Electronic Supplementary Material (ESI) for Chemical Science.

Electronic Supporting Information

Water Enables Diastereodivergency in Bispidine-Based Chiral Amine-Catalyzed Asymmetric Mannich Reaction of Cyclic *N*-Sulfonyl Ketimines with Ketones

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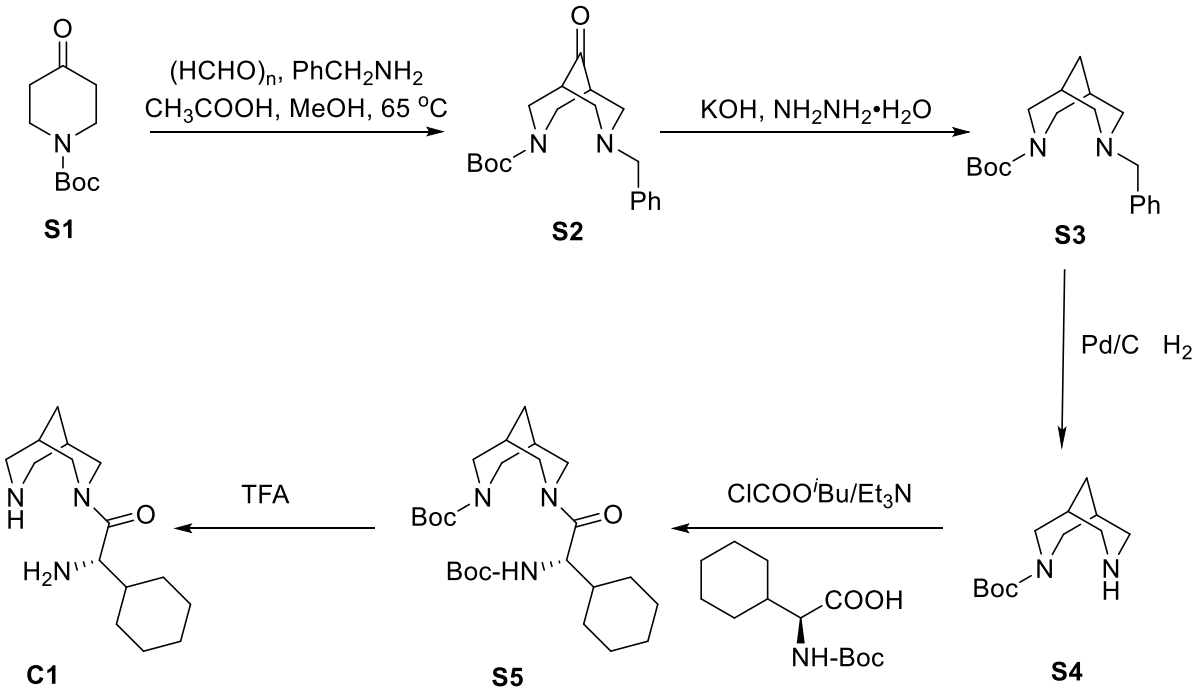
1. General informations

Unless otherwise noted, NMR characterization data were collected on Bruker ASCENDTM operating at 400 MHz or 600 MHz for ^{1}H NMR, 100 MHz or 150 MHz for $^{13}C\{1H\}$ NMR (with complete proton decoupling), and 376 MHz or 565 MHz for $^{19}F\{1H\}$ NMR (with complete proton decoupling). ^{1}H NMR chemical shifts were reported in ppm from tetramethylsilane with the solvent resonance as the internal standard ($CDCl_3$, δ = 7.26). ^{13}C NMR spectra chemical shifts are reported in ppm from the tetramethylsilane with the solvent resonance as internal standard ($CDCl_3$, δ = 77.0). Spectra were reported as follows: chemical shift (δppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz), integration and assignment. High-resolution mass spectra (HRMS) were recorded on a Thermo Q-Exactive Focus (FTMS+c ESI). Enantiomeric excesses were determined by chiral SFC analysis using the corresponding commercial chiralpak column as stated in the experimental procedures at 23 °C with UV detector. Optical rotations were measured on Rudolph Research Analytic Automatic Polarimeter and reported as follows: $[\alpha]_D^T$ (c: g/100 mL, in CH_2Cl_2, λ = 589 nm). Infrared spectra (IR) were recorded on Bruker Tensor II spectrometer with Plantium ATR accessory and the peaks are reported as absorption maxima (v, cm^{-1}). Circular dichroism spectrums (CD) were recorded on Applied Photophysics Chirascan. Melting point ranges were determined on OptiMelt. X-ray crystallographic data were collected by a Bruker D8 Venture Photon II. All the solvents were purified by usual methods before use and reagents obtained from commercial sources were used without further purification. Chiral bispidines,[1] cyclic *N*-sulfonyl ketimines[2] were synthesized according to reported literature procedures.

2. Typical procedure for chiral bispidines preparation.[1]



A solution of 1-Boc-piperidin-4-one **S1** (9.96 g, 50.0 mmol), benzylamine (5.36 g, 50.0 mmol) and acetic acid (3.0 mL) in dry methanol (20 mL) was added dropwise over a period of 1 h at 65 °C in an oil bath to a suspension of paraformaldehyde (3.03 g, 100.0 mmol) in dry methanol (40 mL). Another portion of paraformaldehyde (3.03 g, 100.0 mmol) was added and the mixture was stirred for 8 h at 65 °C in an oil bath. Then 1 *N* KOH solution (100 mL) was added in ice-water bath, the aqueous phase was extracted with CH_2Cl_2 (3×200 mL). The combined organic layers were dried over Na_2SO_4 and the solvent was evaporated in vacuo. and further purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 3/1) to yield a yellow oil **S2** (10.03 g, 30.37 mmol, 61% yield).

To a mixture of **S2** (10.03 g, 30.37 mmol), hydrazine monohydrate (7.3 mL, 151.8 mmol) and diethylene glycol (60 mL) at 60 °C was added powdered KOH (11.77 g, 210.2 mmol) in an oil bath. The mixture was heated to 160 °C for 4 h in an oil bath. After cooling, the mixture was treated with water (200 mL) and extracted with CH_2Cl_2 (3×200 mL). The combined organic layers were dried with Na_2SO_4. The organic solvent was evaporated in vacuo and the residue was purified by flash chromatography on silica gel (petroleum ether /ethyl acetate = 4/1) to yield a white solid **S3** (6.72 g, 21.2 mmol, 70% yield).

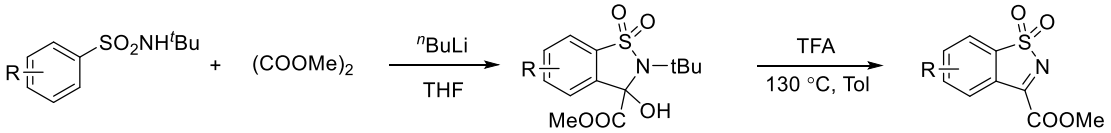
Pd/C (0.51 g, 10%) was added to a suspension of bispidine **S3** (3.16 g, 10.0 mmol) in methanol (15 mL), then acetic acid (10 mL) was added. The atmosphere was exchanged with hydrogen for 3 times. The mixture was stirred under H_2 atmosphere for 12 h. The mixture was filtered over celite and the solvent was alkalized by 1 *N* KOH solution (250 mL) and extracted with CH_2Cl_2 (3×200 mL). The combined organic layers were dried with Na_2SO_4. The organic solvent was evaporated in vacuo and the crude product **S4** was obtained used directly in the next step without purification.

N-tert-Butoxycarbonyl-L-tert-leucine (2.66 g, 11.5 mmol) and TEA (1.60 mL, 11.5 mmol) were dissolved in THF (20 mL). The solution was cooled to 0 °C in ice-water bath. To the solution was added isobutyl chlorocarbonate (1.49 mL, 11.5 mmol) dropwise for 15 min. After the solution was stirred for 30 min, amine **S4** obtained above was added for 15 min. The resulting solution was stirred at 0 °C for 1 h in ice-water bath and then at room temperature for another 16 h. After filtration and removal of solvent under reduced

pressure, the residue was purified through column chromatography on silica gel (petroleum ether/ethyl acetate = 3/1) to yield a white solid **S5** (2.94 g, 67% yield).

To **S5** (2.94 g, 6.7 mmol) in CH_2Cl_2 (5 mL) was added TFA (13.4 mL) and stirred until the reaction was finished. Then the solvent was evaporated, and CH_2Cl_2 (10 mL) was added. The pH value was brought into the range of 8–10 by the addition of 1 *N* NaOH. The aqueous phase was extracted with CH_2Cl_2 (5×20 mL). The combined organic phase was washed with brine, dried over anhydrous $MgSO_4$ and evaporated in vacuo to yield a yellow oil **C1** (1.42 g, 6.0 mmol, 89% yield).

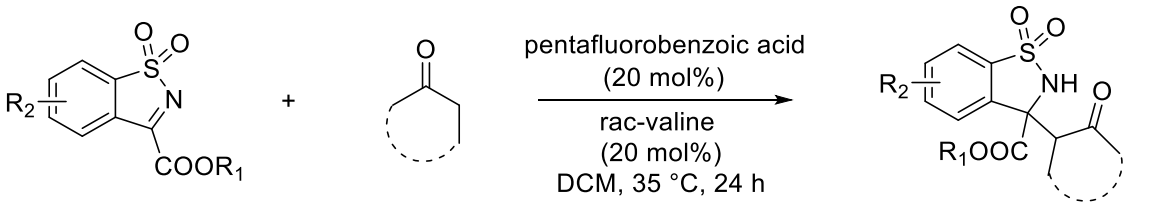
3. General procedure for cyclic *N*-sulfonyl ketimines preparation.[2]



Under a dry nitrogen atmosphere, aryl sulfonamide (15 mmol) was dissolved in anhydrous THF (80 mL), and then the solution was cooled to 0 °C. To the solution was added butyllithium (30.75 mmol) dropwise for 20 min. After stirring an additional 25 min, the suspension was cooled further to -78 °C and dimethyl oxalate (45 mmol) in THF (20 mL) was added dropwise over 10 minutes. The cooling bath was removed and the suspension was stirred at ambient temperature for 2 h. The reaction was quenched with 5% HCl (40 mL) and added to water (200 mL). The organics were extracted with ether (50×3 mL). The ether phase was washed with brine (200 mL). The solvent was removed and the crude product was obtained used directly in the next step without further purification.

To the crude product obtained above, TFA (75 mol) in toluene (20 mL) was added and the resulting mixture was stirred at 130 °C in sealed tube for 10 to 60 minutes, then the solution was concentrated and the resultant solid was dissolved in CH_2Cl_2 (150 mL) and washed with $NaHCO_3$ saturated solution (50×2 mL) to remove traces of TFA. Then the organic phase was washed with brine and dried over Na_2SO_4. The solvent was removed and theobtained crude product was further purified by flash chromatography (DCM/PE = 1/2).

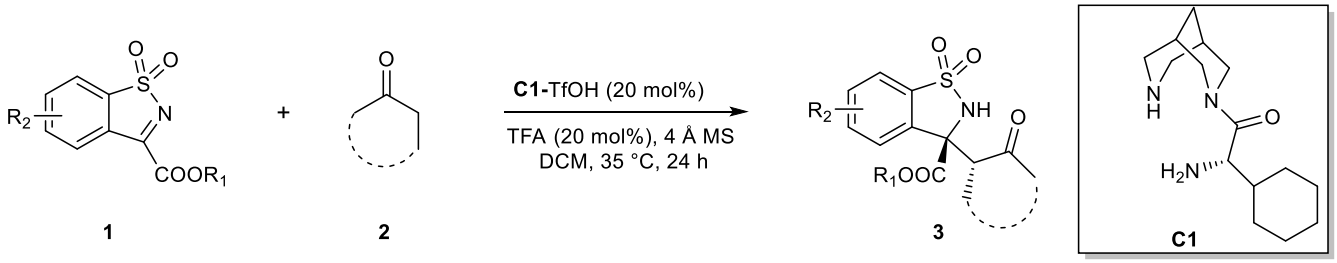
4. General procedure for preparation of the racemic products 3 and 4.



A dry reaction tube was charged with cyclic *N*-sulfonyl ketimines **1** (0.20 mmol), ketones **2** (liquid ketone 0.2 mL, solid ketone 1.0 mmol), rac-valine (4.7 mg, 0.04 mmol, 20 mol%), pentafluorobenzoic acid (8.5 mg, 0.04 mmol, 20 mol%) in anhydrous DCM (0.6 mL). The reaction mixture was stirred at 35 °C for 24 h in water bath. The desire product was purified directly by silica gel column chromatograph (petroleum ether/ethyl acetate = 2/1)) to yield a white solid.

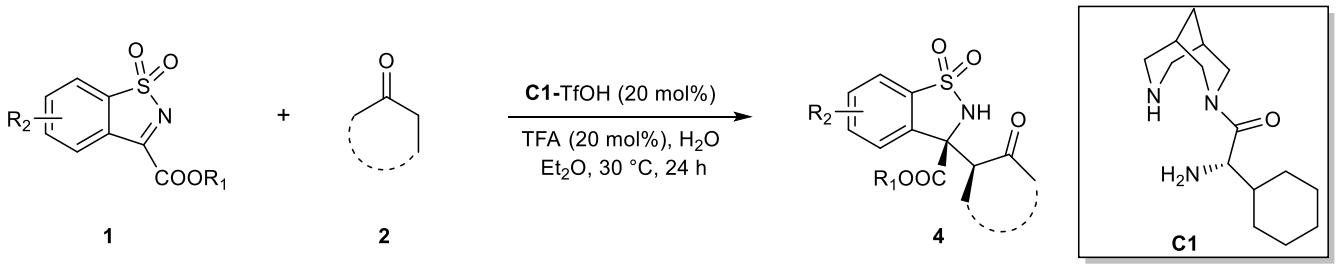
5. General procedure for the catalytic asymmetric Mannich reaction.

***Anti*-selective Mannich reaction:**



A dry reaction tube was charged with cyclic *N*-sulfonyl ketimines **1** (0.20 mmol), ketones **2** (liquid ketone 0.2 mL, solid ketone 1.0 mmol), **C1-TfOH** (16.6 mg, 0.04 mmol, 20 mol%), TFA (4.6 mg, 0.04 mmol, 20 mol%), and 4 Å MS (20 mg) in anhydrous DCM (0.6 mL). The reaction mixture was stirred at 35 °C for 24 h in water bath. The desire product was purified directly by silica gel column chromatograph (petroleum ether/ethyl acetate = 2/1)) to yield a white solid.

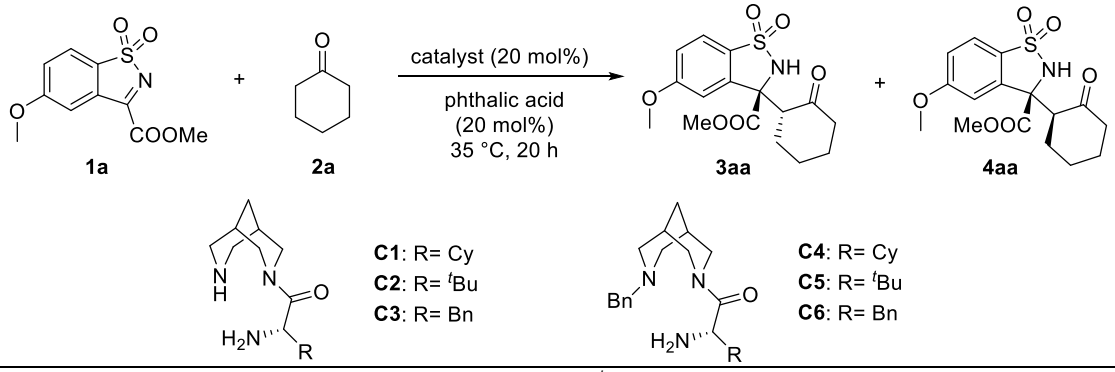
***Syn*-selective Mannich reaction:**



A dry reaction tube was charged with cyclic *N*-sulfonyl ketimines **1** (0.20 mmol), ketones **2** (liquid ketone 0.2 mL, solid ketone 1.0 mmol), **C1-TfOH** (16.6 mg, 0.04 mmol, 20 mol%), TFA (4.6 mg, 0.04 mmol, 20 mol%), and H_2O (0.2 mL) in anhydrous Et_2O (0.6 mL). The reaction mixture was stirred at 30 °C for 24 h in water bath. The desire product was purified directly by silica gel column chromatograph (petroleum ether/ethyl acetate = 2/1)) to yield a white solid.

6. Optimization of the reaction conditions.

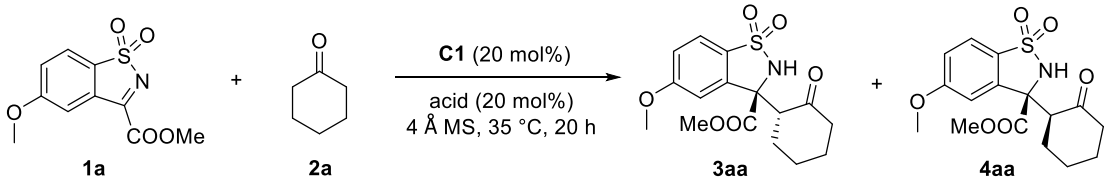
Table S1: Screening of catalysts.



Entry[a]	Catalyst	Yield (%)[b]	dr (**3aa**:**4aa**)[c]	ee (%)[c]
1	**C1**	99	76:24	67/0
2	**C2**	98	62:28	62/-34
3	**C3**	98	60:40	60/20
4	**C4**	98	62:38	33/58
5	**C5**	99	65:35	5/60
6	**C6**	99	60:40	55/20

[a] Unless otherwise noted, catalyst (0.04 mmol, 20 mol%), phthalic acid (0.04 mmol, 20 mol%), **1a** (51.0 mg, 0.20 mmol) and **2a** (0.6 mL) were stirred at 35 °C for 20 h in water bath. The mixture was purified directly by column chromatography on silica gel. [b] Isolated yield. [c] Determined by SFC analysis on a chiral stationary.

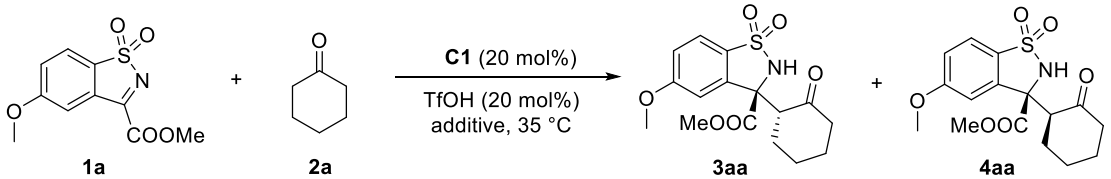
Table S2: Screening of acids with **C1** as catalyst.



Entry[a]	Acid	Yield (%)[b]	dr (**3aa**:**4aa**)[c]	ee (%)[c]
1	benzoic acid	78	>19:1	31
2	salicylic acid	97	>19:1	40
3	phthalic acid	95	>19:1	44
4	pentafluorobenzoic acid	92	>19:1	50
5	trifluoroacetic acid	93	>19:1	72
6	trifluoromethanesulfonic acid	95	85:15	80

[a] Unless otherwise noted, **C1** (0.04 mmol, 20 mol%), acid (0.04 mmol, 20 mol%), **1a** (51.0 mg, 0.20 mmol), **2a** (0.6 mL) and 4 Å MS (20.0 mg) were stirred at 35 °C for 20 h in water bath. The mixture was purified directly by column chromatography on silica gel. [b] Isolated yield. [c] Determined by SFC analysis on a chiral stationary.

Table S3: Screening of additives with **C1** as catalyst.

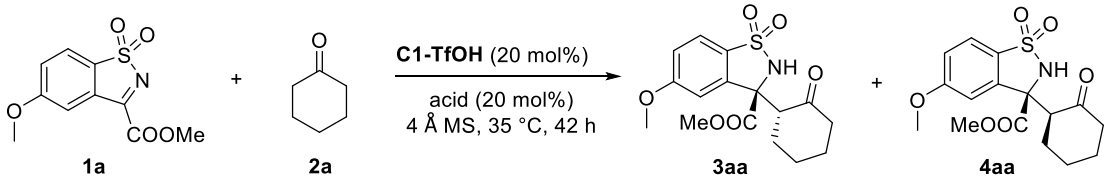


1a **2a** **3aa** **4aa**

Entry[a]	Additive	Time (h)	Yield (%)[b]	dr (**3aa**:**4aa**)[c]	ee (%)[c]
1	H_2O (0.2 mL)	36 h	78	20:80	67/69
2	4 Å MS (20.0 mg)	16 h	95	76:24	80/10
3	4 Å MS (40.0 mg)	36 h	50	87:13	45/23
4	4 Å MS (60.0 mg)	36 h	46	91:9	30/11

[a] Unless otherwise noted, **C1** (0.04 mmol, 20 mol%), TfOH (0.04 mmol, 20 mol%), **1a** (51.0 mg, 0.20 mmol), additive and **2a** (0.6 mL) were stirred at 35 °C in water bath. The mixture was purified directly by column chromatography on silica gel. [b] Isolated yield. [c] Determined by SFC analysis on a chiral stationary.

Table S4: Screening of acids with **C1**-**TfOH** as catalyst.

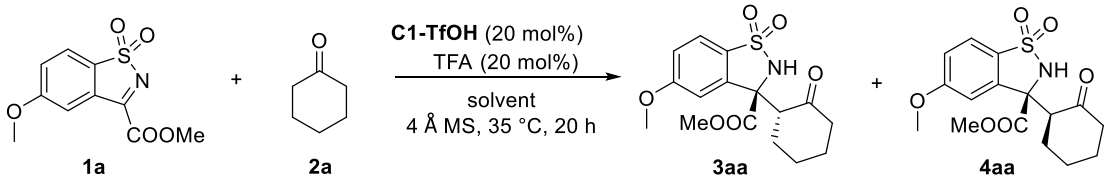


1a **2a** **3aa** **4aa**

Entry[a]	Acid	Yield (%)[b]	dr (**3aa**:**4aa**)[c]	ee (%)[c]
1	-	80	88:12	68
2	benzoic acid	80	89:11	64
3	acetic acid	97	88:12	71
4	salicylic acid	89	93:7	73
5	*ortho*-phthalic acid	98	91:9	71
6[d]	pentafluorobenzoic acid	95	95:5	80
7[d]	trifluoroacetic acid	99	>19:1	83

[a] Unless otherwise noted, **C1**-**TfOH** (0.04 mmol, 20 mol%), acid (0.04 mmol, 20 mol%), **1a** (51.0 mg, 0.20 mmol), **2a** (0.6 mL) and 4 Å MS (20.0 mg) were stirred at 35 °C for 42 h in water bath. The mixture was purified directly by column chromatography on silica gel. [b] Isolated yield. [c] Determined by SFC analysis on a chiral stationary. [d] For 20 h.

Table S5: Screening of solvents for *anti*-selective Mannich reaction.

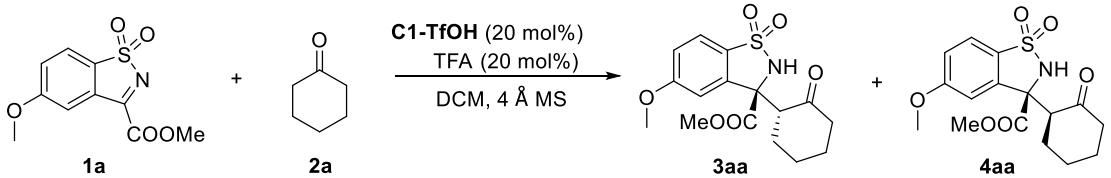


1a **2a** **3aa** **4aa**

Entry[a]	Solvent	Yield (%)[b]	dr (**3aa**:**4aa**)[c]	ee (%)[c]
1	Toluene	97	>19:1	85
2	Et_2O	91	>19:1	83
3	DCM	98	>19:1	92
4	DCE	98	>19:1	89
5	EtOAc	95	>19:1	86
6	THF	90	>19:1	82
7	$CHCl_3$	97	>19:1	88
8	1,4-Dioxane	98	>19:1	83
9	MeOH	85	62:38	85/75

[a] Unless otherwise noted, **C1**-**TfOH** (0.04 mmol, 20 mol%), TFA (0.04 mmol, 20 mol%), **1a** (51.0 mg, 0.20 mmol), **2a** (0.2 mL) and 4 Å MS (20.0 mg) were stirred in 0.6 mL solvent at 35 °C for 20 h in water bath. The mixture was purified directly by column chromatography on silica gel. [b] Isolated yield. [c] Determined by SFC analysis on a chiral stationary.

Table S6: Optimization of temperature for *anti*-selective Mannich reaction.



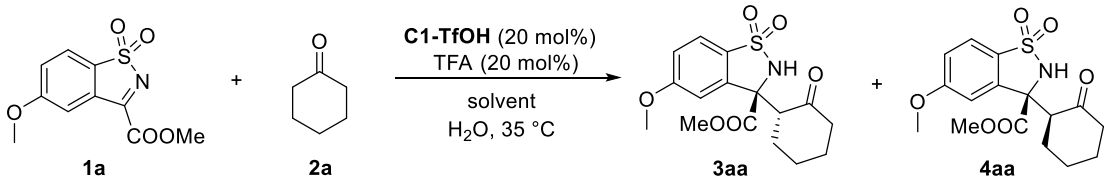
1a **2a** **3aa** **4aa**

Entry[a]	Temp (°C)	Time (h)	Yield (%)[b]	dr (**3aa**:**4aa**)[c]	ee (%)[c]
1	0	48 h	20	>19:1	93
2	10	48 h	25	>19:1	92
3	20	48 h	92	>19:1	92

4	30	20 h	94	>19:1	92
5	35	20 h	98	>19:1	92
6	40	16 h	97	>19:1	90

[a] Unless otherwise noted, **C1-TfOH** (0.04 mmol, 20 mol%), TFA (0.04 mmol, 20 mol%), **1a** (51.0 mg, 0.20 mmol), **2a** (0.2 mL) and 4 Å MS (20.0 mg) were stirred in 0.6 mL DCM in water bath. The mixture was purified directly by column chromatography on silica gel. [b] Isolated yield. [c] Determined by SFC analysis on a chiral stationary.

Table S7: Screening of solvents for *syn*-selective Mannich reaction.

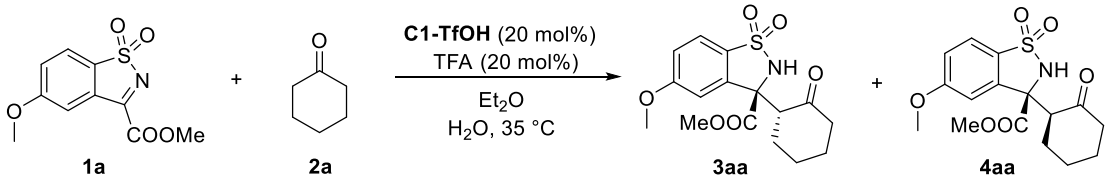


1a **2a** **3aa** **4aa**

Entry[a]	Solvent	Time (h)	Yield (%)[b]	dr (**3aa**:**4aa**)[c]	ee (%)[c]
1	Toluene	12 h	98	23:77	96/96
2	Et_2O	12 h	98	12:88	90/93
3	DCM	12 h	99	21:79	94/93
4	DCE	12 h	97	22:78	94/94
5	EtOAc	12 h	98	15:85	85/90
6	THF	36 h	92	11:89	75/88
7	CH_3CN	36 h	80	20:80	76/80
8	1,4-Dioxane	36 h	88	15:85	77/88
9	MTBE	12 h	98	12:88	85/92

[a] Unless otherwise noted, **C1-TfOH** (0.04 mmol, 20 mol%), TFA (0.04 mmol, 20 mol%), **1a** (51.0 mg, 0.20 mmol), **2a** (0.2 mL) and H_2O (0.2 mL) were stirred in 0.6 mL solvent at 35 °C in water bath. The mixture was purified directly by column chromatography on silica gel. [b] Isolated yield. [c] Determined by SFC analysis on a chiral stationary.

Table S8: Optimization of amount of H_2O for *syn*-selective Mannich reaction.

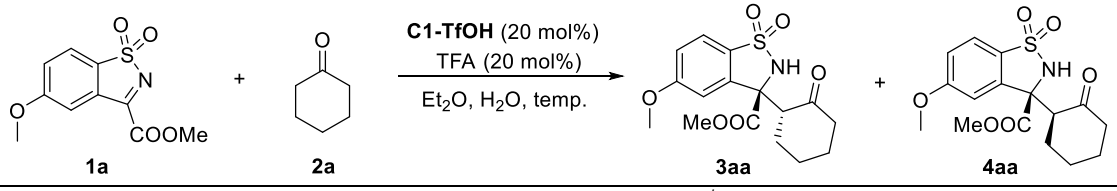


1a **2a** **3aa** **4aa**

Entry[a]	H_2O	Time (h)	Yield (%)[b]	dr (**3aa**:**4aa**)[c]	ee (%)[c]
1	3.6 µL	12 h	98	31:69	95/94
2	10 µL	12 h	98	18:82	92/94
3	50 µL	12 h	98	14:86	84/91
4	0.1 mL	12 h	98	13:87	85/92
5	0.2 mL	12 h	98	12:88	90/93
6	0.4 mL	16 h	98	12:88	88/92
7[d]	0.6 mL	16 h	98	11:89	77/88

[a] Unless otherwise noted, **C1-TfOH** (0.04 mmol, 20 mol%), TFA (0.04 mmol, 20 mol%), **1a** (51.0 mg, 0.20 mmol), **2a** (0.2 mL) and H_2O were stirred in 0.6 mL Et_2O at 35 °C in water bath. The mixture was purified directly by column chromatography on silica gel. [b] Isolated yield. [c] Determined by SFC analysis on a chiral stationary. [d] 0.6 mL H_2O as solvent.

Table S9: Optimization of temperature for *syn*-selective Mannich reaction.



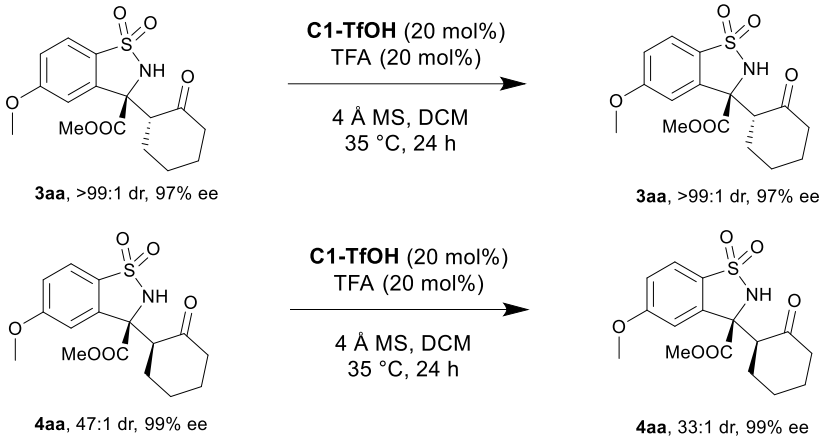
1a **2a** **3aa** **4aa**

Entry[a]	Temp (°C)	Time (h)	Yield (%)[b]	dr (**3aa**:**4aa**)[c]	ee (%)[c]
1	0	72 h	17	10:90	80/93
2	10	72 h	46	9:91	86/94
3	20	40 h	95	10:90	89/93
4	30	24 h	98	10:90 (11:89)[d]	90/94
5	35	16 h	98	12:88 (14:86)[d]	90/93

[a] Unless otherwise noted, **C1-TfOH** (0.04 mmol, 20 mol%), TFA (0.04 mmol, 20 mol%), **1a** (51.0 mg, 0.20 mmol), **2a** (0.2 mL) and H_2O (0.2 mL) were stirred in 0.6 mL Et_2O in water bath. The mixture was purified directly by column chromatography on silica gel. [b] Isolated yield. [c] Determined by SFC analysis on a chiral stationary. [d] Determined by NMR analysis.

7. Control experiments.

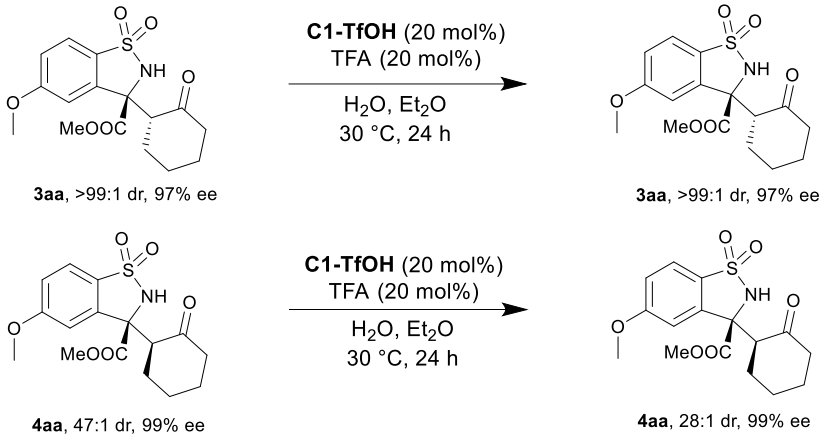
(a)



3aa, >99:1 dr, 97% ee → **3aa**, >99:1 dr, 97% ee

4aa, 47:1 dr, 99% ee → **4aa**, 33:1 dr, 99% ee

(b)



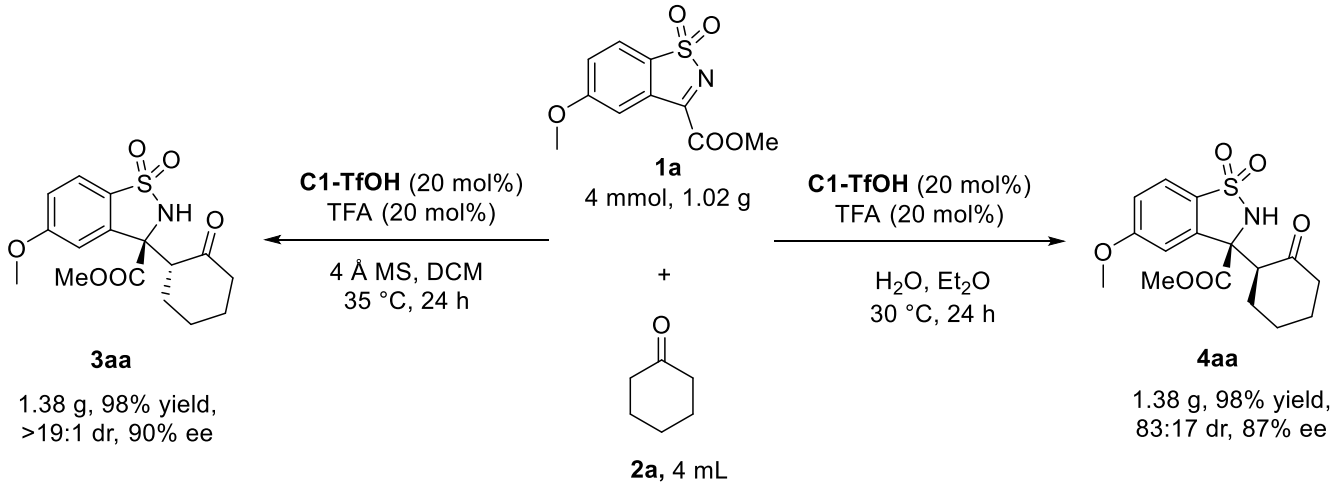
3aa, >99:1 dr, 97% ee → **3aa**, >99:1 dr, 97% ee

4aa, 47:1 dr, 99% ee → **4aa**, 28:1 dr, 99% ee

Control experimens in condition A: A dry reaction flask was charged with **3aa** or **4aa** (0.2 mmol) , **C1-TfOH** (0.04 mmol, 20 mol%), TFA (0.04 mmol, 20 mol%) and 4 Å MS (20 mg) in anhydrous DCM (0.6 mL). The reaction mixture was stirred at 35 °C for 24 h in water bath. The desire product was purified directly by silica gel column chromatograph (petroleum ether/ethyl acetate = 2/1)) to yield a white solid.

Control experimens in condition B: A dry reaction flask was charged with **3aa** or **4aa** (0.2 mmol), **C1-TfOH** (0.04 mmol, 20 mol%), TFA (0.04 mmol, 20 mol%) and H_2O (0.2 mL) in anhydrous Et_2O (0.6 mL). The reaction mixture was stirred at 30 °C for 24 h in water bath. The desire product was purified directly by silica gel column chromatograph (petroleum ether/ethyl acetate = 2/1)) to yield a white solid.

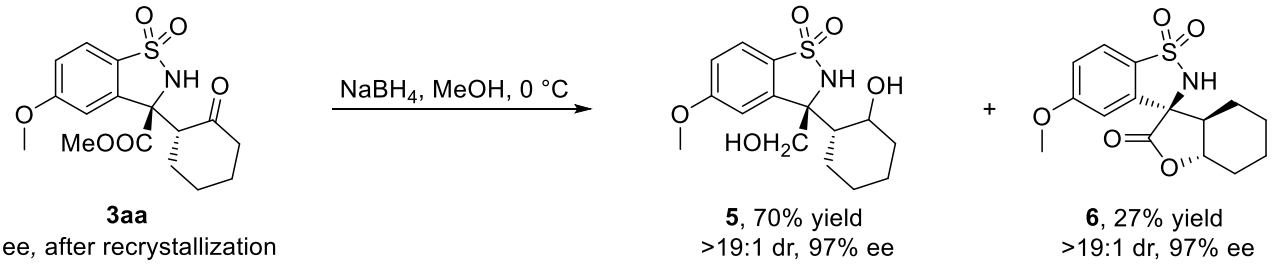
8. Gram-scale synthesis of 3aa and 4aa.



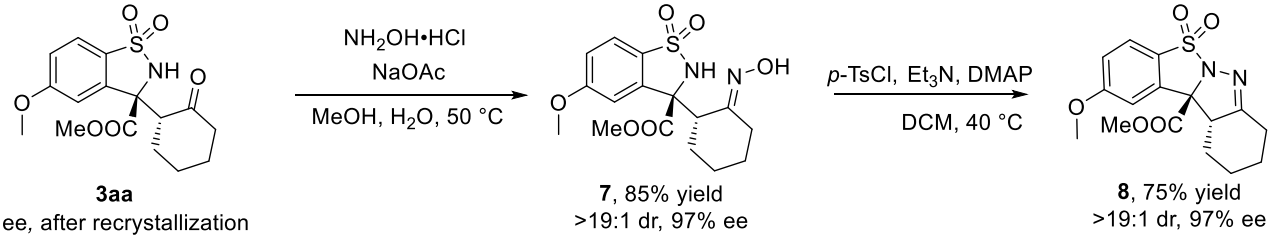
Gram-scale synthesis of **3aa**: A dry reaction flask was charged with cyclic *N*-sulfonyl ketimine **1a** (4.0 mmol, 1.02 g), cyclohexanone **2a** (4.0 mL), **C1-TfOH** (0.8 mmol, 20 mol%), TFA (0.8 mmol, 20 mol%) and 4 Å MS (400 mg) in anhydrous DCM (12.0 mL). The reaction mixture was stirred at 35 °C for 24 h in water bath. The desire product was purified directly by silica gel column chromatograph (petroleum ether/ethyl acetate = 2/1)) to yield a white solid.

Gram-scale synthesis of **4aa**: A dry reaction flask was charged with cyclic *N*-sulfonyl ketimine **1a** (4.0 mmol, 1.02 g), cyclohexanone **2a** (4.0 mL), **C1-TfOH** (0.8 mmol, 20 mol%), TFA (0.8 mmol, 20 mol%) and H_2O (4.0 mL) in anhydrous Et_2O (12.0 mL). The reaction mixture was stirred at 30 °C for 24 h in water bath. The desire product was purified directly by silica gel column chromatograph (petroleum ether/ethyl acetate = 2/1)) to yield a white solid.

9. Transformations of the product.



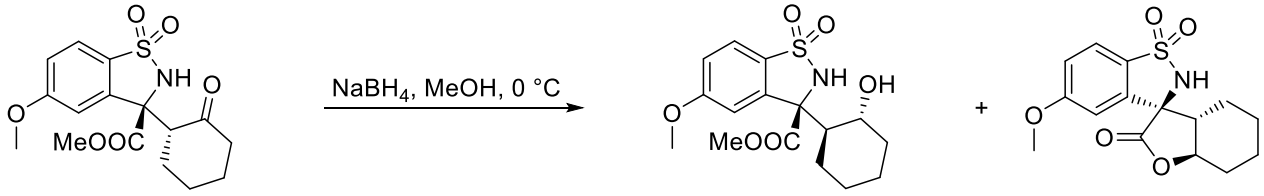
Synthesis of **5 and 6**: To a solution of **3aa** (0.10 mmol, 35.3 mg) in MeOH (1.5 mL) was added $NaBH_4$ (19.9 mg, 0.50 mmol), the solution was stirred at 0 °C for 3 h. After the reaction was completed, 1.0 mL water was added. Then, the mixture was extract by EtOAc, and the aqueous layer was washed with EtOAc (2 x 2.0 mL). The combined organic phases were washed with brine (5.0 mL) and dried over Na_2SO_4. After evaporation of the solvent, the residue was subjected to column chromatography on silica gel with PE/EA = 3:1. The product **5** was obtained in 70% yield with >19:1 dr and 97% ee. The spirocyclic product **6** was also obtained in 27% yield with >19:1 dr and 97% ee.



Synthesis of **7:** To a solution of **3aa** (0.10 mmol, 35.3 mg) in MeOH/H_2O (1:1, 1.0 mL) was added $NH_2OH{\cdot}HCl$ (0.30 mmol, 20.8 mg) and NaOAc (0.30 mmol, 24.6 mg), the solution was stirred at 50 °C for 36 h in water bath. After the reaction was completed, the mixture was extract by EtOAc, and the aqueous layer was washed with EtOAc (2 x 2.0 mL). The combined organic phases were washed with brine (5.0 mL) and dried over Na_2SO_4. After evaporation of the solvent, the residue was subjected to column chromatography on silica gel with PE/EA = 3:1. The product **7** was obtained in 85% yield with >19:1 dr and 97% ee.

Synthesis of **8**: To a solution of **7** (0.10 mmol, 36.8 mg) in DCM (1.0 mL) was added *p*-TsCl (0.30 mmol, 57.2 mg), Et_3N (0.3 mmol) and Dmap (0.02 mmol, 2.4 mg), the solution was stirred at 40 °C for 3 h in water bath. After the reaction was completed, 1.0 mL water was added. Then, the mixture was extract by EtOAc, and the aqueous layer was washed with EtOAc (2 x 2.0 mL). The combined organic

phases were washed with brine (5.0 mL) and dried over Na_2SO_4. After evaporation of the solvent, the residue was subjected to column chromatography on silica gel with PE/EA = 3:1. The product **8** was obtained in 75% yield with >19:1 dr and 97% ee.

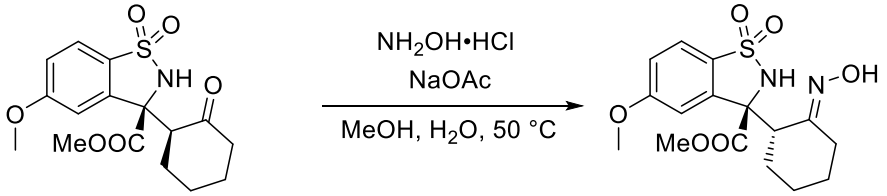


4aa
99% ee, after recrystallization

9, 57% yield
>19:1 dr, 99% ee

10, 38% yield
>19:1 dr, 99% ee

Synthesis of **9 and 10**: To a solution of **4aa** (0.10 mmol, 35.3 mg) in MeOH (1.5 mL) was added $NaBH_4$ (19.9 mg, 0.50 mmol), the solution was stirred at 0 °C for 3 h. After the reaction was completed, 1.0 mL water was added. Then, the mixture was extract by EtOAc, and the aqueous layer was washed with EtOAc (2 x 2.0 mL). The combined organic phases were washed with brine (5.0 mL) and dried over Na_2SO_4. After evaporation of the solvent, the residue was subjected to column chromatography on silica gel with PE/EA = 3:1. The product **9** was obtained in 57% yield with >19:1 dr and 97% ee. The spirocyclic product **10** was also obtained in 35% yield with >19:1 dr and 97% ee.



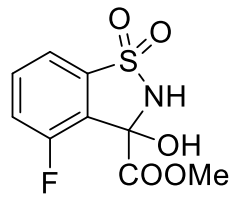
4aa
99% ee, after recrystallization

7, 50% yield
>19:1 dr, 99% ee

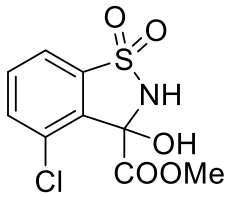
Synthesis of **7:** To a solution of **4aa** (0.10 mmol, 35.3 mg) in MeOH/H_2O (1:1, 1.0 mL) was added $NH_2OH{\cdot}HCl$ (0.30 mmol, 20.8 mg) and NaOAc (0.30 mmol, 24.6 mg), the solution was stirred at 50 °C for 36 h in water bath. After the reaction was completed, the mixture was extract by EtOAc, and the aqueous layer was washed with EtOAc (2 x 2.0 mL). The combined organic phases were washed with brine (5.0 mL) and dried over Na_2SO_4. After evaporation of the solvent, the residue was subjected to column chromatography on silica gel with PE/EA = 3:1. The product **7** was obtained in 50% yield with >19:1 dr and 99% ee.

10. Other substrates.

Other substrates in condition without additional water:

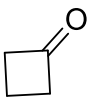


24 h, 97% yield
78:22 dr, 90% ee

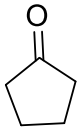


36 h, 46% yield
71:29 dr, 90% *ee*

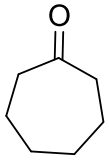
95% yield
40% ee



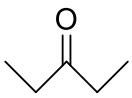
90% yield
2.5:1 dr, 30/7% ee



96% yield
6:1 dr, 17/63% ee



trace



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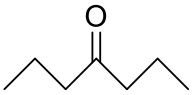

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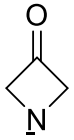
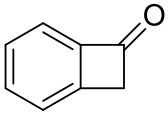


Boc
trace



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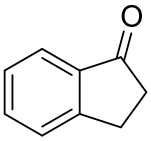

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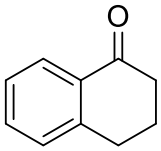
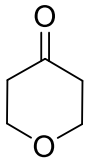
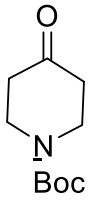


trace

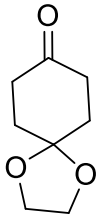
Other substrates in condition with additional water:



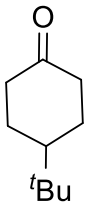
3ab, 88% yield
anti:*syn* = 6:1
77% ee



3ac, 95% yield
anti:*syn* = 2.5:1
94% ee



3af, 75% yield
anti:*syn* = 2.5:1
30% ee



3ah, 75% yield
anti:*syn* = 3.7:1
90% ee

11. DFT Calculations

11.1 Computational methods

All structures in this work were optimized in dichloromethane solvent and characterized by frequency analysis at 308 K, using Gaussian 09 program package[3] and dispersion-included[4,5] M062X-D3 density functional with the 6-31G(d,p) basis set. The self-consistent reaction field (SCRF) and SMD[6] solvation model was adopted to evaluate the effect of solvent. To obtained more accurate energy, single-point calculations were run at the M062X-D3/def2-TZVP(SMD, dichloromethane) theoretical level. Unless specified, the Gibbs free energies obtained at the M062X-D3/def2-TZVP (SMD, dichloromethane)//M062X-D3 /6-31G(d,p) (SMD, dichloromethane) level at 308K are used in the discussion. The conformation search for key intermediates and products were performed using Grimme's XTB code[7] in combination with Molclus software (Version 1.9.9.4)[8]

11.2 Computational results and discussion

As shown in Scheme S1, Scheme S2 and Figure S1, the catalytic reaction occurred *via* three continuous steps, including C-C bond formation, hydrolysis of imine and H-transfer.

When the *Si* or *Re*-face of **1** interacted with the enamine species generated by condensation between the primary amine of catalyst and cyclohexanone, two intermediates (**4-IM1** and **3-IM1**) were formed, alternatively. **3-IM1** was stable than **4-IM1** by 0.8 kcal mol^{-1}. Then, the C-C bonds were constructed *via* transition state **3-TS1** and **4-TS1**, forming **3-IM2** and **4-IM2** respectively. For **3-TS1**, the NH_2 group of catalyst simultaneously interacted with N atom and O atom in **1**, with the distances of 2.124 and 2.329 Å. Due to stronger non-covalent bond interaction (Figure S6), the ΔG of **3-TS1** was lower than that of **4-TS1** by 6.4 kcal mol^{-1}. In the following step, **3** and **4** were obtained by hydrolysis of imine moiety, followed by H-transfer from the catalyst to *N* atom. The energy barrier in the re-generation of catalyst process was predicted to be the rate-determining step (RDS) of reaction, and the relative energy of two competing TSs (**3-TS2** and **4-TS2**) was comparable ($\Delta\Delta G$=0.7 kcal mol^{-1}).

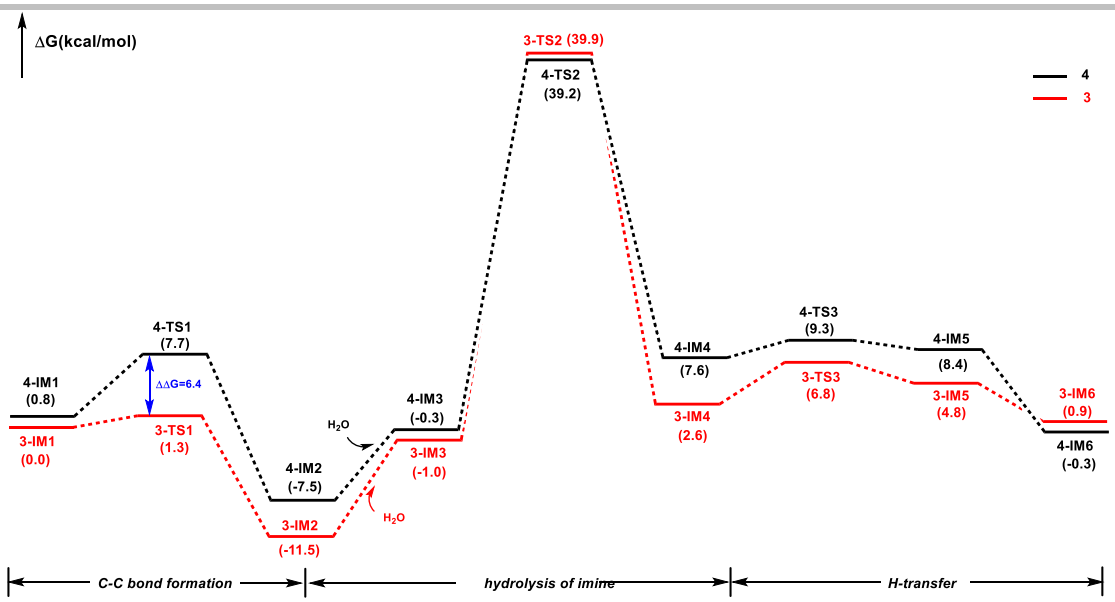
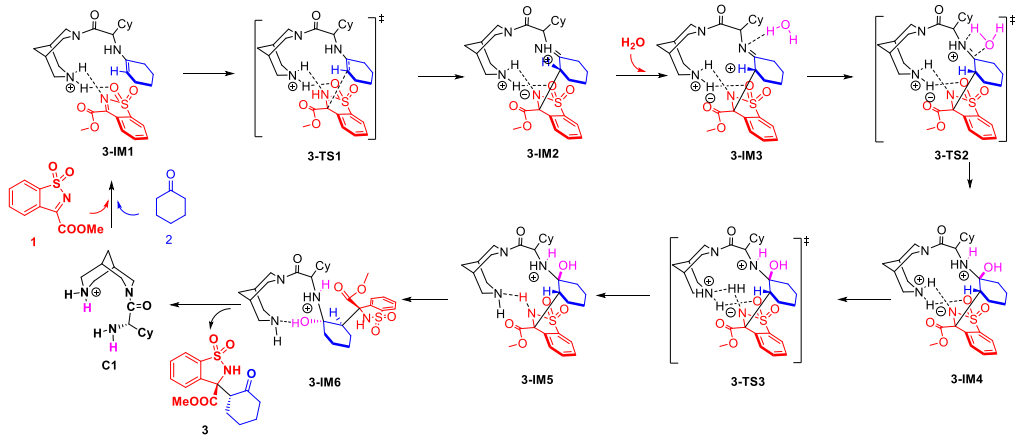
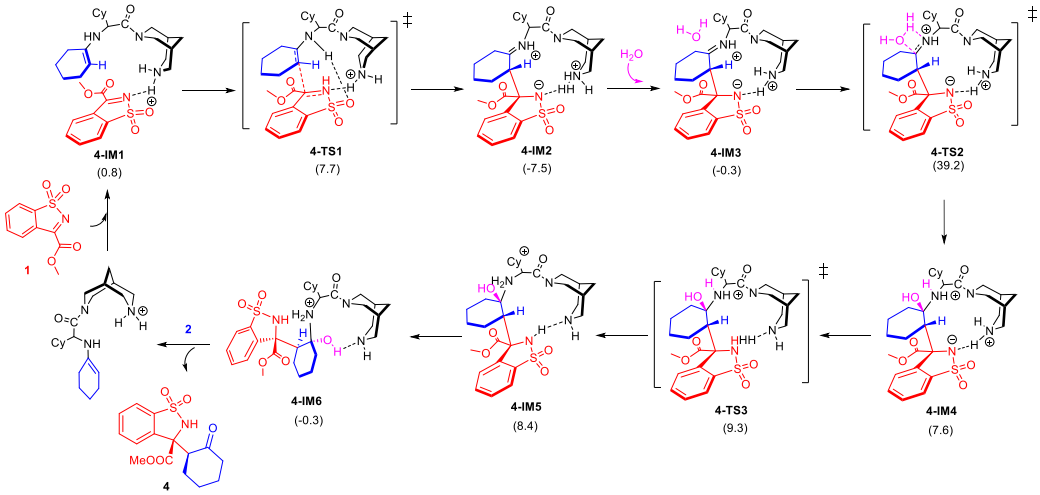


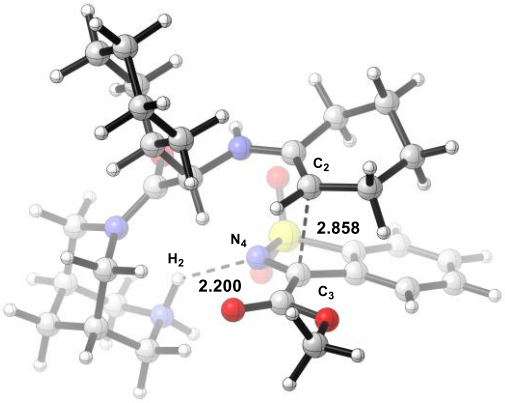
Figure S1. Energy profiles for the formation of **3** and **4** in the absence of H_2O.



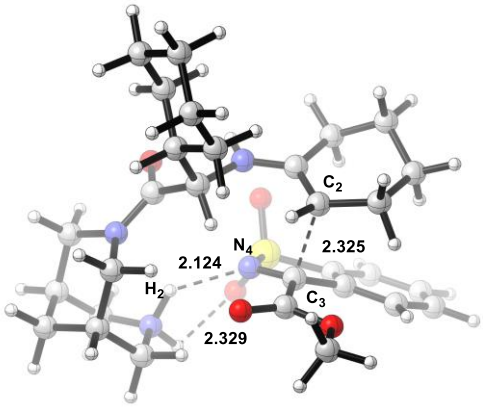
Scheme S1. Reaction mechanism for the formation of **3** without additional water.



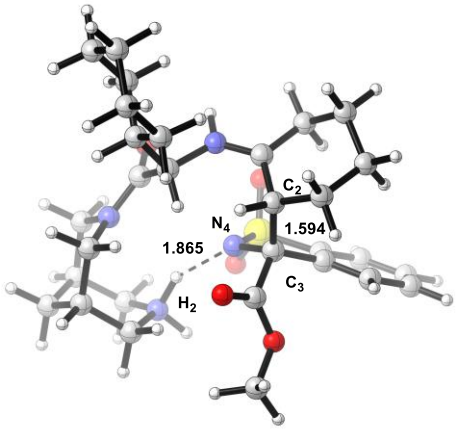
Scheme S2. Reaction mechanism for the formation of **4** without additional water.



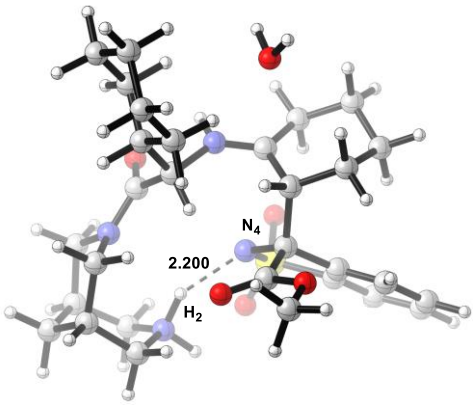
3-IM1
(0.0)



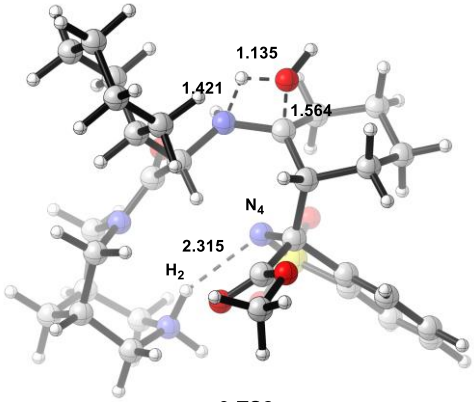
3-TS1
(1.3)



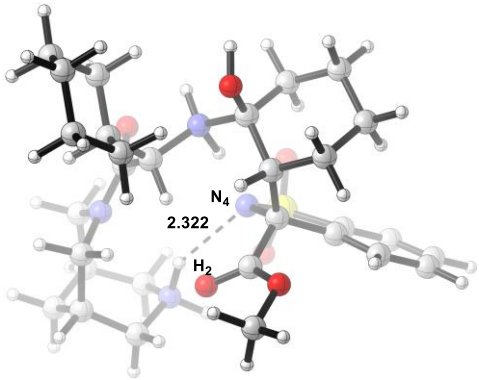
3-IM2
(-11.5)



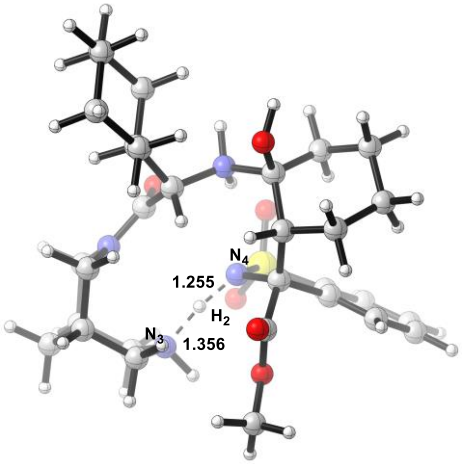
3-IM3
(-1.0)



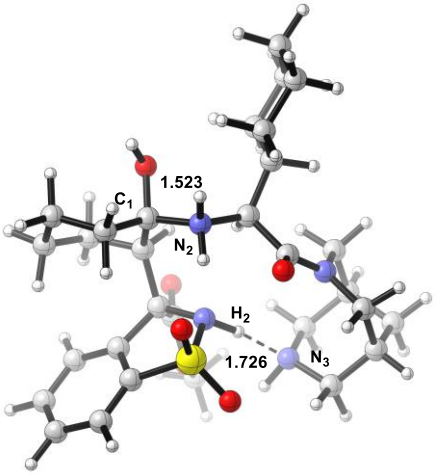
3-TS2
(39.9)



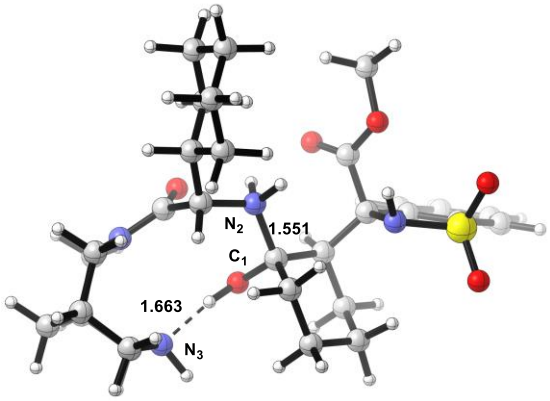
3-IM4
(2.6)



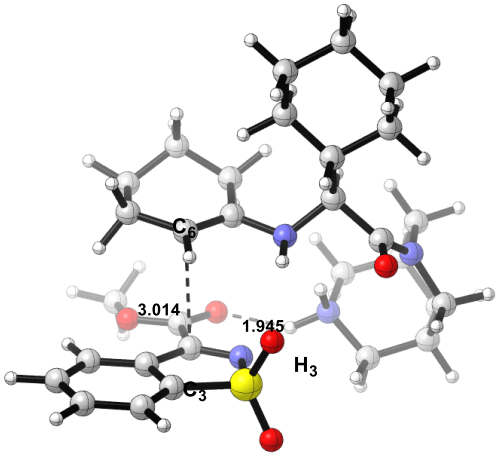
3-TS3
(6.8)



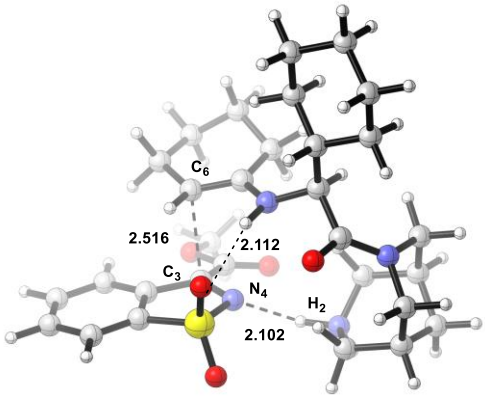
3-IM5
(4.8)



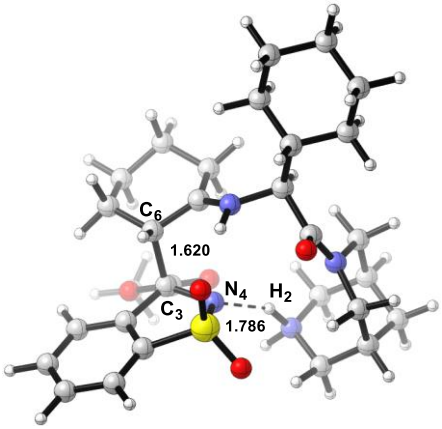
3-IM6
(0.9)



4-IM1
(0.8)



4-TS1
(7.7)



4-IM2
(-7.5)

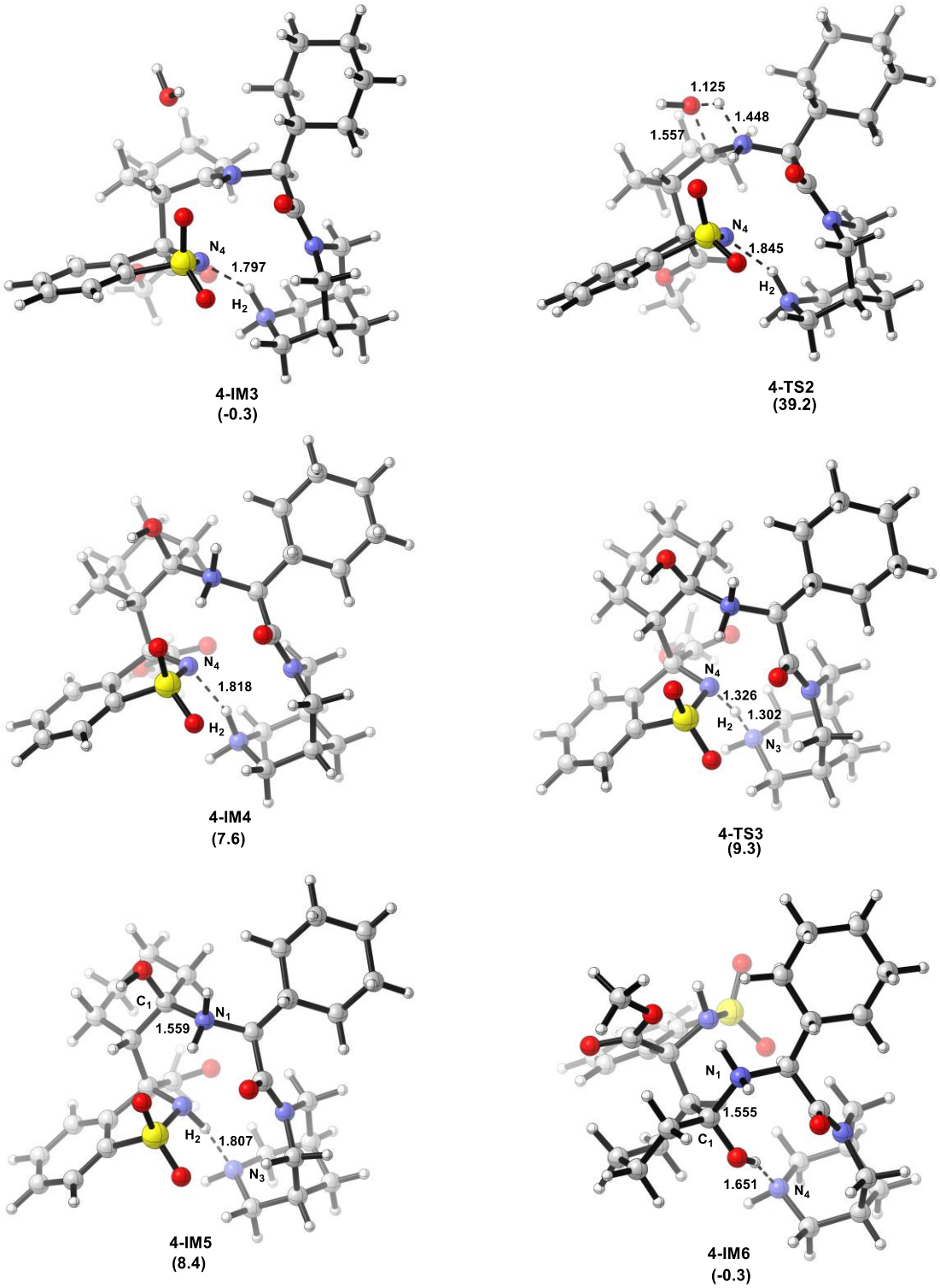


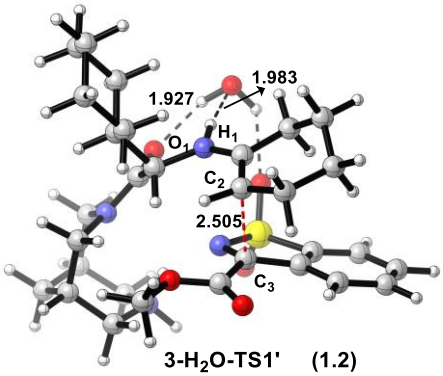
Figure S2. Optimized geometries of all stationary points in the catalytic reactions without additional water.

To get insight into the effect of water on the stereoselectivity of reaction, we studied the reaction mechanism in the presence of water. The optimized geometries of key intermediates and transition states with 1~4 waters in the structures were located. As shown in Table S10, the relative energy difference of the two competing TSs in C-C bond formation decreased, especially for those with four waters. The ΔΔG between **3-TS1′** and **4-TS1′** in the C-C bond formation step decreased from 6.4 kcal mol^{-1}(without water) to 0.4 kcal mol^{-1}(four water). These results indicated that four waters could construct a suitable hydrogen bonding net, stabilizing the two competing transition states in the chiral controlling step well. In addition, water could also accelerate the re-generation of catalyst by decreasing the activation barrier in the hydrolysis of imine step by 5.8-8.4 kcal mol^{-1}. Considering that **4-TS2′** was more stable than that of **3-TS2′** by 3.4 kcal mol^{-1} in the rate-determining step, we assumed that 4 might be predominantly formed in the presence of water.

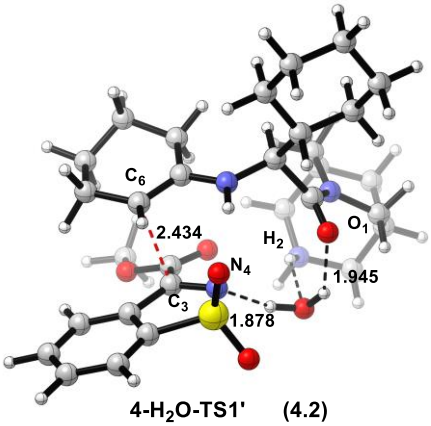
Table S10. Relative Gibbs free energy of transition states in the C-C bond formation step along **3** and **4** pathways.

Path	ΔG (kcal mol^{-1})

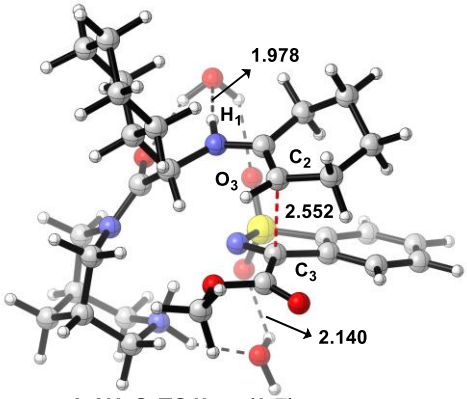
	Without water	H_2O	$2H_2O$	$3H_2O$	$4H_2O$
3	1.3	1.2	0.7	2.1	0.9
4	7.7	4.2	4.6	6.1	1.3



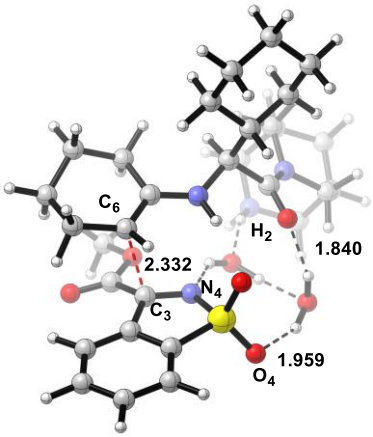
3-H_2O-TS1' (1.2)



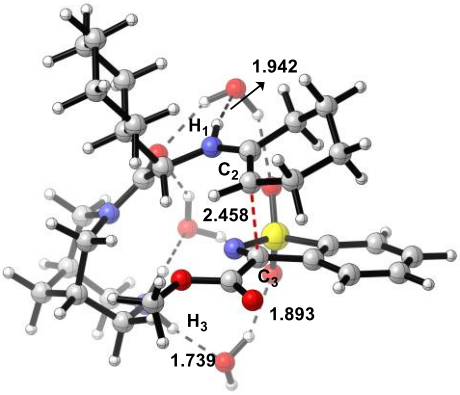
4-H_2O-TS1' (4.2)



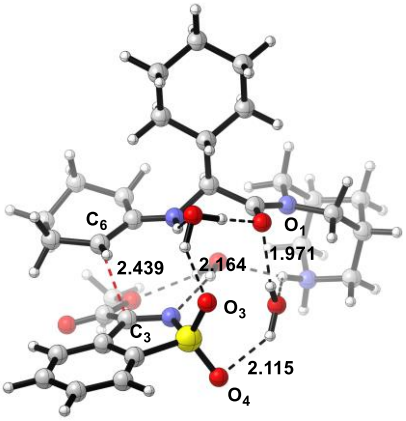
3-$2H_2O$-TS1' (0.7)



4-$2H_2O$-TS1′ (4.6)



3-$3H_2O$-TS1′ (2.1)



4-$3H_2O$-TS1′ (6.1)

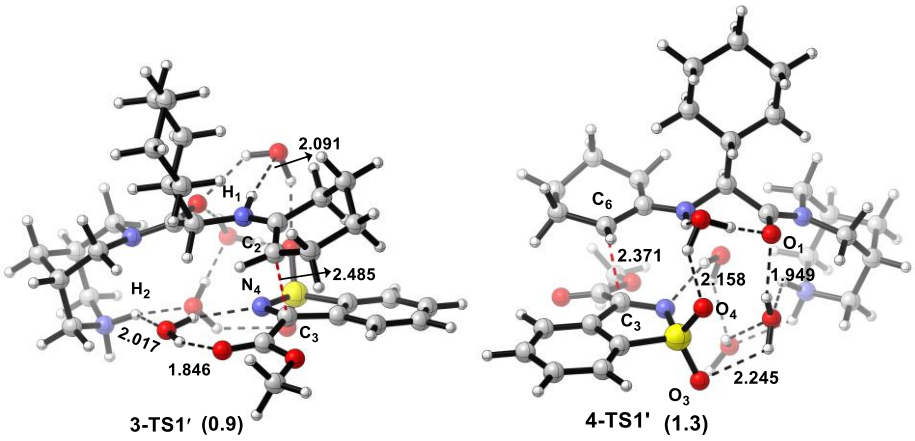


Figure S3. Optimized geometries of all stationary points in the catalytic reactions with different water molecules.

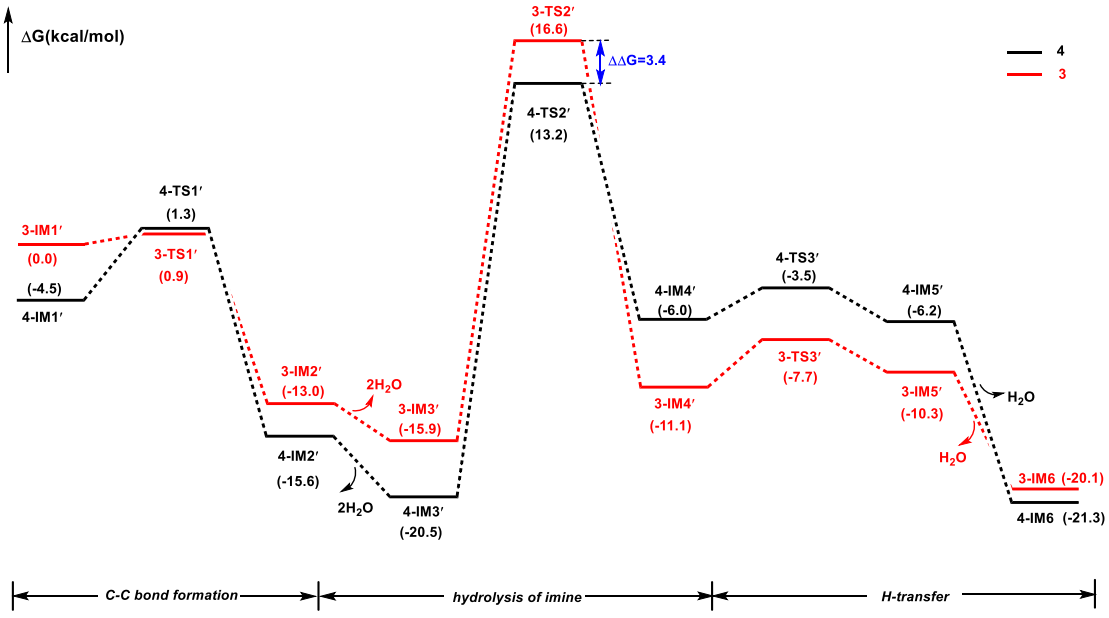
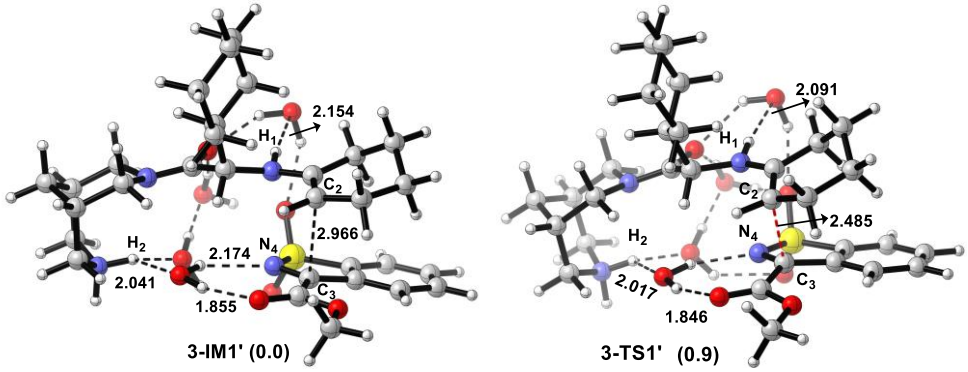
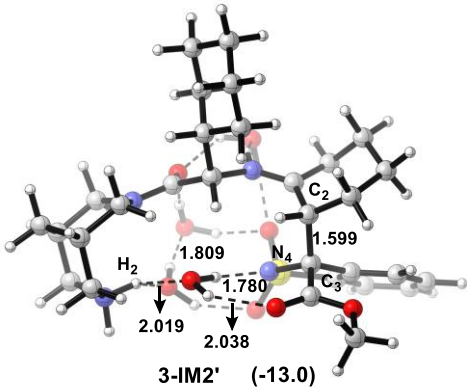
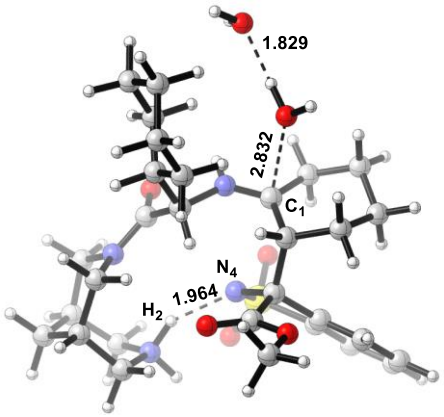


Figure S4. Reaction mechanism for the formation of **3** and **4**. in the presence of four water molecules.

