield. mp 162-163 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.56-7.54 (m, 2H), 7.00 (dd, *J* = 4.0 Hz, *J* = 4.0 Hz, 1H), 3.17 (s, 1H), 3.11 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 145.5, 133.4, 133.0, 127.8, 47.3; HRMS (ESI-TOF) *m/z*: [M+H]⁺ calcd for C₅H₈NOS₂ 162.0042; found 162.0047.

5. H/D Exchange experiment



A mixture of **1f** (0.2 mmol), [RhCp*Cl₂]₂ (1 mol%, 3 mg), AgPF₆ (20 mol %, 34 mg), Cu(OAc)₂ (2 equiv, 80 mg) CD₃OD (1 ml) were added to a 15 mL round-bottomed flask equipped with a stirring bar. Methanol (3 mL) was then added. The resulting mixture was stirred in an oil bath preheated to 90 °C for 1 hours. Upon completion of the reaction, the reaction mixture was cooled to room temperature, extracted with CH₂Cl₂ (3×10 mL). The organic layer was combined, dried over Na₂SO₄, filtered, and then evaporated under a vacuum. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:1, v/v) to obtain the desired products **1f-d₂** in 70% yield. 79 % of the hydrogen in the ortho-position of imine is deuterated.

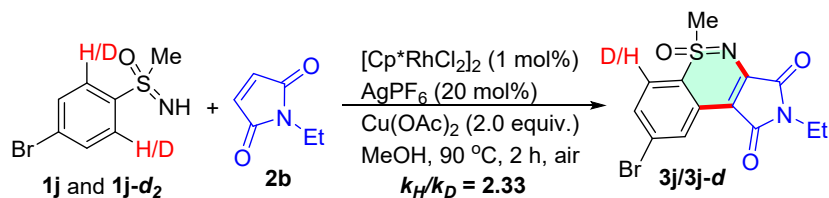
6. General procedure for the competitive experiment



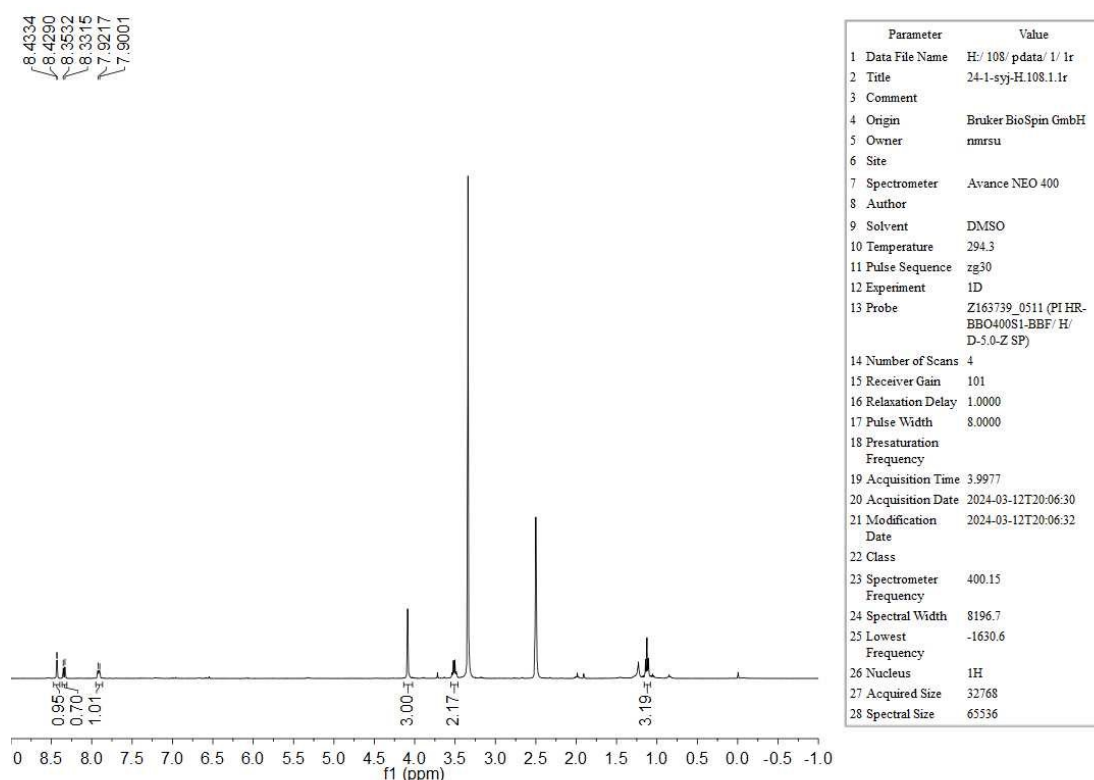
A mixture of **1b** (0.1 mmol), **1d** (0.1 mmol), **2a** (0.25 mmol), [RhCp*Cl₂]₂ (1 mol%, 3 mg), AgPF₆ (20 mol %, 34 mg), Cu(OAc)₂ (2 equiv, 80 mg) were added to a 15 mL round-bottomed flask equipped with a stirring bar. Methanol (3 mL) was then added. The resulting mixture was stirred in an oil bath preheated to 90 °C for 5 hours. Upon completion of the reaction, the reaction mixture was cooled to room temperature, extracted with CH₂Cl₂ (3×10 mL). The organic layer was

combined, dried over Na₂SO₄, filtered, and then evaporated under a vacuum. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:3, v/v) to obtain the desired products **3b** and **3d** in a ratio of 1:1.5.

7. Kinetic Isotope Effect study



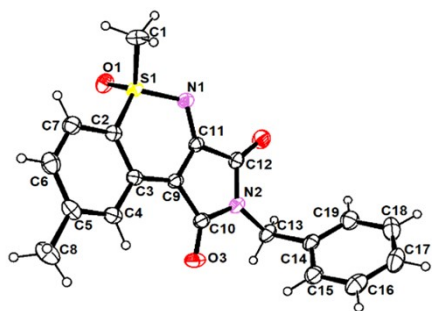
A mixture of **1j** (0.1 mmol), **1j-d₂** (0.1 mmol), **2b** (0.25 mmol), [Cp*RhCl₂]₂ (1 mol%, 3 mg), AgPF₆ (20 mol %, 34 mg), Cu(OAc)₂ (2 equiv., 80 mg) were added to a 15 mL round-bottomed flask equipped with a stirring bar. Methanol (3 mL) was then added. The resulting mixture was stirred in an oil bath preheated to 90 °C for 2 hours. Upon completion of the reaction, the reaction mixture was cooled to room temperature, extracted with CH₂Cl₂ (3×10 mL). The organic layer was combined, dried over Na₂SO₄, filtered, and then evaporated under a vacuum. The residue was purified using flash column chromatography with a silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:3, v/v) to obtain the mixture products **3j** and **3j-d**. The KIE experiment result was detected by NMR. A KIE value (k_H/k_D) was determined to be 2.33 by the ¹H NMR test.



8. References:

- [1] Y. Cheng and C. Bolm, *Angew. Chem. Int. Ed.*, 2015, **54**, 12349-12352.
- [2] L.-Y. Zhang, Y.-H. Wu, N.-X. Wang, X.-W. Gao, Z. Yan, B.-C. Xu, N. Liu, B.-Z. Wang and Y. Xing, *Eur. J. Org. Chem.*, 2021, **2021**, 1446-1451.
- [3] H. Okamura and C. Bolm, *Org. Lett.*, 2004, **6**, 1305-1307.
- [4] Z. Hloušková, M. Klikar, O. Pytela, N. Almonasy, A. Růžička, V. Jandová and F. Bureš, *RSC adv.*, 2019, **9**, 23797-23809.
- [5] C. Kang, M. Li, W. Huang, S. Wang, M. Peng, L. Zhao, G. Jiang and F. Ji, *Green Chem.*, 2023, **25**, 8838-8844.

9. X-ray crystallographic data of compound 3q



The purified compound **3q** is dissolved in a mixed solvent of dichloromethane and *n*-hexane, and placed in a dark cabinet to slowly evaporate. After several days, a colourless bulk crystal is obtained. The X-ray crystal-structure determinations were obtained on a Bruker Smart CCD C APEX-2 diffractometer (graphite-monochromated Mo $K\alpha$ radiation, $\lambda=0.71073$ nm) at 293.15 K.

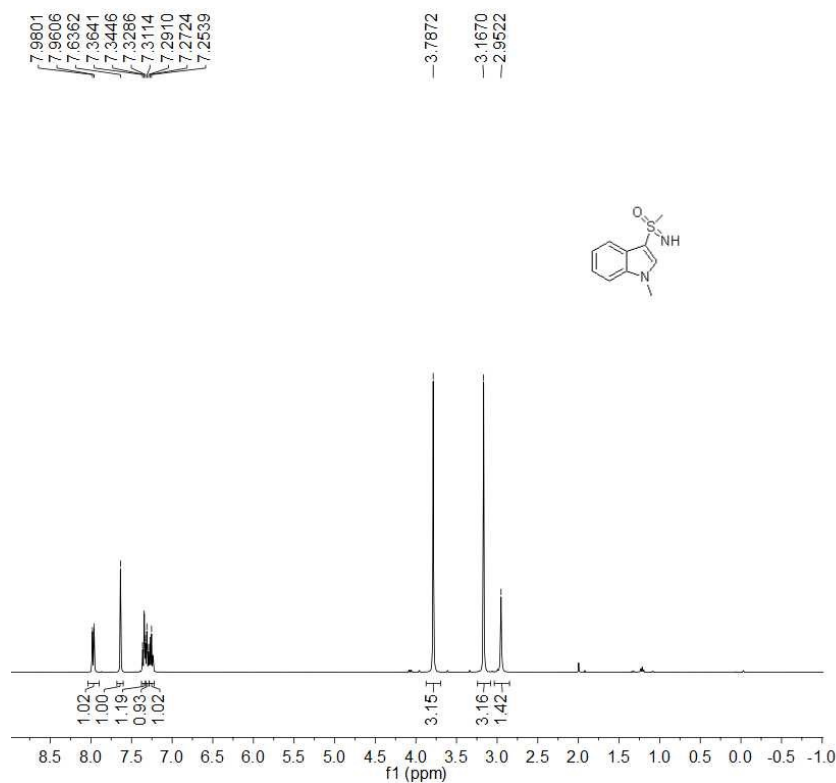
Figure S1. ORTEP drawing of compound **3q** (30% probability for the thermal ellipsoid).

Table S1. Crystal data and structure refinement for compound **3q**.

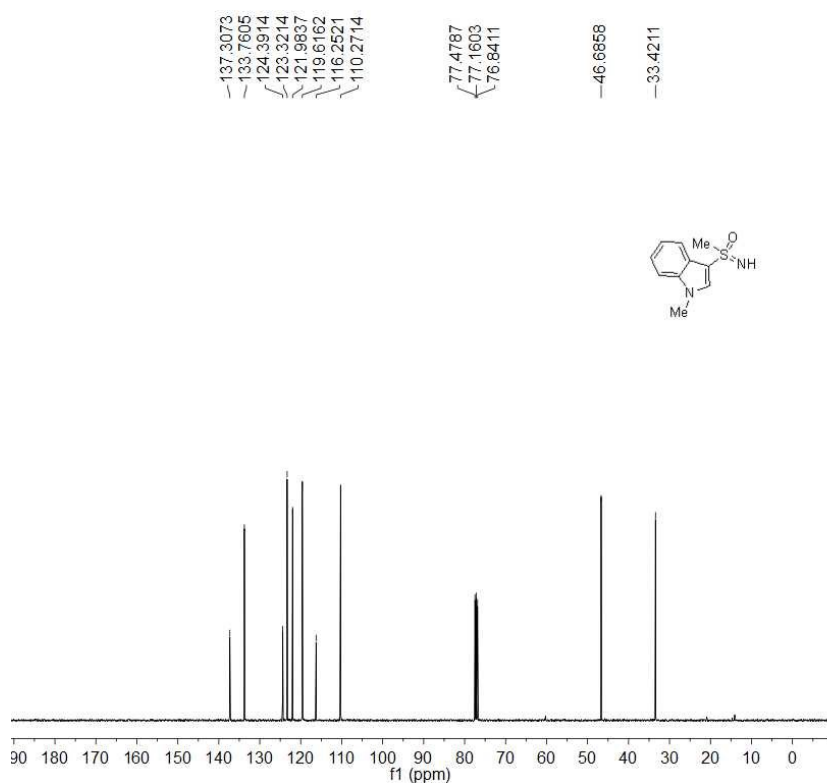
CCDC number	2328549
Identification code	330831d_0m_a
Empirical formula	$C_{19}H_{16}N_2O_3S$
Formula weight	352.40
Temperature	293.15 K
Wavelength	0.71073 Å
Crystal system	orthorhombic
Space group	$P2_1/c$
Unit cell dimensions	$a = 11.45(2)$ Å $\alpha = 90^\circ$. $b = 8.899(16)$ Å $\beta = 101.80(3)^\circ$. $c = 17.03(3)$ Å $\gamma = 90^\circ$.
Volume	$1698(6)$ Å ³
Z	4
Density (calculated)	1.379 Mg/m ³
Absorption coefficient	0.211 mm ⁻¹
F(000)	736.0
Crystal size	$0.16 \times 0.15 \times 0.13$ mm ³
2 θ range for data collection	3.636 to 55.012°.
Index ranges	$-14 \leq h \leq 14, -11 \leq k \leq 11, -21 \leq l \leq 22$
Reflections collected	18605
Independent reflections	3868 [$R_{int} = 0.0336, R_{sigma} = 0.0279$]
Data / restraints / parameters	3868/0/228
Goodness-of-fit on F^2	1.053
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0391, wR_2 = 0.1077$
R indices (all data)	$R_1 = 0.0505, wR_2 = 0.1160$
Largest diff. peak and hole	0.31 and -0.39 e.Å ⁻³

10. ¹H and ¹³C NMR spectra for all compounds

Imino(methyl)(1-methyl-1*H*-indol-3-yl)-λ⁶-sulfanone (4)

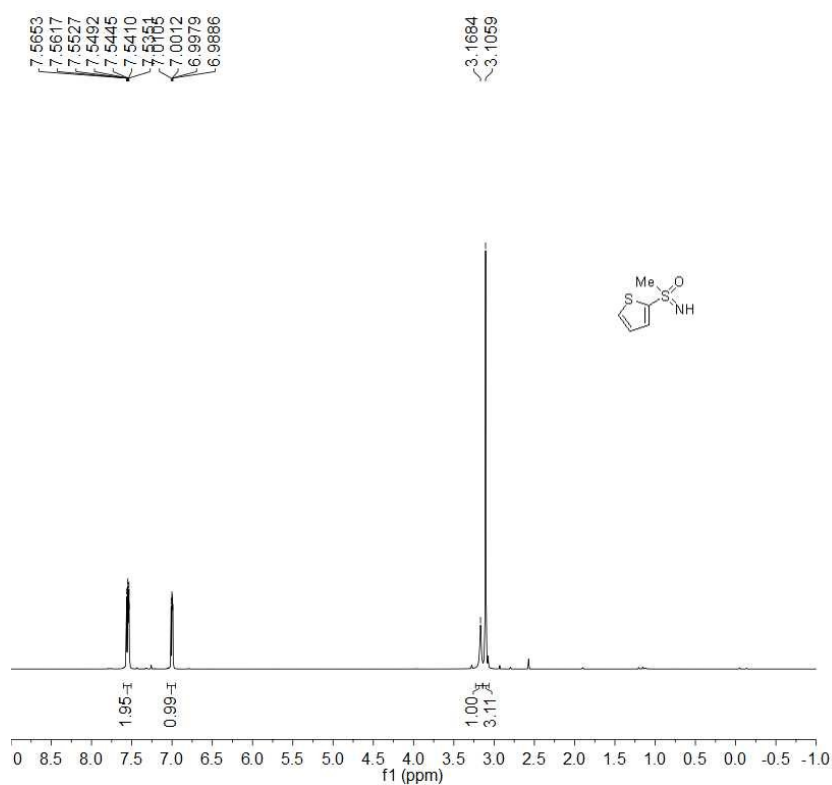


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27 Acquired Size	32768
28 Spectral Size	65536

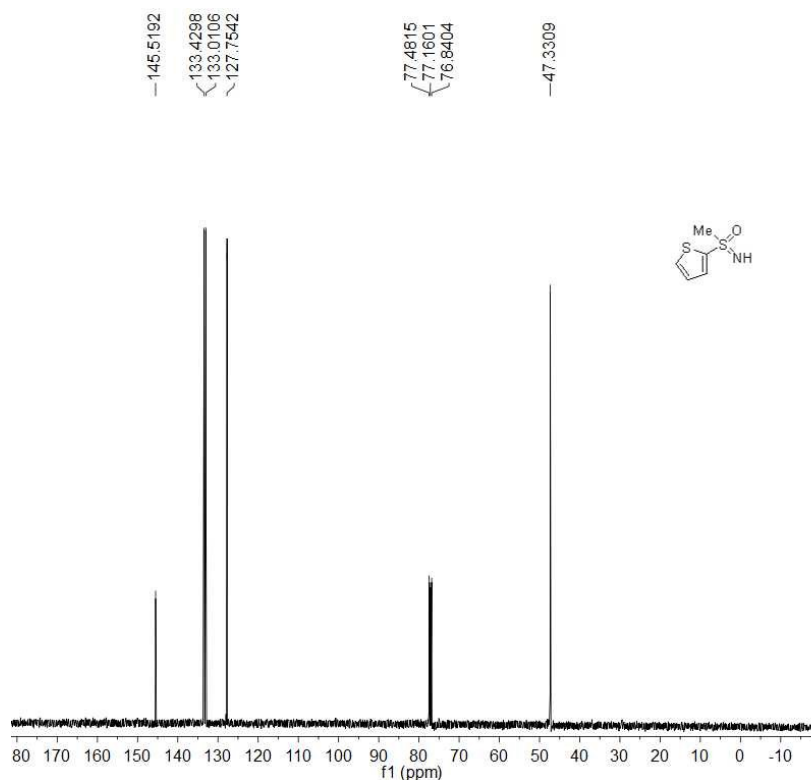


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Imino(methyl)(thiophen-2-yl)-λ⁶-sulfanone (6)

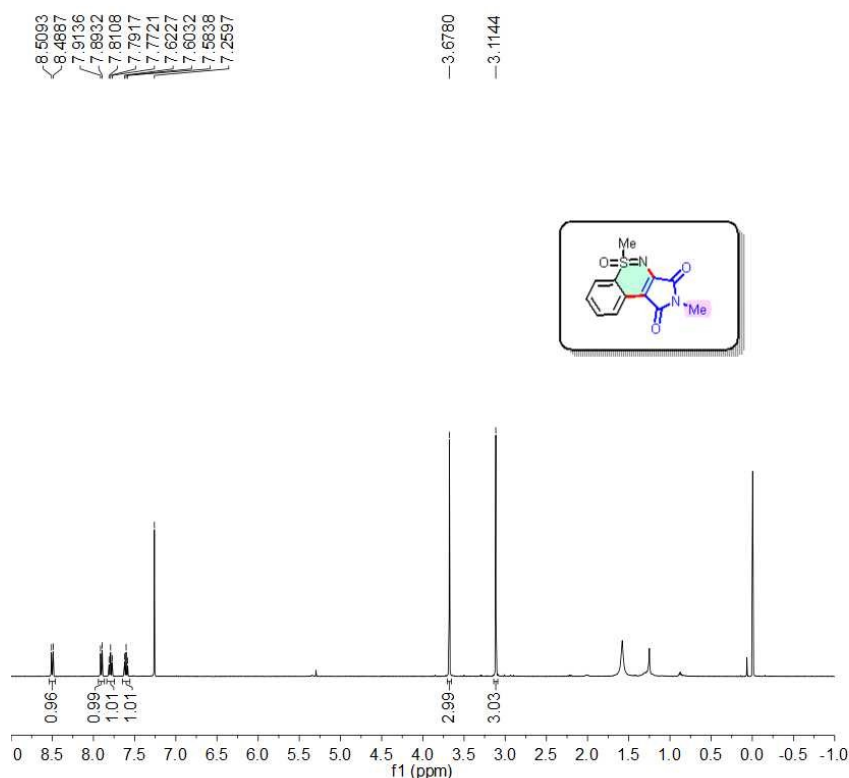


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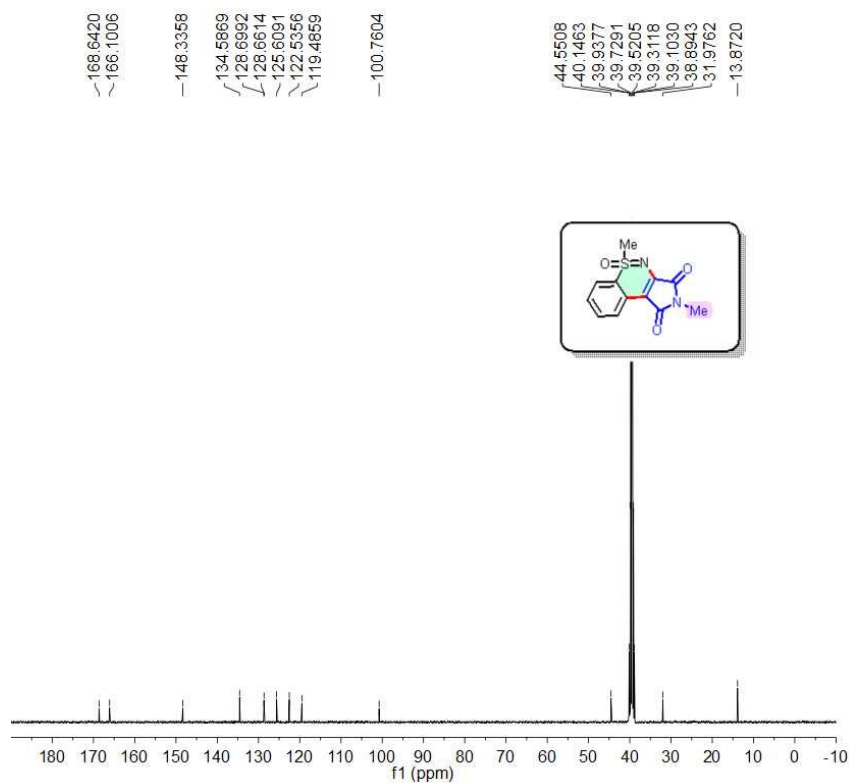


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2,5-Dimethyl-1*H*-5λ⁴-benzo[e]pyrro[3,4-*c*][1,2]thiazine-1,3(2*H*)-dione-5-oxide (product 3a)