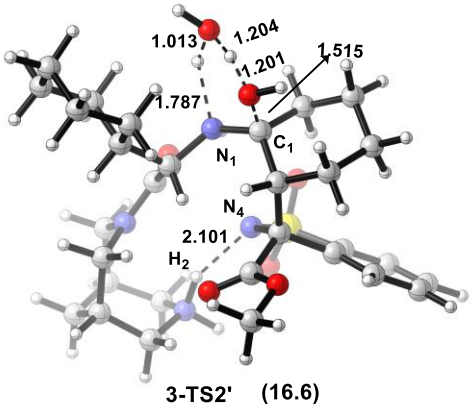




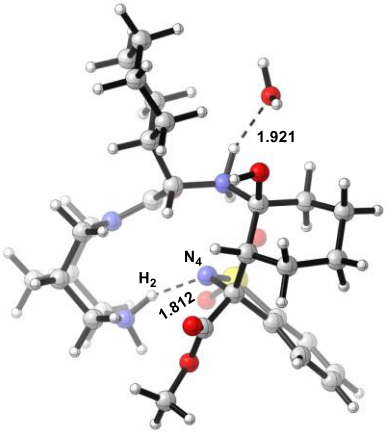
3-IM2' (-13.0)



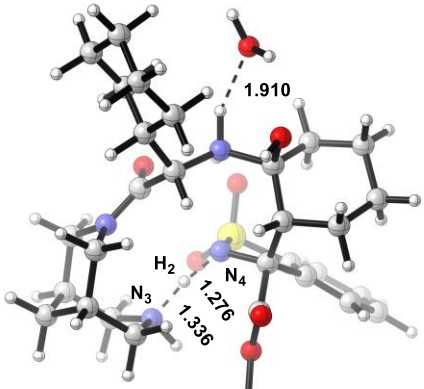
3-IM3' (-15.9)



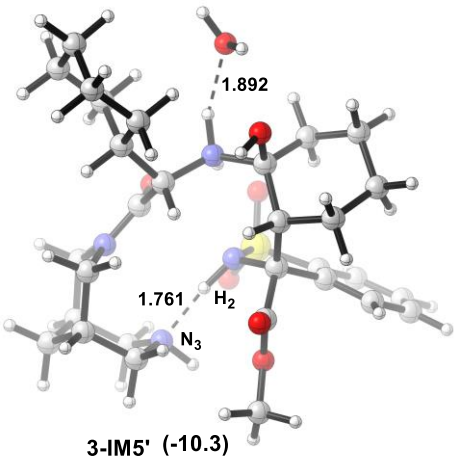
3-TS2' (16.6)



3-IM4' (-11.1)



3-TS3' (-7.7)



3-IM5' (-10.3)

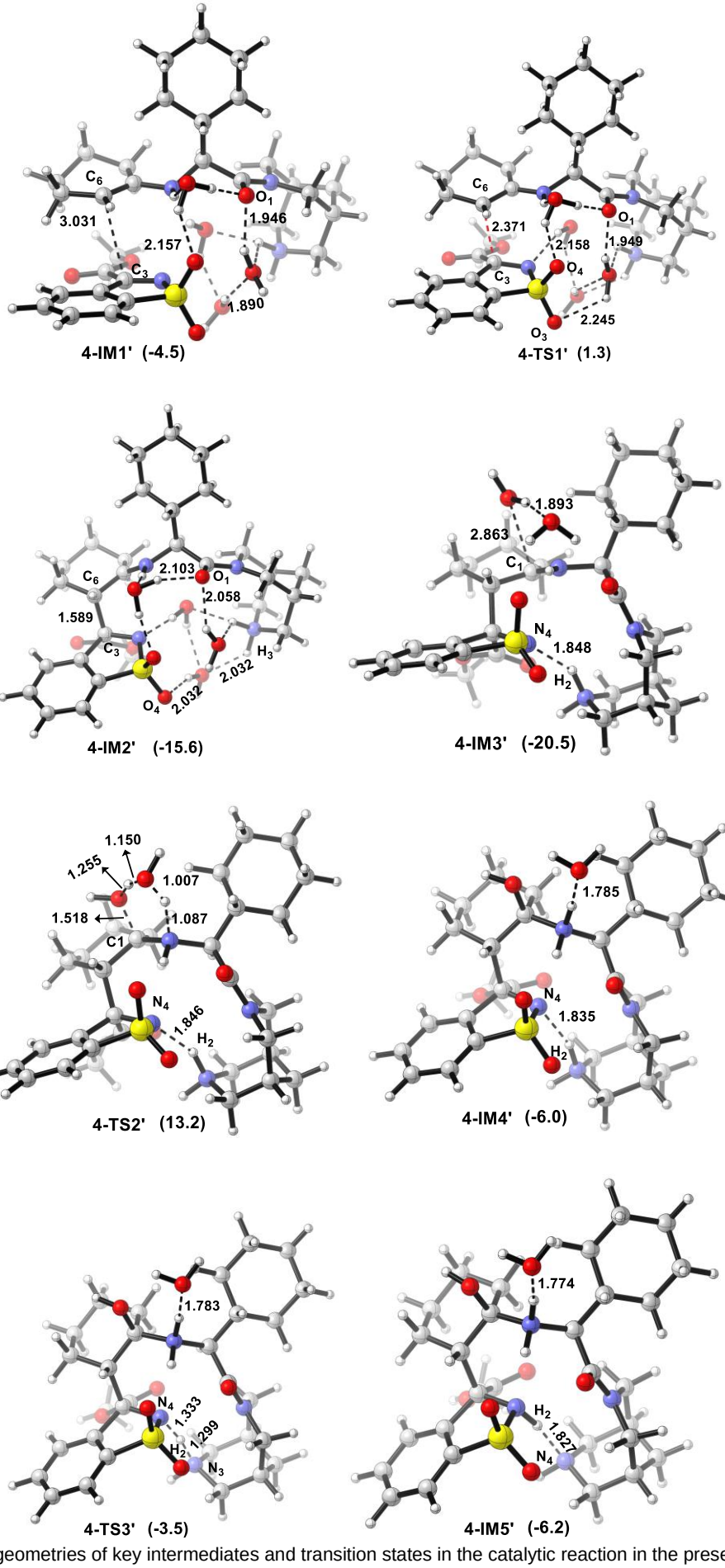


Figure S5. Optimized geometries of key intermediates and transition states in the catalytic reaction in the presence of additioal water.

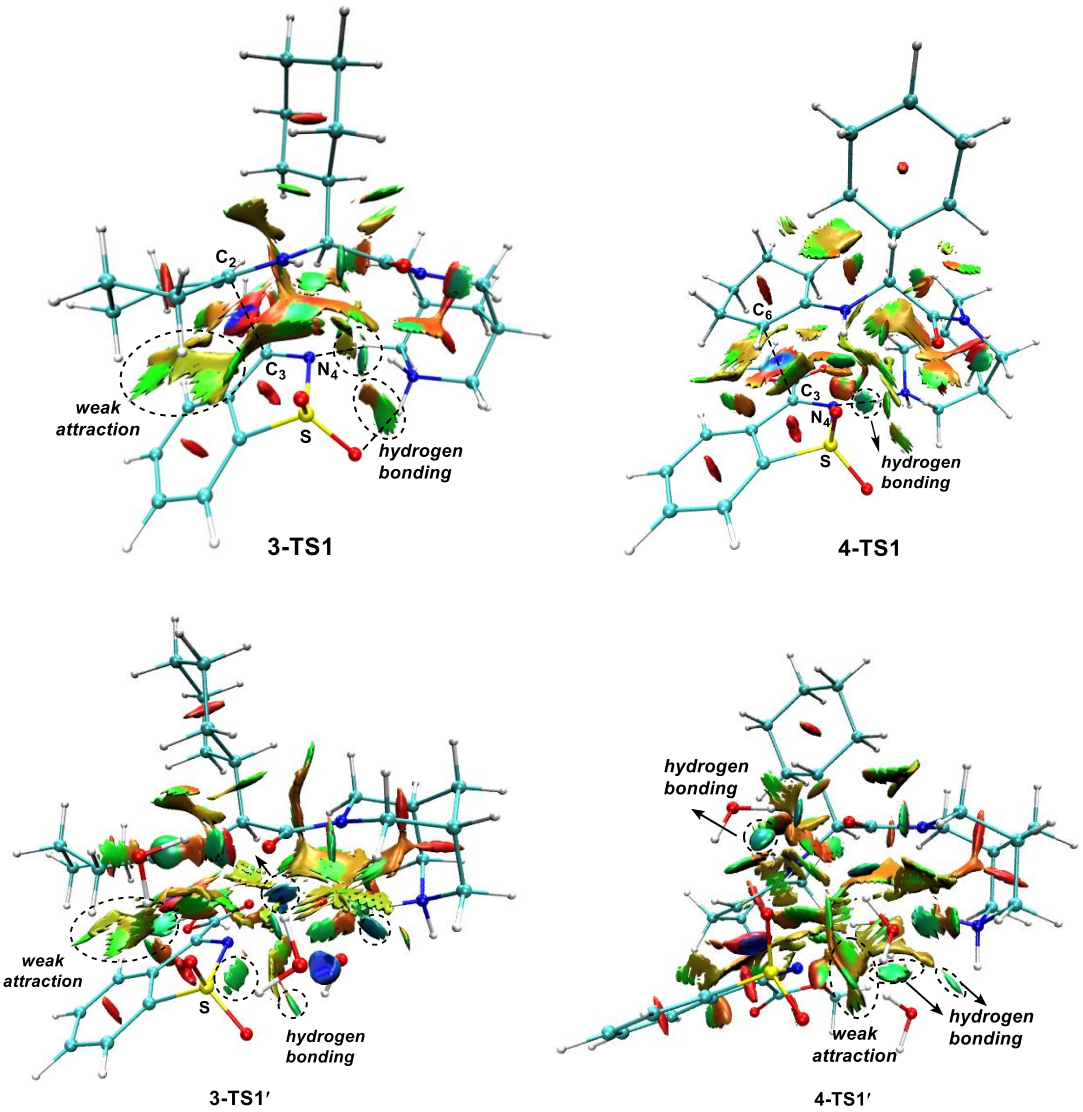


Figure S6. Non-covalent interaction analysis of transition states **3-TS1**, **4-TS1**, **3-TS1′**, and **4-TS1′**, obtained by VMD and Multiwfn software (isovalue = 0.50) (Green color represents attractive interaction, and red color represents repulsive interaction)

Energies and coordinates

3-IM1
Zero-point correction = 0.72610 a.u.
Thermal correction to Gibbs Free Energy = 0.65729 a.u.
Sum of electronic and zero-point Energies = -2160.83419 a.u.
Sum of electronic and thermal Free Energies = -2160.90300 a.u.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.393612	-1.762939	-1.452516
2	6	0	3.056997	-1.479080	-0.907903
3	6	0	3.005306	-0.882471	0.351380
4	6	0	1.582671	-0.733179	0.774151
5	7	0	0.667977	-1.156959	-0.037832
6	6	0	4.228144	-1.751293	-1.587007
7	6	0	5.420119	-1.421787	-0.937460
8	6	0	5.399935	-0.845733	0.332372
9	6	0	4.201544	-0.567679	0.993890
10	8	0	1.084528	-0.946851	-2.612932
11	6	0	1.133734	-0.306419	2.152012
12	8	0	-0.016972	-0.357778	2.523648
13	8	0	2.147342	0.086525	2.904315
14	6	0	1.797924	0.584537	4.207676
15	1	0	1.322527	-0.203646	4.793457
16	1	0	2.736166	0.893189	4.663756
17	1	0	4.210379	-0.113302	1.975627
18	1	0	6.337165	-0.602151	0.821616
19	1	0	6.367971	-1.619848	-1.426307
20	1	0	4.223031	-2.204608	-2.572848
21	8	0	1.039807	-3.181716	-1.490060
22	1	0	1.119252	1.434383	4.107931
23	7	0	-2.821590	-0.948543	-0.261433
24	6	0	-3.030604	-0.909027	1.188802
25	6	0	-3.051184	-2.332509	1.770821
26	6	0	-4.139256	-3.159131	1.079849
27	6	0	-3.744361	-1.823582	-0.998329
28	6	0	-3.781604	-3.235969	-0.407580
29	1	0	-3.995061	-0.429856	1.406102
30	1	0	-2.239835	-0.329632	1.663642
31	1	0	-3.258331	-2.243711	2.841802
32	6	0	-1.708899	-3.055760	1.648003

33	1	0	-5.114019	-2.677506	1.206741
34	1	0	-4.753297	-1.393209	-0.940690
35	1	0	-3.430521	-1.836764	-2.041440
36	6	0	-2.461666	-3.984436	-0.579834
37	1	0	-4.538352	-3.805174	-0.955954
38	7	0	-1.367348	-3.329901	0.212071
39	1	0	-1.753381	-4.025779	2.148460
40	1	0	-0.885494	-2.465677	2.054384
41	1	0	-2.546942	-5.007324	-0.205945
42	1	0	-4.197241	-4.161992	1.516349
43	1	0	-1.112322	-2.436688	-0.223038
44	1	0	-2.124848	-4.003548	-1.618297
45	1	0	-0.519183	-3.904175	0.157450
46	6	0	-2.006811	-0.115441	-0.976370
47	8	0	-1.868004	-0.240265	-2.189639
48	6	0	-1.313419	1.047238	-0.255803
49	6	0	-2.358716	2.178551	-0.068983
50	7	0	-0.181719	1.420576	-1.077888
51	1	0	-3.216187	1.728918	0.457240
52	6	0	-1.828861	3.314657	0.812151
53	1	0	-0.950001	0.725453	0.721081
54	6	0	1.028526	1.886152	-0.663121
55	6	0	1.387623	2.114268	0.633110
56	6	0	2.710289	2.719753	1.031435
57	6	0	3.726531	2.775262	-0.113544
58	6	0	2.008287	2.118172	-1.793608
59	6	0	3.051916	3.168247	-1.423855
60	1	0	0.627606	2.054731	1.407994
61	1	0	2.535445	3.737776	1.410394
62	1	0	3.134327	2.161161	1.878128
63	1	0	4.187893	1.789625	-0.248888
64	1	0	4.530304	3.473786	0.139469
65	1	0	3.788677	3.257112	-2.227807
66	1	0	2.566433	4.146225	-1.315408
67	1	0	2.504861	1.169051	-2.037485
68	1	0	1.448440	2.413848	-2.687178
69	1	0	-0.265236	1.128162	-2.045782
70	1	0	-1.505432	2.912606	1.780971
71	1	0	-0.943473	3.756296	0.334868
72	6	0	-2.863401	2.728135	-1.409123
73	6	0	-3.920444	3.814687	-1.204650
74	6	0	-3.389334	4.944642	-0.322429
75	6	0	-2.889860	4.399397	1.016752
76	1	0	-4.805706	3.371121	-0.727832
77	1	0	-4.245673	4.206197	-2.174397
78	1	0	-2.557985	5.443234	-0.839359
79	1	0	-4.164585	5.701168	-0.161038
80	1	0	-2.482713	5.208430	1.632622
81	1	0	-3.738004	3.972598	1.570100
82	1	0	-2.008695	3.150048	-1.956006
83	1	0	-3.267359	1.919754	-2.028135

3-TS1

Zero-point correction = 0.72566 a.u.
Thermal correction to Gibbs Free Energy = 0.65770 a.u.
Sum of electronic and zero-point Energies = -2160.83331 a.u.
Sum of electronic and thermal Free Energies = -2160.90127 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.380814	-1.706555	-1.410611
2	6	0	3.037156	-1.422576	-0.841115
3	6	0	2.966888	-0.748803	0.377050
4	6	0	1.530596	-0.498088	0.732469
5	7	0	0.636122	-1.078147	-0.067354
6	6	0	4.221114	-1.788488	-1.455470
7	6	0	5.403965	-1.480144	-0.783493
8	6	0	5.363182	-0.839096	0.455426
9	6	0	4.156643	-0.467450	1.050615
10	8	0	1.120372	-0.938302	-2.625968
11	6	0	1.067605	-0.241176	2.140913
12	8	0	-0.090118	-0.316937	2.495623
13	8	0	2.063510	0.098383	2.948965
14	6	0	1.678235	0.490094	4.277056
15	1	0	1.200079	-0.343812	4.792788
16	1	0	2.601220	0.773690	4.778797
17	1	0	4.154538	0.021635	2.015382
18	1	0	6.291668	-0.623163	0.974032
19	1	0	6.358321	-1.753939	-1.220575
20	1	0	4.227666	-2.306487	-2.409119
21	8	0	1.046374	-3.136099	-1.463389
22	1	0	0.990606	1.337406	4.228662
23	7	0	-2.851562	-0.987544	-0.335842
24	6	0	-3.067852	-0.945375	1.116311
25	6	0	-3.057502	-2.358991	1.723078
26	6	0	-4.091772	-3.237553	1.015628
27	6	0	-3.724754	-1.911271	-1.072414
28	6	0	-3.692094	-3.313666	-0.460843
29	1	0	-4.046399	-0.489248	1.318920
30	1	0	-2.297906	-0.339681	1.592620
31	1	0	-3.303543	-2.254288	2.784371
32	6	0	-1.690547	-3.040469	1.657508
33	1	0	-5.090033	-2.798408	1.110762
34	1	0	-4.754360	-1.530816	-1.038426
35	1	0	-3.393644	-1.923146	-2.110183
36	6	0	-2.326237	-3.986097	-0.596095
37	1	0	-4.400379	-3.933680	-1.018856
38	7	0	-1.288537	-3.294502	0.236685
39	1	0	-1.727437	-4.011721	2.156499
40	1	0	-0.902384	-2.425647	2.095270
41	1	0	-2.372035	-5.017554	-0.239099
42	1	0	-4.116780	-4.236751	1.463638
43	1	0	-1.032198	-2.387620	-0.174424
44	1	0	-1.958326	-3.975703	-1.624016
45	1	0	-0.417366	-3.835869	0.207050
46	6	0	-2.121128	-0.090615	-1.057160
47	8	0	-2.069411	-0.124287	-2.283727
48	6	0	-1.370992	1.018581	-0.314448
49	6	0	-2.329035	2.211031	-0.073394
50	7	0	-0.233257	1.350595	-1.160584
51	1	0	-3.231682	1.785032	0.393740
52	6	0	-1.729901	3.217363	0.914804
53	1	0	-0.995613	0.651099	0.638196
54	6	0	0.976770	1.755343	-0.795917
55	6	0	1.400493	1.814844	0.537003
56	6	0	2.683482	2.522960	0.908984
57	6	0	3.671213	2.685706	-0.249575
58	6	0	1.943630	2.035925	-1.919293
59	6	0	2.949972	3.114615	-1.523370
60	1	0	0.617605	1.880657	1.286241
61	1	0	2.412196	3.518918	1.288341
62	1	0	3.159700	2.009302	1.752928
63	1	0	4.183395	1.736420	-0.445279
64	1	0	4.438371	3.414312	0.029496
65	1	0	3.661450	3.264489	-2.339969
66	1	0	2.430108	4.067087	-1.361795
67	1	0	2.477047	1.104925	-2.151795
68	1	0	1.380605	2.308483	-2.816799
69	1	0	-0.401611	1.174355	-2.149216
70	1	0	-1.456198	2.702936	1.845491
71	1	0	-0.805264	3.631757	0.487975
72	6	0	-2.753067	2.913297	-1.369151
73	6	0	-3.724164	4.061355	-1.080537
74	6	0	-3.125080	5.060867	-0.089682
75	6	0	-2.704588	4.361178	1.203416
76	1	0	-4.653445	3.651395	-0.661868
77	1	0	-3.991925	4.564191	-2.015619
78	1	0	-2.244048	5.533977	-0.544868
79	1	0	-3.841725	5.860609	0.124507
80	1	0	-2.248023	5.075468	1.896440
81	1	0	-3.596002	3.956328	1.701881

82	1	0	-1.856488	3.317457	-1.860206
83	1	0	-3.201375	2.195781	-2.064330

3-IM2

Zero-point correction = 0.72786 a.u.
Thermal correction to Gibbs Free Energy = 0.65930 a.u.
Sum of electronic and zero-point Energies = -2160.85007 a.u.
Sum of electronic and thermal Free Energies = -2160.91863 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.644767	-0.848698	-1.560319
2	6	0	3.222680	-0.242150	-1.008266
3	6	0	3.039981	0.379143	0.216836
4	6	0	1.579248	0.326259	0.677289
5	7	0	0.868351	-0.619907	-0.180221
6	6	0	4.453473	-0.328622	-1.645376
7	6	0	5.552590	0.217291	-0.989308
8	6	0	5.399614	0.817561	0.265094
9	6	0	4.151870	0.900085	0.878406
10	8	0	1.204991	-0.000679	-2.683853
11	6	0	1.434012	-0.297632	2.079238
12	8	0	0.460721	-0.137501	2.784517
13	8	0	2.439182	-1.107055	2.386673
14	6	0	2.341334	-1.770739	3.655789
15	1	0	1.490991	-2.456334	3.664962
16	1	0	3.272819	-2.321902	3.770201
17	1	0	4.058193	1.347585	1.862811
18	1	0	6.270313	1.217399	0.775016
19	1	0	6.536017	0.162319	-1.444580
20	1	0	4.554388	-0.817950	-2.609280
21	8	0	1.675103	-2.292704	-1.876238
22	1	0	2.228610	-1.037585	4.456363
23	7	0	-2.343122	-1.672842	-0.546590
24	6	0	-2.707274	-1.855742	0.864792
25	6	0	-2.226270	-3.206894	1.409410
26	6	0	-2.735533	-4.341060	0.517939
27	6	0	-2.681609	-2.785615	-1.441312
28	6	0	-2.161525	-4.110154	-0.881779
29	1	0	-3.800858	-1.812015	0.960401
30	1	0	-2.286562	-1.051464	1.470510
31	1	0	-2.629815	-3.303099	2.421808
32	6	0	-0.706790	-3.298089	1.534863
33	1	0	-3.829995	-4.332667	0.482386
34	1	0	-3.772067	-2.843120	-1.561060
35	1	0	-2.240605	-2.569946	-2.414514
36	6	0	-0.634823	-4.178856	-0.836124
37	1	0	-2.485796	-4.902632	-1.563306
38	7	0	-0.047271	-3.260066	0.193957
39	1	0	-0.424328	-4.238316	2.014847
40	1	0	-0.299844	-2.460423	2.107974
41	1	0	-0.319168	-5.189010	-0.563840
42	1	0	-2.416521	-5.310985	0.913989
43	1	0	-0.009473	-2.263973	-0.118853
44	1	0	-0.173754	-3.898249	-1.784958
45	1	0	0.945874	-3.493530	0.292111
46	6	0	-2.068781	-0.471345	-1.122567
47	8	0	-2.052486	-0.297514	-2.336072
48	6	0	-1.768416	0.712708	-0.202184
49	6	0	-3.049039	1.478001	0.192274
50	7	0	-0.859202	1.571606	-0.966321
51	1	0	-3.734303	0.722884	0.604526
52	6	0	-2.760746	2.502611	1.295751
53	1	0	-1.243183	0.369881	0.684007
54	6	0	0.278285	2.055013	-0.603782
55	6	0	0.850528	1.742314	0.744978
56	6	0	1.657527	2.918906	1.332045
57	6	0	2.472475	3.728273	0.321083
58	6	0	1.051069	2.895409	-1.563078
59	6	0	1.601742	4.143888	-0.860899
60	1	0	0.019411	1.568248	1.427590
61	1	0	0.933066	3.597347	1.797761
62	1	0	2.283290	2.544403	2.148521
63	1	0	3.322229	3.149205	-0.053229
64	1	0	2.878989	4.611935	0.822320
65	1	0	2.178573	4.723656	-1.585577
66	1	0	0.772296	4.775750	-0.521235
67	1	0	1.890659	2.275396	-1.906743
68	1	0	0.439579	3.135763	-2.436891
69	1	0	-1.143497	1.697695	-1.940990
70	1	0	-2.292490	2.002516	2.153137
71	1	0	-2.039688	3.243029	0.918172
72	6	0	-3.744322	2.142366	-1.003011
73	6	0	-5.028593	2.847401	-0.562077
74	6	0	-4.743256	3.874126	0.535509
75	6	0	-4.042062	3.220718	1.727775
76	1	0	-5.738686	2.100038	-0.183494
77	1	0	-5.501436	3.328840	-1.423911
78	1	0	-4.099148	4.665307	0.128144
79	1	0	-5.672540	4.353813	0.859632
80	1	0	-3.809988	3.967734	2.493584
81	1	0	-4.720882	2.490583	2.188445
82	1	0	-3.067690	2.889961	-1.441808
83	1	0	-3.954979	1.402103	-1.781657

3-IM3

Zero-point correction = 0.75235 a.u.
Thermal correction to Gibbs Free Energy = 0.68008 a.u.
Sum of electronic and zero-point Energies = -2237.22564 a.u.
Sum of electronic and thermal Free Energies = -2237.29791 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.744154	-4.331290	-0.803655
2	1	0	1.124246	-4.519771	-1.672602
3	1	0	0.692074	-5.194869	-0.371744
4	16	0	-1.994983	1.395528	-1.274459
5	6	0	-3.452264	0.770072	-0.479382
6	6	0	-3.067311	-0.086568	0.542004
7	6	0	-1.532150	-0.224018	0.606486
8	7	0	-0.941027	0.779166	-0.257731
9	6	0	-4.773579	1.057389	-0.790056
10	6	0	-5.759680	0.463342	-0.008513
11	6	0	-5.400726	-0.373527	1.050768
12	6	0	-4.065648	-0.652943	1.339293
13	8	0	-1.946578	0.870618	-2.654134
14	1	0	-3.823570	-1.286750	2.182657
15	1	0	-6.175919	-0.813929	1.669802
16	1	0	-6.806821	0.661863	-0.212015
17	1	0	-5.022637	1.728501	-1.606418
18	8	0	-1.960721	2.877068	-1.229809
19	6	0	-1.016111	-0.002414	2.035942
20	8	0	-0.073999	0.700721	2.324406
21	8	0	-1.651590	-0.764402	2.921525
22	6	0	-1.154627	-0.706299	4.268606
23	1	0	-0.114933	-1.038083	4.298571
24	1	0	-1.227999	0.312326	4.653176
25	1	0	-1.787606	-1.377674	4.845358
26	7	0	2.402687	1.831357	-0.548049
27	6	0	2.753476	1.928079	0.879502
28	6	0	2.407374	3.299191	1.491164
29	6	0	2.933981	4.431467	0.607394
30	6	0	2.771678	2.971847	-1.393989
31	6	0	2.277523	4.270269	-0.765145
32	1	0	3.835476	1.773257	0.985637
33	1	0	2.240606	1.141117	1.436769
34	1	0	2.879817	3.329296	2.477762
35	6	0	0.911994	3.516506	1.707541

36	1	0	4.022584	4.372502	0.504407
37	1	0	3.862438	3.010416	-1.517321
38	1	0	2.323342	2.811347	-2.373897
39	6	0	0.749403	4.323282	-0.656997
40	1	0	2.567159	5.091557	-1.427753
41	7	0	0.193683	3.414101	0.403955
42	1	0	0.733611	4.521833	2.097979
43	1	0	0.473696	2.779118	2.375752
44	1	0	0.434640	5.331907	-0.377667
45	1	0	2.688550	5.400486	1.054294
46	1	0	0.257414	4.042339	-1.590123
47	1	0	-0.800933	3.643767	0.509203
48	6	0	2.121037	0.669655	-1.192315
49	8	0	2.165104	0.561656	-2.415597
50	6	0	1.713829	-0.551762	-0.360881
51	6	0	2.936890	-1.370978	0.099984
52	7	0	0.840708	-1.307104	-1.266190
53	1	0	3.661367	-0.643984	0.496419
54	6	0	2.547996	-2.317706	1.240282
55	1	0	1.130187	-0.230194	0.498018
56	6	0	-0.349086	-1.759600	-1.067304
57	6	0	-0.976327	-1.720395	0.298317
58	6	0	-1.963019	-2.884670	0.486239
59	6	0	-2.898137	-3.109888	-0.701248
60	6	0	-1.126231	-2.239288	-2.249391
61	6	0	-2.081272	-3.398659	-1.956369
62	1	0	-0.158547	-1.886881	1.006359
63	1	0	-1.362350	-3.790928	0.623020
64	1	0	-2.513019	-2.731747	1.416485
65	1	0	-3.533501	-2.233218	-0.871976
66	1	0	-3.562318	-3.950970	-0.480110
67	1	0	-2.733068	-3.534149	-2.823474
68	1	0	-1.503330	-4.316803	-1.818505
69	1	0	-1.708688	-1.352393	-2.548969
70	1	0	-0.442624	-2.461911	-3.074674
71	1	0	1.186022	-1.300076	-2.229349
72	1	0	2.098175	-1.738555	2.058187
73	1	0	1.789501	-3.017550	0.864734
74	6	0	3.613718	-2.134879	-1.043659
75	6	0	4.825633	-2.917871	-0.533860
76	6	0	4.421699	-3.871221	0.592428
77	6	0	3.757505	-3.109041	1.740957
78	1	0	5.583411	-2.215205	-0.161446
79	1	0	5.283735	-3.471599	-1.359759
80	1	0	3.709269	-4.607985	0.195900
81	1	0	5.293202	-4.426185	0.954716
82	1	0	3.448838	-3.799769	2.532797
83	1	0	4.486192	-2.417410	2.185397
84	1	0	2.889647	-2.847459	-1.461271
85	1	0	3.899781	-1.444986	-1.845792
86	1	0	0.153915	2.417127	0.100261

3-TS2

Zero-point correction = 0.75313 a.u.
Thermal correction to Gibbs Free Energy = 0.68618 a.u.
Sum of electronic and zero-point Energies = -2237.17165 a.u.
Sum of electronic and thermal Free Energies = -2237.23860 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.280621	-3.686916	-0.793457
2	1	0	1.212880	-3.095070	-1.057494
3	1	0	-0.019977	-4.323873	-1.473354
4	16	0	-2.131812	1.190319	-1.282670
5	6	0	-3.490004	0.674733	-0.265878
6	6	0	-3.018186	-0.211424	0.687296
7	6	0	-1.497535	-0.471924	0.520541
8	7	0	-0.986243	0.406244	-0.513030
9	6	0	-4.815312	1.078360	-0.348642
10	6	0	-5.701186	0.571026	0.597464
11	6	0	-5.240881	-0.289568	1.597487
12	6	0	-3.903988	-0.678690	1.660803
13	8	0	-2.354094	0.754778	-2.676293
14	1	0	-3.568558	-1.323535	2.464952
15	1	0	-5.934813	-0.658359	2.346070
16	1	0	-6.747329	0.857792	0.569969
17	1	0	-5.142540	1.770555	-1.118557
18	8	0	-1.987159	2.664349	-1.178742
19	6	0	-0.916681	-0.043891	1.882476
20	8	0	-0.321310	0.990320	2.080614
21	8	0	-1.168685	-0.933861	2.841236
22	6	0	-0.736731	-0.572153	4.162388
23	1	0	0.342245	-0.407220	4.174354
24	1	0	-1.251025	0.333544	4.489551
25	1	0	-1.001296	-1.413230	4.800082
26	7	0	2.236213	1.726420	-0.609816
27	6	0	2.663490	1.906790	0.789000
28	6	0	2.376619	3.321159	1.333802
29	6	0	2.852216	4.390274	0.349390
30	6	0	2.530073	2.823550	-1.542773
31	6	0	2.090275	4.158712	-0.956392
32	1	0	3.746135	1.737932	0.857081
33	1	0	2.159613	1.167423	1.417783
34	1	0	2.913507	3.403568	2.283333
35	6	0	0.900636	3.569769	1.630043
36	1	0	3.928600	4.304291	0.166855
37	1	0	3.607201	2.848797	-1.756824
38	1	0	2.003255	2.611011	-2.471584
39	6	0	0.573611	4.222124	-0.745852
40	1	0	2.330815	4.936536	-1.687649
41	7	0	0.104849	3.350698	0.386496
42	1	0	0.744476	4.611238	1.924144
43	1	0	0.507995	2.909328	2.396725
44	1	0	0.273787	5.239017	-0.480642
45	1	0	2.656773	5.387401	0.757264
46	1	0	0.020371	3.902466	-1.629540
47	1	0	-0.891439	3.541566	0.535459
48	6	0	1.925629	0.532704	-1.181602
49	8	0	1.835873	0.408938	-2.402222
50	6	0	1.717446	-0.717534	-0.306547
51	6	0	3.063876	-1.283831	0.192515
52	7	0	1.035982	-1.690359	-1.179843
53	1	0	3.592556	-0.462792	0.693075
54	6	0	2.849537	-2.379875	1.242011
55	1	0	1.090387	-0.468592	0.548748
56	6	0	-0.302526	-2.249363	-0.988806
57	6	0	-1.084713	-1.999405	0.302624
58	6	0	-2.244080	-3.016715	0.327144
59	6	0	-3.128230	-2.962654	-0.921573
60	6	0	-1.108958	-2.265328	-2.269800
61	6	0	-2.306338	-3.216903	-2.184148
62	1	0	-0.402012	-2.274371	1.112653
63	1	0	-1.807002	-4.018419	0.410484
64	1	0	-2.831833	-2.872359	1.233609
65	1	0	-3.618029	-1.986171	-1.004136
66	1	0	-3.922139	-3.710571	-0.834609
67	1	0	-2.919440	-3.087507	-3.079831
68	1	0	-1.967624	-4.262616	-2.195234
69	1	0	-1.441300	-1.237699	-2.448964
70	1	0	-0.444484	-2.546578	-3.096253
71	1	0	1.128841	-1.322357	-2.135112
72	1	0	2.238075	-1.985859	2.064744
73	1	0	2.287426	-3.214908	0.799730
74	6	0	3.960671	-1.777506	-0.948599
75	6	0	5.296070	-2.294095	-0.408662
76	6	0	5.079282	-3.396260	0.629114
77	6	0	4.186504	-2.906908	1.771221
78	1	0	5.844122	-1.463348	0.056238
79	1	0	5.914646	-2.661389	-1.233873
80	1	0	4.601699	-4.258209	0.143157
81	1	0	6.039972	-3.744258	1.022516

82	1	0	4.012443	-3.709453	2.495094
83	1	0	4.701070	-2.098209	2.307475
84	1	0	3.452675	-2.594526	-1.479465
85	1	0	4.123628	-0.976827	-1.679170
86	1	0	0.103553	2.347825	0.121856

3-IM4

Zero-point correction = 0.75523 a.u.
Thermal correction to Gibbs Free Energy = 0.68607 a.u.
Sum of electronic and zero-point Energies = -2237.23021 a.u.
Sum of electronic and thermal Free Energies = -2237.29936 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.256515	-3.481371	-0.501090
2	1	0	1.044561	-1.455524	-2.151766
3	1	0	0.397034	-3.994754	-1.312065
4	16	0	-1.985449	1.404526	-1.384870
5	6	0	-3.447442	0.850825	-0.561719
6	6	0	-3.099804	-0.003632	0.474617
7	6	0	-1.580351	-0.282330	0.519155
8	7	0	-0.950779	0.542016	-0.512279
9	6	0	-4.746644	1.258917	-0.832114
10	6	0	-5.752517	0.786552	0.002407
11	6	0	-5.428064	-0.032249	1.087595
12	6	0	-4.115082	-0.421831	1.340569
13	8	0	-1.976660	1.022089	-2.804212
14	1	0	-3.898175	-1.029736	2.208719
15	1	0	-6.214006	-0.370113	1.755451
16	1	0	-6.784397	1.071000	-0.174516
17	1	0	-4.960907	1.927564	-1.660130
18	8	0	-1.821841	2.858002	-1.160338
19	6	0	-1.044486	0.148325	1.894922
20	8	0	-0.103797	0.893043	2.060556
21	8	0	-1.668710	-0.471074	2.889104
22	6	0	-1.142808	-0.241044	4.206705
23	1	0	-0.105198	-0.577230	4.256242
24	1	0	-1.200884	0.819393	4.456950
25	1	0	-1.766840	-0.827812	4.877605
26	7	0	2.566918	1.652127	-0.528211
27	6	0	2.928323	1.757657	0.896311
28	6	0	2.658192	3.161080	1.479662
29	6	0	3.230692	4.246992	0.566702
30	6	0	2.992748	2.757572	-1.396050
31	6	0	2.551338	4.086806	-0.794787
32	1	0	4.001232	1.549929	1.001277
33	1	0	2.379726	1.007120	1.470652
34	1	0	3.139242	3.189350	2.461934
35	6	0	1.178434	3.466588	1.698967
36	1	0	4.313316	4.131451	0.450369
37	1	0	4.084421	2.743926	-1.512366
38	1	0	2.543606	2.596834	-2.374926
39	6	0	1.024579	4.193792	-0.682823
40	1	0	2.864010	4.882926	-1.477294
41	7	0	0.442904	3.328038	0.404758
42	1	0	1.053875	4.503637	2.021632
43	1	0	0.710038	2.801758	2.417894
44	1	0	0.740984	5.216842	-0.424695
45	1	0	3.040370	5.235135	0.997826
46	1	0	0.521403	3.907713	-1.608292
47	1	0	-0.546871	3.580883	0.506680
48	6	0	2.206265	0.503403	-1.160182
49	8	0	2.220104	0.397877	-2.384459
50	6	0	1.712188	-0.697738	-0.338050
51	6	0	2.898594	-1.607316	0.030090
52	7	0	0.644326	-1.246092	-1.232583
53	1	0	3.718386	-0.910716	0.271279
54	6	0	2.650531	-2.430962	1.298807
55	1	0	1.208196	-0.353034	0.566483
56	6	0	-0.366839	-2.274034	-0.826391
57	6	0	-1.113592	-1.825814	0.453339
58	6	0	-2.219235	-2.863481	0.723414
59	6	0	-3.164163	-3.084679	-0.461913
60	6	0	-1.306985	-2.440548	-2.023636
61	6	0	-2.387914	-3.477801	-1.717174
62	1	0	-0.369176	-1.951918	1.250210
63	1	0	-1.712755	-3.808452	0.943977
64	1	0	-2.766760	-2.592503	1.627288
65	1	0	-3.742234	-2.178806	-0.673537
66	1	0	-3.884581	-3.867058	-0.202771
67	1	0	-3.059819	-3.560082	-2.575828
68	1	0	-1.924128	-4.460800	-1.574658
69	1	0	-1.762498	-1.471334	-2.262487
70	1	0	-0.707833	-2.740254	-2.893899
71	1	0	-0.029190	-0.355590	-1.279140
72	1	0	2.344452	-1.759343	2.112567
73	1	0	1.827646	-3.131670	1.121503
74	6	0	3.389538	-2.479993	-1.130055
75	6	0	4.643750	-3.258252	-0.724359
76	6	0	4.394649	-4.087597	0.537239
77	6	0	3.911353	-3.205124	1.690585
78	1	0	5.460999	-2.549078	-0.535905
79	1	0	4.964316	-3.902335	-1.549553
80	1	0	3.630304	-4.847325	0.323045
81	1	0	5.305304	-4.623578	0.824438
82	1	0	3.716024	-3.811403	2.581215
83	1	0	4.705671	-2.493447	1.955125
84	1	0	2.600744	-3.193408	-1.399089
85	1	0	3.586653	-1.859493	-2.011902
86	1	0	0.400949	2.333266	0.123089

3-TS3

Zero-point correction = 0.75398 a.u.
Thermal correction to Gibbs Free Energy = 0.68839 a.u.
Sum of electronic and zero-point Energies = -2237.22846 a.u.
Sum of electronic and thermal Free Energies = -2237.29405 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.022208	-3.169447	0.591620
2	1	0	1.559039	-2.069058	-1.560107
3	1	0	1.272679	-3.942554	0.060476
4	16	0	-1.686997	0.535506	-1.764108
5	6	0	-3.196117	-0.138355	-1.148852
6	6	0	-2.993117	-0.583611	0.144863
7	6	0	-1.548726	-0.371613	0.645674
8	7	0	-0.893904	0.529919	-0.331087
9	6	0	-4.419781	-0.187683	-1.804154
10	6	0	-5.500804	-0.688431	-1.088051
11	6	0	-5.336998	-1.098358	0.239043
12	6	0	-4.094904	-1.045690	0.865515
13	8	0	-1.093133	-0.426291	-2.711924
14	1	0	-3.997869	-1.353521	1.902764
15	1	0	-6.196659	-1.454344	0.797474
16	1	0	-6.479863	-0.738963	-1.552271
17	1	0	-4.527420	0.171948	-2.822540
18	8	0	-1.843127	1.905402	-2.254289
19	6	0	-1.685567	0.403381	1.984196
20	8	0	-1.211533	0.058518	3.039040
21	8	0	-2.416852	1.507589	1.831159
22	6	0	-2.708969	2.235283	3.036832
23	1	0	-3.342645	1.628436	3.686838
24	1	0	-1.789456	2.495697	3.563596
25	1	0	-3.240150	3.130691	2.718342
26	7	0	2.113460	1.958599	-0.608643
27	6	0	2.537610	2.184773	0.773968
28	6	0	1.808233	3.376547	1.402474
29	6	0	2.002104	4.617146	0.529508

30	6	0	2.130488	3.136260	-1.479903
31	6	0	1.383873	4.302487	-0.833480
32	1	0	3.617802	2.387616	0.782750
33	1	0	2.366772	1.290601	1.375030
34	1	0	2.249507	3.531065	2.392255
35	6	0	0.314584	3.128212	1.616374
36	1	0	3.068387	4.845783	0.424221
37	1	0	3.171960	3.428503	-1.671766
38	1	0	1.673410	2.850519	-2.427266
39	6	0	-0.115279	4.048917	-0.669131
40	1	0	1.483982	5.160546	-1.506068
41	7	0	-0.444653	3.003975	0.342966
42	1	0	-0.095662	3.959239	2.203159
43	1	0	0.166152	2.204106	2.187460
44	1	0	-0.583910	4.988811	-0.352758
45	1	0	1.513000	5.485199	0.985195
46	1	0	-0.571192	3.733891	-1.610066
47	1	0	-1.430198	3.142888	0.573704
48	6	0	1.895938	0.752669	-1.173827
49	8	0	1.711743	0.590096	-2.378646
50	6	0	1.881514	-0.477931	-0.263437
51	6	0	3.334568	-0.962948	-0.019120
52	7	0	0.984688	-1.455547	-0.970577
53	1	0	3.950451	-0.053950	-0.096818
54	6	0	3.576160	-1.520313	1.388545
55	1	0	1.398319	-0.246235	0.682835
56	6	0	0.118254	-2.376059	-0.124801
57	6	0	-0.706098	-1.658356	0.974234
58	6	0	-1.501994	-2.762915	1.715815
59	6	0	-2.290951	-3.727550	0.819307
60	6	0	-0.726944	-3.223540	-1.076329
61	6	0	-1.429163	-4.330722	-0.287823
62	1	0	0.038401	-1.309110	1.694707
63	1	0	-0.772235	-3.341936	2.288465
64	1	0	-2.157501	-2.291669	2.452639
65	1	0	-3.138420	-3.220811	0.351277
66	1	0	-2.706857	-4.522191	1.446878
67	1	0	-2.045747	-4.920919	-0.970894
68	1	0	-0.685011	-5.012161	0.139477
69	1	0	-1.459297	-2.584865	-1.581114
70	1	0	-0.075960	-3.646932	-1.852570
71	1	0	0.398048	-0.936954	-1.652349
72	1	0	3.207712	-0.802890	2.132983
73	1	0	3.004880	-2.444806	1.521473
74	6	0	3.859450	-1.923911	-1.092115
75	6	0	5.352302	-2.189745	-0.880765
76	6	0	5.617783	-2.731777	0.525353
77	6	0	5.068313	-1.788641	1.598582
78	1	0	5.904576	-1.251283	-1.021823
79	1	0	5.715003	-2.892506	-1.637318
80	1	0	5.134590	-3.713020	0.628405
81	1	0	6.691304	-2.888932	0.672309
82	1	0	5.235936	-2.207651	2.595987
83	1	0	5.614739	-0.836524	1.554599
84	1	0	3.329958	-2.885990	-1.018506
85	1	0	3.676180	-1.514206	-2.093567
86	1	0	-0.580929	1.709622	-0.037029

3-IM5

Zero-point correction = 0.75641 a.u.
Thermal correction to Gibbs Free Energy = 0.68839 a.u.
Sum of electronic and zero-point Energies = -2237.22840 a.u.
Sum of electronic and thermal Free Energies = -2237.29641 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.922890	-3.210318	0.619864
2	1	0	1.492867	-2.160532	-1.530799
3	1	0	1.146305	-3.998566	0.098898
4	16	0	-1.722511	0.559831	-1.798601
5	6	0	-3.238480	-0.043477	-1.134145
6	6	0	-3.028285	-0.514702	0.150839
7	6	0	-1.577770	-0.356823	0.649471
8	7	0	-0.890965	0.480586	-0.359491
9	6	0	-4.474194	-0.038958	-1.768662
10	6	0	-5.560075	-0.511017	-1.041340
11	6	0	-5.387780	-0.949590	0.275163
12	6	0	-4.134756	-0.950235	0.880844
13	8	0	-1.190181	-0.437542	-2.734231
14	1	0	-4.031625	-1.278278	1.911098
15	1	0	-6.249378	-1.285000	0.842985
16	1	0	-6.547859	-0.517900	-1.489244
17	1	0	-4.586323	0.338793	-2.779838
18	8	0	-1.791878	1.943452	-2.251712
19	6	0	-1.677937	0.466312	1.964103
20	8	0	-1.212910	0.129176	3.024312
21	8	0	-2.371107	1.585485	1.775047
22	6	0	-2.639482	2.364570	2.954638
23	1	0	-3.276148	1.792481	3.632648
24	1	0	-1.709897	2.631005	3.460395
25	1	0	-3.158947	3.254938	2.604859
26	7	0	2.164311	1.875872	-0.619981
27	6	0	2.616296	2.078902	0.758958
28	6	0	2.003114	3.332041	1.393105
29	6	0	2.279082	4.543518	0.501561
30	6	0	2.201248	3.049607	-1.499465
31	6	0	1.580869	4.278407	-0.833217
32	1	0	3.710392	2.184496	0.759549
33	1	0	2.370734	1.207677	1.368093
34	1	0	2.485800	3.456385	2.368027
35	6	0	0.496498	3.216488	1.640113
36	1	0	3.357288	4.676171	0.355635
37	1	0	3.246271	3.266790	-1.759486
38	1	0	1.668815	2.787218	-2.413662
39	6	0	0.073257	4.151267	-0.600581
40	1	0	1.734063	5.119028	-1.518154
41	7	0	-0.265551	3.101881	0.382870
42	1	0	0.180205	4.100715	2.215004
43	1	0	0.287147	2.329999	2.252592
44	1	0	-0.293016	5.128894	-0.251580
45	1	0	1.886812	5.455035	0.965851
46	1	0	-0.444301	3.906103	-1.532498
47	1	0	-1.252340	3.221660	0.608085
48	6	0	1.870384	0.684756	-1.173193
49	8	0	1.618819	0.530050	-2.369132
50	6	0	1.851243	-0.550503	-0.264793
51	6	0	3.298784	-1.057724	-0.035248
52	7	0	0.932042	-1.517772	-0.959565
53	1	0	3.927785	-0.159046	-0.120707
54	6	0	3.544902	-1.619739	1.369498
55	1	0	1.384792	-0.314641	0.688827
56	6	0	0.037008	-2.401933	-0.100450
57	6	0	-0.764827	-1.653089	0.995400
58	6	0	-1.582897	-2.727183	1.754440
59	6	0	-2.402564	-3.679692	0.872697
60	6	0	-0.837895	-3.232710	-1.039430
61	6	0	-1.564054	-4.313760	-0.235726
62	1	0	-0.012228	-1.307072	1.709514
63	1	0	-0.863849	-3.318590	2.327544
64	1	0	-2.217875	-2.228553	2.491438
65	1	0	-3.241424	-3.157456	0.406146
66	1	0	-2.832340	-4.458570	1.510388
67	1	0	-2.200313	-4.893694	-0.909364
68	1	0	-0.834123	-5.009953	0.191913
69	1	0	-1.557591	-2.577296	-1.541806
70	1	0	-0.204420	-3.677907	-1.817924
71	1	0	0.376128	-0.989837	-1.656664
72	1	0	3.193413	-0.898625	2.118540
73	1	0	2.961703	-2.536544	1.506149
74	6	0	3.797162	-2.028926	-1.111358
75	6	0	5.289011	-2.313092	-0.917179

76	6	0	5.563354	-2.857386	0.486322
77	6	0	5.035195	-1.908585	1.565293
78	1	0	5.850930	-1.381525	-1.065713
79	1	0	5.634425	-3.020763	-1.677231
80	1	0	5.070915	-3.833442	0.594337
81	1	0	6.636594	-3.025811	0.622227
82	1	0	5.206481	-2.330758	2.560714
83	1	0	5.592911	-0.963263	1.517556
84	1	0	3.256383	-2.983705	-1.024597
85	1	0	3.606479	-1.621353	-2.112171
86	1	0	-0.573862	1.467130	-0.075940

3-IM6

Zero-point correction = 0.75721 a.u.
Thermal correction to Gibbs Free Energy = 0.68870 a.u.
Sum of electronic and zero-point Energies = -2237.22982 a.u.
Sum of electronic and thermal Free Energies = -2237.29832 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.476898	0.731777	-1.105129
2	7	0	-4.021423	-0.129994	-0.861994
3	6	0	-4.874963	0.141409	0.297938
4	6	0	-5.467025	-1.135706	0.900261
5	6	0	-6.183370	-1.926642	-0.196034
6	6	0	-4.596019	-1.000815	-1.888119
7	6	0	-5.132023	-2.287361	-1.248913
8	1	0	-5.698900	0.785643	-0.037534
9	1	0	-4.322964	0.697677	1.056429
10	1	0	-6.177339	-0.821726	1.672408
11	6	0	-4.426792	-2.035103	1.570185
12	1	0	-6.983402	-1.326249	-0.643778
13	1	0	-5.415015	-0.480885	-2.402178
14	1	0	-3.810881	-1.210411	-2.615362
15	6	0	-4.052547	-3.166376	-0.601964
16	1	0	-5.586840	-2.876904	-2.052156
17	7	0	-3.441091	-2.561332	0.605894
18	1	0	-4.963418	-2.858817	2.063458
19	1	0	-3.881776	-1.484812	2.346049
20	1	0	-4.521567	-4.127797	-0.347689
21	1	0	-6.635462	-2.832123	0.223810
22	1	0	-3.244836	-3.365729	-1.314554
23	1	0	-2.940258	-3.312653	1.080932
24	6	0	-2.803546	0.401028	-1.069789
25	8	0	-2.221232	0.402045	-2.153806
26	6	0	-2.063959	0.968766	0.148425
27	6	0	-2.219548	2.492356	0.301633
28	7	0	-0.634232	0.606266	-0.089102
29	1	0	-3.301715	2.686313	0.277310
30	6	0	-1.694108	2.974271	1.660858
31	1	0	-2.370616	0.471660	1.068842
32	1	0	-2.193188	2.424535	2.467227
33	1	0	-0.616856	2.761671	1.748099
34	6	0	-1.577047	3.274985	-0.852205
35	6	0	-1.780684	4.780694	-0.672507
36	6	0	-1.252619	5.257729	0.681298
37	6	0	-1.903121	4.481234	1.826946
38	1	0	-2.852584	5.007680	-0.743210
39	1	0	-1.286438	5.317528	-1.488384
40	1	0	-0.164070	5.109674	0.718160
41	1	0	-1.431734	6.330733	0.802056
42	1	0	-1.502151	4.808026	2.791475
43	1	0	-2.980962	4.690944	1.839705
44	1	0	-0.495018	3.068948	-0.877802
45	1	0	-1.982067	2.938470	-1.811275
46	8	0	-1.160751	-1.661012	-0.378236
47	1	0	-2.030815	-1.821197	0.126215
48	16	0	4.315681	-0.203876	1.505942
49	6	0	4.681979	-0.794811	-0.114024
50	6	0	3.557559	-0.752522	-0.917905
51	6	0	2.303493	-0.189006	-0.233144
52	7	0	2.686018	0.089754	1.158782
53	6	0	5.914151	-1.266201	-0.551277
54	6	0	5.996797	-1.694893	-1.871306
55	6	0	4.873893	-1.649163	-2.704026
56	6	0	3.648023	-1.178383	-2.240749
57	8	0	4.438113	-1.279454	2.480173
58	1	0	2.784924	-1.142047	-2.898885
59	1	0	4.958286	-1.983651	-3.732629
60	1	0	6.939584	-2.067082	-2.256819
61	1	0	6.773845	-1.294687	0.110392
62	8	0	4.969483	1.061868	1.818365
63	6	0	2.072646	1.116357	-1.027887
64	8	0	1.371582	1.178019	-2.014262
65	8	0	2.787760	2.121325	-0.551416
66	6	0	2.764018	3.336822	-1.325928
67	1	0	3.144517	3.138825	-2.329189
68	1	0	1.745664	3.726210	-1.384557
69	1	0	3.412771	4.030068	-0.795473
70	6	0	-0.253429	-0.855926	0.261250
71	6	0	1.122541	-1.193961	-0.384017
72	6	0	1.485286	-2.627180	0.067510
73	6	0	1.447018	-2.848359	1.582855
74	6	0	-0.273691	-1.011608	1.782305
75	6	0	0.092332	-2.447820	2.163303
76	1	0	0.916127	-1.224304	-1.460137
77	1	0	0.755528	-3.293087	-0.402607
78	1	0	2.464410	-2.901668	-0.333249
79	1	0	2.242049	-2.283648	2.077053
80	1	0	1.636696	-3.907573	1.784658
81	1	0	0.094522	-2.540748	3.252840
82	1	0	-0.682857	-3.123616	1.781657
83	1	0	0.432698	-0.305831	2.230082
84	1	0	-1.274227	-0.773133	2.160177
85	1	0	2.471609	1.039359	1.461031
86	1	0	-0.035279	1.258581	0.426030

4-IM1

Zero-point correction = 0.72612 a.u.
Thermal correction to Gibbs Free Energy = 0.65563 a.u.
Sum of electronic and zero-point Energies = -2160.82179 a.u.
Sum of electronic and thermal Free Energies = -2160.89229 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.919234	-1.250871	-2.020259
2	6	0	3.403612	-0.281831	-1.914561
3	6	0	3.606742	0.052812	-0.576203
4	6	0	2.527564	-0.548571	0.251826
5	7	0	1.649504	-1.284521	-0.336494
6	6	0	4.231936	0.123320	-2.940830
7	6	0	5.338958	0.899559	-2.583469
8	6	0	5.573669	1.235141	-1.251230
9	6	0	4.717046	0.818407	-0.229254
10	8	0	0.840360	-0.484505	-2.626136
11	6	0	2.418086	-0.492426	1.756418
12	8	0	1.543485	-1.077365	2.354735
13	8	0	3.397023	0.192294	2.316327
14	6	0	3.440690	0.155213	3.757065
15	1	0	4.232750	0.843984	4.042265
16	1	0	2.483645	0.469410	4.175335
17	1	0	4.918140	1.080706	0.801231
18	1	0	6.443129	1.831940	-0.997487
19	1	0	6.023227	1.239627	-3.353235
20	1	0	4.040730	-0.149914	-3.973304
21	1	0	3.673811	-0.860013	4.083583

22	8	0	2.169921	-2.609918	-2.469770
23	6	0	0.198774	3.126307	2.582957
24	6	0	1.712374	3.116121	2.395539
25	1	0	-0.060189	3.250444	3.638973
26	1	0	2.164352	4.013584	2.829127
27	1	0	2.124262	2.257268	2.936851
28	1	0	-0.233519	3.977792	2.041001
29	6	0	-0.418038	1.833101	2.051192
30	1	0	-1.507511	1.899188	2.103245
31	1	0	-0.125245	0.980531	2.683681
32	7	0	-3.142227	-1.723729	-0.156886
33	6	0	-3.524445	-1.777559	1.250229
34	6	0	-2.596417	-2.736383	2.012377
35	6	0	-2.667249	-4.124420	1.362649
36	6	0	-3.199061	-3.030000	-0.813685
37	6	0	-2.232087	-3.989496	-0.103153
38	1	0	-4.555467	-2.146227	1.308667
39	1	0	-3.506183	-0.785203	1.696838
40	1	0	-2.937612	-2.789550	3.049373
41	6	0	-1.149829	-2.207002	1.988214
42	1	0	-3.695000	-4.497986	1.404598
43	1	0	-4.222073	-3.417086	-0.746239
44	1	0	-2.935380	-2.897106	-1.861658
45	6	0	-0.789844	-3.438098	-0.192052
46	1	0	-2.275836	-4.962409	-0.598782
47	7	0	-0.250371	-3.078005	1.160866
48	1	0	-0.704324	-2.170514	2.981777
49	1	0	-1.070396	-1.212565	1.538931
50	1	0	-0.093043	-4.162716	-0.613968
51	1	0	-2.043339	-4.846323	1.900370
52	1	0	0.631991	-2.559915	1.028633
53	1	0	-0.740274	-2.522926	-0.788556
54	1	0	-0.025630	-3.931799	1.679629
55	6	0	-2.516171	-0.701462	-0.805747
56	8	0	-2.151775	-0.801781	-1.974590
57	6	0	-2.194566	0.613652	-0.085687
58	6	0	-2.907363	1.764974	-0.823945
59	7	0	-0.730833	0.672219	-0.122654
60	1	0	-2.502937	1.781297	-1.846499
61	6	0	-4.417450	1.498596	-0.907608
62	1	0	-2.518198	0.605843	0.954425
63	6	0	0.034447	1.546952	0.637747
64	6	0	1.199581	2.048470	0.161292
65	6	0	2.081588	3.007525	0.915867
66	1	0	3.135111	2.714024	0.815080
67	1	0	2.006266	3.998634	0.445200
68	1	0	1.451171	1.855247	-0.881991
69	1	0	-0.389111	0.527765	-1.071889
70	1	0	-4.607092	0.544584	-1.413145
71	1	0	-4.818145	1.406861	0.113694
72	6	0	-2.651423	3.126547	-0.168583
73	6	0	-3.374768	4.251843	-0.913536
74	6	0	-4.877639	3.982459	-0.992685
75	6	0	-5.150290	2.624871	-1.640832
76	1	0	-2.966584	4.328646	-1.930316
77	1	0	-3.181945	5.209913	-0.419072
78	1	0	-5.297734	3.987964	0.022863
79	1	0	-5.380877	4.779286	-1.550489
80	1	0	-6.225596	2.418282	-1.662528
81	1	0	-4.808414	2.648861	-2.684273
82	1	0	-3.017039	3.095376	0.868882
83	1	0	-1.576829	3.335859	-0.126906

4-TS1

Zero-point correction = 0.72615 a.u.
Thermal correction to Gibbs Free Energy = 0.65779 a.u.
Sum of electronic and zero-point Energies = -2160.82062 a.u.
Sum of electronic and thermal Free Energies = -2160.88898 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.773088	-1.158836	-1.979300
2	6	0	3.372000	-0.393720	-1.894204
3	6	0	3.552002	0.073764	-0.593956
4	6	0	2.378072	-0.320985	0.240721
5	7	0	1.476888	-1.086498	-0.322993
6	6	0	4.281392	-0.201234	-2.915709
7	6	0	5.452649	0.488502	-2.594188
8	6	0	5.665460	0.955017	-1.297459
9	6	0	4.726641	0.756460	-0.282358
10	8	0	0.859796	-0.259420	-2.682952
11	6	0	2.347967	-0.288658	1.739633
12	8	0	1.497810	-0.865979	2.384447
13	8	0	3.371477	0.365778	2.266834
14	6	0	3.476234	0.303493	3.700731
15	1	0	4.300793	0.963367	3.962438
16	1	0	2.549353	0.639117	4.168316
17	1	0	4.920303	1.112985	0.720758
18	1	0	6.584303	1.483428	-1.065831
19	1	0	6.204122	0.653952	-3.358554
20	1	0	4.100394	-0.578442	-3.917056
21	1	0	3.691652	-0.722559	4.005020
22	8	0	1.819682	-2.555621	-2.386692
23	6	0	0.241679	3.268581	2.414794
24	6	0	1.760729	3.217746	2.301337
25	1	0	-0.063556	3.452885	3.449047
26	1	0	2.207782	4.141163	2.681871
27	1	0	2.130903	2.402097	2.931237
28	1	0	-0.149152	4.096281	1.809012
29	6	0	-0.381224	1.958702	1.928652
30	1	0	-1.468449	2.037408	1.964523
31	1	0	-0.098972	1.132059	2.598852
32	7	0	-3.027956	-1.737519	-0.099484
33	6	0	-3.430206	-1.729462	1.303293
34	6	0	-2.508117	-2.655606	2.110995
35	6	0	-2.579454	-4.073096	1.529764
36	6	0	-3.100145	-3.071217	-0.699104
37	6	0	-2.150183	-4.011541	0.057300
38	1	0	-4.462323	-2.094109	1.363151
39	1	0	-3.417487	-0.719206	1.708109
40	1	0	-2.848947	-2.657977	3.149390
41	6	0	-1.062398	-2.130749	2.064466
42	1	0	-3.605458	-4.447601	1.597020
43	1	0	-4.130286	-3.436178	-0.620532
44	1	0	-2.829076	-2.990122	-1.750700
45	6	0	-0.702621	-3.488258	-0.064289
46	1	0	-2.210761	-5.005356	-0.392776
47	7	0	-0.158799	-3.014047	1.252231
48	1	0	-0.612474	-2.076279	3.054565
49	1	0	-0.982483	-1.139512	1.609044
50	1	0	-0.012417	-4.256662	-0.413051
51	1	0	-1.946531	-4.761939	2.100329
52	1	0	0.694530	-2.465662	1.057286
53	1	0	-0.636057	-2.636777	-0.744891
54	1	0	0.115749	-3.823421	1.815409
55	6	0	-2.372573	-0.754700	-0.776136
56	8	0	-1.962725	-0.910169	-1.922932
57	6	0	-2.124793	0.612006	-0.124373
58	6	0	-2.973646	1.667677	-0.865323
59	7	0	-0.692388	0.855373	-0.267270
60	1	0	-2.630920	1.663943	-1.910404
61	6	0	-4.461204	1.290055	-0.844206
62	1	0	-2.381279	0.619405	0.932416
63	6	0	0.094818	1.608563	0.538197
64	6	0	1.358237	1.977037	0.121790
65	6	0	2.197746	2.992670	0.853637
66	1	0	3.256151	2.704802	0.822264
67	1	0	2.136027	3.943909	0.305426
68	1	0	1.587833	1.827644	-0.931895
69	1	0	-0.345110	0.647891	-1.204192
70	1	0	-4.610949	0.301475	-1.293073

71	1	0	-4.795205	1.222674	0.202679
72	6	0	-2.777390	3.072191	-0.286673
73	6	0	-3.612096	4.105479	-1.046897
74	6	0	-5.095050	3.732172	-1.024945
75	6	0	-5.309805	2.326138	-1.585669
76	1	0	-3.264318	4.153567	-2.087514
77	1	0	-3.460291	5.099174	-0.612630
78	1	0	-5.457903	3.767223	0.011600
79	1	0	-5.681584	4.461577	-1.593392
80	1	0	-6.367594	2.048038	-1.532064
81	1	0	-5.030495	2.315863	-2.647703
82	1	0	-3.092813	3.069677	0.767319
83	1	0	-1.717252	3.351554	-0.307975

4-IM2

Zero-point correction = 0.72858 a.u.
Thermal correction to Gibbs Free Energy = 0.66128 a.u.
Sum of electronic and zero-point Energies = -2160.84393 a.u.
Sum of electronic and thermal Free Energies = -2160.91123 a.u.

Standard orientation:

Center umber	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-1.633309	0.969156	-1.850657
2	6	0	-3.268261	0.271973	-1.885755
3	6	0	-3.473290	-0.390228	-0.679709
4	6	0	-2.221752	-0.260291	0.221763
5	7	0	-1.444226	0.863964	-0.267309
6	6	0	-4.190877	0.301961	-2.917431
7	6	0	-5.398449	-0.363748	-2.714436
8	6	0	-5.631681	-1.037782	-1.515910
9	6	0	-4.679163	-1.065594	-0.494484
10	8	0	-0.758129	0.030854	-2.600688
11	6	0	-2.538000	0.021900	1.689767
12	8	0	-1.872247	0.755782	2.386348
13	8	0	-3.597672	-0.644872	2.131071
14	6	0	-3.924108	-0.456685	3.517607
15	1	0	-4.775172	-1.106967	3.709857
16	1	0	-3.076566	-0.735823	4.147334
17	1	0	-4.899302	-1.584607	0.429940
18	1	0	-6.578001	-1.547805	-1.366115
19	1	0	-6.159246	-0.354206	-3.488315
20	1	0	-3.982809	0.836278	-3.839364
21	1	0	-4.187174	0.586624	3.700149
22	8	0	-1.590307	2.357578	-2.319138
23	6	0	-0.155389	-3.156742	2.334447
24	6	0	-1.664730	-3.181098	2.135812
25	1	0	0.109758	-3.348778	3.377058
26	1	0	-2.068811	-4.157827	2.417016
27	1	0	-2.125791	-2.443226	2.801051
28	1	0	0.320246	-3.935638	1.726450
29	6	0	0.410922	-1.785222	1.938197
30	1	0	1.489087	-1.755534	2.088635
31	1	0	-0.043747	-1.014045	2.579112
32	7	0	2.903330	1.874528	0.028846
33	6	0	3.161264	1.903070	1.467533
34	6	0	2.096307	2.760094	2.167984
35	6	0	2.119433	4.179415	1.590550
36	6	0	2.932820	3.213338	-0.568939
37	6	0	1.848871	4.082589	0.084945
38	1	0	4.153437	2.342264	1.622320
39	1	0	3.178838	0.897718	1.884722
40	1	0	2.333919	2.784181	3.234834
41	6	0	0.707194	2.124976	1.986298
42	1	0	3.100288	4.633854	1.762832
43	1	0	3.924034	3.646989	-0.396404
44	1	0	2.768137	3.113599	-1.640705
45	6	0	0.463340	3.461012	-0.180690
46	1	0	1.886917	5.075982	-0.369334
47	7	0	-0.180830	2.868162	1.037859
48	1	0	0.160429	2.067213	2.925522
49	1	0	0.777570	1.109406	1.587225
50	1	0	-0.247268	4.192940	-0.563697
51	1	0	1.374752	4.813264	2.084439
52	1	0	-0.886514	2.147478	0.658924
53	1	0	0.525803	2.657152	-0.917380
54	1	0	-0.681718	3.598478	1.546844
55	6	0	2.418790	0.846224	-0.710770
56	8	0	2.083699	0.960898	-1.885672
57	6	0	2.276767	-0.555620	-0.093665
58	6	0	3.207333	-1.545007	-0.816257
59	7	0	0.865303	-0.913195	-0.306915
60	1	0	2.907428	-1.565340	-1.873079
61	6	0	4.657250	-1.050178	-0.725796
62	1	0	2.486970	-0.580550	0.970859
63	6	0	0.032107	-1.425890	0.536229
64	6	0	-1.388537	-1.630849	0.073786
65	6	0	-2.019037	-2.902541	0.675551
66	1	0	-3.101660	-2.860739	0.536560
67	1	0	-1.664525	-3.747457	0.074327
68	1	0	-1.345486	-1.756092	-1.012202
69	1	0	0.501880	-0.643521	-1.240944
70	1	0	4.751525	-0.063410	-1.192719
71	1	0	4.924846	-0.935321	0.335741
72	6	0	3.080466	-2.951915	-0.222291
73	6	0	4.044092	-3.929952	-0.897768
74	6	0	5.487675	-3.435995	-0.798151
75	6	0	5.621737	-2.033733	-1.391976
76	1	0	3.768002	-4.030579	-1.955919
77	1	0	3.942694	-4.921227	-0.444388
78	1	0	5.789073	-3.412244	0.258153
79	1	0	6.163444	-4.130442	-1.307930
80	1	0	6.648559	-1.668391	-1.290194
81	1	0	5.401136	-2.073876	-2.466797
82	1	0	3.310388	-2.900110	0.852730
83	1	0	2.051224	-3.317197	-0.318021

4-IM3

Zero-point correction = 0.75221 a.u.
Thermal correction to Gibbs Free Energy = 0.68110 a.u.
Sum of electronic and zero-point Energies = -2237.22644 a.u.
Sum of electronic and thermal Free Energies = -2237.29754 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.628944	-4.048959	-0.678389
2	1	0	0.783409	-5.000926	-0.611525
3	1	0	1.075518	-3.788229	-1.495896
4	6	0	0.018236	-3.189571	2.471300
5	6	0	-1.497691	-3.175106	2.319692
6	1	0	0.307862	-3.310605	3.518249
7	1	0	-1.926536	-4.102639	2.710329
8	1	0	-1.910427	-2.359965	2.925707
9	1	0	0.444714	-4.025068	1.906210
10	6	0	0.620795	-1.878791	1.951577
11	1	0	1.708783	-1.892923	2.023535
12	1	0	0.253452	-1.042843	2.566639
13	7	0	1.899050	2.129147	-0.091835
14	6	0	2.437895	2.352425	1.255936
15	6	0	1.662425	3.443713	1.996166
16	6	0	1.661537	4.728652	1.167943
17	6	0	1.666632	3.328676	-0.913673
18	6	0	0.927923	4.419837	-0.138061
19	1	0	3.490349	2.660225	1.182055
20	1	0	2.395458	1.427834	1.831610
21	1	0	2.171814	3.603970	2.951545
22	6	0	0.229228	3.041580	2.337011
23	1	0	2.689815	5.043257	0.960577

24	1	0	2.629806	3.721428	-1.267564
25	1	0	1.084346	3.014058	-1.781594
26	6	0	-0.528624	4.063480	0.156384
27	1	0	0.902668	5.305153	-0.780793
28	7	0	-0.643141	2.927159	1.125975
29	1	0	-0.220420	3.806370	2.975753
30	1	0	0.179949	2.079404	2.847935
31	1	0	-1.035334	4.919545	0.609245
32	1	0	1.162449	5.538261	1.710942
33	1	0	-1.061719	3.751199	-0.745419
34	1	0	-1.614610	2.878381	1.446411
35	6	0	2.077952	0.976217	-0.795127
36	8	0	2.007353	0.927186	-2.014730
37	6	0	2.254099	-0.366743	-0.057021
38	6	0	3.439240	-1.146168	-0.638512
39	7	0	0.965147	-1.031377	-0.309560
40	1	0	3.215345	-1.330458	-1.698442
41	6	0	4.716622	-0.300256	-0.553380
42	1	0	2.377830	-0.256687	1.017496
43	6	0	0.183937	-1.592898	0.550755
44	6	0	-1.237125	-1.841701	0.123921
45	6	0	-1.892611	-3.028111	0.849922
46	1	0	-2.977722	-2.957603	0.747584
47	1	0	-1.578985	-3.930194	0.317561
48	1	0	-1.211652	-2.055038	-0.949224
49	1	0	4.582861	0.645060	-1.091673
50	1	0	4.908115	-0.053203	0.501766
51	6	0	3.640075	-2.485143	0.079381
52	6	0	4.832147	-3.246886	-0.504699
53	6	0	6.108673	-2.407580	-0.429878
54	6	0	5.917529	-1.058413	-1.124235
55	1	0	4.621359	-3.493553	-1.554177
56	1	0	4.964904	-4.195557	0.025744
57	1	0	6.364373	-2.237218	0.624931
58	1	0	6.948049	-2.948427	-0.879091
59	1	0	6.821200	-0.447443	-1.031742
60	1	0	5.752685	-1.224866	-2.196995
61	1	0	3.833694	-2.285406	1.144203
62	1	0	2.729176	-3.091742	0.022379
63	1	0	0.582331	-0.848745	-1.253591
64	16	0	-1.464933	0.726231	-1.914641
65	6	0	-3.113646	0.059275	-1.912512
66	6	0	-3.304463	-0.582058	-0.692443
67	6	0	-2.043963	-0.439305	0.194363
68	7	0	-1.257734	0.660292	-0.337296
69	6	0	-4.050023	0.074251	-2.932206
70	6	0	-5.257559	-0.582546	-2.702131
71	6	0	-5.477247	-1.235183	-1.489221
72	6	0	-4.511539	-1.248053	-0.480353
73	8	0	-0.635358	-0.251646	-2.665591
74	6	0	-2.343825	-0.100273	1.654858
75	8	0	-1.614681	0.584312	2.342328
76	8	0	-3.460313	-0.651817	2.110045
77	6	0	-3.778279	-0.384065	3.485882
78	1	0	-4.674060	-0.963675	3.698938
79	1	0	-2.955521	-0.692584	4.134093
80	1	0	-4.724036	-1.748133	0.456141
81	1	0	-6.422741	-1.740158	-1.318235
82	1	0	-6.028089	-0.584684	-3.466435
83	1	0	-3.851469	0.589256	-3.867128
84	1	0	-3.968900	0.682169	3.621580
85	8	0	-1.392121	2.106609	-2.415385
86	1	0	-0.545101	2.005742	0.617560

4-TS2

Zero-point correction = 0.75158 a.u.
Thermal correction to Gibbs Free Energy = 0.68527 a.u.
Sum of electronic and zero-point Energies = -2237.175179 a.u.
Sum of electronic and thermal Free Energies = -2237.24150 a.u.

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	8	0	0.396960	-3.520636	-0.873241
2	1	0	-0.327031	-3.804176	-1.470899
3	1	0	1.099179	-2.790296	-1.361875
4	6	0	-0.236143	-3.735007	1.906066
5	6	0	-1.742683	-3.504993	1.847199
6	1	0	0.085653	-3.901125	2.937505
7	1	0	-2.274300	-4.402693	2.176296
8	1	0	-2.008929	-2.714730	2.554888
9	1	0	0.030762	-4.631625	1.336178
10	6	0	0.528537	-2.538418	1.336484
11	1	0	1.601783	-2.744233	1.329223
12	1	0	0.360517	-1.645211	1.947373
13	7	0	1.870236	1.938934	-0.056102
14	6	0	2.490729	1.993082	1.270129
15	6	0	1.835198	3.054440	2.159506
16	6	0	1.864787	4.412511	1.455198
17	6	0	1.712212	3.228856	-0.743566
18	6	0	1.055000	4.265740	0.167063
19	1	0	3.555516	2.243669	1.163884
20	1	0	2.422652	1.016688	1.751690
21	1	0	2.408833	3.092208	3.090847
22	6	0	0.400960	2.708282	2.545812
23	1	0	2.896857	4.694099	1.220918
24	1	0	2.698116	3.597841	-1.061738
25	1	0	1.103708	3.050257	-1.630240
26	6	0	-0.400251	3.931016	0.498420
27	1	0	1.033469	5.212313	-0.382148
28	7	0	-0.513699	2.707023	1.360133
29	1	0	0.013466	3.461539	3.237222
30	1	0	0.320459	1.724532	3.006506
31	1	0	-0.852047	4.753106	1.059797
32	1	0	1.438670	5.189080	2.099525
33	1	0	-0.983098	3.726866	-0.401688
34	1	0	-1.475785	2.653554	1.706793
35	6	0	1.844027	0.834554	-0.855819
36	8	0	1.664013	0.911257	-2.065185
37	6	0	2.050340	-0.576459	-0.283407
38	6	0	3.444565	-1.064655	-0.733219
39	7	0	0.991688	-1.427560	-0.884620
40	1	0	3.404396	-1.107199	-1.831631
41	6	0	4.546459	-0.073568	-0.333858
42	1	0	1.966580	-0.615149	0.802256
43	6	0	0.068646	-2.225891	-0.072695
44	6	0	-1.445878	-1.990384	-0.241892
45	6	0	-2.210903	-3.153838	0.429931
46	1	0	-3.279262	-2.927552	0.424936
47	1	0	-2.098409	-4.047113	-0.197281
48	1	0	-1.633010	-2.024176	-1.323955
49	1	0	4.328604	0.925255	-0.730805
50	1	0	4.569253	0.010681	0.762563
51	6	0	3.792669	-2.458252	-0.199679
52	6	0	5.157845	-2.924931	-0.711497
53	6	0	6.257054	-1.932966	-0.331527
54	6	0	5.917805	-0.530275	-0.835529
55	1	0	5.115664	-3.018631	-1.804773
56	1	0	5.383248	-3.919747	-0.313705
57	1	0	6.357570	-1.909084	0.762283
58	1	0	7.221582	-2.260397	-0.733503
59	1	0	6.684301	0.185957	-0.521850
60	1	0	5.910993	-0.531932	-1.933615
61	1	0	3.813046	-2.421346	0.899799
62	1	0	3.025660	-3.189825	-0.480638
63	1	0	0.490731	-0.891130	-1.606682
64	16	0	-1.475694	0.870649	-1.839926
65	6	0	-3.200742	0.487110	-1.655681
66	6	0	-3.337351	-0.323752	-0.536189
67	6	0	-1.954801	-0.536867	0.148009
68	7	0	-1.056403	0.504853	-0.344198
69	6	0	-4.248035	0.843460	-2.489761
70	6	0	-5.515143	0.363577	-2.168020

71	6	0	-5.684753	-0.458858	-1.053954
72	6	0	-4.609965	-0.813528	-0.235964
73	8	0	-0.967273	-0.076603	-2.861897
74	6	0	-2.030161	-0.346045	1.666986
75	8	0	-1.122435	0.104820	2.332070
76	8	0	-3.188092	-0.725322	2.193124
77	6	0	-3.305856	-0.589898	3.617888
78	1	0	-4.274306	-1.014792	3.874124
79	1	0	-2.501436	-1.132008	4.118993
80	1	0	-4.789496	-1.433139	0.633454
81	1	0	-6.675903	-0.826180	-0.807037
82	1	0	-6.369853	0.629473	-2.781394
83	1	0	-4.081571	1.482033	-3.352190
84	1	0	-3.265238	0.464590	3.897007
85	8	0	-1.248252	2.293398	-2.139841
86	1	0	-0.427641	1.837051	0.767033

4-IM4

Zero-point correction = 0.75808 a.u.
Thermal correction to Gibbs Free Energy = 0.69089 a.u.
Sum of electronic and zero-point Energies = -2237.22345 a.u.
Sum of electronic and thermal Free Energies = -2237.29064 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.249496	-3.578761	-1.300044
2	1	0	-0.341543	-3.460500	-2.061994
3	1	0	1.610681	-1.968110	-1.749685
4	6	0	-0.092566	-4.129930	1.447841
5	6	0	-1.564043	-3.758677	1.591456
6	1	0	0.327640	-4.425859	2.413398
7	1	0	-2.144023	-4.628812	1.914003
8	1	0	-1.675769	-3.006289	2.379458
9	1	0	0.011475	-4.982366	0.769181
10	6	0	0.717406	-2.952114	0.899257
11	1	0	1.749630	-3.263464	0.737868
12	1	0	0.712182	-2.135792	1.622549
13	7	0	1.699799	2.001274	-0.059390
14	6	0	1.993557	1.959617	1.378061
15	6	0	1.269137	3.071503	2.150284
16	6	0	1.567705	4.429265	1.513931
17	6	0	1.746261	3.315535	-0.717448
18	6	0	1.013831	4.385876	0.089092
19	1	0	3.072040	2.090253	1.536951
20	1	0	1.696039	0.990387	1.779890
21	1	0	1.646804	3.037016	3.176850
22	6	0	-0.242727	2.874798	2.238607
23	1	0	2.647410	4.611966	1.493903
24	1	0	2.795849	3.616694	-0.844559
25	1	0	1.297595	3.197911	-1.703635
26	6	0	-0.498037	4.172826	0.117796
27	1	0	1.180017	5.342185	-0.416808
28	7	0	-0.876571	2.938051	0.883650
29	1	0	-0.687434	3.676877	2.833844
30	1	0	-0.502315	1.911072	2.675650
31	1	0	-0.981890	5.009036	0.629574
32	1	0	1.098135	5.233878	2.089842
33	1	0	-0.914901	4.057779	-0.882122
34	1	0	-1.894328	2.947626	1.003799
35	6	0	1.699021	0.922240	-0.882942
36	8	0	1.585584	1.015148	-2.101881
37	6	0	1.949776	-0.492000	-0.336846
38	6	0	3.421331	-0.845263	-0.674486
39	7	0	1.030120	-1.409981	-1.113596
40	1	0	3.510737	-0.713920	-1.764067
41	6	0	4.396430	0.132854	-0.001627
42	1	0	1.726398	-0.608668	0.721242
43	6	0	0.133273	-2.485639	-0.431724
44	6	0	-1.365535	-2.073963	-0.372147
45	6	0	-2.136490	-3.253762	0.264447
46	1	0	-3.186636	-2.978801	0.377933
47	1	0	-2.114771	-4.082643	-0.450973
48	1	0	-1.677833	-2.006311	-1.423674
49	1	0	4.159737	1.165245	-0.282338
50	1	0	4.276552	0.054977	1.088319
51	6	0	3.813613	-2.287387	-0.330649
52	6	0	5.260645	-2.581779	-0.734268
53	6	0	6.227120	-1.613078	-0.056110
54	6	0	5.849087	-0.169591	-0.380497
55	1	0	5.356231	-2.488216	-1.824140
56	1	0	5.506653	-3.617328	-0.478666
57	1	0	6.186588	-1.764397	1.031158
58	1	0	7.256008	-1.817259	-0.369521
59	1	0	6.513568	0.529752	0.137158
60	1	0	5.978197	0.004411	-1.456994
61	1	0	3.706838	-2.438403	0.752264
62	1	0	3.154283	-3.010550	-0.827289
63	1	0	0.442187	-0.820366	-1.730097
64	16	0	-1.596954	0.805010	-1.840148
65	6	0	-3.269500	0.391083	-1.396828
66	6	0	-3.227574	-0.382338	-0.240966
67	6	0	-1.756448	-0.641791	0.180516
68	7	0	-0.947631	0.414622	-0.433379
69	6	0	-4.438950	0.734827	-2.056412
70	6	0	-5.638787	0.283805	-1.511188
71	6	0	-5.630070	-0.487872	-0.348297
72	6	0	-4.437582	-0.831015	0.290871
73	8	0	-1.182563	-0.088166	-2.947687
74	6	0	-1.494983	-0.534851	1.681954
75	8	0	-0.405816	-0.267344	2.145738
76	8	0	-2.561762	-0.775515	2.433044
77	6	0	-2.351062	-0.749315	3.854209
78	1	0	-3.290010	-1.077788	4.295327
79	1	0	-1.537641	-1.423908	4.128753
80	1	0	-4.466651	-1.418940	1.199738
81	1	0	-6.570247	-0.828283	0.074052
82	1	0	-6.580295	0.536044	-1.988056
83	1	0	-4.416285	1.341979	-2.956055
84	1	0	-2.112086	0.265351	4.178749
85	8	0	-1.447206	2.244231	-2.107960
86	1	0	-0.698456	2.038676	0.345597

4-TS3

Zero-point correction = 0.75270 a.u.
Thermal correction to Gibbs Free Energy = 0.68550 a.u.
Sum of electronic and zero-point Energies = -2237.22363 a.u.
Sum of electronic and thermal Free Energies = -2237.29082 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.331199	-3.520498	-1.407340
2	1	0	-0.268763	-3.362277	-2.155146
3	1	0	1.768364	-1.937480	-1.729304
4	6	0	0.088555	-4.165650	1.360174
5	6	0	-1.370287	-3.784480	1.581338
6	1	0	0.552854	-4.488141	2.296321
7	1	0	-1.940993	-4.651773	1.926912
8	1	0	-1.439837	-3.034706	2.377416
9	1	0	0.147615	-5.003588	0.658030
10	6	0	0.884808	-2.985966	0.797517
11	1	0	1.898866	-3.311647	0.564117
12	1	0	0.941170	-2.191096	1.542083
13	7	0	1.563993	2.074300	-0.121388
14	6	0	1.949157	2.106501	1.293814
15	6	0	1.122979	3.107357	2.109313
16	6	0	1.154671	4.479192	1.434369
17	6	0	1.313377	3.360811	-0.790633

18	6	0	0.482172	4.309912	0.072796
19	1	0	3.003831	2.400511	1.373861
20	1	0	1.839658	1.109618	1.723784
21	1	0	1.586533	3.157432	3.099950
22	6	0	-0.327140	2.678811	2.319653
23	1	0	2.187115	4.825534	1.312312
24	1	0	2.275195	3.839229	-1.022810
25	1	0	0.802157	3.140518	-1.727944
26	6	0	-0.968106	3.858930	0.262416
27	1	0	0.443857	5.266939	-0.457851
28	7	0	-1.066619	2.581331	1.030423
29	1	0	-0.828402	3.428729	2.943938
30	1	0	-0.381730	1.713725	2.822365
31	1	0	-1.505017	4.632348	0.824561
32	1	0	0.619798	5.216105	2.043344
33	1	0	-1.461941	3.706590	-0.696586
34	1	0	-2.056414	2.460317	1.263692
35	6	0	1.655209	0.993145	-0.926822
36	8	0	1.505745	1.053089	-2.147136
37	6	0	2.001342	-0.396539	-0.363726
38	6	0	3.495841	-0.663993	-0.680417
39	7	0	1.140540	-1.373982	-1.144322
40	1	0	3.591909	-0.561494	-1.772715
41	6	0	4.390302	0.401780	-0.028263
42	1	0	1.770120	-0.518550	0.692568
43	6	0	0.244546	-2.466877	-0.487553
44	6	0	-1.261968	-2.080553	-0.373133
45	6	0	-1.995992	-3.273800	0.282816
46	1	0	-3.044751	-3.011553	0.434982
47	1	0	-1.989135	-4.095454	-0.440764
48	1	0	-1.611668	-2.027106	-1.410286
49	1	0	4.092297	1.402660	-0.358379
50	1	0	4.249755	0.360262	1.061015
51	6	0	3.978784	-2.063670	-0.279802
52	6	0	5.458909	-2.269239	-0.615390
53	6	0	6.334121	-1.210222	0.049695
54	6	0	5.869700	0.185825	-0.356709
55	1	0	5.589776	-2.214720	-1.704367
56	1	0	5.763252	-3.274552	-0.307100
57	1	0	6.264916	-1.314018	1.141072
58	1	0	7.384565	-1.358301	-0.220549
59	1	0	6.467494	0.954982	0.142718
60	1	0	6.018282	0.316328	-1.436812
61	1	0	3.828110	-2.196923	0.800431
62	1	0	3.402563	-2.845520	-0.787713
63	1	0	0.576874	-0.824318	-1.819014
64	16	0	-1.613570	0.713242	-1.891119
65	6	0	-3.256724	0.275874	-1.379381
66	6	0	-3.170540	-0.448835	-0.193288
67	6	0	-1.688793	-0.672639	0.198680
68	7	0	-0.926874	0.420823	-0.439065
69	6	0	-4.445387	0.575276	-2.024691
70	6	0	-5.622548	0.126707	-1.430537
71	6	0	-5.571337	-0.597093	-0.238858
72	6	0	-4.358396	-0.897002	0.384385
73	8	0	-1.157636	-0.260559	-2.901282
74	6	0	-1.368963	-0.586842	1.688235
75	8	0	-0.244306	-0.389148	2.096232
76	8	0	-2.414754	-0.770406	2.478505
77	6	0	-2.142541	-0.772810	3.892021
78	1	0	-3.093435	-0.996642	4.370997
79	1	0	-1.398613	-1.535375	4.131183
80	1	0	-4.354976	-1.453306	1.313452
81	1	0	-6.494964	-0.934888	0.220186
82	1	0	-6.579611	0.345426	-1.892303
83	1	0	-4.453670	1.148447	-2.946389
84	1	0	-1.776945	0.206918	4.204063
85	8	0	-1.510398	2.126870	-2.252009
86	1	0	-0.879543	1.523365	0.295182

4-IM5

Zero-point correction = 0.75646 a.u.
Thermal correction to Gibbs Free Energy = 0.69008 a.u.
Sum of electronic and zero-point Energies = -2237.22563 a.u.
Sum of electronic and thermal Free Energies = -2237.29202 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.355562	-3.592630	-1.291088
2	1	0	-0.225078	-3.473353	-2.061084
3	1	0	1.767524	-2.010254	-1.683130
4	6	0	0.059464	-4.130880	1.474508
5	6	0	-1.410891	-3.763504	1.640206
6	1	0	0.498834	-4.412646	2.435376
7	1	0	-1.979630	-4.628613	1.994093
8	1	0	-1.513810	-2.992364	2.412154
9	1	0	0.152076	-4.991947	0.805074
10	6	0	0.855688	-2.958220	0.896320
11	1	0	1.883738	-3.270361	0.706592
12	1	0	0.875011	-2.138279	1.614245
13	7	0	1.551914	2.036774	-0.143419
14	6	0	1.965559	2.089244	1.266460
15	6	0	1.218999	3.151846	2.082096
16	6	0	1.290876	4.497240	1.358869
17	6	0	1.276766	3.309105	-0.835555
18	6	0	0.539535	4.321722	0.040731
19	1	0	3.035356	2.329854	1.312840
20	1	0	1.815860	1.109562	1.723191
21	1	0	1.734827	3.210487	3.046599
22	6	0	-0.244459	2.807600	2.362779
23	1	0	2.333014	4.783629	1.174094
24	1	0	2.230646	3.745867	-1.163709
25	1	0	0.690361	3.070044	-1.723401
26	6	0	-0.918564	3.943990	0.325377
27	1	0	0.526633	5.262421	-0.520124
28	7	0	-1.009752	2.696604	1.109947
29	1	0	-0.661801	3.601127	3.004160
30	1	0	-0.315021	1.860832	2.902104
31	1	0	-1.382348	4.778699	0.875227
32	1	0	0.826837	5.281246	1.967370
33	1	0	-1.462670	3.800207	-0.610442
34	1	0	-1.990776	2.560038	1.355296
35	6	0	1.649411	0.950807	-0.935956
36	8	0	1.474098	0.990636	-2.156163
37	6	0	2.010126	-0.430605	-0.359282
38	6	0	3.498454	-0.707407	-0.690526
39	7	0	1.143021	-1.427014	-1.113553
40	1	0	3.577301	-0.647183	-1.787355
41	6	0	4.405903	0.380372	-0.096705
42	1	0	1.794244	-0.536827	0.702132
43	6	0	0.243759	-2.498833	-0.424762
44	6	0	-1.268583	-2.117650	-0.357908
45	6	0	-2.009536	-3.298682	0.310921
46	1	0	-3.064343	-3.043507	0.427684
47	1	0	-1.976200	-4.138708	-0.389846
48	1	0	-1.595852	-2.085815	-1.405484
49	1	0	4.100252	1.369443	-0.454743
50	1	0	4.291683	0.375975	0.996094
51	6	0	3.983944	-2.090769	-0.238907
52	6	0	5.455375	-2.316645	-0.598732
53	6	0	6.348120	-1.232113	-0.000816
54	6	0	5.876513	0.147899	-0.452245
55	1	0	5.560607	-2.309152	-1.691820
56	1	0	5.765243	-3.308451	-0.254486
57	1	0	6.306437	-1.290273	1.095328
58	1	0	7.391202	-1.393932	-0.291038
59	1	0	6.488117	0.934171	0.001656
60	1	0	5.998839	0.234872	-1.539971
61	1	0	3.856664	-2.172693	0.849551
62	1	0	3.392414	-2.892619	-0.695724
63	1	0	0.586667	-0.888987	-1.802448

64	16	0	-1.678099	0.707154	-1.956423
65	6	0	-3.294223	0.266686	-1.382920
66	6	0	-3.183520	-0.468311	-0.205301
67	6	0	-1.706307	-0.705759	0.180853
68	7	0	-0.927546	0.341767	-0.513153
69	6	0	-4.495785	0.579690	-1.998917
70	6	0	-5.660004	0.128388	-1.384072
71	6	0	-5.584805	-0.608807	-0.201674
72	6	0	-4.360813	-0.917177	0.393069
73	8	0	-1.232015	-0.257282	-2.964654
74	6	0	-1.374295	-0.534372	1.663281
75	8	0	-0.254788	-0.269832	2.041675
76	8	0	-2.406158	-0.725457	2.465177
77	6	0	-2.126848	-0.650874	3.876497
78	1	0	-3.052058	-0.938234	4.371413
79	1	0	-1.318884	-1.338447	4.133964
80	1	0	-4.339072	-1.480451	1.317581
81	1	0	-6.499009	-0.948776	0.273951
82	1	0	-6.625903	0.355683	-1.822238
83	1	0	-4.522206	1.163554	-2.913393
84	1	0	-1.847995	0.369700	4.144396
85	8	0	-1.557530	2.128619	-2.248296
86	1	0	-0.834120	1.226779	0.072943

4-IM6

Zero-point correction = 0.75732 a.u.
Thermal correction to Gibbs Free Energy = 0.69056 a.u.
Sum of electronic and zero-point Energies = -2237.23848 a.u.
Sum of electronic and thermal Free Energies = -2237.30524 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.258802	1.449575	1.644153
2	7	0	3.241376	-0.683802	0.044281
3	6	0	3.033232	-0.629107	-1.407320
4	6	0	2.953557	-2.021211	-2.039885
5	6	0	4.188388	-2.833773	-1.646640
6	6	0	4.301936	-1.580031	0.510177
7	6	0	4.165002	-2.967437	-0.122410
8	1	0	3.880425	-0.089584	-1.853575
9	1	0	2.127212	-0.071308	-1.641335
10	1	0	2.922253	-1.869919	-3.124047
11	6	0	1.691987	-2.792248	-1.648733
12	1	0	5.103606	-2.326337	-1.972661
13	1	0	5.282213	-1.157034	0.250176
14	1	0	4.230041	-1.631627	1.597094
15	6	0	2.896980	-3.718083	0.300477
16	1	0	5.019783	-3.559947	0.221001
17	7	0	1.655144	-3.087305	-0.202958
18	1	0	1.668918	-3.724254	-2.232678
19	1	0	0.798398	-2.210985	-1.901235
20	1	0	2.978294	-4.748367	-0.075971
21	1	0	4.163086	-3.820746	-2.122330
22	1	0	2.823619	-3.764000	1.392364
23	1	0	0.908935	-3.766933	-0.058009
24	6	0	2.692154	0.155647	0.943782
25	8	0	3.099928	0.295325	2.096143
26	6	0	1.453499	0.972738	0.548801
27	6	0	1.840087	2.463814	0.497107
28	7	0	0.476806	0.733978	1.662954
29	1	0	2.241351	2.713872	1.491047
30	6	0	2.962346	2.674383	-0.532244
31	1	0	0.975359	0.652854	-0.373844
32	1	0	3.815033	2.022800	-0.307675
33	1	0	2.585265	2.387136	-1.524556
34	6	0	0.676422	3.414632	0.184937
35	6	0	1.146521	4.871497	0.195578
36	6	0	2.267696	5.090244	-0.819747
37	6	0	3.428869	4.131567	-0.557864
38	1	0	1.506775	5.128473	1.200810
39	1	0	0.299917	5.531204	-0.019928
40	1	0	1.873951	4.915843	-1.830179
41	1	0	2.616140	6.127583	-0.785929
42	1	0	4.207136	4.254188	-1.317735
43	1	0	3.886324	4.373184	0.410792
44	1	0	0.276273	3.177706	-0.810093
45	1	0	-0.149486	3.297665	0.898772
46	1	0	1.024652	0.859924	2.528679
47	8	0	0.865306	-1.579180	1.811988
48	1	0	1.130049	-1.989842	0.912471
49	6	0	-1.442082	-2.082719	3.441994
50	6	0	-2.423277	-2.478131	2.338395
51	1	0	-1.939714	-2.070556	4.415606
52	1	0	-2.765430	-3.505428	2.497228
53	1	0	-3.311008	-1.839164	2.379176
54	1	0	-0.633864	-2.819366	3.493964
55	6	0	-0.821838	-0.708780	3.178755
56	1	0	-0.038535	-0.500552	3.915494
57	1	0	-1.575970	0.076891	3.280589
58	6	0	-0.163679	-0.676941	1.793115
59	6	0	-1.151907	-1.006166	0.637416
60	6	0	-1.758374	-2.388031	0.964123
61	1	0	-2.445261	-2.685408	0.170296
62	1	0	-0.931682	-3.103779	0.937039
63	1	0	-0.538742	-1.131007	-0.266084
64	16	0	-1.341876	0.863073	-2.134975
65	6	0	-2.805969	-0.125322	-2.150374
66	6	0	-3.164357	-0.451528	-0.847065
67	6	0	-2.188762	0.102972	0.203371
68	7	0	-1.423939	1.179949	-0.477842
69	6	0	-3.515062	-0.529317	-3.272589
70	6	0	-4.654527	-1.297889	-3.056696
71	6	0	-5.038340	-1.640728	-1.758203
72	6	0	-4.301253	-1.231295	-0.647641
73	8	0	-0.167119	0.033969	-2.395201
74	6	0	-2.957439	0.745031	1.367801
75	8	0	-3.988277	0.329685	1.826042
76	8	0	-2.326086	1.834667	1.824889
77	6	0	-2.954644	2.503516	2.939524
78	1	0	-2.296153	3.332960	3.188160
79	1	0	-3.938825	2.865711	2.640711
80	1	0	-4.614454	-1.501902	0.354054
81	1	0	-5.933514	-2.234696	-1.605409
82	1	0	-5.249840	-1.625438	-3.902063
83	1	0	-3.201958	-0.241930	-4.270999
84	1	0	-3.048967	1.814252	3.780741
85	8	0	-1.474226	2.123141	-2.849780
86	1	0	-1.867692	2.094691	-0.369840

3-H_2O-TS1′

Zero-point correction = 0.75068 a.u.
Thermal correction to Gibbs Free Energy = 0.67949 a.u.
Sum of electronic and zero-point Energies = -2237.21946 a.u.
Sum of electronic and thermal Free Energies = -2237.29065 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.615526	-1.098881	-0.438338
2	6	0	-3.032767	-1.113915	0.970335
3	6	0	-3.107146	-2.543924	1.527481
4	6	0	-4.010608	-3.403817	0.639848
5	6	0	-3.341492	-2.019124	-1.328128
6	6	0	-3.380063	-3.435142	-0.754259
7	1	0	-4.029063	-0.659700	1.057061
8	1	0	-2.335977	-0.521384	1.563876
9	1	0	-3.520011	-2.471194	2.538336
10	6	0	-1.744573	-3.222009	1.660581
11	1	0	-5.013433	-2.968028	0.585126

12	1	0	-4.369254	-1.655401	-1.460379
13	1	0	-2.844883	-2.001856	-2.297545
14	6	0	-1.998975	-4.086748	-0.692627
15	1	0	-3.980473	-4.047808	-1.433378
16	7	0	-1.113285	-3.410797	0.314027
17	1	0	-1.856305	-4.215304	2.101178
18	1	0	-1.041477	-2.635158	2.252822
19	1	0	-2.082290	-5.129180	-0.376537
20	1	0	-4.102043	-4.414267	1.051522
21	1	0	-0.807100	-2.487496	-0.027834
22	1	0	-1.473752	-4.039088	-1.648717
23	1	0	-0.248897	-3.953788	0.410449
24	6	0	-1.912240	-0.090998	-1.028958
25	8	0	-1.781847	-0.042336	-2.251729
26	6	0	-1.305955	1.013251	-0.158033
27	6	0	-2.360341	2.124049	0.072156
28	7	0	-0.115249	1.481067	-0.847386
29	1	0	-3.269413	1.621651	0.440217
30	6	0	-1.898407	3.099498	1.159999
31	1	0	-0.997910	0.607161	0.803441
32	6	0	1.041726	1.890839	-0.312236
33	6	0	1.345148	1.841908	1.038094
34	6	0	2.593746	2.468333	1.605118
35	6	0	3.662268	2.789230	0.555589
36	6	0	2.078866	2.335592	-1.317701
37	6	0	3.034847	3.360747	-0.711638
38	1	0	0.517707	1.730718	1.732821
39	1	0	2.305152	3.395238	2.121684
40	1	0	3.006059	1.816922	2.388184
41	1	0	4.210701	1.879258	0.287605
42	1	0	4.389320	3.488459	0.979723
43	1	0	3.806402	3.618384	-1.442893
44	1	0	2.484823	4.281118	-0.478848
45	1	0	2.641596	1.449929	-1.646939
46	1	0	1.569523	2.729534	-2.202174
47	1	0	-0.178387	1.513968	-1.865816
48	1	0	-1.672417	2.545466	2.081328
49	1	0	-0.964102	3.577647	0.834091
50	6	0	-2.725255	2.877619	-1.213007
51	6	0	-3.777367	3.955755	-0.939911
52	6	0	-3.310175	4.926216	0.145893
53	6	0	-2.951487	4.176240	1.429669
54	1	0	-4.710664	3.475064	-0.615608
55	1	0	-4.003079	4.496465	-1.864797
56	1	0	-2.424294	5.467767	-0.212785
57	1	0	-4.083446	5.675436	0.345356
58	1	0	-2.586821	4.872197	2.192457
59	1	0	-3.855708	3.701832	1.835248
60	1	0	-1.818601	3.352000	-1.614575
61	1	0	-3.083940	2.178903	-1.976534
62	8	0	-0.061247	1.501539	-3.845781
63	1	0	0.689247	0.894703	-3.784035
64	1	0	-0.806445	0.929778	-3.599673
65	16	0	1.487753	-1.562188	-1.395349
66	6	0	3.132999	-1.308390	-0.784794
67	6	0	3.036242	-0.792115	0.505387
68	6	0	1.601418	-0.645522	0.887367
69	7	0	0.715087	-1.080464	0.015113
70	6	0	4.331227	-1.551602	-1.430221
71	6	0	5.497199	-1.280841	-0.711856
72	6	0	5.428602	-0.798626	0.596297
73	6	0	4.206512	-0.549285	1.223741
74	8	0	1.232537	-0.673862	-2.524759
75	6	0	1.232081	-0.484442	2.330593
76	8	0	2.045055	-0.336025	3.213132
77	8	0	-0.088035	-0.545391	2.537211
78	6	0	-0.505656	-0.324897	3.894139
79	1	0	-1.593601	-0.383029	3.882018
80	1	0	-0.088234	-1.091437	4.549425
81	1	0	4.168390	-0.181920	2.240903
82	1	0	6.347557	-0.608693	1.141157
83	1	0	6.463297	-1.457630	-1.172422
84	1	0	4.364812	-1.943186	-2.441664
85	8	0	1.152927	-2.977016	-1.580113
86	1	0	-0.181162	0.661925	4.231600

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Zero-point correction = 0.75156 a.u.
Thermal correction to Gibbs Free Energy = 0.67940 a.u.
Sum of electronic and zero-point Energies = -2237.21075 a.u.
Sum of electronic and thermal Free Energies = -2237.28291 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.448064	-1.911129	-2.408829
2	1	0	0.321486	-1.480398	-1.991747
3	1	0	-0.970435	-1.128532	-2.651146
4	6	0	0.742492	0.480095	4.032200
5	6	0	2.181638	0.047581	3.784888
6	1	0	0.292734	-0.099124	4.843910
7	1	0	2.771263	0.126061	4.703034
8	1	0	2.192620	-1.005767	3.485527
9	1	0	0.724479	1.533060	4.338573
10	6	0	-0.107370	0.313977	2.770940
11	1	0	-1.094390	0.750232	2.946084
12	1	0	-0.263959	-0.753159	2.549693
13	7	0	-2.757441	-0.894309	-0.454815
14	6	0	-3.159808	-1.261743	0.909093
15	6	0	-3.367429	-2.772962	1.040220
16	6	0	-4.405504	-3.246807	0.022732
17	6	0	-3.565890	-1.481872	-1.541518
18	6	0	-3.822037	-2.982514	-1.366487
19	1	0	-4.092691	-0.748252	1.181059
20	1	0	-2.377910	-0.962123	1.606662
21	1	0	-3.717755	-2.957556	2.060451
22	6	0	-2.069125	-3.566920	0.882169
23	1	0	-5.340694	-2.693267	0.156790
24	1	0	-4.538248	-0.969045	-1.553374
25	1	0	-3.070736	-1.276035	-2.489083
26	6	0	-2.579603	-3.846953	-1.563732
27	1	0	-4.533581	-3.275781	-2.144210
28	7	0	-1.551465	-3.531157	-0.522623
29	1	0	-2.247840	-4.618659	1.118835
30	1	0	-1.269656	-3.183490	1.518579
31	1	0	-2.833224	-4.904931	-1.459606
32	1	0	-4.620137	-4.312448	0.154339
33	1	0	-2.098531	-3.673999	-2.526651
34	1	0	-0.779860	-4.199726	-0.605082
35	6	0	-2.019627	0.217400	-0.748180
36	8	0	-1.702517	0.509165	-1.899809
37	6	0	-1.661570	1.208052	0.374217
38	6	0	-2.287514	2.568559	0.008469
39	7	0	-0.221749	1.324330	0.517277
40	1	0	-1.828444	2.894794	-0.936210
41	6	0	-3.799092	2.425420	-0.209807
42	1	0	-2.085114	0.902683	1.326021
43	6	0	0.538507	0.952367	1.564808
44	6	0	1.914964	1.107741	1.499664
45	6	0	2.816011	0.901164	2.688264
46	1	0	3.764076	0.455876	2.361626
47	1	0	3.080924	1.885777	3.099973
48	1	0	2.292520	1.761246	0.716254
49	1	0	-4.001838	1.711558	-1.016752
50	1	0	-4.250414	2.018361	0.708136
51	6	0	-2.001421	3.611815	1.093386
52	6	0	-2.646905	4.957984	0.756283
53	6	0	-4.153609	4.811486	0.541447
54	6	0	-4.447555	3.771554	-0.540185
55	1	0	-2.189223	5.354173	-0.160087
56	1	0	-2.440983	5.679919	1.553403
57	1	0	-4.622907	4.495423	1.483618

58	1	0	-4.596240	5.776150	0.271464
59	1	0	-5.527599	3.642971	-0.667112
60	1	0	-4.053143	4.128853	-1.500822
61	1	0	-2.404695	3.245851	2.050174
62	1	0	-0.921002	3.731837	1.225061
63	1	0	0.251574	1.764658	-0.269958
64	1	0	-1.128957	-2.619198	-0.782732
65	16	0	2.127859	0.968264	-2.189346
66	6	0	3.766616	0.743288	-1.537626
67	6	0	3.678468	-0.127203	-0.450638
68	6	0	2.255403	-0.537521	-0.261525
69	7	0	1.414369	-0.172727	-1.202574
70	6	0	4.949514	1.306276	-1.974552
71	6	0	6.110564	0.955283	-1.280940
72	6	0	6.051479	0.075135	-0.201182
73	6	0	4.842213	-0.476481	0.230136
74	8	0	1.607615	2.289716	-1.819805
75	6	0	1.763330	-1.652305	0.608682
76	8	0	0.619330	-2.057785	0.564285
77	8	0	2.709080	-2.161715	1.386514
78	6	0	2.313608	-3.286651	2.189398
79	1	0	3.176751	-3.524052	2.807764
80	1	0	1.454530	-3.029000	2.812063
81	1	0	4.816291	-1.168491	1.062406
82	1	0	6.965870	-0.192971	0.317796
83	1	0	7.065764	1.362363	-1.594585
84	1	0	4.977800	1.977785	-2.826572
85	1	0	2.061402	-4.130406	1.543717
86	8	0	2.023791	0.561765	-3.582651

3-2H₂O-TS1′

Zero-point correction = 0.77559 a.u.
Thermal correction to Gibbs Free Energy = 0.70074 a.u.
Sum of electronic and zero-point Energies = -2313.60593 a.u.
Sum of electronic and thermal Free Energies = -2313.68078 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.454165	1.408963	-0.524663
2	6	0	2.936592	1.571504	0.854545
3	6	0	2.790267	3.018753	1.357289
4	6	0	3.430603	3.991388	0.363210
5	6	0	2.915495	2.414039	-1.494203
6	6	0	2.691247	3.830167	-0.967550
7	1	0	4.000577	1.302554	0.897075
8	1	0	2.389699	0.893379	1.512539
9	1	0	3.295501	3.071581	2.326777
10	6	0	1.342504	3.447138	1.585444
11	1	0	4.492033	3.759600	0.227995
12	1	0	3.985181	2.265207	-1.694566
13	1	0	2.369083	2.249159	-2.421809
14	6	0	1.207173	4.171708	-0.806086
15	1	0	3.089960	4.524341	-1.713407
16	7	0	0.572352	3.395285	0.306566
17	1	0	1.307137	4.481352	1.937661
18	1	0	0.815285	2.809646	2.293397
19	1	0	1.086077	5.228136	-0.553447
20	1	0	3.352412	5.018173	0.735703
21	1	0	0.448568	2.406841	0.033461
22	1	0	0.633886	3.948801	-1.708892
23	1	0	-0.397449	3.719302	0.483242
24	6	0	1.948705	0.251570	-1.038145
25	8	0	1.822680	0.105004	-2.253882
26	6	0	1.550896	-0.886908	-0.093412
27	6	0	2.780124	-1.792130	0.170548
28	7	0	0.451489	-1.590956	-0.732872
29	1	0	3.595746	-1.128110	0.499428
30	6	0	2.507446	-2.783471	1.307606
31	1	0	1.190585	-0.477386	0.849290
32	6	0	-0.611012	-2.172985	-0.153823
33	6	0	-0.930897	-2.077281	1.185086
34	6	0	-2.065672	-2.850037	1.806489
35	6	0	-3.042450	-3.445764	0.787363
36	6	0	-1.533514	-2.884019	-1.118099
37	6	0	-2.302212	-4.005708	-0.423200
38	1	0	-0.157906	-1.735998	1.867413
39	1	0	-1.638172	-3.660005	2.415103
40	1	0	-2.600711	-2.203699	2.516715
41	1	0	-3.736364	-2.673646	0.436594
42	1	0	-3.643953	-4.221883	1.270328
43	1	0	-3.003333	-4.461277	-1.128336
44	1	0	-1.600900	-4.788323	-0.107418
45	1	0	-2.239936	-2.150107	-1.533643
46	1	0	-0.942909	-3.260197	-1.958987
47	1	0	0.530496	-1.703076	-1.743940
48	1	0	2.206223	-2.235623	2.210557
49	1	0	1.663148	-3.427958	1.026311
50	6	0	3.249974	-2.528242	-1.090179
51	6	0	4.473543	-3.399859	-0.799452
52	6	0	4.195282	-4.387180	0.335117
53	6	0	3.733674	-3.652882	1.594799
54	1	0	5.317539	-2.755354	-0.517307
55	1	0	4.771890	-3.934850	-1.706977
56	1	0	3.409033	-5.085608	0.017475
57	1	0	5.087777	-4.984578	0.549130
58	1	0	3.506668	-4.366336	2.393838
59	1	0	4.550050	-3.014215	1.959286
60	1	0	2.430872	-3.164815	-1.453217
61	1	0	3.473380	-1.813104	-1.888875
62	8	0	0.468559	-1.868653	-3.713691
63	1	0	-0.390141	-1.424750	-3.731311
64	1	0	1.071628	-1.137939	-3.498530
65	16	0	-1.654429	1.054918	-1.579668
66	6	0	-3.230477	0.522266	-0.969018
67	6	0	-3.072551	0.177596	0.370687
68	6	0	-1.644948	0.337425	0.767433
69	7	0	-0.825265	0.806585	-0.143797
70	6	0	-4.438021	0.473902	-1.640994
71	6	0	-5.551034	0.072578	-0.900019
72	6	0	-5.426399	-0.244274	0.453955
73	6	0	-4.194395	-0.195795	1.108972
74	8	0	-1.196525	0.205200	-2.671556
75	6	0	-1.280914	0.398820	2.218172
76	8	0	-2.075956	0.220937	3.111016
77	8	0	0.009894	0.684085	2.415614
78	6	0	0.435648	0.665587	3.788144
79	1	0	1.505085	0.875347	3.768951
80	1	0	-0.094571	1.428661	4.361031
81	1	0	-4.112545	-0.437933	2.160501
82	1	0	-6.308308	-0.536850	1.014266
83	1	0	-6.522590	0.019010	-1.379375
84	1	0	-4.518324	0.743958	-2.689108
85	8	0	-1.631080	2.506794	-1.811679
86	1	0	0.249657	-0.317999	4.225433
87	8	0	-2.148157	3.369305	0.885694
88	1	0	-2.469508	3.343526	-0.029280
89	1	0	-2.729250	3.986399	1.350766

4-2H₂O-TS1′

Zero-point correction = 0.77650 a.u.
Thermal correction to Gibbs Free Energy = 0.70279 a.u.
Sum of electronic and zero-point Energies = -2313.59807 a.u.
Sum of electronic and thermal Free Energies = -2313.67179 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.250337	2.595366	3.218268
2	6	0	2.652102	2.001365	3.224247

3	1	0	0.847139	2.666684	4.232531
4	1	0	3.312841	2.575260	3.880869
5	1	0	2.612237	0.980230	3.621619
6	1	0	1.284877	3.613960	2.811392
7	6	0	0.306141	1.748718	2.364722
8	1	0	-0.648132	2.268391	2.262956
9	1	0	0.095056	0.790872	2.861352
10	7	0	-3.095081	-0.566273	-0.379867
11	6	0	-4.013297	-0.027408	0.634020
12	6	0	-4.804119	-1.134540	1.331461
13	6	0	-5.577950	-1.940229	0.287186
14	6	0	-3.678443	-1.548586	-1.313404
15	6	0	-4.541173	-2.606279	-0.617305
16	1	0	-4.730046	0.650945	0.153945
17	1	0	-3.453271	0.542264	1.375879
18	1	0	-5.494751	-0.641115	2.022040
19	6	0	-3.936326	-2.060461	2.181893
20	1	0	-6.223074	-1.274571	-0.295327
21	1	0	-4.297124	-1.012654	-2.046481
22	1	0	-2.863582	-2.032451	-1.850066
23	6	0	-3.736729	-3.610067	0.203469
24	1	0	-5.033594	-3.178083	-1.409641
25	7	0	-3.052350	-2.938452	1.353185
26	1	0	-4.574386	-2.723850	2.770619
27	1	0	-3.286443	-1.500882	2.858928
28	1	0	-4.400048	-4.374408	0.615535
29	1	0	-6.211694	-2.693566	0.766743
30	1	0	-2.953072	-4.092501	-0.385479
31	1	0	-2.663059	-3.666111	1.959815
32	6	0	-1.966795	0.067903	-0.799970
33	8	0	-1.369258	-0.253590	-1.827212
34	6	0	-1.400481	1.267243	-0.028706
35	6	0	-1.758641	2.565954	-0.798207
36	7	0	0.049017	1.112448	0.002748
37	1	0	-1.257228	2.482047	-1.774475
38	6	0	-3.264270	2.712226	-1.048731
39	1	0	-1.778216	1.317200	0.989305
40	6	0	0.880517	1.450935	0.999618
41	6	0	2.258643	1.457847	0.777645
42	6	0	3.226626	1.987538	1.807832
43	1	0	4.153405	1.402218	1.786628
44	1	0	3.515420	3.009402	1.524605
45	1	0	2.565288	1.543704	-0.262455
46	1	0	-3.652918	1.838425	-1.586804
47	1	0	-3.783762	2.758827	-0.081115
48	6	0	-1.225131	3.810641	-0.080739
49	6	0	-1.524503	5.081182	-0.880167
50	6	0	-3.023057	5.225890	-1.146032
51	6	0	-3.571687	3.982794	-1.846016
52	1	0	-0.988885	5.034780	-1.837781
53	1	0	-1.143212	5.955924	-0.343117
54	1	0	-3.546294	5.362862	-0.189583
55	1	0	-3.220176	6.119091	-1.747870
56	1	0	-4.652436	4.072017	-1.997595
57	1	0	-3.114830	3.895986	-2.840658
58	1	0	-1.707298	3.884426	0.905615
59	1	0	-0.146335	3.723675	0.090836
60	1	0	0.454655	0.923331	-0.914752
61	1	0	-2.195395	-2.459583	0.954044
62	16	0	2.208263	-0.914367	-2.036759
63	6	0	3.911568	-0.665002	-1.609907
64	6	0	3.991146	-0.624225	-0.220299
65	6	0	2.626894	-0.807849	0.363473
66	7	0	1.677263	-1.171677	-0.483107
67	6	0	5.000582	-0.521623	-2.447741
68	6	0	6.244399	-0.346803	-1.836426
69	6	0	6.354474	-0.326345	-0.446104
70	6	0	5.237267	-0.465305	0.381350
71	8	0	1.621625	0.324525	-2.558978
72	6	0	2.453381	-1.120637	1.814093
73	8	0	3.362463	-1.131047	2.612807
74	8	0	1.184774	-1.406418	2.110655
75	6	0	0.942163	-1.778283	3.473918
76	1	0	-0.126805	-1.977536	3.536674
77	1	0	1.512496	-2.673543	3.728300
78	1	0	5.339357	-0.474888	1.458884
79	1	0	7.332859	-0.207362	0.007615
80	1	0	7.132979	-0.240652	-2.449584
81	1	0	4.897138	-0.559569	-3.527228
82	1	0	1.219199	-0.963976	4.147545
83	8	0	2.032278	-2.122879	-2.845364
84	8	0	-0.707240	-2.821738	-2.512065
85	1	0	0.224824	-2.876240	-2.776064
86	1	0	-0.917229	-1.872782	-2.576125
87	8	0	-0.743697	-2.573237	0.205647
88	1	0	-0.732582	-2.757502	-0.760932
89	1	0	-0.017450	-1.937856	0.321733

3-3H_2O-TS1′

Zero-point correction = 0.80148 a.u.
Thermal correction to Gibbs Free Energy = 0.72524 a.u.
Sum of electronic and zero-point Energies = -2389.99223 a.u.
Sum of electronic and thermal Free Energies = -2390.06846 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.851642	-0.438751	-0.264765
2	6	0	-3.085570	-0.358232	1.182151
3	6	0	-3.374452	-1.744675	1.760405
4	6	0	-4.630869	-2.302064	1.088689
5	6	0	-3.895612	-1.150368	-1.030955
6	6	0	-4.299550	-2.490155	-0.393500
7	1	0	-3.948512	0.294151	1.372586
8	1	0	-2.216632	0.072005	1.674026
9	1	0	-3.537813	-1.619715	2.835911
10	6	0	-2.199072	-2.715121	1.603891
11	1	0	-5.460661	-1.598533	1.214393
12	1	0	-4.781470	-0.503299	-1.072743
13	1	0	-3.527488	-1.298023	-2.045092
14	6	0	-3.228378	-3.571844	-0.517401
15	1	0	-5.177926	-2.845590	-0.940742
16	7	0	-1.982887	-3.142488	0.185627
17	1	0	-2.395764	-3.628932	2.170624
18	1	0	-1.258015	-2.276990	1.942859
19	1	0	-3.566819	-4.494854	-0.038990
20	1	0	-4.925889	-3.257076	1.535733
21	1	0	-1.546494	-2.398504	-0.377916
22	1	0	-2.954249	-3.767107	-1.552704
23	1	0	-1.270845	-3.907519	0.202460
24	6	0	-1.957807	0.330342	-0.929389
25	8	0	-1.867414	0.308090	-2.164812
26	6	0	-1.107157	1.319170	-0.130494
27	6	0	-1.954363	2.599288	0.106481
28	7	0	0.110363	1.567087	-0.876563
29	1	0	-2.915911	2.262242	0.524312
30	6	0	-1.308539	3.526352	1.141315
31	1	0	-0.822817	0.882473	0.824372
32	6	0	1.315216	1.856870	-0.375161
33	6	0	1.637596	1.790331	0.974075
34	6	0	2.945287	2.322947	1.504434
35	6	0	4.018304	2.526163	0.430942
36	6	0	2.369063	2.188167	-1.406477
37	6	0	3.420873	3.135474	-0.832522
38	1	0	0.815391	1.794612	1.682021
39	1	0	2.742818	3.285383	1.996510
40	1	0	3.315661	1.663482	2.301190
41	1	0	4.474626	1.565578	0.165965
42	1	0	4.815324	3.160242	0.831034
43	1	0	4.197348	3.315051	-1.581295
44	1	0	2.956017	4.102771	-0.604000
45	1	0	2.849104	1.253756	-1.729792

46	1	0	1.880073	2.609690	-2.289794
47	1	0	0.018424	1.602613	-1.893585
48	1	0	-1.132861	2.973886	2.073960
49	1	0	-0.328008	3.855833	0.770744
50	6	0	-2.248026	3.359403	-1.193204
51	6	0	-3.117340	4.590828	-0.926701
52	6	0	-2.476223	5.512262	0.111369
53	6	0	-2.184365	4.752910	1.406682
54	1	0	-4.099846	4.263321	-0.559592
55	1	0	-3.291820	5.130740	-1.863109
56	1	0	-1.535351	5.910097	-0.292420
57	1	0	-3.125994	6.370595	0.312500
58	1	0	-1.696761	5.408827	2.135332
59	1	0	-3.133109	4.426094	1.854144
60	1	0	-1.294747	3.676853	-1.638825
61	1	0	-2.736280	2.701671	-1.920430
62	8	0	0.077979	1.513391	-3.833319
63	1	0	0.659795	0.745237	-3.742031
64	1	0	-0.795863	1.149913	-3.622575
65	16	0	1.522916	-1.602058	-1.296263
66	6	0	3.166282	-1.350327	-0.692799
67	6	0	3.064933	-0.879863	0.612488
68	6	0	1.628366	-0.667820	0.958453
69	7	0	0.731293	-1.096369	0.084012
70	6	0	4.363117	-1.636180	-1.323915
71	6	0	5.525073	-1.450651	-0.573379
72	6	0	5.449822	-1.025565	0.754374
73	6	0	4.229087	-0.737701	1.367560
74	8	0	1.220502	-0.771308	-2.461741
75	6	0	1.242812	-0.456877	2.392245
76	8	0	2.047502	-0.357568	3.288666
77	8	0	-0.079217	-0.399813	2.571146
78	6	0	-0.505102	-0.185043	3.926469
79	1	0	-1.594489	-0.174644	3.895239
80	1	0	-0.150723	-0.995157	4.565919
81	1	0	4.188284	-0.422077	2.401299
82	1	0	6.364415	-0.915074	1.327866
83	1	0	6.491219	-1.658304	-1.020660
84	1	0	4.396562	-1.997885	-2.346391
85	8	0	1.272687	-3.042741	-1.486351
86	1	0	-0.123705	0.769771	4.294280
87	8	0	-1.338595	-2.370670	-2.436645
88	1	0	-0.484397	-2.759771	-2.666383
89	1	0	-1.276691	-1.431243	-2.671852
90	8	0	0.239790	-4.696216	0.546465
91	1	0	0.810994	-4.245025	-0.098838
92	1	0	0.309024	-5.638430	0.342492

4-3H$_2$O-TS1′

Zero-point correction = 0.80153 a.u.
Thermal correction to Gibbs Free Energy = 0.72507 a.u.
Sum of electronic and zero-point Energies = -2389.98465 a.u.
Sum of electronic and thermal Free Energies = -2390.06111 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.274127	3.147593	2.594699
2	6	0	2.753125	2.786672	2.539609
3	1	0	0.968527	3.370047	3.621549
4	1	0	3.362436	3.598941	2.947501
5	1	0	2.933255	1.910875	3.171574
6	1	0	1.089155	4.051754	2.000240
7	6	0	0.408687	2.011403	2.046560
8	1	0	-0.632388	2.331894	2.023909
9	1	0	0.448823	1.134134	2.705640
10	7	0	-3.123006	-0.697715	-0.265111
11	6	0	-3.731073	-0.343660	1.028317
12	6	0	-4.434934	-1.532929	1.693698
13	6	0	-5.422328	-2.179825	0.722917
14	6	0	-3.917893	-1.547831	-1.172993
15	6	0	-4.604021	-2.709823	-0.455061
16	1	0	-4.470310	0.453072	0.877396
17	1	0	-2.947755	0.011695	1.696506
18	1	0	-4.961584	-1.130077	2.564305
19	6	0	-3.468759	-2.587946	2.226820
20	1	0	-6.151275	-1.440913	0.373767
21	1	0	-4.686470	-0.922043	-1.647575
22	1	0	-3.251634	-1.915913	-1.951342
23	6	0	-3.630536	-3.783897	0.026186
24	1	0	-5.256408	-3.192066	-1.189483
25	7	0	-2.737645	-3.263471	1.109961
26	1	0	-4.019156	-3.365718	2.761726
27	1	0	-2.710043	-2.157460	2.880682
28	1	0	-4.180470	-4.627203	0.450952
29	1	0	-5.969293	-2.991533	1.213962
30	1	0	-2.976021	-4.129479	-0.773812
31	1	0	-2.200907	-4.046755	1.494703
32	6	0	-2.106825	-0.000669	-0.827216
33	8	0	-1.709501	-0.256557	-1.973578
34	6	0	-1.468112	1.192423	-0.111599
35	6	0	-1.955421	2.472927	-0.843742
36	7	0	-0.016716	1.052015	-0.198340
37	1	0	-1.600961	2.390036	-1.880262
38	6	0	-3.487240	2.571649	-0.862446
39	1	0	-1.754538	1.230389	0.934195
40	6	0	0.869869	1.579022	0.675454
41	6	0	2.210372	1.654417	0.328673
42	6	0	3.198754	2.486508	1.107022
43	1	0	4.179071	1.995480	1.120883
44	1	0	3.346943	3.432131	0.566337
45	1	0	2.443187	1.483585	-0.721726
46	1	0	-3.930996	1.672797	-1.308847
47	1	0	-3.851244	2.633013	0.173858
48	6	0	-1.361014	3.752456	-0.245270
49	6	0	-1.810294	4.984965	-1.033959
50	6	0	-3.335062	5.087800	-1.072080
51	6	0	-3.951715	3.808095	-1.637707
52	1	0	-1.424880	4.911292	-2.059655
53	1	0	-1.375270	5.887788	-0.592622
54	1	0	-3.710775	5.248900	-0.052233
55	1	0	-3.645017	5.953549	-1.666592
56	1	0	-5.044994	3.868450	-1.619319
57	1	0	-3.654743	3.698475	-2.689171
58	1	0	-1.697139	3.853456	0.797240
59	1	0	-0.266386	3.698678	-0.234677
60	1	0	0.315259	0.943718	-1.158497
61	1	0	-2.024798	-2.621165	0.719425
62	16	0	1.970424	-1.824894	-1.501118
63	6	0	3.641972	-1.251922	-1.583497
64	6	0	3.945405	-0.654178	-0.363947
65	6	0	2.751594	-0.714361	0.537098
66	7	0	1.703087	-1.364578	0.081054
67	6	0	4.529668	-1.351421	-2.638327
68	6	0	5.804754	-0.820384	-2.436633
69	6	0	6.142241	-0.233263	-1.216645
70	6	0	5.227725	-0.145251	-0.165167
71	8	0	1.118786	-1.073508	-2.426490
72	6	0	2.934373	-0.527006	2.011314
73	8	0	3.982158	-0.181232	2.507495
74	8	0	1.843864	-0.836094	2.716136
75	6	0	1.992954	-0.749356	4.143812
76	1	0	1.040317	-1.075348	4.559049
77	1	0	2.799188	-1.405436	4.476023
78	1	0	5.515051	0.288075	0.783595
79	1	0	7.143314	0.160784	-1.076112
80	1	0	6.541046	-0.876772	-3.231315
81	1	0	4.253140	-1.829208	-3.572815
82	1	0	2.205767	0.278014	4.445904
83	8	0	1.882357	-3.284010	-1.589794
84	8	0	-0.951871	-2.768121	-0.994800
85	1	0	-0.200054	-3.332247	-1.225823

86	1	0	-0.942743	-2.042041	-1.641104
87	8	0	-0.813996	-1.240450	1.584893
88	1	0	-0.222382	-1.329972	2.342831
89	1	0	-0.186475	-1.268844	0.838144
90	8	0	0.217697	1.424234	-3.202491
91	1	0	0.977954	0.858988	-3.390251
92	1	0	-0.480483	0.777381	-3.000021

3-IM1′

Zero-point correction = 0.82874 a.u.
Thermal correction to Gibbs Free Energy = 0.74807 a.u.
Sum of electronic and zero-point Energies = -2466.36720 a.u.
Sum of electronic and thermal Free Energies = -2466.44788 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.107283	-0.102667	-0.293680
2	6	0	-3.606264	0.674984	0.856135
3	6	0	-4.776400	0.002353	1.583783
4	6	0	-5.862468	-0.382305	0.577795
5	6	0	-4.096499	-0.784721	-1.151990
6	6	0	-5.249110	-1.413202	-0.368541
7	1	0	-3.969554	1.648677	0.503377
8	1	0	-2.778516	0.833821	1.548111
9	1	0	-5.159194	0.743701	2.291807
10	6	0	-4.387062	-1.218513	2.410489
11	1	0	-6.189447	0.498301	0.014884
12	1	0	-4.502624	-0.061460	-1.871300
13	1	0	-3.571521	-1.553487	-1.720233
14	6	0	-4.841720	-2.664136	0.408605
15	1	0	-5.984779	-1.742498	-1.108888
16	7	0	-3.909324	-2.324211	1.527592
17	1	0	-5.256595	-1.598346	2.952905
18	1	0	-3.574840	-1.007146	3.104070
19	1	0	-5.719959	-3.136005	0.855775
20	1	0	-6.734304	-0.798593	1.093194
21	1	0	-2.981252	-2.095802	1.135752
22	1	0	-4.318209	-3.386287	-0.220992
23	1	0	-3.749562	-3.161622	2.095805
24	6	0	-1.921634	0.177020	-0.895085
25	8	0	-1.679022	-0.242332	-2.036243
26	6	0	-0.911292	1.112658	-0.219167
27	6	0	-1.440684	2.576948	-0.430409
28	7	0	0.375470	0.851485	-0.837372
29	1	0	-2.522702	2.509296	-0.613366
30	6	0	-1.270675	3.472218	0.801386
31	1	0	-0.857065	0.875776	0.848788
32	6	0	1.558525	1.444829	-0.482806
33	6	0	1.849139	1.911557	0.759683
34	6	0	3.113100	2.666548	1.086448
35	6	0	4.194587	2.520323	0.013856
36	6	0	2.580734	1.490991	-1.600797
37	6	0	3.593769	2.613562	-1.385464
38	1	0	1.073154	1.894561	1.521395
39	1	0	2.865356	3.731648	1.212756
40	1	0	3.507850	2.339295	2.056238
41	1	0	4.682627	1.544092	0.117578
42	1	0	4.966435	3.282804	0.158012
43	1	0	4.376237	2.556160	-2.148514
44	1	0	3.091926	3.582281	-1.507615
45	1	0	3.102735	0.523759	-1.655126
46	1	0	2.054768	1.612090	-2.553710
47	1	0	0.305402	0.609142	-1.819020
48	1	0	-1.679168	2.970957	1.688405
49	1	0	-0.202355	3.636588	0.986239
50	6	0	-0.855535	3.254889	-1.674495
51	6	0	-1.530014	4.610300	-1.904712
52	6	0	-1.402763	5.510128	-0.672806
53	6	0	-1.954388	4.822559	0.578952
54	1	0	-2.593971	4.450745	-2.127487
55	1	0	-1.091808	5.100746	-2.780165
56	1	0	-0.341741	5.744994	-0.510280
57	1	0	-1.917403	6.461711	-0.843290
58	1	0	-1.821575	5.463671	1.456796
59	1	0	-3.035549	4.664108	0.458636
60	1	0	0.222637	3.408237	-1.532236
61	1	0	-0.974306	2.607479	-2.552421
62	8	0	0.398195	0.217756	-3.934830
63	1	0	0.851636	-0.557650	-3.577183
64	1	0	-0.494600	0.132730	-3.569267
65	16	0	1.445891	-2.404416	-0.722360
66	6	0	3.190432	-2.121468	-0.620510
67	6	0	3.436098	-1.333227	0.501839
68	6	0	2.142584	-1.010187	1.174400
69	7	0	1.056252	-1.455962	0.636040
70	6	0	4.170472	-2.570753	-1.483542
71	6	0	5.484201	-2.205378	-1.182008
72	6	0	5.763319	-1.432181	-0.055263
73	6	0	4.752793	-0.989273	0.801113
74	8	0	0.904449	-1.865906	-1.965752
75	6	0	2.017761	-0.335838	2.518772
76	8	0	0.974571	-0.218150	3.122900
77	8	0	3.189638	0.057831	2.986364
78	6	0	3.162170	0.697808	4.274718
79	1	0	4.192239	0.980949	4.481267
80	1	0	2.517348	1.578013	4.242127
81	1	0	4.994674	-0.387540	1.666932
82	1	0	6.791264	-1.163336	0.163708
83	1	0	6.292657	-2.529892	-1.828179
84	1	0	3.931464	-3.176430	-2.351509
85	8	0	1.090820	-3.779782	-0.384676
86	1	0	2.796045	-0.002225	5.027539
87	8	0	-1.660973	-2.912224	-2.763190
88	1	0	-0.743350	-3.173848	-2.924290
89	1	0	-1.614834	-1.940228	-2.707651
90	8	0	-1.676162	-2.910050	-0.047732
91	1	0	-1.704103	-2.982701	-1.029120
92	1	0	-1.015616	-3.561893	0.225935
93	8	0	-1.448714	-1.166287	2.111925
94	1	0	-1.013891	-1.472252	1.300517
95	1	0	-0.703621	-0.844744	2.640583

3-TS1′

Zero-point correction = 0.82744 a.u.
Thermal correction to Gibbs Free Energy = 0.74719 a.u.
Sum of electronic and zero-point Energies = -2466.36745 a.u.
Sum of electronic and thermal Free Energies = -2466.44770 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.142241	0.001486	-0.157092
2	6	0	-3.587617	0.574587	1.125964
3	6	0	-4.722541	-0.219074	1.786787
4	6	0	-5.858516	-0.417796	0.782287
5	6	0	-4.171217	-0.534598	-1.071561
6	6	0	-5.301398	-1.273969	-0.355948
7	1	0	-3.981685	1.583252	0.951280
8	1	0	-2.726995	0.632748	1.793244
9	1	0	-5.062006	0.389572	2.630429
10	6	0	-4.315700	-1.569081	2.369389
11	1	0	-6.199241	0.548582	0.395985
12	1	0	-4.595946	0.297991	-1.648098
13	1	0	-3.675451	-1.205194	-1.774296
14	6	0	-4.880189	-2.642802	0.175257
15	1	0	-6.073384	-1.460169	-1.108519
16	7	0	-3.891423	-2.506614	1.287865
17	1	0	-5.170767	-2.029579	2.871060
18	1	0	-3.476410	-1.490461	3.057654

19	1	0	-5.744328	-3.176865	0.577833
20	1	0	-6.711347	-0.913094	1.257861
21	1	0	-2.974477	-2.219561	0.904831
22	1	0	-4.399276	-3.250927	-0.593442
23	1	0	-3.718769	-3.430747	1.694154
24	6	0	-1.958449	0.306698	-0.741777
25	8	0	-1.736335	-0.007387	-1.920060
26	6	0	-0.907053	1.169409	-0.015172
27	6	0	-1.400714	2.648147	-0.042793
28	7	0	0.334769	1.018683	-0.765303
29	1	0	-2.411142	2.655982	0.382118
30	6	0	-0.557031	3.583909	0.830731
31	1	0	-0.770639	0.813835	1.011290
32	6	0	1.576511	1.378082	-0.410646
33	6	0	2.003452	1.521990	0.896260
34	6	0	3.298939	2.219140	1.237770
35	6	0	4.267736	2.377912	0.059233
36	6	0	2.553317	1.544882	-1.553042
37	6	0	3.529655	2.680820	-1.240401
38	1	0	1.239169	1.543399	1.668478
39	1	0	3.036353	3.215403	1.624846
40	1	0	3.798947	1.706024	2.069066
41	1	0	4.839880	1.454890	-0.082203
42	1	0	4.989013	3.167859	0.289800
43	1	0	4.237168	2.795515	-2.066523
44	1	0	2.974408	3.623807	-1.152770
45	1	0	3.118217	0.612567	-1.697079
46	1	0	1.998852	1.729545	-2.477219
47	1	0	0.190069	0.868255	-1.761480
48	1	0	-0.485415	3.182892	1.849304
49	1	0	0.463348	3.638764	0.430700
50	6	0	-1.502514	3.202171	-1.470638
51	6	0	-2.080105	4.620228	-1.467188
52	6	0	-1.265084	5.554420	-0.571423
53	6	0	-1.154472	4.993344	0.847010
54	1	0	-3.115945	4.584706	-1.102553
55	1	0	-2.116939	5.007390	-2.490611
56	1	0	-0.256238	5.665238	-0.991868
57	1	0	-1.715316	6.552520	-0.553389
58	1	0	-0.539945	5.649652	1.471945
59	1	0	-2.153167	4.959326	1.303853
60	1	0	-0.500467	3.220312	-1.921363
61	1	0	-2.120931	2.548095	-2.096374
62	8	0	0.233578	0.725272	-3.847623
63	1	0	0.608793	-0.126516	-3.582201
64	1	0	-0.695650	0.648183	-3.589804
65	16	0	1.418353	-2.206184	-0.971534
66	6	0	3.165993	-1.995197	-0.793912
67	6	0	3.396384	-1.276599	0.376461
68	6	0	2.089481	-0.957173	1.034805
69	7	0	1.006712	-1.410584	0.435929
70	6	0	4.161691	-2.430879	-1.649109
71	6	0	5.474797	-2.131721	-1.286973
72	6	0	5.738832	-1.426164	-0.111781
73	6	0	4.714905	-0.993030	0.732096
74	8	0	0.946865	-1.529297	-2.185000
75	6	0	1.968488	-0.608619	2.491638
76	8	0	0.921083	-0.541600	3.101090
77	8	0	3.150319	-0.393636	3.051334
78	6	0	3.123323	0.018801	4.428155
79	1	0	4.163111	0.186334	4.701560
80	1	0	2.545220	0.939744	4.529200
81	1	0	4.946621	-0.442382	1.634207
82	1	0	6.766987	-1.204248	0.154897
83	1	0	6.294696	-2.453000	-1.920256
84	1	0	3.930962	-2.984650	-2.553526
85	8	0	1.017672	-3.608908	-0.839613
86	1	0	2.681941	-0.764959	5.045459
87	8	0	-1.595965	-2.503040	-3.101265
88	1	0	-0.643473	-2.652441	-3.191989
89	1	0	-1.648106	-1.558158	-2.872346
90	8	0	-1.751485	-2.922606	-0.408929
91	1	0	-1.744156	-2.845366	-1.388042
92	1	0	-1.001068	-3.502157	-0.213850
93	8	0	-1.433173	-1.449575	1.953062
94	1	0	-0.940047	-1.633730	1.137992
95	1	0	-0.729276	-1.160812	2.552665

3-IM2′

Zero-point correction = 0.83185 a.u.
Thermal correction to Gibbs Free Energy = 0.75357 a.u.
Sum of electronic and zero-point Energies = -2466.39030 a.u.
Sum of electronic and thermal Free Energies = -2466.46859 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.241259	-0.167262	-0.178624
2	6	0	-3.662349	0.280373	1.162743
3	6	0	-4.628775	-0.689666	1.853385
4	6	0	-5.789021	-1.015770	0.912653
5	6	0	-4.248815	-0.799004	-1.052742
6	6	0	-5.193214	-1.733779	-0.298970
7	1	0	-4.190430	1.237349	1.067552
8	1	0	-2.770633	0.413217	1.777653
9	1	0	-4.994650	-0.169748	2.744133
10	6	0	-3.986649	-1.984660	2.342422
11	1	0	-6.293644	-0.096306	0.597317
12	1	0	-4.834192	-0.011454	-1.545007
13	1	0	-3.714587	-1.349445	-1.828214
14	6	0	-4.523718	-3.036120	0.137927
15	1	0	-5.981991	-2.015328	-1.003150
16	7	0	-3.491531	-2.790779	1.190573
17	1	0	-4.728406	-2.592513	2.867259
18	1	0	-3.131236	-1.802256	2.990366
19	1	0	-5.263822	-3.713940	0.570249
20	1	0	-6.525093	-1.651638	1.415590
21	1	0	-2.649226	-2.347439	0.776810
22	1	0	-4.009548	-3.532320	-0.686038
23	1	0	-3.148230	-3.693474	1.532059
24	6	0	-2.158274	0.331031	-0.816308
25	8	0	-1.985593	0.170024	-2.030248
26	6	0	-1.148657	1.196626	-0.050079
27	6	0	-1.694614	2.634447	0.162663
28	7	0	0.052780	1.289263	-0.887175
29	1	0	-2.654561	2.533189	0.680700
30	6	0	-0.777075	3.454016	1.075403
31	1	0	-0.907003	0.718121	0.899338
32	6	0	1.294873	1.328339	-0.547104
33	6	0	1.785354	1.052327	0.844605
34	6	0	2.802472	2.119735	1.314076
35	6	0	3.750899	2.668884	0.240349
36	6	0	2.304231	1.716528	-1.578336
37	6	0	3.018137	2.980359	-1.059119
38	1	0	0.933184	1.083937	1.527870
39	1	0	2.211400	2.955634	1.705105
40	1	0	3.369359	1.719928	2.161092
41	1	0	4.549758	1.955760	0.022585
42	1	0	4.227892	3.571957	0.632682
43	1	0	3.715996	3.324380	-1.826552
44	1	0	2.280330	3.778865	-0.909848
45	1	0	3.038846	0.910925	-1.691260
46	1	0	1.822370	1.889963	-2.540700
47	1	0	-0.133693	1.362949	-1.903990
48	1	0	-0.631039	2.925917	2.026328
49	1	0	0.212138	3.558900	0.606981
50	6	0	-1.955851	3.366746	-1.160739
51	6	0	-2.535071	4.759884	-0.905273
52	6	0	-1.614764	5.579494	0.000367
53	6	0	-1.355943	4.850537	1.319734
54	1	0	-3.519144	4.660475	-0.427726
55	1	0	-2.693194	5.274100	-1.858429

56	1	0	-0.657509	5.742796	-0.514073
57	1	0	-2.048350	6.566538	0.190662
58	1	0	-0.674391	5.428739	1.951781
59	1	0	-2.300771	4.755321	1.871422
60	1	0	-1.012140	3.475928	-1.714796
61	1	0	-2.631688	2.780358	-1.793891
62	8	0	0.099744	0.997531	-3.740126
63	1	0	0.488454	0.151213	-3.460972
64	1	0	-0.841732	0.803519	-3.844522
65	16	0	1.579836	-1.949190	-1.039640
66	6	0	3.322597	-1.678018	-0.886794
67	6	0	3.538557	-0.842670	0.200427
68	6	0	2.222706	-0.484671	0.909264
69	7	0	1.158310	-1.290619	0.332087
70	6	0	4.328807	-2.135879	-1.725265
71	6	0	5.630235	-1.742115	-1.431313
72	6	0	5.881600	-0.915897	-0.332345
73	6	0	4.850816	-0.463365	0.489280
74	8	0	1.139464	-1.225799	-2.272145
75	6	0	2.268011	-0.777686	2.426571
76	8	0	1.287759	-1.030820	3.088693
77	8	0	3.480024	-0.647782	2.952258
78	6	0	3.565446	-0.821146	4.376803
79	1	0	4.604755	-0.624717	4.632934
80	1	0	2.902959	-0.115131	4.880577
81	1	0	5.076989	0.165002	1.342409
82	1	0	6.902320	-0.623519	-0.107606
83	1	0	6.452675	-2.080066	-2.053076
84	1	0	4.103551	-2.779381	-2.570094
85	8	0	1.220985	-3.379856	-1.110893
86	1	0	3.290781	-1.842429	4.645294
87	8	0	-1.282411	-2.198819	-3.342529
88	1	0	-0.331008	-2.107354	-3.159233
89	1	0	-1.636407	-1.347018	-3.037203
90	8	0	-1.576888	-2.992312	-0.708858
91	1	0	-1.570441	-2.838348	-1.674844
92	1	0	-0.684321	-3.329565	-0.534914
93	8	0	-1.170273	-1.388024	1.761299
94	1	0	-0.440128	-1.453377	1.098562
95	1	0	-0.660198	-1.351818	2.581709

3-IM3′

Zero-point correction = 0.77821 a.u.
Thermal correction to Gibbs Free Energy = 0.70286 a.u.
Sum of electronic and zero-point Energies = -2313.60646 a.u.
Sum of electronic and thermal Free Energies = -2313.68180 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	4.770945	-2.815171	-2.660044
2	16	0	-2.362836	0.340741	-1.431148
3	6	0	-3.449845	-0.866547	-0.717952
4	6	0	-2.858575	-1.370781	0.432605
5	6	0	-1.462284	-0.755017	0.654147
6	7	0	-1.321257	0.385319	-0.229976
7	6	0	-4.691409	-1.268308	-1.188349
8	6	0	-5.384061	-2.216858	-0.442182
9	6	0	-4.829397	-2.717049	0.738077
10	6	0	-3.575760	-2.303032	1.186806
11	8	0	-1.854484	-0.179643	-2.716103
12	1	0	-3.183737	-2.696855	2.115347
13	1	0	-5.386076	-3.441201	1.324483
14	1	0	-6.360590	-2.557795	-0.769950
15	1	0	-5.107711	-0.846879	-2.098225
16	8	0	-3.040359	1.650778	-1.573798
17	6	0	-1.249005	-0.269696	2.095175
18	8	0	-0.686724	0.761593	2.390061
19	8	0	-1.632727	-1.169685	2.995037
20	6	0	-1.314891	-0.863106	4.362693
21	1	0	-0.237580	-0.724636	4.473880
22	1	0	-1.837113	0.042229	4.676440
23	1	0	-1.653693	-1.719805	4.941942
24	7	0	1.126597	2.830043	-0.531460
25	6	0	1.279409	3.143754	0.899913
26	6	0	0.291174	4.220982	1.386068
27	6	0	0.302040	5.428506	0.446665
28	6	0	0.994947	3.972290	-1.442023
29	6	0	-0.090534	4.919851	-0.942125
30	1	0	2.298950	3.514016	1.071826
31	1	0	1.138432	2.235620	1.489885
32	1	0	0.614602	4.511433	2.390129
33	6	0	-1.144247	3.716747	1.510025
34	1	0	1.298359	5.880941	0.406247
35	1	0	1.951407	4.508350	-1.509663
36	1	0	0.752883	3.577734	-2.428516
37	6	0	-1.475185	4.266081	-0.915851
38	1	0	-0.156251	5.750995	-1.651032
39	7	0	-1.631056	3.249952	0.179511
40	1	0	-1.802096	4.528157	1.832414
41	1	0	-1.232118	2.874825	2.194581
42	1	0	-2.238291	5.025835	-0.729464
43	1	0	-0.400415	6.188313	0.805045
44	1	0	-1.708226	3.747739	-1.847735
45	1	0	-2.623336	2.994122	0.221564
46	6	0	1.449061	1.637368	-1.095592
47	8	0	1.611448	1.495459	-2.305424
48	6	0	1.609515	0.418521	-0.184330
49	6	0	3.050582	0.296201	0.357633
50	7	0	1.243892	-0.713863	-1.043010
51	1	0	3.340799	1.301896	0.697151
52	6	0	3.086040	-0.641549	1.569990
53	1	0	0.896534	0.477962	0.633656
54	6	0	0.425982	-1.683750	-0.818586
55	6	0	-0.241027	-1.829647	0.519228
56	6	0	-0.569014	-3.301761	0.822136
57	6	0	-1.165117	-4.072710	-0.355425
58	6	0	0.077631	-2.592394	-1.953014
59	6	0	-0.208404	-4.037822	-1.542342
60	1	0	0.503320	-1.514865	1.257345
61	1	0	0.376128	-3.782277	1.097516
62	1	0	-1.208847	-3.348566	1.705384
63	1	0	-2.131501	-3.650510	-0.652792
64	1	0	-1.349034	-5.106994	-0.048082
65	1	0	-0.637807	-4.559751	-2.401774
66	1	0	0.732940	-4.527172	-1.280298
67	1	0	-0.834879	-2.142765	-2.375186
68	1	0	0.852140	-2.527022	-2.722965
69	1	0	1.598295	-0.604754	-1.995955
70	1	0	2.396167	-0.266629	2.338141
71	1	0	2.737416	-1.632507	1.251561
72	6	0	4.044927	-0.144850	-0.722798
73	6	0	5.455978	-0.303024	-0.152977
74	6	0	5.459843	-1.263397	1.038534
75	6	0	4.503595	-0.776334	2.128196
76	1	0	5.834895	0.675608	0.170761
77	1	0	6.132838	-0.657421	-0.939469
78	1	0	5.123847	-2.254758	0.701929
79	1	0	6.473345	-1.377395	1.436382
80	1	0	4.506133	-1.467489	2.977409
81	1	0	4.847718	0.196653	2.504574
82	1	0	3.728499	-1.118807	-1.117181
83	1	0	4.037228	0.565644	-1.557344
84	8	0	4.848332	-3.299319	-1.826620
85	1	0	3.349336	-3.362693	-0.781262
86	1	0	5.639952	-2.939530	-1.403543
87	8	0	2.577702	-3.411834	-0.184899
88	1	0	2.699917	-4.236289	0.302988
89	1	0	-1.182898	2.335666	-0.047301

3-TS2′

Zero-point correction = 0.77895 a.u.
Thermal correction to Gibbs Free Energy = 0.71056 a.u.
Sum of electronic and zero-point Energies = -2313.57291 a.u.
Sum of electronic and thermal Free Energies = -2313.64130 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.767509	-2.868865	-1.788662
2	16	0	-1.895542	1.082631	-1.523767
3	6	0	-3.429119	0.643103	-0.746089
4	6	0	-3.152064	-0.018562	0.441244
5	6	0	-1.624686	-0.221712	0.631818
6	7	0	-0.942696	0.592754	-0.356321
7	6	0	-4.711138	0.942582	-1.184724
8	6	0	-5.774083	0.573254	-0.366594
9	6	0	-5.524083	-0.051254	0.857592
10	6	0	-4.226784	-0.344269	1.274580
11	8	0	-1.774275	0.364638	-2.809114
12	1	0	-4.073600	-0.804344	2.242277
13	1	0	-6.356247	-0.308427	1.505346
14	1	0	-6.794056	0.789381	-0.667384
15	1	0	-4.871554	1.458722	-2.126546
16	8	0	-1.820985	2.554196	-1.694413
17	6	0	-1.230084	0.284896	2.029437
18	8	0	-0.360358	1.095531	2.251667
19	8	0	-1.894839	-0.342998	2.999113
20	6	0	-1.523136	0.004611	4.341449
21	1	0	-0.466826	-0.214820	4.508909
22	1	0	-1.712202	1.064141	4.522510
23	1	0	-2.147745	-0.609232	4.987553
24	7	0	2.218823	1.816988	-0.458459
25	6	0	2.483663	2.068850	0.966082
26	6	0	2.110612	3.505200	1.399618
27	6	0	2.701258	4.536010	0.434527
28	6	0	2.657755	2.863561	-1.387852
29	6	0	2.129556	4.223189	-0.950282
30	1	0	3.556101	1.932417	1.162117
31	1	0	1.924931	1.350780	1.569227
32	1	0	2.518117	3.641497	2.405721
33	6	0	0.607124	3.758601	1.487248
34	1	0	3.793818	4.465862	0.404879
35	1	0	3.756304	2.888659	-1.412748
36	1	0	2.293664	2.598311	-2.378156
37	6	0	0.597615	4.272211	-0.952472
38	1	0	2.462910	4.965881	-1.682023
39	7	0	-0.023016	3.475955	0.164608
40	1	0	0.418870	4.812099	1.711348
41	1	0	0.115140	3.134543	2.226499
42	1	0	0.256004	5.300024	-0.805709
43	1	0	2.436232	5.547701	0.759440
44	1	0	0.173488	3.881007	-1.878089
45	1	0	-1.022824	3.700743	0.179898
46	6	0	1.812704	0.640661	-1.016288
47	8	0	1.684807	0.527456	-2.233792
48	6	0	1.609274	-0.607222	-0.140635
49	6	0	2.997125	-1.107190	0.322735
50	7	0	0.855190	-1.553934	-0.992950
51	1	0	3.387521	-0.307900	0.968323
52	6	0	2.922274	-2.361709	1.197078
53	1	0	1.031734	-0.340029	0.746195
54	6	0	-0.315211	-2.267342	-0.521797
55	6	0	-1.119763	-1.752400	0.697347
56	6	0	-2.237565	-2.771382	1.021436
57	6	0	-3.118315	-3.149507	-0.175034
58	6	0	-1.201968	-2.622064	-1.714854
59	6	0	-2.287364	-3.639320	-1.358964
60	1	0	-0.409087	-1.802783	1.530750
61	1	0	-1.779338	-3.681745	1.432017
62	1	0	-2.841878	-2.385174	1.842731
63	1	0	-3.705924	-2.285455	-0.499823
64	1	0	-3.830995	-3.919628	0.136654
65	1	0	-2.925391	-3.792358	-2.233519
66	1	0	-1.844577	-4.621813	-1.140829
67	1	0	-1.658038	-1.691633	-2.068832
68	1	0	-0.566266	-2.995299	-2.526102
69	1	0	0.582734	-1.019281	-1.822773
70	1	0	2.179058	-2.222064	1.992366
71	1	0	2.582244	-3.210872	0.594135
72	6	0	4.024495	-1.290128	-0.801949
73	6	0	5.397798	-1.649789	-0.226876
74	6	0	5.327051	-2.886149	0.671531
75	6	0	4.293846	-2.701202	1.784342
76	1	0	5.767885	-0.799482	0.362024
77	1	0	6.114077	-1.808101	-1.039698
78	1	0	5.044924	-3.758143	0.063707
79	1	0	6.312463	-3.103205	1.096671
80	1	0	4.227112	-3.605758	2.397862
81	1	0	4.616548	-1.887006	2.447084
82	1	0	3.706460	-2.090468	-1.483846
83	1	0	4.097818	-0.380573	-1.408215
84	8	0	1.760342	-3.881425	-1.828717
85	1	0	1.037278	-3.940779	-0.867497
86	1	0	2.660248	-4.230701	-1.709594
87	8	0	0.280599	-3.564634	-0.014151
88	1	0	-0.405616	-4.217914	0.207278
89	1	0	-0.021536	2.452365	-0.028034

3-IM4′

Zero-point correction = 0.78284 a.u.
Thermal correction to Gibbs Free Energy = 0.71228 a.u.
Sum of electronic and zero-point Energies = -2313.60477 a.u.
Sum of electronic and thermal Free Energies = -2313.67532 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.406178	-2.224326	-1.255394
2	16	0	-1.642340	0.865209	-1.669190
3	6	0	-3.272922	0.455474	-1.108268
4	6	0	-3.184805	-0.048271	0.182314
5	6	0	-1.713219	-0.145446	0.650668
6	7	0	-0.895972	0.610976	-0.289244
7	6	0	-4.464850	0.639381	-1.795145
8	6	0	-5.643076	0.315037	-1.131760
9	6	0	-5.592175	-0.162797	0.180037
10	6	0	-4.380850	-0.346650	0.844184
11	8	0	-1.256114	-0.057574	-2.760120
12	1	0	-4.388941	-0.706138	1.864863
13	1	0	-6.516267	-0.393147	0.700844
14	1	0	-6.600345	0.447053	-1.625263
15	1	0	-4.471136	1.035236	-2.806176
16	8	0	-1.567415	2.290244	-2.058753
17	6	0	-1.497134	0.483484	2.038180
18	8	0	-0.464770	1.027296	2.365957
19	8	0	-2.494662	0.259898	2.885562
20	6	0	-2.274941	0.688396	4.239488
21	1	0	-1.406086	0.176112	4.656985
22	1	0	-2.116860	1.767704	4.271950
23	1	0	-3.178081	0.418257	4.783115
24	7	0	2.188354	1.848104	-0.360808
25	6	0	2.387563	2.142186	1.064009
26	6	0	1.939398	3.571095	1.434089
27	6	0	2.553079	4.594878	0.475787
28	6	0	2.630017	2.877837	-1.309343
29	6	0	2.063812	4.241113	-0.930555
30	1	0	3.455092	2.050714	1.305392
31	1	0	1.828416	1.419595	1.660752
32	1	0	2.279389	3.751441	2.458319
33	6	0	0.424632	3.764912	1.432925
34	1	0	3.646811	4.550294	0.507573

35	1	0	3.727564	2.924128	-1.299041
36	1	0	2.302666	2.573045	-2.301614
37	6	0	0.535855	4.279771	-1.013504
38	1	0	2.430260	4.969466	-1.660593
39	7	0	-0.131565	3.482315	0.074133
40	1	0	0.182623	4.805571	1.665466
41	1	0	-0.080601	3.104549	2.133404
42	1	0	0.181970	5.306068	-0.887729
43	1	0	2.247878	5.607186	0.761068
44	1	0	0.163106	3.880635	-1.957542
45	1	0	-1.129783	3.712254	0.053455
46	6	0	1.805878	0.657280	-0.885484
47	8	0	1.674123	0.487150	-2.095460
48	6	0	1.649979	-0.568827	0.028398
49	6	0	3.065798	-1.079586	0.376947
50	7	0	0.800978	-1.520095	-0.785431
51	1	0	3.481266	-0.270301	0.996239
52	6	0	3.098795	-2.347035	1.237332
53	1	0	1.098110	-0.327469	0.936300
54	6	0	-0.310838	-2.334471	-0.161297
55	6	0	-1.158158	-1.625239	0.926840
56	6	0	-2.234832	-2.631800	1.401900
57	6	0	-3.046935	-3.294964	0.281471
58	6	0	-1.152936	-2.897556	-1.308105
59	6	0	-2.148407	-3.929012	-0.778386
60	1	0	-0.454782	-1.518018	1.761636
61	1	0	-1.739123	-3.414302	1.990966
62	1	0	-2.892500	-2.128239	2.113776
63	1	0	-3.685790	-2.557760	-0.212602
64	1	0	-3.709809	-4.045713	0.722985
65	1	0	-2.750181	-4.303841	-1.610432
66	1	0	-1.617459	-4.799504	-0.370772
67	1	0	-1.688544	-2.075300	-1.791868
68	1	0	-0.479738	-3.342318	-2.048927
69	1	0	0.392190	-0.952728	-1.551493
70	1	0	2.413428	-2.247546	2.086421
71	1	0	2.745510	-3.195279	0.642514
72	6	0	3.999033	-1.235474	-0.835091
73	6	0	5.424850	-1.557390	-0.378756
74	6	0	5.470752	-2.792405	0.520562
75	6	0	4.524464	-2.635769	1.712199
76	1	0	5.821276	-0.694869	0.174605
77	1	0	6.069155	-1.695999	-1.253086
78	1	0	5.168914	-3.674302	-0.062044
79	1	0	6.494373	-2.974035	0.864783
80	1	0	4.533742	-3.539912	2.329635
81	1	0	4.872015	-1.809808	2.347777
82	1	0	3.629848	-2.044469	-1.480132
83	1	0	4.006501	-0.325798	-1.442940
84	8	0	1.916847	-3.926454	-1.817411
85	1	0	1.629018	-4.361664	-1.001377
86	1	0	2.796859	-4.274081	-2.014576
87	8	0	0.414941	-3.370275	0.475954
88	1	0	-0.202905	-4.000433	0.872677
89	1	0	-0.120921	2.454364	-0.109082