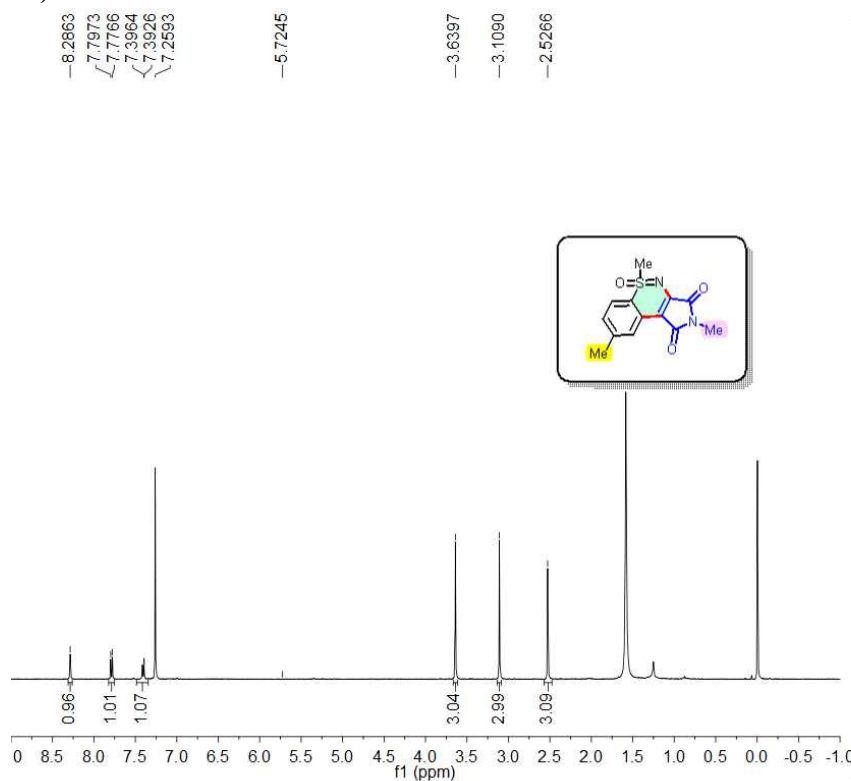


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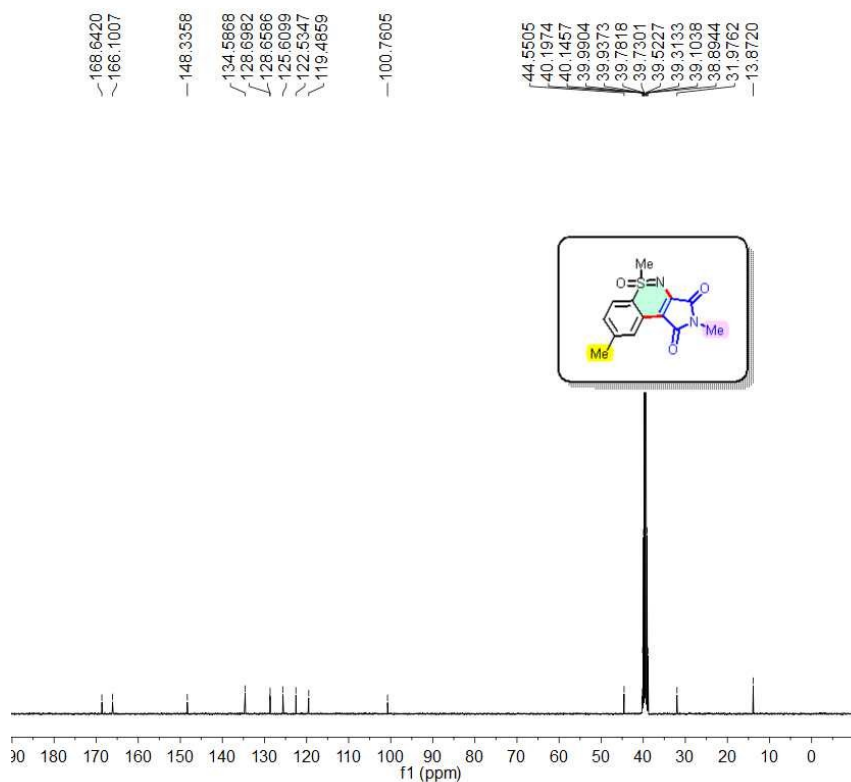


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28 Spectral Size	32768

2,5,8-Trimethyl-1*H*-5 λ^4 -benzo[*e*]pyrrolo[3,4-*c*][1,2]thiazine-1,3(2*H*)-dione 5-oxide (product 3b)

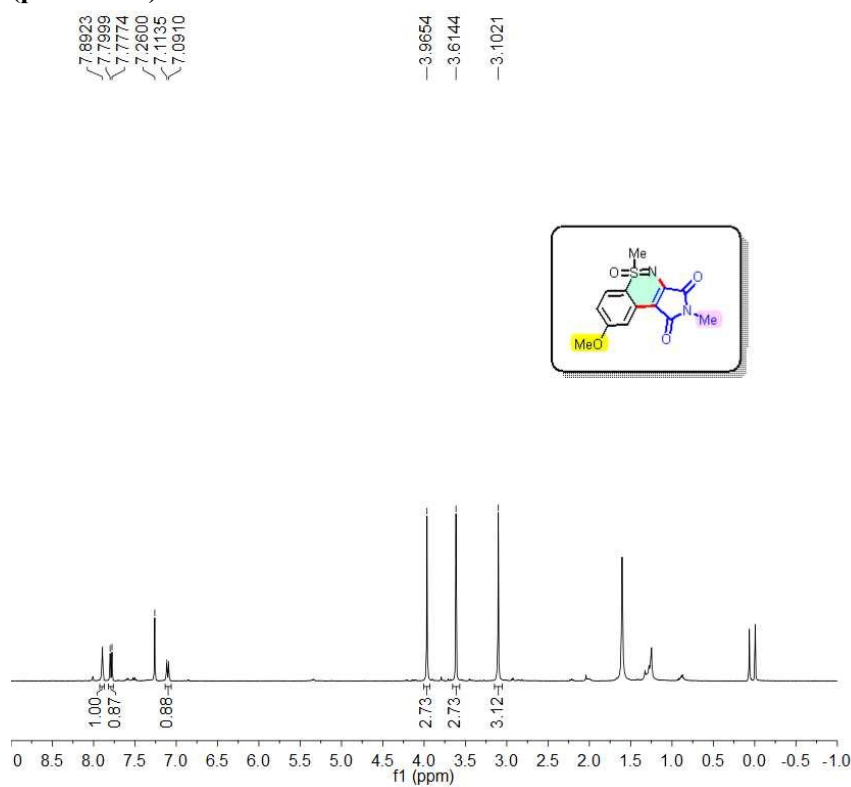


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27 Acquired Size	32768
28 Spectral Size	65536

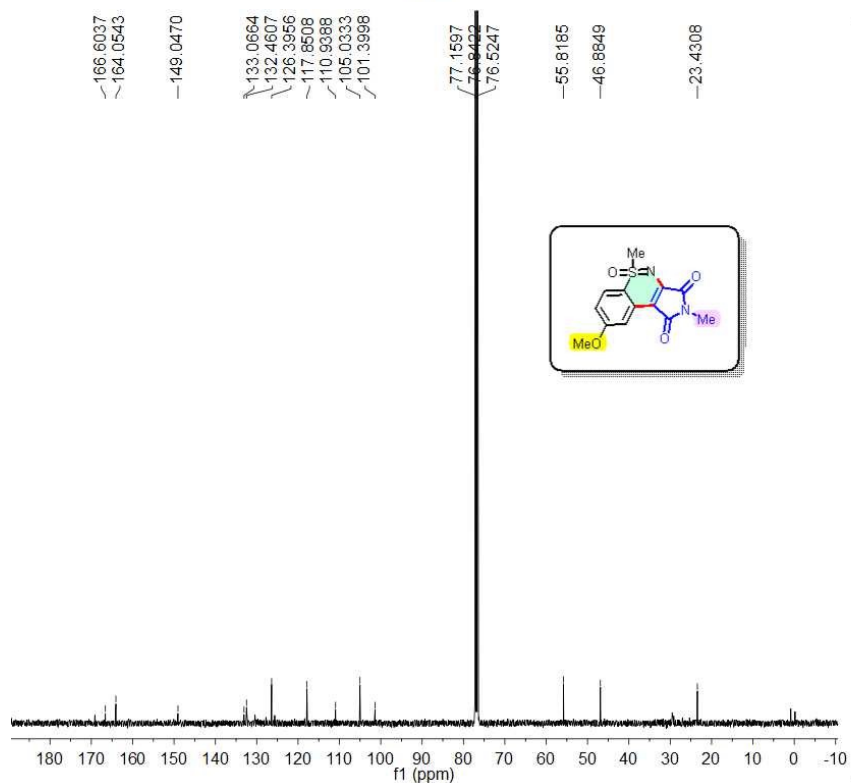


Parameter	Value
1 Data File Name	D:/3/pdata/1/1r
2 Title	22-2-syj-C.3.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	DMSO
10 Temperature	295.1
11 Pulse Sequence	zpgp30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	2500
15 Receiver Gain	32
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-07-10T03:55:15
21 Modification Date	2022-07-10T03:55:20
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1887.1
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

8-Methoxy-2,5-dimethyl-1H-5(4-benzo[e]pyrrolo[3,4-c][1,2]thiazine-1,3(2H)-dione 5-oxide
(product 3c)

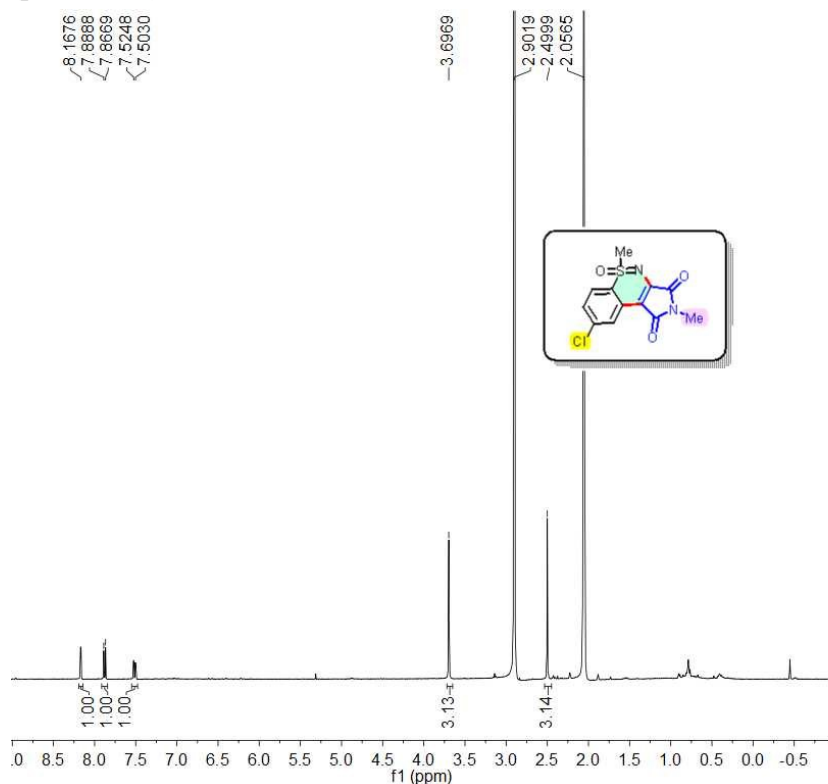


Parameter	Value
1 Data File Name	D:/ / 625/ pdata/ 1/ 1r
2 Title	22-1-syj-H.625.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.8
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2022-06-25T18:39:41
21 Modification Date	2022-06-25T18:39:48
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.0
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

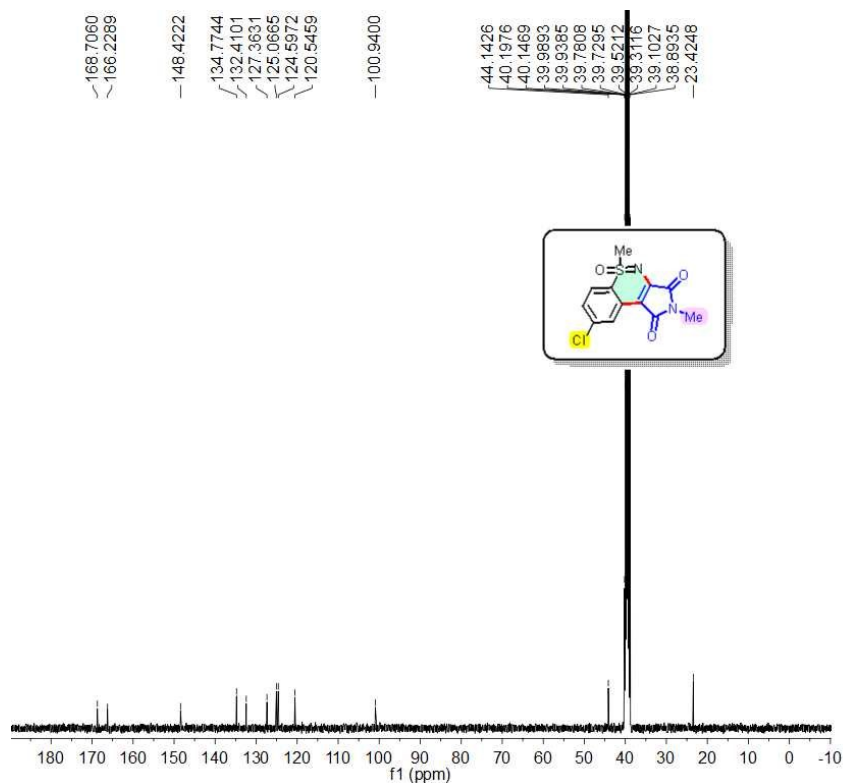


Parameter	Value
1 Data File Name	D:/ 134/ pdata/ 1/ 1r
2 Title	22-1-syj-C.134.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	296.5
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	1500
15 Receiver Gain	15
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-06-26T14:42:22
21 Modification Date	2022-06-26T14:42:28
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1861.9
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

8-Chloro-2,5-dimethyl-1*H*-5λ⁴-benzo[*e*]pyrrolo[3,4-*c*][1,2]thiazine-1,3(2*H*)-dione 5-oxide
(product 3d)

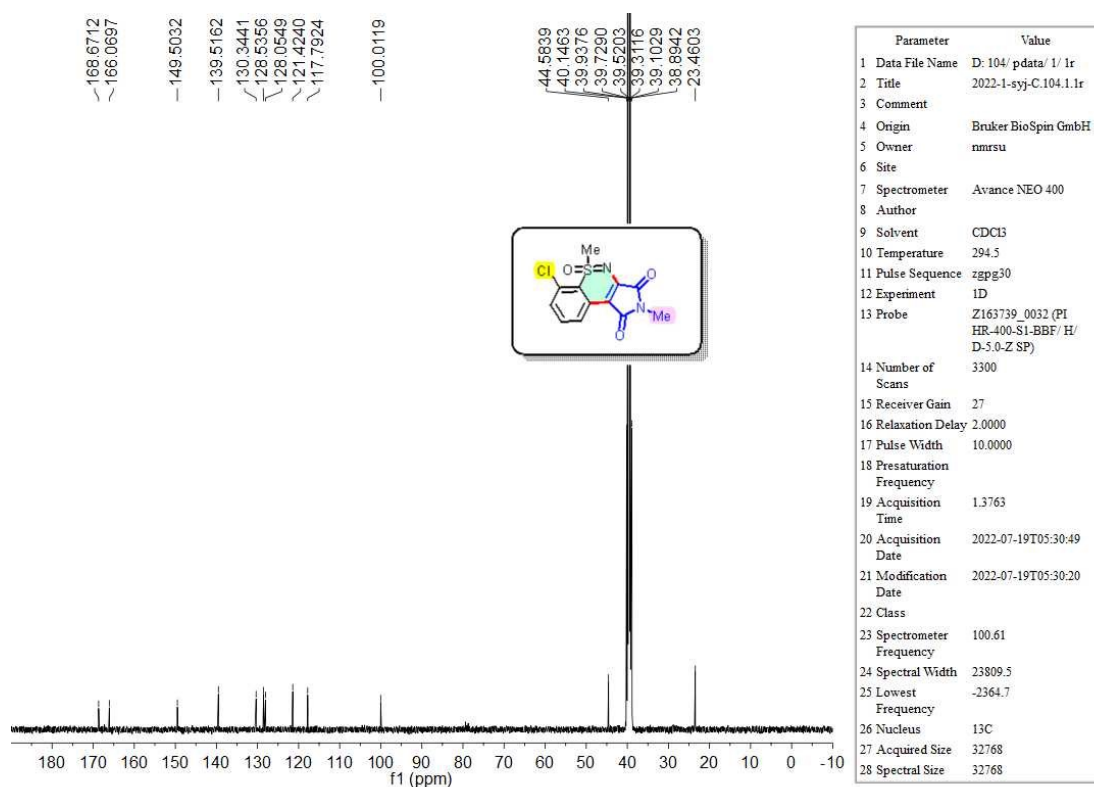
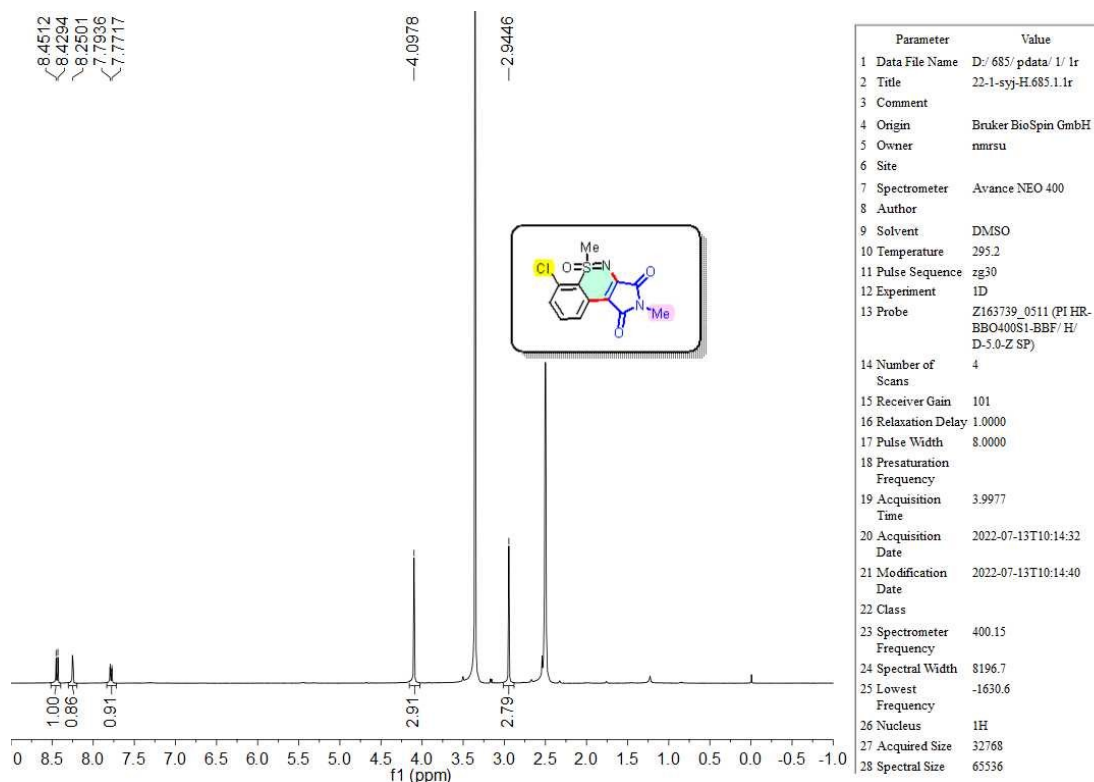


Parameter	Value
1 Data File Name	D:/ 675/ pdata/ 1/ 1r
2 Title	22-1-syj-H.675.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	DMSO
10 Temperature	294.8
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR- BB0400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2022-07-08T21:12:44
21 Modification Date	2022-07-08T21:12:48
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1807.9
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

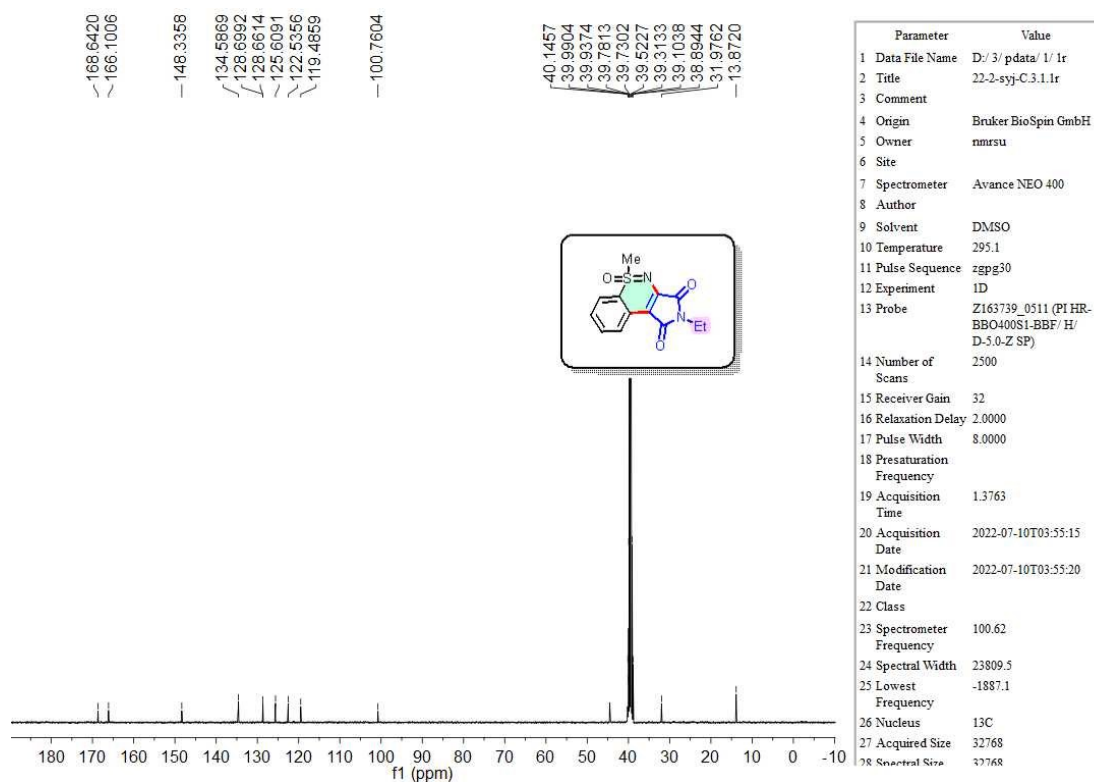
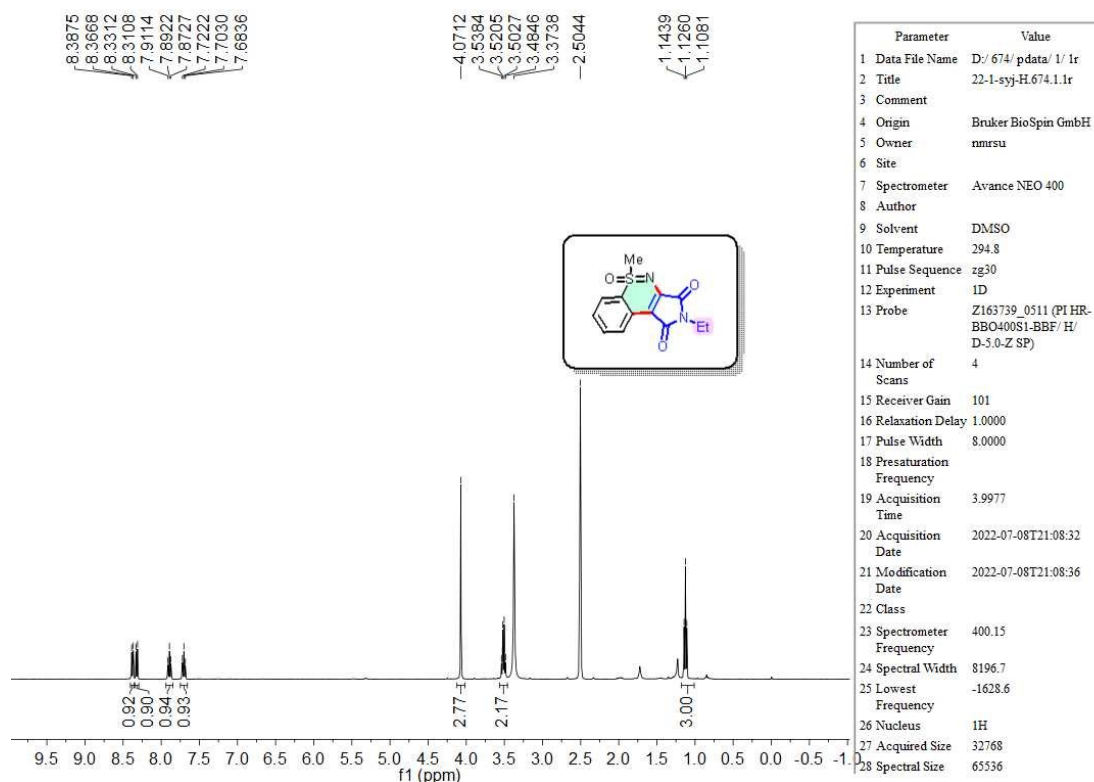