3-TS3′

Zero-point correction = 0.77891 a.u.
Thermal correction to Gibbs Free Energy = 0.71067 a.u.
Sum of electronic and zero-point Energies = -2313.61244 a.u.
Sum of electronic and thermal Free Energies = -2313.68068 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.973638	-1.979631	-0.965819
2	16	0	-1.606848	0.231424	-1.829981
3	6	0	-3.098131	-0.558648	-1.305994
4	6	0	-2.990329	-0.874128	0.035586
5	6	0	-1.641515	-0.449350	0.651496
6	7	0	-0.993237	0.453986	-0.323867
7	6	0	-4.231924	-0.801208	-2.070840
8	6	0	-5.324456	-1.365756	-1.422679
9	6	0	-5.262043	-1.647485	-0.053755
10	6	0	-4.108082	-1.400520	0.684278
11	8	0	-0.830206	-0.736948	-2.621679
12	1	0	-4.097164	-1.603283	1.751369
13	1	0	-6.133820	-2.055790	0.447170
14	1	0	-6.236958	-1.565843	-1.974105
15	1	0	-4.266720	-0.537553	-3.123233
16	8	0	-1.855974	1.527877	-2.462504
17	6	0	-2.003960	0.388671	1.908976
18	8	0	-1.539169	0.222382	3.011347
19	8	0	-2.913278	1.322372	1.630316
20	6	0	-3.410649	2.063325	2.758553
21	1	0	-3.909976	1.383445	3.451807
22	1	0	-2.596454	2.575347	3.274389
23	1	0	-4.120611	2.779794	2.349979
24	7	0	1.686685	2.289208	-0.440584
25	6	0	1.945508	2.677085	0.946706
26	6	0	1.002477	3.794185	1.405308
27	6	0	1.098722	4.981124	0.446903
28	6	0	1.598564	3.388114	-1.408748
29	6	0	0.647163	4.482116	-0.925720
30	1	0	2.981673	3.033319	1.029735
31	1	0	1.835298	1.815075	1.606178
32	1	0	1.321365	4.086404	2.411089
33	6	0	-0.452934	3.338443	1.517394
34	1	0	2.128713	5.351527	0.400001
35	1	0	2.600124	3.815459	-1.553040
36	1	0	1.262735	2.964534	-2.354604
37	6	0	-0.809749	4.027331	-0.853591
38	1	0	0.689396	5.293121	-1.660243
39	7	0	-1.058911	3.002646	0.200706
40	1	0	-1.036190	4.138659	1.988741
41	1	0	-0.514569	2.450155	2.155756
42	1	0	-1.431606	4.902762	-0.630706
43	1	0	0.460306	5.802250	0.791020
44	1	0	-1.140452	3.595960	-1.800033
45	1	0	-2.071281	2.982882	0.337598
46	6	0	1.681378	1.028818	-0.922612
47	8	0	1.565367	0.768851	-2.118177
48	6	0	1.899059	-0.139959	0.046806
49	6	0	3.418657	-0.288377	0.288704
50	7	0	1.245503	-1.332632	-0.605115
51	1	0	3.718886	0.686660	0.700721
52	6	0	3.778078	-1.339489	1.344437
53	1	0	1.389556	0.024836	0.995898
54	6	0	0.340910	-2.260623	0.216381
55	6	0	-0.685303	-1.585522	1.160844
56	6	0	-1.421417	-2.739029	1.896084
57	6	0	-1.984199	-3.846123	0.994011
58	6	0	-0.297286	-3.246784	-0.764148
59	6	0	-0.947996	-4.391417	0.013172
60	1	0	-0.086771	-1.080056	1.926772
61	1	0	-0.706909	-3.189979	2.590690
62	1	0	-2.209520	-2.313245	2.522531
63	1	0	-2.837704	-3.478655	0.419021
64	1	0	-2.360759	-4.651324	1.633336
65	1	0	-1.424487	-5.077101	-0.693101
66	1	0	-0.173663	-4.953341	0.543703
67	1	0	-1.041181	-2.717725	-1.366159
68	1	0	0.473596	-3.622640	-1.444177
69	1	0	0.732990	-0.994769	-1.444369
70	1	0	3.193967	-1.165068	2.258707
71	1	0	3.521666	-2.334697	0.964888
72	6	0	4.236886	-0.499467	-0.995188
73	6	0	5.736997	-0.507214	-0.686022
74	6	0	6.089132	-1.544727	0.380119
75	6	0	5.276286	-1.311961	1.653530
76	1	0	6.033300	0.488550	-0.329359
77	1	0	6.299237	-0.696207	-1.606018

78	1	0	5.868645	-2.550012	-0.006479
79	1	0	7.161205	-1.515963	0.599897
80	1	0	5.512816	-2.070096	2.406959
81	1	0	5.542486	-0.336755	2.082566
82	1	0	3.964585	-1.458833	-1.454359
83	1	0	4.009765	0.279765	-1.728108
84	8	0	2.838250	-3.669226	-1.175527
85	1	0	2.650564	-4.023134	-0.293702
86	1	0	3.763746	-3.879598	-1.359309
87	8	0	1.216741	-3.011712	1.016824
88	1	0	1.445960	-2.519820	1.821720
89	1	0	-0.923052	1.708041	-0.098353

3-IM5′

Zero-point correction = 0.78141 a.u.
Thermal correction to Gibbs Free Energy = 0.71079 a.u.
Sum of electronic and zero-point Energies = -2313.61303 a.u.
Sum of electronic and thermal Free Energies = -2313.68366 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.889228	-2.074640	-0.933608
2	16	0	-1.675996	0.265362	-1.861152
3	6	0	-3.175224	-0.456874	-1.274666
4	6	0	-3.050486	-0.777143	0.065757
5	6	0	-1.676197	-0.424032	0.667112
6	7	0	-0.983206	0.398005	-0.345657
7	6	0	-4.338222	-0.643986	-2.011532
8	6	0	-5.440732	-1.154185	-1.337005
9	6	0	-5.360274	-1.435226	0.030726
10	6	0	-4.178626	-1.244962	0.740725
11	8	0	-0.961489	-0.721119	-2.672889
12	1	0	-4.153310	-1.443221	1.808265
13	1	0	-6.239264	-1.796649	0.554417
14	1	0	-6.374239	-1.309557	-1.866897
15	1	0	-4.385932	-0.379995	-3.063271
16	8	0	-1.867777	1.598039	-2.420184
17	6	0	-1.985836	0.471178	1.899159
18	8	0	-1.586593	0.262933	3.018462
19	8	0	-2.783409	1.481920	1.568270
20	6	0	-3.258869	2.292118	2.658462
21	1	0	-3.937345	1.703010	3.279145
22	1	0	-2.426559	2.652005	3.264768
23	1	0	-3.789722	3.122836	2.197202
24	7	0	1.821240	2.205068	-0.432295
25	6	0	2.078525	2.576633	0.961737
26	6	0	1.249577	3.789062	1.404411
27	6	0	1.472625	4.947879	0.431773
28	6	0	1.800165	3.300380	-1.410746
29	6	0	0.961727	4.485419	-0.933300
30	1	0	3.143910	2.821575	1.072692
31	1	0	1.861086	1.731023	1.616454
32	1	0	1.601667	4.057815	2.406064
33	6	0	-0.249871	3.497533	1.506107
34	1	0	2.536478	5.206646	0.378649
35	1	0	2.833240	3.634176	-1.579531
36	1	0	1.413095	2.894212	-2.344660
37	6	0	-0.533359	4.173018	-0.841011
38	1	0	1.085659	5.279817	-1.676920
39	7	0	-0.834390	3.166671	0.195637
40	1	0	-0.736953	4.381204	1.948510
41	1	0	-0.418894	2.652458	2.185521
42	1	0	-1.059841	5.115461	-0.622959
43	1	0	0.925889	5.835697	0.768332
44	1	0	-0.907621	3.785384	-1.792500
45	1	0	-1.847518	3.145355	0.301448
46	6	0	1.690697	0.950902	-0.899783
47	8	0	1.496360	0.688119	-2.087642
48	6	0	1.875385	-0.227259	0.069725
49	6	0	3.390768	-0.427196	0.294770
50	7	0	1.183816	-1.398302	-0.579582
51	1	0	3.728693	0.530786	0.715311
52	6	0	3.722280	-1.504442	1.332467
53	1	0	1.381927	-0.047932	1.024993
54	6	0	0.238738	-2.295848	0.233157
55	6	0	-0.768108	-1.593306	1.181093
56	6	0	-1.549400	-2.724171	1.901659
57	6	0	-2.153213	-3.796098	0.983301
58	6	0	-0.434932	-3.244173	-0.759576
59	6	0	-1.133735	-4.370963	0.001698
60	1	0	-0.155521	-1.113004	1.952239
61	1	0	-0.853049	-3.210976	2.589929
62	1	0	-2.319540	-2.271641	2.531089
63	1	0	-2.987445	-3.386190	0.408557
64	1	0	-2.566411	-4.592437	1.610646
65	1	0	-1.632918	-5.029410	-0.714738
66	1	0	-0.384901	-4.968497	0.530173
67	1	0	-1.158292	-2.680375	-1.356328
68	1	0	0.321537	-3.641892	-1.443183
69	1	0	0.704099	-1.031911	-1.424079
70	1	0	3.161300	-1.314351	2.258013
71	1	0	3.417330	-2.483958	0.947693
72	6	0	4.182680	-0.647069	-1.004582
73	6	0	5.684975	-0.727103	-0.717315
74	6	0	6.004496	-1.797586	0.326419
75	6	0	5.224929	-1.545453	1.616938
76	1	0	6.029982	0.247846	-0.347469
77	1	0	6.225922	-0.924027	-1.648303
78	1	0	5.726570	-2.784451	-0.070435
79	1	0	7.080223	-1.824296	0.527310
80	1	0	5.440031	-2.322871	2.356936
81	1	0	5.541217	-0.588471	2.052702
82	1	0	3.862020	-1.582149	-1.481780
83	1	0	3.981108	0.157808	-1.717638
84	8	0	2.694346	-3.768314	-1.183757
85	1	0	2.510940	-4.154842	-0.314888
86	1	0	3.612264	-3.991590	-1.389461
87	8	0	1.082146	-3.086855	1.028216
88	1	0	1.336608	-2.607354	1.833221
89	1	0	-0.844592	1.435620	-0.129805

4-IM1′

Zero-point correction = 0.82873 a.u.
Thermal correction to Gibbs Free Energy = 0.74811 a.u.
Sum of electronic and zero-point Energies = -2466.37636 a.u.
Sum of electronic and thermal Free Energies = -2466.45697 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.169362	3.122468	2.896684
2	6	0	2.654538	2.797417	2.774075
3	1	0	0.880716	3.219284	3.948172
4	1	0	3.256699	3.554605	3.286032
5	1	0	2.856029	1.843164	3.272929
6	1	0	0.965210	4.088675	2.416598
7	6	0	0.309732	2.050014	2.227635
8	1	0	-0.728965	2.388218	2.206688
9	1	0	0.311626	1.115467	2.806294
10	7	0	-3.204985	-0.541576	-0.364196
11	6	0	-3.857836	-0.269997	0.927227
12	6	0	-4.514443	-1.521141	1.528209
13	6	0	-5.451709	-2.165339	0.506007
14	6	0	-3.941580	-1.380581	-1.328864
15	6	0	-4.589058	-2.603958	-0.678110
16	1	0	-4.631870	0.495334	0.787714
17	1	0	-3.111258	0.100350	1.627694
18	1	0	-5.076934	-1.185640	2.404714
19	6	0	-3.506287	-2.556290	2.028332

20	1	0	-6.207127	-1.444320	0.176108
21	1	0	-4.727433	-0.767051	-1.790189
22	1	0	-3.240620	-1.680653	-2.106481
23	6	0	-3.570738	-3.647128	-0.221015
24	1	0	-5.204396	-3.082996	-1.445682
25	7	0	-2.719487	-3.114189	0.885429
26	1	0	-4.024775	-3.392306	2.504141
27	1	0	-2.785093	-2.123349	2.721973
28	1	0	-4.081881	-4.529601	0.172067
29	1	0	-5.970307	-3.022939	0.947391
30	1	0	-2.895797	-3.940479	-1.024699
31	1	0	-2.074720	-3.844006	1.217398
32	6	0	-2.149915	0.160979	-0.836597
33	8	0	-1.671173	-0.081368	-1.957678
34	6	0	-1.527446	1.321533	-0.052428
35	6	0	-1.935139	2.629461	-0.775895
36	7	0	-0.082188	1.055539	-0.027960
37	1	0	-1.494423	2.584009	-1.781274
38	6	0	-3.461258	2.738882	-0.918321
39	1	0	-1.891595	1.354119	0.972867
40	6	0	0.793947	1.741866	0.831514
41	6	0	2.057382	2.012316	0.443266
42	6	0	3.080664	2.700471	1.307531
43	1	0	4.042341	2.175121	1.237404
44	1	0	3.262557	3.707493	0.905670
45	1	0	2.334834	1.796009	-0.589645
46	1	0	-3.865001	1.868211	-1.450648
47	1	0	-3.912497	2.740619	0.085729
48	6	0	-1.387953	3.879634	-0.077446
49	6	0	-1.777080	5.150702	-0.836740
50	6	0	-3.294266	5.261899	-0.986262
51	6	0	-3.864648	4.014914	-1.661786
52	1	0	-1.314146	5.127079	-1.832650
53	1	0	-1.376935	6.029361	-0.319751
54	1	0	-3.746497	5.372562	0.009035
55	1	0	-3.558460	6.157680	-1.558131
56	1	0	-4.956024	4.078496	-1.727380
57	1	0	-3.485285	3.957422	-2.690809
58	1	0	-1.799776	3.932004	0.941522
59	1	0	-0.298344	3.819630	0.012758
60	1	0	0.280759	1.014210	-0.980929
61	1	0	-2.082470	-2.366363	0.555713
62	16	0	2.132564	-1.755592	-1.689472
63	6	0	3.746137	-1.013666	-1.681160
64	6	0	4.009942	-0.592052	-0.380627
65	6	0	2.849607	-0.913070	0.491728
66	7	0	1.832173	-1.502168	-0.028292
67	6	0	4.623253	-0.844020	-2.733227
68	6	0	5.836069	-0.213117	-2.439183
69	6	0	6.126731	0.210250	-1.142794
70	6	0	5.222615	0.027006	-0.093440
71	8	0	1.196498	-0.950247	-2.468252
72	6	0	2.881849	-0.662617	1.978726
73	8	0	3.869686	-0.266729	2.550061
74	8	0	1.736419	-0.987372	2.552140
75	6	0	1.695692	-0.894153	3.984859
76	1	0	0.676696	-1.161450	4.259040
77	1	0	2.410595	-1.594666	4.421056
78	1	0	5.459232	0.347799	0.913074
79	1	0	7.077058	0.693278	-0.941844
80	1	0	6.560556	-0.056769	-3.231045
81	1	0	4.388322	-1.181170	-3.737302
82	1	0	1.926573	0.121269	4.311631
83	8	0	2.180686	-3.190516	-1.924911
84	8	0	-0.798469	-2.683125	-1.249662
85	1	0	-0.780421	-1.774597	-1.603496
86	1	0	-0.555645	-3.242698	-2.001163
87	8	0	0.038761	-3.765242	1.158723
88	1	0	0.092920	-3.362310	0.271671
89	1	0	0.919469	-4.114080	1.344699
90	8	0	0.309916	1.625964	-3.073165
91	1	0	1.066451	1.054433	-3.254060
92	1	0	-0.402026	0.988909	-2.890416
93	8	0	-0.880060	-1.178340	1.517000
94	1	0	-0.338933	-0.573325	0.971553
95	1	0	-0.275695	-1.918118	1.699505

4-TS1′

Zero-point correction = 0.82794 a.u.
Thermal correction to Gibbs Free Energy = 0.74939 a.u.
Sum of electronic and zero-point Energies = -2466.37086 a.u.
Sum of electronic and thermal Free Energies = -2466.44940 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.208321	3.094784	2.774104
2	6	0	2.690195	2.752416	2.689853
3	1	0	0.903236	3.240961	3.814629
4	1	0	3.293293	3.542385	3.147706
5	1	0	2.882226	1.838531	3.261593
6	1	0	1.012132	4.036511	2.245389
7	6	0	0.353293	1.989182	2.152427
8	1	0	-0.692438	2.295471	2.156686
9	1	0	0.408246	1.066833	2.745870
10	7	0	-3.153906	-0.606249	-0.355345
11	6	0	-3.782561	-0.361020	0.954541
12	6	0	-4.402815	-1.629860	1.556597
13	6	0	-5.352888	-2.279859	0.550020
14	6	0	-3.901674	-1.447163	-1.311539
15	6	0	-4.510103	-2.689991	-0.658283
16	1	0	-4.576292	0.387888	0.839524
17	1	0	-3.028435	0.017854	1.642169
18	1	0	-4.949562	-1.313765	2.450089
19	6	0	-3.364349	-2.652524	2.018848
20	1	0	-6.129510	-1.569759	0.246632
21	1	0	-4.710304	-0.842202	-1.743949
22	1	0	-3.217550	-1.727099	-2.111006
23	6	0	-3.461775	-3.718868	-0.235931
24	1	0	-5.134155	-3.171963	-1.416980
25	7	0	-2.592317	-3.176350	0.852319
26	1	0	-3.856213	-3.506639	2.490985
27	1	0	-2.644626	-2.217057	2.712344
28	1	0	-3.946610	-4.613000	0.164079
29	1	0	-5.844784	-3.151732	0.994020
30	1	0	-2.802024	-3.991055	-1.058865
31	1	0	-1.915453	-3.888768	1.157153
32	6	0	-2.136598	0.133311	-0.854818
33	8	0	-1.705463	-0.055447	-2.002606
34	6	0	-1.525192	1.294998	-0.063940
35	6	0	-2.028388	2.605575	-0.726077
36	7	0	-0.068241	1.184527	-0.154205
37	1	0	-1.690988	2.573926	-1.771177
38	6	0	-3.560999	2.689496	-0.714840
39	1	0	-1.814515	1.268866	0.982228
40	6	0	0.812339	1.656986	0.753509
41	6	0	2.157927	1.752288	0.409150
42	6	0	3.131647	2.556134	1.238143
43	1	0	4.123919	2.091924	1.212769
44	1	0	3.250366	3.538091	0.759085
45	1	0	2.380412	1.680177	-0.655024
46	1	0	-4.001775	1.810182	-1.201279
47	1	0	-3.907742	2.689660	0.329029
48	6	0	-1.429974	3.858902	-0.079228
49	6	0	-1.905172	5.122511	-0.800416
50	6	0	-3.431140	5.214842	-0.802620
51	6	0	-4.050372	3.959075	-1.417047
52	1	0	-1.541300	5.098199	-1.836220
53	1	0	-1.466772	6.007452	-0.327558
54	1	0	-3.787226	5.325260	0.230803
55	1	0	-3.758646	6.104969	-1.349927
56	1	0	-5.143405	4.009058	-1.373574

57	1	0	-3.774563	3.903917	-2.478555
58	1	0	-1.742432	3.908029	0.974174
59	1	0	-0.335025	3.813080	-0.096449
60	1	0	0.267187	1.144013	-1.120065
61	1	0	-1.983941	-2.418705	0.497395
62	16	0	2.002908	-1.590805	-1.651485
63	6	0	3.654447	-0.955022	-1.686127
64	6	0	3.932452	-0.426733	-0.429407
65	6	0	2.726847	-0.549573	0.449004
66	7	0	1.695868	-1.202153	-0.062301
67	6	0	4.559081	-0.979877	-2.731193
68	6	0	5.822972	-0.444345	-2.479187
69	6	0	6.137153	0.067557	-1.219549
70	6	0	5.206687	0.079861	-0.178648
71	8	0	1.136145	-0.846165	-2.571085
72	6	0	2.899560	-0.507782	1.936935
73	8	0	3.939585	-0.205726	2.477835
74	8	0	1.798255	-0.884690	2.578373
75	6	0	1.891495	-0.927125	4.008939
76	1	0	0.911975	-1.253886	4.355117
77	1	0	2.662295	-1.637353	4.314200
78	1	0	5.476386	0.451306	0.801272
79	1	0	7.132432	0.460633	-1.039759
80	1	0	6.570974	-0.440990	-3.265087
81	1	0	4.303407	-1.405784	-3.696263
82	1	0	2.124712	0.061834	4.409460
83	8	0	1.984185	-3.048960	-1.793374
84	8	0	-0.832509	-2.620421	-1.273200
85	1	0	-0.842631	-1.788763	-1.779965
86	1	0	-0.254531	-3.212471	-1.775955
87	8	0	0.162429	-3.682834	1.233814
88	1	0	0.338226	-3.160978	0.432690
89	1	0	0.987313	-4.147269	1.424655
90	8	0	0.227438	1.714555	-3.089797
91	1	0	0.989182	1.169798	-3.327871
92	1	0	-0.474524	1.051853	-2.969570
93	8	0	-0.812750	-1.112123	1.515205
94	1	0	-0.134334	-0.859792	0.862737
95	1	0	-0.352980	-1.829743	1.980459

4-IM2′

Zero-point correction = 0.83078 a.u.
Thermal correction to Gibbs Free Energy = 0.75394 a.u.
Sum of electronic and zero-point Energies = -2466.40034 a.u.
Sum of electronic and thermal Free Energies = -2466.47719 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.708562	3.247932	2.565851
2	6	0	2.213782	3.302237	2.330094
3	1	0	0.474698	3.368076	3.626950
4	1	0	2.600029	4.285792	2.614572
5	1	0	2.705883	2.565687	2.969072
6	1	0	0.205990	4.060833	2.028036
7	6	0	0.136811	1.901475	2.090639
8	1	0	-0.929658	1.828863	2.297014
9	1	0	0.625009	1.077396	2.628808
10	7	0	-3.072405	-0.936123	-0.320362
11	6	0	-3.619183	-0.822202	1.042178
12	6	0	-3.972786	-2.184431	1.652034
13	6	0	-4.876330	-2.965857	0.698238
14	6	0	-3.700878	-1.905316	-1.241759
15	6	0	-4.062269	-3.231873	-0.568842
16	1	0	-4.527985	-0.207906	1.021404
17	1	0	-2.872239	-0.347202	1.676634
18	1	0	-4.495847	-1.974986	2.590249
19	6	0	-2.747370	-3.025298	2.012852
20	1	0	-5.770219	-2.379796	0.459098
21	1	0	-4.618665	-1.452905	-1.641194
22	1	0	-3.009929	-2.067750	-2.067664
23	6	0	-2.843345	-4.089819	-0.232432
24	1	0	-4.654225	-3.798822	-1.293732
25	7	0	-1.990018	-3.407821	0.785962
26	1	0	-3.057642	-3.951980	2.503182
27	1	0	-2.060111	-2.485532	2.665445
28	1	0	-3.159629	-5.041812	0.202267
29	1	0	-5.198976	-3.906727	1.155868
30	1	0	-2.216233	-4.267180	-1.104632
31	1	0	-1.172039	-3.984050	1.031754
32	6	0	-2.243610	-0.022327	-0.871203
33	8	0	-1.824536	-0.121009	-2.030818
34	6	0	-1.869146	1.253909	-0.100589
35	6	0	-2.614339	2.451588	-0.731945
36	7	0	-0.426493	1.444939	-0.261686
37	1	0	-2.280912	2.529051	-1.777189
38	6	0	-4.131187	2.219963	-0.722263
39	1	0	-2.107535	1.197191	0.955376
40	6	0	0.449741	1.705482	0.643621
41	6	0	1.893557	1.822407	0.200817
42	6	0	2.555479	3.054573	0.858318
43	1	0	3.635796	3.008460	0.712891
44	1	0	2.208022	3.920197	0.281276
45	1	0	1.887148	1.980295	-0.882377
46	1	0	-4.384524	1.307038	-1.275032
47	1	0	-4.458230	2.073873	0.317735
48	6	0	-2.266974	3.753630	-0.002146
49	6	0	-3.015517	4.945147	-0.602872
50	6	0	-4.526393	4.711176	-0.597740
51	6	0	-4.876168	3.413001	-1.325201
52	1	0	-2.675636	5.095141	-1.636242
53	1	0	-2.764968	5.855516	-0.049009
54	1	0	-4.878858	4.649036	0.441002
55	1	0	-5.043687	5.557404	-1.061334
56	1	0	-5.954837	3.229828	-1.289235
57	1	0	-4.602676	3.505988	-2.384658
58	1	0	-2.540552	3.645992	1.058575
59	1	0	-1.186998	3.936168	-0.040916
60	1	0	-0.074108	1.337607	-1.248729
61	1	0	-1.542004	-2.565097	0.381138
62	16	0	2.264927	-1.382180	-1.457235
63	6	0	3.862424	-0.622875	-1.463843
64	6	0	3.904300	0.321493	-0.448258
65	6	0	2.572087	0.390750	0.321699
66	7	0	1.645533	-0.542990	-0.281143
67	6	0	4.931686	-0.904530	-2.301751
68	6	0	6.108635	-0.193246	-2.091314
69	6	0	6.188304	0.742270	-1.056165
70	6	0	5.101295	1.001855	-0.222608
71	8	0	1.598540	-1.159077	-2.771832
72	6	0	2.918174	0.036742	1.780469
73	8	0	3.771517	0.616168	2.414390
74	8	0	2.208287	-0.979973	2.258392
75	6	0	2.510681	-1.366379	3.604654
76	1	0	1.860983	-2.213859	3.818206
77	1	0	3.559410	-1.657735	3.688430
78	1	0	5.205731	1.691894	0.605343
79	1	0	7.120490	1.271948	-0.887590
80	1	0	6.972366	-0.378510	-2.721243
81	1	0	4.849201	-1.654468	-3.082359
82	1	0	2.304687	-0.543015	4.292399
83	8	0	2.347478	-2.838086	-1.162851
84	8	0	-0.579761	-2.606845	-1.434874
85	1	0	-0.613565	-1.782309	-1.944006
86	1	0	0.265412	-3.013602	-1.673875
87	8	0	0.788435	-3.515237	1.285130
88	1	0	1.225684	-3.121988	0.507278
89	1	0	1.480158	-4.042644	1.705227
90	8	0	0.420302	1.321170	-2.877567
91	1	0	0.927434	0.482068	-2.915356
92	1	0	-0.470419	1.043840	-3.141697
93	8	0	-0.527347	-1.035473	1.310429

94	1	0	0.158488	-0.907862	0.605213
95	1	0	-0.048330	-1.650568	1.887600

4-IM3′

Zero-point correction = 0.77972 a.u.
Thermal correction to Gibbs Free Energy = 0.70591 a.u.
Sum of electronic and zero-point Energies = -2313.61731 a.u.
Sum of electronic and thermal Free Energies = -2313.69112 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.011942	-3.199237	2.525535
2	6	0	-1.502225	-3.265110	2.363344
3	1	0	0.308180	-3.389182	3.560181
4	1	0	-1.873623	-4.246199	2.673660
5	1	0	-1.966237	-2.526120	3.026021
6	1	0	0.492541	-3.956440	1.895131
7	6	0	0.524554	-1.809159	2.118411
8	1	0	1.604708	-1.733886	2.239756
9	1	0	0.056757	-1.049164	2.760338
10	7	0	1.947971	2.187416	-0.137045
11	6	0	2.499033	2.498067	1.189023
12	6	0	1.708711	3.611925	1.877578
13	6	0	1.687616	4.851827	0.983103
14	6	0	1.702930	3.339503	-1.022788
15	6	0	0.954347	4.462967	-0.301508
16	1	0	3.540688	2.825788	1.072212
17	1	0	2.494404	1.607239	1.815418
18	1	0	2.221078	3.826890	2.820444
19	6	0	0.283267	3.205062	2.246619
20	1	0	2.711050	5.169080	0.757490
21	1	0	2.664404	3.719588	-1.392022
22	1	0	1.126021	2.977097	-1.874842
23	6	0	-0.498153	4.112899	0.020133
24	1	0	0.917815	5.310811	-0.992498
25	7	0	-0.600445	3.028131	1.049926
26	1	0	-0.172049	3.990492	2.855006
27	1	0	0.250233	2.264459	2.798291
28	1	0	-1.004928	4.988943	0.432753
29	1	0	1.177723	5.681869	1.483236
30	1	0	-1.038025	3.752173	-0.859001
31	1	0	-1.568677	2.989678	1.382909
32	6	0	2.040974	0.979381	-0.736458
33	8	0	1.908929	0.830915	-1.951955
34	6	0	2.198989	-0.304904	0.099823
35	6	0	3.406655	-1.117635	-0.384584
36	7	0	0.914838	-0.975029	-0.142520
37	1	0	3.247537	-1.351704	-1.445124
38	6	0	4.679718	-0.271284	-0.260249
39	1	0	2.283923	-0.120346	1.167732
40	6	0	0.119669	-1.518735	0.711572
41	6	0	-1.281014	-1.785880	0.244318
42	6	0	-1.903669	-3.026217	0.906754
43	1	0	-2.990197	-2.988017	0.804754
44	1	0	-1.557594	-3.880561	0.315705
45	1	0	-1.226265	-1.968548	-0.833709
46	1	0	4.579718	0.658443	-0.834187
47	1	0	4.817429	0.009689	0.794625
48	6	0	3.555161	-2.435198	0.381974
49	6	0	4.772801	-3.215613	-0.118815
50	6	0	6.049136	-2.380319	-0.004352
51	6	0	5.903152	-1.051017	-0.746449
52	1	0	4.610575	-3.491493	-1.169590
53	1	0	4.872690	-4.149374	0.444099
54	1	0	6.253370	-2.180125	1.056395
55	1	0	6.906625	-2.938488	-0.394412
56	1	0	6.804678	-0.442060	-0.624246
57	1	0	5.792366	-1.247476	-1.820996
58	1	0	3.688214	-2.213030	1.451186
59	1	0	2.645492	-3.036982	0.269859
60	1	0	0.554697	-0.851084	-1.097263
61	16	0	-1.650865	0.746605	-1.844982
62	6	0	-3.287069	0.064186	-1.729495
63	6	0	-3.399673	-0.553128	-0.488226
64	6	0	-2.093116	-0.388318	0.319921
65	7	0	-1.328167	0.686942	-0.289732
66	6	0	-4.286500	0.055759	-2.687892
67	6	0	-5.473992	-0.600145	-2.369151
68	6	0	-5.615730	-1.227141	-1.130891
69	6	0	-4.588454	-1.216457	-0.185505
70	8	0	-0.865686	-0.214369	-2.662855
71	6	0	-2.318386	-0.005378	1.781507
72	8	0	-1.610762	0.772197	2.386983
73	8	0	-3.338582	-0.644726	2.337802
74	6	0	-3.568902	-0.367844	3.729185
75	1	0	-4.424767	-0.977300	4.011704
76	1	0	-2.691491	-0.639781	4.319904
77	1	0	-4.736957	-1.695496	0.774003
78	1	0	-6.545840	-1.732406	-0.890933
79	1	0	-6.289995	-0.621481	-3.084095
80	1	0	-4.150237	0.551272	-3.644125
81	1	0	-3.789138	0.692082	3.867184
82	8	0	-1.624311	2.123876	-2.357907
83	1	0	-0.506192	2.085980	0.593794
84	1	0	0.445724	-1.552972	-3.310813
85	8	0	1.356956	-1.762859	-3.056095
86	1	0	1.716498	-0.877982	-2.866989
87	1	0	1.060991	-3.093276	-1.742813
88	8	0	0.698288	-3.690756	-1.061590
89	1	0	0.671272	-4.559860	-1.480490

4-TS2′

Zero-point correction = 0.77719 a.u.
Thermal correction to Gibbs Free Energy = 0.70743 a.u.
Sum of electronic and zero-point Energies = -2313.57623 a.u.
Sum of electronic and thermal Free Energies = -2313.64600 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.082193	-3.310708	2.466065
2	6	0	-1.597158	-3.160440	2.359516
3	1	0	0.225132	-3.281322	3.515033
4	1	0	-2.097826	-4.012556	2.829081
5	1	0	-1.899825	-2.277932	2.930148
6	1	0	0.233521	-4.286767	2.079060
7	6	0	0.639940	-2.197352	1.704583
8	1	0	1.720273	-2.355436	1.745094
9	1	0	0.423035	-1.227491	2.163207
10	7	0	1.748906	2.131073	-0.155202
11	6	0	2.285337	2.349345	1.191305
12	6	0	1.551099	3.481627	1.916307
13	6	0	1.587737	4.752075	1.066868
14	6	0	1.581481	3.327869	-0.991049
15	6	0	0.851989	4.439322	-0.236961
16	1	0	3.349746	2.615934	1.123882
17	1	0	2.206549	1.429311	1.771578
18	1	0	2.066319	3.641054	2.868765
19	6	0	0.105739	3.136043	2.260208
20	1	0	2.623907	5.037810	0.856287
21	1	0	2.567085	3.692363	-1.314771
22	1	0	1.017064	3.026486	-1.873887
23	6	0	-0.609053	4.093769	0.051798
24	1	0	0.836165	5.318580	-0.888525
25	7	0	-0.737953	2.965415	1.033777
26	1	0	-0.341773	3.953186	2.832797
27	1	0	0.028250	2.211801	2.829958
28	1	0	-1.113484	4.954176	0.499435
29	1	0	1.107886	5.582284	1.596244

30	1	0	-1.136161	3.777927	-0.850771
31	1	0	-1.717263	2.920799	1.329683
32	6	0	1.810348	0.945434	-0.828624
33	8	0	1.685329	0.887279	-2.046893
34	6	0	2.031400	-0.384084	-0.093473
35	6	0	3.445421	-0.876560	-0.467464
36	7	0	0.990839	-1.296961	-0.617164
37	1	0	3.438630	-0.979342	-1.564539
38	6	0	4.522841	0.154787	-0.107876
39	1	0	1.944910	-0.280623	0.987771
40	6	0	0.202152	-2.143149	0.245564
41	6	0	-1.341165	-1.980306	0.059652
42	6	0	-2.075523	-3.048350	0.905662
43	1	0	-3.148056	-2.850529	0.883353
44	1	0	-1.978056	-4.030325	0.422752
45	1	0	-1.518356	-2.192322	-1.002992
46	1	0	4.294205	1.123704	-0.568963
47	1	0	4.520978	0.307705	0.981498
48	6	0	3.803058	-2.234538	0.144503
49	6	0	5.178879	-2.707013	-0.332122
50	6	0	6.259138	-1.680713	0.012775
51	6	0	5.910243	-0.306155	-0.559290
52	1	0	5.152350	-2.852861	-1.421043
53	1	0	5.416692	-3.678119	0.114339
54	1	0	6.344308	-1.605952	1.105556
55	1	0	7.233498	-2.012304	-0.361165
56	1	0	6.662823	0.432865	-0.265147
57	1	0	5.925337	-0.357400	-1.656269
58	1	0	3.821119	-2.138537	1.239969
59	1	0	3.037047	-2.981998	-0.095243
60	1	0	0.375463	-0.765491	-1.231331
61	16	0	-1.582694	0.699707	-1.904143
62	6	0	-3.264354	0.169156	-1.688848
63	6	0	-3.347389	-0.503256	-0.475458
64	6	0	-1.960759	-0.518158	0.238823
65	7	0	-1.155264	0.539048	-0.375792
66	6	0	-4.322112	0.315549	-2.572072
67	6	0	-5.548114	-0.230964	-2.202631
68	6	0	-5.668650	-0.903859	-0.986371
69	6	0	-4.583646	-1.048679	-0.120510
70	8	0	-0.962735	-0.287605	-2.817370
71	6	0	-2.071208	-0.130269	1.718377
72	8	0	-1.181401	0.416344	2.334231
73	8	0	-3.236986	-0.443624	2.273702
74	6	0	-3.381321	-0.102765	3.660828
75	1	0	-4.376000	-0.441155	3.944675
76	1	0	-2.619189	-0.606845	4.259743
77	1	0	-4.731775	-1.551370	0.826471
78	1	0	-6.629580	-1.317178	-0.696257
79	1	0	-6.408707	-0.130211	-2.855956
80	1	0	-4.195324	0.847806	-3.509897
81	1	0	-3.291601	0.977203	3.792255
82	8	0	-1.482475	2.101588	-2.345016
83	1	0	-0.597449	2.034184	0.552603
84	1	0	1.564369	-2.204214	-2.070816
85	8	0	1.474147	-3.143706	-2.422741
86	1	0	2.358976	-3.520094	-2.579273
87	1	0	0.984295	-3.512376	-1.449449
88	8	0	0.507481	-3.531398	-0.287946
89	1	0	-0.193919	-4.176741	-0.102230

4-IM4′

Zero-point correction = 0.78290 a.u.
Thermal correction to Gibbs Free Energy = 0.71279 a.u.
Sum of electronic and zero-point Energies = -2313.60285 a.u.
Sum of electronic and thermal Free Energies = -2313.67296 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.098304	-3.904145	1.868815
2	6	0	-1.407932	-3.670448	1.908895
3	1	0	0.487063	-4.089790	2.873663
4	1	0	-1.923681	-4.567279	2.265433
5	1	0	-1.628606	-2.879518	2.633018
6	1	0	0.326827	-4.800528	1.278806
7	6	0	0.824746	-2.692166	1.277173
8	1	0	1.892382	-2.900889	1.214727
9	1	0	0.679813	-1.834392	1.936945
10	7	0	1.441251	2.205373	-0.084200
11	6	0	1.671421	2.320171	1.360398
12	6	0	0.834102	3.439111	1.995624
13	6	0	1.059392	4.749438	1.241373
14	6	0	1.404068	3.450104	-0.866890
15	6	0	0.563823	4.529994	-0.188263
16	1	0	2.728929	2.546692	1.549637
17	1	0	1.424568	1.372203	1.840130
18	1	0	1.168119	3.530457	3.033900
19	6	0	-0.660896	3.132342	2.048060
20	1	0	2.124031	5.006692	1.235670
21	1	0	2.429673	3.823000	-0.999676
22	1	0	0.996416	3.202006	-1.847045
23	6	0	-0.928143	4.201502	-0.189426
24	1	0	0.676541	5.445031	-0.778275
25	7	0	-1.236142	3.010396	0.671383
26	1	0	-1.191028	3.951179	2.541776
27	1	0	-0.863709	2.198790	2.571308
28	1	0	-1.494549	5.036866	0.231674
29	1	0	0.514650	5.568080	1.723419
30	1	0	-1.295329	3.967284	-1.187629
31	1	0	-2.254953	2.934240	0.751042
32	6	0	1.568682	1.059559	-0.802014
33	8	0	1.506447	1.033749	-2.027676
34	6	0	1.910491	-0.274289	-0.119235
35	6	0	3.420849	-0.522631	-0.362163
36	7	0	1.114740	-1.326744	-0.857247
37	1	0	3.544235	-0.523113	-1.455742
38	6	0	4.280251	0.618468	0.200793
39	1	0	1.645411	-0.317994	0.934631
40	6	0	0.295420	-2.387339	-0.125350
41	6	0	-1.240547	-2.120874	-0.173356
42	6	0	-1.951598	-3.304688	0.524955
43	1	0	-3.021756	-3.098932	0.576705
44	1	0	-1.872747	-4.187951	-0.122008
45	1	0	-1.483331	-2.173061	-1.241375
46	1	0	3.956934	1.581810	-0.208473
47	1	0	4.143265	0.661589	1.290418
48	6	0	3.927039	-1.864814	0.179616
49	6	0	5.404666	-2.074295	-0.161114
50	6	0	6.264792	-0.938551	0.390166
51	6	0	5.762417	0.410496	-0.120509
52	1	0	5.516870	-2.115156	-1.253888
53	1	0	5.740564	-3.039373	0.231538
54	1	0	6.217144	-0.951798	1.487588
55	1	0	7.313851	-1.084591	0.113366
56	1	0	6.348714	1.228167	0.311003
57	1	0	5.898397	0.459169	-1.209069
58	1	0	3.801803	-1.879341	1.271127
59	1	0	3.342338	-2.696058	-0.230116
60	1	0	0.495392	-0.833750	-1.523187
61	16	0	-1.679178	0.608874	-1.880729
62	6	0	-3.326170	0.089027	-1.451812
63	6	0	-3.258715	-0.597246	-0.243671
64	6	0	-1.785829	-0.691304	0.242191
65	7	0	-1.049267	0.379290	-0.431447
66	6	0	-4.498596	0.296117	-2.161097
67	6	0	-5.676799	-0.206883	-1.614463
68	6	0	-5.643512	-0.895146	-0.401247
69	6	0	-4.447214	-1.102074	0.287842
70	8	0	-1.163102	-0.317033	-2.913116
71	6	0	-1.605077	-0.430177	1.736936
72	8	0	-0.578603	0.007199	2.214567

73	8	0	-2.666650	-0.739279	2.472027
74	6	0	-2.514099	-0.581941	3.891631
75	1	0	-3.436684	-0.957687	4.329339
76	1	0	-1.655939	-1.156985	4.245903
77	1	0	-4.461335	-1.627665	1.234533
78	1	0	-6.567268	-1.276516	0.022289
79	1	0	-6.621001	-0.058110	-2.128046
80	1	0	-4.495194	0.841823	-3.099690
81	1	0	-2.375370	0.472006	4.140346
82	8	0	-1.641194	2.035024	-2.244957
83	1	0	-0.952613	2.089217	0.226774
84	1	0	1.773562	-1.857994	-1.469229
85	8	0	2.668089	-2.782120	-2.706439
86	1	0	3.615781	-2.963748	-2.645509
87	1	0	2.227036	-3.622502	-2.515734
88	8	0	0.560277	-3.491753	-0.979100
89	1	0	-0.016553	-4.231971	-0.745380

4-TS3′

Zero-point correction = 0.77845 a.u.
Thermal correction to Gibbs Free Energy = 0.70909 a.u.
Sum of electronic and zero-point Energies = -2313.60258 a.u.
Sum of electronic and thermal Free Energies = -2313.67194 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.256429	-3.836929	1.924770
2	6	0	-1.252421	-3.620358	1.970693
3	1	0	0.656128	-3.988229	2.930881
4	1	0	-1.751680	-4.515108	2.354616
5	1	0	-1.479300	-2.816536	2.678736
6	1	0	0.486915	-4.755203	1.368482
7	6	0	0.970156	-2.636407	1.293366
8	1	0	2.035749	-2.847324	1.204968
9	1	0	0.844608	-1.770893	1.944846
10	7	0	1.316996	2.266479	-0.143809
11	6	0	1.619003	2.452366	1.278723
12	6	0	0.683614	3.461173	1.954732
13	6	0	0.664332	4.764844	1.157739
14	6	0	1.019084	3.464667	-0.942823
15	6	0	0.082281	4.428183	-0.214730
16	1	0	2.646708	2.824706	1.385074
17	1	0	1.549073	1.492315	1.791983
18	1	0	1.085090	3.631686	2.958958
19	6	0	-0.745659	2.953846	2.129640
20	1	0	1.677615	5.168708	1.053841
21	1	0	1.958280	3.985837	-1.176046
22	1	0	0.573110	3.123714	-1.877423
23	6	0	-1.342995	3.893809	-0.059041
24	1	0	0.013370	5.329382	-0.832721
25	7	0	-1.401600	2.686346	0.819126
26	1	0	-1.328730	3.723730	2.649856
27	1	0	-0.767717	2.039924	2.720513
28	1	0	-1.962549	4.673564	0.400613
29	1	0	0.050737	5.514937	1.668550
30	1	0	-1.768221	3.619908	-1.023921
31	1	0	-2.393300	2.521101	1.013342
32	6	0	1.538138	1.128611	-0.840395
33	8	0	1.462325	1.071844	-2.066493
34	6	0	1.950965	-0.174012	-0.133218
35	6	0	3.469740	-0.360812	-0.364746
36	7	0	1.203036	-1.278227	-0.850716
37	1	0	3.600959	-0.370651	-1.457717
38	6	0	4.270735	0.826948	0.188203
39	1	0	1.678115	-0.212042	0.919239
40	6	0	0.411520	-2.345643	-0.101343
41	6	0	-1.133474	-2.114538	-0.144325
42	6	0	-1.810084	-3.301757	0.581115
43	1	0	-2.886312	-3.129555	0.630797
44	1	0	-1.697547	-4.190754	-0.051396
45	1	0	-1.375812	-2.206509	-1.207636
46	1	0	3.907767	1.767493	-0.240591
47	1	0	4.118368	0.883178	1.275392
48	6	0	4.032579	-1.671631	0.198347
49	6	0	5.520331	-1.815332	-0.130210
50	6	0	6.322468	-0.635522	0.415761
51	6	0	5.764022	0.683479	-0.115175
52	1	0	5.641275	-1.861585	-1.221903
53	1	0	5.897838	-2.759852	0.274360
54	1	0	6.264342	-0.639285	1.512703
55	1	0	7.379828	-0.736190	0.150500
56	1	0	6.307390	1.532021	0.312792
57	1	0	5.909162	0.726090	-1.202793
58	1	0	3.898250	-1.680425	1.288894
59	1	0	3.493335	-2.534889	-0.206613
60	1	0	0.585069	-0.841664	-1.557671
61	16	0	-1.647720	0.513227	-1.935559
62	6	0	-3.274124	-0.046664	-1.497619
63	6	0	-3.205186	-0.672790	-0.256053
64	6	0	-1.741957	-0.707428	0.256016
65	7	0	-1.043743	0.404919	-0.423138
66	6	0	-4.437602	0.097096	-2.235386
67	6	0	-5.609856	-0.412948	-1.682751
68	6	0	-5.576785	-1.044422	-0.439484
69	6	0	-4.387530	-1.186689	0.278096
70	8	0	-1.027996	-0.481114	-2.829434
71	6	0	-1.562270	-0.451547	1.749097
72	8	0	-0.510523	-0.071860	2.218746
73	8	0	-2.640046	-0.703384	2.476454
74	6	0	-2.489693	-0.547597	3.898890
75	1	0	-3.419727	-0.909381	4.332038
76	1	0	-1.640926	-1.134143	4.256003
77	1	0	-4.403321	-1.669018	1.247287
78	1	0	-6.496681	-1.430862	-0.012573
79	1	0	-6.549426	-0.312307	-2.215683
80	1	0	-4.432372	0.602012	-3.196409
81	1	0	-2.338131	0.505228	4.144312
82	8	0	-1.657538	1.899609	-2.403532
83	1	0	-1.112353	1.577963	0.207122
84	1	0	1.892534	-1.808042	-1.430344
85	8	0	2.819801	-2.717904	-2.651756
86	1	0	3.771473	-2.874208	-2.581415
87	1	0	2.399033	-3.571382	-2.473869
88	8	0	0.677073	-3.450072	-0.955137
89	1	0	0.303338	-4.254631	-0.569383

4-IM5′

Zero-point correction = 0.78154 a.u.
Thermal correction to Gibbs Free Energy = 0.71140 a.u.
Sum of electronic and zero-point Energies = -2313.60566 a.u.
Sum of electronic and thermal Free Energies = -2313.67580 a.u.

Standard orientation:

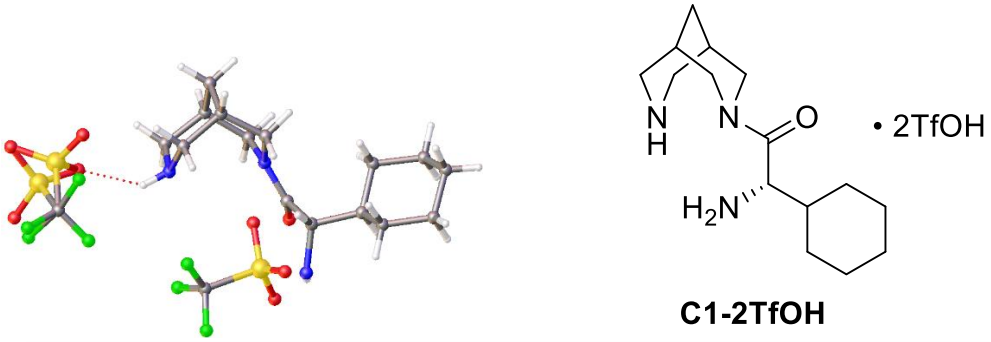
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.237386	-3.793569	2.029118
2	6	0	-1.273823	-3.583957	2.035683
3	1	0	0.617827	-3.901375	3.048061
4	1	0	-1.774646	-4.465062	2.447578
5	1	0	-1.522338	-2.751403	2.702795
6	1	0	0.480770	-4.734300	1.517391
7	6	0	0.961209	-2.617514	1.362772
8	1	0	2.029130	-2.829517	1.294394
9	1	0	0.829419	-1.729025	1.980729
10	7	0	1.299164	2.232074	-0.169422
11	6	0	1.601283	2.431824	1.254614
12	6	0	0.737292	3.513408	1.916043
13	6	0	0.782582	4.790926	1.078338
14	6	0	0.989673	3.413440	-0.993571

15	6	0	0.137348	4.452382	-0.265350
16	1	0	2.650907	2.737166	1.357022
17	1	0	1.464238	1.488887	1.785712
18	1	0	1.177854	3.688807	2.903390
19	6	0	-0.720494	3.102014	2.128697
20	1	0	1.816604	5.127492	0.936713
21	1	0	1.933627	3.881066	-1.307840
22	1	0	0.477331	3.053481	-1.886558
23	6	0	-1.312232	4.007720	-0.043113
24	1	0	0.111892	5.337387	-0.909971
25	7	0	-1.384331	2.829826	0.842774
26	1	0	-1.228451	3.921655	2.662869
27	1	0	-0.774160	2.205403	2.749204
28	1	0	-1.862515	4.855082	0.397681
29	1	0	0.232501	5.594143	1.580730
30	1	0	-1.780281	3.748987	-0.995350
31	1	0	-2.370323	2.649675	1.032944
32	6	0	1.522524	1.089663	-0.849469
33	8	0	1.410824	1.004005	-2.074399
34	6	0	1.966832	-0.196310	-0.128532
35	6	0	3.481949	-0.378584	-0.380565
36	7	0	1.222758	-1.324678	-0.815780
37	1	0	3.596308	-0.429015	-1.474256
38	6	0	4.288611	0.831170	0.112969
39	1	0	1.717068	-0.219289	0.929703
40	6	0	0.420212	-2.372970	-0.047738
41	6	0	-1.128226	-2.153490	-0.118684
42	6	0	-1.803019	-3.329755	0.622133
43	1	0	-2.883740	-3.181176	0.634376
44	1	0	-1.649623	-4.233979	0.021860
45	1	0	-1.356306	-2.265404	-1.184452
46	1	0	3.917478	1.753613	-0.347664
47	1	0	4.154216	0.930230	1.199092
48	6	0	4.051684	-1.666350	0.227258
49	6	0	5.536448	-1.823687	-0.107713
50	6	0	6.342681	-0.620065	0.377373
51	6	0	5.777197	0.673583	-0.205976
52	1	0	5.648192	-1.917851	-1.197285
53	1	0	5.918655	-2.749300	0.334448
54	1	0	6.295673	-0.574825	1.473914
55	1	0	7.397280	-0.732062	0.105798
56	1	0	6.326835	1.540607	0.174128
57	1	0	5.906731	0.665642	-1.296419
58	1	0	3.925169	-1.631780	1.318457
59	1	0	3.508804	-2.545568	-0.137074
60	1	0	0.625096	-0.895492	-1.541486
61	16	0	-1.724118	0.468005	-2.008878
62	6	0	-3.321887	-0.080306	-1.482700
63	6	0	-3.212413	-0.707604	-0.244497
64	6	0	-1.747643	-0.751081	0.248414
65	7	0	-1.032888	0.306379	-0.498955
66	6	0	-4.509169	0.068376	-2.182270
67	6	0	-5.661536	-0.443124	-1.593119
68	6	0	-5.587854	-1.079177	-0.353548
69	6	0	-4.377411	-1.221792	0.325708
70	8	0	-1.131797	-0.530462	-2.899560
71	6	0	-1.545284	-0.400775	1.722490
72	8	0	-0.487031	0.013522	2.141668
73	8	0	-2.610070	-0.611288	2.476227
74	6	0	-2.435733	-0.372703	3.885912
75	1	0	-3.367877	-0.685944	4.351092
76	1	0	-1.596155	-0.959830	4.263983
77	1	0	-4.360784	-1.704639	1.294658
78	1	0	-6.493137	-1.467928	0.101177
79	1	0	-6.617437	-0.340417	-2.095284
80	1	0	-4.535379	0.575600	-3.141487
81	1	0	-2.254508	0.688987	4.062149
82	8	0	-1.719669	1.865682	-2.416597
83	1	0	1.915894	-1.874324	-1.374122
84	8	0	2.827807	-2.797610	-2.583607
85	1	0	3.782797	-2.939168	-2.526803
86	1	0	2.422591	-3.656700	-2.397808
87	8	0	0.692785	-3.500416	-0.865995
88	1	0	0.397320	-4.305815	-0.418509
89	1	0	-1.049477	1.246371	-0.003917

12. Crystal data of catalyst and product.

Crystals suitable for the X-ray crystal structure analysis were obtained from a solution of compound **C1-2TfOH** in THF and Et_2O at rt. The colourless and block-shape crystals were selected and mounted for the single-crystal X-ray diffraction. The data set was collected by a Bruker D8 Venture Photon II at 170(2)K equipped with micro-focus Cu radiation source (Kα = 1.54178Å). Applied with face-indexed numerical absorption correction, the structure solution was solved and refinement was processed by SHELXTL (version 6.14) program package.[9,10,11] The structure was analyzed by ADDSYM routine implemented in PLATON suite and no higher symmetry was suggested.[12]

The crystal data and further details are listed below. CCDC 2058446 which contains the crystallographic data for the structure have been deposited with the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK, which can be obtained free of charge via Fax: +44 (0)1223 336033; E-Mail: deposit@ccdc.cam.ac.uk, https://www.ccdc.cam.ac.uk/structures/.



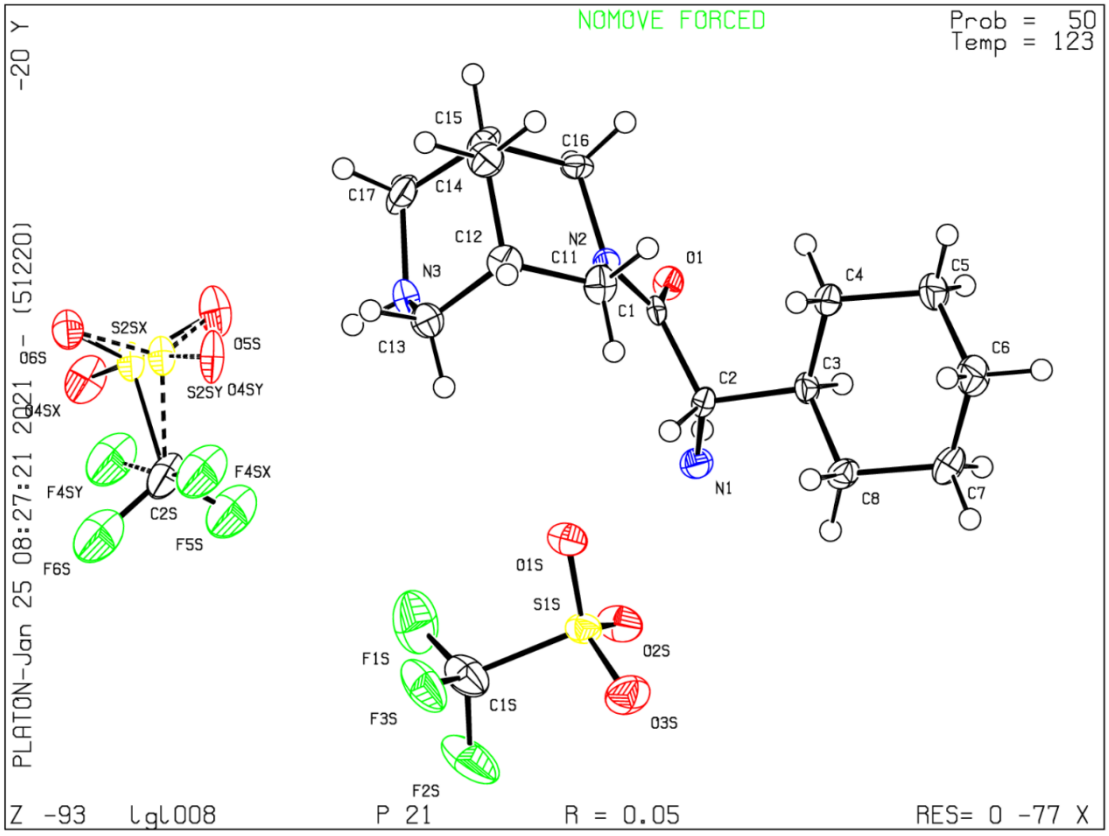


Figure S7. the thermal ellipsoid figure of **C1-2TfOH** with 50% probabilities.

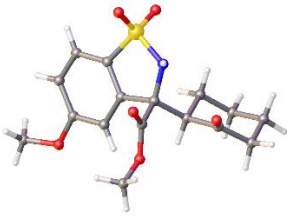
Crystallographic Data for $C_{17}H_{26}F_6N_3O_7S_2$.

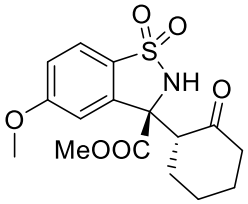
Formula	$C_{17}H_{26}F_6N_3O_7S_2$
Formula mass (amu)	562.53
Space group	P 21 21 21
a (Å)	11.0402 (9)
b (Å)	9.5966 (8)
c (Å)	15.5085 (10)
α (deg)	90
β (deg)	115.079 (2)
γ (deg)	90
V (Å^3)	1200.31 (17)
Z	2
λ (Å)	1.54178
T (K)	123 K

ρ_{calcd} (g cm^{-3})	1.556
μ (mm^{-1})	2.853
Transmission factors	0.691–0.896
$2\theta_{max}$ (deg)	68.274
No. of unique data, including $F_o^2 < 0$	4282
No. of unique data, with $F_o^2 > 2\sigma(F_o^2)$	4214
No. of variables	328
$R(F)$ for $F_o^2 > 2\sigma(F_o^2)$ [a]	0.0464
$R_w(F_o^2)$ [b]	0.1203
Goodness of fit	1.037

Crystals suitable for the X-ray crystal structure analysis were obtained from a solution of compound **3aa** in DCM and petroleum ether at rt. The colourless and block-shape crystals were selected and mounted for the single-crystal X-ray diffraction. The data set was collected by a Bruker D8 Venture Photon II at 170(2)K equipped with micro-focus Cu radiation source (Kα = 1.54178Å). Applied with face-indexed numerical absorption correction, the structure solution was solved and refinement was processed by SHELXTL (version 6.14) program package.[9,10,11] The structure was analyzed by ADDSYM routine implemented in PLATON suite and no higher symmetry was suggested.[12]

The crystal data and further details are listed below. CCDC 2002650 which contains the crystallographic data for the structure have been deposited with the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK, which can be obtained free of charge via Fax: +44 (0)1223 336033; E-Mail: deposit@ccdc.cam.ac.uk, https://www.ccdc.cam.ac.uk/structures/.





3aa

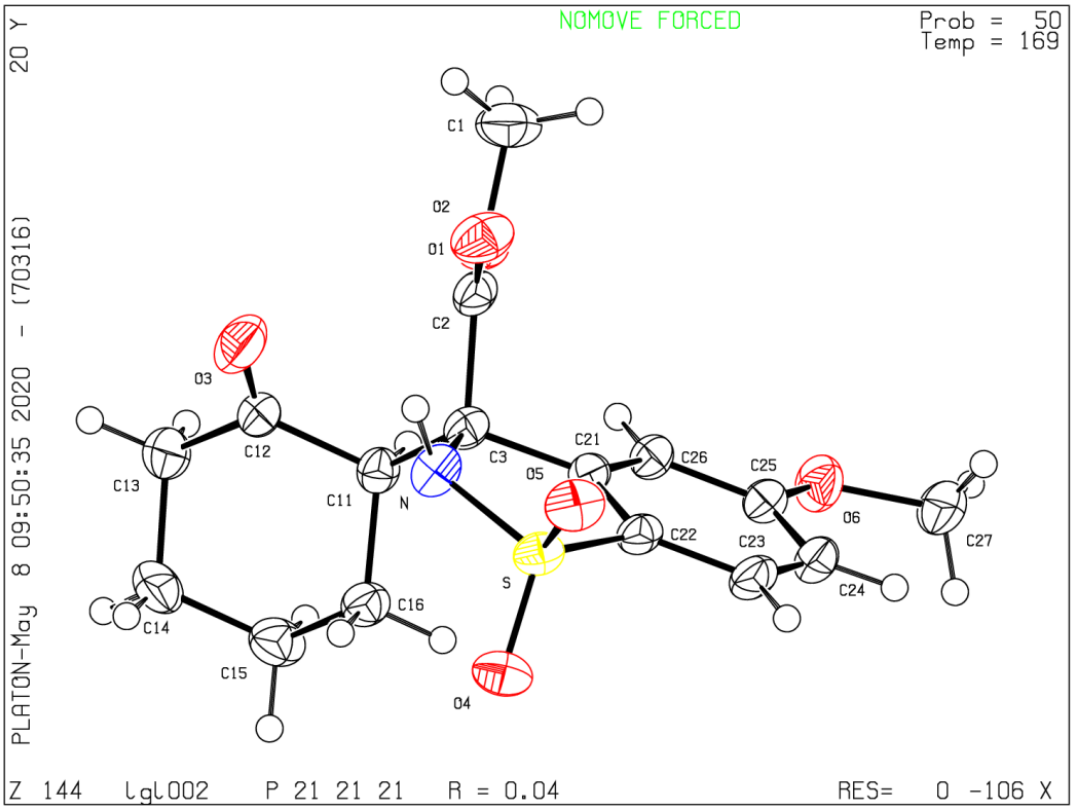


Figure S8. the thermal ellipsoid figure of **3aa** with 50% probabilities.

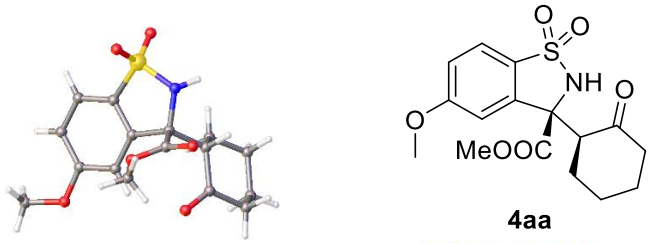
Crystallographic Data for $C_{16}H_{19}NO_6S$.

Formula	$C_{16}H_{19}NO_6S$
Formula mass (amu)	353.38
Space group	P 21 21 21
a (Å)	8.0346 (3)
b (Å)	12.6210 (5)
c (Å)	16.5455 (6)
α (deg)	90
β (deg)	90
γ (deg)	90

V (Å^3)	1677.79 (11)
Z	4
λ (Å)	1.54178
T (K)	169 K
ρ_{calcd} (g cm^{-3})	1.399
μ (mm^{-1})	2.007
Transmission factors	0.721–0.915
$2\theta_{max}$ (deg)	80.536
No. of unique data, including $F_o^2 < 0$	3542
No. of unique data, with $F_o^2 > 2\sigma(F_o^2)$	3353
No. of variables	223
$R(F)$ for $F_o^2 > 2\sigma(F_o^2)$ [a]	0.0426
$R_w(F_o^2)$ [b]	0.1184
Goodness of fit	1.140

Crystals suitable for the X-ray crystal structure analysis were obtained from a solution of compound **4aa** in DCM and petroleum ether at rt. The colourless and block-shape crystals were selected and mounted for the single-crystal X-ray diffraction. The data set was collected by a Bruker D8 Venture Photon II at 173(2)K equipped with micro-focus Cu radiation source (Kα = 1.54178Å). Applied with face-indexed numerical absorption correction, the structure solution was solved and refinement was processed by SHELXTL (version 6.14) program package.[9,10,11] The structure was analyzed by ADDSYM routine implemented in PLATON suite and no higher symmetry was suggested.[12]

The crystal data and further details are listed below. CCDC 2084361 which contains the crystallographic data for the structure have been deposited with the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK, which can be obtained free of charge via Fax: +44 (0)1223 336033; E-Mail: deposit@ccdc.cam.ac.uk, https://www.ccdc.cam.ac.uk/structures/.



4aa

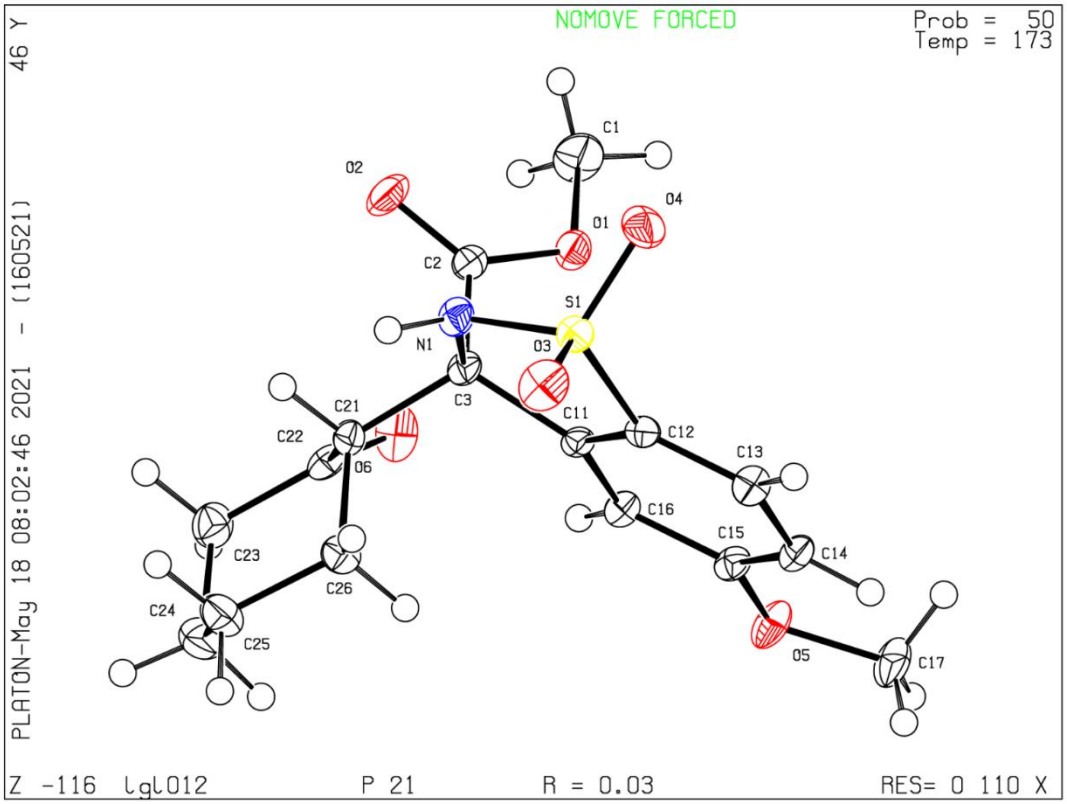


Figure S9. the thermal ellipsoid figure of **4aa** with 50% probabilities.

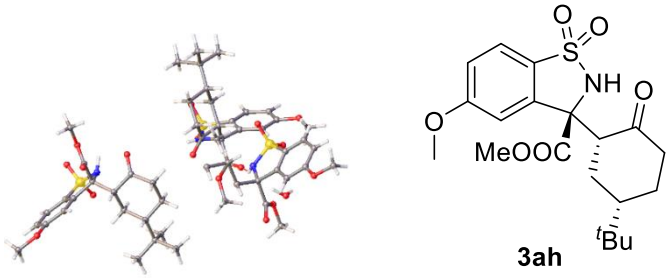
Crystallographic Data for $C_{16}H_{19}NO_6S$.

Formula	$C_{16}H_{19}NO_6S$
Formula mass (amu)	353.38
Space group	P 21
a (Å)	10.1269 (6)
b (Å)	8.0430 (5)

c (Å)	10.8756 (7)
α (deg)	90
β (deg)	114.408 (2)
γ (deg)	90
V (Å^3)	806.65 (9)
Z	2
λ (Å)	1.54178
T (K)	173 K
ρ_{calcd} (g cm^{-3})	1.455
μ (mm^{-1})	2.087
Transmission factors	0.564–0.928
$2\theta_{max}$ (deg)	72.362
No. of unique data, including $F_o^2 < 0$	3036
No. of unique data, with $F_o^2 > 2\sigma(F_o^2)$	2976
No. of variables	223
$R(F)$ for $F_o^2 > 2\sigma(F_o^2)$ [a]	0.0296
$R_w(F_o^2)$ [b]	0.0764
Goodness of fit	1.090

Crystals suitable for the X-ray crystal structure analysis were obtained from a solution of compound **3ah** in DCM and petroleum ether at rt. The colourless and block-shape crystals were selected and mounted for the single-crystal X-ray diffraction. The data set was collected by a Bruker D8 Venture Photon II at 173(2)K equipped with micro-focus Cu radiation source (Kα = 1.54178Å). Applied with face-indexed numerical absorption correction, the structure solution was solved and refinement was processed by SHELXTL (version 6.14) and OLEX 2.3 program package.[9,10,11] The structure was analyzed by ADDSYM routine implemented in PLATON suite and no higher symmetry was suggested.[12]

The crystal data and further details are listed below. CCDC 2097127 which contains the crystallographic data for the structure have been deposited with the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK, which can be obtained free of charge via Fax: +44 (0)1223 336033; E-Mail: deposit@ccdc.cam.ac.uk, https://www.ccdc.cam.ac.uk/structures/.



3ah

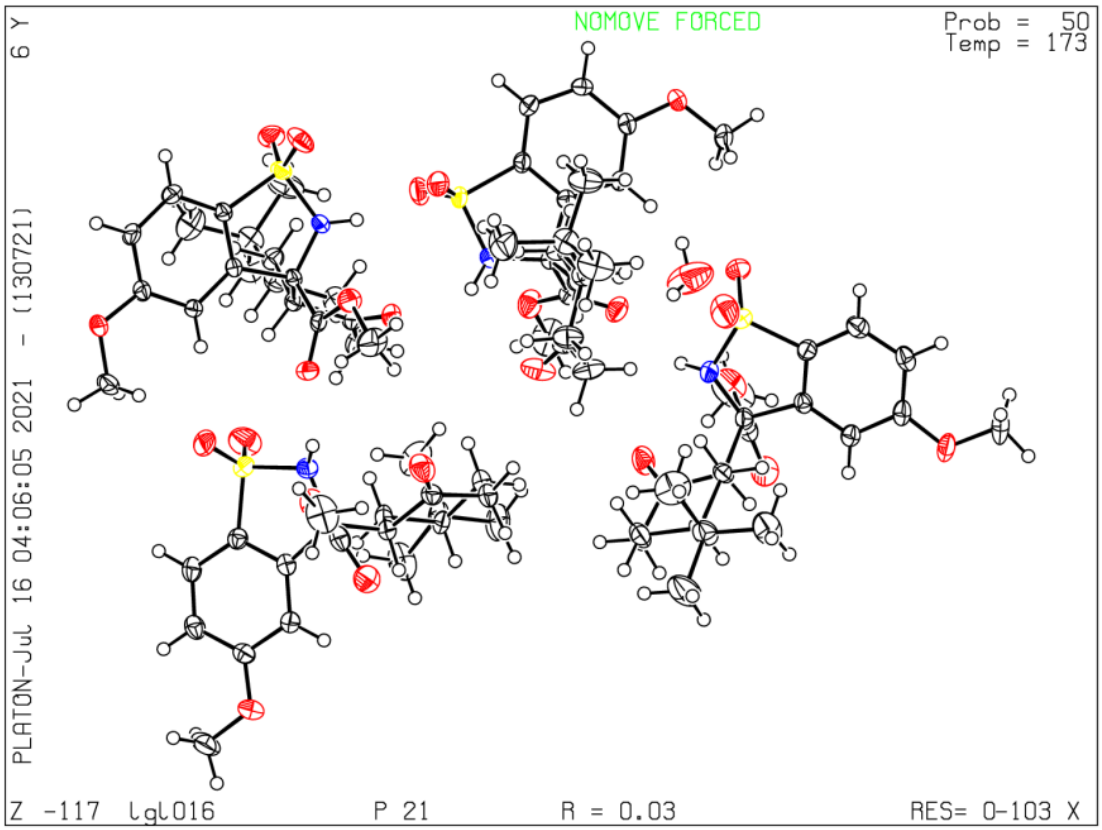


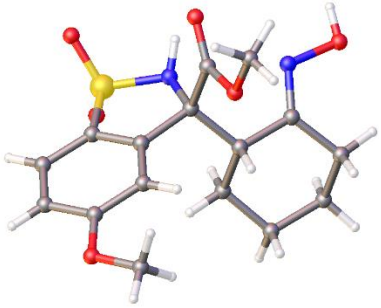
Figure S10. the thermal ellipsoid figure of **3ah** with 50% probabilities.

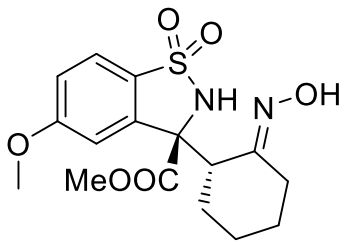
Crystallographic Data for $C_{160}H_{218}N_8O_{49}S_8$.

Formula	$C_{160}H_{218}N_8O_{49}S_8$
Formula mass (amu)	3293.89
Space group	P 21
a (Å)	13.5261 (7)
b (Å)	12.6740 (6)
c (Å)	25.4683(12)
α (deg)	90
β (deg)	99.780 (2)
γ (deg)	90
V (Å^3)	4302.6 (4)
Z	1
λ (Å)	1.54178
T (K)	173 K
ρ_{calcd} (g cm^{-3})	1.271
μ (mm^{-1})	1.640
Transmission factors	0.623–0.831
$2\theta_{max}$ (deg)	68.518
No. of unique data, including $F_o^2 < 0$	15375
No. of unique data, with $F_o^2 > 2\sigma(F_o^2)$	14653
No. of variables	1060
$R(F)$ for $F_o^2 > 2\sigma(F_o^2)$ [a]	0.0300
$R_w(F_o^2)$ [b]	0.0710
Goodness of fit	1.050

Crystals suitable for the X-ray crystal structure analysis were obtained from a solution of compound **7** in DCM and petroleum ether at rt. The colourless and block-shape crystals were selected and mounted for the single-crystal X-ray diffraction. The data set was collected by a Bruker D8 Venture Photon II at 173(2)K equipped with micro-focus Cu radiation source (Kα = 1.54178Å). Applied with face-indexed numerical absorption correction, the structure solution was solved and refinement was processed by SHELXTL (version 6.14) and OLEX 2.3 program package.[9,10,11] The structure was analyzed by ADDSYM routine implemented in PLATON suite and no higher symmetry was suggested.[12]

The crystal data and further details are listed below. CCDC 2090581 which contains the crystallographic data for the structure have been deposited with the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK, which can be obtained free of charge via Fax: +44 (0)1223 336033; E-Mail: deposit@ccdc.cam.ac.uk, https://www.ccdc.cam.ac.uk/structures/.





7

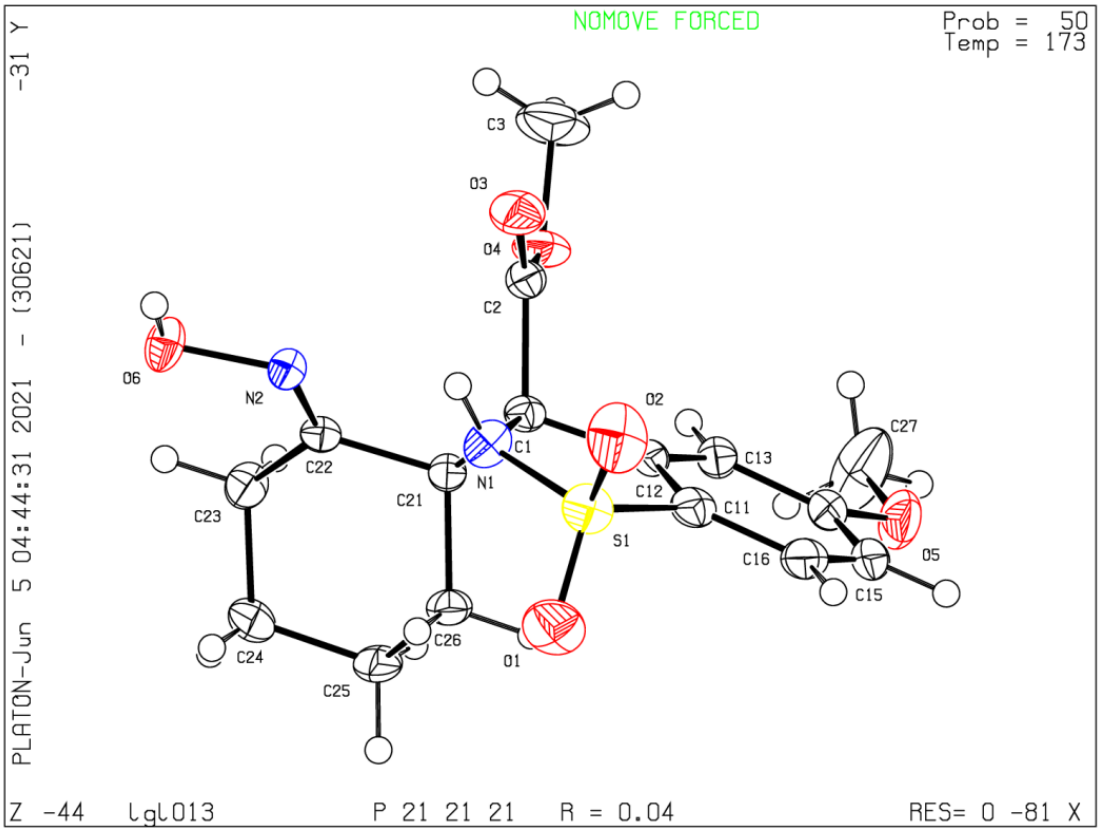


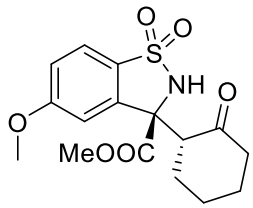
Figure S11. the thermal ellipsoid figure of **7** with 50% probabilities.

Crystallographic Data for $C_{16}H_{20}N_2O_6S$.

Formula	$C_{16}H_{20}N_2O_6S$
Formula mass (amu)	368.40
Space group	P 21 21 21
a (Å)	8.1051 (4)
b (Å)	14.1921 (6)
c (Å)	15.2659 (7)
α (deg)	90
β (deg)	90
γ (deg)	90
V (Å^3)	1756.01 (14)
Z	4
λ (Å)	1.54178
T (K)	173 K
ρ_{calcd} (g cm^{-3})	1.393
μ (mm^{-1})	1.957
Transmission factors	0.555–0.990
$2\theta_{max}$ (deg)	68.361
No. of unique data, including $F_o^2 < 0$	3201
No. of unique data, with $F_o^2 > 2\sigma(F_o^2)$	3065
No. of variables	237
$R(F)$ for $F_o^2 > 2\sigma(F_o^2)$ [a]	0.0406
$R_w(F_o^2)$ [b]	0.1054
Goodness of fit	1.109

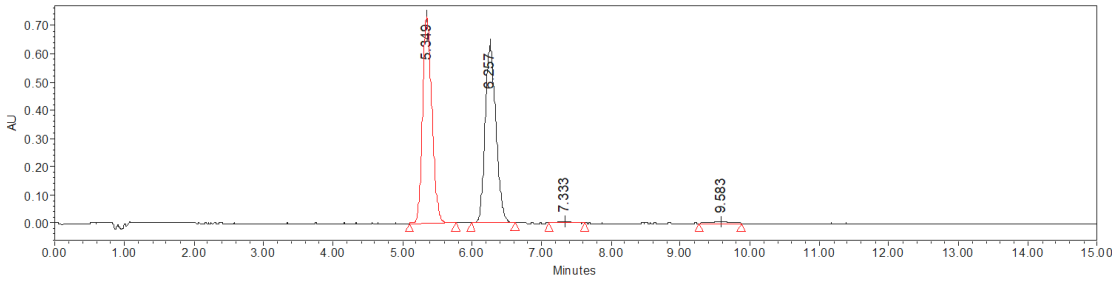
13. Spectral characterization data for the products.