Parameter	Value
1 Data File Name	D:/ 2/ pdata/ 1/ 1r
2 Title	22-2-syj-C.2.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	DMSO
10 Temperature	295.3
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR- BB0400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	3000
15 Receiver Gain	15
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-07-10T01:27:51
21 Modification Date	2022-07-10T01:27:56
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1888.0
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

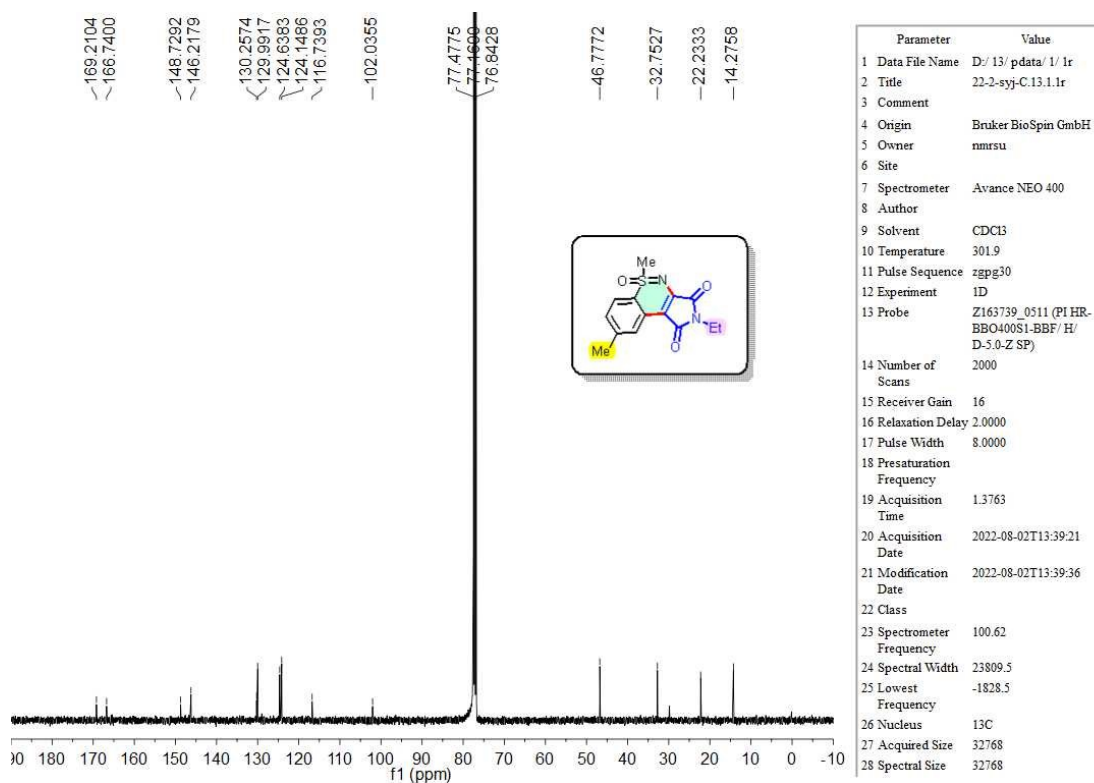
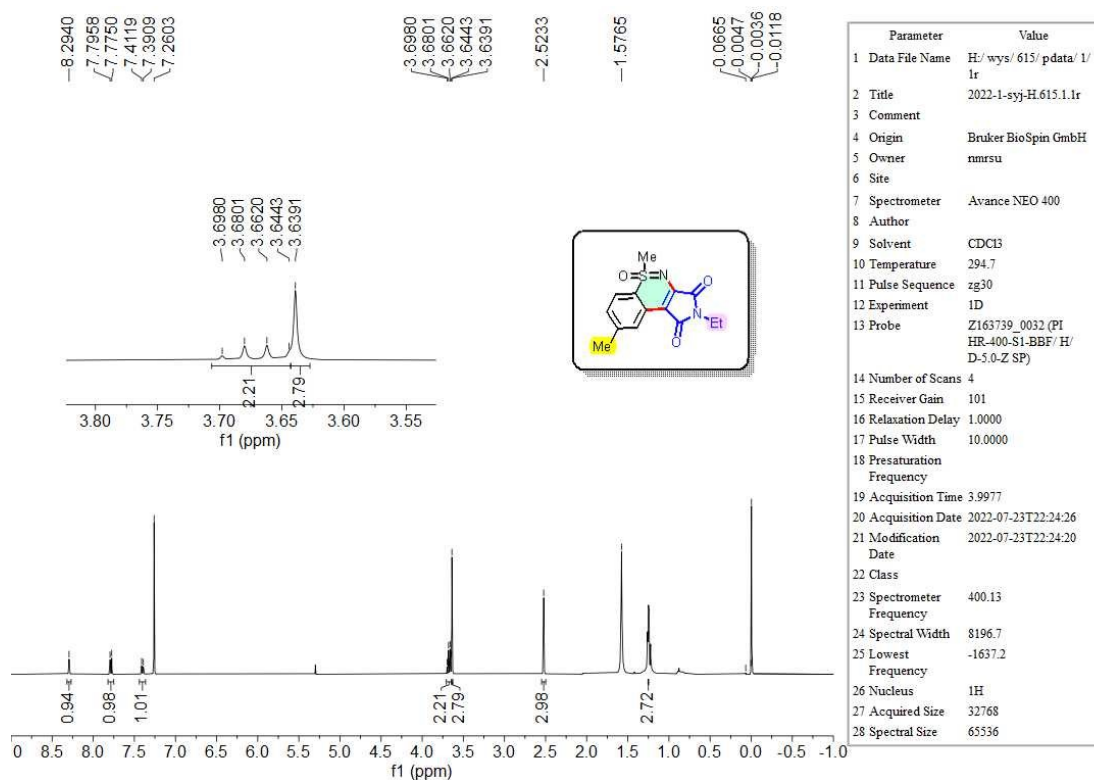
6-Chloro-2,5-dimethyl-1*H*-5λ⁴-benzo[e]pyrrolo[3,4-*c*][1,2]thiazine-1,3(2*H*)-dione 5-oxide
(product 3e)



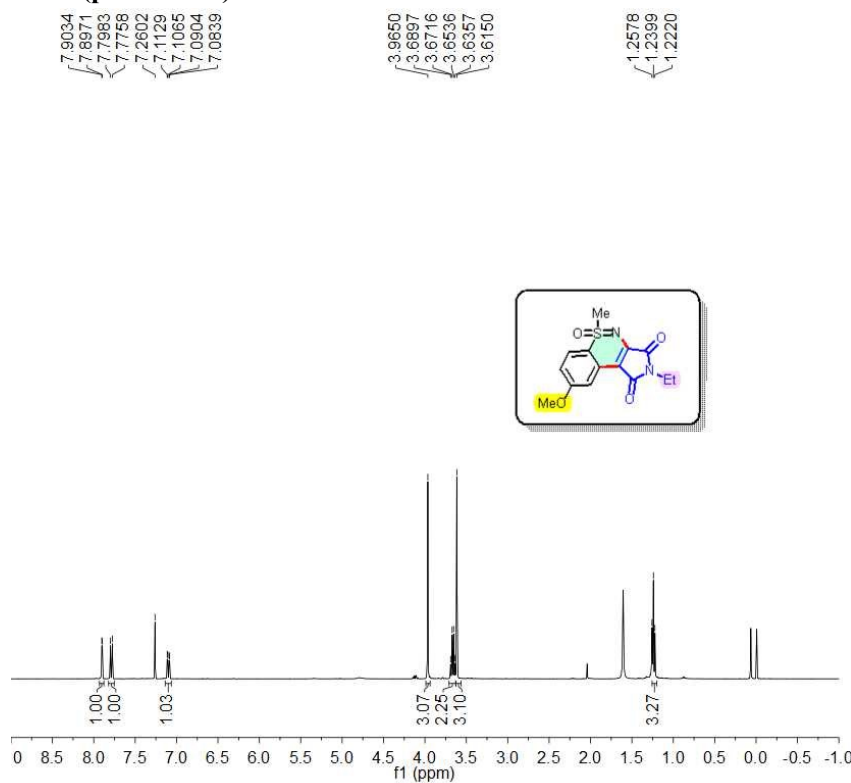
2-Ethyl-5-methyl-1*H*-5λ⁴-benzo[e]pyrrolo[3,4-*c*][1,2]thiazine-1,3(2*H*)-dione 5-oxide (product 3f)



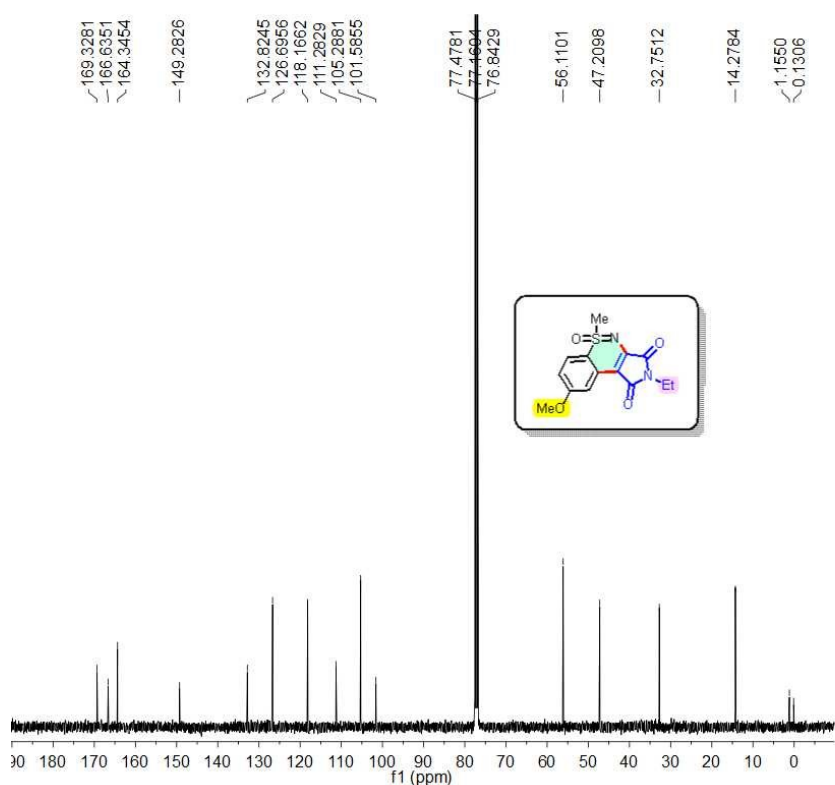
2-Ethyl-5,8-dimethyl-1*H*-5λ⁴-benzo[*e*]pyrrolo[3,4-*c*][1,2]thiazine-1,3(2*H*)-dione 5-oxide
(product 3g)



2-Ethyl-8-methoxy-5-methyl-1*H*-5λ⁴-benzo[*e*]pyrrolo[3,4-*c*][1,2]thiazine-1,3(2*H*)-dione 5-oxide (product 3h)

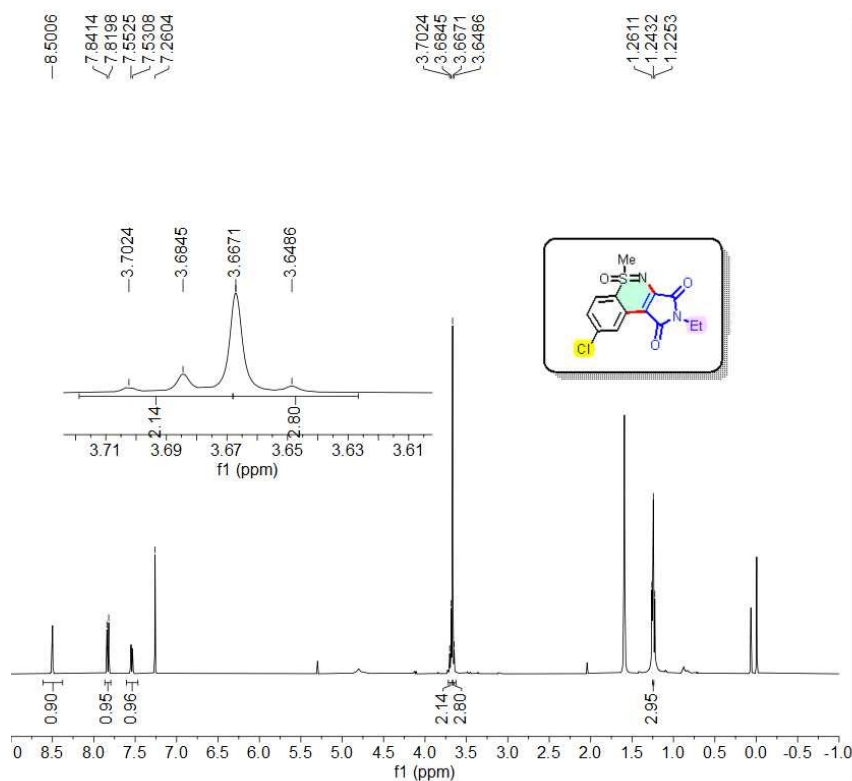


Parameter	Value
1 Data File Name	D:/ 626 /pdata/ 1/ 1r
2 Title	22-1-syj-H.626.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.3
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2022-06-25T18:44:53
21 Modification Date	2022-06-25T18:44:58
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.0
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

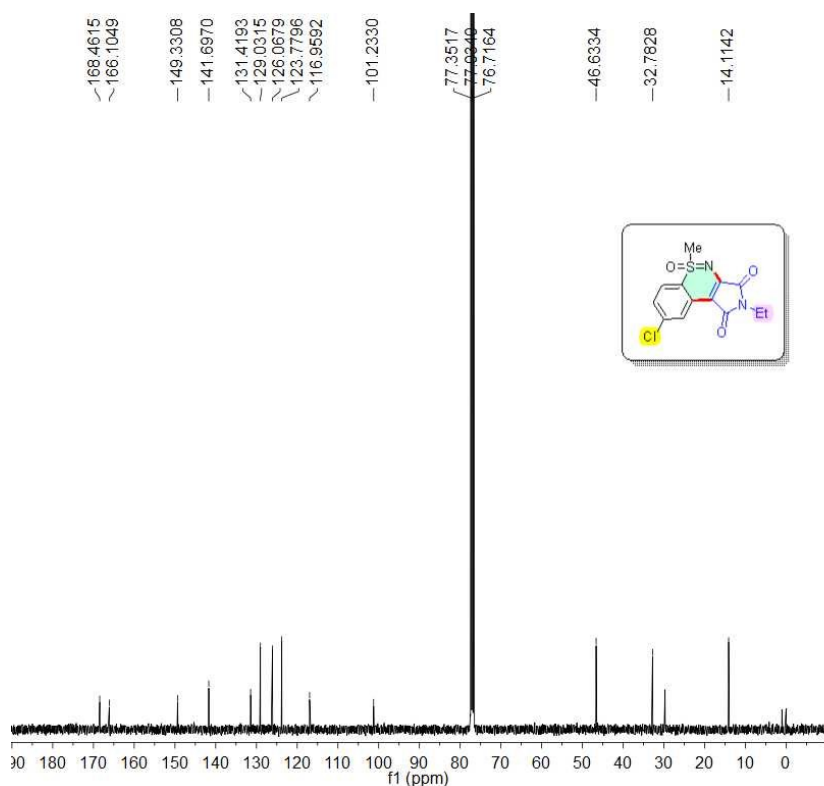


Parameter	Value
1 Data File Name	D:/ 132 /pdata/ 1/ 1r
2 Title	22-1-syj-C.132.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	296.5
11 Pulse Sequence	zpgp30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	1200
15 Receiver Gain	15
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-06-25T21:31:24
21 Modification Date	2022-06-25T21:31:30
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.3
25 Lowest Frequency	-1830.4
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

8-Chloro-2-ethyl-5-methyl-1H-5(4-benzo[e]pyrrolo[3,4-c][1,2]thiazine-1,3(2H)-dione 5-oxide
(product 3i)

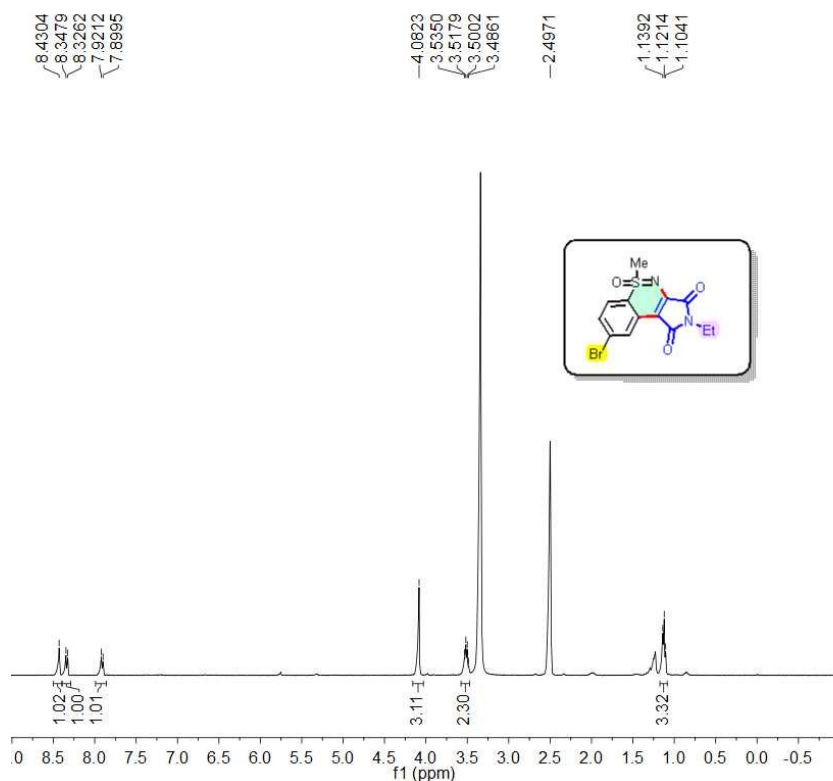


Parameter	Value
1 Data File Name	D:/642/pdata/1/ 1r
2 Title	22-1-syj-H.642.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2022-06-29T11:17:12
21 Modification Date	2022-06-29T11:17:20
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.0
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

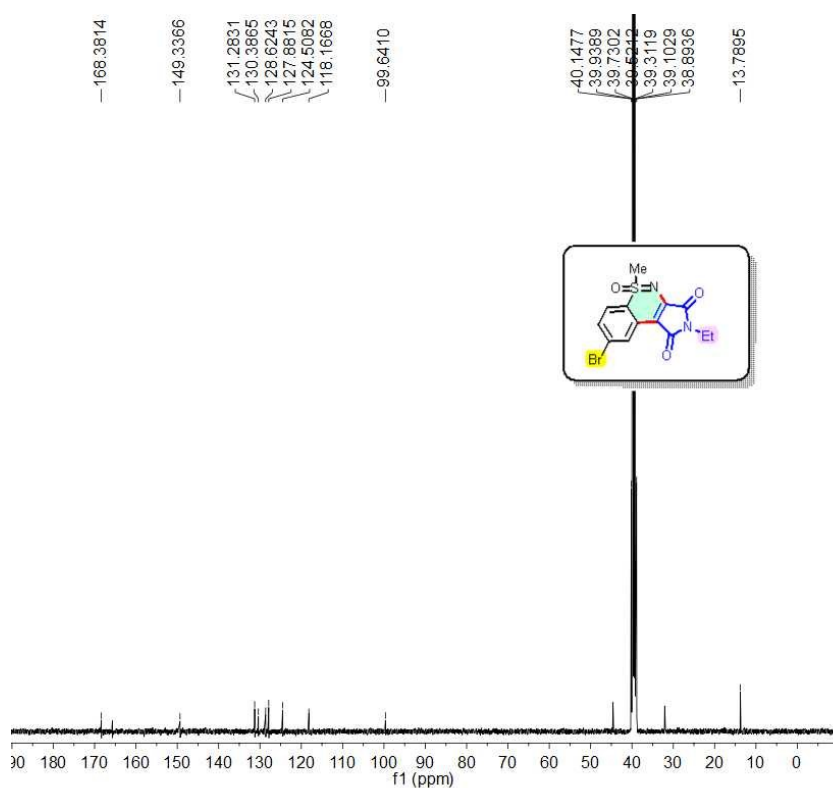


Parameter	Value
1 Data File Name	D:/ 142/pdata/1/ 1r
2 Title	22-1-syj-C.142.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	296.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	1500
15 Receiver Gain	15
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-06-29T13:04:53
21 Modification Date	2022-06-29T13:05:02
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.0
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