Methyl (*R*)-5-methoxy-3-((*R*)-2-oxocyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **3aa**

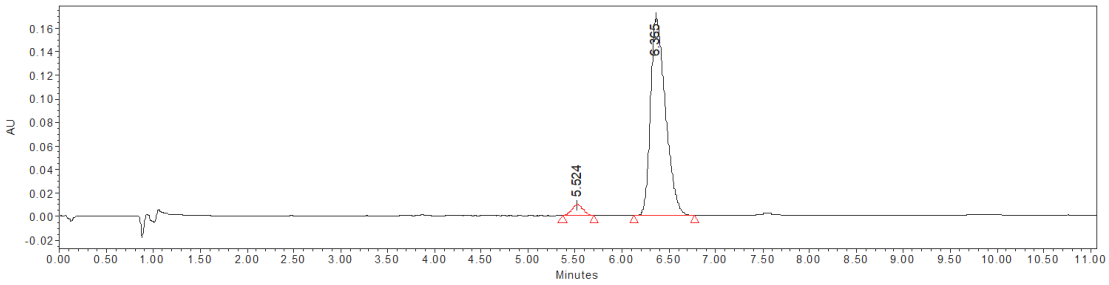


Result: white solid, m.p. 176 - 180 °C, 98% yield, 92% ee, >19:1 dr; $[\alpha]^{26.1}_{D}$ = +155.6 (c = 1.17, CH_2Cl_2); SFC (Daicel chiralcel IC-3, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 230 nm), t_1 = 5.52 min, t_2 = 6.36 min.

^{1}H NMR (400 MHz, Chloroform-d) δ 7.68 (d, J = 8.8 Hz, 1H), 7.09 (dd, J = 8.8, 2.4 Hz, 1H), 6.95 (d, J = 2.4 Hz, 1H), 5.72 (s, 1H), 3.88 (s, 3H), 3.78 (s, 3H), 3.53 (dd, J = 12.8, 5.6 Hz, 1H), 2.51 – 2.42 (m, 1H), 2.42 – 2.29 (m, 1H), 2.11 – 2.01 (m, 1H), 1.89 – 1.81 (m, 1H), 1.77 – 1.56 (m, 3H), 1.49 – 1.41 (m, 1H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 210.1, 170.9, 164.0, 137.3, 127.3, 123.3, 117.3, 107.9, 68.2, 58.5, 56.0, 54.0, 41.8, 26.7, 26.6, 24.3.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{16}H_{19}NO_6S+Na^+]$: 376.0825, found 376.0807.
IR (film): ν (cm^{-1}) 3293, 2947, 2868, 1743, 1706, 1599, 1485, 1289, 1248, 1133, 1020, 894, 735, 576.

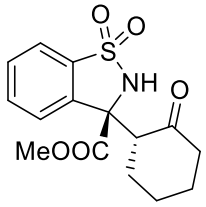


Name	Retention Time	Area	% Area
1	5.349	6839316	49.30
2	6.257	6848656	49.37
3	7.333	92225	0.66
4	9.583	92476	0.67



Name	Retention Time	Area	% Area
1	5.524	78094	3.98
2	6.365	1884806	96.02

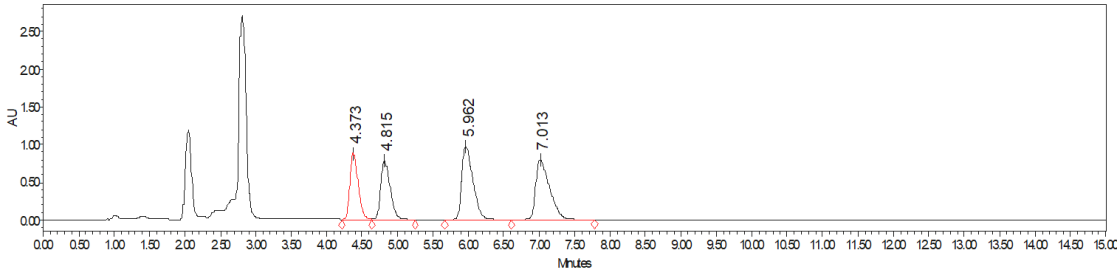
Methyl (*R*)-3-((*R*)-2-oxocyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **3ba**



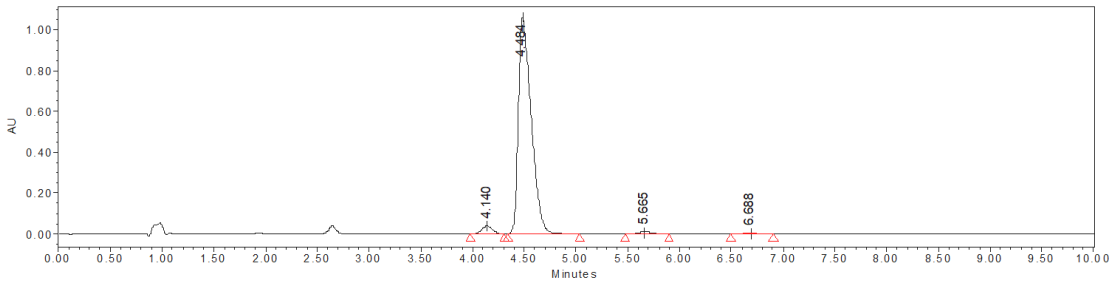
Result: white solid, m.p. 169 - 171 °C, 98% yield, 94% ee, >19:1 d.; $[\alpha]^{26.9}_{D}$ = +173.1 (c = 1.12, CH_2Cl_2); SFC (Daicel chiralcel IC-3, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 210 nm), t_1 = 4.14 min, t_2 = 4.48 min, t_3 = 5.66 min, t_4 = 6.69 min.

^{1}H NMR (400 MHz, Chloroform-d) δ 7.78 (d, J = 7.6 Hz, 1H), 7.70 – 7.64 (m, 1H), 7.63 – 7.54 (m, 2H), 5.81 (s, 1H), 3.76 (s, 3H), 3.59 (dd, J = 12.8, 5.6 Hz, 1H), 2.51 – 2.43 (m, 1H), 2.43 – 2.32 (m, 1H), 2.11 – 2.03 (m, 1H), 1.87 – 1.79 (m, 1H), 1.75 – 1.53 (m, 3H), 1.45 – 1.35 (m, 1H).

^{13}C NMR (100 MHz, Chloroform-d) δ 210.1, 170.9, 135.2, 134.7, 133.8, 130.8, 123.8, 121.9, 68.6, 58.3, 53.9, 41.8, 26.7, 26.6, 24.2.
HRMS (FTMS+c ESI) m/z: [M + Na]$^+$ calcd for [$C_{15}H_{17}NO_5S$+Na$^+$]: 346.0720, found 346.0716.
IR (film): ν (cm^{-1}) 3288, 2948, 2869, 1738, 1706, 1587, 1451, 1302, 1249, 1210, 1172, 1133, 879, 760, 567.

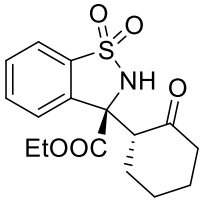


Name	Retention Time	Area	% Area
1	4.373	7366220	19.88
2	4.815	7547147	20.37
3	5.962	11008677	29.72
4	7.013	11122363	30.02



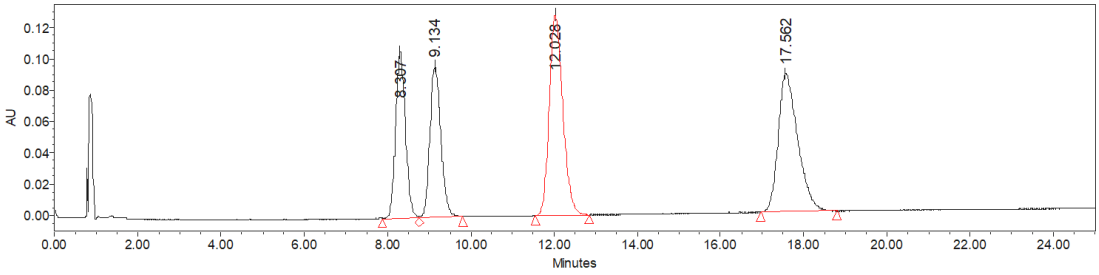
Name	Retention Time	Area	% Area
1	4.140	270974	2.84
2	4.484	9147872	95.80
3	5.665	87222	0.91
4	6.688	42685	0.45

Ethyl (*R*)-3-((*R*)-2-oxocyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **3ca**



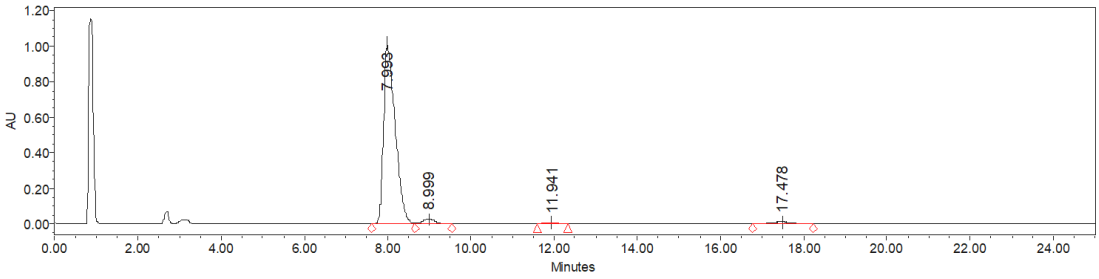
Result: white solid, m.p. 148 - 151 °C, 98% yield, 94% ee, >19:1 dr; [α]$^{27.2}_D$ = +164.6 (c = 1.14, CH_2Cl_2); SFC (Daicel chiralcel OX-3, CO_2/EtOH = 90/10, flow rate = 1.5 mL/min, λ = 210 nm), t_1 = 7.99 min, t_2 = 9.00 min, t_3 = 11.94 min, t_4 = 17.48 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.79 – 7.75 (m, 1H), 7.69 – 7.64 (m, 1H), 7.62 – 7.55 (m, 2H), 5.78 (s, 1H), 4.31 – 4.21 (m, 1H), 4.21 – 4.10 (m, 1H), 3.57 (dd, *J* = 12.8, 5.6 Hz, 1H), 2.52 – 2.42 (m, 1H), 2.41 – 2.30 (m, 1H), 2.10 – 2.02 (m, 1H), 1.87 – 1.79 (m, 1H), 1.76 – 1.56 (m, 3H), 1.43 – 1.35 (m, 1H), 1.25 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 209.9, 170.2, 135.2, 134.9, 133.7, 130.7, 123.7, 121.8, 68.7, 63.2, 58.2, 41.8, 26.7, 26.6, 24.3, 13.8.
HRMS (FTMS+c ESI) m/z: [M + Na]$^+$ calcd for [$C_{16}H_{19}NO_5S$+Na$^+$]: 360.0876, found 360.0866.
IR (film): ν (cm^{-1}) 3289, 2941, 2868, 1736, 1707, 1451, 1366, 1301, 1240, 1209, 1133, 886, 760, 567.



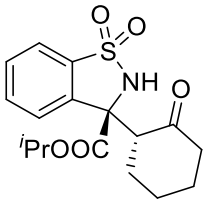
Name	Retention Time	Area	% Area
1	8.307	1753188	18.86

2	9.134	1765302	18.99
3	12.028	2895441	31.15
4	17.562	2881460	31.00



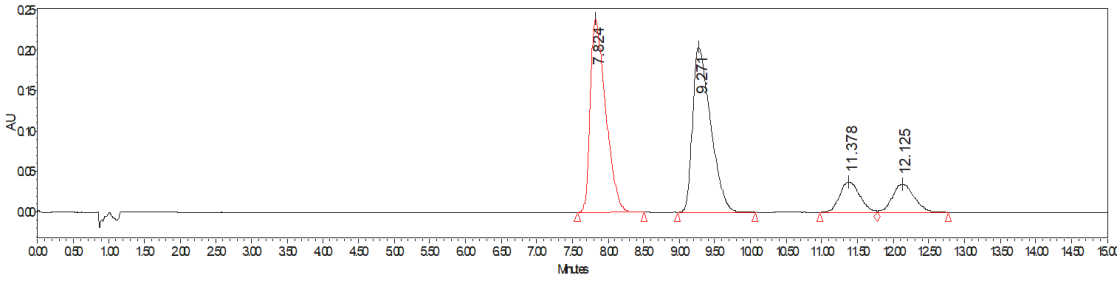
Name	Retention Time	Area	% Area
1	7.993	19835348	94.25
2	8.999	634354	3.01
3	11.941	134092	0.64
4	17.478	441464	2.10

Isopropyl (*R*)-3-((*R*)-2-oxocyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **3da**

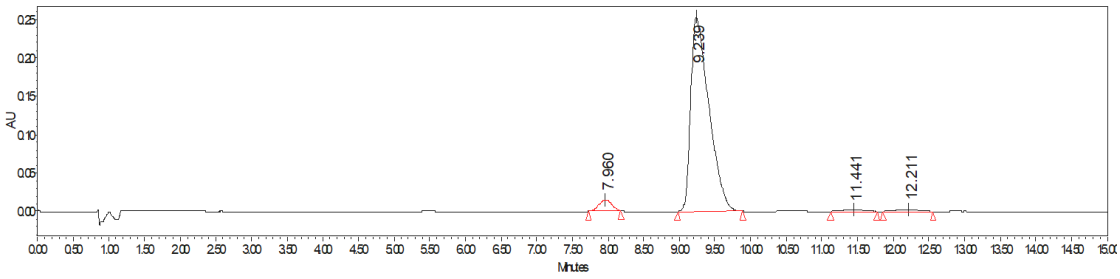


Result: white solid, m.p. 153 - 156 °C, 99% yield, 92% ee, >19:1 dr; $[\alpha]^{27.5}_{D}$ = +154.6 (c = 1.20, CH_2Cl_2); SFC (Daicel chiralcel IC-3, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm), t_1 = 7.96 min, t_2 = 9.24 min, t_3 = 11.44 min, t_4 = 12.21 min.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.78 (d, *J* = 7.8 Hz, 1H), 7.66 (t, *J* = 7.8 Hz, 1H), 7.59 (t, *J* = 7.8 Hz, 1H), 7.56 (d, *J* = 7.8 Hz, 1H), 5.75 (s, 1H), 5.03 – 4.97 (m, 1H), 3.54 (dd, *J* = 12.6, 5.4 Hz, 1H), 2.48 – 2.42 (m, 1H), 2.37 – 2.29 (m, 1H), 2.07 – 2.02 (m, 1H), 1.84 – 1.79 (m, 1H), 1.77 – 1.54 (m, 3H), 1.42 – 1.35 (m, 1H), 1.28 (d, *J* = 6.0 Hz, 3H), 1.17 (d, *J* = 6.0 Hz, 3H).
^{13}C NMR (150 MHz, Chloroform-*d*) δ 209.7, 169.6, 135.4, 135.2, 133.7, 130.7, 123.7, 121.9, 71.3, 58.2, 41.8, 26.7, 26.7, 24.3, 21.4, 21.3.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{17}H_{21}NO_5S+Na^+]$: 374.1033, found 374.1014.
IR (film): ν (cm^{-1}) 3291, 2942, 2870, 1733, 1708, 1468, 1376, 1211, 1172, 1103, 882, 760, 567.

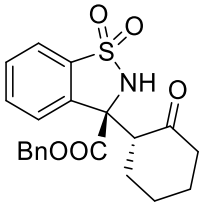


Name	Retention Time	Area	% Area
1	7.824	3584503	41.34
2	9.271	3603920	41.56
3	11.378	739379	8.53
4	12.125	742831	8.57



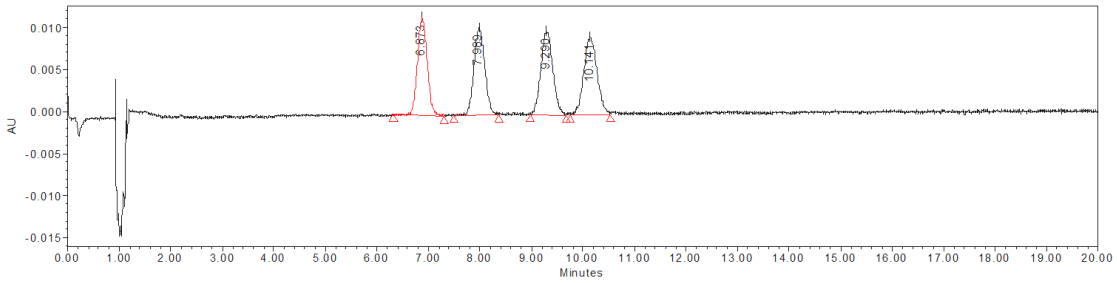
Name	Retention Time	Area	% Area
1	7.960	189081	3.95
2	9.239	4488337	93.73
3	11.441	51434	1.07
4	12.211	59948	1.25

Benzyl (*R*)-3-((*R*)-2-oxocyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **3ea**

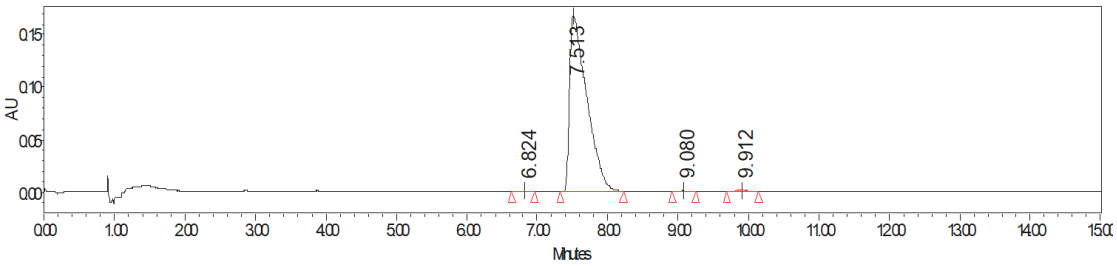


Result: Colorless oil, 96% yield, 99% ee, >19:1 dr; $[\alpha]^{26.7}_{D}$ = +174.5 (c = 1.11, CH_2Cl_2); SFC (Daicel chiralcel IC-3, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm), t_1 = 6.82 min, t_2 = 7.51 min, t_3 = 9.08 min, t_4 = 9.91 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.77 – 7.71 (m, 1H), 7.60 – 7.51 (m, 2H), 7.46 – 7.41 (m, 1H), 7.30 – 7.17 (m, 5H), 5.76 (s, 1H), 5.16 (d, *J* = 12.4 Hz, 1H), 5.08 (d, *J* = 12.4 Hz, 1H), 3.51 (dd, *J* = 12.4, 5.2 Hz, 1H), 2.47 – 2.38 (m, 1H), 2.35 – 2.21 (m, 1H), 2.05 – 1.96 (m, 1H), 1.82 – 1.73 (m, 1H), 1.72 – 1.48 (m, 3H), 1.40 – 1.31 (m, 1H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 210.0, 170.2, 135.4, 134.7, 134.6, 133.7, 130.8, 128.6, 128.6, 128.1, 123.8, 122.0, 68.8, 68.8, 58.2, 41.8, 26.8, 26.8, 24.3.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{21}H_{21}NO_5S+Na^+]$: 422.1033, found 422.1027.
IR (film): v (cm^{-1}) 3291, 2943, 2869, 1739, 1706, 1452, 1363, 1303, 1209, 1047, 884, 758, 736, 700, 566.

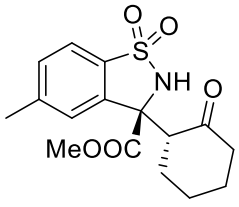


Name	Retention Time	Area	% Area
1	6.873	155695	24.48
2	7.989	154614	24.31
3	9.290	162463	25.54
4	10.141	163218	25.66



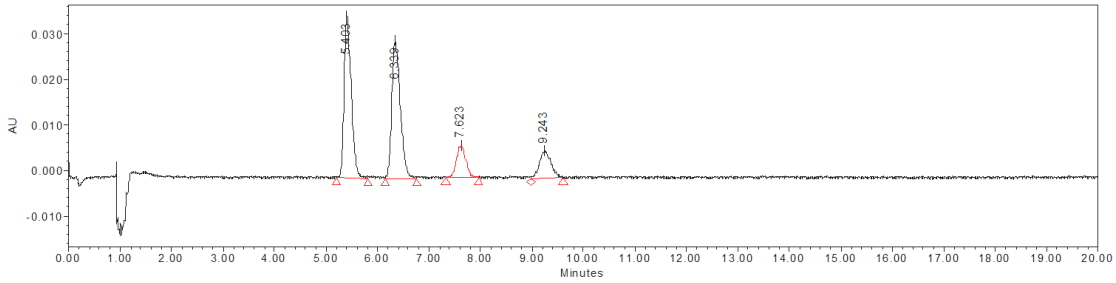
Name	Retention Time	Area	% Area
1	6.824	7815	0.27
2	7.513	2834768	98.65
3	9.080	12372	0.43
4	9.912	18488	0.64

Methyl (*R*)-5-methyl-3-((*R*)-2-oxocyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **3fa**

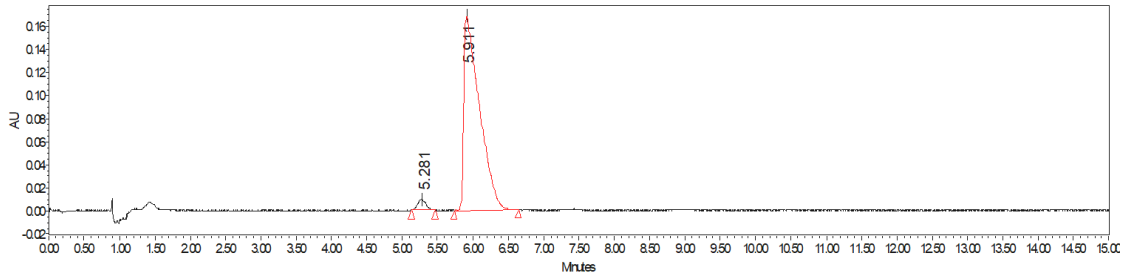


Result: white solid, m.p. 167 - 171 °C, 98% yield, 94% ee, >19:1 dr; $[\alpha]^{27.1}_D$ = +156.6 (c = 1.34, CH_2Cl_2); SFC (Daicel chiralcel IC-3, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm), t_1 = 5.28 min, t_2 = 5.91 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.65 (d, *J* = 8.0 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.32 (s, 1H), 5.73 (s, 1H), 3.77 (s, 3H), 3.56 (dd, *J* = 12.4, 4.4 Hz, 1H), 2.47 (s, 4H), 2.51 – 2.43 (m, 1H), 2.41 – 2.32 (m, 1H), 2.10 – 2.02 (m, 1H), 1.88 – 1.80 (m, 1H), 1.77 – 1.56 (m, 3H), 1.45 – 1.38 (m, 1H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 210.2, 171.0, 145.0, 135.0, 132.6, 131.8, 123.8, 121.6, 68.4, 58.4, 53.9, 41.8, 26.7, 26.6, 24.3, 21.8.
HRMS (FTMS+c ESI) m/z: $[M + H]^+$ calcd for $[C_{16}H_{19}NO_5S+H^+]$: 338.1056, found 338.1059.
IR (film): ν (cm^{-1}) 3280, 2947, 2868, 1739, 1706, 1599, 1451, 1364, 1301, 1247, 1188, 1144, 1046, 894, 734, 661, 570.

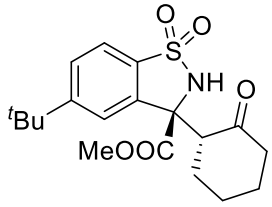


Name	Retention Time	Area	% Area
1	5.403	344024	39.54
2	6.339	345230	39.68
3	7.623	89889	10.33
4	9.243	90899	10.45



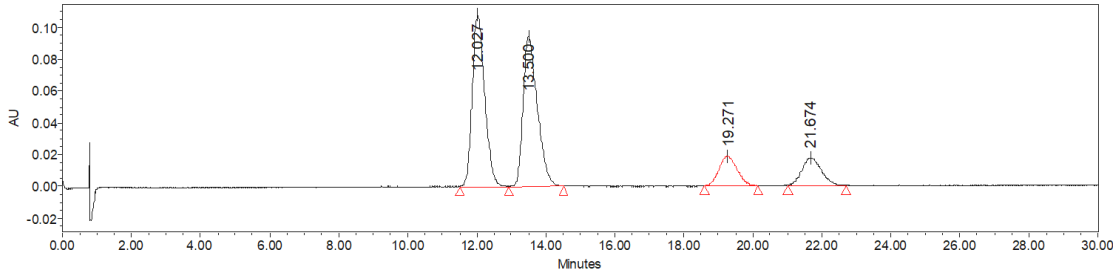
Name	Retention Time	Area	% Area
1	5.281	74280	2.80
2	5.911	2581941	97.20

Methyl (*R*)-5-(tert-butyl)-3-((*R*)-2-oxocyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **3ga**

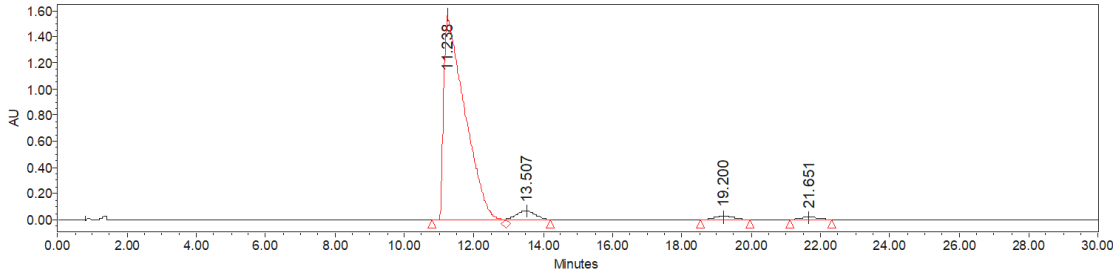


Result: white solid, m.p. 156 - 158 °C, 98% yield, 93% ee, >19:1 dr; $[\alpha]^{26.5}_D$ = +141.4 (c = 0.90, CH_2Cl_2); SFC (Daicel chiralcel OX-3, CO_2/EtOH = 90/10, flow rate = 1.5 mL/min, λ = 230 nm), t_1 = 11.24 min, t_2 = 13.51 min, t_3 = 19.20 min, t_4 = 21.65 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.72 – 7.67 (m, 1H), 7.66 – 7.60 (m, 1H), 7.52 – 7.47 (m, 1H), 5.74 (s, 1H), 3.77 (s, 3H), 3.59 (dd, *J* = 12.0, 5.2 Hz, 1H), 2.52 – 2.44 (m, 1H), 2.42 – 2.33 (m, 1H), 2.10 – 2.02 (m, 1H), 1.88 – 1.81 (m, 1H), 1.78 – 1.56 (dd, *J* = 42.3, 11.4 Hz, 4H), 1.44 – 1.37 (m, 1H), 1.34 (s, 9H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 210.2, 171.0, 158.4, 134.8, 132.5, 128.5, 121.4, 119.9, 68.6, 58.41, 53.8, 41.8, 31.1, 26.7, 26.6, 24.3.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{19}H_{25}NO_5S+Na^+]$: 402.1346, found 402.1335.
IR (film): ν (cm^{-1}) 3288, 2956, 2870, 1740, 1707, 1597, 1366, 1302, 1248, 1199, 1149, 1100, 836, 735, 628.

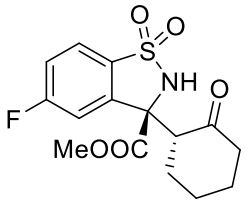


Name	Retention Time	Area	% Area
1	12.027	2702111	39.97
2	13.500	2702176	39.97
3	19.271	679441	10.05
4	21.674	676660	10.01



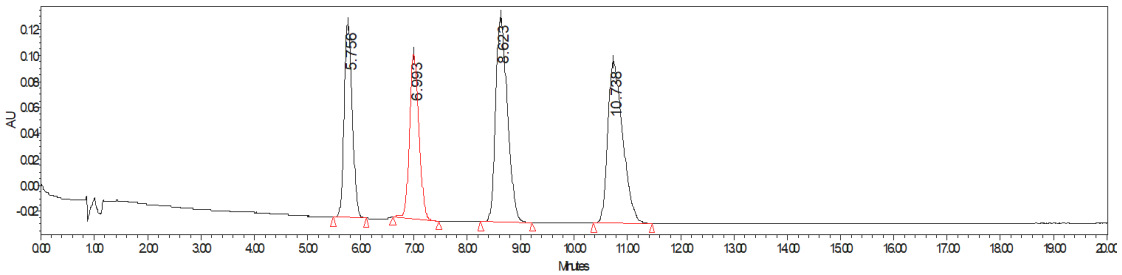
Name	Retention Time	Area	% Area
1	11.238	65374313	94.23
2	13.507	2446955	3.53
3	19.200	984653	1.42
4	21.651	573283	0.83

Methyl (*R*)-5-fluoro-3-((*R*)-2-oxocyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **3ha**



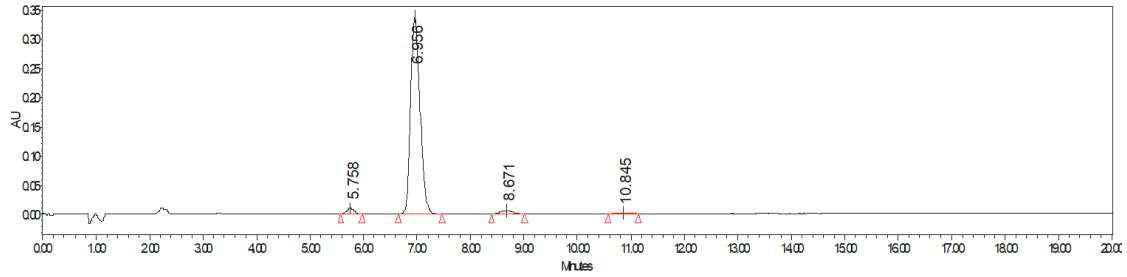
Result: white solid, m.p. 159 - 163 °C, 98% yield, 95% ee, >19:1 dr; $[\alpha]^{27.3}_{D}$ = +151.5 (c = 1.25, CH_2Cl_2); SFC (Daicel chiralcel IC-3, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 230 nm), t_1 = 5.76 min, t_2 = 6.96 min, t_3 = 8.67 min, t_4 = 10.85 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.78 (dd, *J* = 8.8, 4.8 Hz, 1H), 7.29 (td, *J* = 8.4, 2.0 Hz, 1H), 7.24 (dd, *J* = 8.0, 2.0 Hz, 1H), 5.92 (s, 1H), 3.78 (s, 3H), 3.53 (dd, *J* = 12.8, 5.6 Hz, 1H), 2.51 – 2.43 (m, 1H), 2.42 – 2.32 (m, 1H), 2.13 – 2.03 (m, 1H), 1.89 – 1.81 (m, 1H), 1.79 – 1.57 (m, 3H), 1.47 – 1.39 (m, 1H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 209.8, 170.4, 165.7 (d, *J* = 254.7 Hz), 137.9 (d, *J* = 9.3 Hz), 131.3 (d, *J* = 2.7 Hz), 124.2 (d, *J* = 9.8 Hz), 118.9 (d, *J* = 24.0 Hz), 111.0 (d, *J* = 24.6 Hz), 68.1 (d, *J* = 2.1 Hz), 58.4, 54.1 (d, *J* = 2.6 Hz), 41.7, 26.6, 26.5, 24.2.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -102.6.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{15}H_{16}FNO_5S+Na^+]$: 364.0625, found 364.0608.
IR (film): ν (cm^{-1}) 3280, 2949, 2869, 1737, 1706, 1593, 1477, 1362, 1305, 1237, 1178, 1128, 873, 735, 570.



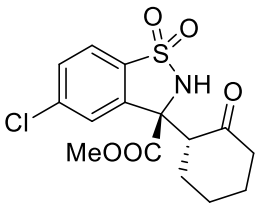
Name	Retention Time	Area	% Area
1	5.756	1561533	19.61
2	6.993	1552411	19.49
3	8.623	2423769	30.43

4	10.738	2426155	30.46



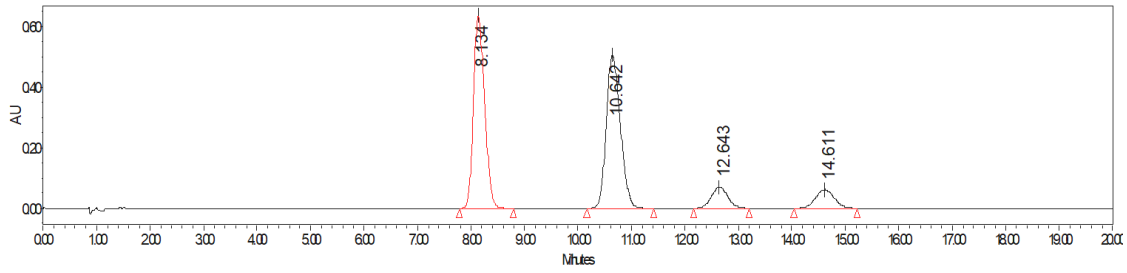
Name	Retention Time	Area	% Area
1	5.758	98465	2.26
2	6.956	4127015	94.93
3	8.671	92896	2.14
4	10.845	29072	0.67

Methyl (*R*)-5-chloro-3-((*R*)-2-oxocyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **3ia**

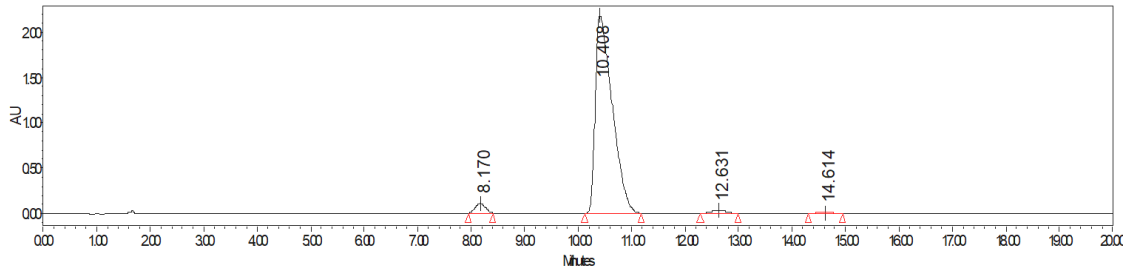


Result: white solid, m.p. 175 - 179 °C, 98% yield, 94% ee, >19:1 dr; $[\alpha]^{27.3}_{D}$ = +136.6 (c = 1.26, CH_2Cl_2); SFC (Daicel chiralcel IC-3, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 230 nm), t_1 = 8.17 min, t_2 = 10.41 min, t_3 = 12.63 min, t_4 = 14.61 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.75 – 7.69 (m, 1H), 7.60 – 7.52 (m, 2H), 5.87 (s, 1H), 3.79 (s, 3H), 3.55 (dd, *J* = 12.4, 4.8 Hz, 1H), 2.54 – 2.44 (m, 1H), 2.42 – 2.31 (m, 1H), 2.13 – 2.04 (m, 1H), 1.92 – 1.80 (m, 1H), 1.80 – 1.56 (m, 3H), 1.48 – 1.38 (m, 1H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 209.8, 170.4, 140.3, 136.8, 133.8, 131.4, 124.0, 123.1, 68.2, 58.4, 54.2, 41.8, 26.7, 26.6, 24.2.
HRMS (FTMS+c ESI) m/z: $[M + H]^+$ calcd for $[C_{15}H_{16}Cl^{34.9689}NO_5S+H^+]$: 358.0510, found 358.0509.
HRMS (FTMS+c ESI) m/z: $[M + H]^+$ calcd for $[C_{15}H_{16}Cl^{36.9659}NO_5S+H^+]$: 360.0481, found 360.0474.
IR (film): ν (cm^{-1}) 3271, 2948, 2869, 1737, 1706, 1587, 1306, 1204, 1174, 1137, 1088, 883, 826, 735, 610, 570.



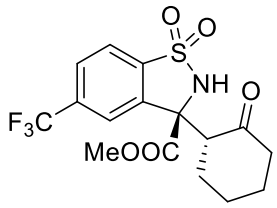
Name	Retention Time	Area	% Area
1	8.134	9198199	42.96
2	10.642	9228550	43.10
3	12.643	1493652	6.98
4	14.611	1492171	6.97



Name	Retention Time	Area	% Area
1	8.170	1388502	2.77
2	10.408	47917207	95.48

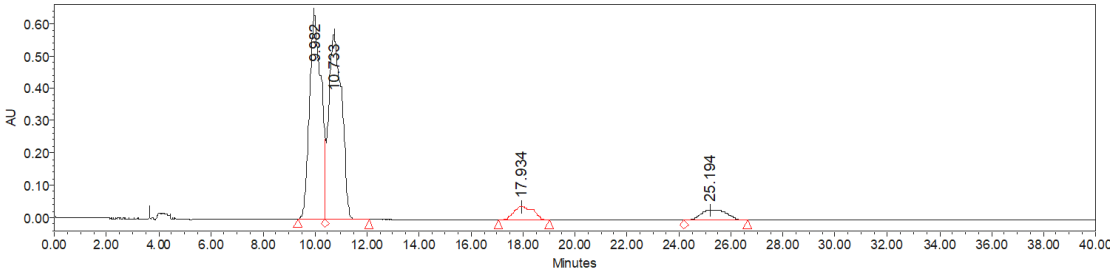
3	12.631	630869	1.26
4	14.614	247943	0.49

Methyl (*R*)-3-((*R*)-2-oxocyclohexyl)-5-(trifluoromethyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **3ja**

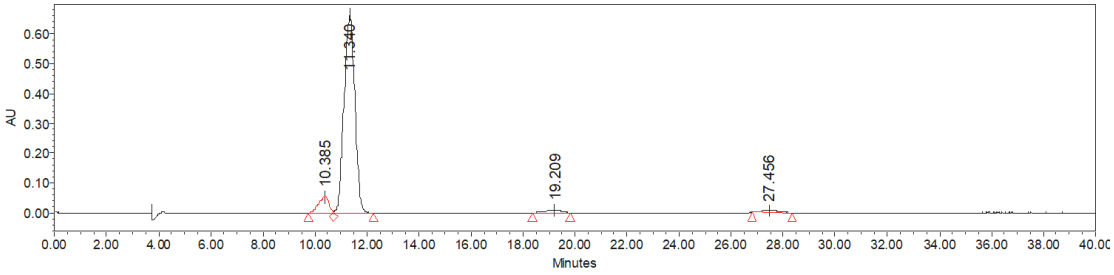


Result: white solid, m.p. 158 - 162 °C, 98% yield, 86% ee, >19:1 dr; $[\alpha]^{27.1}_{D}$ = +125.8 (c = 1.11, CH_2Cl_2); SFC (Lux 5u Cellulose-1, CO_2/EtOH = 95/5, flow rate = 0.8 mL/min, λ = 230 nm), t_1 = 10.38 min, t_2 = 11.34 min, t_3 = 19.21 min, t_4 = 27.46 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.94 (d, *J* = 8.0 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.83 (s, 1H), 5.97 (s, 1H), 3.80 (s, 3H), 3.63 (dd, *J* = 12.4, 4.8 Hz, 1H), 2.55 – 2.46 (m, 1H), 2.46 – 2.35 (m, 1H), 2.15 – 2.05 (m, 1H), 1.92 – 1.82 (m, 1H), 1.81 – 1.59 (m, 4H), 1.43 – 1.34 (m, 1H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 209.8, 170.2, 138.5, 135.9, 135.9 (q, *J* = 33.2 Hz), 128.2 (q, *J* = 3.4 Hz), 122.9, 122.8 (q, *J* = 271.9 Hz), 121.2 (q, *J* = 3.8 Hz), 68.6, 58.4, 54.3, 41.8, 26.6, 24.2.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.7.
HRMS (FTMS+c ESI) m/z: $[M + H]^+$ calcd for $[C_{16}H_{16}F_3NO_5S+H^+]$: 392.0774, found 392.0771.
IR (film): ν (cm^{-1}) 3270, 2951, 2871, 1737, 1707, 1423, 1329, 1253, 1173, 1134, 1086, 1077, 823, 710.

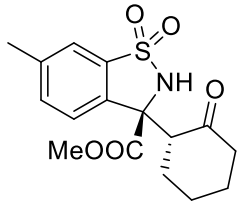


Name	Retention Time	Area	% Area
1	9.982	19662423	44.83
2	10.733	19785727	45.11
3	17.934	2196231	5.01
4	25.194	2213040	5.05



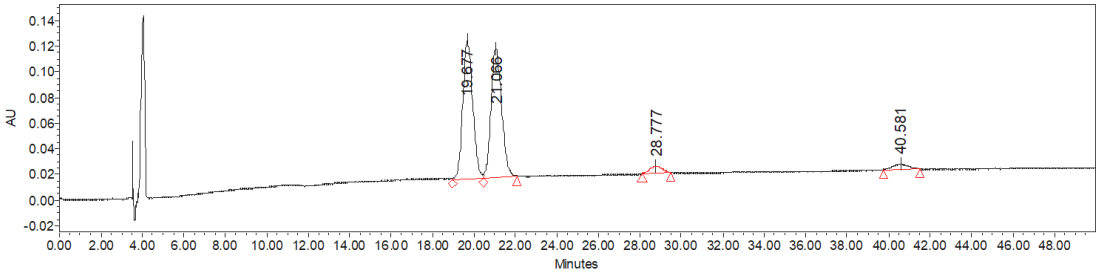
Name	Retention Time	Area	% Area
1	10.385	1475428	6.88
2	11.340	19347315	90.20
3	19.209	326301	1.52
4	27.456	299294	1.40

Methyl (*R*)-6-methyl-3-((*R*)-2-oxocyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **3ka**

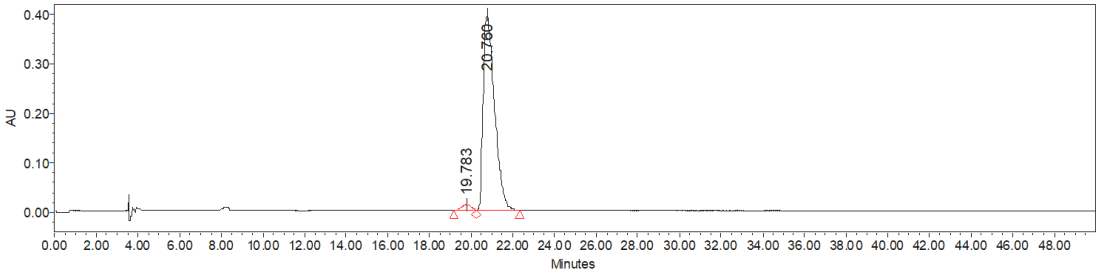


Result: white solid, m.p. 194 - 197 °C, 99% yield, 95% ee, >19:1 dr; $[\alpha]^{24.5}_{D}$ = +168.2 (c = 0.98, CH_2Cl_2); SFC (Lux 5u Cellulose-1, CO_2/^{i}PrOH = 90/10, flow rate = 0.8 mL/min, λ = 230 nm), t_1 = 19.78 min, t_2 = 20.76 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.57 (s, 1H), 7.44 (q, *J* = 8.0 Hz, 2H), 5.75 (s, 1H), 3.75 (s, 3H), 3.56 (dd, *J* = 12.0, 4.8 Hz, 1H), 2.44 (s, 3H), 2.50 – 2.42 (m, 1H), 2.40 – 2.31 (m, 1H), 2.10 – 2.02 (m, 1H), 1.87 – 1.79 (m, 1H), 1.78 – 1.54 (m, 3H), 1.46 – 1.38 (m, 1H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 210.2, 171.0, 141.6, 135.2, 134.9, 131.9, 123.4, 121.8, 68.3, 58.2, 53.8, 41.8, 26.7, 26.6, 24.3, 21.2.
HRMS (FTMS+c ESI) m/z: [M + Na]$^{+}$ calcd for [$C_{16}H_{19}NO_5S$+Na^{+}]: 360.0876, found 360.0870.
IR (film): ν (cm^{-1}) 3285, 2948, 2868, 1744, 1705, 1490, 1451, 1363, 1301, 1165, 1022, 891, 787, 735, 571.

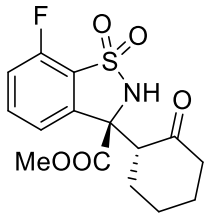


Name	Retention Time	Area	% Area
1	19.677	3586177	47.17
2	21.066	3583042	47.13
3	28.777	218093	2.87
4	40.581	214711	2.82



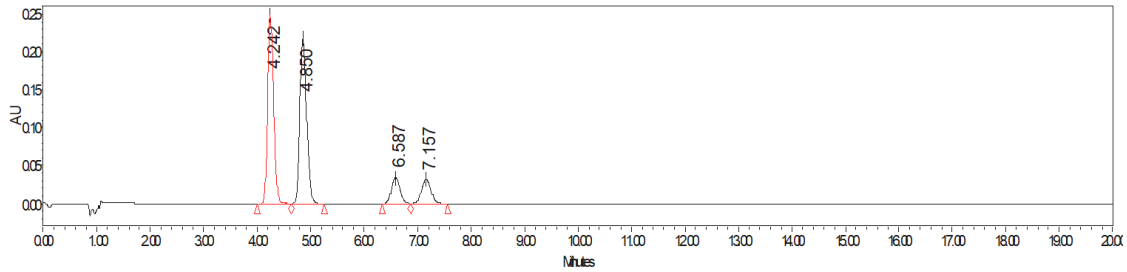
Name	Retention Time	Area	% Area
1	19.783	374308	2.47
2	20.760	14783435	97.53

Methyl (*R*)-7-fluoro-3-((*R*)-2-oxocyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **3la**

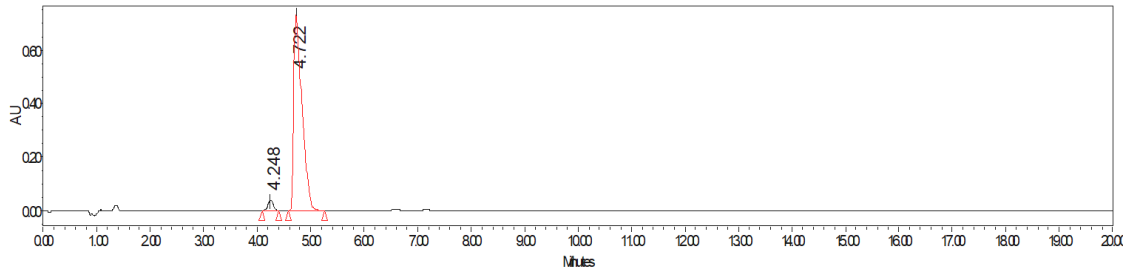


Result: white solid, m.p. 137 - 141 °C, 98% yield, 93% ee, >19:1 dr; [α]$^{24.4}_{D}$ = +135.9 (c = 1.01, CH_2Cl_2); SFC (Daicel chiralcel IC-3, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 230 nm), t_1 = 4.25 min, t_2 = 4.72 min.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.68 (td, *J* = 7.8, 4.8 Hz, 1H), 7.37 (d, *J* = 7.8 Hz, 1H), 7.27 (d, *J* = 7.8 Hz, 1H), 5.88 (s, 1H), 3.80 (s, 3H), 3.59 (dd, *J* = 13.2, 5.4 Hz, 1H), 2.52 – 2.47 (m, 1H), 2.42 – 2.35 (m, 1H), 2.11 – 2.07 (m, 1H), 1.91 – 1.85 (m, 1H), 1.81 – 1.74 (m, 1H), 1.69 – 1.58 (m, 2H), 1.49 – 1.43 (m, 1H).
^{13}C NMR (150 MHz, Chloroform-*d*) δ 209.8, 170.4, 156.5 (d, *J* = 258.6 Hz), 138.0, 136.2 (d, *J* = 7.3 Hz), 123.4 (d, *J* = 19.6 Hz), 119.5 (d, *J* = 4.0 Hz), 117.6 (d, *J* = 18.0 Hz), 68.7, 58.4, 54.1, 41.8, 26.7, 24.2.
^{19}F NMR (564 MHz, Chloroform-*d*) δ -113.9.
HRMS (FTMS+c ESI) m/z: [M + H]$^{+}$ calcd for [$C_{15}H_{16}FNO_5S$+H^{+}]: 342.0806, found 342.0802.
IR (film): ν (cm^{-1}) 3270, 2949, 2869, 1745, 1706, 1594, 1473, 1311, 1232, 1179, 771, 735, 592.

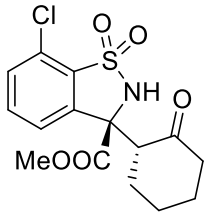


Name	Retention Time	Area	% Area
1	4.242	1930230	41.44
2	4.850	1927503	41.38
3	6.587	396326	8.51
4	7.157	404068	8.67



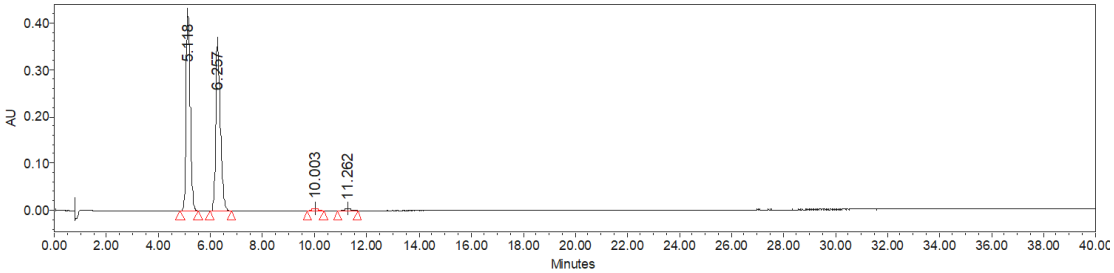
Name	Retention Time	Area	% Area
1	4.248	286765	3.54
2	4.722	7803373	96.46

Methyl (*R*)-7-chloro-3-((*R*)-2-oxocyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **3ma**

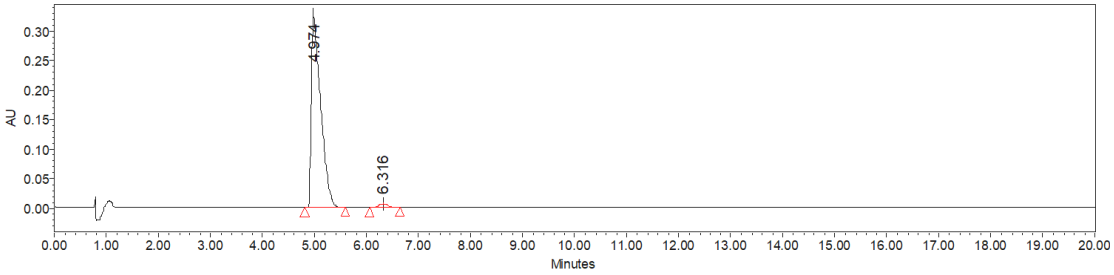


Result: white solid, m.p. 189 - 192 °C, 97% yield, 95% ee, >19:1 dr; $[\alpha]^{24.3}_{D}$ = +170.7 (c = 1.12, CH_2Cl_2); SFC (Daicel chiralcel OX-3, CO_2/EtOH = 80/20, flow rate = 1.5 mL/min, λ = 230 nm), t_1 = 4.97 min, t_2 = 6.32 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.60 (t, *J* = 7.6 Hz, 1H), 7.53 (d, *J* = 7.6 Hz, 1H), 7.47 (d, *J* = 7.6 Hz, 1H), 5.88 (s, 1H), 3.78 (s, 3H), 3.57 (dd, *J* = 12.8, 5.2 Hz, 1H), 2.52 – 2.43 (m, 1H), 2.42 – 2.31 (m, 1H), 2.13 – 2.03 (m, 1H), 1.89 – 1.81 (m, 1H), 1.81 – 1.56 (m, 3H), 1.47 – 1.39 (m, 1H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 209.8, 170.4, 137.4, 134.8, 133.1, 131.5, 129.6, 122.1, 67.7, 58.3, 54.1, 41.8, 26.6, 24.2.
HRMS (FTMS+c ESI) m/z: $[M + H]^+$ calcd for $[C_{15}H_{16}Cl^{34.9689}NO_5S+H^+]$: 358.0510, found 358.0512.
HRMS (FTMS+c ESI) m/z: $[M + H]^+$ calcd for $[C_{15}H_{16}Cl^{36.9659}NO_5S+H^+]$: 360.0481, found 360.0478.
IR (film): ν (cm^{-1}) 3270, 2948, 2869, 1744, 1706, 1588, 1454, 1263, 1229, 1172, 1137, 881, 735, 580.

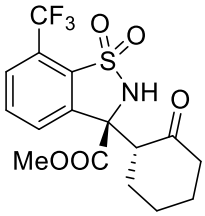


Name	Retention Time	Area	% Area
1	5.118	4576090	49.07
2	6.257	4575973	49.06
3	10.003	89653	0.96
4	11.262	84828	0.91



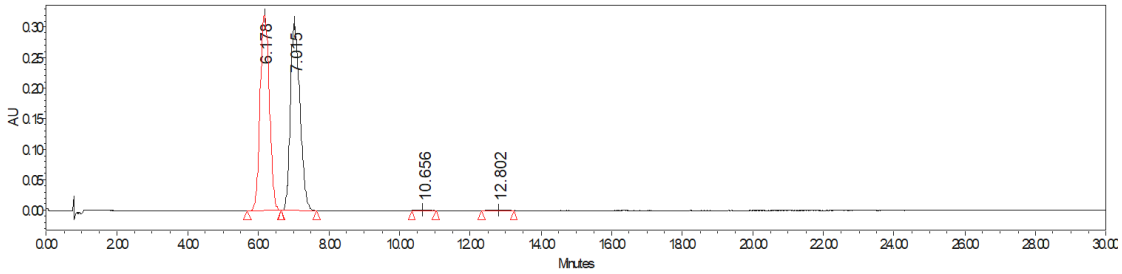
Name	Retention Time	Area	% Area
1	4.974	4065404	97.64
2	6.316	98398	2.36

Methyl (*R*)-3-((*R*)-2-oxocyclohexyl)-7-(trifluoromethyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **3na**

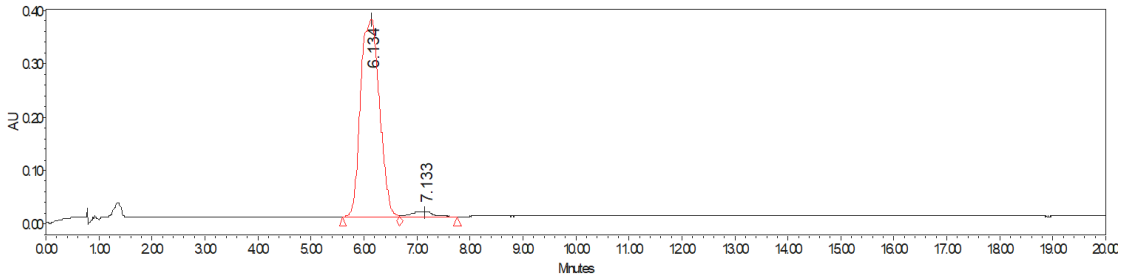


Result: white solid, m.p. 174 - 177 °C, 97% yield, 95% ee, >19:1 dr; $[\alpha]^{25.1}_{D}$ = +151.2 (c = 1.34, CH_2Cl_2); SFC (Daicel chiralcel OX-3, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 230 nm), t_1 = 6.13 min, t_2 = 7.13 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.89 – 7.79 (m, 3H), 5.95 (s, 1H), 3.79 (s, 3H), 3.60 (dd, *J* = 12.4, 4.4 Hz, 1H), 2.54 – 2.45 (m, 1H), 2.44 – 2.32 (m, 1H), 2.13 – 2.04 (m, 1H), 1.91 – 1.82 (m, 1H), 1.81 – 1.54 (m, 3H), 1.45 – 1.36 (m, 1H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 209.6, 170.4, 137.3, 134.1, 133.1, 128.7 (q, *J* = 4.6 Hz), 127.8, 126.3 (d, *J* = 35.9 Hz), 122.1 (d, *J* = 272.9 Hz), 68.1, 58.4, 54.2, 41.7, 26.7, 26.6, 24.2.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -59.5.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{16}H_{16}F_3NO_5S+Na^+]$: 414.0593, found 414.0586.
IR (film): ν (cm^{-1}) 3286, 2950, 2870, 1739, 1704, 1589, 1438, 1327, 1267, 1234, 1019, 882, 773, 737, 583.

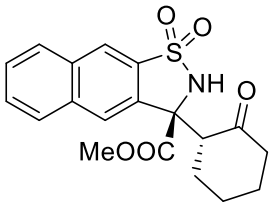


Name	Retention Time	Area	% Area
1	6.178	5838818	49.76
2	7.015	5830271	49.69
3	10.656	31961	0.27
4	12.802	32441	0.28



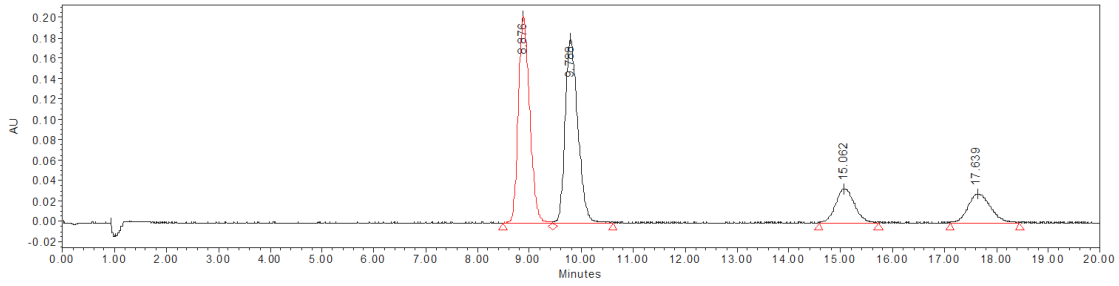
Name	Retention Time	Area	% Area
1	6.134	9140954	97.33
2	7.133	250801	2.67

Methyl (*R*)-3-((*R*)-2-oxocyclohexyl)-2,3-dihydronaphtho[2,3-d]isothiazole-3-carboxylate 1,1-dioxide **3oa**

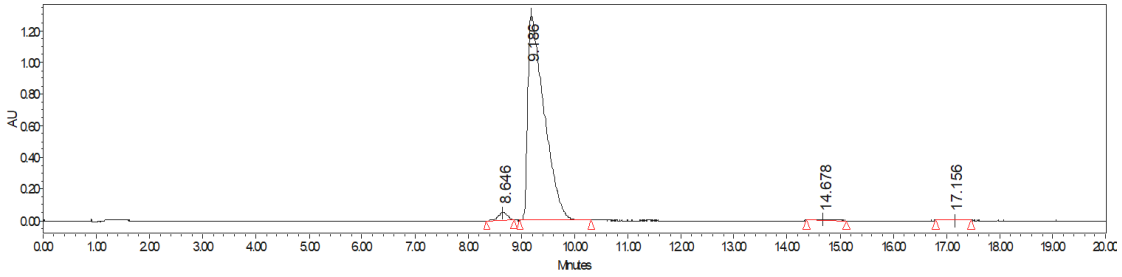


Result: white solid, m.p. 204 - 207 °C, 99% yield, 96% ee, >19:1 dr; $[\alpha]^{25.4}_{D}$ = +200.0 (c = 1.42, CH_2Cl_2); SFC (Daicel chiralcel IC-3, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm), t_1 = 8.65 min, t_2 = 9.19 min, t_3 = 14.68 min, t_2 = 17.16 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.39 (d, *J* = 8.0 Hz, 1H), 8.11 (d, *J* = 8.4 Hz, 1H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.70 (dt, *J* = 25.6, 7.2 Hz, 2H), 7.56 (d, *J* = 8.4 Hz, 1H), 5.94 (s, 1H), 3.78 (s, 3H), 3.70 (dd, *J* = 12.4, 4.8 Hz, 1H), 2.54 – 2.46 (m, 1H), 2.45 – 2.34 (m, 1H), 2.11 – 2.02 (m, 1H), 1.87 – 1.56 (m, 4H), 1.45 – 1.37 (m, 1H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 210.0, 170.7, 135.0, 133.9, 133.7, 130.7, 129.4, 128.6, 128.4, 125.3, 123.1, 119.1, 68.6, 57.9, 54.0, 41.8, 26.6, 24.2.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{19}H_{19}NO_5S+Na^+]$: 396.0876, found 396.0872.
IR (film): v (cm^{-1}) 3280, 2947, 2868, 1741, 1706, 1434, 1356, 1253, 1220, 1158, 1132, 867, 828, 763, 735, 577.

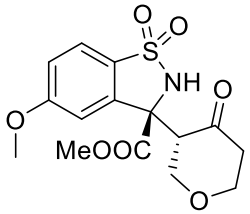


Name	Retention Time	Area	% Area
1	8.876	3046795	39.23
2	9.788	3047838	39.25
3	15.062	828433	10.67
4	17.639	843019	10.86



Name	Retention Time	Area	% Area
1	8.646	587263	2.05
2	9.186	27921331	97.42
3	14.678	102545	0.36
4	17.156	50226	0.18

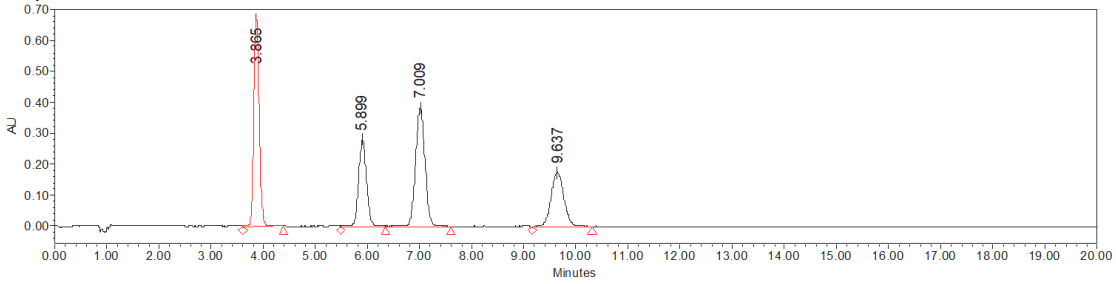
Methyl (*R*)-5-methoxy-3-((*S*)-4-oxotetrahydro-2H-pyran-3-yl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **3ab**



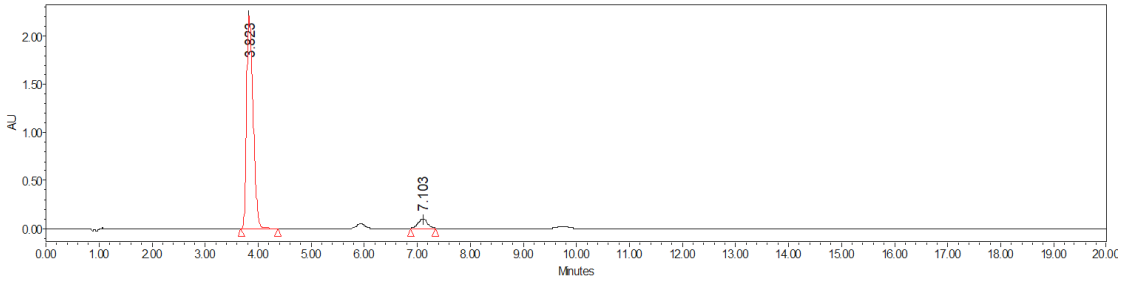
Result: colorless oil, 98% yield, 88% ee, >19:1 dr; $[\alpha]^{24.3}_{D}$ = +117.6 (c = 1.43, CH_2Cl_2); SFC (Daicel chiralcel IC-3, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 230 nm), t_1 = 3.82 min, t_2 = 7.10 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.68 (d, *J* = 8.8 Hz, 1H), 7.11 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.01 (d, *J* = 2.4 Hz, 1H), 5.78 (s, 1H), 4.26 (dd, *J* = 11.6, 7.6 Hz, 1H), 3.89 (s, 3H), 3.82 (s, 3H), 3.83 – 3.78 (m, 1H), 3.72 – 3.62 (m, 3H), 2.77 – 2.67 (m, 1H), 2.48 – 2.42 (m, 1H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 205.4, 170.0, 164.2, 136.1, 127.0, 123.4, 117.9, 107.9, 67.7, 66.0, 57.9, 56.1, 54.2, 42.3.

HRMS (FTMS+c ESI) m/z: $[M + H]^+$ calcd for $[C_{15}H_{17}NO_7S+H^+]$: 356.0798, found 356.0792.
IR (film): v (cm^{-1}) 3274, 2957, 2872, 1746, 1713, 1599, 1486, 1290, 1241, 1187, 1136, 900, 735, 577.

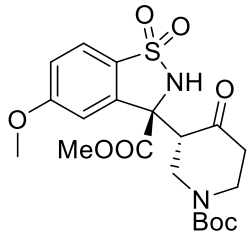


Name	Retention Time	Area	% Area
3.865	4786874	30.97	3.865
5.899	2929258	18.95	5.899
7.009	4796812	31.04	7.009
9.637	2941725	19.03	9.637



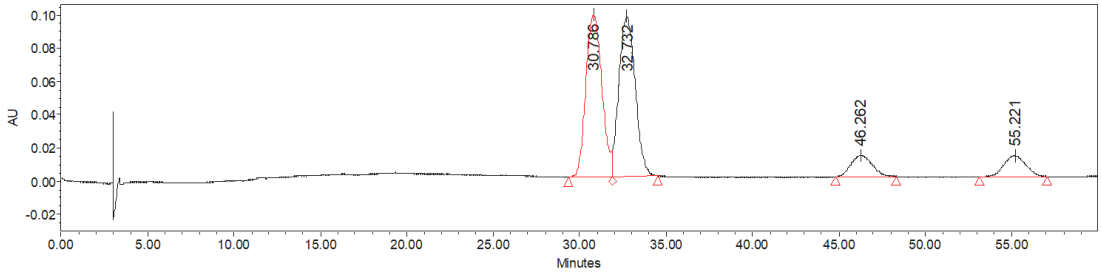
Name	Retention Time	Area	% Area
3.823	18875201	93.98	3.823
7.103	1208679	6.02	7.103

Methyl (*R*)-3-((*R*)-1-(tert-butoxycarbonyl)-4-oxopiperidin-3-yl)-5-methoxy-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide
3ac

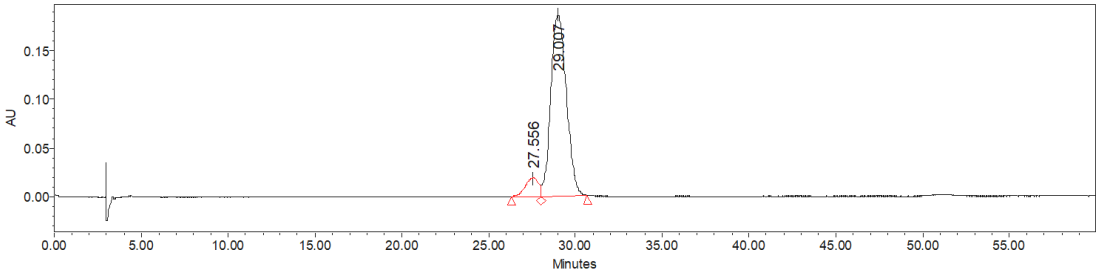


Result: colorless oil, 97% yield, 84% ee, >19:1 dr; $[\alpha]^{24.7}_D$ = +100.3 (c = 1.21, CH_2Cl_2); SFC (Lux 5u Cellulose-1, CO_2/EtOH = 95/5, flow rate = 1.0 mL/min, λ = 230 nm), t_1 = 27.55 min, t_2 = 29.00 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.78 – 7.61 (m, 1H), 7.11 (d, *J* = 8.4 Hz, 1H), 7.03 (d, *J* = 2.4 Hz, 1H), 5.78 (s, 1H), 4.50 – 4.20 (m, 1H), 3.88 (s, 3H), 3.81 (s, 3H), 3.86 – 3.46 (m, 2H), 3.16 – 2.88 (m, 2H), 2.62 – 2.47 (m, 1H), 2.46 – 2.39 (m, 1H), 1.37 (s, 9H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 206.4, 170.1, 164.2, 154.1, 136.3, 127.0, 123.4, 117.0, 108.2, 80.7, 66.5, 57.8, 56.0, 54.2, 43.9, 43.1, 41.2, 28.1.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{20}H_{26}N_2O_8S+Na^+]$: 477.1302, found 477.1294.
IR (film): v (cm^{-1}) 3273, 2976, 1740, 1699, 1599, 1484, 1423, 1367, 1305, 1249, 1137, 1020, 855, 735, 578.

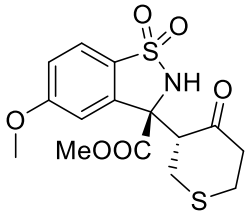


Name	Retention Time	Area	% Area
1	30.786	6311936	42.49
2	32.732	6356623	42.79
3	46.262	1093055	7.36
4	55.221	1093472	7.36



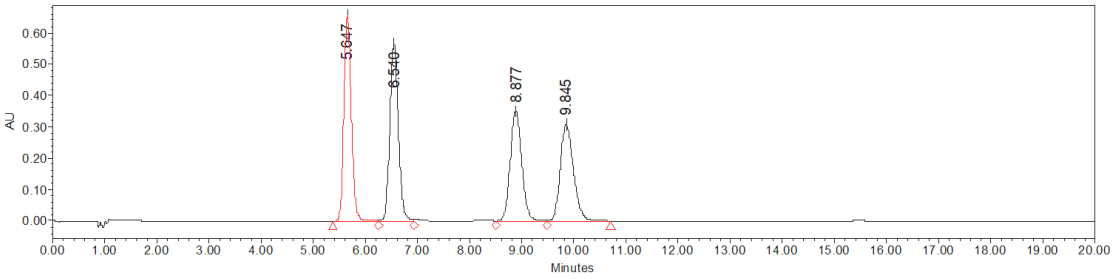
Name	Retention Time	Area	% Area
1	27.556	1017479	8.06
2	29.007	11602076	91.94

Methyl (*R*)-5-methoxy-3-((*R*)-4-oxotetrahydro-2H-thiopyran-3-yl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **3ad**

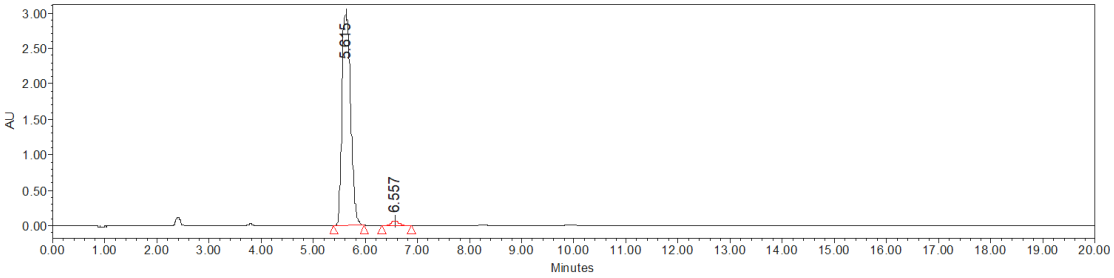


Result: colorless oil, 95% yield, 96% ee, >19:1 dr; $[\alpha]^{24.1}_{D}$ = +142.7 (c = 1.46, CH_2Cl_2); SFC (Daicel chiralcel IC-3, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 230 nm), t_1 = 5.61 min, t_2 = 6.56 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.69 (d, *J* = 8.8 Hz, 1H), 7.11 (dd, *J* = 8.8, 1.6 Hz, 1H), 7.00 – 6.97 (m, 1H), 5.80 (s, 1H), 3.89 (s, 3H), 3.90 – 3.84 (m, 1H), 3.78 (s, 3H), 3.04 – 2.92 (m, 2H), 2.91 – 2.72 (m, 3H), 2.24 (dt, *J* = 13.6, 3.6 Hz, 1H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 207.4, 170.2, 164.2, 136.4, 127.3, 123.5, 117.6, 107.9, 67.9, 60.6, 56.0, 54.1, 44.5, 29.8, 29.5.
HRMS (FTMS+c ESI) m/z: [M + Na]$^+$ calcd for [$C_{15}H_{17}NO_6S_2$+Na$^+$]: 394.0389, found 394.0369.
IR (film): ν (cm^{-1}) 3280, 2954, 2843, 1748, 1707, 1599, 1486, 1434, 1302, 1257, 1185, 1133, 1017, 897, 832, 735, 710, 757.

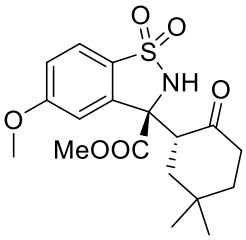


Name	Retention Time	Area	% Area
1	5.647	6475799	27.29
2	6.540	6457352	27.21
3	8.877	5403142	22.77
4	9.845	5396951	22.74



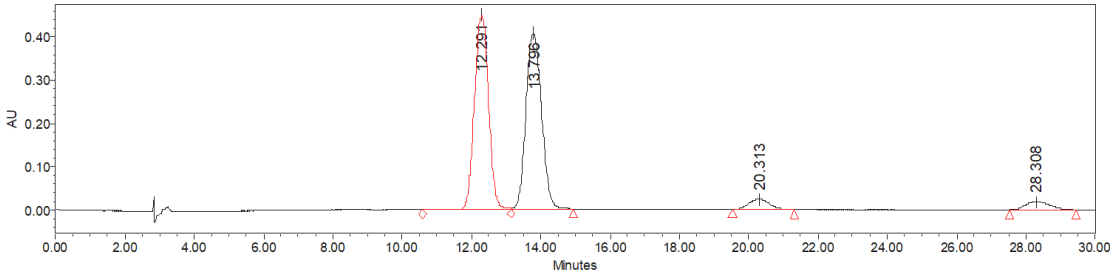
Name	Retention Time	Area	% Area
1	5.615	34854222	97.96
2	6.557	725922	2.04

Methyl (*R*)-3-((*R*)-5,5-dimethyl-2-oxocyclohexyl)-5-methoxy-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **3ae**

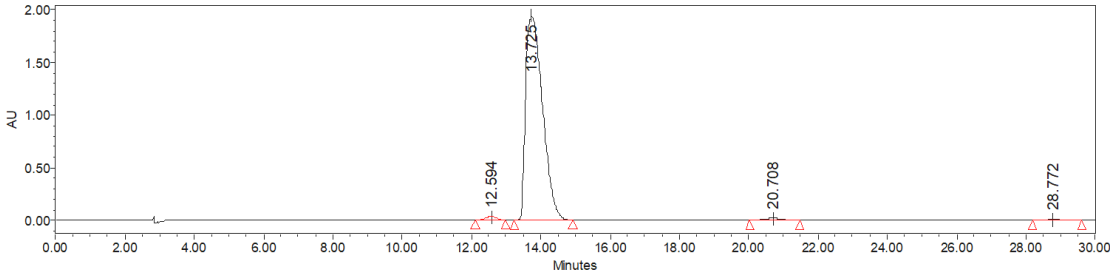


Result: colorless oil, 99% yield, 97% ee, >19:1 dr; $[\alpha]^{24.9}_{D}$ = +168.2 (c = 1.28, CH_2Cl_2); SFC ((Lux 5u Cellulose-1, CO_2/^{i}PrOH = 90/10, flow rate = 1.0 mL/min, λ = 230 nm), t_1 = 12.59 min, t_2 = 13.72 min, t_3 = 20.71 min, t_2 = 28.77 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.67 (d, *J* = 8.8 Hz, 1H), 7.09 (dd, *J* = 8.8, 2.0 Hz, 1H), 6.92 (d, *J* = 2.0 Hz, 1H), 5.72 (s, 1H), 3.87 (s, 3H), 3.77 (s, 3H), 3.67 (dd, *J* = 13.6, 5.2 Hz, 1H), 2.58 – 2.46 (m, 1H), 2.36 – 2.28 (m, 1H), 1.74 – 1.58 (m, 3H), 1.14 (s, 3H), 1.07 – 1.00 (m, 1H), 0.92 (s, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 210.5, 171.0, 164.1, 137.1, 127.2, 123.3, 117.3, 107.6, 68.2, 56.0, 54.4, 54.0, 38.7, 38.6, 37.8, 31.2, 30.4, 24.4.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{18}H_{23}NO_6S+Na^+]$: 378.1597, found 378.1588.
IR (film): ν (cm^{-1}) 3285, 2956, 1737, 1598, 1485, 1301, 1249, 1182, 1133, 1020, 903, 735, 577.

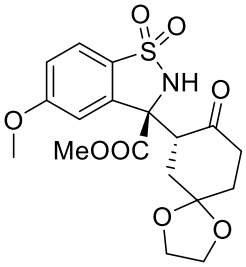


Name	Retention Time	Area	% Area
1	12.291	12753543	46.67
2	13.796	12696128	46.46
3	20.313	954946	3.49
4	28.308	920296	3.37



Name	Retention Time	Area	% Area
1	12.594	883924	1.29
2	13.725	66217231	96.63
3	20.708	932107	1.36
4	28.772	496704	0.72

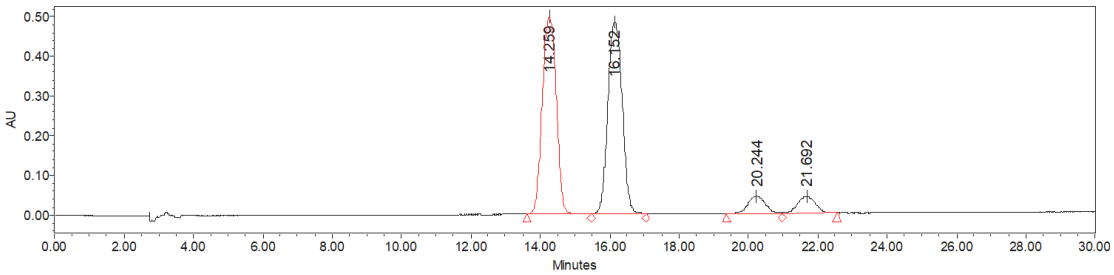
Methyl (R)-5-methoxy-3-((R)-8-oxo-1,4-dioxaspiro[4.5]decan-7-yl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **3af**



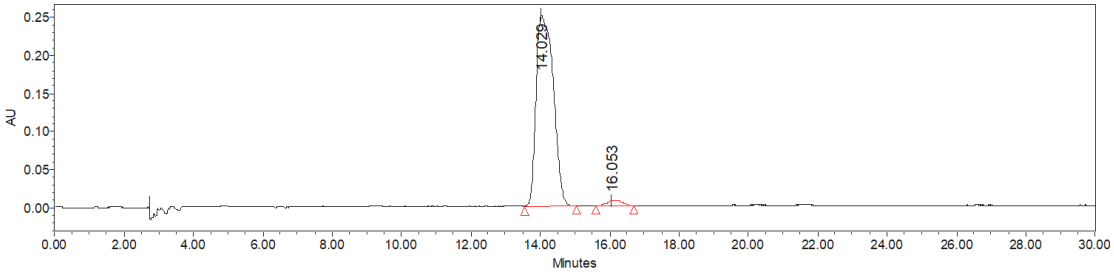
Result: colorless oil, 99% yield, 95% ee, >19:1 dr; $[\alpha]^{24.8}_{D}$ = +142.5 (c = 1.21, CH_2Cl_2); SFC ((Lux 5u Cellulose-1, CO_2/MeOH = 90/10, flow rate = 1.0 mL/min, λ = 254 nm), t_1 = 14.03 min, t_2 = 16.05 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.67 (d, *J* = 8.8 Hz, 1H), 7.09 (dd, *J* = 8.8, 1.6 Hz, 1H), 6.96 (s, 1H), 5.74 (s, 1H), 4.00 – 3.95 (m, 1H), 3.95 – 3.82 (m, 4H), 3.88 (s, 3H), 3.78 (s, 3H), 2.77 – 2.65 (m, 1H), 2.47 – 2.38 (m, 1H), 2.12 – 1.92 (m, 3H), 1.42 – 1.35 (m, 1H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 208.7, 170.5, 164.1, 136.8, 127.3, 123.4, 117.5, 107.8, 107.1, 67.9, 64.7, 64.5, 56.1, 54.9, 54.0, 37.8, 34.0, 33.6.
HRMS (FTMS+c ESI) m/z: [M + Na]$^+$ calcd for [$C_{18}H_{21}NO_8S$+Na$^+$]: 434.0880, found 434.0875.
IR (film): ν (cm^{-1}) 3280, 2959, 2895, 1746, 1714, 1598, 1485, 1438, 1250, 1137, 1054, 1022, 839, 734, 578.