8-Bromo-2-ethyl-5-methyl-1*H*-5λ⁴-benzo[*e*]pyrrolo[3,4-*c*][1,2]thiazine-1,3(2*H*)-dione 5-oxide
(product 3j)

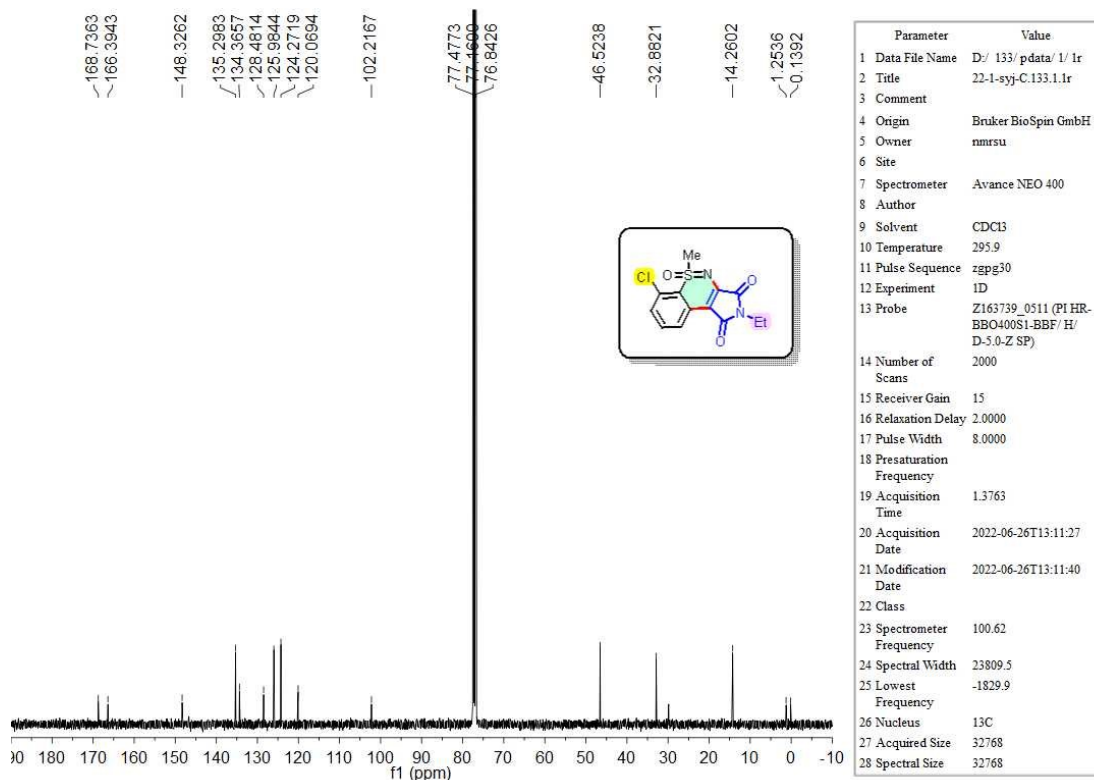
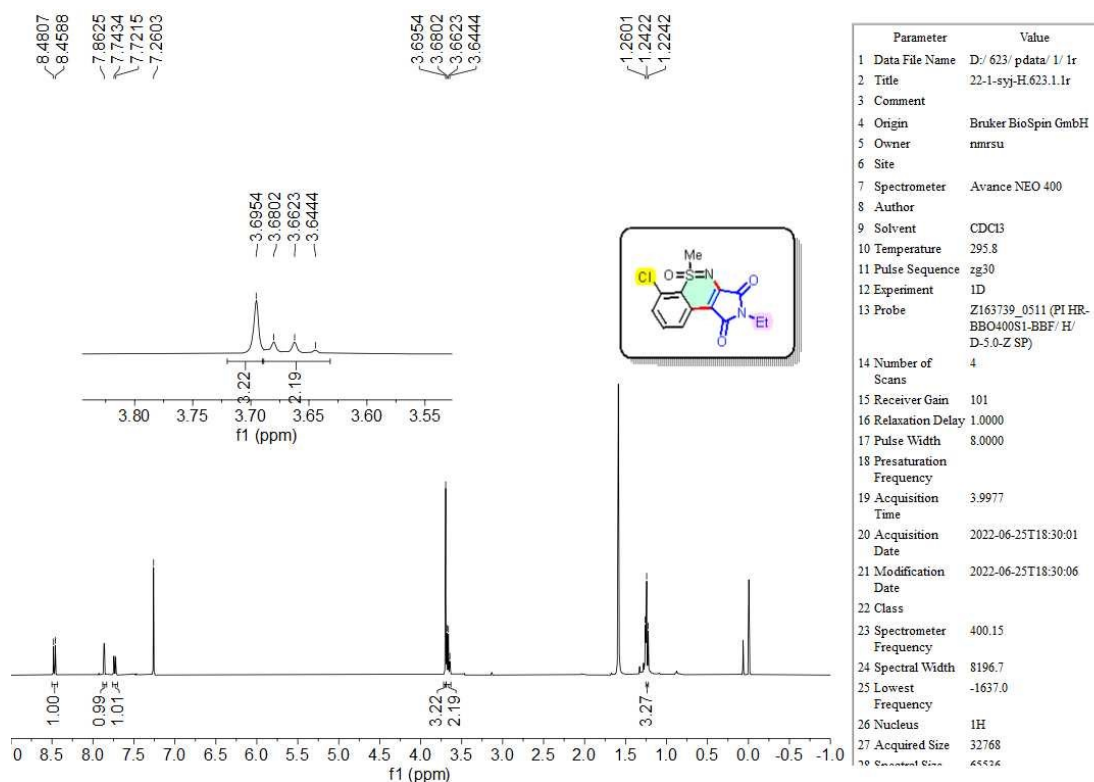


Parameter	Value
1 Data File Name	H:/ 599/ pdata/ 1/ 1r
2 Title	2023-2-syj-H.599.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	DMSO
10 Temperature	295.3
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-11-13T22:02:17
21 Modification Date	2023-11-13T22:01:32
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1630.4
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536

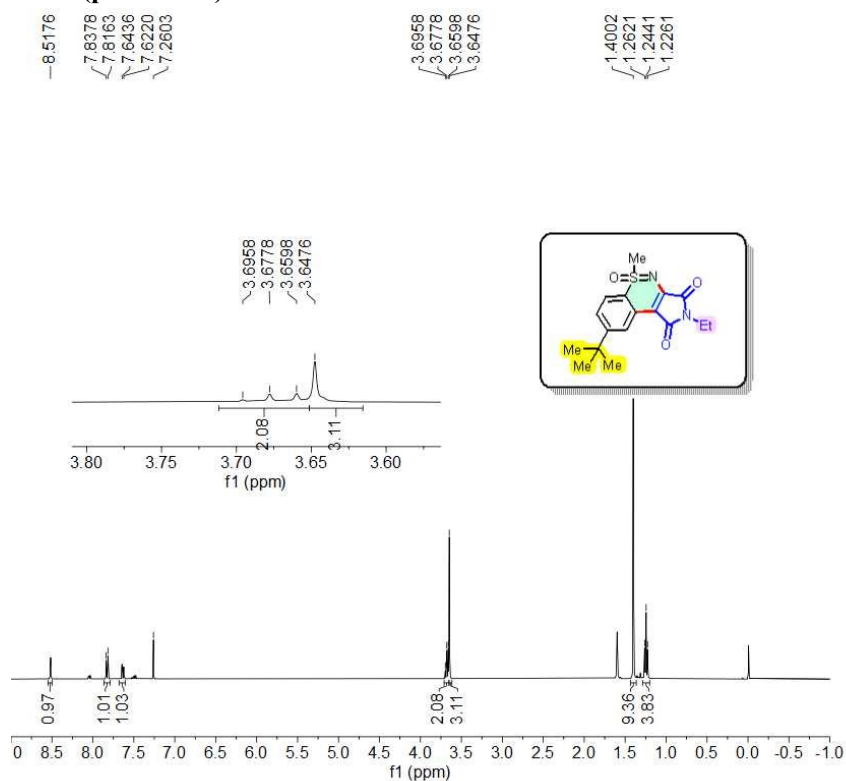


Parameter	Value
1 Data File Name	H:/ 95/ pdata/ 1/ 1r
2 Title	2023-2-syj-C.95.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	DMSO-D6
10 Temperature	296.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	2000
15 Receiver Gain	13
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-11-14T01:20:29
21 Modification Date	2023-11-14T01:19:42
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1889.6
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	32768

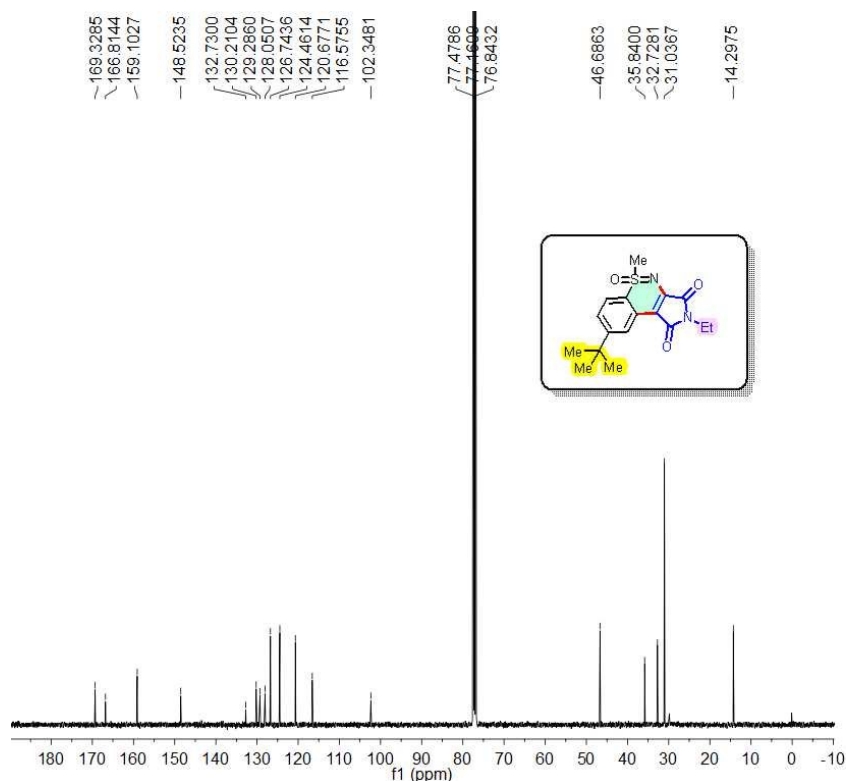
6-Chloro-2-ethyl-5-methyl-1*H*-5λ⁴-benzo[e]pyrrolo[3,4-*c*][1,2]thiazine-1,3(2*H*)-dione 5-oxide
(product 3k)



8-(*tert*-Butyl)-2-ethyl-5-methyl-1*H*-5λ⁴-benzo[*e*]pyrrolo[3,4-*c*][1,2]thiazine-1,3(2*H*)-dione 5-oxide (product 3l)

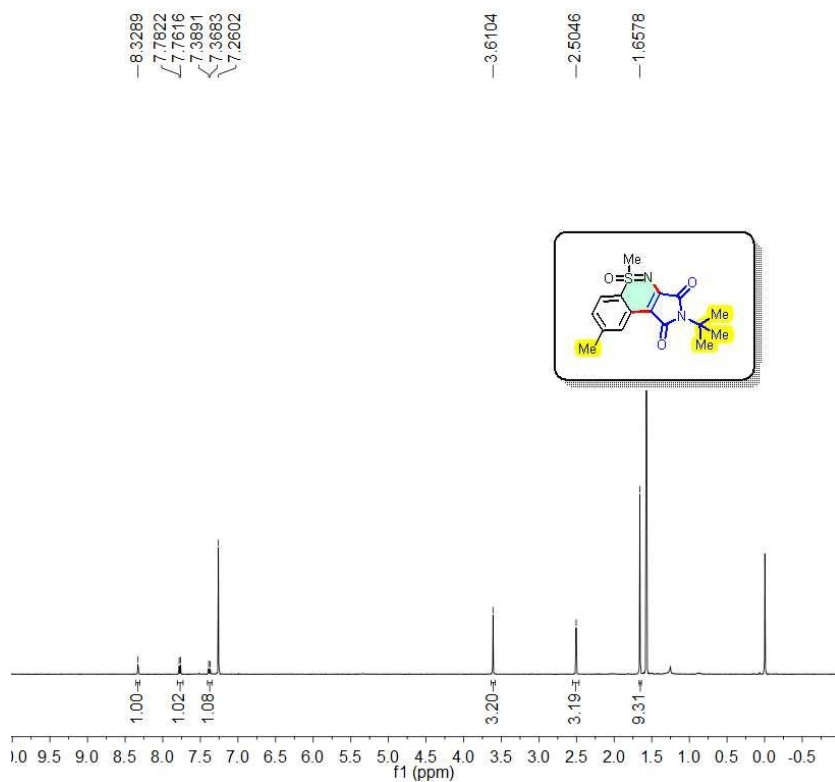


Parameter	Value
1 Data File Name	D:/580/pdata/1/1r
2 Title	2022-1-syj-H.580.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2022-07-15T11:50:52
21 Modification Date	2022-07-15T11:50:44
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

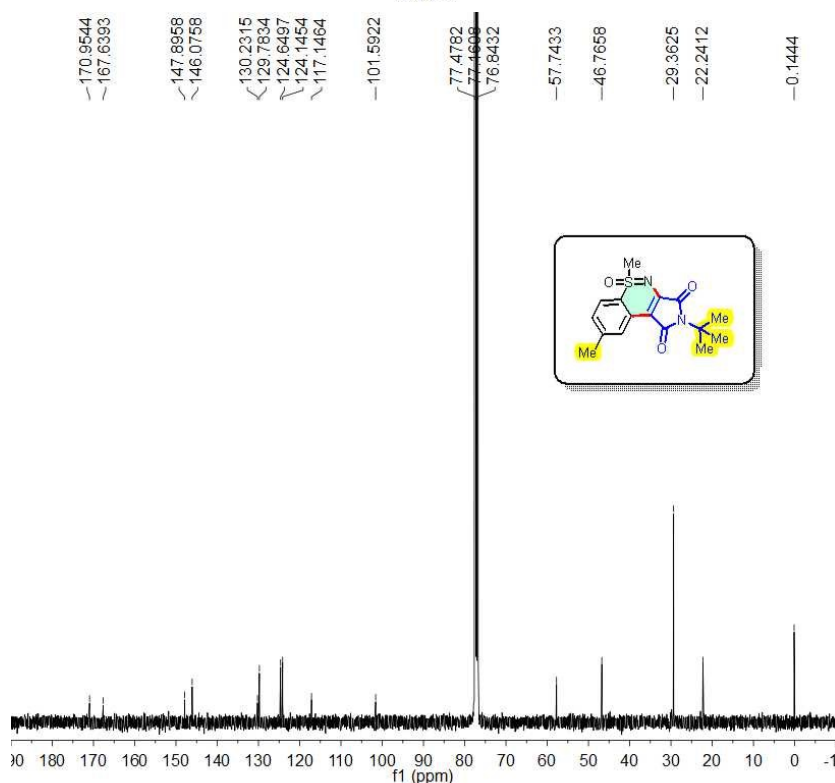


Parameter	Value
1 Data File Name	D:/176/pdata/1/1r
2 Title	22-1-syj-C.176.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	294.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	2200
15 Receiver Gain	15
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-07-20T01:35:15
21 Modification Date	2022-07-20T01:35:28
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1831.1
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2-(*tert*-Butyl)-5,8-dimethyl-1*H*-5λ⁴-benzo[e]pyrrolo[3,4-*c*][1,2]thiazine-1,3(2*H*)-dione 5-oxide
(product 3m)

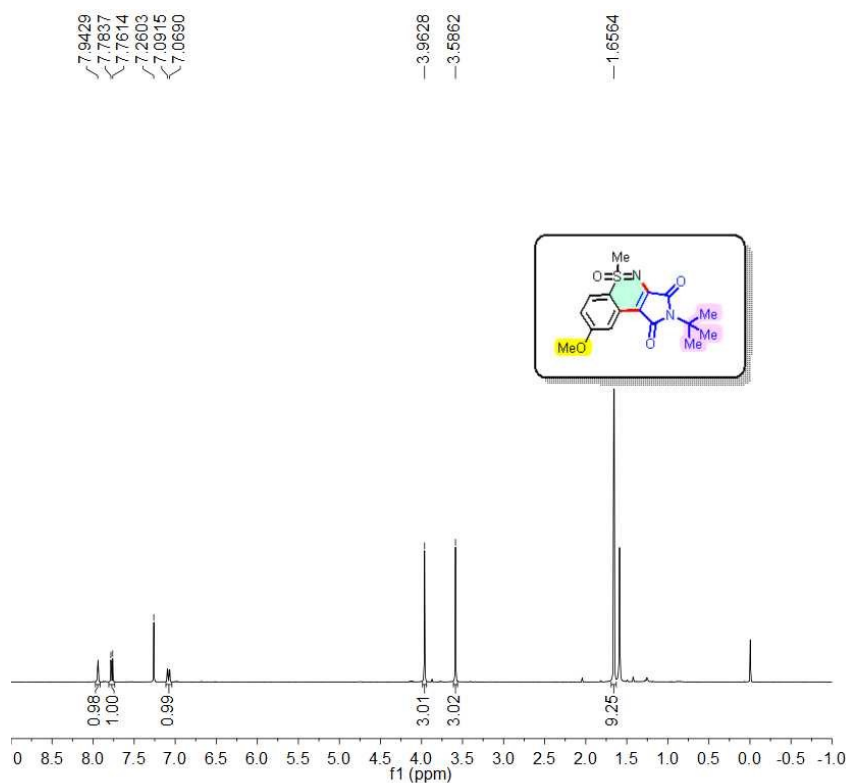


Parameter	Value
1 Data File Name	D:/373/pdata/1/1r
2 Title	22-1-syj-H.573.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	294.5
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2022-07-23T22:31:30
21 Modification Date	2022-07-23T22:31:34
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.0
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

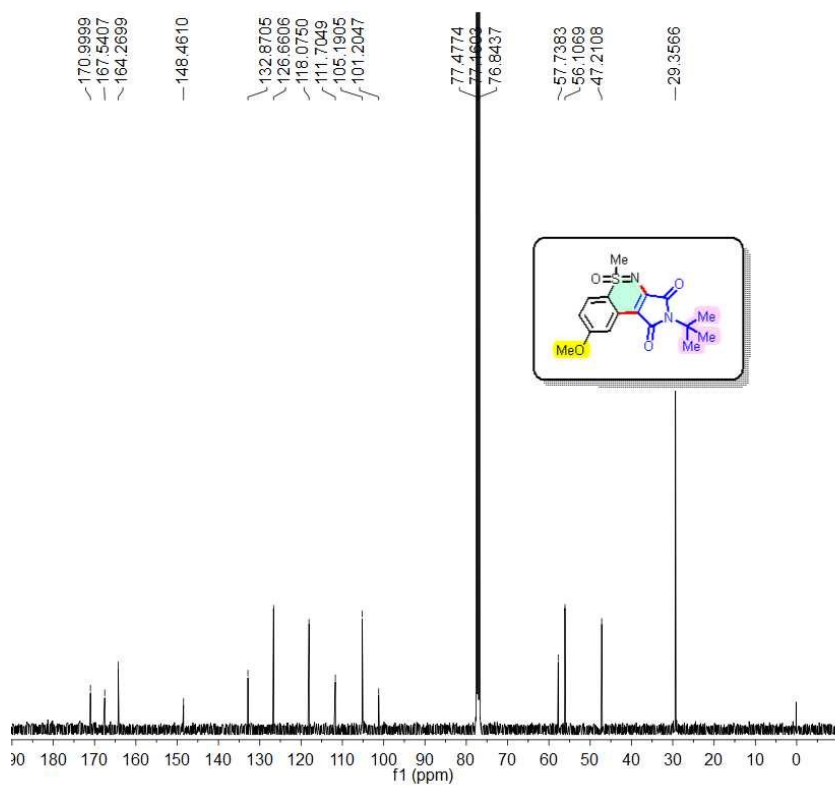


Parameter	Value
1 Data File Name	D:/183/pdata/1/1r
2 Title	22-1-syj-C.185.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	294.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	9000
15 Receiver Gain	15
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-07-24T07:28:19
21 Modification Date	2022-07-24T07:28:22
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1829.6
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2-(*tert*-Butyl)-8-methoxy-5-methyl-1*H*-5λ⁴-benzo[*e*]pyrrolo[3,4-*c*][1,2]thiazine-1,3(2*H*)-dione 5-oxide (product 3n)

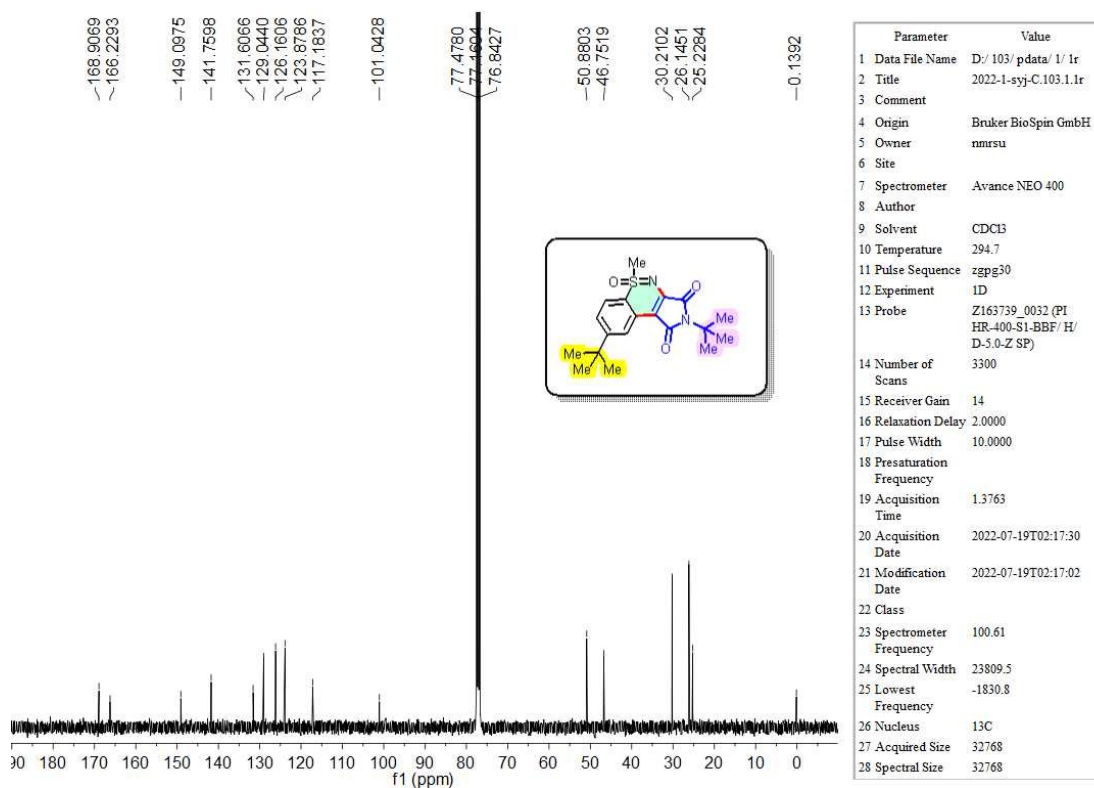
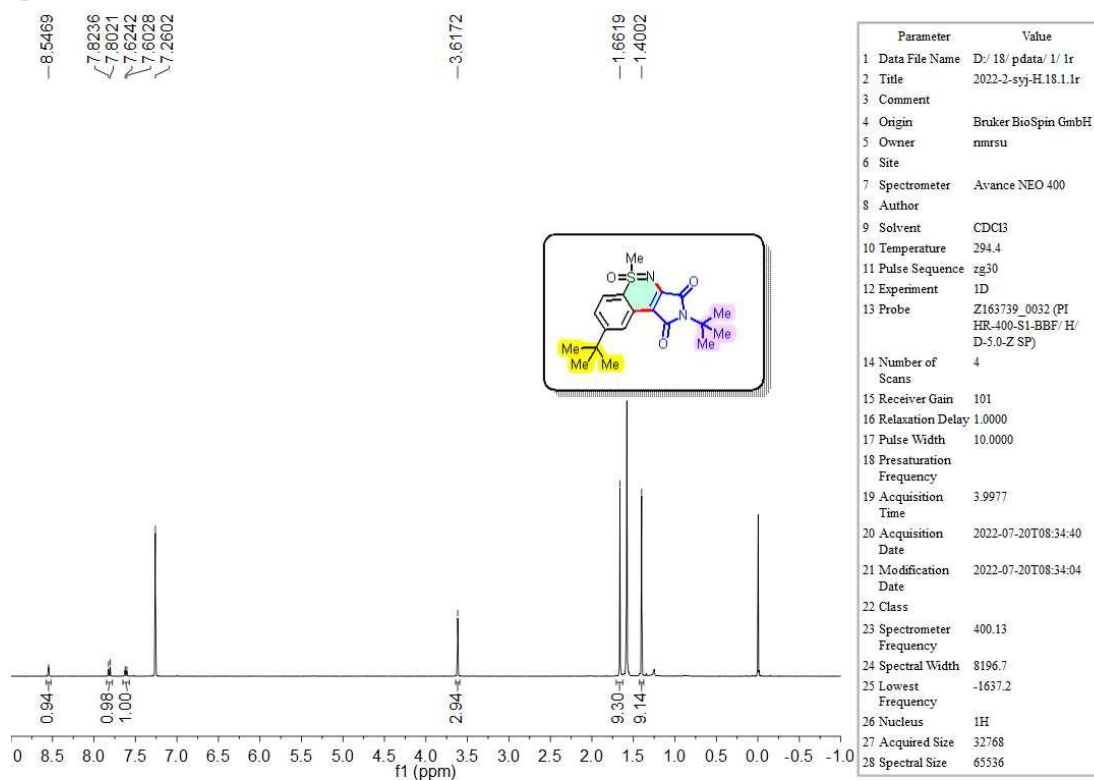


Parameter	Value
1 Data File Name	D:/ 578/ pdata/ 1/ 1r
2 Title	2022-1-syj-H.578.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2022-07-15T11:40:58
21 Modification Date	2022-07-15T11:40:50
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65336



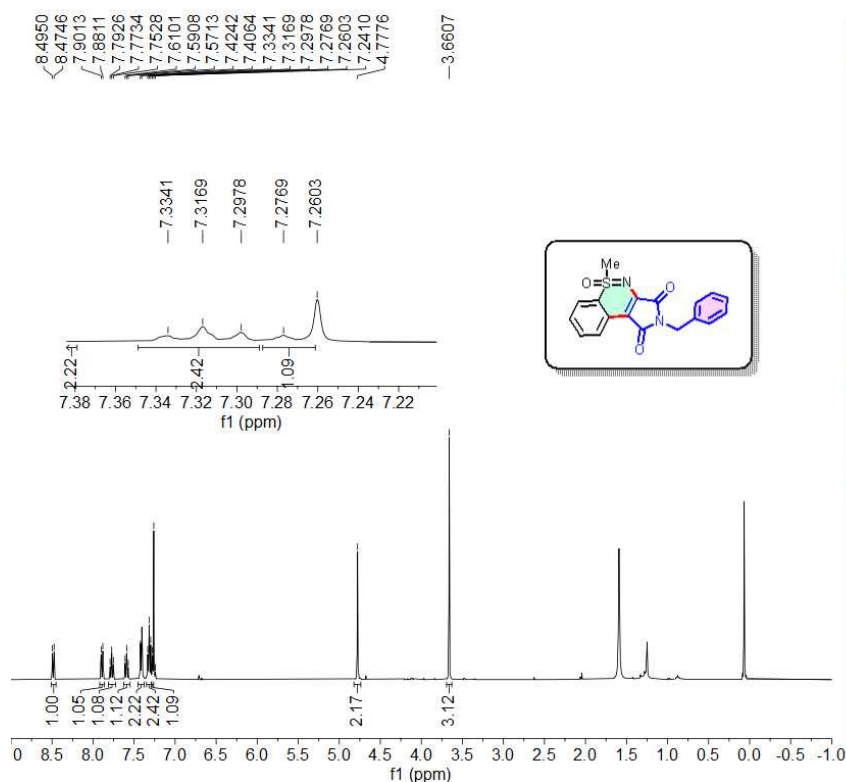
Parameter	Value
1 Data File Name	D:/ 177/ pdata/ 1/ 1r
2 Title	22-1-syj-C.177.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	294.5
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	2200
15 Receiver Gain	15
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-07-20T03:46:08
21 Modification Date	2022-07-20T03:46:22
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1830.8
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2,8-Di-*tert*-butyl-5-methyl-1*H*-5λ4-benzo[e]pyrrolo[3,4-*c*][1,2]thiazine-1,3(2*H*)-dione 5-oxide (product 3o)

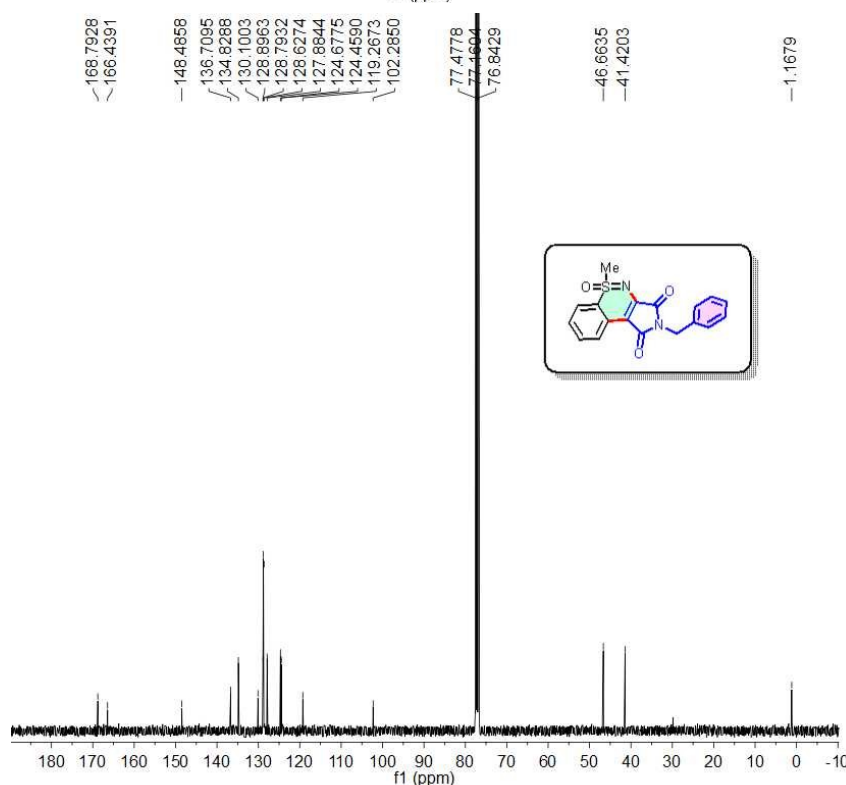


2-Benzyl-5-methyl-1*H*-5λ⁴-benzo[e]pyrrolo[3,4-*c*][1,2]thiazine-1,3(2*H*)-dione
(product 3p)

5-oxide

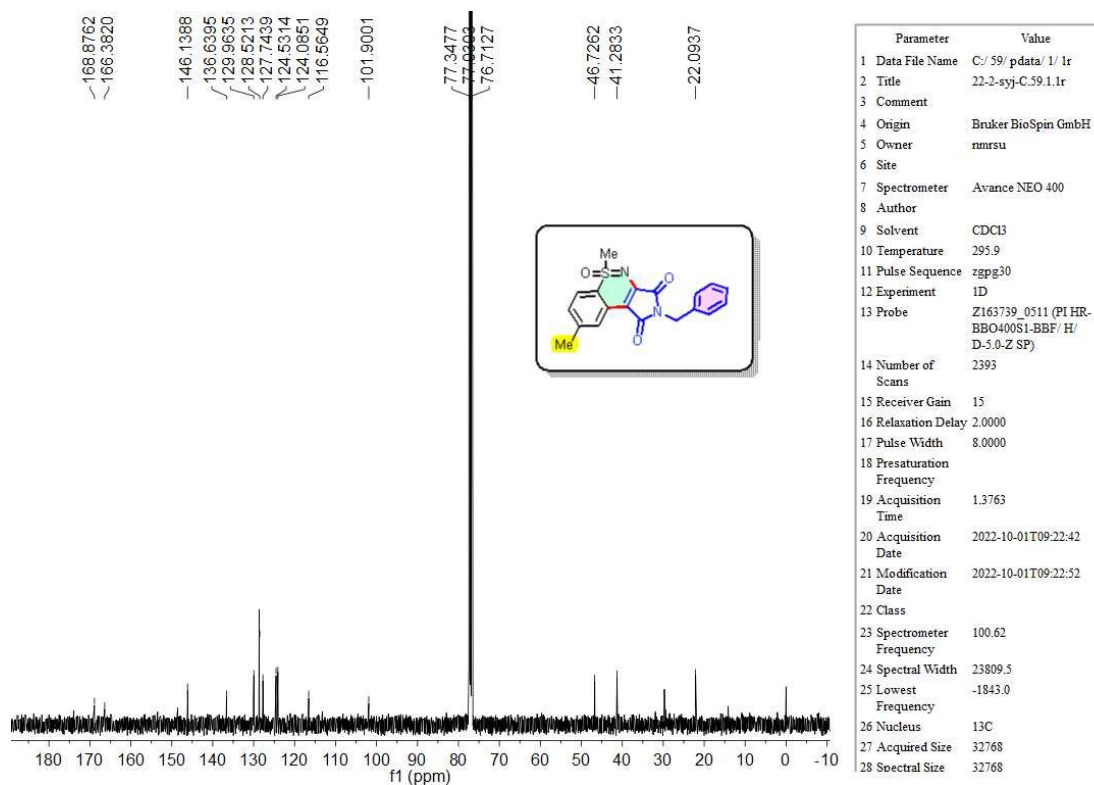
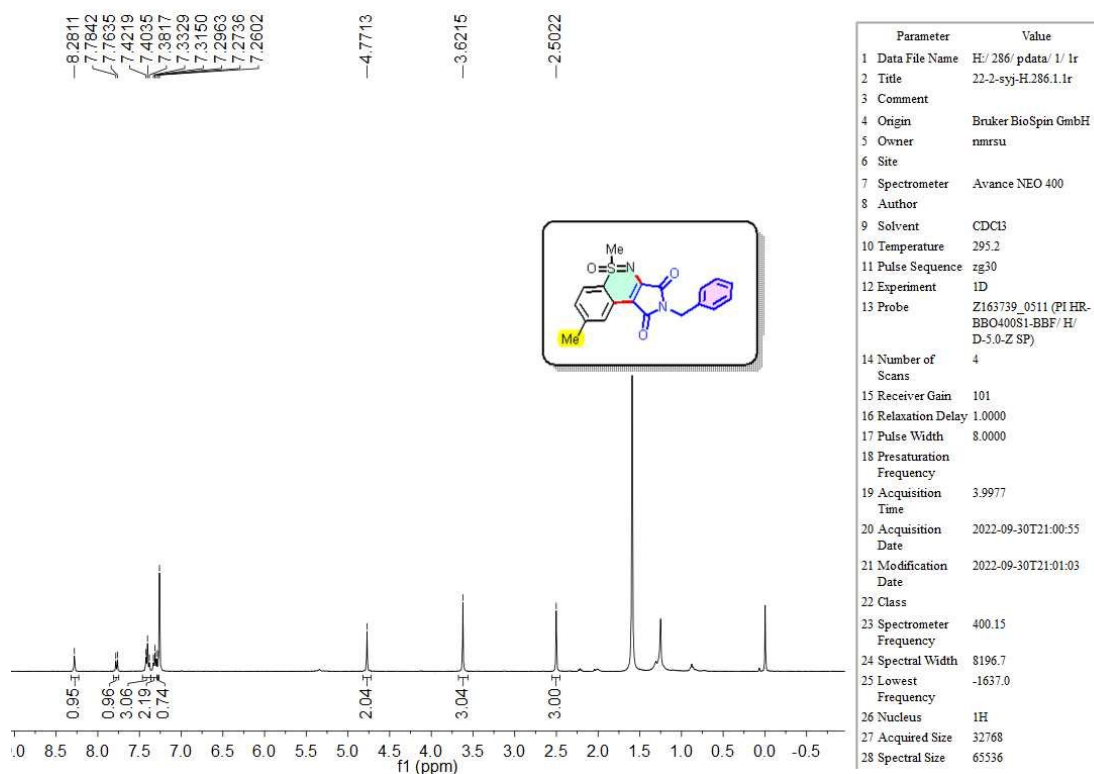


Parameter	Value
1 Data File Name	D:/536/pdata/1/1r
2 Title	22-1-syj-H.536.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	294.1
11 Pulse Sequence	zg30
12 Experiment	ID
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2022-06-14T20:05:36
21 Modification Date	2022-06-14T20:04:00
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.0
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536

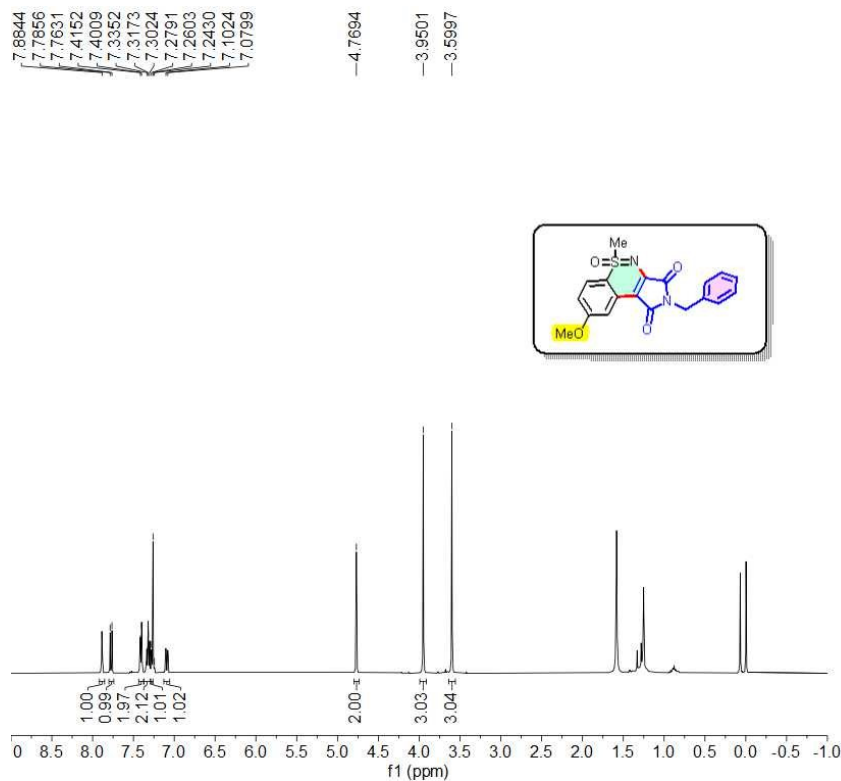


Parameter	Value
1 Data File Name	D:/96/pdata/1/1r
2 Title	22-1-syj-C.96.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.5
11 Pulse Sequence	zpgp30
12 Experiment	ID
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	1500
15 Receiver Gain	15
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-06-15T20:09:40
21 Modification Date	2022-06-15T20:08:06
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1830.5
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	32768

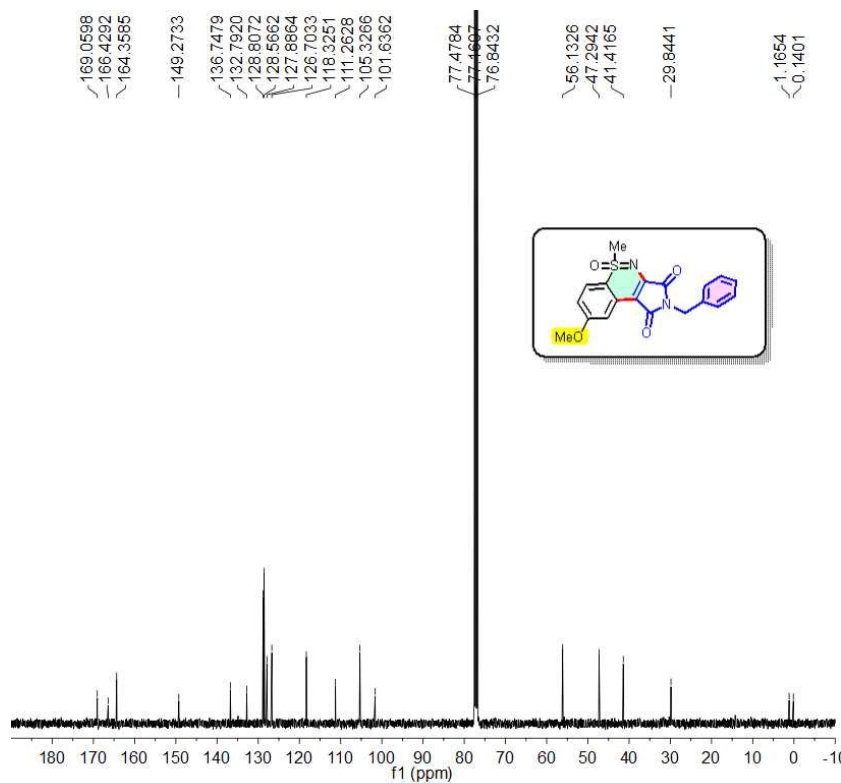
2-Benzyl-5,8-dimethyl-1*H*-5λ⁴-benzo[e]pyrrolo[3,4-*c*][1,2]thiazine-1,3(2*H*)-dione 5-oxide
(product 3q)



2-Benzyl-8-methoxy-5-methyl-1H-5λ⁴-benzo[e]pyrrolo[3,4-c][1,2]thiazine-1,3(2H)-dione 5-oxide (product 3r)

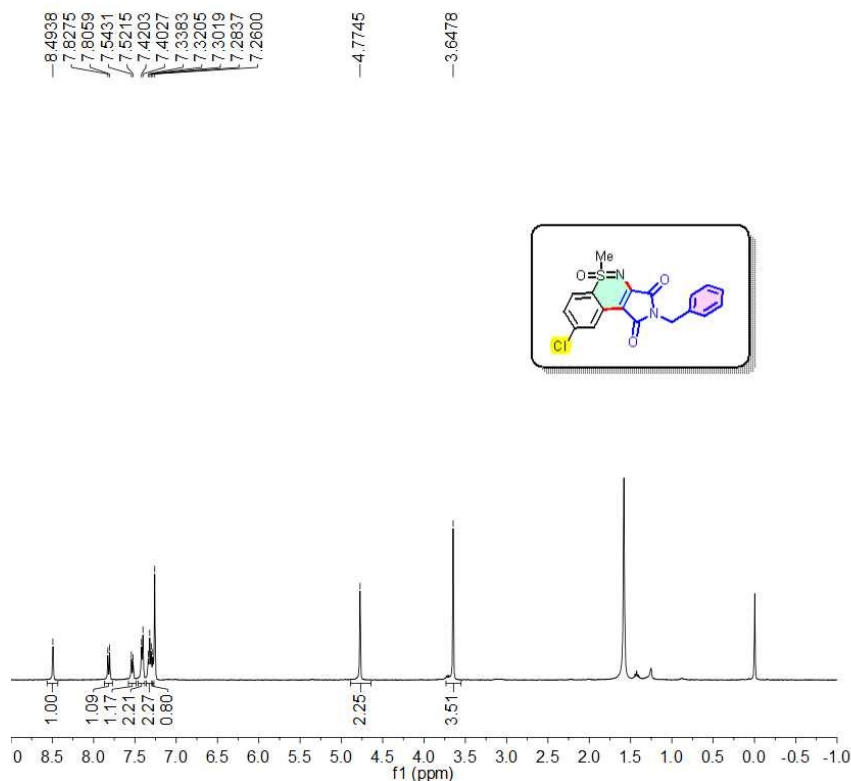


Parameter	Value
1 Data File Name	D:/519/pdata/1/1r
2 Title	2022-1-syj-H.519.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.6
11 Pulse Sequence	zg30
12 Experiment	ID
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2022-06-26T11:19:48
21 Modification Date	2022-06-26T11:17:52
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