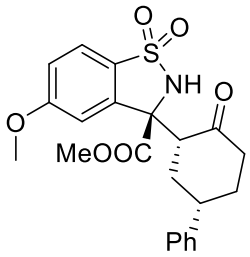


Name	Retention Time	Area	% Area
1	14.259	13941025	45.20
2	16.152	13865305	44.96
3	20.244	1529633	4.96
4	21.692	1506586	4.88



Name	Retention Time	Area	% Area
1	14.029	8638518	97.41
2	16.053	229305	2.59

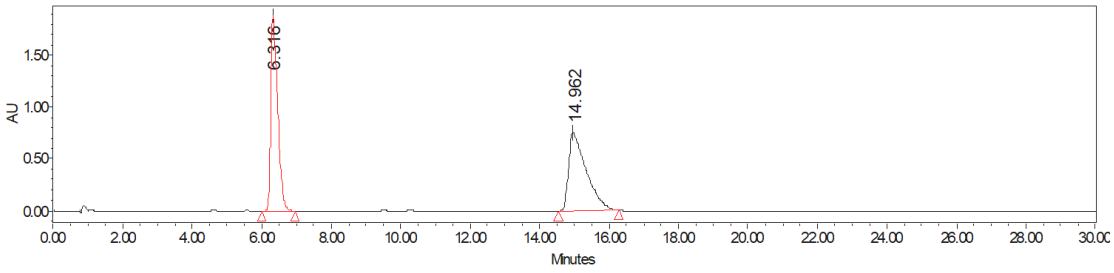
Methyl (*R*)-5-methoxy-3-((1*R*,5*S*)-2-oxo-5-phenylcyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **3ag**



Result: colorless oil, 88% yield, 93% ee, >19:1 dr; [α]$^{24.8}_D$ = +169.0 (c = 0.98, CH_2Cl_2); SFC ((Daicel chiralcel OX-3, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 230 nm), t_1 = 6.28 min, t_2 = 15.44 min.

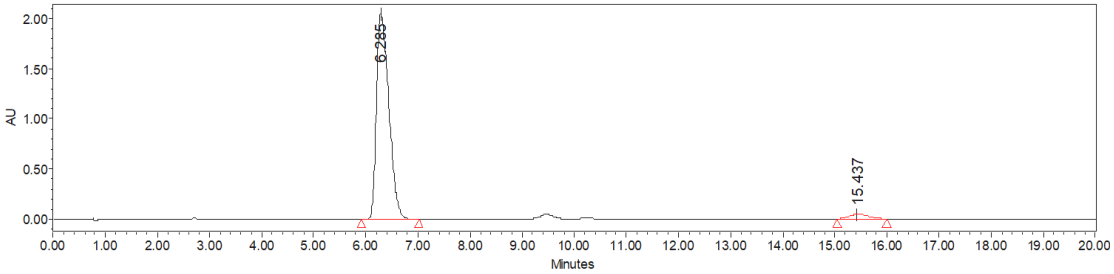
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.65 (d, *J* = 8.4 Hz, 1H), 7.27 – 7.23 (m, 2H), 7.19 – 7.13 (m, 3H), 7.05 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.97 (d, *J* = 1.8 Hz, 1H), 5.80 (s, 1H), 3.87 (s, 3H), 3.83 – 3.74 (m, 1H), 3.81 (s, 1H), 3.11 – 3.03 (m, 1H), 2.66 – 2.54 (m, 2H), 2.25 – 2.17 (m, 1H), 2.13 (q, *J* = 13.2 Hz, 1H), 1.94 – 1.84 (m, 1H), 1.62 – 1.56 (m, 1H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 209.3, 170.8, 164.0, 143.6, 137.0, 128.6, 127.3, 126.8, 126.7, 123.4, 117.1, 108.1, 68.2, 57.9, 56.0, 54.0, 42.5, 41.3, 34.6, 32.7.
HRMS (FTMS+c ESI) m/z: [M + Na]$^+$ calcd for [$C_{22}H_{23}NO_6S$+H$^+$]: 430.1318, found 430.1315.
IR (film): ν (cm^{-1}) 3287, 2950, 2870, 1743, 1710, 1599, 1485, 1287, 1249, 1135, 1020, 896, 849, 759, 735, 702, 574.



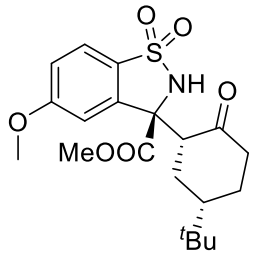
Name	Retention Time	Area	% Area

1	6.316	25721926	49.39
2	14.962	26354762	50.61



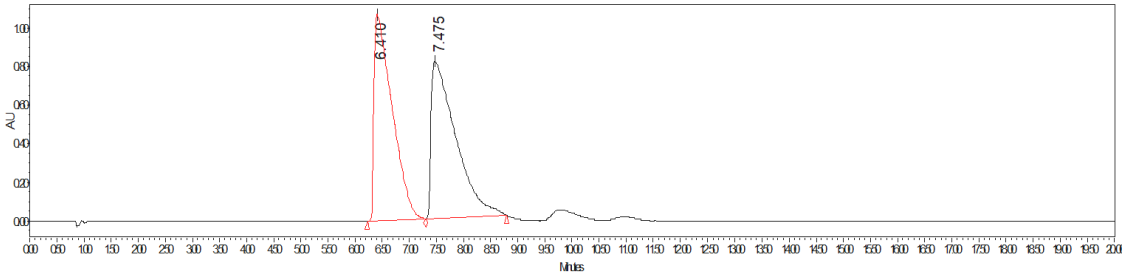
Name	Retention Time	Area	% Area
1	6.285	33663845	96.55
2	15.437	1201909	3.45

Methyl (*R*)-3-((1*R*,5*S*)-5-(tert-butyl)-2-oxocyclohexyl)-5-methoxy-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **3ah**

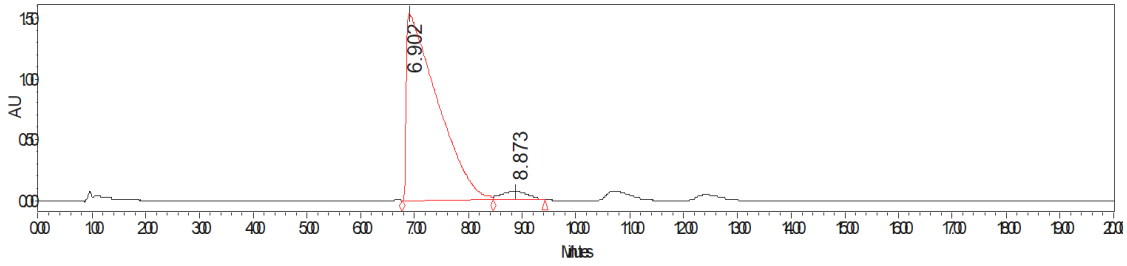


Result: white solid, m.p. 159 - 162 °C, 99% yield, 93% ee, >19:1 dr; $[\alpha]^{26.6}_{D}$ = +139.8 (c = 1.36, CH_2Cl_2); SFC ((Daicel chiralcel ID-3, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 230 nm), t_1 = 6.90 min, t_2 = 8.87 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.68 (d, *J* = 8.8 Hz, 1H), 7.09 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.95 (d, *J* = 2.4 Hz, 1H), 5.72 (s, 1H), 3.88 (s, 3H), 3.77 (s, 3H), 3.55 (dd, *J* = 12.0, 5.6 Hz, 1H), 2.54 – 2.43 (m, 1H), 2.43 – 2.32 (m, 1H), 2.13 – 2.03 (m, 1H), 1.61 – 1.38 (m, 4H), 0.77 (s, 9H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 210.4, 170.9, 164.0, 137.4, 127.4, 123.3, 117.2, 107.8, 68.4, 57.8, 56.0, 53.9, 46.2, 41.1, 32.5, 27.6, 27.5, 27.4.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{20}H_{27}NO_6S+H^+]$: 410.1631, found 410.1630.
IR (film): ν (cm^{-1}) 3287, 2959, 2871, 1741, 1710, 1598, 1484, 1368, 1250, 1185, 1136, 1021, 898, 736, 577.

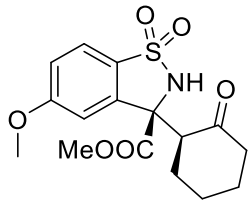


Name	Retention Time	Area	% Area
1	6.410	24593296	49.27
2	7.475	25323265	50.73



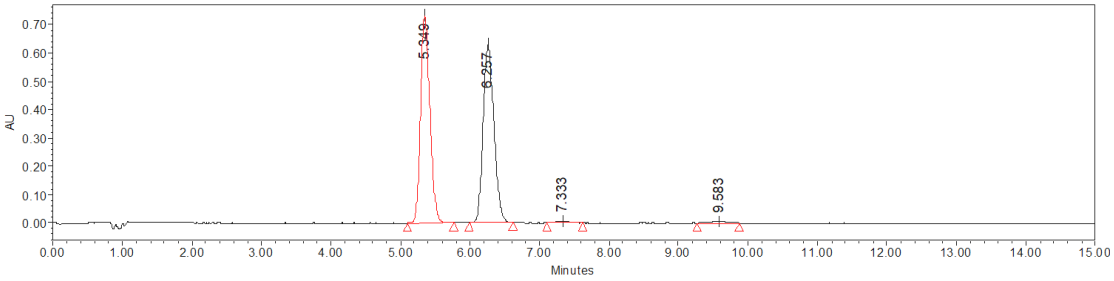
Name	Retention Time	Area	% Area
1	6.902	61961511	96.46
2	8.873	2272565	3.54

Methyl (*R*)-5-methoxy-3-((*S*)-2-oxocyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **4aa**

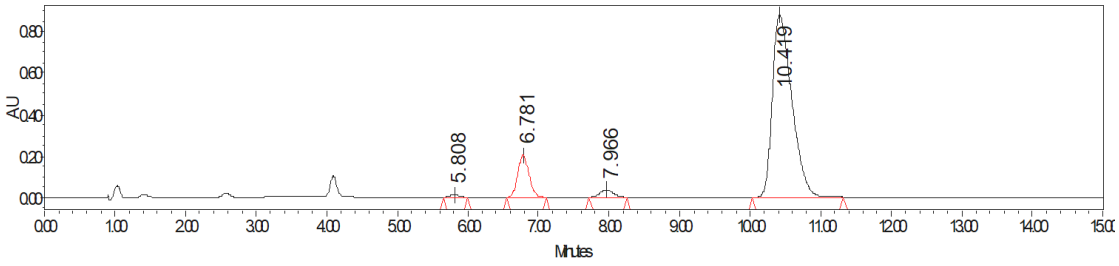


Result: white solid, 98% yield, 94% ee, 89:11 dr; SFC (Daicel chiralcel IC-3, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 230 nm), t_1 = 5.81 min, t_2 = 6.78 min, t_3 = 7.96 min, t_4 = 10.42 min.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.68 (d, *J* = 8.4 Hz, 1H), 7.06 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.95 (d, *J* = 2.4 Hz, 1H), 5.91 (s, 1H), 3.86 (s, 3H), 3.82 (s, 3H), 3.14 (dd, *J* = 12.0, 6.6 Hz, 1H), 2.48 – 2.41 (m, 1H), 2.40 – 2.32 (m, 1H), 2.15 – 2.04 (m, 3H), 1.97 – 1.89 (m, 1H), 1.77 – 1.54 (m, 2H).
^{13}C NMR (150 MHz, Chloroform-*d*) δ 209.0, 169.9, 162.9, 138.5, 128.5, 122.9, 116.1, 111.1, 67.2, 59.6, 55.9, 53.7, 42.3, 30.5, 27.2, 25.1.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{16}H_{19}NO_6S+Na^+]$: 376.0825, found 376.0823.
IR (film): ν (cm^{-1}) 3274, 2952, 2866, 1740, 1710, 1596, 1484, 1435, 1288, 1250, 1184, 1135, 1019, 898, 832, 736, 579.

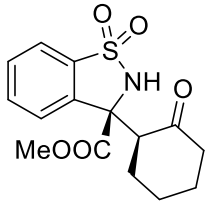


Name	Retention Time	Area	% Area
1	5.349	6839316	49.30
2	6.257	6848656	49.37
3	7.333	92225	0.66
4	9.583	92476	0.67



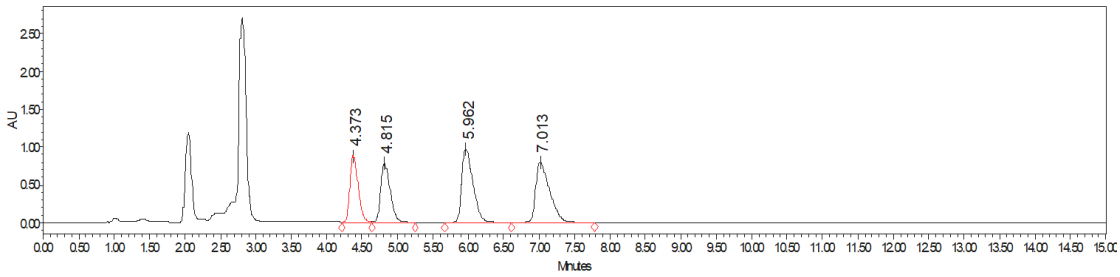
Name	Retention Time	Area	% Area
1	5.808	121537	0.62
2	6.781	2306892	11.75
3	7.966	491206	2.50
4	10.419	16713162	85.13

Methyl (*R*)-3-((*S*)-2-oxocyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **4ba**

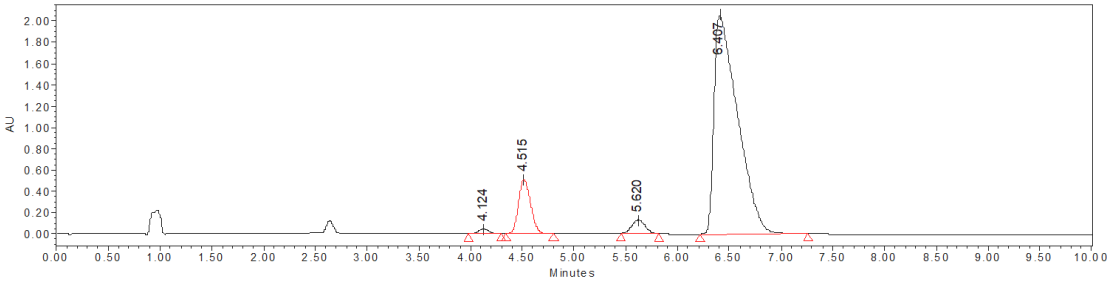


Result: white solid, 99% yield, 93% ee, 90:10 dr; SFC (Daicel chiralcel IC-3, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 210 nm), t_1 = 4.12 min, t_2 = 4.52 min, t_3 = 5.62 min, t_4 = 6.41 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.81 – 7.75 (m, 1H), 7.63 – 7.55 (m, 2H), 7.55 – 7.50 (m, 1H), 5.98 (s, 1H), 3.81 (s, 3H), 3.14 (dd, *J* = 12.4, 6.4 Hz, 1H), 2.48 – 2.41 (m, 1H), 2.40 – 2.30 (m, 1H), 2.16 – 2.02 (m, 3H), 1.96 – 1.88 (m, 1H), 1.74 – 1.51 (m, 2H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 209.0, 170.0, 136.4, 135.9, 132.6, 130.3, 126.1, 121.5, 67.6, 59.5, 53.7, 42.2, 30.6, 27.1, 25.0.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{15}H_{17}NO_5S+Na^+]$: 346.0720, found 346.0701.
IR (film): ν (cm^{-1}) 3275, 2953, 2866, 1740, 1710, 1452, 1303, 1250, 1172, 1134, 1050, 883, 761, 735, 567.

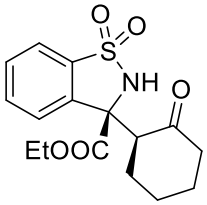


Name	Retention Time	Area	% Area
1	4.373	7366220	19.88
2	4.815	7547147	20.37
3	5.962	11008677	29.72
4	7.013	11122363	30.02



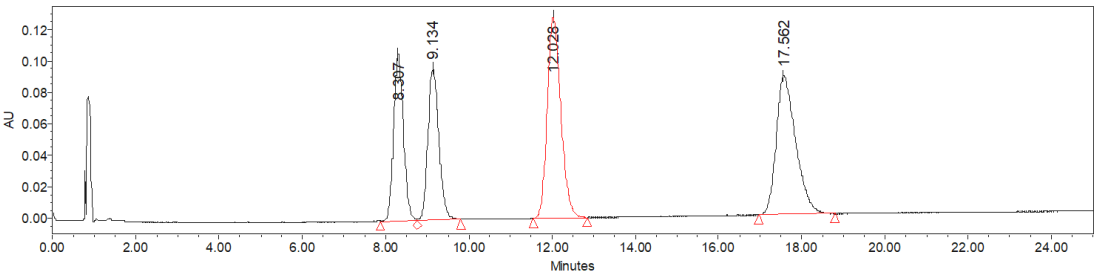
Name	Retention Time	Area	% Area
1	4.124	345079	0.91
2	4.515	4172655	10.96
3	5.620	1166078	3.06
4	6.407	32390075	85.07

Ethyl (*R*)-3-((*S*)-2-oxocyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **4ca**

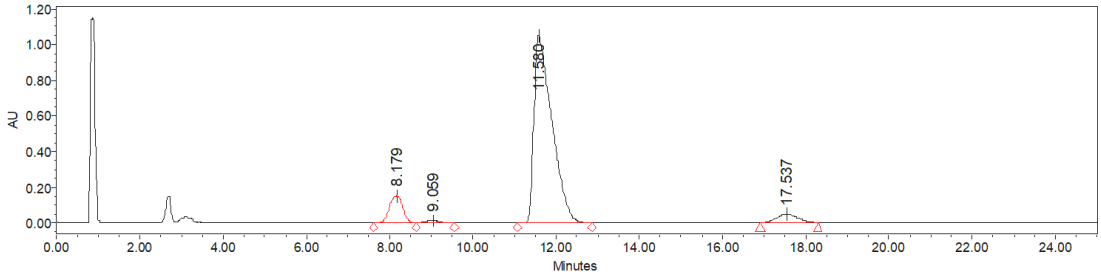


Result: white solid, 97% yield, 90% ee, 91:9 dr; SFC (Daicel chiralcel OX-3, CO_2/EtOH = 90/10, flow rate = 1.5 mL/min, λ = 210 nm), t_1 = 8.18 min, t_2 = 9.06 min, t_3 = 11.58 min, t_4 = 17.54 min.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.80 – 7.75 (m, 1H), 7.63 – 7.56 (m, 2H), 7.55 – 7.50 (m, 1H), 5.97 (s, 1H), 4.33 – 4.23 (m, 2H), 3.13 (dd, *J* = 13.2, 5.4 Hz, 1H), 2.49 – 2.41 (m, 1H), 2.39 – 2.31 (m, 1H), 2.17 – 2.01 (m, 3H), 1.96 – 1.89 (m, 1H), 1.76 – 1.53 (m, 3H), 1.30 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (150 MHz, Chloroform-*d*) δ 208.7, 169.4, 136.6, 136.2, 132.5, 130.3, 126.0, 121.5, 67.6, 63.1, 59.4, 42.2, 30.7, 27.2, 25.1, 13.9.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{16}H_{19}NO_5S+Na^+]$: 360.0876, found 360.0860.
IR (film): ν (cm^{-1}) 3275, 2940, 2866, 1735, 1712, 1451, 1363, 1303, 1244, 1172, 1134, 1025, 857, 760, 566.

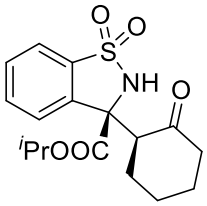


Name	Retention Time	Area	% Area
1	8.307	1753188	18.86
2	9.134	1765302	18.99
3	12.028	2895441	31.15
4	17.562	2881460	31.00



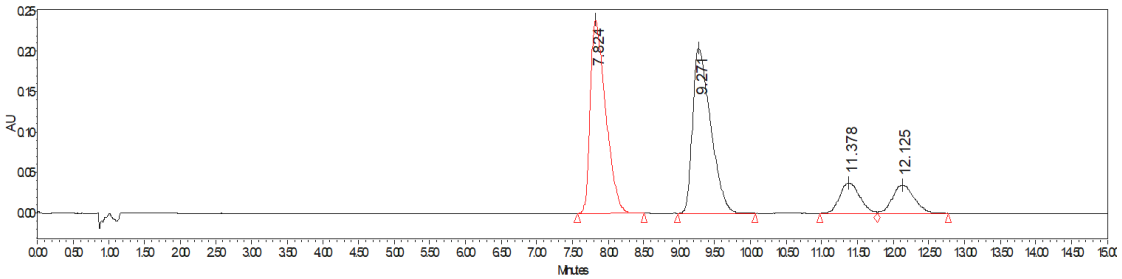
Name	Retention Time	Area	% Area
1	8.179	3447856	9.33
2	9.059	372409	1.01
3	11.580	31474293	85.16
4	17.537	1663054	4.50

Isopropyl (*R*)-3-((*S*)-2-oxocyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **4da**

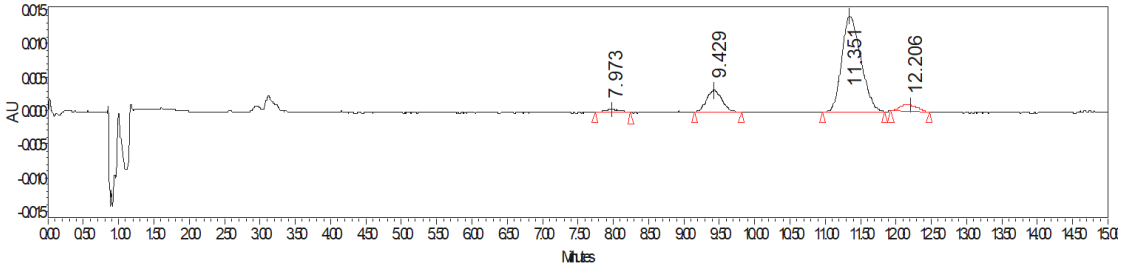


Result: white solid, 98% yield, 88% ee, 86:14 dr; SFC (Daicel chiralcel IC-3, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 254 nm), t_1 = 7.97 min, t_2 = 9.43 min, t_3 = 11.35 min, t_4 = 12.21 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.80 – 7.74 (m, 1H), 7.76 – 7.56 (m, 2H), 7.56 – 7.50 (m, 1H), 5.98 (s, 1H), 5.12 (m, 1H), 3.12 (dd, *J* = 13.2, 5.6 Hz, 1H), 2.50 – 2.41 (m, 1H), 2.41 – 2.30 (m, 1H), 2.21 – 1.97 (m, 3H), 1.97 – 1.88 (m, 1H), 1.75 – 1.50 (m, 2H), 1.31 (d, *J* = 6.4 Hz, 3H), 1.26 (d, *J* = 6.4 Hz, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 208.4, 168.5, 136.7, 136.5, 132.4, 130.3, 125.8, 121.5, 71.5, 67.6, 59.2, 42.2, 30.8, 27.3, 25.1, 21.5.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{17}H_{21}NO_5S+Na^+]$: 374.1033, found 374.1031.
IR (film): ν (cm^{-1}) 3278, 2939, 2866, 1732, 1583, 1452, 1305, 1249, 1173, 1135, 1102, 1049, 882, 761, 735, 566.

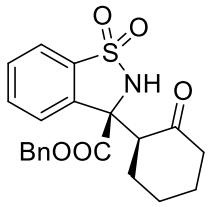


Name	Retention Time	Area	% Area
1	7.824	3584503	41.34
2	9.271	3603920	41.56
3	11.378	739379	8.53
4	12.125	742831	8.57



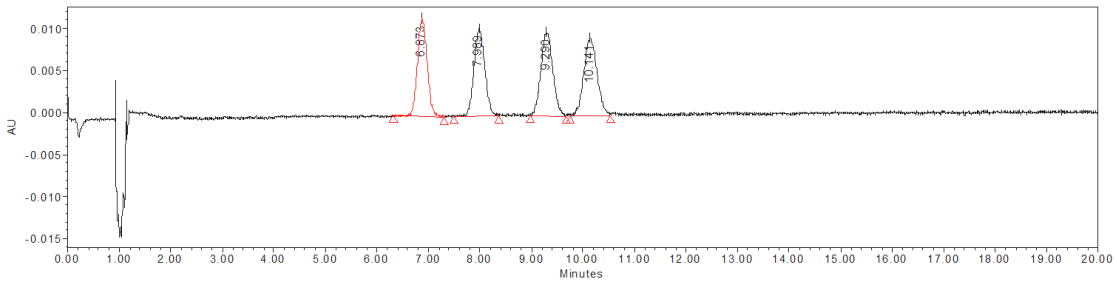
Name	Retention Time	Area	% Area
1	7.973	6951	2.01
2	9.429	51595	14.94
3	11.351	269348	77.99
4	12.206	17484	5.06

Benzyl (*R*)-3-((*S*)-2-oxocyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **4ea**

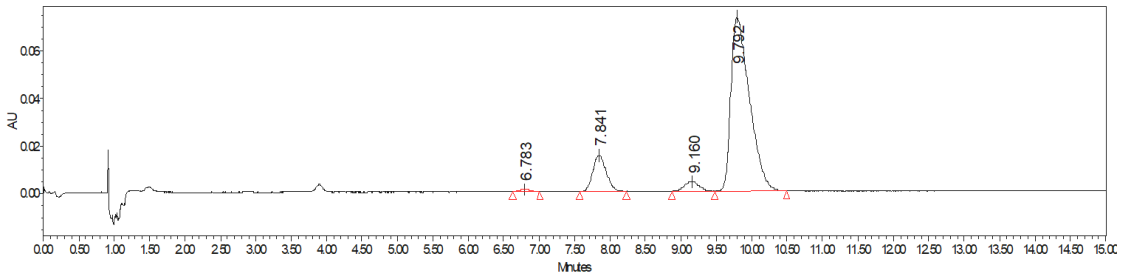


Result: Colorless oil, 97% yield, 92% ee, 88:12 dr; SFC (Daicel chiralcel IC-3, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm), t_1 = 6.78 min, t_2 = 7.84 min, t_3 = 9.16 min, t_4 = 9.79 min.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.80 – 7.76 (m, 1H), 7.63 – 7.52 (m, 2H), 7.47 – 7.43 (m, 1H), 7.38 – 7.28 (m, 5H), 5.99 (s, 1H), 5.24 (d, *J* = 3.6 Hz, 2H), 3.14 (dd, *J* = 13.8, 5.4 Hz, 1H), 2.49 – 2.42 (m, 1H), 2.38 – 2.30 (m, 1H), 2.10 – 2.02 (m, 2H), 2.01 – 1.94 (m, 1H), 1.89 – 1.83 (m, 1H), 1.65 – 1.49 (m, 2H).
^{13}C NMR (150 MHz, Chloroform-*d*) δ 208.7, 169.3, 136.6, 136.0, 134.3, 132.4, 130.3, 128.7, 128.6, 126.0, 121.5, 68.8, 67.6, 59.3, 42.2, 30.6, 27.1, 25.0.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{21}H_{21}NO_5S+Na^+]$: 422.1033, found 422.1046.
IR (film): ν (cm^{-1}) 3277, 2946, 2866, 1739, 1710, 1452, 1360, 1304, 1227, 1172, 1134, 892, 758, 736, 699, 581.

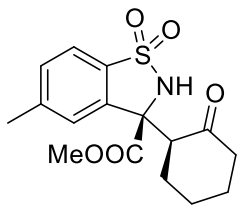


Name	Retention Time	Area	% Area
1	6.873	155695	24.48
2	7.989	154614	24.31
3	9.290	162463	25.54
4	10.141	163218	25.66



Name	Retention Time	Area	% Area
1	6.783	12646	0.79
2	7.841	199195	12.46
3	9.160	58639	3.67
4	9.792	1328515	83.08

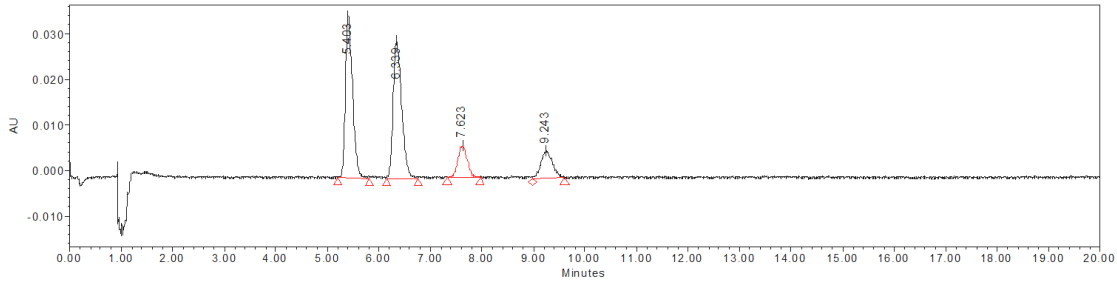
Methyl (*R*)-5-methyl-3-((*S*)-2-oxocyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **4fa**



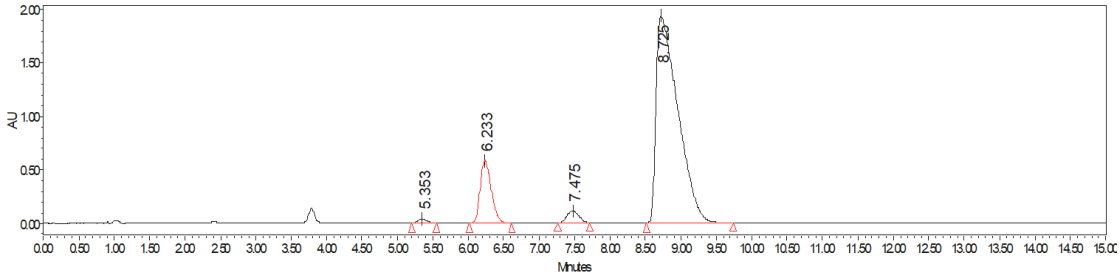
Result: white solid, 98% yield, 94% ee, 89:11 dr; SFC (Daicel chiralcel IC-3, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm), t_1 = 5.35 min, t_2 = 6.23 min, t_3 = 7.47 min, t_4 = 8.72 min.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.65 (d, *J* = 7.8 Hz, 1H), 7.38 (d, *J* = 7.8 Hz, 1H), 7.30 (d, *J* = 23.4 Hz, 1H), 5.91 (s, 1H), 3.82 (s, 3H), 3.12 (dd, *J* = 12.6, 5.4 Hz, 1H), 2.45 (s, 3H), 2.48 – 2.43 (m, 1H), 2.40 – 2.32 (m, 1H), 2.17 – 2.04 (m, 3H), 1.97 – 1.91 (m, 1H), 1.73 – 1.54 (m, 2H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 209.1, 170.0, 143.6, 136.3, 133.8, 131.3, 126.2, 121.3, 67.4, 59.7, 53.6, 42.3, 30.6, 27.2, 25.1, 21.9.
HRMS (FTMS+c ESI) m/z: $[M + H]^+$ calcd for $[C_{16}H_{19}NO_5S+H^+]$: 338.1056, found 338.1058.
IR (film): ν (cm^{-1}) 3279, 2953, 2866, 1739, 1710, 1599, 1451, 1301, 1249, 1187, 1144, 1046, 900, 820, 736, 666, 566.

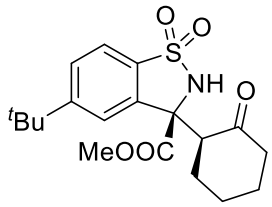


Name	Retention Time	Area	% Area
1	5.403	344024	39.54
2	6.339	345230	39.68
3	7.623	89889	10.33
4	9.243	90899	10.45



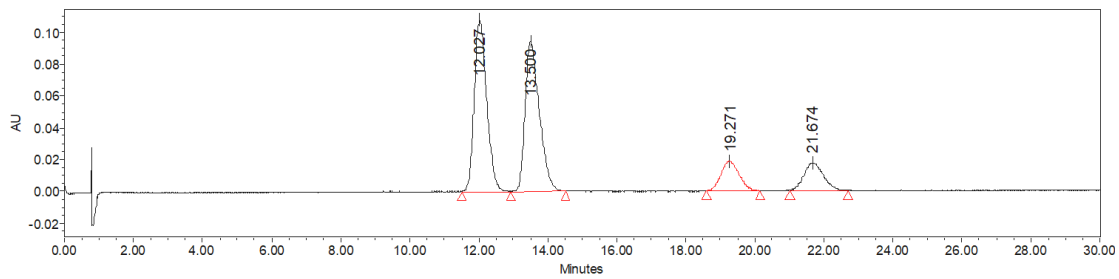
Name	Retention Time	Area	% Area
1	5.353	384987	0.77
2	6.233	6373805	12.82
3	7.475	1358429	2.73
4	8.725	41611805	83.68

Methyl (*R*)-5-(tert-butyl)-3-((*S*)-2-oxocyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **4ga**



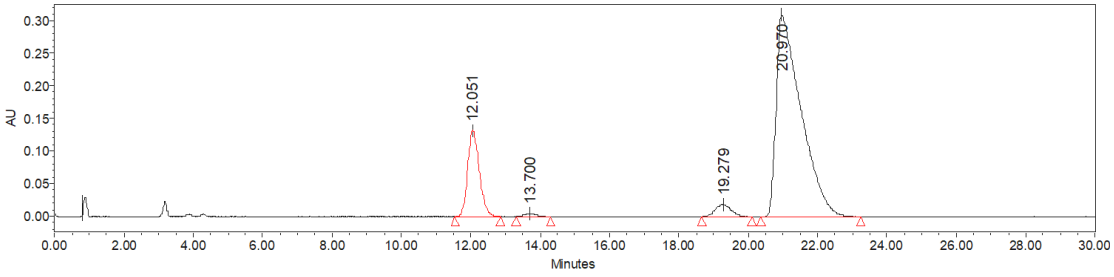
Result: white solid, 98% yield, 92% ee, 85:15 dr; SFC (Daicel chiralcel OX-3, CO_2/EtOH = 90/10, flow rate = 1.5 mL/min, λ = 230 nm), t_1 = 12.05 min, t_2 = 13.70 min, t_3 = 19.28 min, t_4 = 20.97 min.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.70 (d, *J* = 8.4 Hz, 1H), 7.61 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.47 (d, *J* = 1.2 Hz, 1H), 5.97 (s, 1H), 3.82 (s, 3H), 3.09 (dd, *J* = 13.2, 5.4 Hz, 1H), 2.49 – 2.43 (m, 1H), 2.41 – 2.33 (m, 1H), 2.22 – 2.13 (m, 1H), 2.13 – 2.01 (m, 2H), 1.96 – 1.90 (m, 1H), 1.72 – 1.53 (m, 2H), 1.32 (s, 9H).
^{13}C NMR (150 MHz, Chloroform-*d*) δ 209.2, 170.1, 156.8, 135.9, 133.7, 127.9, 122.7, 121.1, 67.4, 59.9, 53.6, 42.3, 35.4, 31.1, 30.7, 27.2, 25.2.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{19}H_{25}NO_5S+Na^+]$: 402.1346, found 402.1351.
IR (film): ν (cm^{-1}) 3282, 2958, 2869, 1740, 1711, 1596, 1302, 1249, 1194, 1150, 1108, 835, 736, 626, 572.



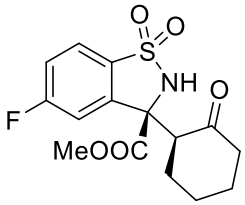
Name	Retention Time	Area	% Area

1	12.027	2702111	39.97
2	13.500	2702176	39.97
3	19.271	679441	10.05
4	21.674	676660	10.01



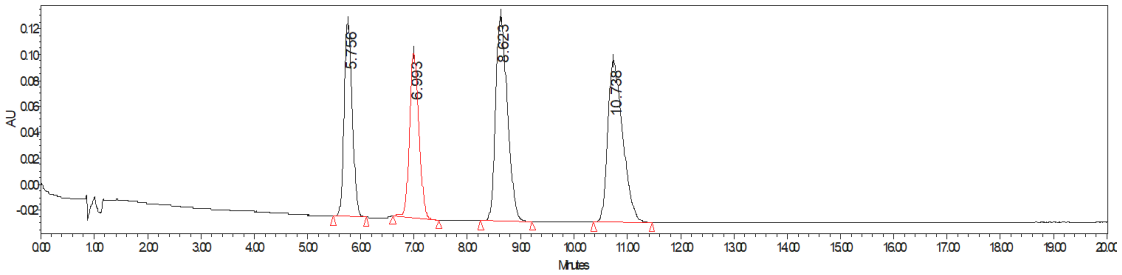
Name	Retention Time	Area	% Area
1	12.051	3106436	16.00
2	13.700	147023	0.76
3	19.279	644543	3.32
4	20.970	15516079	79.92

Methyl (*R*)-5-fluoro-3-((*S*)-2-oxocyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **4ha**

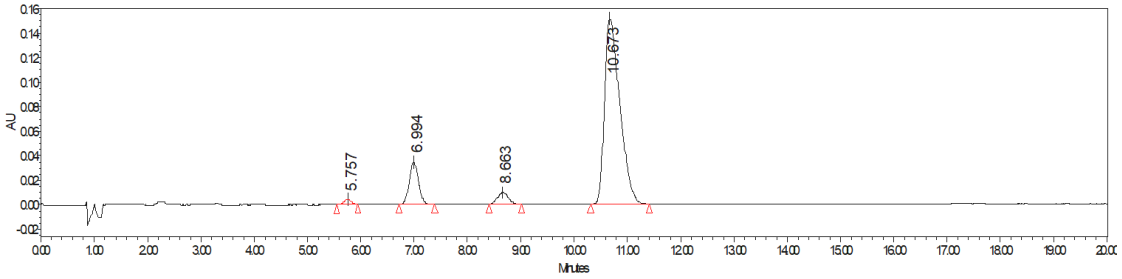


Result: white solid, 98% yield, 91% ee, 91:9 dr; SFC (Daicel chiralcel IC-3, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 230 nm), t_1 = 5.76 min, t_2 = 6.99 min, t_3 = 8.66 min, t_4 = 10.67 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.77 (dd, *J* = 8.4, 4.8 Hz, 1H), 7.33 – 7.18 (m, 2H), 6.02 (s, 1H), 3.83 (s, 3H), 3.18 (dd, *J* = 13.2, 5.6 Hz, 1H), 2.50 – 2.41 (m, 1H), 2.41 – 2.30 (m, 1H), 2.15 – 1.89 (m, 4H), 1.73 – 1.56 (m, 2H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 208.7, 169.6, 164.8 (d, *J* = 253.6 Hz), 139.2 (d, *J* = 9.3 Hz), 132.4 (d, *J* = 2.6 Hz), 123.7 (d, *J* = 10.0 Hz), 118.3 (d, *J* = 23.9 Hz), 113.4 (d, *J* = 25.3 Hz), 67.3, 59.2, 53.9, 42.2, 30.2, 27.0, 24.9.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -103.9.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{15}H_{16}FNO_5S+Na^+]$: 364.0625, found 364.0615.
IR (film): ν (cm^{-1}) 3270, 2954, 2867, 1744, 1710, 1591, 1475, 1306, 1253, 1179, 1127, 1046, 831, 737, 570.



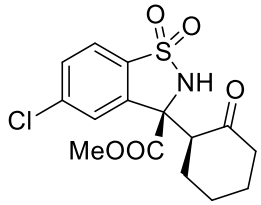
Name	Retention Time	Area	% Area
1	5.756	1561533	19.61
2	6.993	1552411	19.49
3	8.623	2423769	30.43
4	10.738	2426155	30.46



Name	Retention Time	Area	% Area

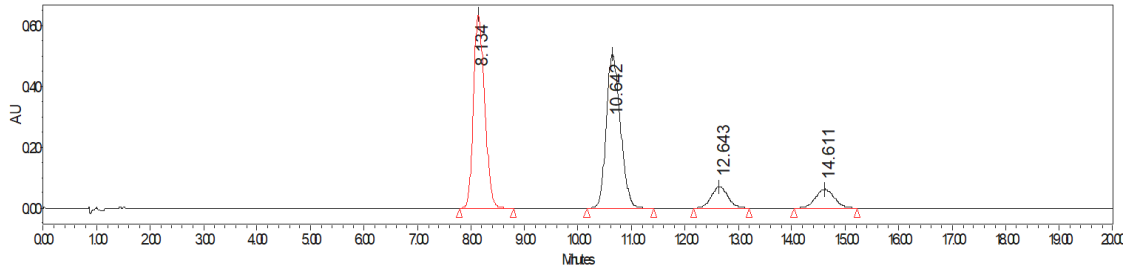
1	5.757	44898	1.24
2	6.994	425355	11.73
3	8.663	141205	3.89
4	10.673	3013917	83.13

Methyl (*R*)-5-chloro-3-((*S*)-2-oxocyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **4ia**

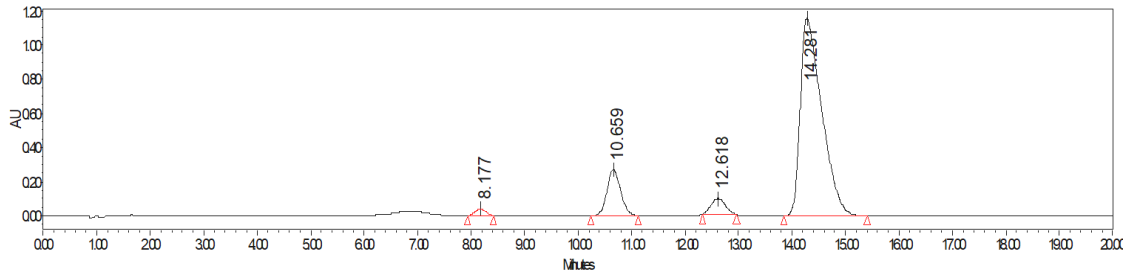


Result: white solid, 98% yield, 90% ee, 88:12 dr; SFC (Daicel chiralcel IC-3, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 230 nm), t_1 = 8.18 min, t_2 = 10.66 min, t_3 = 12.62 min, t_4 = 14.28 min.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.71 (d, *J* = 8.4 Hz, 1H), 7.55 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.50 (d, *J* = 1.2 Hz, 1H), 5.99 (s, 1H), 3.84 (s, 3H), 3.16 (dd, *J* = 11.4, 7.2 Hz, 1H), 2.49 – 2.42 (m, 1H), 2.40 – 2.32 (m, 1H), 2.14 – 2.00 (m, 3H), 1.98 – 1.92 (m, 1H), 1.77 – 1.56 (m, 2H).
^{13}C NMR (150 MHz, Chloroform-*d*) δ 208.6, 169.5, 139.2, 138.1, 134.9, 130.8, 126.1, 122.7, 67.4, 59.2, 53.9, 42.2, 30.4, 27.1, 25.0.
HRMS (FTMS+c ESI) m/z: [M + H]$^+$ calcd for [$C_{15}H_{16}Cl^{34.9689}NO_5S+H^+$]: 358.0510, found 358.0514.
HRMS (FTMS+c ESI) m/z: [M + H]$^+$ calcd for [$C_{15}H_{16}Cl^{36.9659}NO_5S+H^+$]: 360.0481, found 360.0474.
IR (film): ν (cm^{-1}) 3271, 2953, 1743, 1710, 1590, 1451, 1307, 1264, 1173, 1139, 1088, 890, 825, 736, 615, 565.

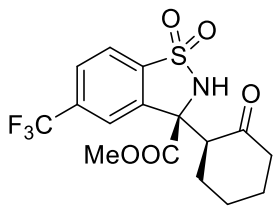


Name	Retention Time	Area	% Area
1	8.134	9198199	42.96
2	10.642	9228550	43.10
3	12.643	1493652	6.98
4	14.611	1492171	6.97



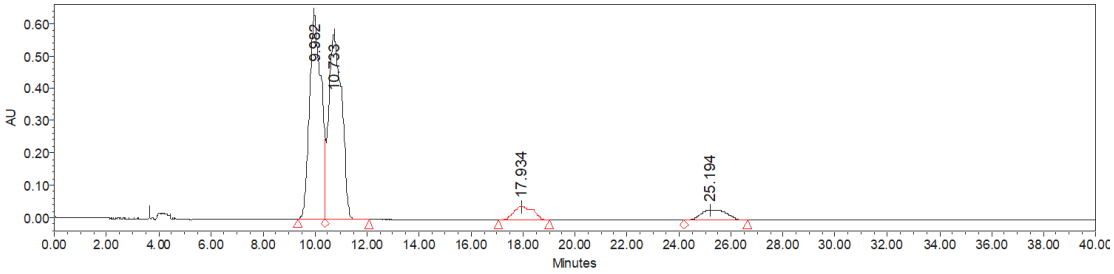
Name	Retention Time	Area	% Area
1	8.177	532362	1.36
2	10.659	4732005	12.09
3	12.618	1722636	4.40
4	14.281	32141288	82.14

Methyl (*R*)-3-((*S*)-2-oxocyclohexyl)-5-(trifluoromethyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **4ja**

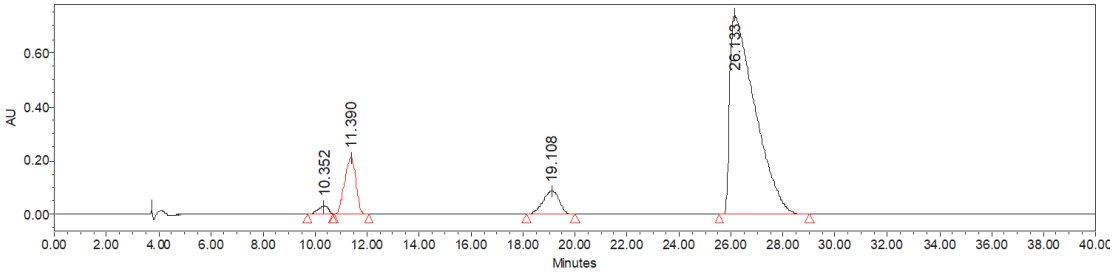


Result: white solid, 98% yield, 86% ee, 90:10 dr; SFC (Lux 5u Cellulose-1, CO_2/EtOH = 95/5, flow rate = 0.8 mL/min, λ = 230 nm), t_1 = 10.35 min, t_2 = 11.39 min, t_3 = 19.11 min, t_4 = 26.13 min.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.92 (d, *J* = 8.4 Hz, 1H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.78 (s, 1H), 6.08 (s, 1H), 3.85 (s, 3H), 3.19 (dd, *J* = 12.6, 5.4 Hz, 1H), 2.52 – 2.43 (m, 1H), 2.42 – 2.33 (m, 1H), 2.15 – 1.92 (m, 4H), 1.78 – 1.56 (m, 2H).
^{13}C NMR (150 MHz, Chloroform-*d*) δ 208.5, 169.4, 139.7, 137.2, 134.8 (q, *J* = 33.0 Hz), 127.7 (q, *J* = 3.3 Hz), 123.2 (q, *J* = 3.6 Hz), 122.9 (q, *J* = 271.9 Hz), 122.5, 67.7, 59.1, 54.1, 42.2, 30.4, 27.0, 25.0.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.6.
HRMS (FTMS+c ESI) m/z: $[M + H]^+$ calcd for $[C_{16}H_{16}F_3NO_5S+H^+]$: 392.0774, found 392.0779.
IR (film): ν (cm^{-1}) 3274, 2955, 2868, 1745, 1712, 1423, 1329, 1253, 1172, 1135, 1080, 895, 835, 737, 717, 561.

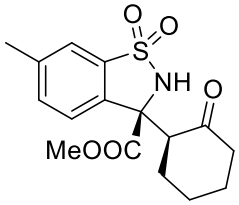


Name	Retention Time	Area	% Area
1	9.982	19662423	44.83
2	10.733	19785727	45.11
3	17.934	2196231	5.01
4	25.194	2213040	5.05



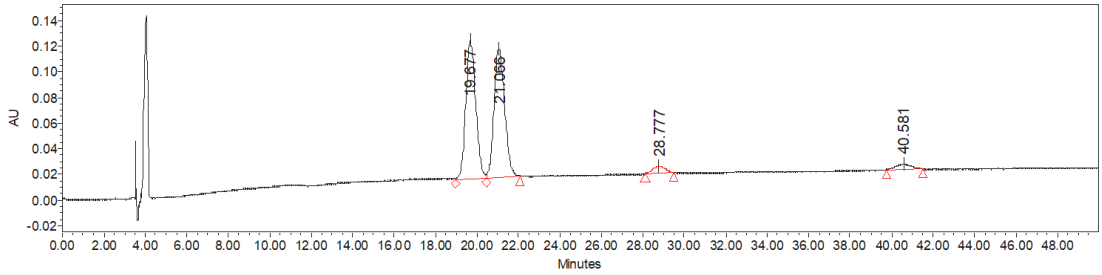
Name	Retention Time	Area	% Area
1	10.352	843476	1.39
2	11.390	6380996	10.55
3	19.108	3760258	6.22
4	26.133	49498776	81.84

Methyl (*R*)-6-methyl-3-((*S*)-2-oxocyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **4ka**

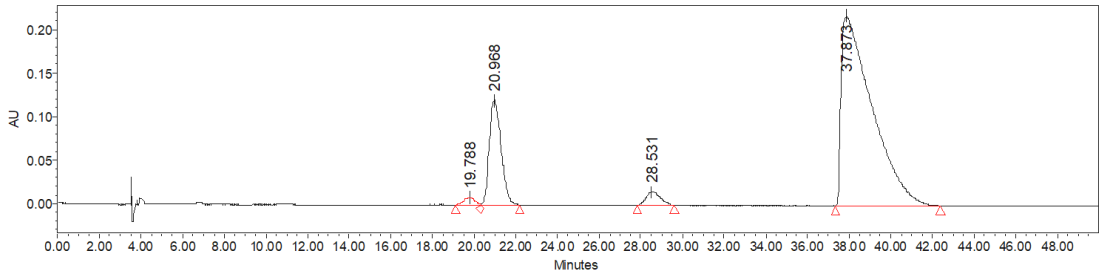


Result: white solid, 99% yield, 94% ee, 88:12 dr; SFC (Lux 5u Cellulose-1, CO_2/^{i}PrOH = 90/10, flow rate = 0.8 mL/min, λ = 230 nm), t_1 = 19.79 min, t_2 = 20.97 min, t_3 = 28.53 min, t_4 = 37.87 min.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.57 (s, 1H), 7.39 (s, 2H), 5.93 (s, 1H), 3.80 (s, 3H), 3.11 (dd, *J* = 12.6, 6.0 Hz, 1H), 2.44 (s, 3H), 2.47 – 2.41 (m, 1H), 2.39 – 2.31 (m, 1H), 2.14 – 2.04 (m, 3H), 1.95 – 1.88 (m, 1H), 1.76 – 1.52 (m, 2H).
^{13}C NMR (150 MHz, Chloroform-*d*) δ 209.1, 170.1, 141.2, 136.5, 133.6, 133.1, 125.8, 121.5, 67.3, 59.7, 53.6, 42.2, 30.6, 27.1, 25.0, 21.1.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{16}H_{19}NO_5S+Na^+]$: 360.0876, found 360.0860.
IR (film): ν (cm^{-1}) 3280, 2953, 2866, 1740, 1710, 1490, 1451, 1301, 1251, 1161, 1049, 897, 837, 736, 570.

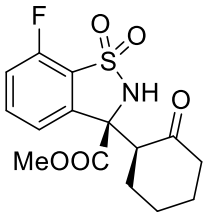


Name	Retention Time	Area	% Area
1	19.677	3586177	47.17
2	21.066	3583042	47.13
3	28.777	218093	2.87
4	40.581	214711	2.82



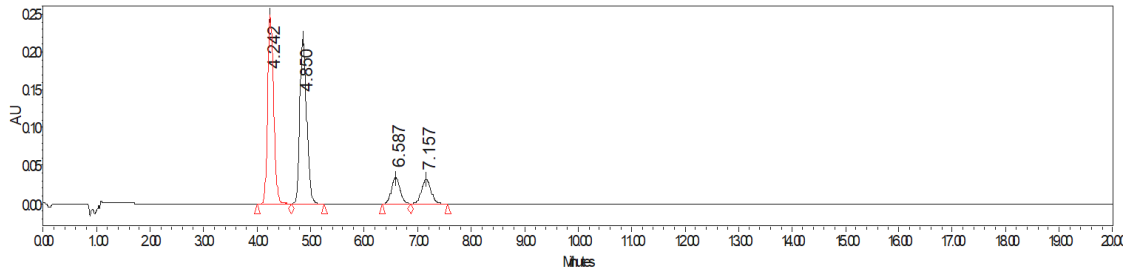
Name	Retention Time	Area	% Area
1	19.788	298585	1.06
2	20.968	4682811	16.63
3	28.531	711874	2.53
4	37.873	22469147	79.78

Methyl (*R*)-7-fluoro-3-((*S*)-2-oxocyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **4la**

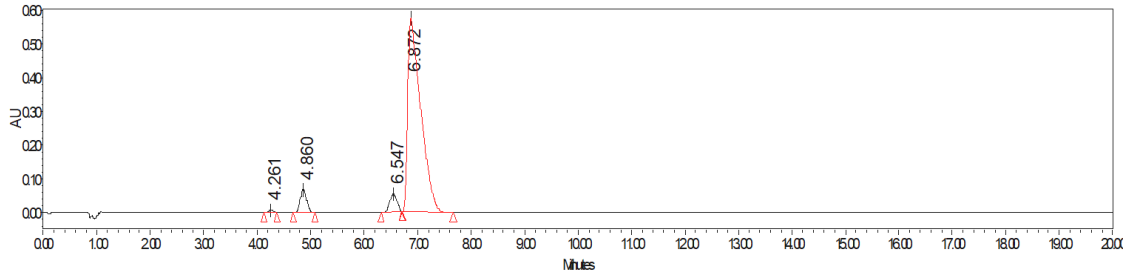


Result: white solid, 98% yield, 90% ee, 95:5 dr; SFC (Daicel chiralcel IC-3, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 230 nm), t_1 = 4.26 min, t_2 = 4.86 min, t_3 = 6.55 min, t_4 = 6.87 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.59 (td, *J* = 8.0, 5.2 Hz, 1H), 7.31 (d, *J* = 7.6 Hz, 1H), 7.22 (t, *J* = 8.4 Hz, 1H), 6.09 (s, 1H), 3.83 (s, 3H), 3.16 (dd, *J* = 11.6, 6.8 Hz, 1H), 2.49 – 2.30 (m, 2H), 2.14 – 1.97 (m, 3H), 1.97 – 1.88 (m, 1H), 1.74 – 1.53 (m, 2H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 208.6, 169.5, 156.1 (d, *J* = 257.3 Hz), 139.2 (d, *J* = 0.9 Hz), 135.1 (d, *J* = 7.0 Hz), 124.5 (d, *J* = 19.9 Hz), 121.7 (d, *J* = 4.0 Hz), 117.3 (d, *J* = 18.3 Hz), 67.7, 59.2, 53.9, 42.2, 30.5, 27.1, 25.0.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -114.6.
HRMS (FTMS+c ESI) m/z: $[M + H]^+$ calcd for $[C_{15}H_{16}FNO_5S+H^+]$: 342.0806, found 342.0818.
IR (film): ν (cm^{-1}) 3274, 2954, 1742, 1712, 1592, 1473, 1314, 1260, 1179, 1111, 909, 808, 769, 736, 590.

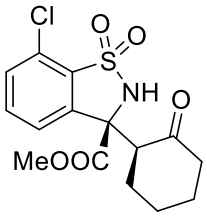


Name	Retention Time	Area	% Area
1	4.242	1930230	41.44
2	4.850	1927503	41.38
3	6.587	396326	8.51
4	7.157	404068	8.67



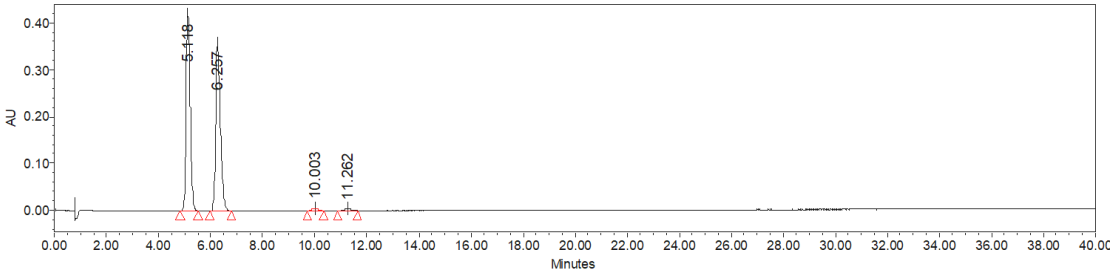
Name	Retention Time	Area	% Area
1	4.261	52940	0.49
2	4.860	581300	5.43
3	6.547	505175	4.72
4	6.872	9561852	89.35

Methyl (*R*)-7-chloro-3-((*S*)-2-oxocyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **4ma**

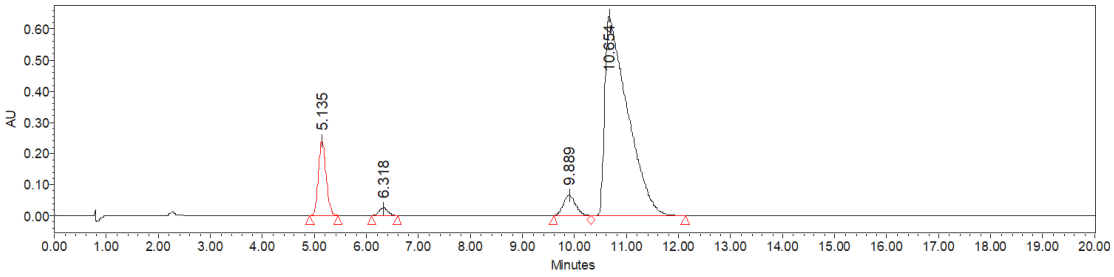


Result: white solid, 97% yield, 90% ee, 91:9 dr; SFC (Daicel chiralcel OX-3, CO_2/EtOH = 80/20, flow rate = 1.5 mL/min, λ = 230 nm), t_1 = 5.14 min, t_2 = 6.32 min, t_3 = 9.89 min, t_4 = 10.65 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.57 – 7.48 (m, 2H), 7.43 (dd, *J* = 7.2, 1.6 Hz, 1H), 6.05 (s, 1H), 3.83 (s, 3H), 3.13 (dd, *J* = 12.8, 6.0 Hz, 1H), 2.49 – 2.41 (m, 1H), 2.40 – 2.31 (m 1H), 2.15 – 1.97 (m, 3H), 1.96 – 1.88 (m, 1H), 1.73 – 1.52 (m, 2H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 208.7, 169.5, 138.7, 134.4, 133.7, 131.2, 129.1, 124.3, 66.6, 59.4, 53.9, 42.2, 30.6, 27.1, 25.0.
HRMS (FTMS+c ESI) m/z: $[M + H]^+$ calcd for $[C_{15}H_{16}Cl^{34.9689}NO_5S+H^+]$: 358.0510, found 358.0514.
HRMS (FTMS+c ESI) m/z: $[M + H]^+$ calcd for $[C_{15}H_{16}Cl^{36.9659}NO_5S+H^+]$: 360.0481, found 360.0479.
IR (film): ν (cm^{-1}) 3273, 2953, 2866, 1741, 1711, 1588, 1454, 1311, 1256, 1172, 879, 736, 579.



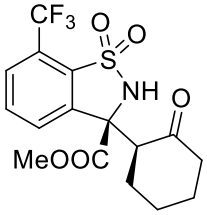
Name	Retention Time	Area	% Area
1	5.118	4576090	49.07
2	6.257	4575973	49.06
3	10.003	89653	0.96
4	11.262	84828	0.91



Name	Retention Time	Area	% Area
1	5.135	2505623	10.84
2	6.318	278332	1.20
3	9.889	1053496	4.56

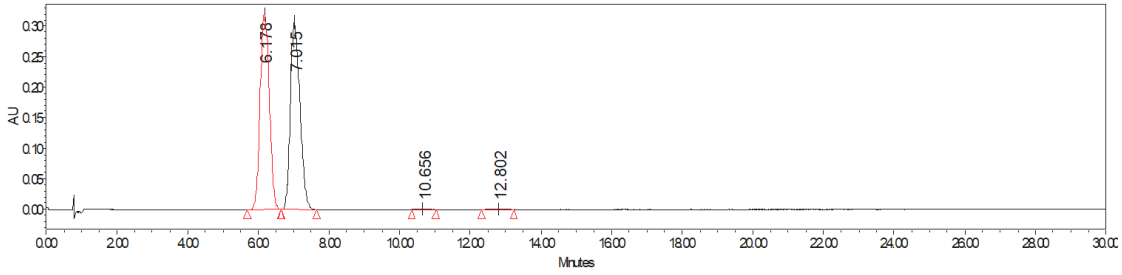
4	10.654	19271344	83.39

Methyl (*R*)-3-((*S*)-2-oxocyclohexyl)-7-(trifluoromethyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **4na**

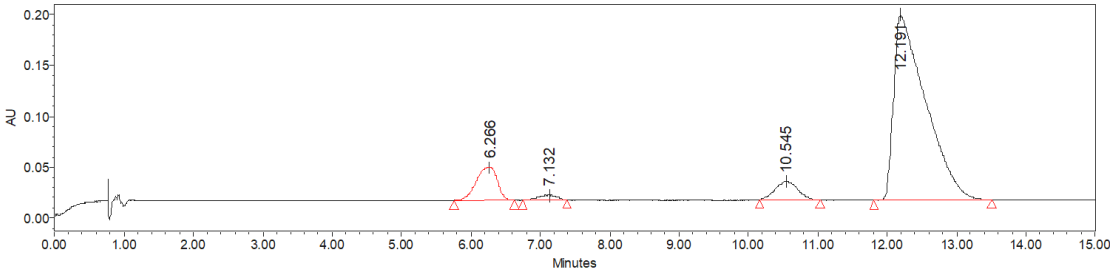


Result: white solid, 96% yield, 87% ee, 92:8 dr; SFC (Daicel chiralcel OX-3, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 230 nm), t_1 = 6.27 min, t_2 = 7.13 min, t_3 = 10.55 min, t_4 = 12.19 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.87 – 7.79 (m, 1H), 7.78 – 7.70 (m, 2H), 6.15 (s, 1H), 3.85 (s, 3H), 3.19 (dd, *J* = 13.2, 5.2 Hz, 1H), 2.53 – 2.43 (m, 1H), 2.42 – 2.32 (m, 1H), 2.20 – 2.06 (m, 2H), 2.00 – 1.89 (m, 2H), 1.77 – 1.52 (m, 2H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 208.6, 169.4, 138.8, 134.8, 132.8, 129.8, 128.1 (q, *J* = 4.6 Hz), 125.8 (q, *J* = 35.7 Hz), 122.2 (d, *J* = 272.6 Hz), 66.9, 59.1, 54.0, 42.2, 30.8, 27.2, 25.0.
^{19}F NMR (376 MHz, Chloroform-*d*) δ -59.5.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{16}H_{16}F_3NO_5S+Na^+]$: 414.0593, found 414.0585.
IR (film): ν (cm^{-1}) 3273, 2955, 2867, 1743, 1713, 1438, 1377, 1324, 1260, 1177, 1142, 880, 737, 585, 527.

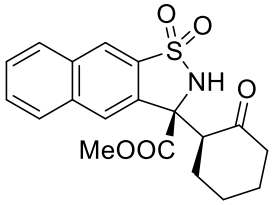


Name	Retention Time	Area	% Area
1	6.178	5838818	49.76
2	7.015	5830271	49.69
3	10.656	31961	0.27
4	12.802	32441	0.28



Name	Retention Time	Area	% Area
1	6.266	681168	9.71
2	7.132	88868	1.27
3	10.545	405194	5.78
4	12.191	5838611	83.24

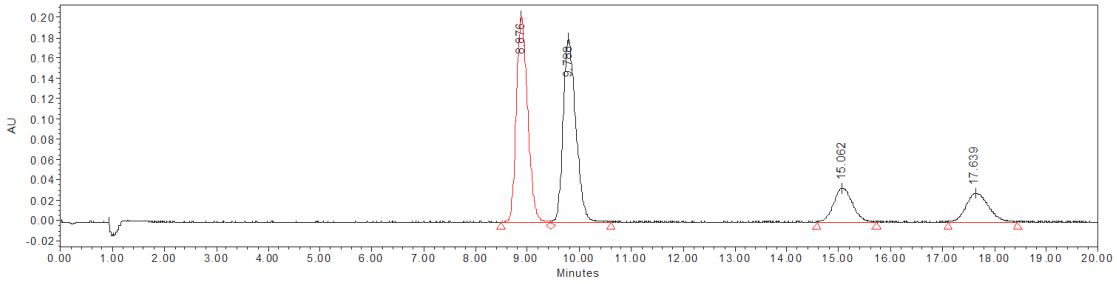
Methyl (*R*)-3-((*S*)-2-oxocyclohexyl)-2,3-dihydronaphtho[2,3-d]isothiazole-3-carboxylate 1,1-dioxide **4oa**



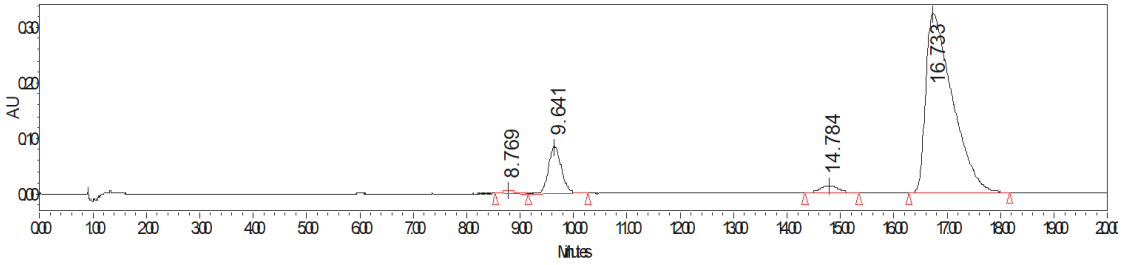
Result: white solid, 96% yield, 95% ee, 88:12 dr; SFC (Daicel chiralcel IC-3, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 254 nm), t_1 = 8.77 min, t_2 = 9.64 min, t_3 = 14.78 min, t_4 = 16.73 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.40 (d, *J* = 8.4 Hz, 1H), 8.04 (d, *J* = 8.4 Hz, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.75 – 7.62 (m, 2H), 7.56 (d, *J* = 8.8 Hz, 1H), 6.12 (s, 1H), 3.84 (s, 3H), 3.23 (dd, *J* = 11.2, 7.6 Hz, 1H), 2.54 – 2.44 (m, 1H), 2.43 – 2.32 (m, 1H), 2.21 – 2.05 (m, 3H), 1.97 – 1.88 (m, 1H), 1.73 – 1.50 (m, 2H).

^{13}C NMR (100 MHz, Chloroform-*d*) δ 209.0, 169.6, 135.2, 133.7, 133.5, 132.0, 129.2, 128.4, 128.3, 125.3, 123.0, 121.7, 67.6, 60.0, 53.7, 42.2, 30.7, 27.1, 25.0.
HRMS (FTMS+c ESI) m/z: [M + Na]$^+$ calcd for [$C_{19}H_{19}NO_5S$+Na$^+$]: 396.0876 found 396.0871.
IR (film): ν (cm^{-1}) 3274, 3061, 2953, 2866, 1742, 1709, 1630, 1595, 1509, 1450, 1357, 1303, 1133, 1056, 975, 897, 869, 829, 765, 736, 702, 553.

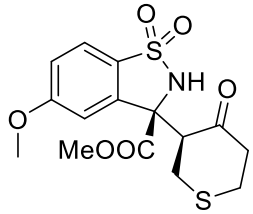


Name	Retention Time	Area	% Area
1	8.876	3046795	39.23
2	9.788	3047838	39.25
3	15.062	828433	10.67
4	17.639	843019	10.86



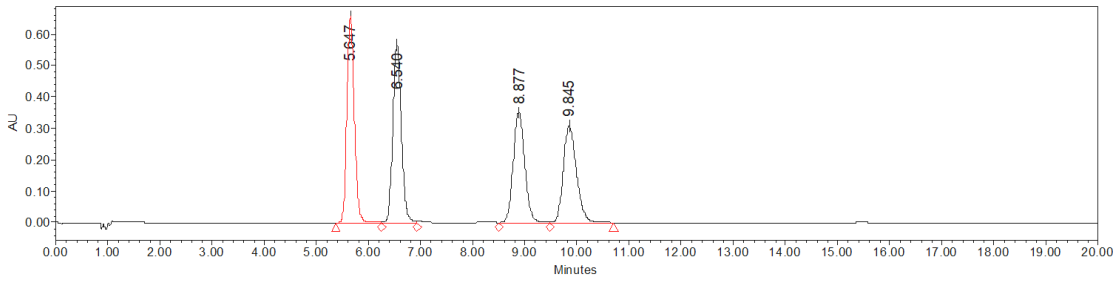
Name	Retention Time	Area	% Area
1	8.769	74645	0.58
2	9.641	1377657	10.61
3	14.784	318208	2.45
4	16.733	11209410	86.36

Methyl (*R*)-5-methoxy-3-((*S*)-4-oxotetrahydro-2H-thiopyran-3-yl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **4ad**



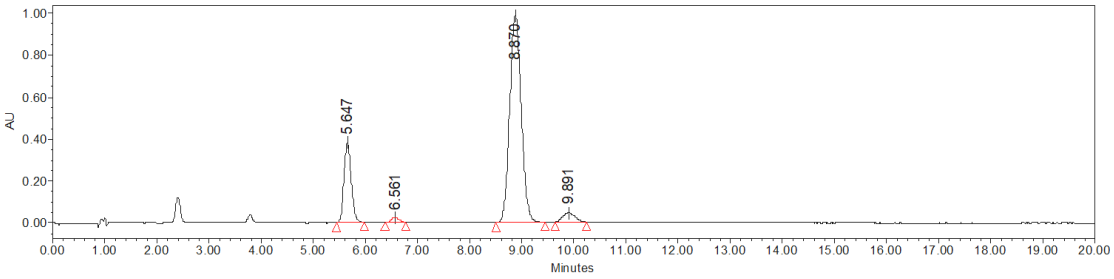
Result: colorless oil, 91% yield, 92% ee, 84:16 dr; SFC (Daicel chiralcel IC-3, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 230 nm), t_1 = 5.65 min, t_2 = 6.56 min, t_3 = 8.87 min, t_4 = 9.89 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.72 (d, *J* = 8.8 Hz, 1H), 7.10 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.93 (d, *J* = 2.4 Hz, 1H), 5.92 (s, 1H), 3.88 (s, 3H), 3.85 (s, 3H), 3.52 (dd, *J* = 12.0, 4.0 Hz, 1H), 3.41 (t, *J* = 12.8 Hz, 1H), 3.07 – 2.88 (m, 3H), 2.86 – 2.76 (m, 2H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 206.7, 169.5, 163.1, 137.8, 128.7, 123.3, 116.4, 111.1, 67.0, 61.9, 56.1, 53.9, 45.1, 32.6, 30.4.
HRMS (FTMS+c ESI) m/z: [M + Na]$^+$ calcd for [$C_{15}H_{17}NO_6S_2$+Na$^+$]: 394.0389 found 394.0386.
IR (film): ν (cm^{-1}) 3271, 2955, 2842, 1740, 1710, 1595, 1484, 1435, 1287, 1246, 1183, 1135, 1019, 827, 736.



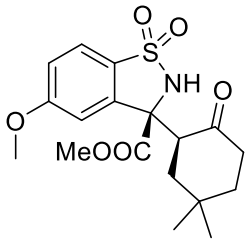
Name	Retention Time	Area	% Area

1	5.647	6475799	27.29
2	6.540	6457352	27.21
3	8.877	5403142	22.77
4	9.845	5396951	22.74



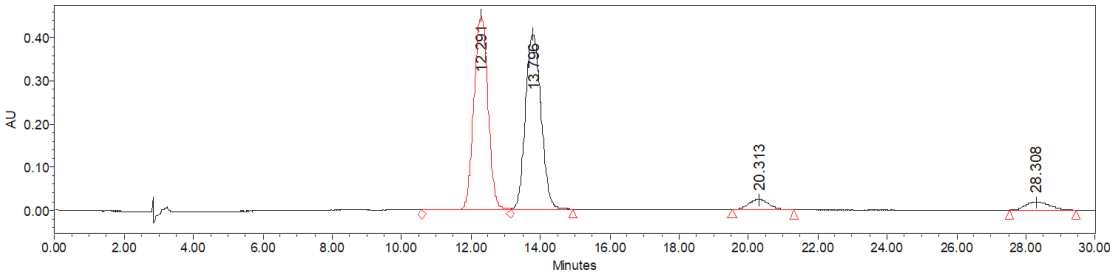
Name	Retention Time	Area	% Area
1	5.647	3731884	18.74
2	6.562	250345	1.26
3	8.870	15278513	76.70
4	9.891	658143	3.30

Methyl (*R*)-3-((*S*)-5,5-dimethyl-2-oxocyclohexyl)-5-methoxy-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **4ae**

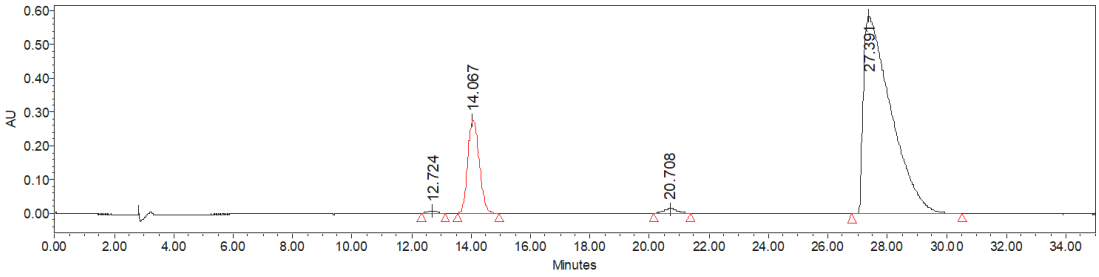


Result: colorless oil, 99% yield, 97% ee, 86:14 dr; SFC ((Lux 5u Cellulose-1, CO_2/^{i}PrOH = 90/10, flow rate = 1.0 mL/min, λ = 230 nm), t_1 = 12.72 min, t_2 = 14.06 min, t_3 = 20.71 min, t_4 = 27.39 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.68 (d, *J* = 8.4 Hz, 1H), 7.06 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.94 (d, *J* = 2.4 Hz, 1H), 5.82 (s, 1H), 3.86 (s, 3H), 3.81 (s, 3H), 3.30 (dd, *J* = 13.6, 5.2 Hz, 1H), 2.58 – 2.43 (m, 1H), 2.36 – 2.26 (m, 1H), 2.01 (t, *J* = 13.2 Hz, 1H), 1.77 – 1.60 (m, 3H), 1.12 (s, 3H), 1.02 (s, 3H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 209.2, 170.0, 163.0, 138.4, 128.3, 122.9, 115.9, 111.1, 67.6, 55.9, 55.2, 53.7, 42.3, 39.1, 38.3, 31.4, 30.9, 24.1.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{18}H_{23}NO_6S+Na^+]$: 378.1597, found 378.1588.
IR (film): ν (cm^{-1}) 3280, 2956, 2856, 1743, 1710, 1598, 1486, 1287, 1248, 1184, 1134, 1019, 738.

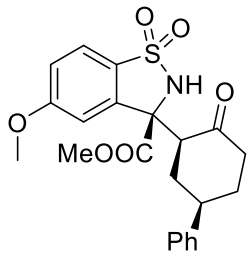


Name	Retention Time	Area	% Area
1	12.291	12753543	46.67
2	13.796	12696128	46.46
3	20.313	954946	3.49
4	28.308	920296	3.37



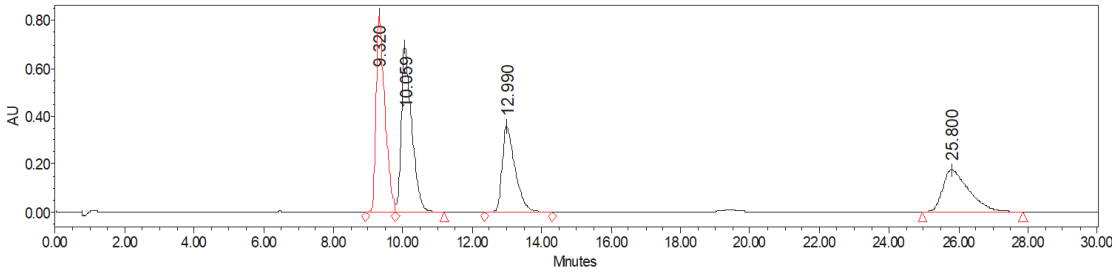
Name	Retention Time	Area	% Area
1	12.724	180688	0.39
2	14.067	7398011	16.16
3	20.708	459206	1.00
4	27.391	37748314	82.44

Methyl (*R*)-5-methoxy-3-((1*S*,5*R*)-2-oxo-5-phenylcyclohexyl)-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **4ag**

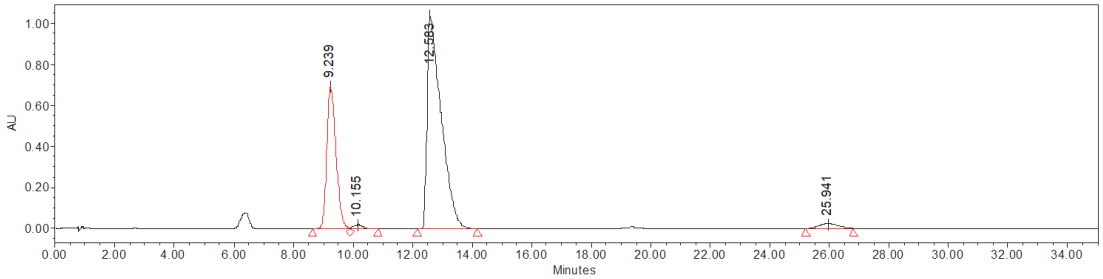


Result: colorless oil, 80% yield, 94% ee, 86:14 dr; SFC (Daicel chiralcel OX, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 230 nm), t_1 = 9.24 min, t_2 = 10.15 min, t_3 = 12.58 min, t_4 = 25.94 min.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.72 – 7.68 (m, 1H), 7.37 – 7.30 (m, 2H), 7.26 – 7.20 (m, 3H), 7.04 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.91 (d, *J* = 2.4 Hz, 1H), 5.95 (s, 1H), 3.85 (s, 3H), 3.80 (s, 3H), 3.38 (dd, *J* = 13.2, 4.8 Hz, 1H), 3.08 – 3.01 (m, 1H), 2.66 – 2.53 (m, 2H), 2.47 – 2.40 (m, 1H), 2.25 – 2.18 (m, 2H), 2.02 – 1.94 (m, 1H).
^{13}C NMR (150 MHz, Chloroform-*d*) δ 208.2, 169.8, 162.9, 143.8, 138.3, 128.6, 126.8, 126.6, 126.5, 123.0, 115.8, 111.2, 67.1, 58.9, 55.9, 53.8, 43.2, 41.6, 37.3, 34.3.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{22}H_{23}NO_6S+H^+]$: 430.1318, found 430.1319.
IR (film): ν (cm^{-1}) 3274, 2953, 1739, 1714, 1598, 1484, 1287, 1247, 1185, 1137, 1020, 736, 702, 579.