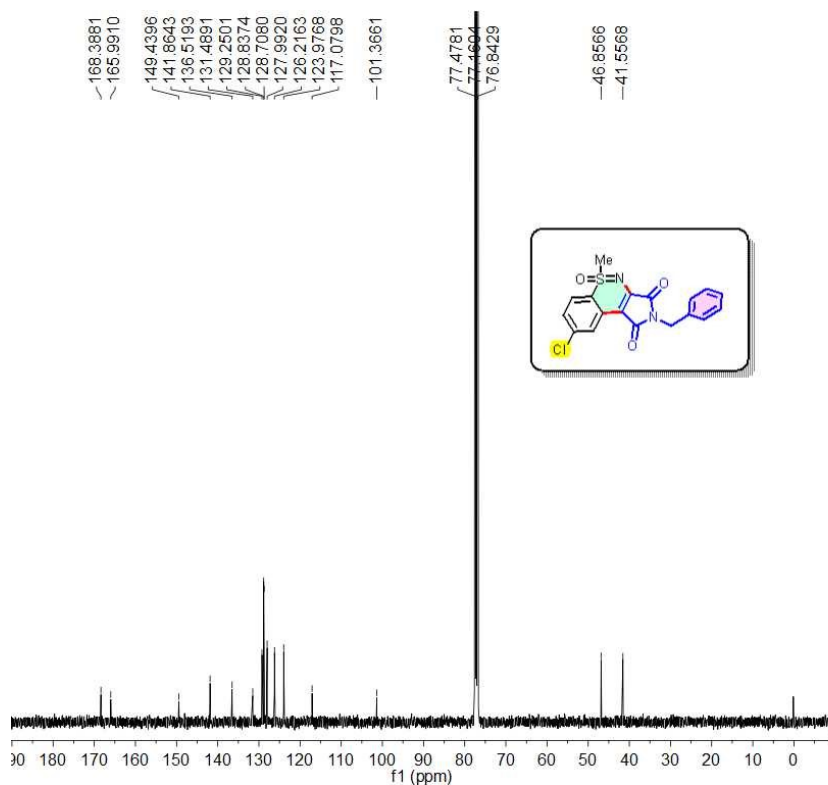


Parameter	Value
1 Data File Name	D:/519/pdata/1/1r
2 Title	2022-1-syj-C.89.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	296.4
11 Pulse Sequence	zpgp30
12 Experiment	ID
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	1600
15 Receiver Gain	14
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-06-26T13:02:13
21 Modification Date	2022-06-26T13:00:18
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1830.7
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2-Benzyl-8-chloro-5-methyl-1*H*-5λ⁴-benzo[e]pyrrolo[3,4-*c*][1,2]thiazine-1,3(2*H*)-dione oxide (product 3s) 5-

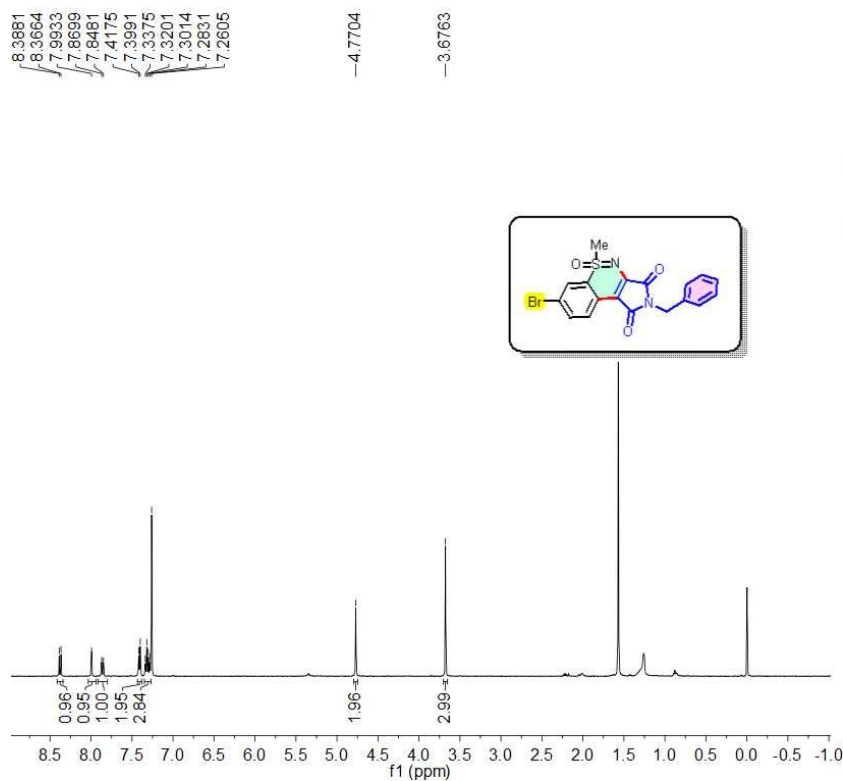


Parameter	Value
1 Data File Name	D:/159/pdata/1/1r
2 Title	22-2-syj-H.159.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2022-08-27T22:09:12
21 Modification Date	2022-08-27T22:09:16
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.4
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

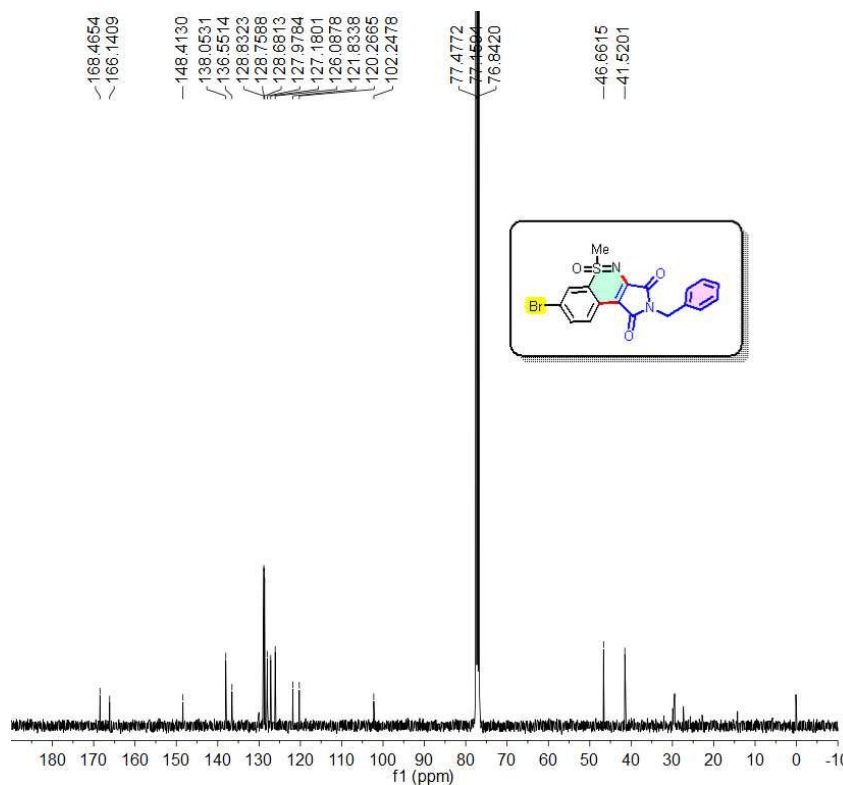


Parameter	Value
1 Data File Name	D:/16/pdata/1/1r
2 Title	22-2-syj-C.16.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	3000
15 Receiver Gain	14
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-08-28T01:17:48
21 Modification Date	2022-08-28T01:17:56
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1830.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2-Benzyl-7-bromo-5-methyl-1H-5λ⁴-benzo[e]pyrrolo[3,4-c][1,2]thiazine-1,3(2H)-dione oxide (3t) 5-

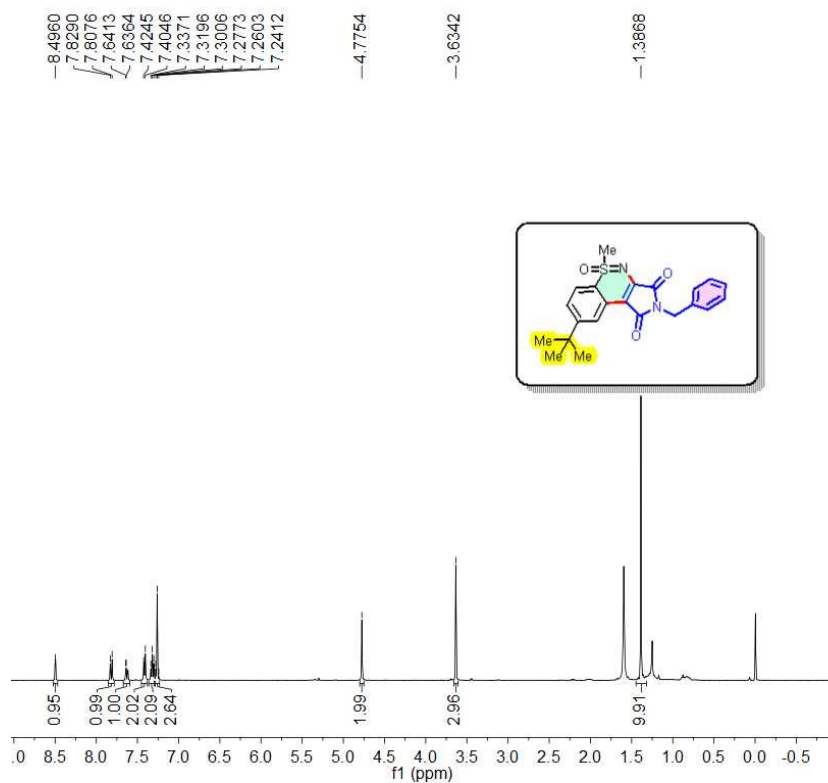


Parameter	Value
1 Data File Name	C:/ 164/ pdata/ 1/ 1r
2 Title	23-1-syj-H.164.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	294.6
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BB0400S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-04-11T21:46:32
21 Modification Date	2023-04-11T21:46:44
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1627.4
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

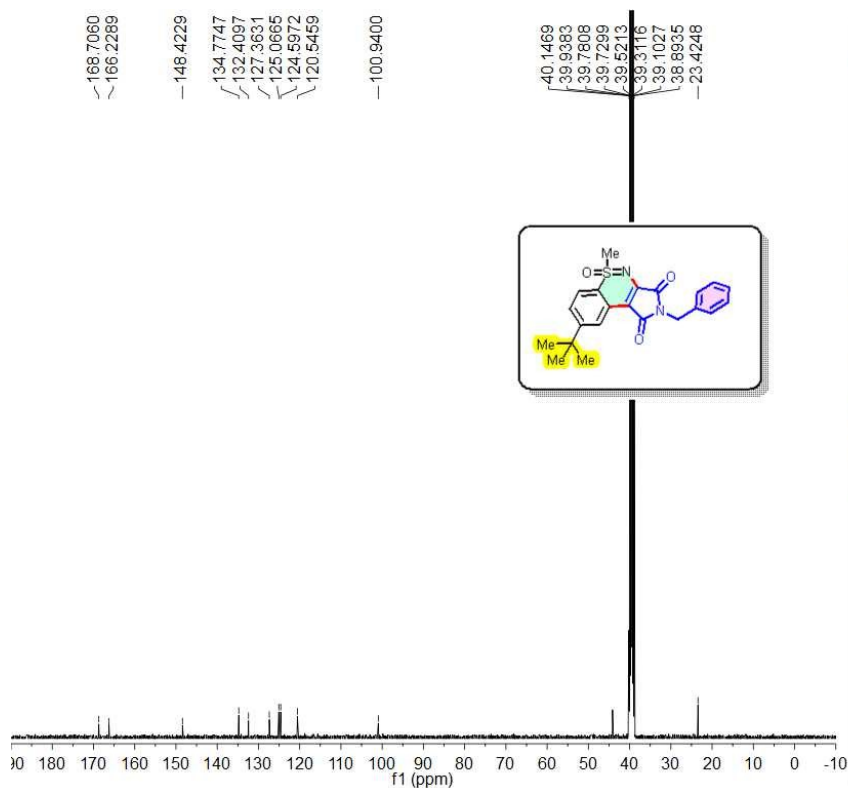


Parameter	Value
1 Data File Name	C:/ 36/ pdata/ 1/ 1r
2 Title	2023-1-syj-C.36.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	296.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	10000
15 Receiver Gain	16
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-04-18T07:47:11
21 Modification Date	2023-04-18T07:46:12
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1830.2
26 Nucleus	13C
27 Acquired Size	32768

2-Benzyl-8-(*tert*-butyl)-5-methyl-1*H*-5λ⁴-benzo[e]pyrrolo[3,4-*c*][1,2]thiazine-1,3(2*H*)-dione 5-oxide (product 3u)

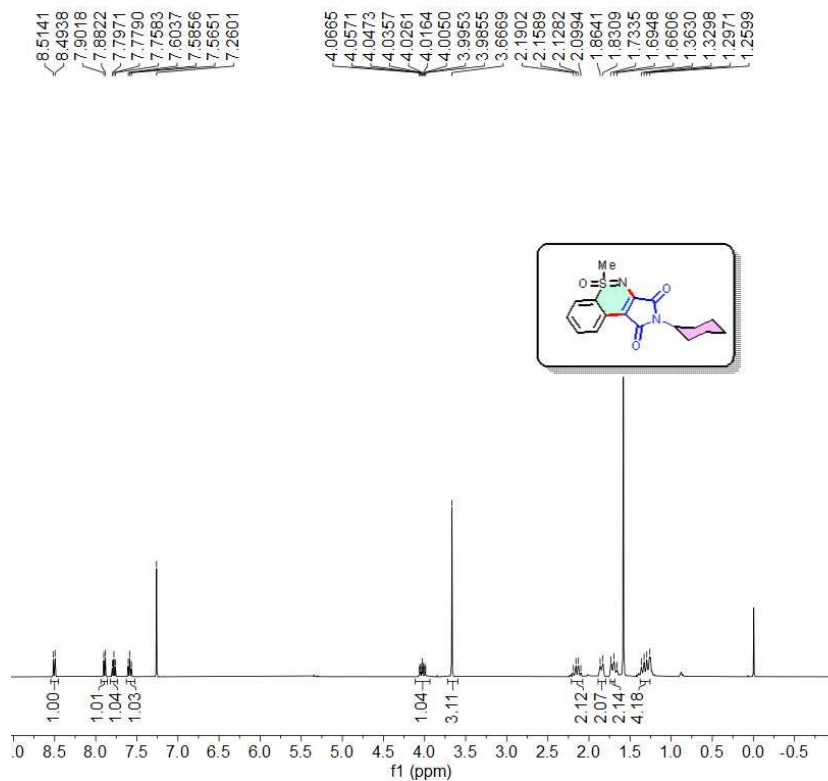


Parameter	Value
1 Data File Name	D:/ 122/ pdata/ 1/ 1r
2 Title	22-2-syj-H.122.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	294.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2022-07-31T15:50:40
21 Modification Date	2022-07-31T15:50:50
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.0
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536

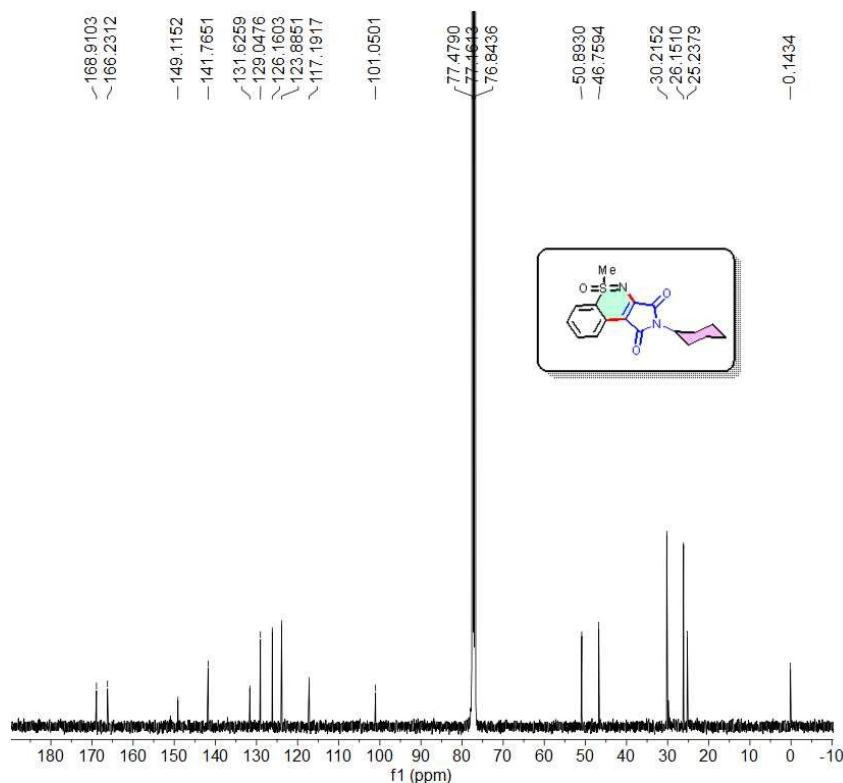


Parameter	Value
1 Data File Name	D:/ 2/ pdata/ 1/ 1r
2 Title	22-2-syj-C.2.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	DMSO
10 Temperature	295.3
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	3000
15 Receiver Gain	15
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-07-10T01:27:51
21 Modification Date	2022-07-10T01:27:56
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1888.0
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	32768

2-Cyclohexyl-5-methyl-1*H*-5λ⁴-benzo[e]pyrrolo[3,4-*c*][1,2]thiazine-1,3(2*H*)-dione 5-oxide (product 3v)

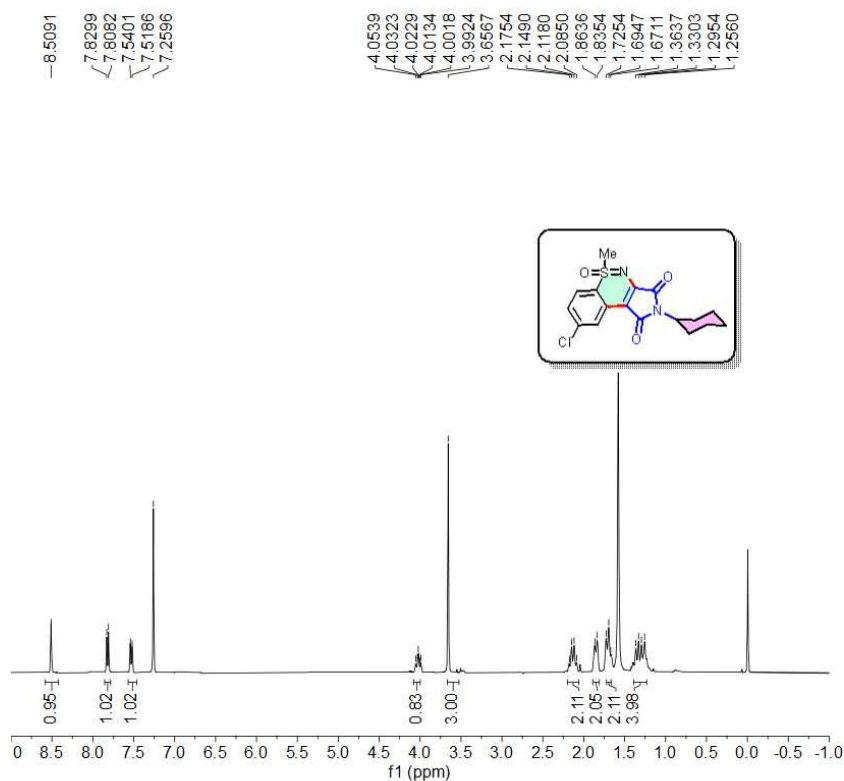


Parameter	Value
1 Data File Name	H:/heci/229/pdata/1/lr
2 Title	23-1-syj-H.229.1.lr
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	296.5
11 Pulse Sequence	zg30
12 Experiment	ID
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-05-04T22:17:47
21 Modification Date	2023-05-04T22:17:54
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.0
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

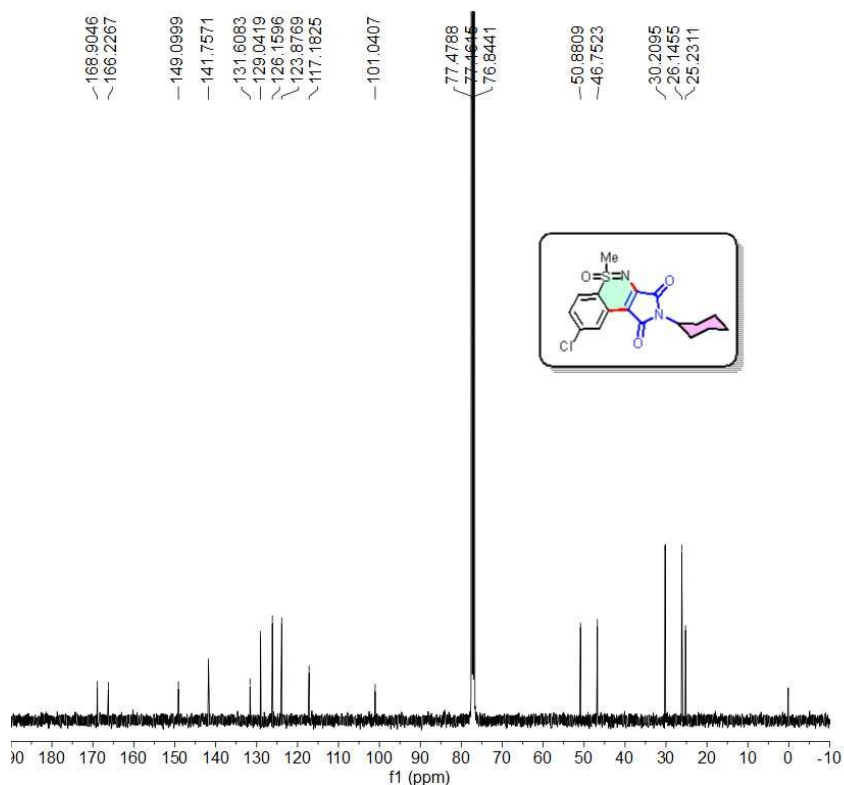


Parameter	Value
1 Data File Name	H:/heci/55/pdata/1/lr
2 Title	22-2-syj-C.55.1.lr
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	296.0
11 Pulse Sequence	zgpg30
12 Experiment	ID
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	10000
15 Receiver Gain	14
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-10-01T06:59:17
21 Modification Date	2022-10-01T06:59:34
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1829.6
26 Nucleus	13C
27 Acquired Size	32768

8-Chloro-2-cyclohexyl-5-methyl-1*H*-5λ⁴-benzo[*e*]pyrrolo[3,4-*c*][1,2]thiazine-1,3(2*H*)-dione 5-oxide (product 3w)



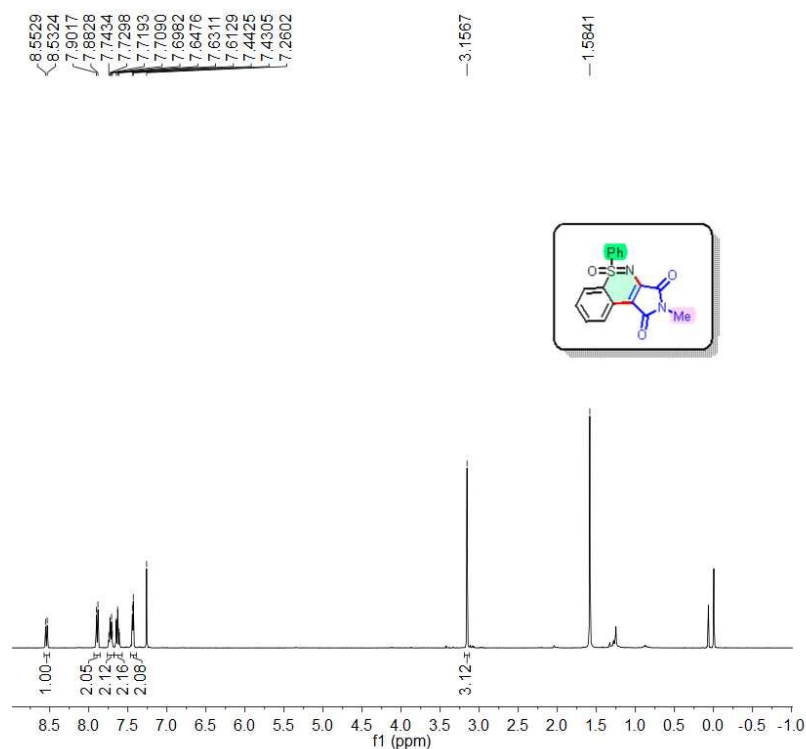
Parameter	Value
1 Data File Name	D:/161/pdata/1/1r
2 Title	22-2-syj-H.161.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/H/D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2022-08-27T22:19:58
21 Modification Date	2022-08-27T22:20:02
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.4
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536



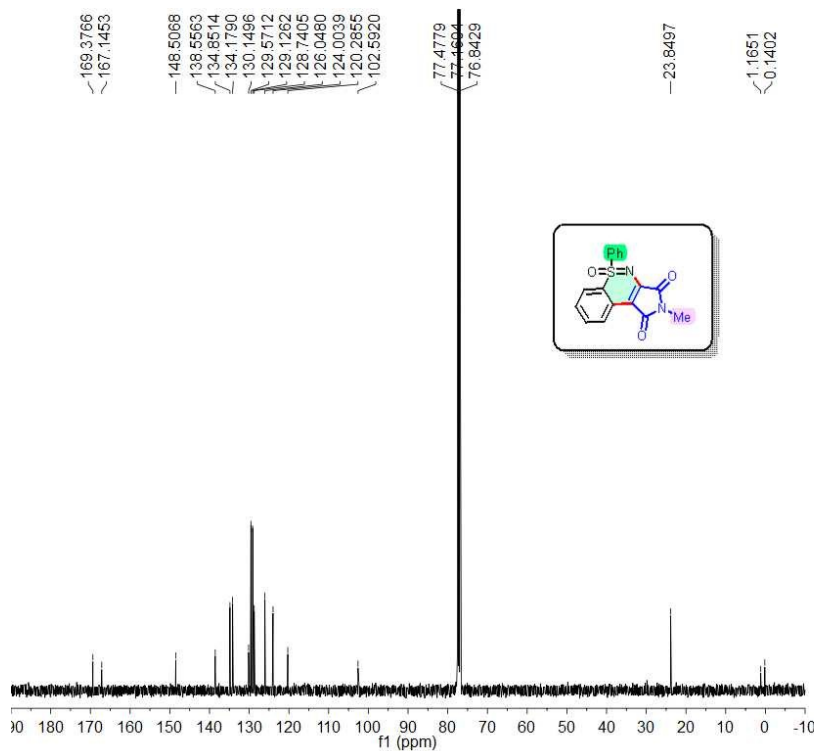
Parameter	Value
1 Data File Name	D:/17/pdata/1/1r
2 Title	22-2-syj-C.17.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/H/D-5.0-Z SP)
14 Number of Scans	4500
15 Receiver Gain	14
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-08-28T05:40:48
21 Modification Date	2022-08-28T05:40:53
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1830.3
26 Nucleus	¹³ C
27 Acquired Size	32768

2-Methyl-5-phenyl-1*H*-5 λ^4 -benzo[e]pyrrolo[3,4-*c*][1,2]thiazine-1,3(2*H*)-dione
(product 3x)

5-oxide

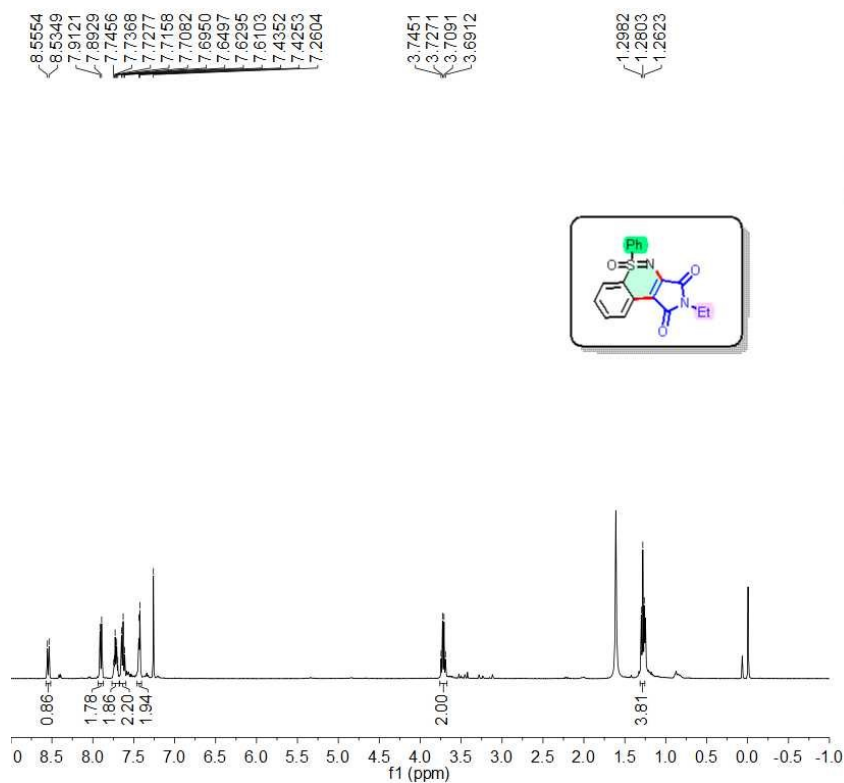


Parameter	Value
1 Data File Name	D:/22/pdata/1/1r
2 Title	22-1-syj-H.622.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsru
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.8
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/H/D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2022-06-25T18:25:20
21 Modification Date	2022-06-25T18:25:26
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.0
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65336

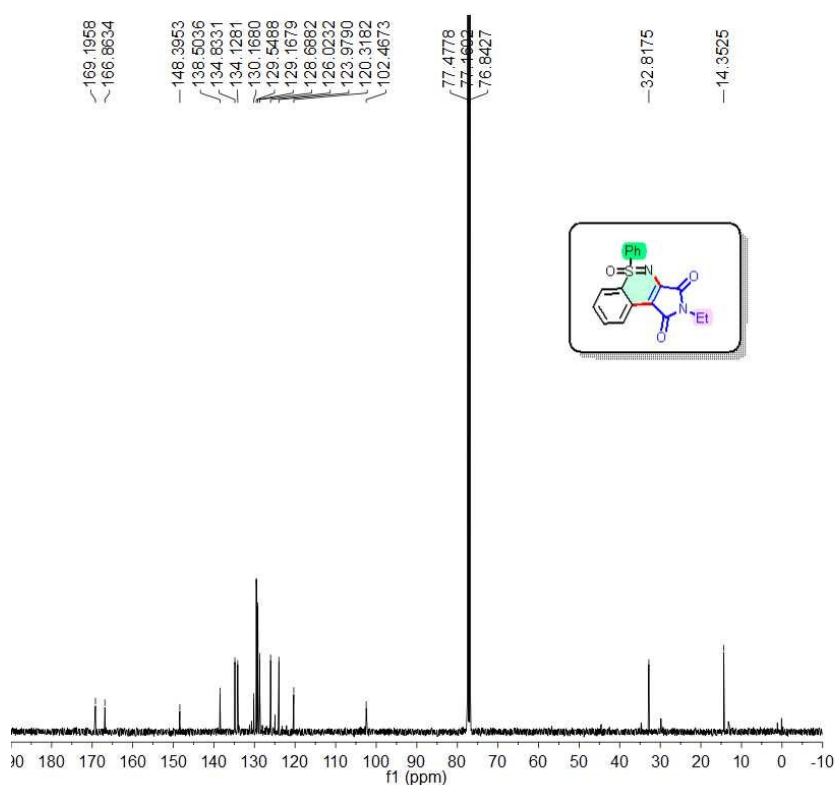


Parameter	Value
1 Data File Name	D:/131/pdata/1/1r
2 Title	22-1-syj-C.131.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsru
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	296.5
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/H/D-5.0-Z SP)
14 Number of Scans	1200
15 Receiver Gain	14
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-06-25T20:17:54
21 Modification Date	2022-06-25T20:18:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1829.9
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2-Ethyl-5-phenyl-1*H*-5λ⁴-benzo[e]pyrrolo[3,4-*c*][1,2]thiazine-1,3(2*H*)-dione 5-oxide (product 3y)

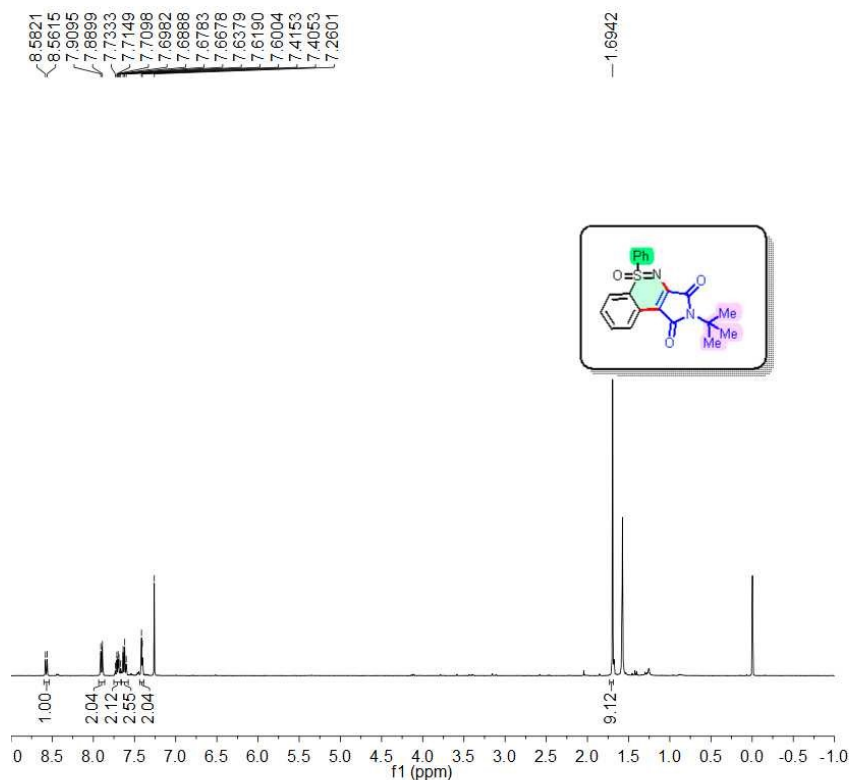


Parameter	Value
1 Data File Name	H:/287/pdata/1/1r
2 Title	22-2-syj-H.287.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI.HR-BBO400S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2022-09-30T21:05:52
21 Modification Date	2022-09-30T21:06:01
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.0
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

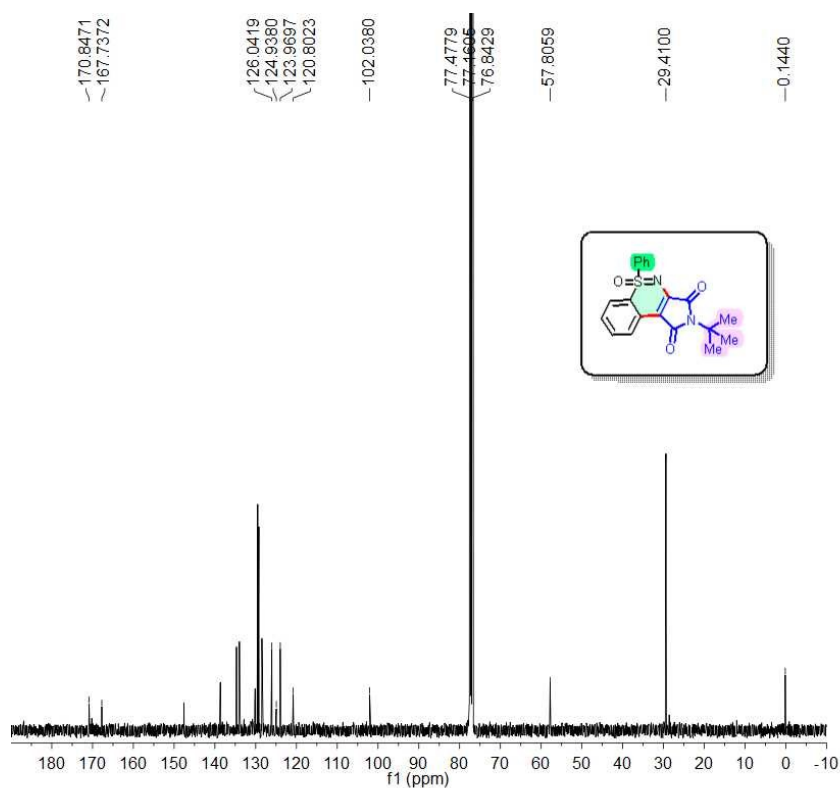


Parameter	Value
1 Data File Name	D:/ 94/pdata/1/1r
2 Title	2022-1-syj-C.94.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.6
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI.HR-400-S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	1024
15 Receiver Gain	11
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-07-02T15:17:53
21 Modification Date	2022-07-02T15:17:22
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1831.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2-(*tert*-Butyl)-5-phenyl-1*H*-5 λ^4 -benzo[e]pyrrolo[3,4-*c*][1,2]thiazine-1,3(2*H*)-dione 5-oxide
(product 3z)

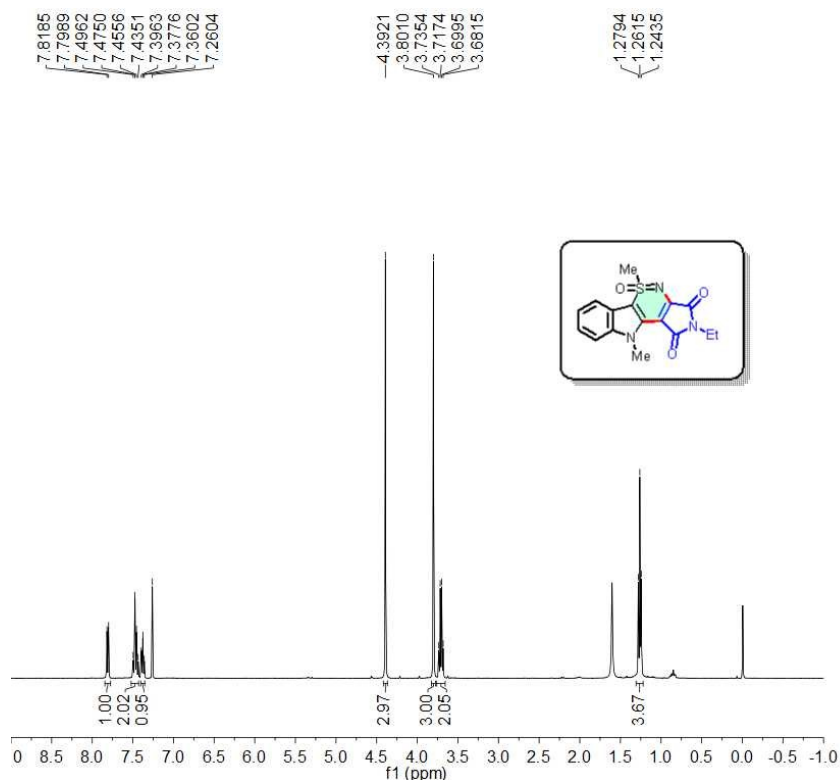


Parameter	Value
1 Data File Name	D:/ 682/ pdata/ 1/ 1r
2 Title	22-1-syj-H.682.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsru
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PIHR-BBO400S1-BBF/ H/ D-5.0-Z.SP)
14 Number of Scans	4
15 Receiver Gain	101
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2022-07-13T10:00:48
21 Modification Date	2022-07-13T10:00:56
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.0
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

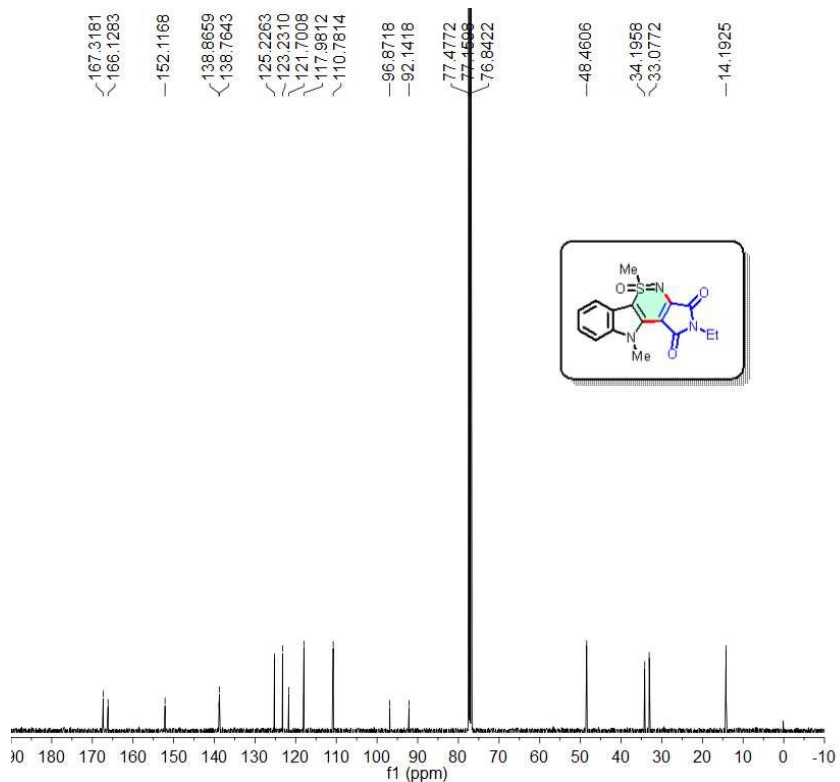


Parameter	Value
1 Data File Name	D:/ 105/ pdata/ 1/ 1r
2 Title	2022-1-syj-C.105.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsru
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	294.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PIHR-400-S1-BBF/ H/ D-5.0-Z.SP)
14 Number of Scans	2500
15 Receiver Gain	13
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-07-19T07:58:52
21 Modification Date	2022-07-19T07:58:22
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2-Ethyl-5,10-dimethyl-5λ⁴-pyrrolo[3',4':3,4][1,2]thiazino[5,6-*b*]indole-1,3(2*H*,10*H*)-dione 5-oxide (5a)

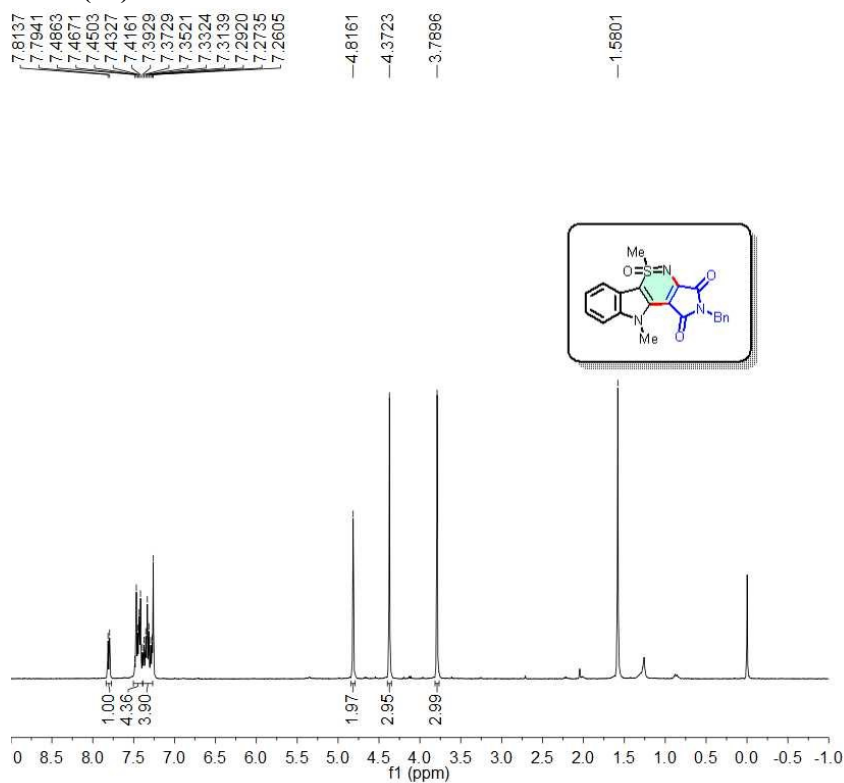


Parameter	Value
1 Data File Name	C:/ 补充产物/ 170/ pdata/ 1/ 1r
2 Title	23-1-syj-H170.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	294.4
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PIHR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-04-15T09:59:14
21 Modification Date	2023-04-15T09:59:28
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.0
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