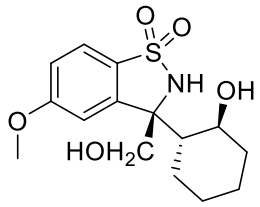


Name	Retention Time	Area	% Area
1	9.320	14468582	30.60
2	10.059	14333832	30.31
3	12.990	9271607	19.61
4	25.800	9211086	19.48



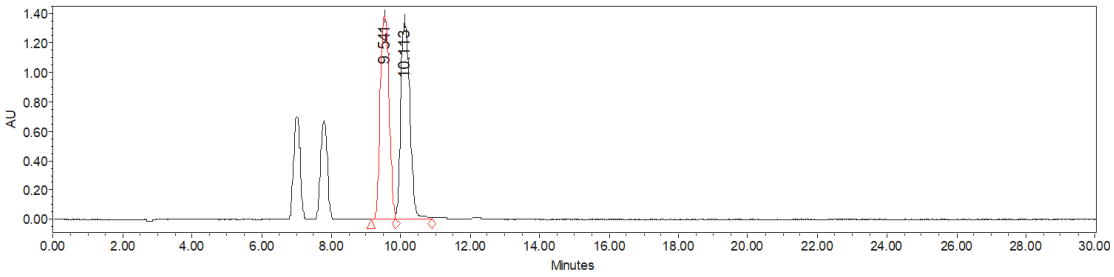
Name	Retention Time	Area	% Area
1	9.239	14874311	29.53
2	10.155	395980	0.79
3	12.583	34116845	67.72
4	25.941	989735	1.96

(*R*)-3-((1*R*,2*S*)-2-hydroxycyclohexyl)-3-(hydroxymethyl)-5-methoxy-2,3-dihydrobenzo[d]isothiazole 1,1-dioxide **5**

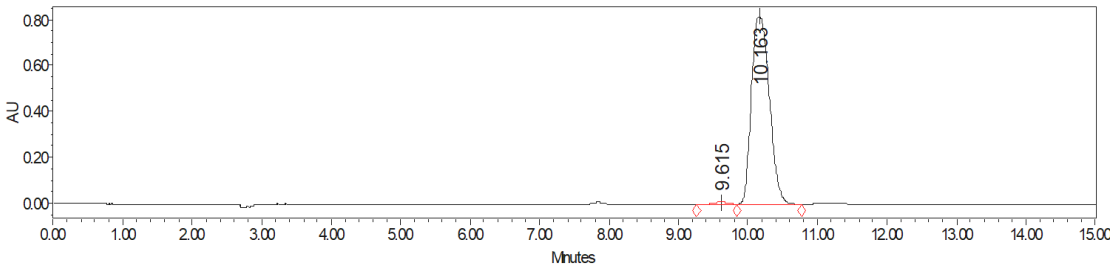


Result: colorless oil, 70% yield, 97% ee, >19:1 dr; $[\alpha]^{24.3}_D$ = +94.6 (c = 0.20, CH_2Cl_2); SFC (Lux 5u Cellulose-1, CO_2/MeOH = 80/20, flow rate = 1.0 mL/min, λ = 230 nm), t_1 = 9.62 min, t_2 = 10.16 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.66 (d, *J* = 8.8 Hz, 1H), 7.03 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.77 (d, *J* = 2.0 Hz, 1H), 5.88 (s, 1H), 4.01 (d, *J* = 11.6 Hz, 1H), 3.88 (s, 3H), 3.67 (td, *J* = 10.0, 4.8 Hz, 1H), 3.58 (d, *J* = 11.6 Hz, 1H), 2.08 – 2.00 (m, 1H), 1.92 – 1.83 (m, 1H), 1.72 – 1.63 (m, 1H), 1.60 – 1.52 (m, 1H), 1.42 – 1.18 (m, 3H), 1.14 – 0.98 (m, 2H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 164.0, 144.3, 126.6, 123.3, 116.0, 107.3, 71.1, 69.5, 68.6, 55.9, 50.6, 36.6, 25.9, 25.0, 24.2.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{15}H_{21}NO_5S+Na^+]$: 350.1032, found 350.1027
IR (film): ν (cm^{-1}) 3272, 2935, 2858, 1596, 1483, 1283, 1245, 1163, 1126, 1051, 1019, 738, 463.

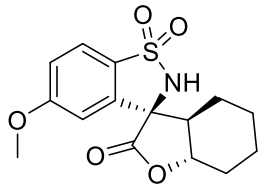


Name	Retention Time	Area	% Area
1	9.541	24098120	49.72
2	10.113	24368930	50.28



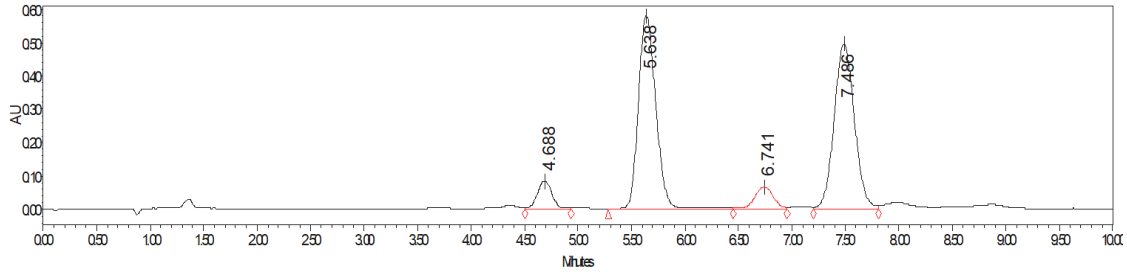
Name	Retention Time	Area	% Area
1	9.615	243044	1.61
2	10.163	14888153	98.39

(3*R*,3a*R*,7a*S*)-5'-methoxy-3a,4,5,6,7,7a-hexahydro-2H,2'H-spiro[benzofuran-3,3'-benzo[d]isothiazol]-2-one 1',1'-dioxide **6**

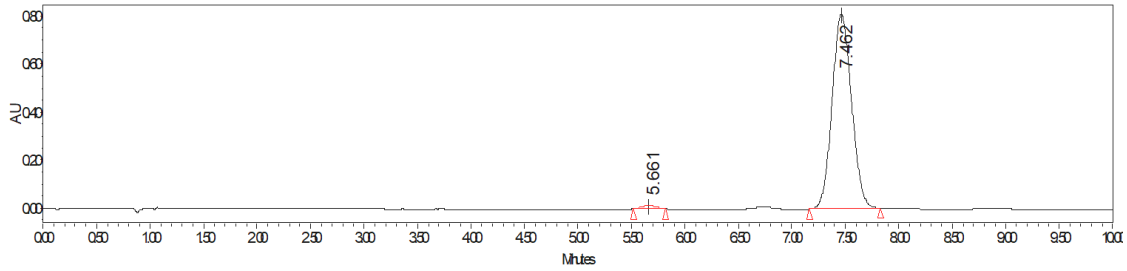


Result: colorless oil, 27% yield, 97% ee, >19:1 dr; $[\alpha]^{24.0}_D$ = +80.9 (c = 0.08, CH_2Cl_2); SFC (Daicel chiralcel IC-3, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 230 nm), t_1 = 5.66 min, t_2 = 7.46 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.70 (d, *J* = 8.8 Hz, 1H), 7.10 (d, *J* = 8.8 Hz, 1H), 6.73 (s, 1H), 5.10 (s, 1H), 4.23 (td, *J* = 11.2, 4.0 Hz, 1H), 3.89 (s, 3H), 2.42 – 2.34 (m, 1H), 2.17 – 2.07 (m, 1H), 2.00 – 1.91 (m, 1H), 1.88 – 1.79 (m, 1H), 1.71 – 1.56 (m, 3H), 1.51 – 1.37 (m, 1H), 1.34 – 1.18 (m, 1H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 173.0, 164.1 , 139.8, 129.0, 122.8, 117.4, 108.1, 82.6, 68.2, 56.0, 55.9, 30.2, 24.7, 23.6, 23.0.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{15}H_{17}NO_5S+Na^+]$: 346.0719, found 346.0717.
IR (film): ν (cm^{-1}) 3256, 2941, 2867, 1780, 1598, 1484, 1289, 1254, 1187, 1133, 1075, 1018, 981, 860, 828, 742.

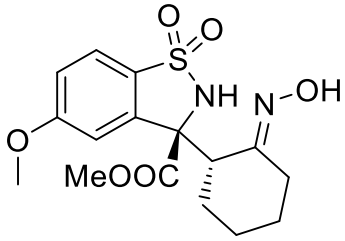


Name	Retention Time	Area	% Area
1	4.688	774907	5.31
2	5.638	6509757	44.65
3	6.741	781415	5.36
4	7.486	6514625	44.68



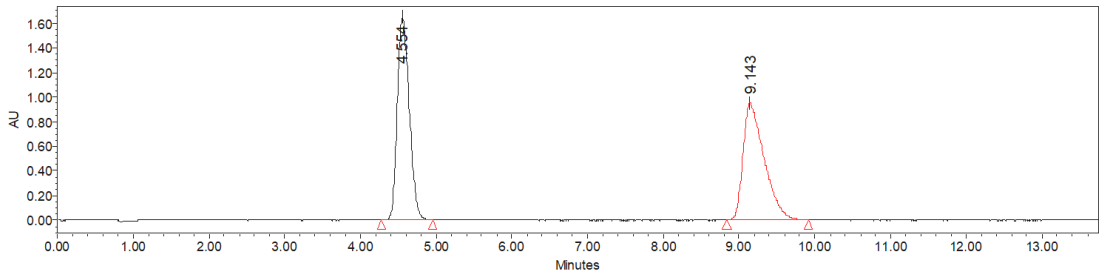
Name	Retention Time	Area	% Area
1	5.661	116186	1.12
2	7.462	10238736	98.88

Methyl (*R*)-3-((*R*, *E*)-2-(hydroxyimino)cyclohexyl)-5-methoxy-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **7**

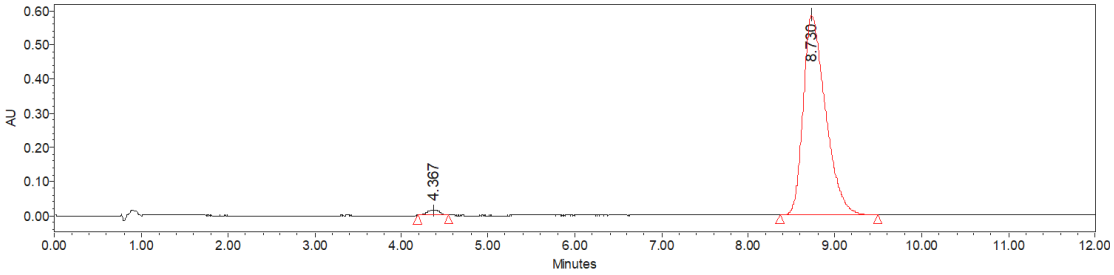


Result: white solid, m.p. 219 - 212 °C, 85% yield, 97% ee, >19:1 dr; $[\alpha]^{21.0}_{D}$ = +98.3 (c = 1.21, CH_2Cl_2); SFC (Daicel chiralcel OX-3, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 230 nm), t_1 = 4.36 min, t_2 = 8.73 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.69 (d, *J* = 8.8 Hz, 1H), 7.52 (s, 1H), 7.09 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.01 (d, *J* = 2.4 Hz, 1H), 5.91 (s, 1H), 3.89 (s, 3H), 3.75 (s, 3H), 3.45 – 3.38 (m, 1H), 3.29 (dd, *J* = 12.4, 4.4 Hz, 1H), 1.88 – 1.81 (m, 1H), 1.80 – 1.73 (m, 1H), 1.71 – 1.62 (m, 1H), 1.59 – 1.48 (m, 1H), 1.44 – 1.32 (m, 2H), 1.29 – 1.22 (m, 1H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 171.3, 164.0, 159.1, 138.0, 127.2, 123.2, 117.0, 108.2, 69.2, 56.0, 53.8, 49.8, 26.2, 25.2, 24.9, 24.5.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{16}H_{20}N_2O_6S+Na^+]$: 391.0934, found 391.0928.
IR (film): ν (cm^{-1}) 3431, 2941, 2861, 1731, 1595, 1483, 1438, 1285, 1247, 1187, 1127, 1023, 896.

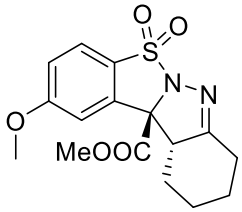


Name	Retention Time	Area	% Area
1	4.554	18164863	49.67
2	9.143	18408566	50.33



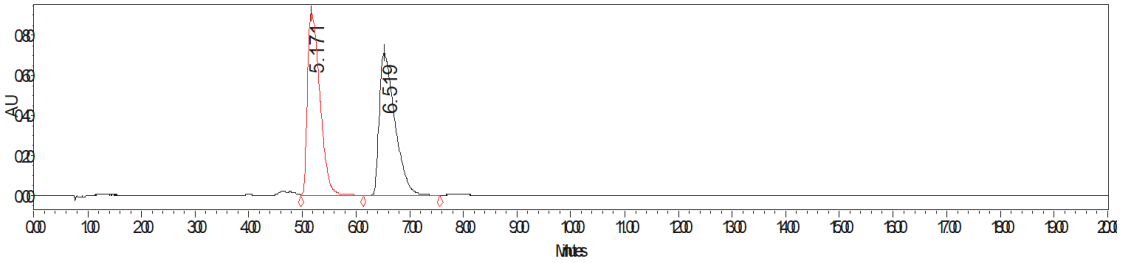
Name	Retention Time	Area	% Area
1	4.367	155068	1.46
2	8.730	10458872	98.54

Methyl (11*aR*,11*bR*)-2-methoxy-9,10,11,11a-tetrahydrobenzo[4,5]isothiazolo[2,3-b]indazole-11b(8H)-carboxylate 5,5-dioxide **8**

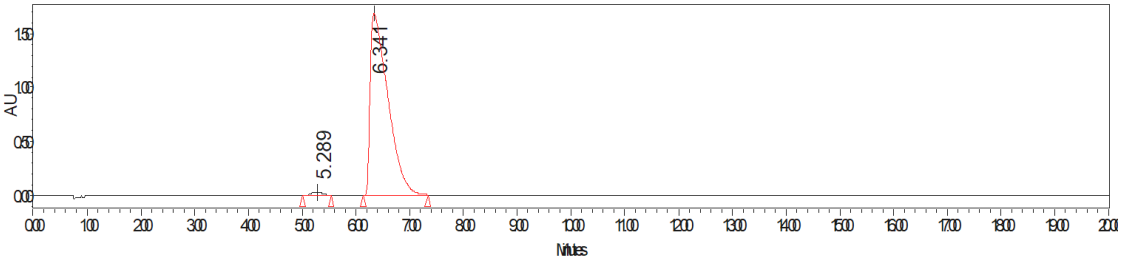


Result: colorless oil, 75% yield, 97% ee, >19:1 dr; $[\alpha]^{22.5}_{D}$ = +16.3 (c = 0.39, CH_2Cl_2); SFC (Daicel chiralcel IA-3, CO_2/MeOH = 90/10, flow rate = 1.5 mL/min, λ = 230 nm), t_1 = 5.29 min, t_2 = 6.34 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.72 (d, *J* = 8.8 Hz, 1H), 7.11 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.85 (d, *J* = 2.0 Hz, 1H), 3.88 (s, 3H), 3.78 (s, 3H), 3.73 (dd, *J* = 12.8, 6.0 Hz, 1H), 2.88 – 2.79 (m, 1H), 2.32 – 2.21 (m, 1H), 2.18 – 2.10 (m, 1H), 2.02 – 1.94 (m, 1H), 1.93 – 1.86 (m, 1H), 1.59 – 1.46 (m, 1H), 1.43 – 1.27 (m, 1H), 1.05 – 0.93 (m, 1H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.4, 165.2, 163.6, 135.7, 126.7, 124.1, 117.3, 111.2, 56.0, 54.7, 54.0, 30.5, 27.9, 25.6, 24.3.
HRMS (FTMS+c ESI) m/z: [M + Na]$^+$ calcd for [$C_{16}H_{18}N_2O_5S$+Na$^+$]: 351.1009, found 351.1005.
IR (film): ν (cm^{-1}) 2927, 2857, 1742, 1592, 1481, 1435, 1333, 1247, 1187, 1172, 1016, 962, 738, 701, 644.

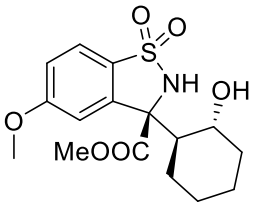


Name	Retention Time	Area	% Area
1	5.171	14704491	49.99
2	6.519	14710346	50.01



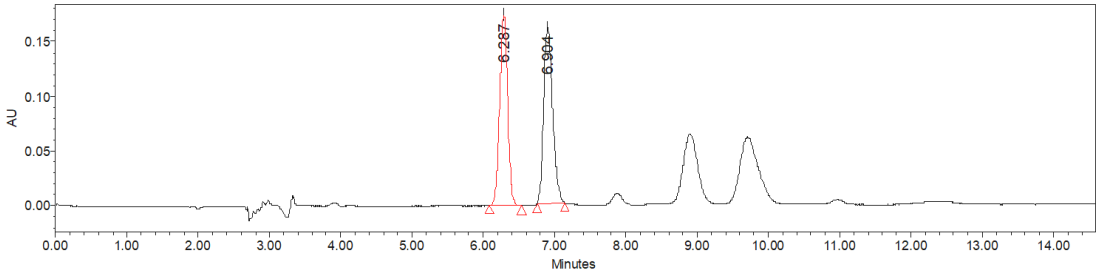
Name	Retention Time	Area	% Area
1	5.289	512896	1.30
2	6.341	38867964	98.70

Methyl (*R*)-3-((1*S*,2*R*)-2-hydroxycyclohexyl)-5-methoxy-2,3-dihydrobenzo[d]isothiazole-3-carboxylate 1,1-dioxide **9**

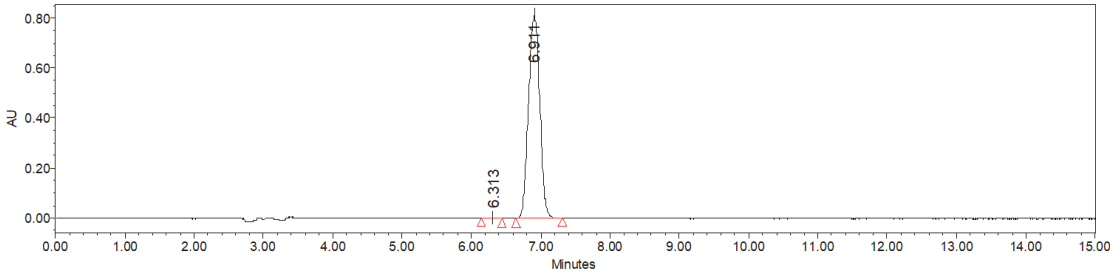


Result: colorless oil, 57% yield, 99% ee, >19:1 dr; $[\alpha]^{20.7}_D$ = -3.1 (c = 0.36, CH_2Cl_2); SFC (Lux 5u Cellulose-1, CO_2/MeOH = 80/20, flow rate = 1.0 mL/min, λ = 230 nm), t_1 = 6.31 min, t_2 = 6.91 min.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.59 (d, *J* = 8.4 Hz, 1H), 7.20 (d, *J* = 2.4 Hz, 1H), 7.02 (dd, *J* = 8.4, 2.4 Hz, 1H), 5.90 (s, 1H), 3.88 (s, 3H), 3.87 (s, 3H), 3.86 – 3.81(m, 1H), 2.34 – 2.28 (m, 1H), 1.89 – 1.83 (m, 1H), 1.83 – 1.66 (m, 3H), 1.49 – 1.42 (m, 1H), 1.33 – 1.18 (m, 4H).
^{13}C NMR (150 MHz, Chloroform-*d*) δ 170.8, 163.5, 141.8, 126.0, 122.3, 116.3, 110.3, 71.8, 70.5, 55.8, 54.1, 52.3, 35.6, 27.8, 25.3, 24.6.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{16}H_{21}NO_6S+Na^+]$: 378.0981, found 378.0978
IR (film): ν (cm^{-1}) 2934, 2858, 1736, 1596, 1483, 1443, 1286, 1250, 1185, 1129, 1071, 1021, 965, 669.

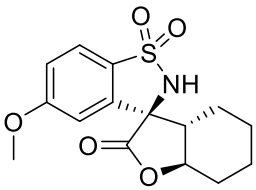


Name	Retention Time	Area	% Area
1	6.287	1353481	49.13
2	6.904	1401478	50.87



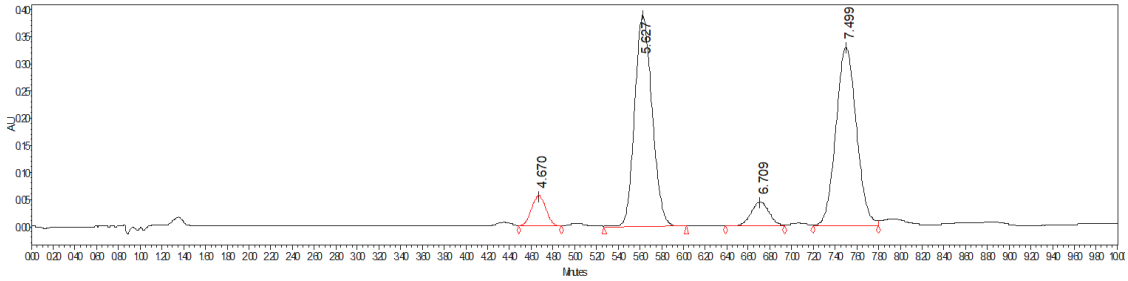
Name	Retention Time	Area	% Area
1	6.313	33352	0.36
2	6.911	9190175	99.64

(3*R*,3a*S*,7a*R*)-5'-methoxy-3a,4,5,6,7,7a-hexahydro-2H,2'H-spiro[benzofuran-3,3'-benzo[d]isothiazol]-2-one 1',1'-dioxide **10**

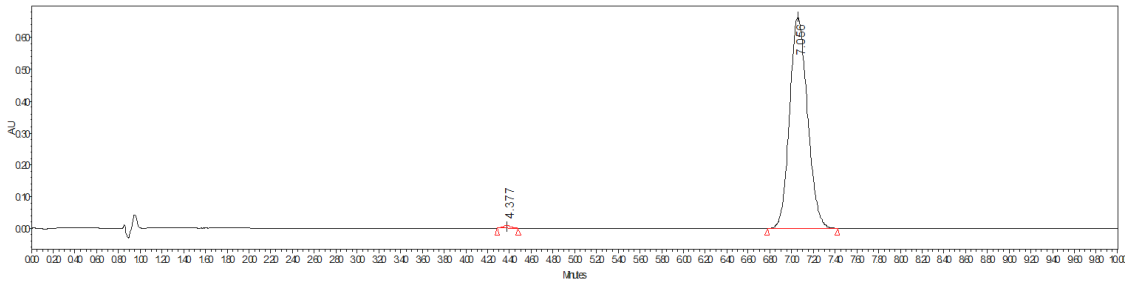


Result: colorless oil, 35% yield, 99% ee, >19:1 dr; $[\alpha]^{20.4}_D$ = -84.2 (c = 0.40, CH_2Cl_2); SFC (Daicel chiralcel IC-3, CO_2/MeOH = 80/20, flow rate = 1.5 mL/min, λ = 230 nm), t_1 = 4.38 min, t_2 = 7.06 min.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.68 (d, J = 8.4 Hz, 1H), 7.05 (dd, J = 8.4, 2.4 Hz, 1H), 6.77 (d, J = 2.4 Hz, 1H), 5.09 (s, 2H), 3.88 (s, 3H), 2.89 – 2.75 (m, 1H), 2.42 – 2.33 (m, 1H), 1.79 – 1.61 (m, 3H), 1.48 – 1.13 (m, 4H).
^{13}C NMR (100 MHz, Chloroform-*d*) δ 172.7, 139.4, 130.4, 122.6, 116.1, 111.6, 79.1, 71.6, 56.0, 45.6, 26.9, 24.2, 22.9, 19.34.
HRMS (FTMS+c ESI) m/z: $[M + Na]^+$ calcd for $[C_{15}H_{17}NO_5S+Na^+]$: 346.0719, found 346.0709.
IR (film): ν (cm^{-1}) 3211, 2940, 2863, 1772, 1592, 1480, 1319, 1289, 1240, 1208, 1180, 1140, 950, 847, 731.

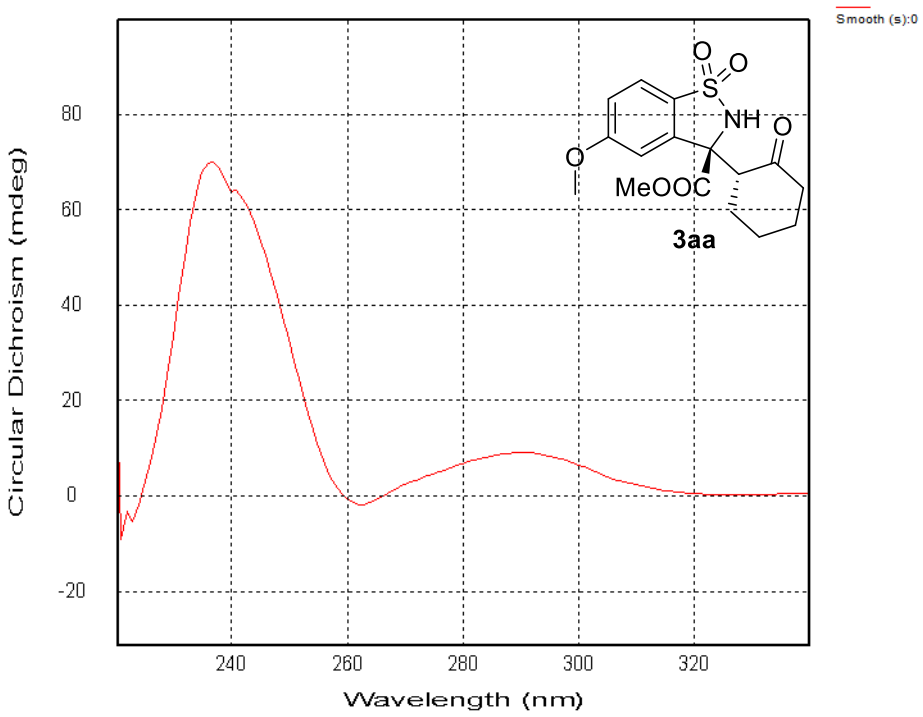


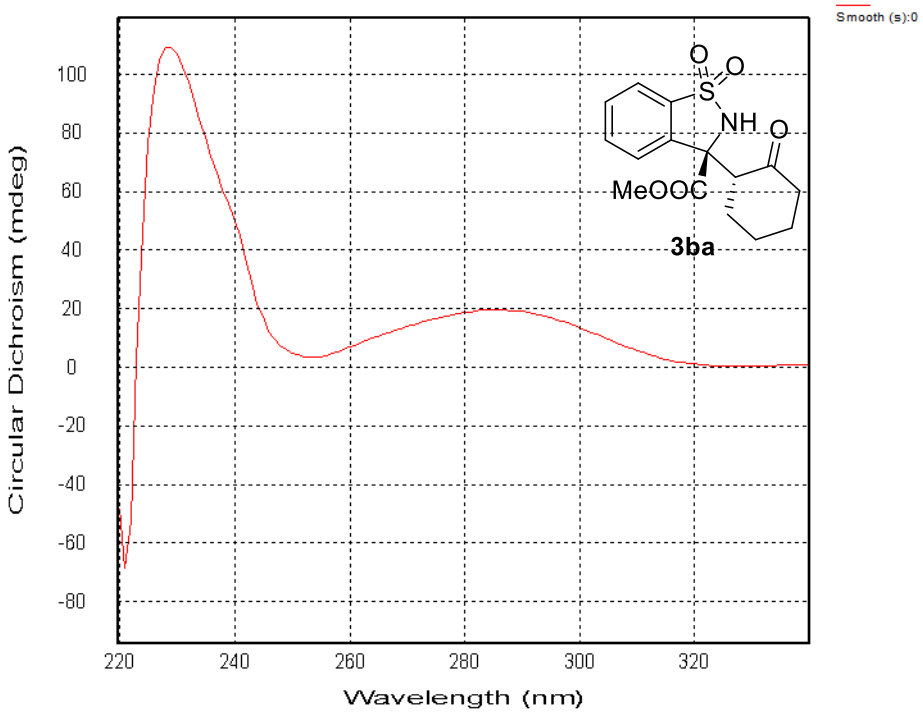
Name	Retention Time	Area	% Area
1	4.670	522184	5.37
2	5.627	4330032	44.49
3	6.709	525056	5.40
4	7.499	4354376	44.74

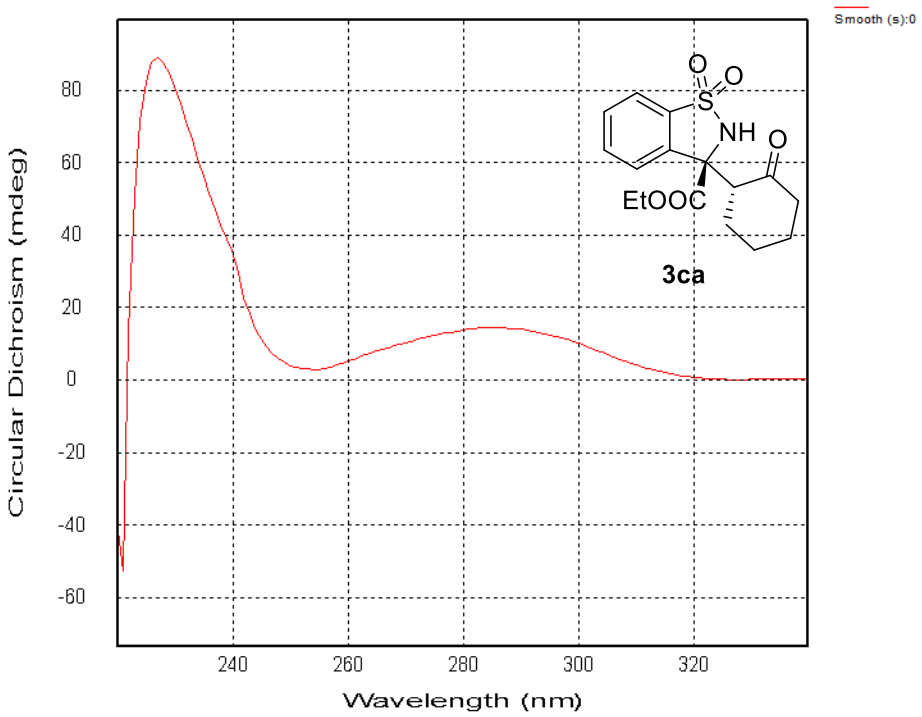


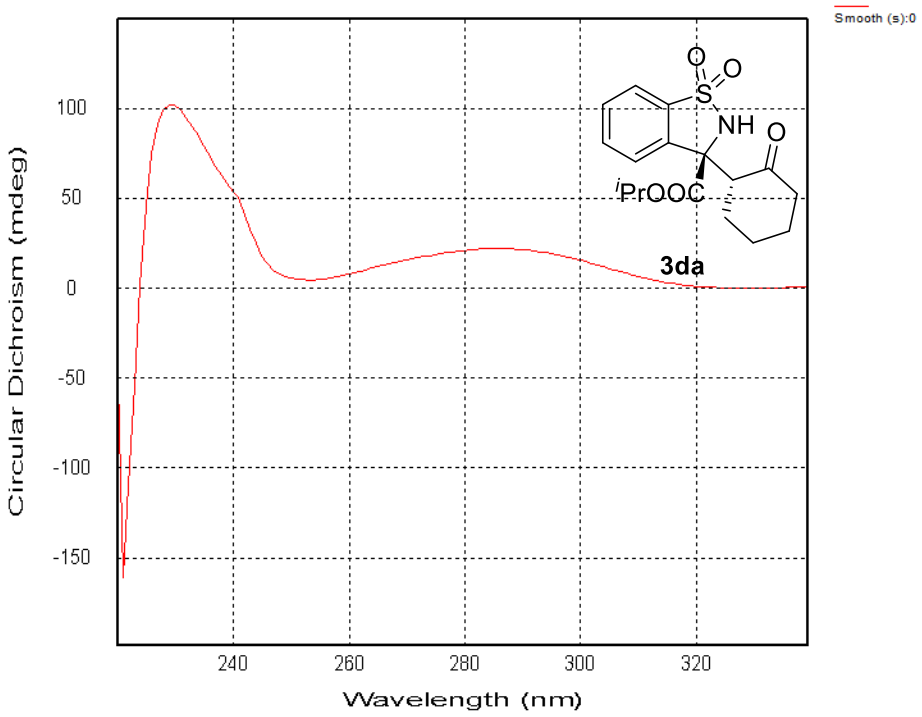
Name	Retention Time	Area	% Area
1	4.377	42339	0.55
2	7.056	7599529	99.45

14. Copies of CD spectra for the products.






Smooth (s):0
Circular Dichroism (mdeg)
80
60
40
20
0
-20
-40
-60
240
260
280
300
320
Wavelength (nm)
O
O
S
NH
O
EtOOC
3ca


Smooth (s):0
Circular Dichroism (mdeg)
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50
0
-50
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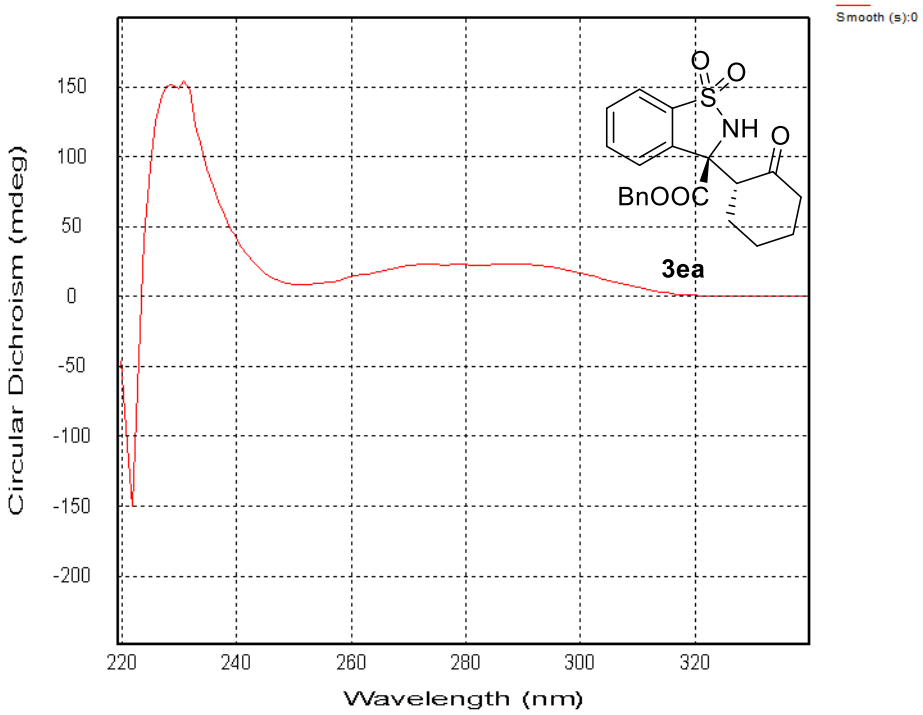
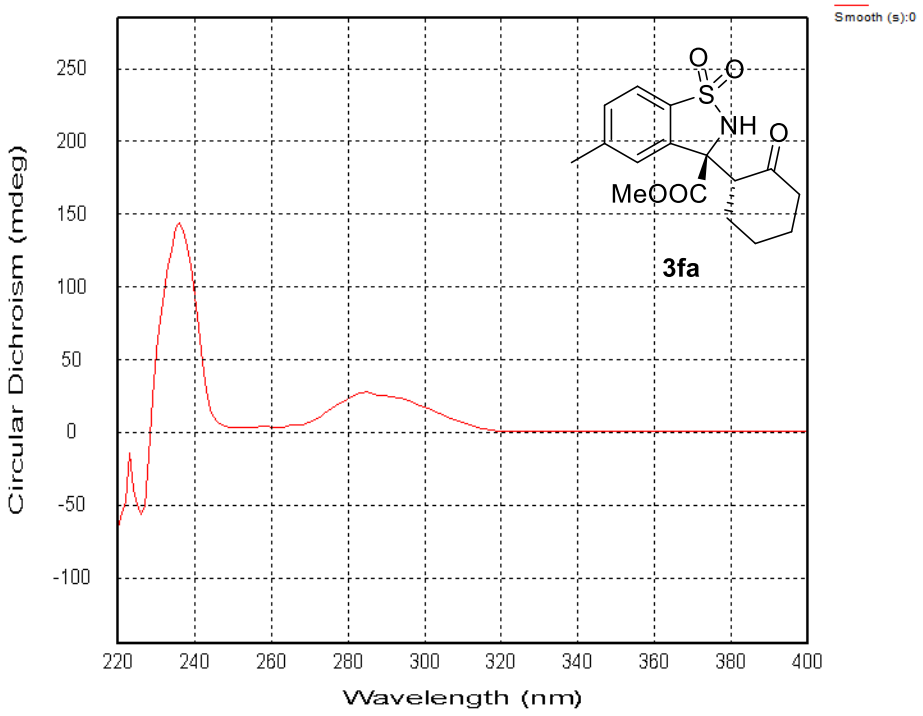
240
260
280
300
320
Wavelength (nm)
O
O
S
NH
O
iPrOOC
3da


Smooth (s):0
Circular Dichroism (mdeg)
150
100
50
0
-50
-100
-150
-200
220
240
260
280
300
320
Wavelength (nm)
O
O
S
NH
O
BnOOC
3ea


Smooth (s):0
Circular Dichroism (mdeg)
250
200
150
100
50
0
-50
-100
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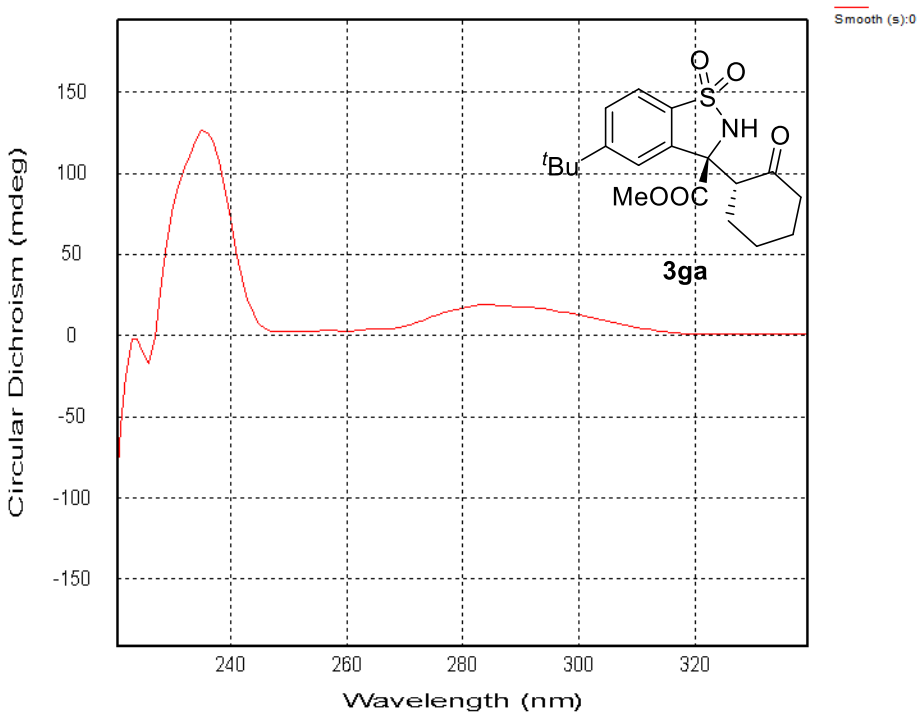
300
320
340
360
380
400
Wavelength (nm)
O
O
S
NH
O
MeOOC
3fa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Circular Dichroism (mdeg)
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100
50
0
-50
-100
-150
240
260
280
300
320
Wavelength (nm)
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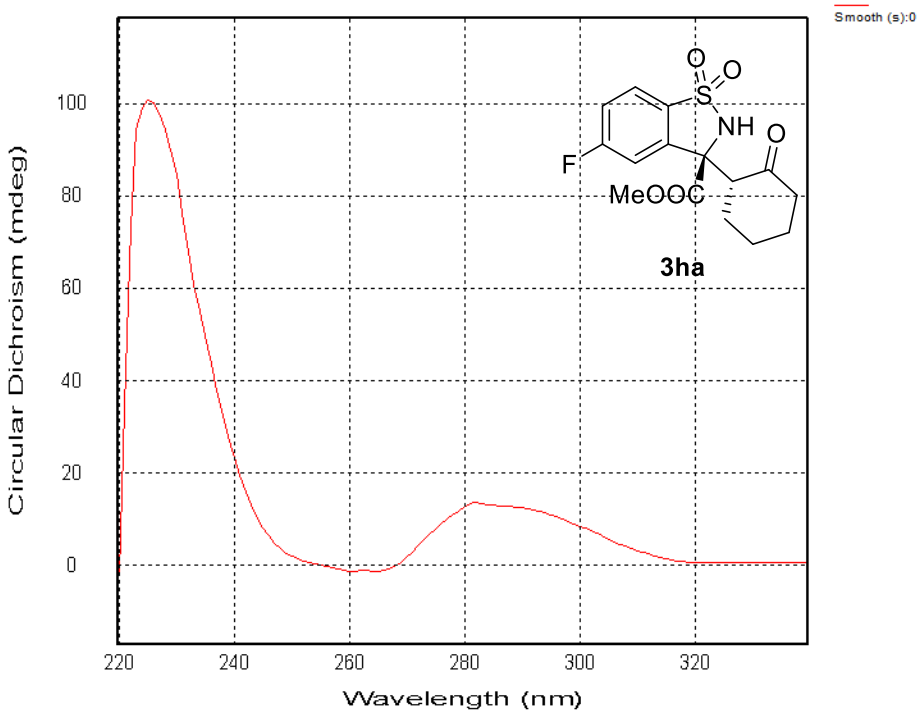
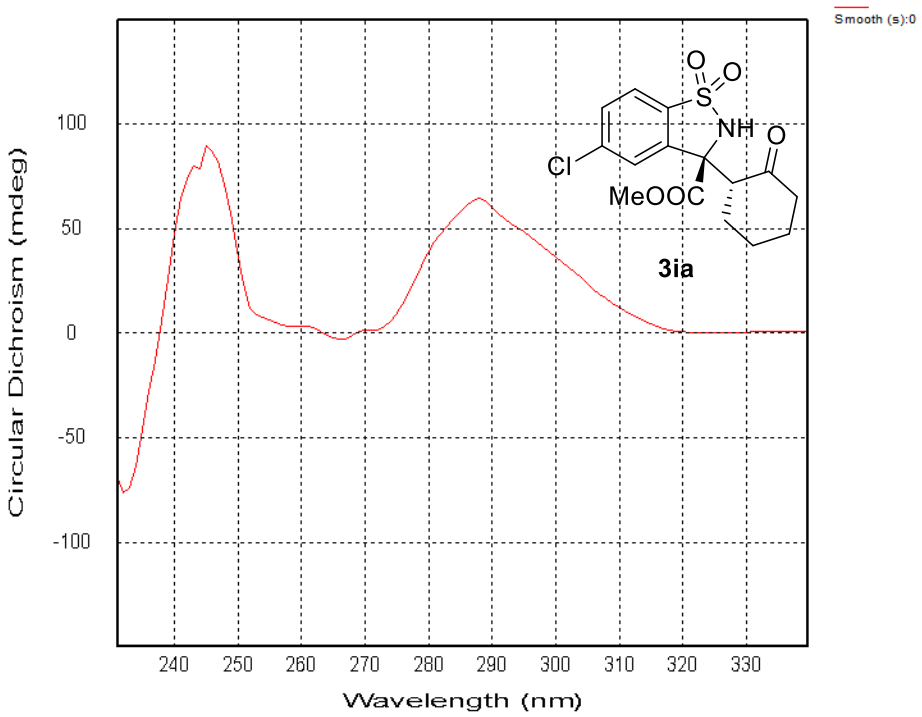
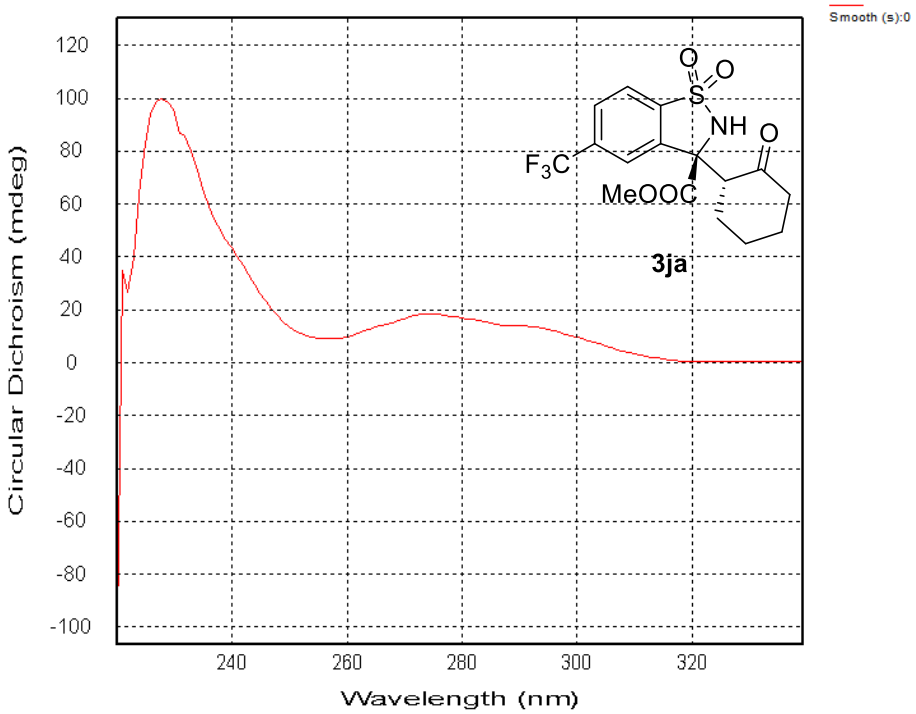
O
S
NH
O
tBu
MeOOC
3ga


Smooth (s):0
Circular Dichroism (mdeg)
100
80
60
40
20
0
220
240
260
280
300
320
Wavelength (nm)
O
O
S
NH
O
F
MeOOC
3ha


Smooth (s):0
Circular Dichroism (mdeg)
100
50
0
-50
-100
240
250
260
270
280
290
300
310
320
330
Wavelength (nm)
O
O
S
NH
O
Cl
MeOOC
3ia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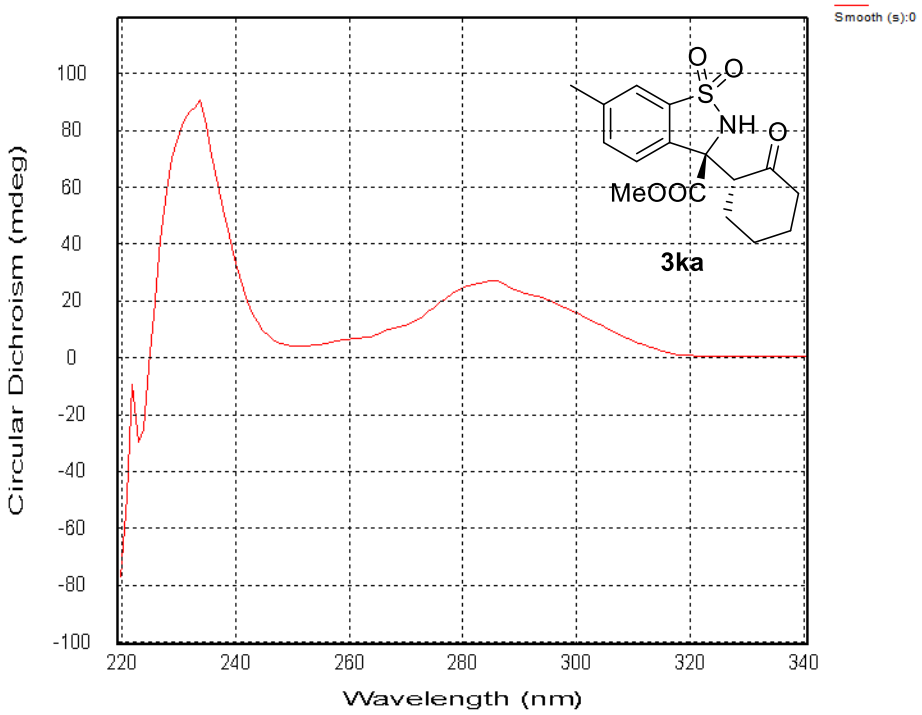
Circular Dichroism (mdeg)
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
240
260
280
300
320
Wavelength (nm)
O
O
S
NH
O
F3C
MeOOC
3ja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Circular Dichroism (mdeg)
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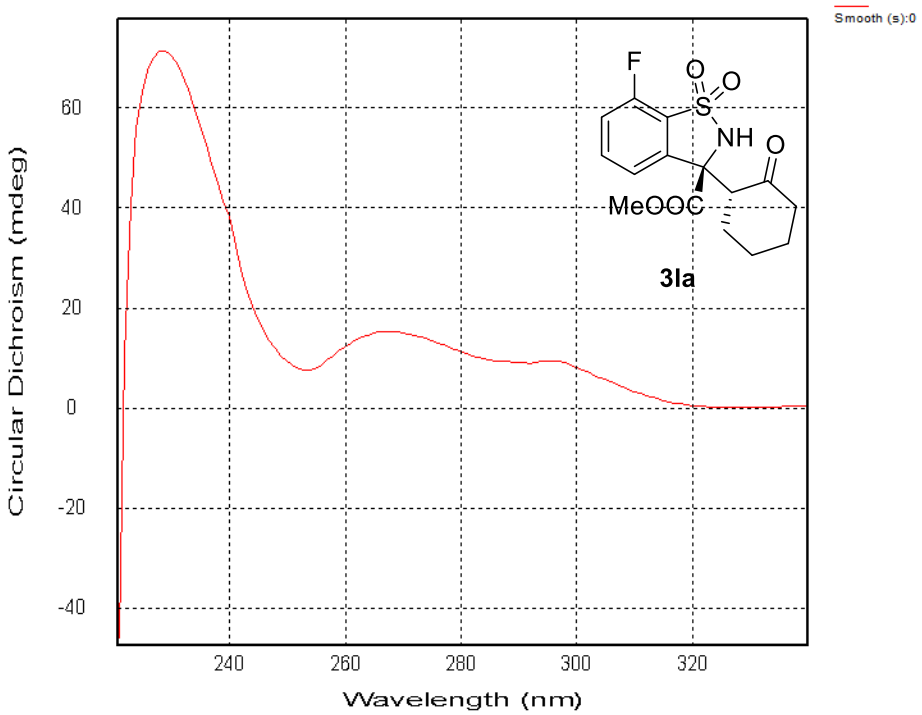
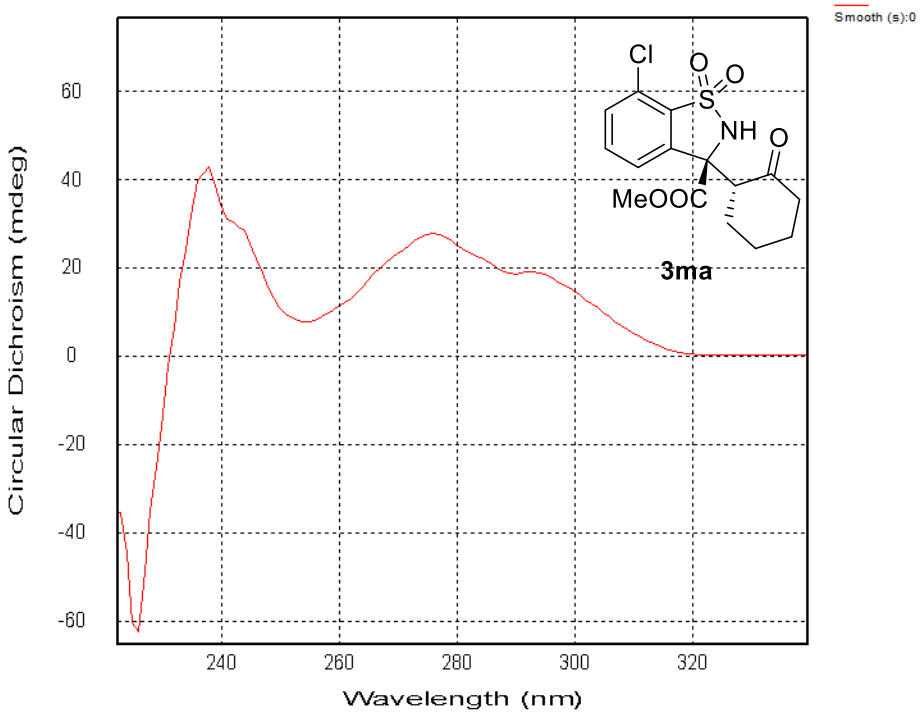
80
60
40
20
0
-20
-40
-60
-80
-100
220
240
260
280
300
320
340
Wavelength (nm)
O
O
S
NH
O
MeOOC
3ka


Smooth (s):0
Circular Dichroism (mdeg)
60
40
20
0
-20
-40
240
260
280
300
320
Wavelength (nm)
F
O
O
S
NH
O
MeOOC
3la


Smooth (s):0
Cl
O
O
S
NH
O
MeOOC
3ma
Circular Dichroism (mdeg)
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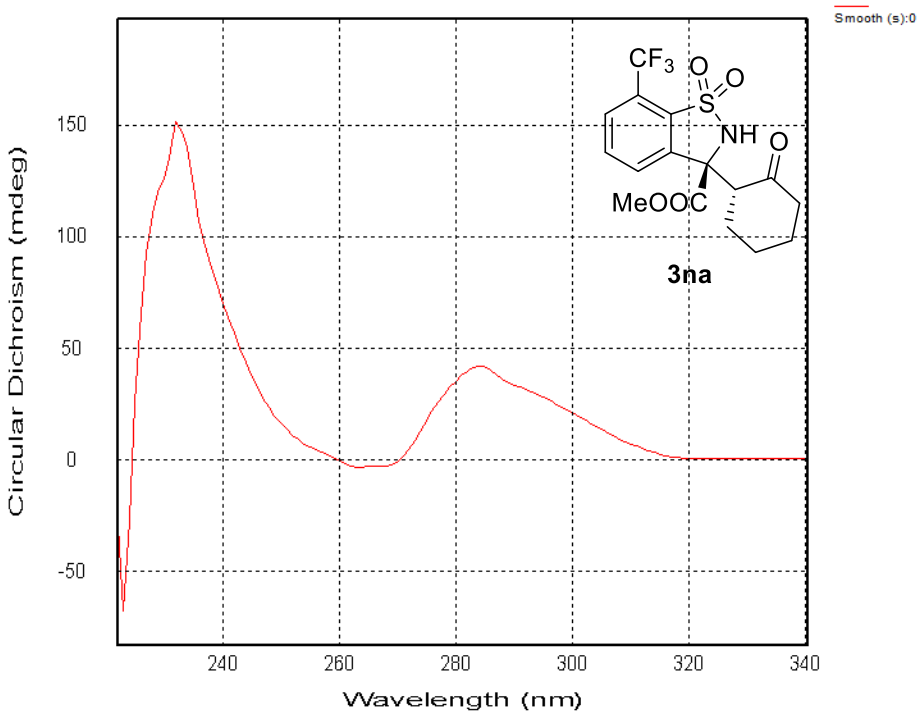
40
20
0
-20
-40
-60
240
260
280
300
320
Wavelength (nm)


Smooth (s):0
CF3
O
O
S
NH
O
MeOOC
3na
Circular Dichroism (mdeg)
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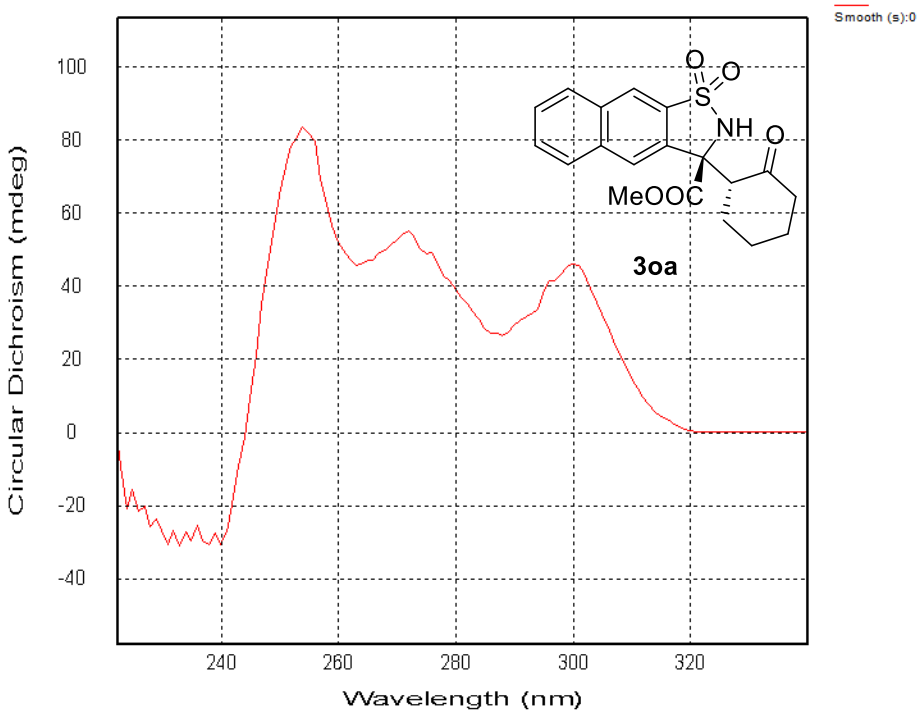
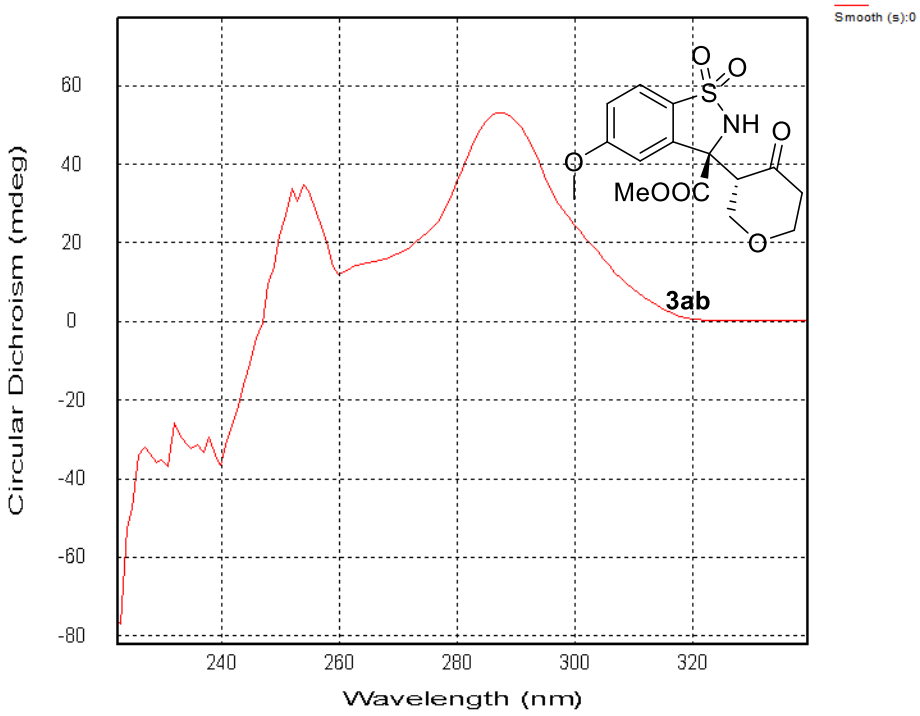
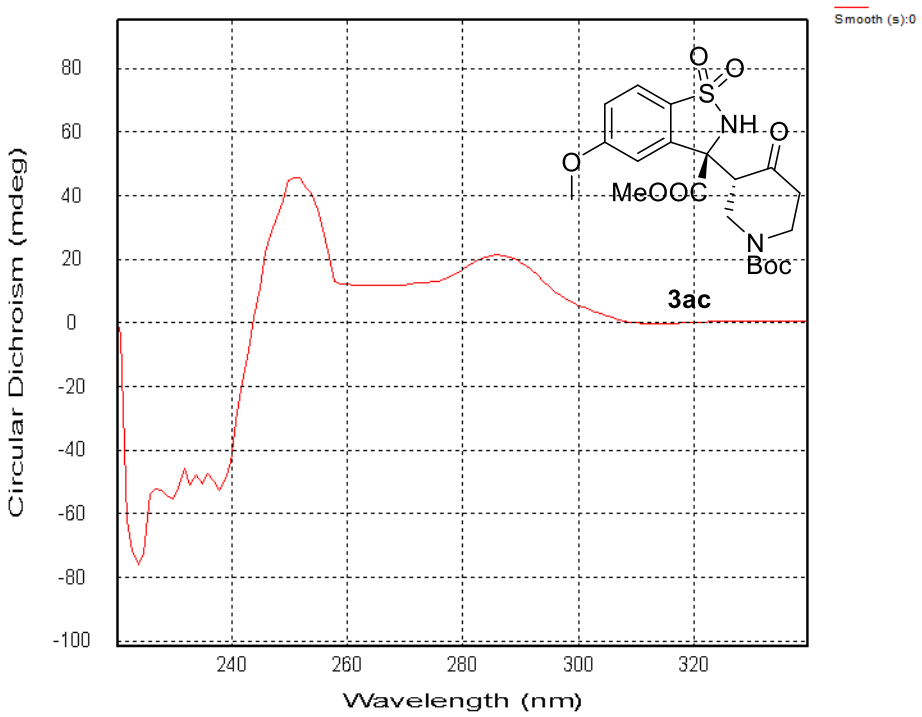
100
50
0
-50
240
260
280
300
320
340
Wavelength (nm)


Smooth (s):0
Circular Dichroism (mdeg)
100
80
60
40
20
0
-20
-40
240
260
280
300
320
Wavelength (nm)
O
O
S
NH
O
MeOOC
3oa


Smooth (s):0
Circular Dichroism (mdeg)
60
40
20
0
-20
-40
-60
-80
240
260
280
300
320
Wavelength (nm)
O
O
S
NH
O
O
MeOOC
O
3ab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Circular Dichroism (mdeg)
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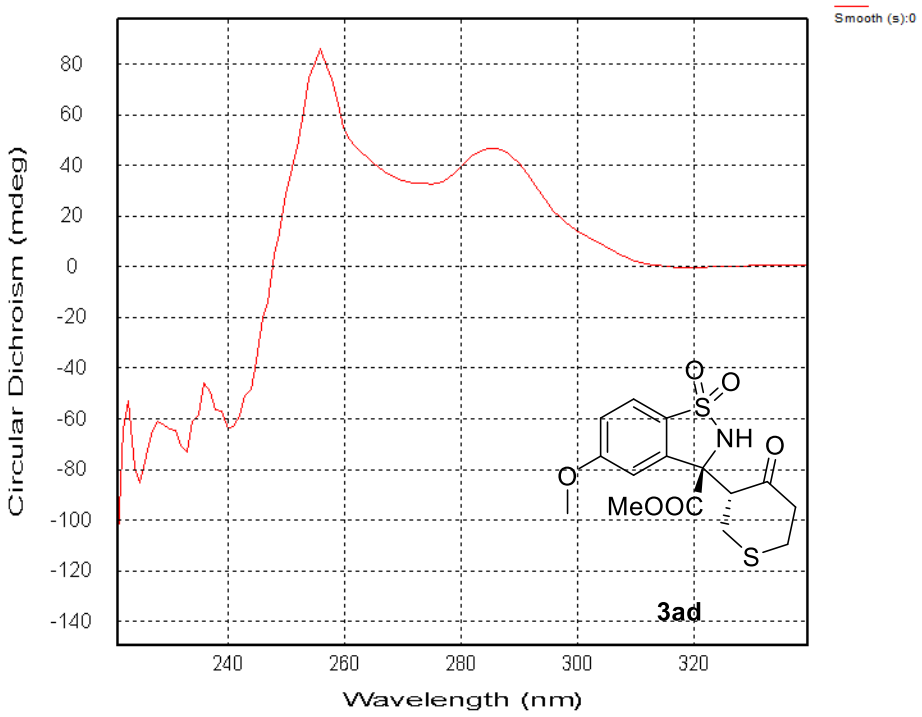
60
40
20
0
-20
-40
-60
-80
-100
240
260
280
300
320
Wavelength (nm)
O
O
S
NH
O
O
MeOOC
N
Boc
3ac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Circular Dichroism (mdeg)
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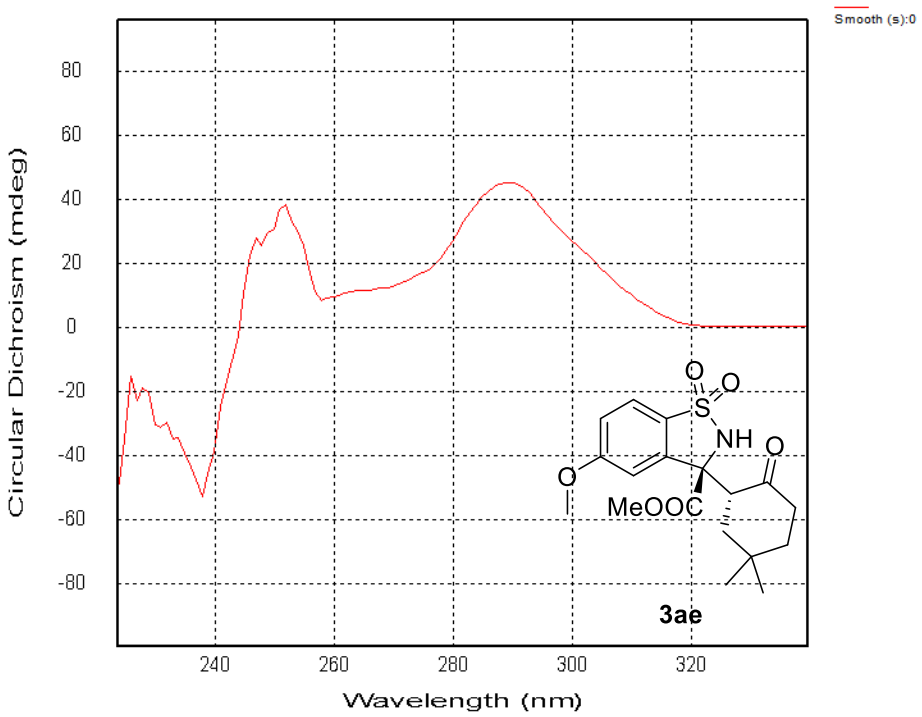
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
240
260
280
300
320
Wavelength (nm)
O
O
S
NH
O
O
MeOOC
S
3ad


Smooth (s):0
Circular Dichroism (mdeg)
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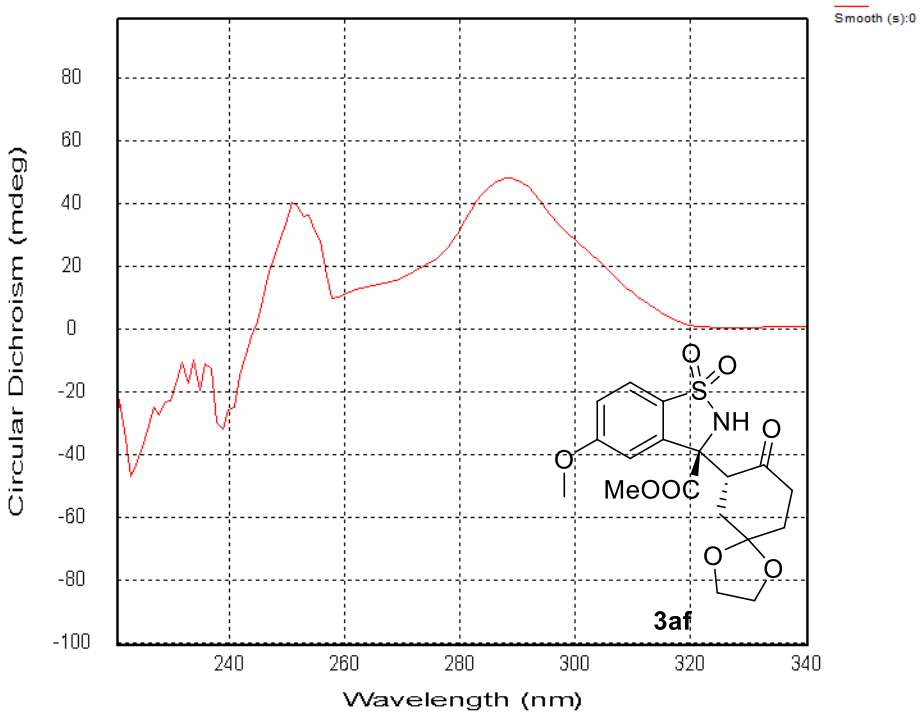
60
40
20
0
-20
-40
-60
-80
240
260
280
300
320
Wavelength (nm)
O
O
S
NH
O
O
MeOOC
3ae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Circular Dichroism (mdeg)
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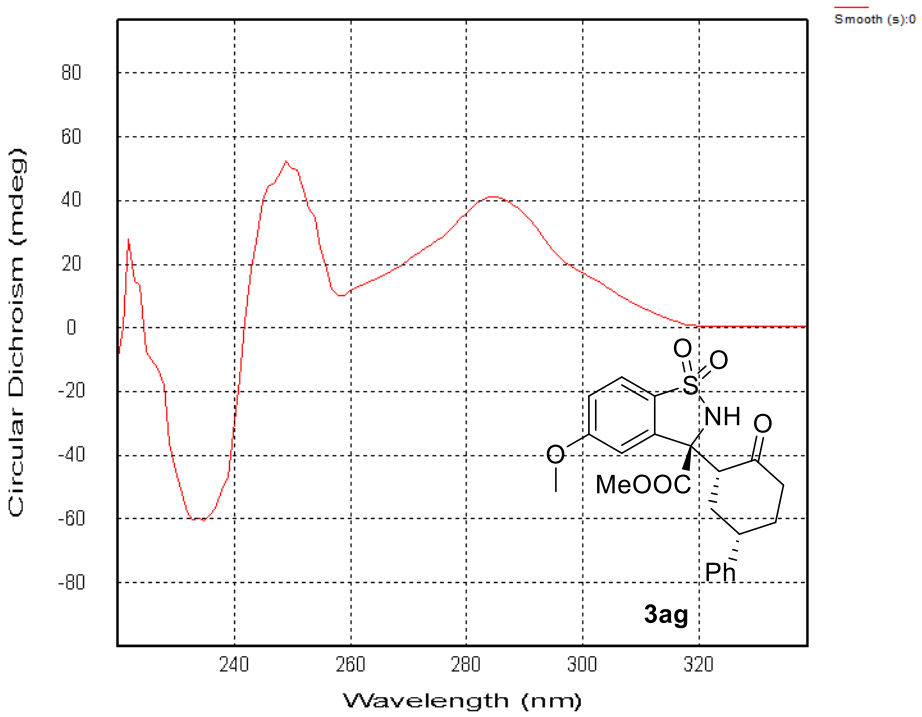
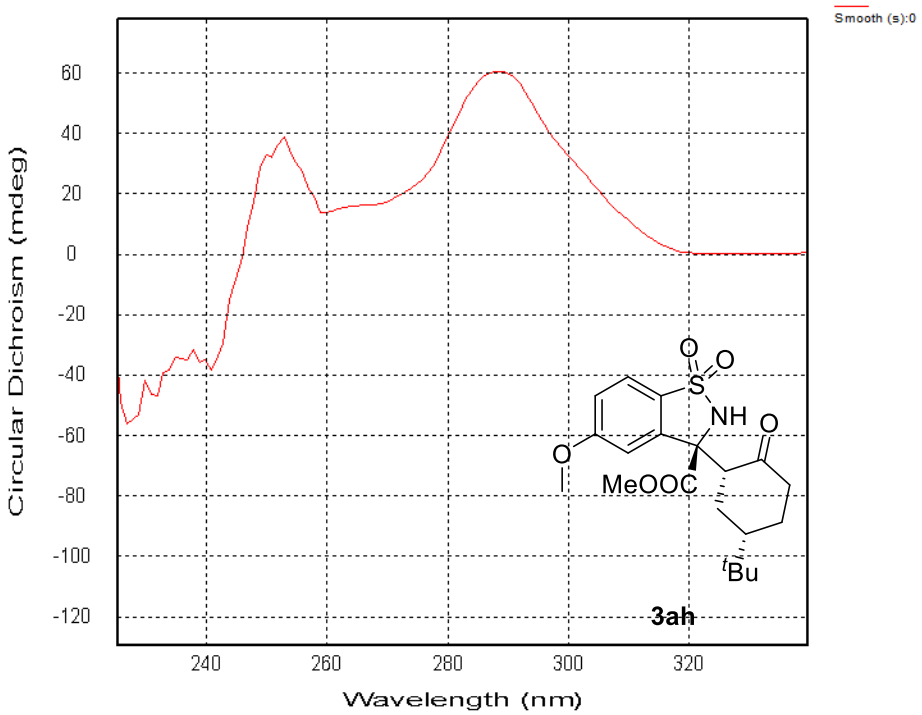
60
40
20
0
-20
-40
-60
-80
-100
240
260
280
300
320
340
Wavelength (nm)
O
O
S
NH
O
O
MeOOC
O
O
3af


Smooth (s):0
Circular Dichroism (mdeg)
80
60
40
20
0
-20
-40
-60
-80
240
260
280
300
320
Wavelength (nm)
O
O
S
NH
O
O
MeOOC
Ph
3ag