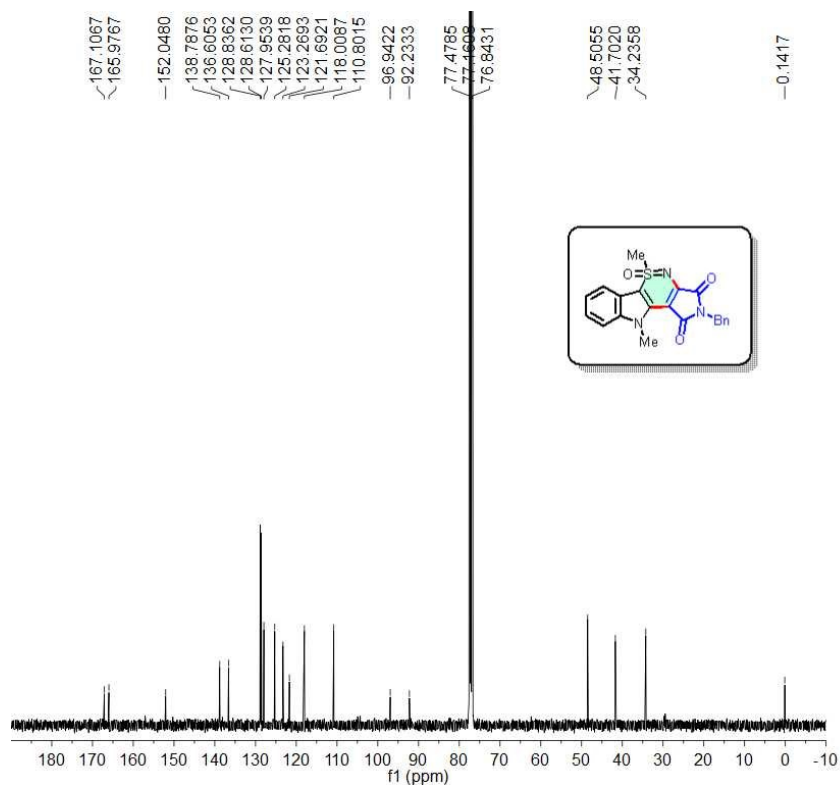


Parameter	Value
1 Data File Name	C:/ 补充产物/ 45/ pdata/ 1/ 1r
2 Title	23-1-syj-C45.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.0
11 Pulse Sequence	zpgg30
12 Experiment	1D
13 Probe	Z163739_0511 (PIHR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	1024
15 Receiver Gain	12
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-04-15T13:25:20
21 Modification Date	2023-04-15T13:25:34
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1831.4
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2-Benzyl-5,10-dimethyl-5λ⁴-pyrrolo[3',4':3,4][1,2]thiazino[5,6-*b*]indole-1,3(2*H*,10*H*)-dione 5-oxide (5b)

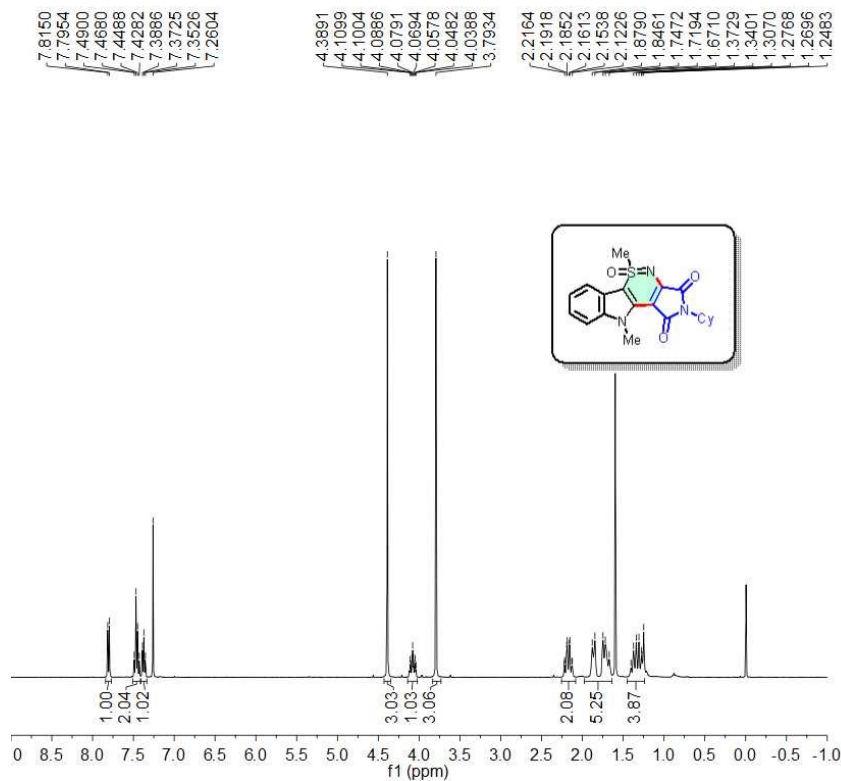


Parameter	Value
1 Data File Name	C:/235/pdata/1/1r
2 Title	2023-1-syj-H.235.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	294.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-04-15T09:58:29
21 Modification Date	2023-04-15T09:57:46
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

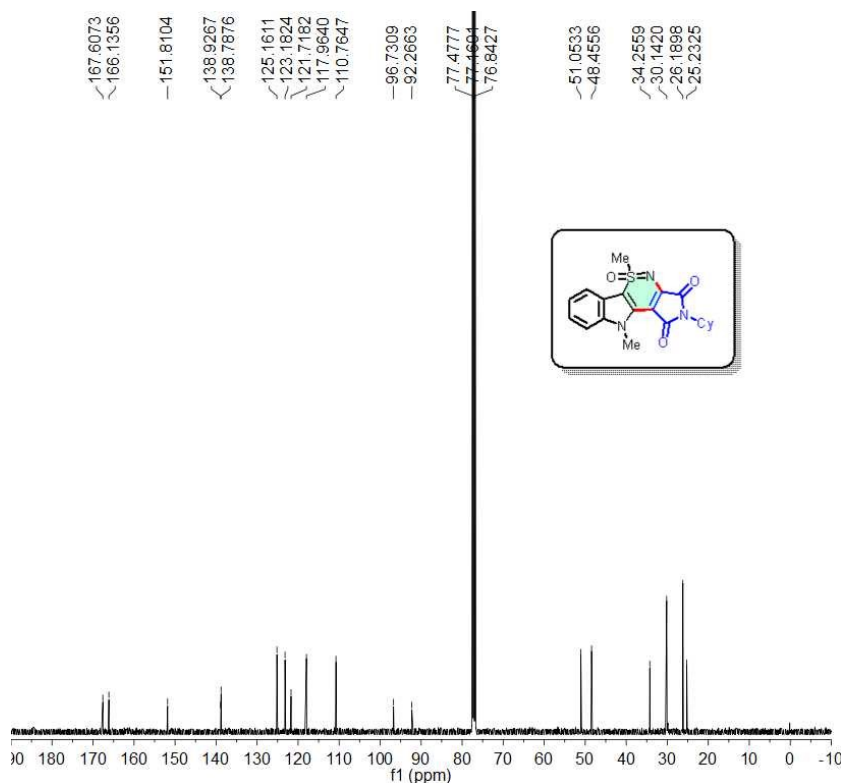


Parameter	Value
1 Data File Name	C:/95/pdata/1/1r
2 Title	2023-1-syj-C.35.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.8
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	5000
15 Receiver Gain	17
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-04-17T03:18:07
21 Modification Date	2023-04-17T03:17:16
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1830.6
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2-Cyclohexyl-5,10-dimethyl-5 λ -4-pyrrolo[3',4':3,4][1,2]thiazino[5,6-*b*]indole-1,3(2*H*,10*H*)-dione 5-oxide (5c)

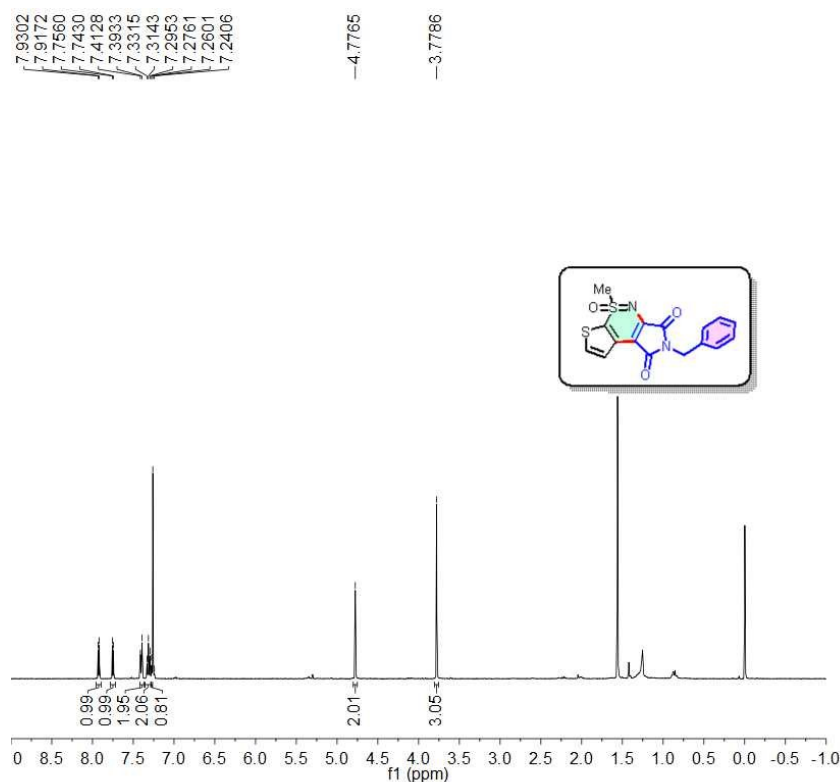


Parameter	Value
1 Data File Name	C:/171/pdata/1/1r
2 Title	23-1-syj-H.171.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	294.3
11 Pulse Sequence	zg30
12 Experiment	ID
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-04-15T10:04:01
21 Modification Date	2023-04-15T10:04:16
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.0
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

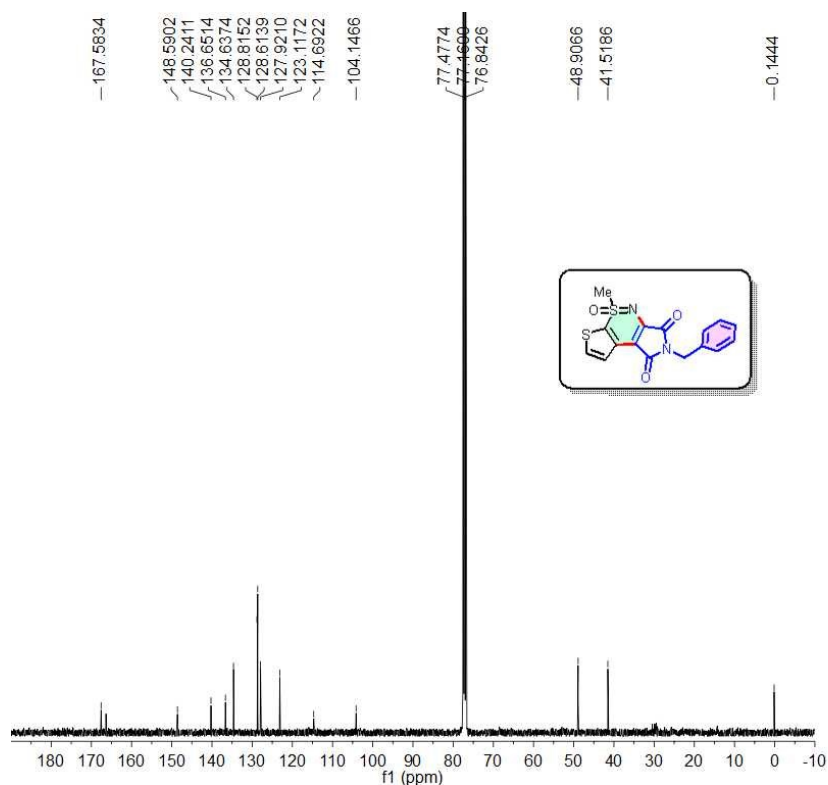


Parameter	Value
1 Data File Name	C:/46/pdata/1/1r
2 Title	23-1-syj-C.46.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.1
11 Pulse Sequence	zgpg30
12 Experiment	ID
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	1024
15 Receiver Gain	16
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-04-15T14:29:01
21 Modification Date	2023-04-15T14:29:16
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1831.2
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2-Benzyl-5-methyl-1*H*-5λ⁴-pyrrolo[3,4-*c*]thieno[3,2-*e*][1,2]thiazine-1,3(2*H*)-dione 5-oxide (7)

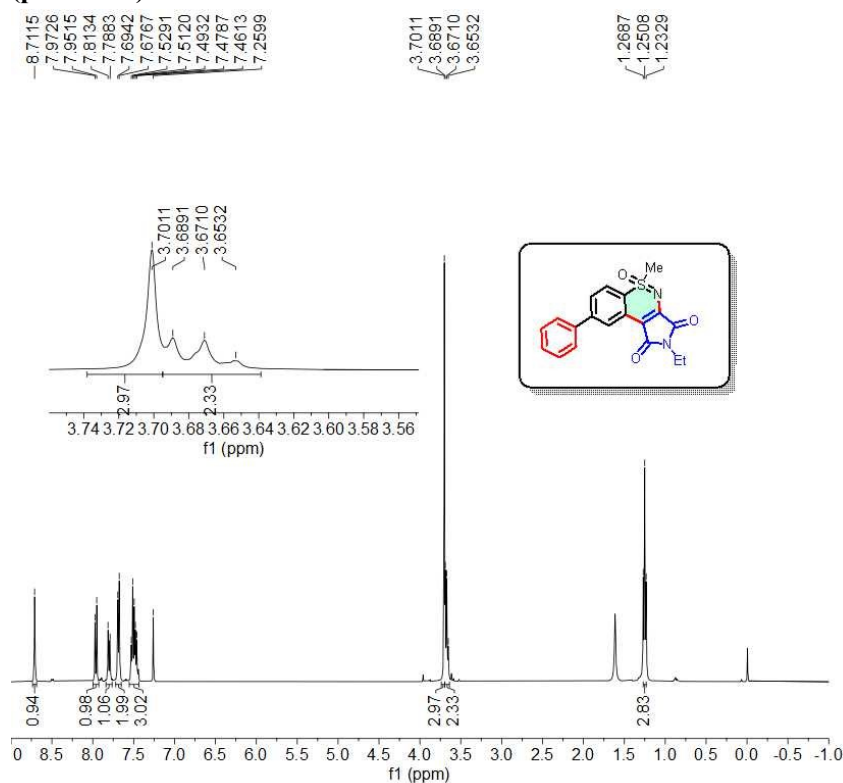


Parameter	Value
1 Data File Name	C:/Users/Administrator/Desktop/补充产物/184/pdata/1/1r
2 Title	23-1-syj-H.184.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.3
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/H/D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-04-21T21:33:04
21 Modification Date	2023-04-21T21:33:24
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.0
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

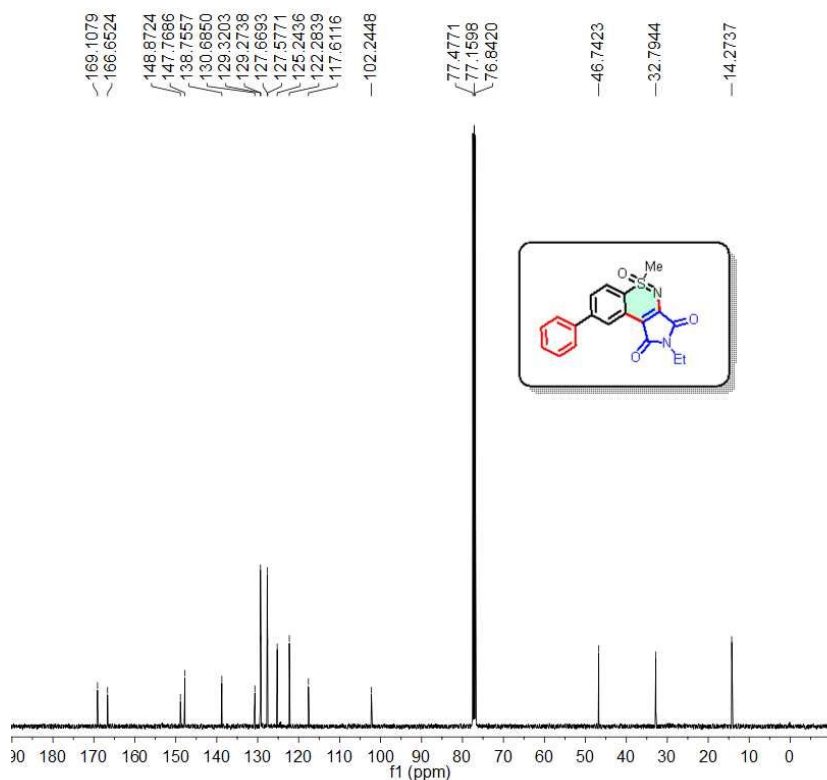


Parameter	Value
1 Data File Name	C:/Users/Administrator/Desktop/补充产物/40/pdata/1/1r
2 Title	2023-1-syj-C.40.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	296.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/H/D-5.0-Z SP)
14 Number of Scans	8210
15 Receiver Gain	16
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-04-22T08:06:07
21 Modification Date	2023-04-22T08:05:48
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1830.3
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2-Ethyl-5-methyl-8-phenyl-1*H*-5λ⁴-benzo[e]pyrrolo[3,4-*c*][1,2]thiazine-1,3(2*H*)-dione 5-oxide (product 8)

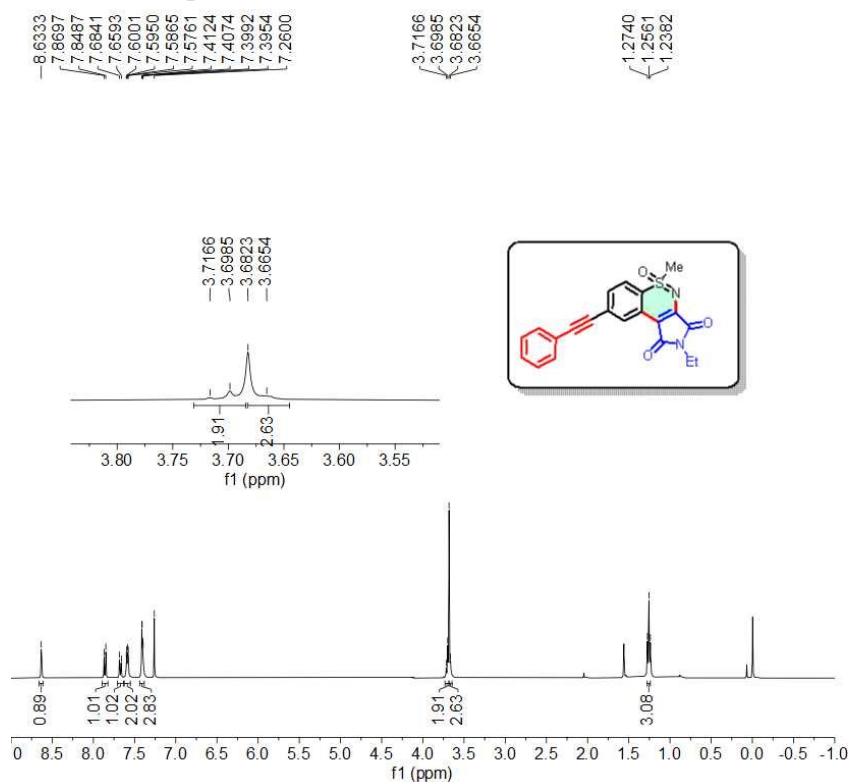


Parameter	Value
1 Data File Name	H:/wys/264/pdata/1/lr
2 Title	23-2-syj-H264.1.lr
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	296.4
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-11-07T21:49:45
21 Modification Date	2023-11-07T21:49:50
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.0
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65336

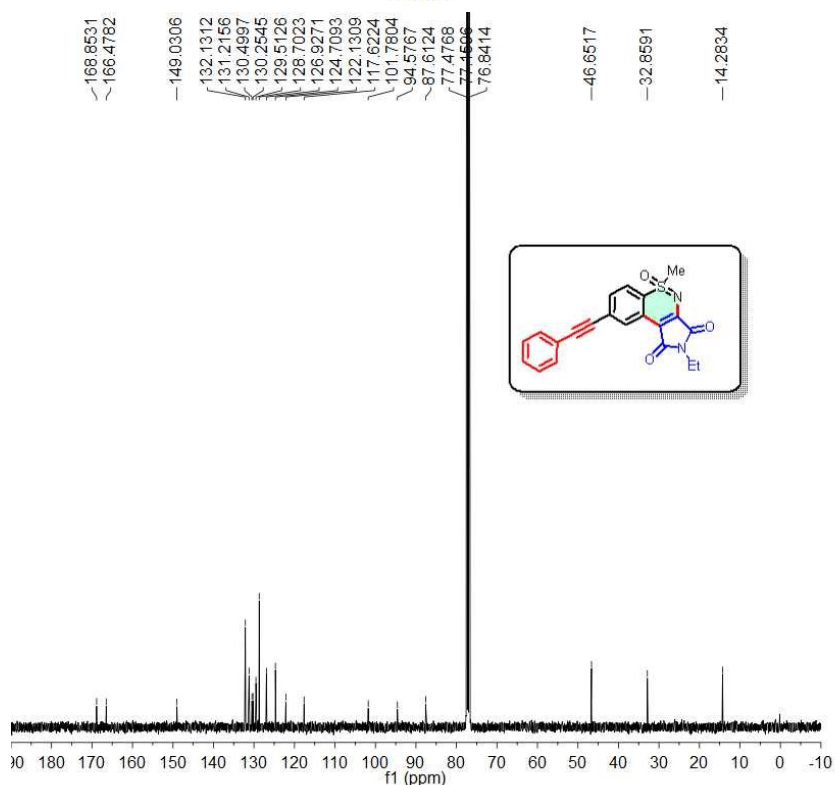


Parameter	Value
1 Data File Name	H:/wys/71/pdata/1/lr
2 Title	23-2-syj-C.71.1.lr
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	297.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/D-5.0-Z SP)
14 Number of Scans	1024
15 Receiver Gain	25
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-11-08T00:59:29
21 Modification Date	2023-11-08T00:59:34
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1831.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2-Ethyl-5-methyl-8-(phenylethynyl)-1*H*-5λ⁴-benzo[e]pyrrolo[3,4-*c*][1,2]thiazine-1,3(2*H*)-dione 5-oxide (product 9)



Parameter	Value
1 Data File Name	H:/ wvs/ 48/ pdata/ 1/ lr
2 Title	23-2-hvw-H.48.1.Ir
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.8
11 Pulse Sequence	zg30
12 Experiment	ID
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-11-24T07:23:57
21 Modification Date	2023-11-24T07:23:14
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.0
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65526



Parameter	Value
1 Data File Name	H:/ wvs/ 50/ pdata/ 1/ lr
2 Title	23-2-hvw-C.50.1.Ir
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	296.5
11 Pulse Sequence	zgpg30
12 Experiment	ID
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	901
15 Receiver Gain	25
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-11-24T08:17:07
21 Modification Date	2023-11-24T08:16:24
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1830.2
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768