Smooth (s):0
Circular Dichroism (mdeg)
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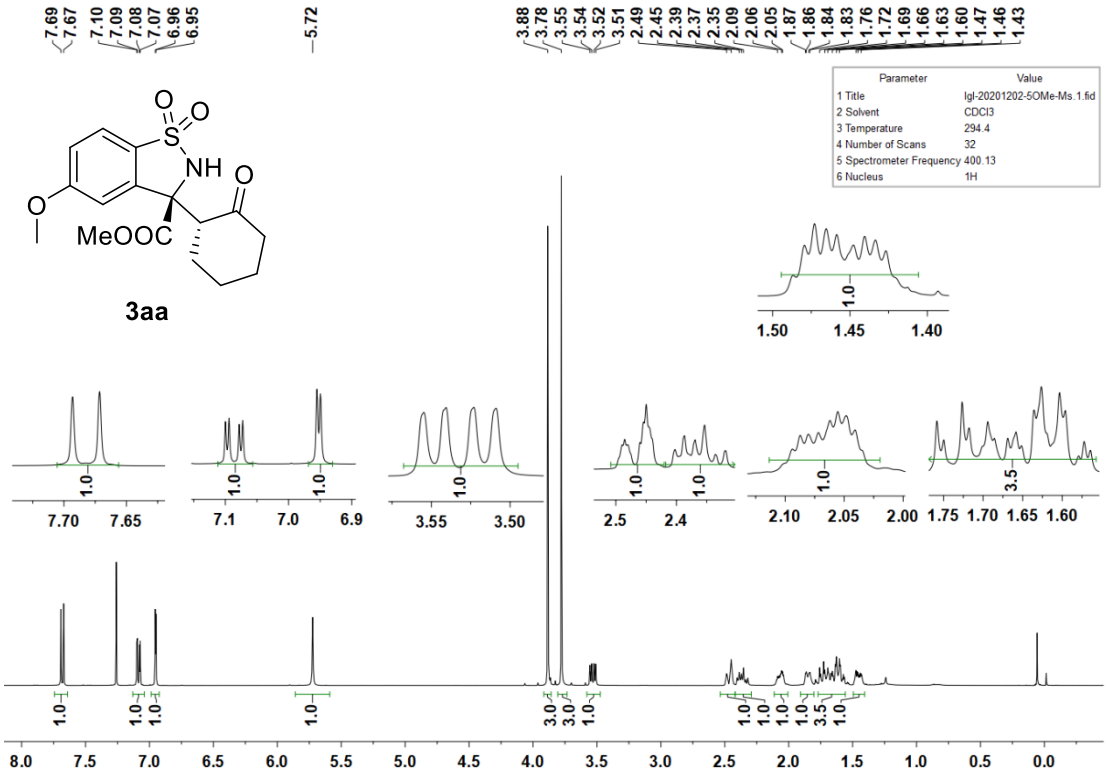
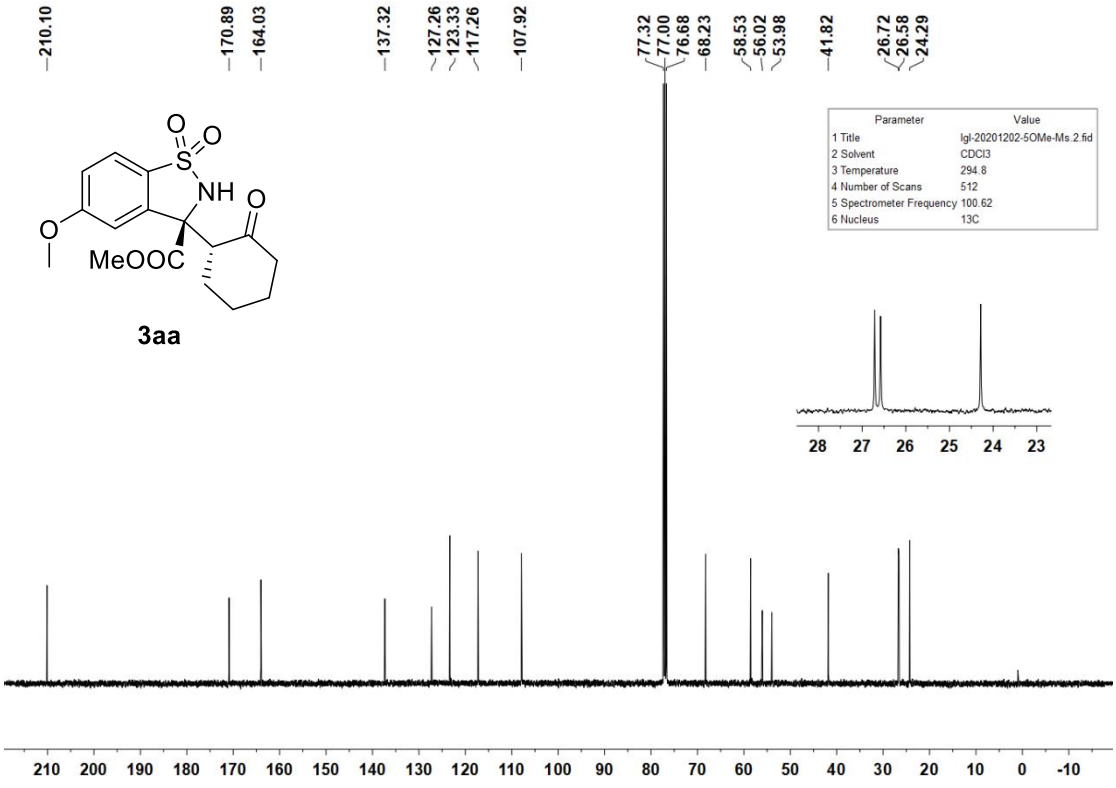
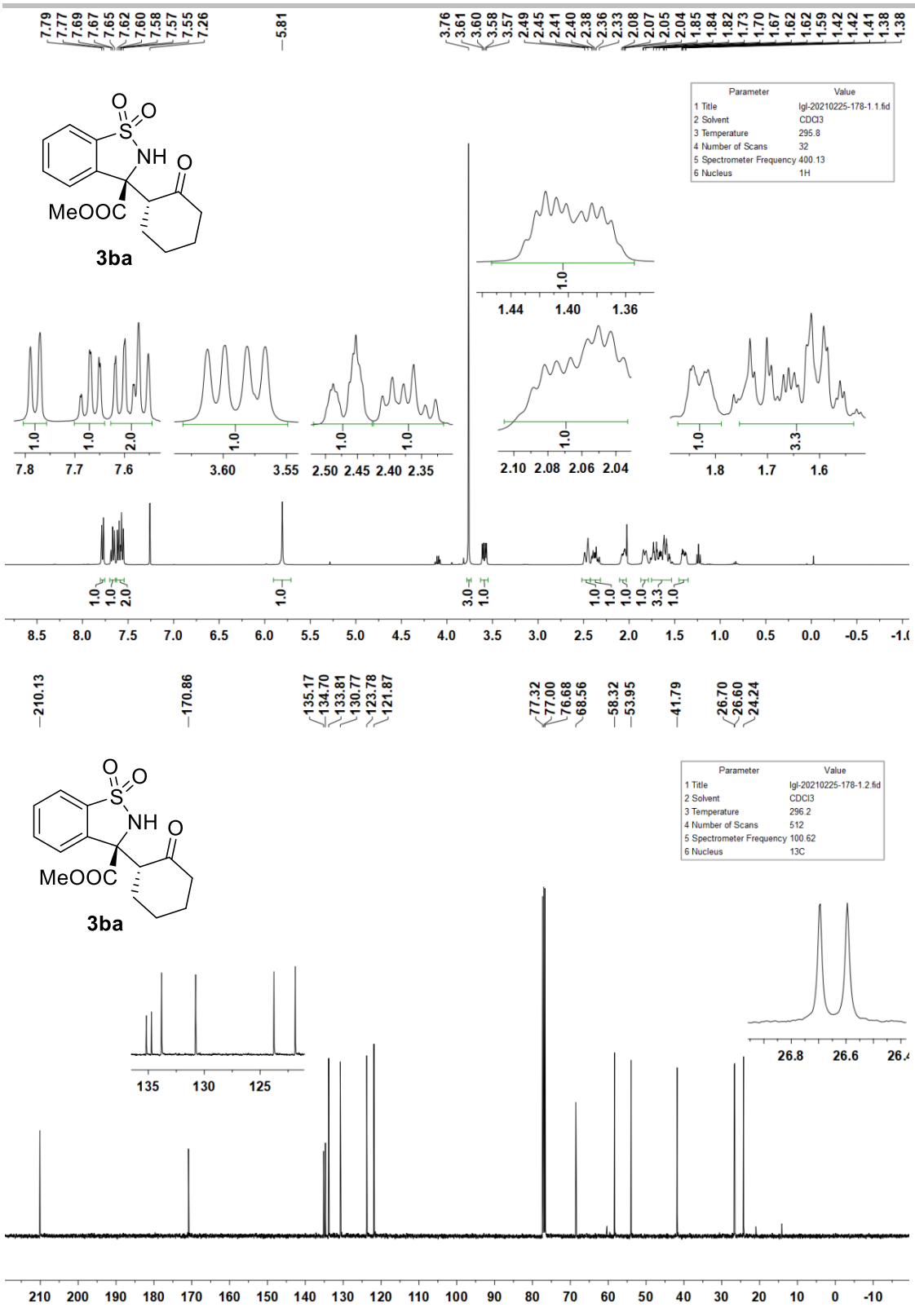
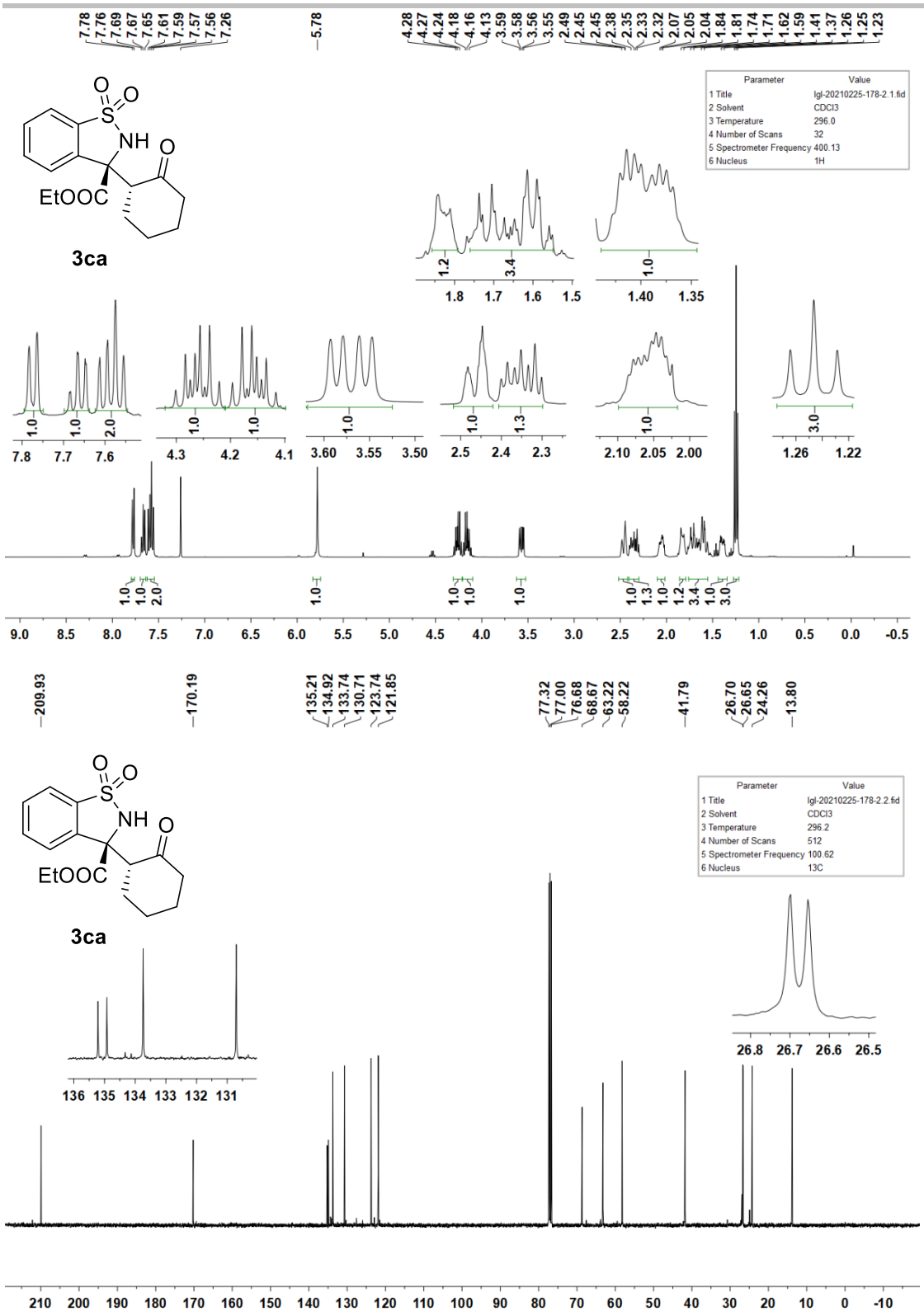
40
20
0
-20
-40
-60
-80
-100
-120
240
260
280
300
320
Wavelength (nm)
O
O
S
NH
O
O
MeOOC
tBu
3ah

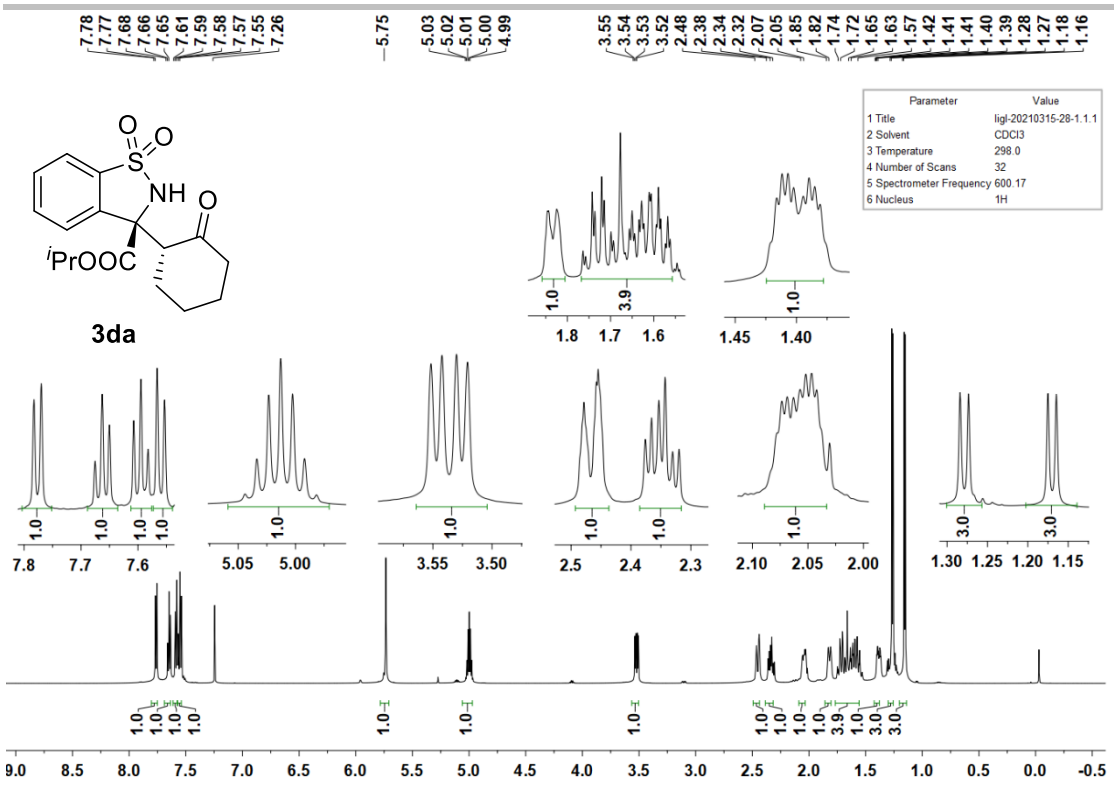
15. Copies of NMR spectra for the products

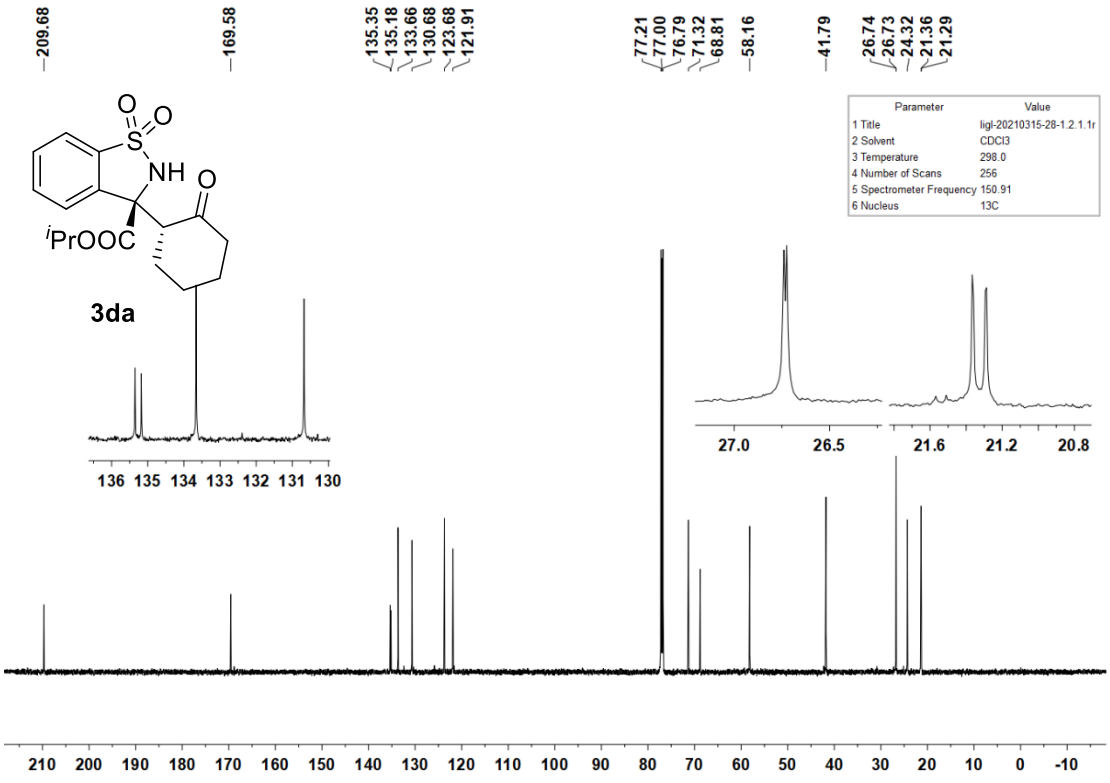


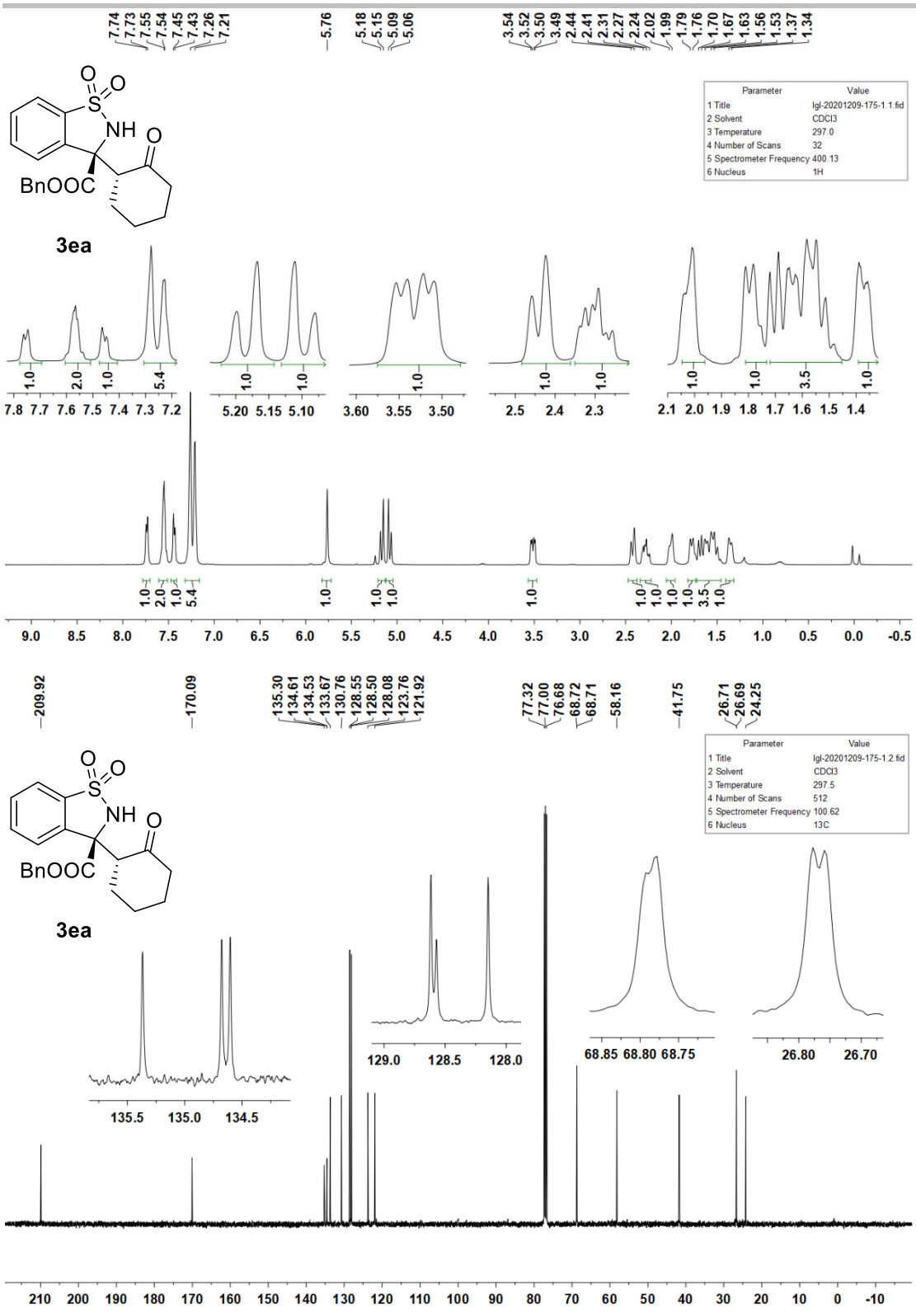



7.79 7.77 7.69 7.67 7.65 7.62 7.60 7.58 7.57 7.55 7.26
5.81
3.76 3.61 3.60 3.58 3.57 2.49 2.45 2.41 2.40 2.38 2.36 2.33 2.08 2.07 2.05 2.04 1.85 1.84 1.82 1.73 1.70 1.67 1.62 1.62 1.59 1.42 1.42 1.41 1.38 1.38
Parameter Value
1 Title lgl-20210225-178-1.1.fid
2 Solvent CDCl3
3 Temperature 295.8
4 Number of Scans 32
5 Spectrometer Frequency 400.13
6 Nucleus 1H
MeOOC
3ba
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
210.13
170.86
135.17 134.70 133.81 130.77 123.78 121.87
77.32 77.00 76.68
68.56
58.32 53.95
41.79
26.70 26.60 24.24
Parameter Value
1 Title lgl-20210225-178-1.2.fid
2 Solvent CDCl3
3 Temperature 296.2
4 Number of Scans 512
5 Spectrometer Frequency 100.62
6 Nucleus 13C
MeOOC
3ba
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


7.78 7.76 7.69 7.67 7.65 7.61 7.59 7.57 7.56 7.26
5.78
4.28 4.27 4.24 4.18 4.16 4.13 3.59 3.58 3.56 3.55 2.49 2.45 2.45 2.38 2.35 2.33 2.32 2.07 2.05 2.04 1.84 1.81 1.74 1.71 1.62 1.59 1.41 1.37 1.26 1.25 1.23
O
O
S
NH
O
EtOOC
3ca
Parameter Value
1 Title lgl-20210225-178-2.1.fid
2 Solvent CDCl3
3 Temperature 296.0
4 Number of Scans 32
5 Spectrometer Frequency 400.13
6 Nucleus 1H
209.93
170.19
135.21 134.92 133.74 130.71 123.74 121.85
77.32 77.00 76.68 68.67 63.22 58.22
41.79
26.70 26.65 24.26
13.80
Parameter Value
1 Title lgl-20210225-178-2.2.fid
2 Solvent CDCl3
3 Temperature 296.2
4 Number of Scans 512
5 Spectrometer Frequency 100.62
6 Nucleus 13C


7.78 7.77 7.68 7.66 7.65 7.61 7.59 7.58 7.57 7.55 7.26
5.75
5.03 5.02 5.01 5.00 4.99
3.55 3.54 3.53 3.52 2.48 2.38 2.34 2.32 2.07 2.05 1.85 1.82 1.74 1.72 1.65 1.63 1.57 1.42 1.41 1.41 1.40 1.39 1.28 1.27 1.18 1.16
Parameter Value
1 Title ligl-20210315-28-1.1.1
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 32
5 Spectrometer Frequency 600.17
6 Nucleus 1H
3da


209.68
169.58
135.35 135.18 133.66 130.68 123.68 121.91
77.21 77.00 76.79 71.32 68.81
58.16
41.79
26.74 26.73 24.32 21.36 21.29
Parameter Value
1 Title ligl-20210315-28-1.2.1.1r
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 256
5 Spectrometer Frequency 150.91
6 Nucleus 13C
3da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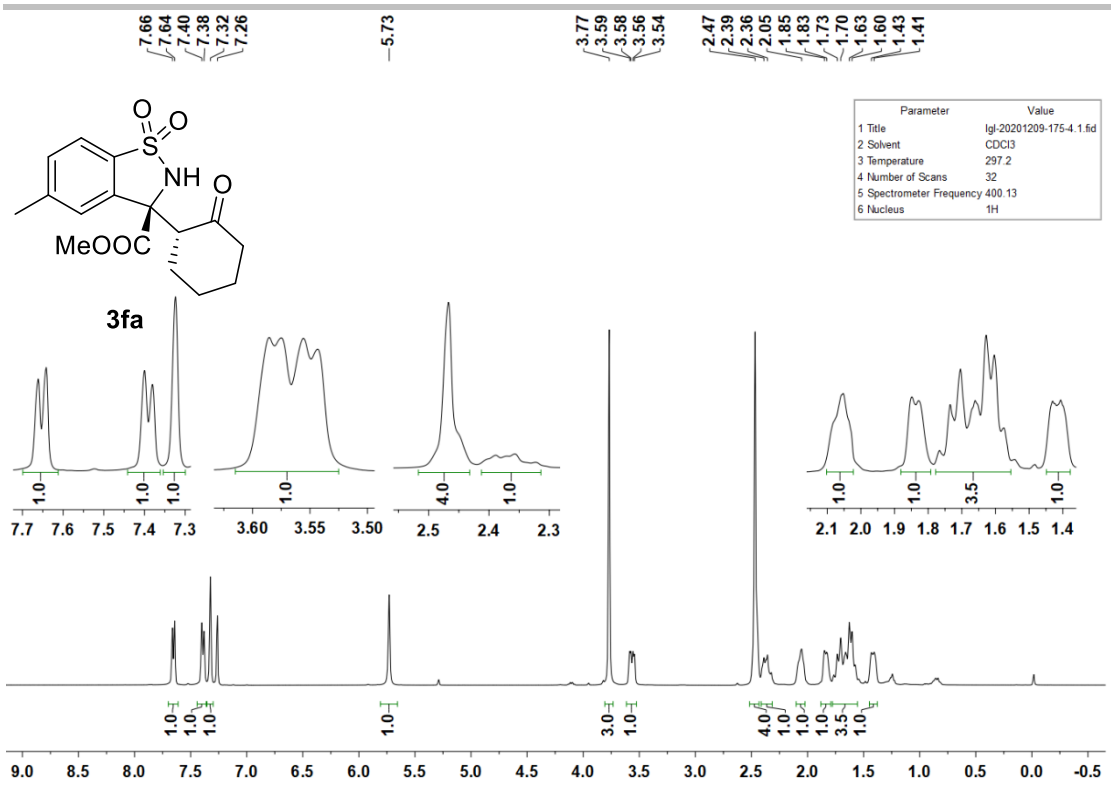
5.76
5.18 5.15 5.09 5.06
3.54 3.52 3.50 3.49
2.44 2.41 2.31 2.27 2.24 2.02 1.99 1.79 1.76 1.70 1.67 1.63 1.56 1.53 1.37 1.34
Parameter Value
1 Title lgl-20201209-175-1.1.fid
2 Solvent CDCl3
3 Temperature 297.0
4 Number of Scans 32
5 Spectrometer Frequency 400.13
6 Nucleus 1H
BnOOC
3ea
209.92
170.09
135.30 134.61 134.53 133.67 130.76 128.55 128.50 128.08 123.76 121.92
77.32 77.00 76.68 68.72 68.71
58.16
41.75
26.71 26.69 24.25
Parameter Value
1 Title lgl-20201209-175-1.2.fid
2 Solvent CDCl3
3 Temperature 297.5
4 Number of Scans 512
5 Spectrometer Frequency 100.62
6 Nucleus 13C
BnOOC
3ea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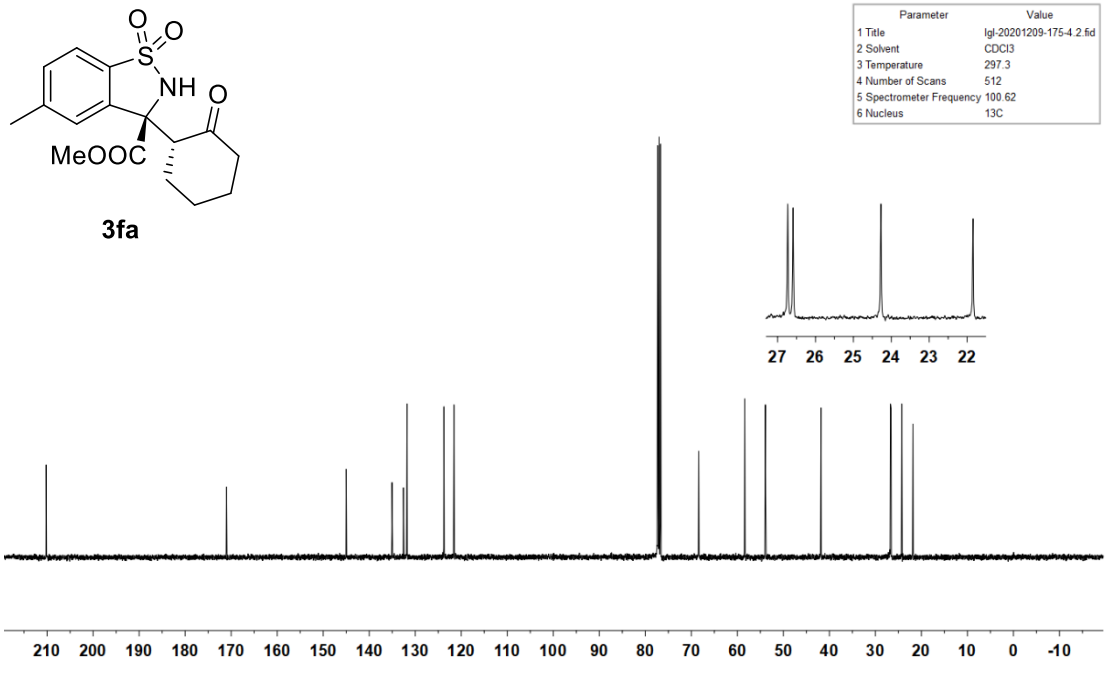
7.64
7.40
7.38
7.32
7.26
5.73
3.77
3.59
3.58
3.56
3.54
2.47
2.39
2.36
2.05
1.85
1.83
1.73
1.70
1.63
1.60
1.43
1.41
Parameter Value
1 Title lgl-20201209-175-4.1.fid
2 Solvent CDCl3
3 Temperature 297.2
4 Number of Scans 32
5 Spectrometer Frequency 400.13
6 Nucleus 1H
MeOOC
3fa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171.00
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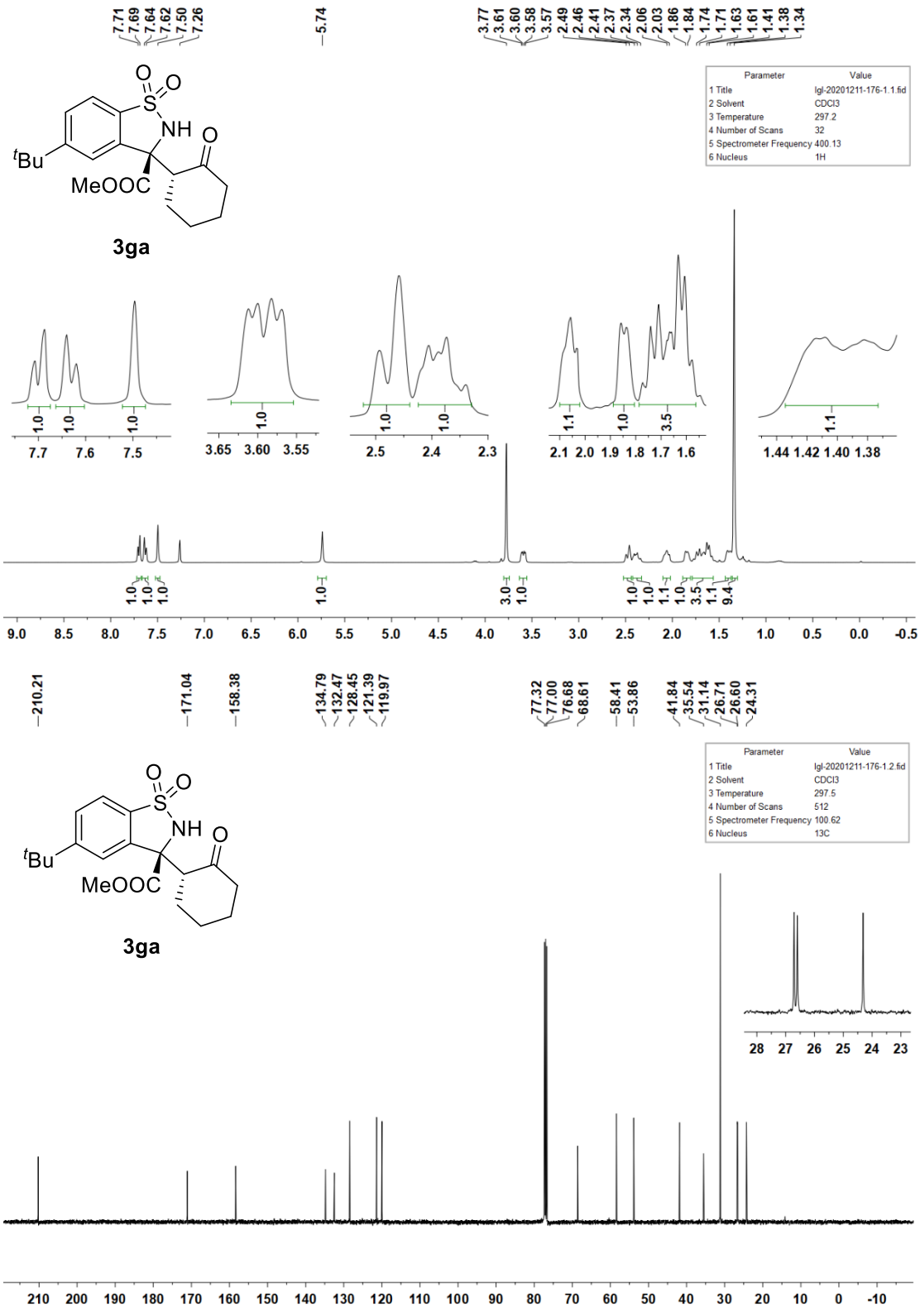
135.04
132.56
131.77
123.77
121.58
77.32
77.00
76.68
68.39
58.39
53.91
41.83
26.73
26.59
24.27
21.84
Parameter Value
1 Title lgl-20201209-175-4.2.fid
2 Solvent CDCl3
3 Temperature 297.3
4 Number of Scans 512
5 Spectrometer Frequency 100.62
6 Nucleus 13C
MeOOC
3fa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7.64
7.62
7.50
7.26
5.74
3.77
3.61
3.60
3.58
3.57
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2.46
2.41
2.37
2.34
2.06
2.03
1.86
1.84
1.74
1.71
1.63
1.61
1.41
1.38
1.34
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1 Title lgl-20201211-176-1.1.fid
2 Solvent CDCl3
3 Temperature 297.2
4 Number of Scans 32
5 Spectrometer Frequency 400.13
6 Nucleus 1H
tBu
MeOOC
3ga
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
210.21
171.04
158.38
134.79
132.47
128.45
121.39
119.97
77.32
77.00
76.68
68.61
58.41
53.86
41.84
35.54
31.14
26.71
26.60
24.31
Parameter Value
1 Title lgl-20201211-176-1.2.fid
2 Solvent CDCl3
3 Temperature 297.5
4 Number of Scans 512
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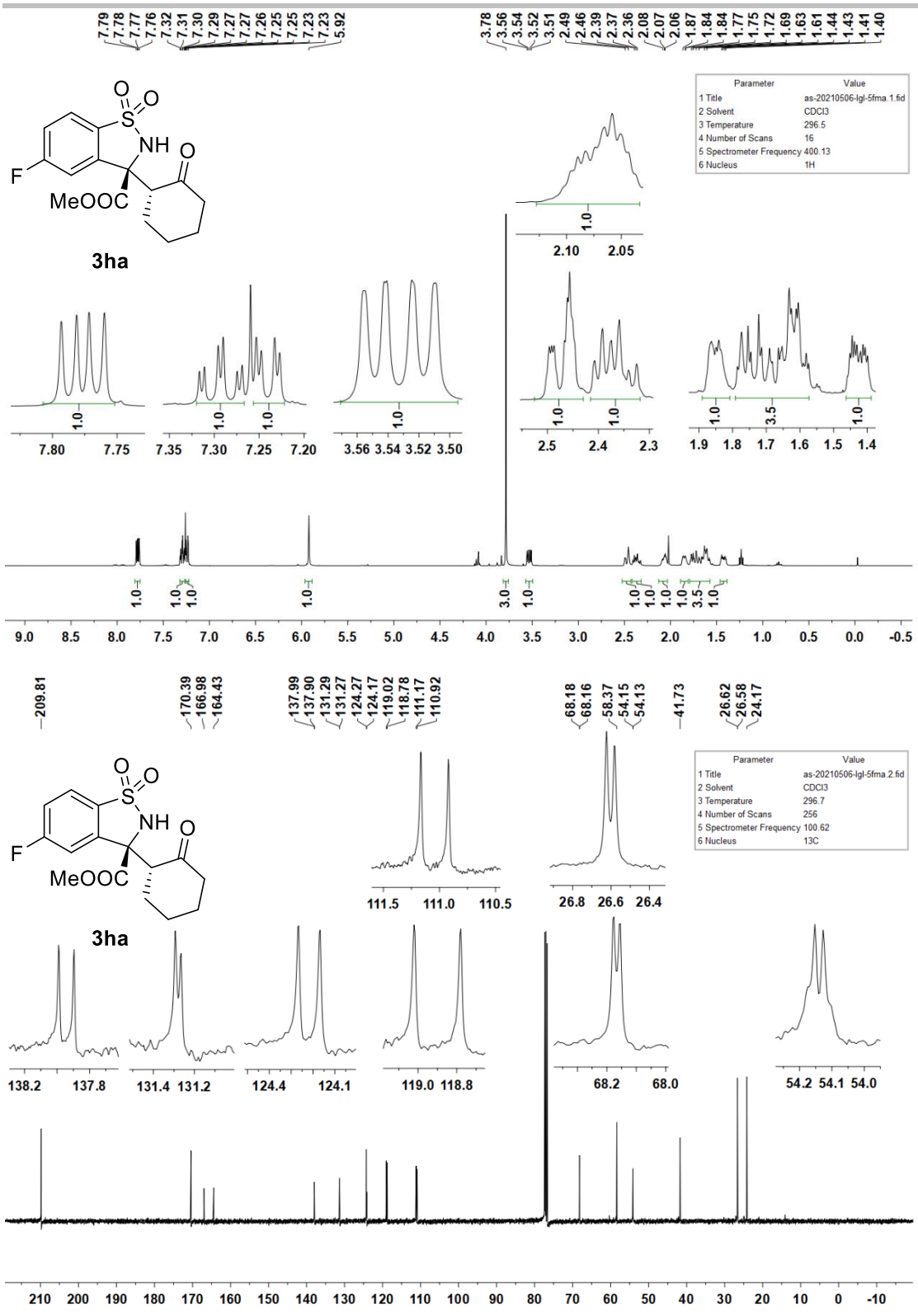
6 Nucleus 13C
tBu
MeOOC
3ga
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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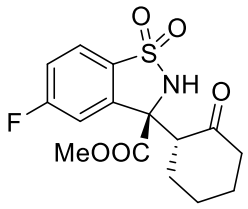
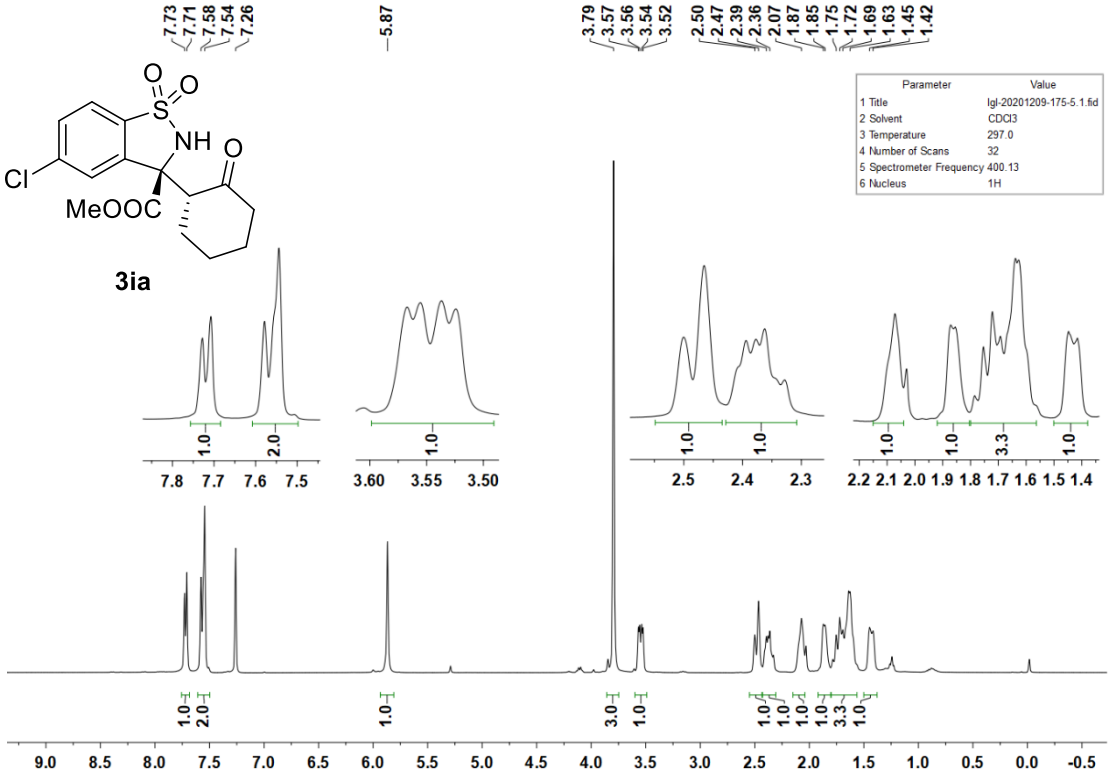
3.78 3.56 3.54 3.52 3.51 2.49 2.46 2.39 2.37 2.36 2.08 2.07 2.06 1.87 1.84 1.84 1.77 1.75 1.72 1.69 1.63 1.61 1.44 1.43 1.41 1.40
Parameter Value
1 Title as-20210506-lgl-5fma.1.fid
2 Solvent CDCl3
3 Temperature 296.5
4 Number of Scans 16
5 Spectrometer Frequency 400.13
6 Nucleus 1H
3ha
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
209.81 170.39 166.98 164.43 137.99 137.90 131.29 131.27 124.27 124.17 119.02 118.78 111.17 110.92 68.18 68.16 58.37 54.15 54.13 41.73 26.62 26.58 24.17
Parameter Value
1 Title as-20210506-lgl-5fma.2.fid
2 Solvent CDCl3
3 Temperature 296.7
4 Number of Scans 256
5 Spectrometer Frequency 100.62
6 Nucleus 13C
3ha
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10



3ha

Parameter	Value
1 Title	as-20210506-lgl-5fma.3.fid
2 Solvent	CDCl3
3 Temperature	296.6
4 Number of Scans	16
5 Spectrometer Frequency	376.46
6 Nucleus	19F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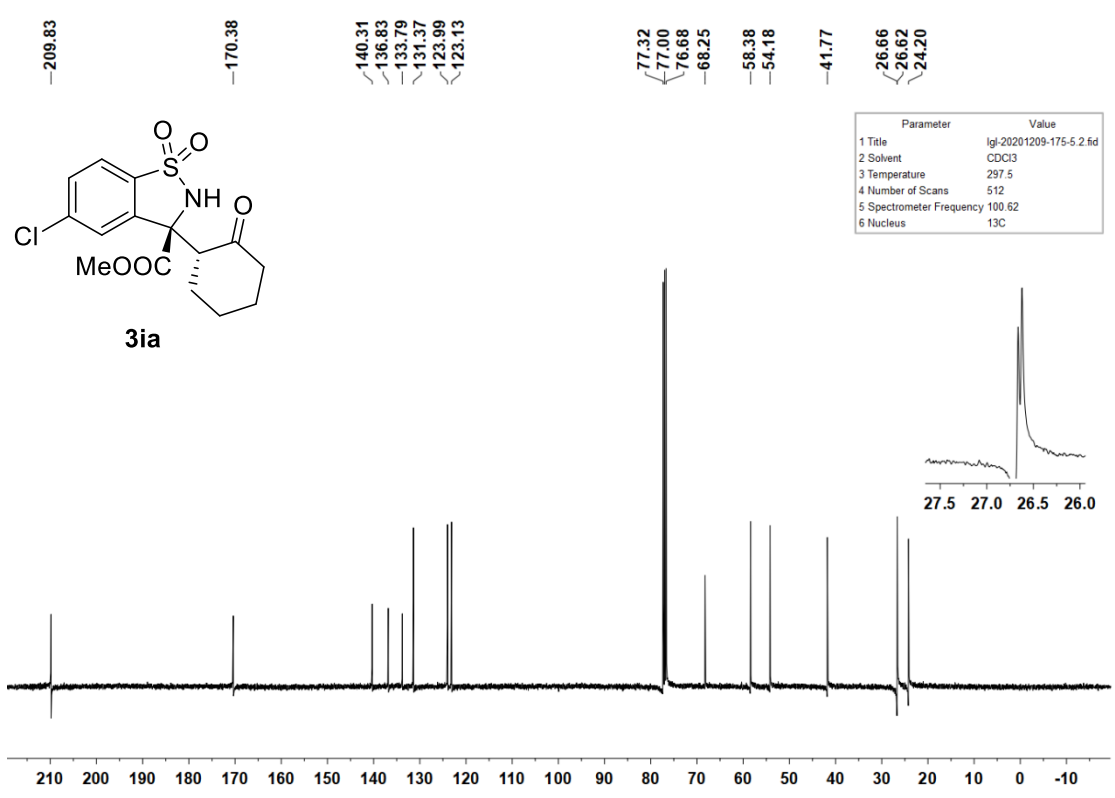
7.58
7.54
7.26
5.87
3.79
3.57
3.56
3.54
3.52
2.50
2.47
2.39
2.36
2.07
1.87
1.85
1.75
1.72
1.69
1.63
1.45
1.42
Parameter Value
1 Title lgl-20201209-175-5.1.fid
2 Solvent CDCl3
3 Temperature 297.0
4 Number of Scans 32
5 Spectrometer Frequency 400.13
6 Nucleus 1H
Cl
MeOOC
NH
O
O
O
3ia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136.83
133.79
131.37
123.99
123.13
77.32
77.00
76.68
68.25
58.38
54.18
41.77
26.66
26.62
24.20
Parameter Value
1 Title lgl-20201209-175-5.2.fid
2 Solvent CDCl3
3 Temperature 297.5
4 Number of Scans 512
5 Spectrometer Frequency 100.62
6 Nucleus 13C
Cl
MeOOC
NH
O
O
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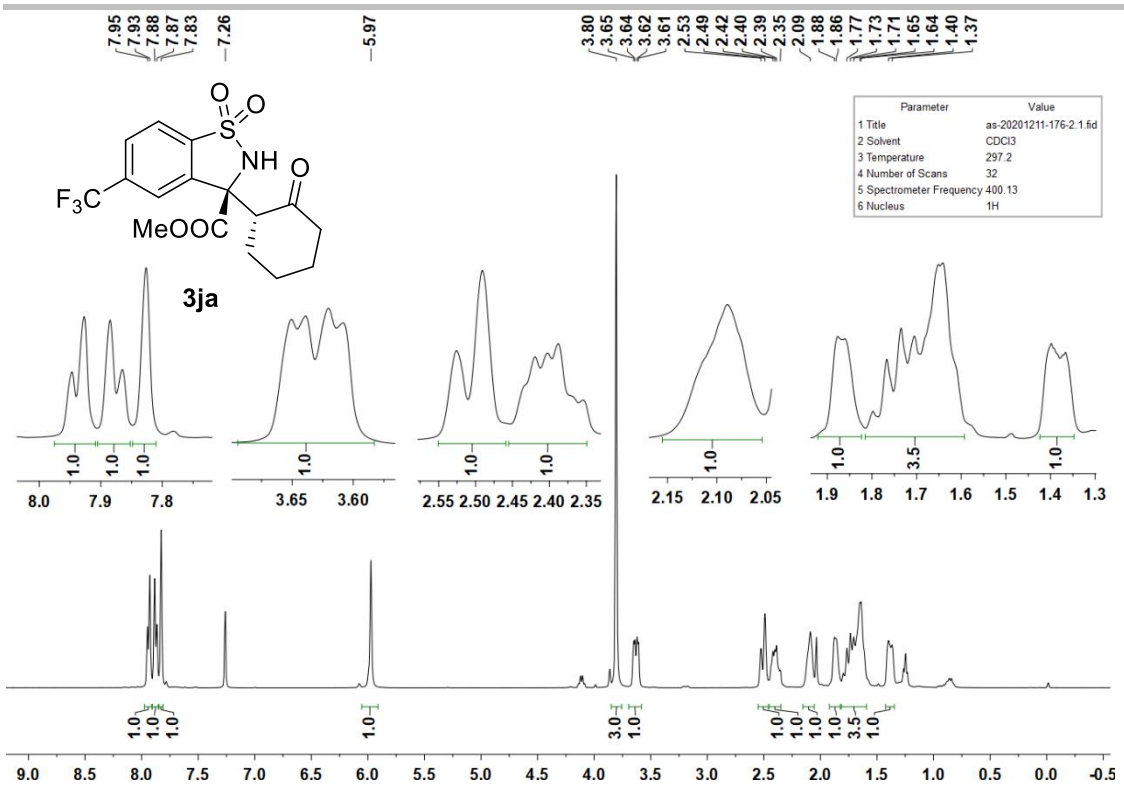
3ia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Parameter Value
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2 Solvent CDCl3
3 Temperature 297.2
4 Number of Scans 32
5 Spectrometer Frequency 400.13
6 Nucleus 1H
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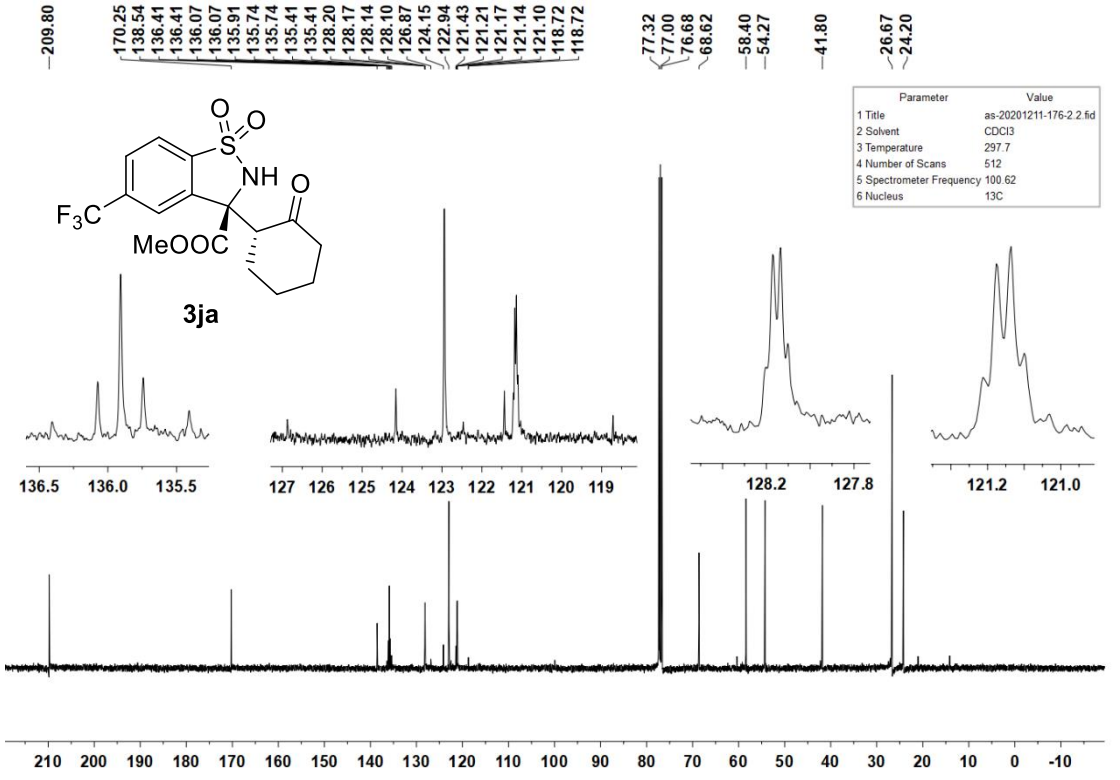
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Parameter Value
1 Title as-20201211-176-2.2.fid
2 Solvent CDCl3
3 Temperature 297.7
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5 Spectrometer Frequency 100.62
6 Nucleus 13C
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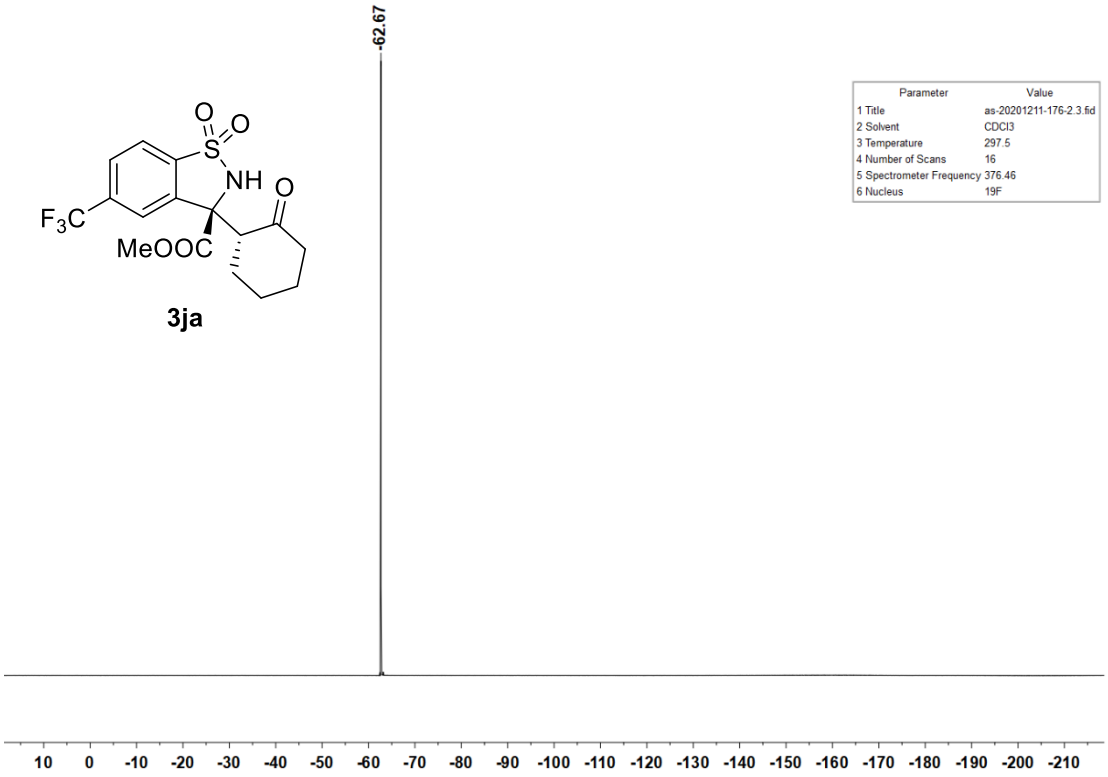
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4 Number of Scans 16
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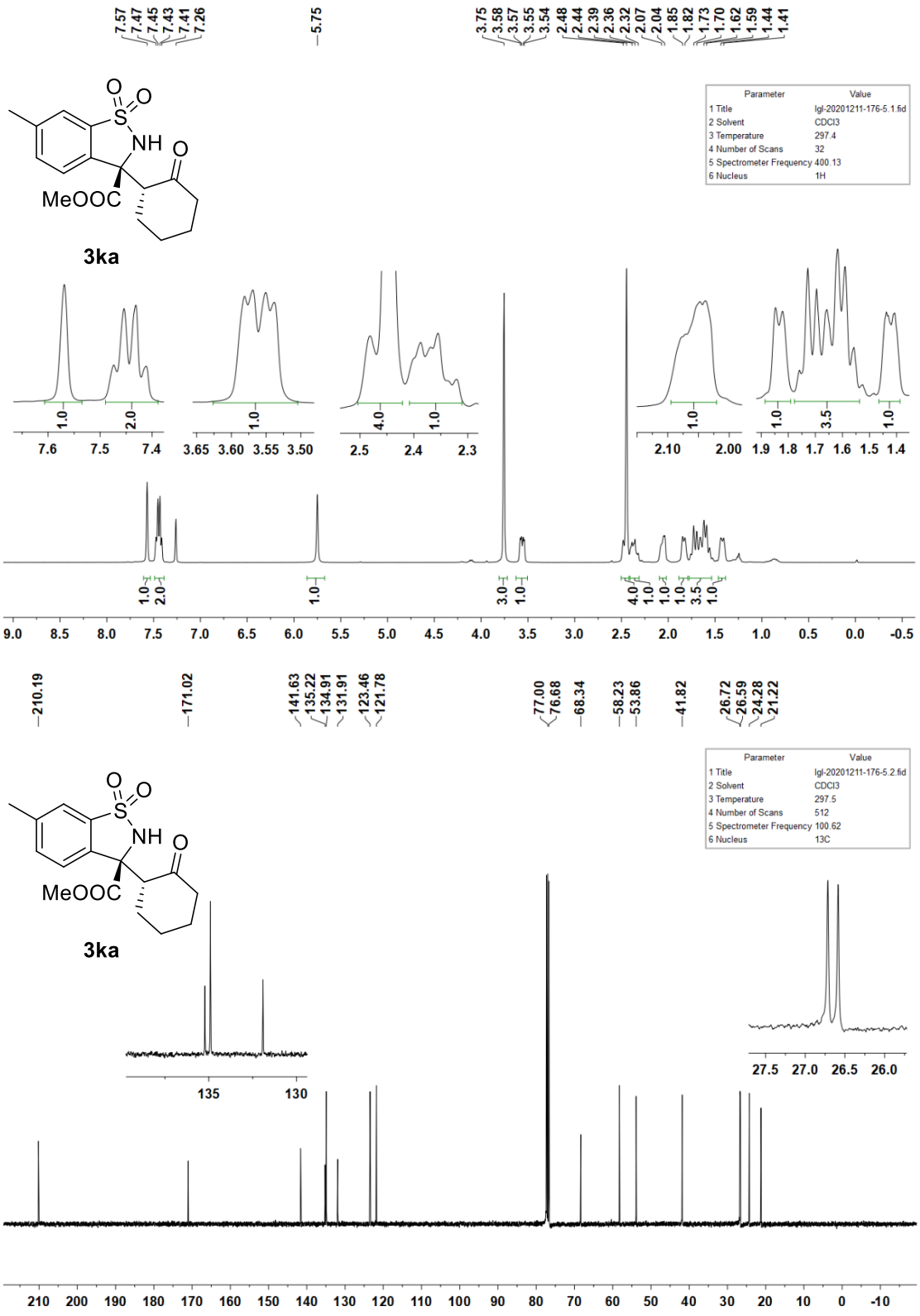
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3.75 3.58 3.57 3.55 3.54 2.48 2.44 2.39 2.36 2.32 2.07 2.04 1.85 1.82 1.73 1.70 1.62 1.59 1.44 1.41
Parameter Value
1 Title lgl-20201211-176-5.1.fid
2 Solvent CDCl3
3 Temperature 297.4
4 Number of Scans 32
5 Spectrometer Frequency 400.13
6 Nucleus 1H
MeOOC
3ka
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210.19 171.02 141.63 135.22 134.91 131.91 123.46 121.78 77.00 76.68 68.34 58.23 53.86 41.82 26.72 26.59 24.28 21.22
Parameter Value
1 Title lgl-20201211-176-5.2.fid
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3 Temperature 297.5
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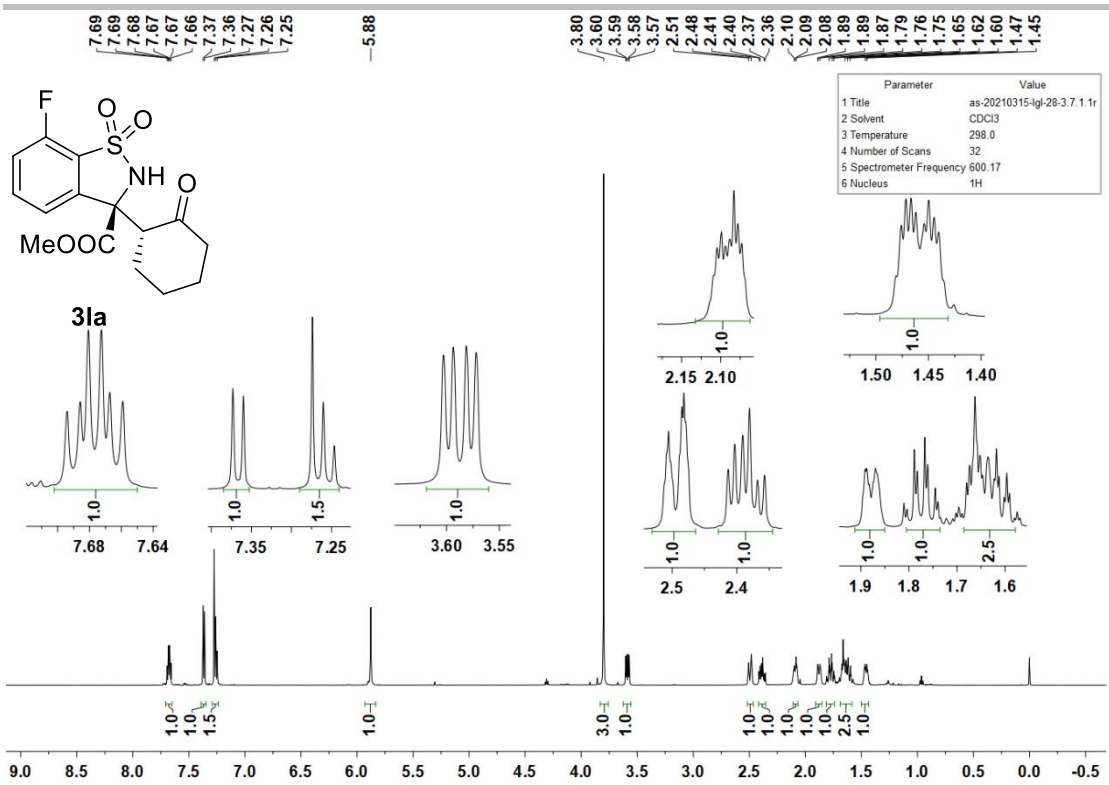
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5.88
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1 Title as-20210315-lgl-28-3.7.1.1r
2 Solvent CDCl3
3 Temperature 298.0
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5 Spectrometer Frequency 600.17
6 Nucleus 1H
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NH
O
MeOOC
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7.35 7.25
3.60 3.55
2.15 2.10
1.50 1.45 1.40
2.5 2.4
1.9 1.8 1.7 1.6
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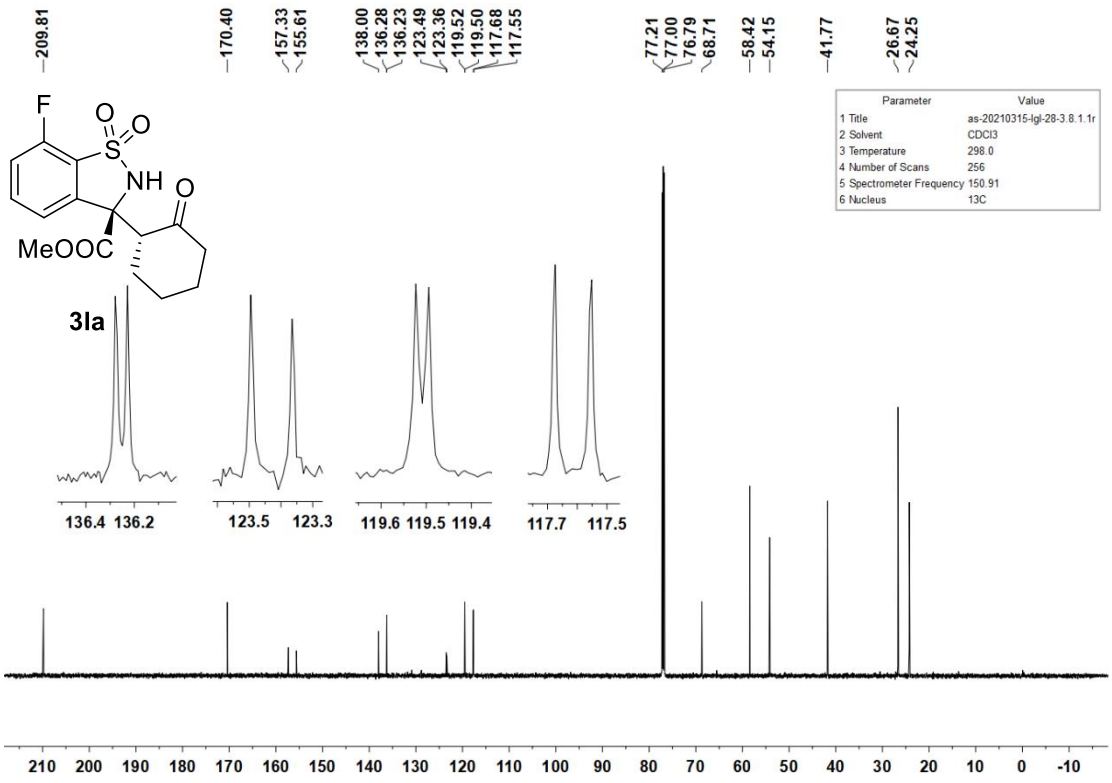
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170.40
157.33 155.61
138.00 136.28 136.23 123.49 123.36 119.52 119.50 117.68 117.55
77.21 77.00 76.79 68.71
58.42 54.15
41.77
26.67 24.25
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2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 256
5 Spectrometer Frequency 150.91
6 Nucleus 13C
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O
S
NH
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MeOOC
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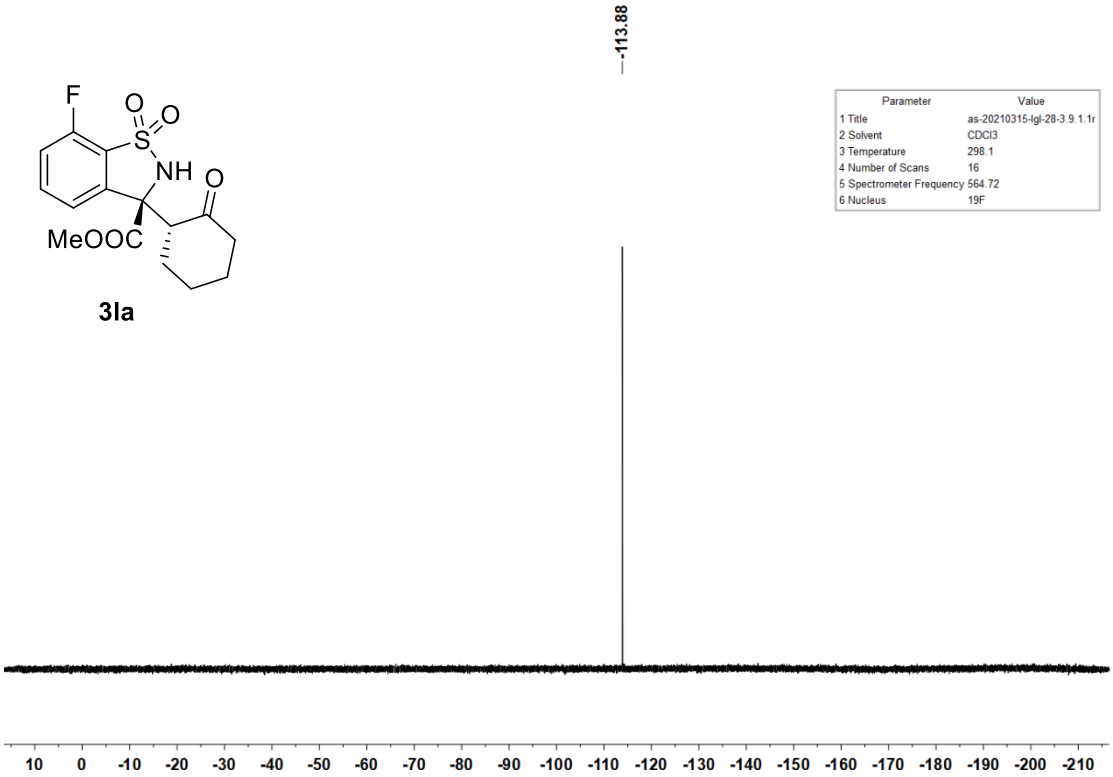
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3 Temperature 298.1
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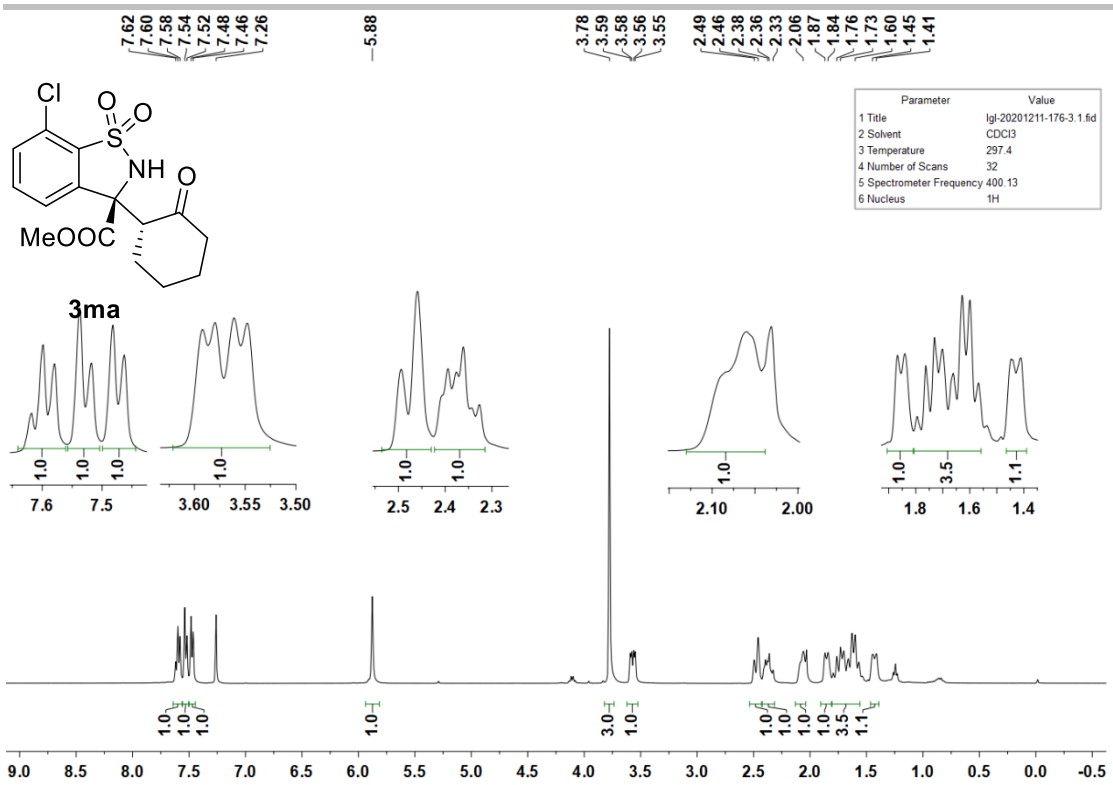
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3.55
2.49
2.46
2.38
2.36
2.33
2.06
1.87
1.84
1.76
1.73
1.60
1.45
1.41
Cl
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O
S
NH
O
MeOOC
3ma
Parameter Value
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2 Solvent CDCl3
3 Temperature 297.4
4 Number of Scans 32
5 Spectrometer Frequency 400.13
6 Nucleus 1H
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7.6 7.5
1.0
3.60 3.55 3.50
1.0 1.0
2.5 2.4 2.3
1.0
2.10 2.00
1.0 3.5 1.1
1.8 1.6 1.4
1.0 1.0 1.0 1.0 3.0 1.0 1.0 1.0 1.0 1.0 3.5 1.1
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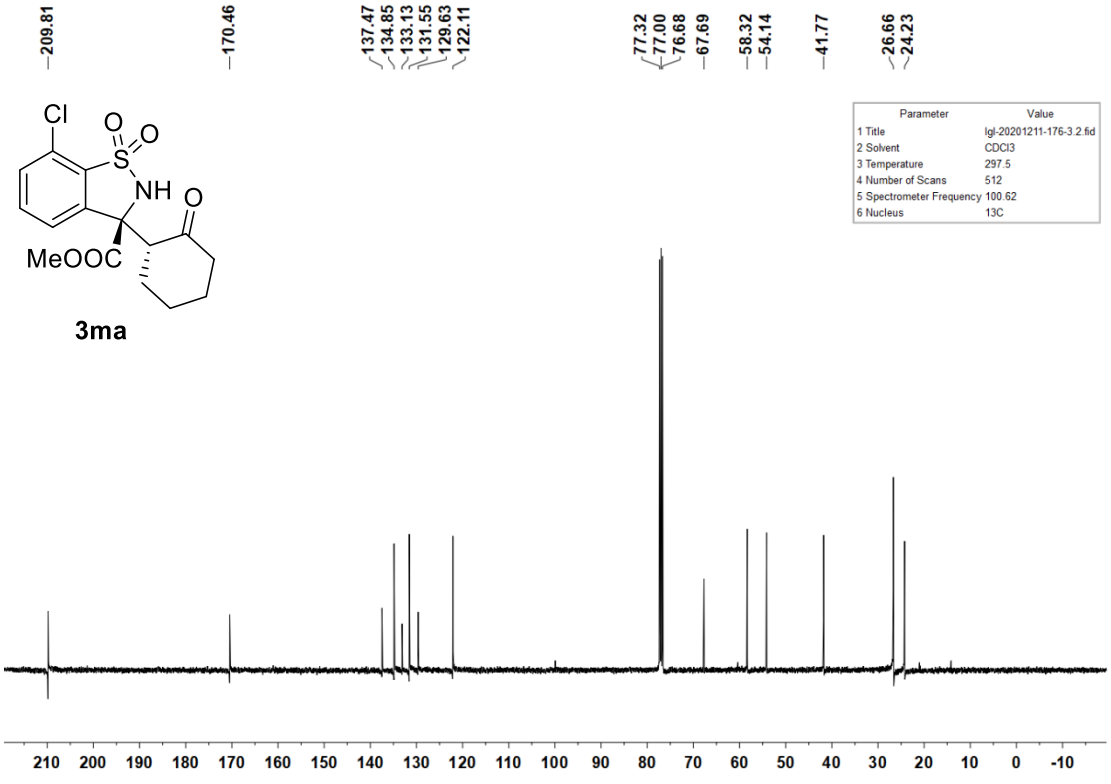
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76.68
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54.14
41.77
26.66
24.23
Cl
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O
S
NH
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MeOOC
3ma
Parameter Value
1 Title lgl-20201211-176-3.2.fid
2 Solvent CDCl3
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4 Number of Scans 512
5 Spectrometer Frequency 100.62
6 Nucleus 13C
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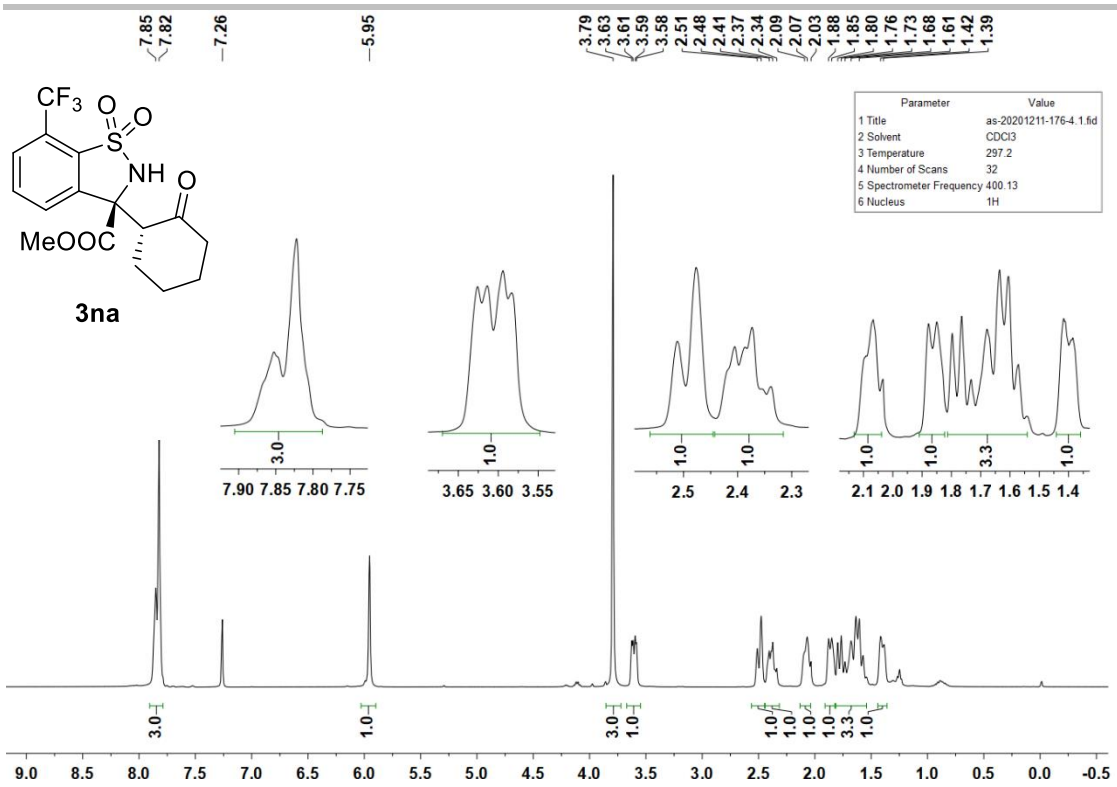
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3.63
3.61
3.59
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2.51
2.48
2.41
2.37
2.34
2.09
2.07
2.03
1.88
1.85
1.80
1.76
1.73
1.68
1.61
1.42
1.39
CF3
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O
S
NH
O
MeOOC
3na
Parameter Value
1 Title as-20201211-176-4.1.fid
2 Solvent CDCl3
3 Temperature 297.2
4 Number of Scans 32
5 Spectrometer Frequency 400.13
6 Nucleus 1H
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1.0
1.0
1.0
1.0
1.0
3.3
1.0
7.90 7.85 7.80 7.75
3.65 3.60 3.55
2.5 2.4 2.3
2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4
3.0
1.0
3.0
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1.0
1.0
1.0
3.3
1.0
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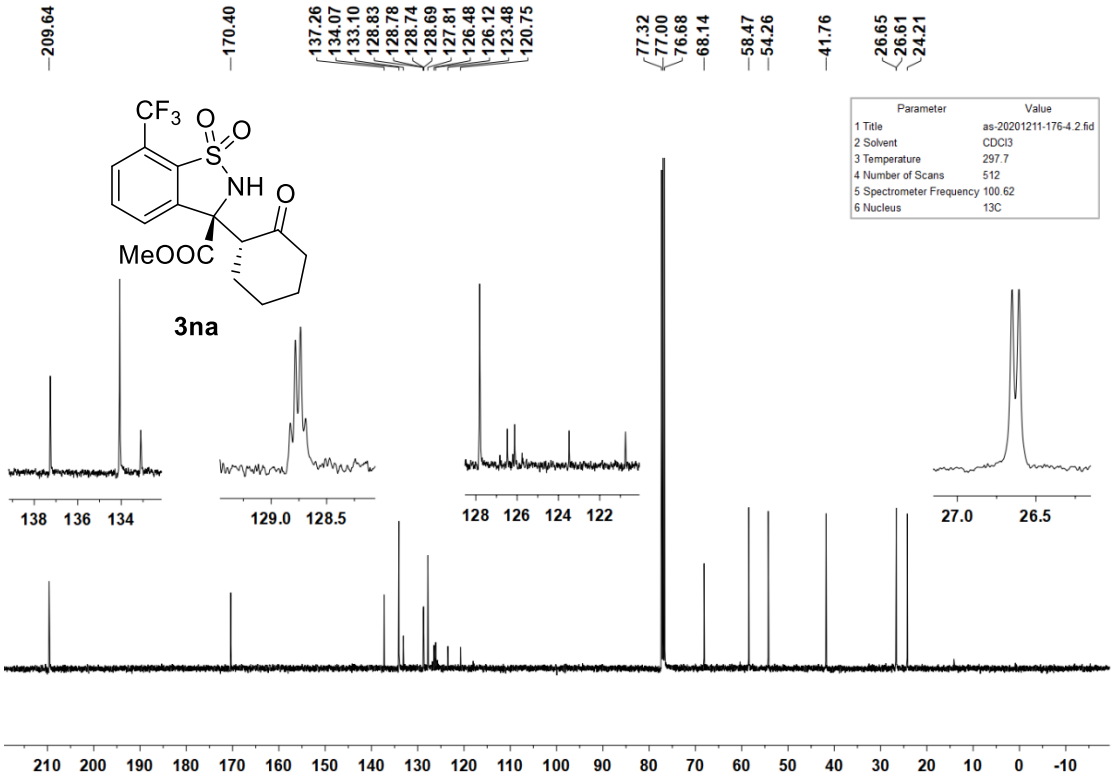
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126.48
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77.00
76.68
68.14
58.47
54.26
41.76
26.65
26.61
24.21
CF3
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O
S
NH
O
MeOOC
3na
Parameter Value
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2 Solvent CDCl3
3 Temperature 297.7
4 Number of Scans 512
5 Spectrometer Frequency 100.62
6 Nucleus 13C
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129.0 128.5
128 126 124 122
27.0 26.5
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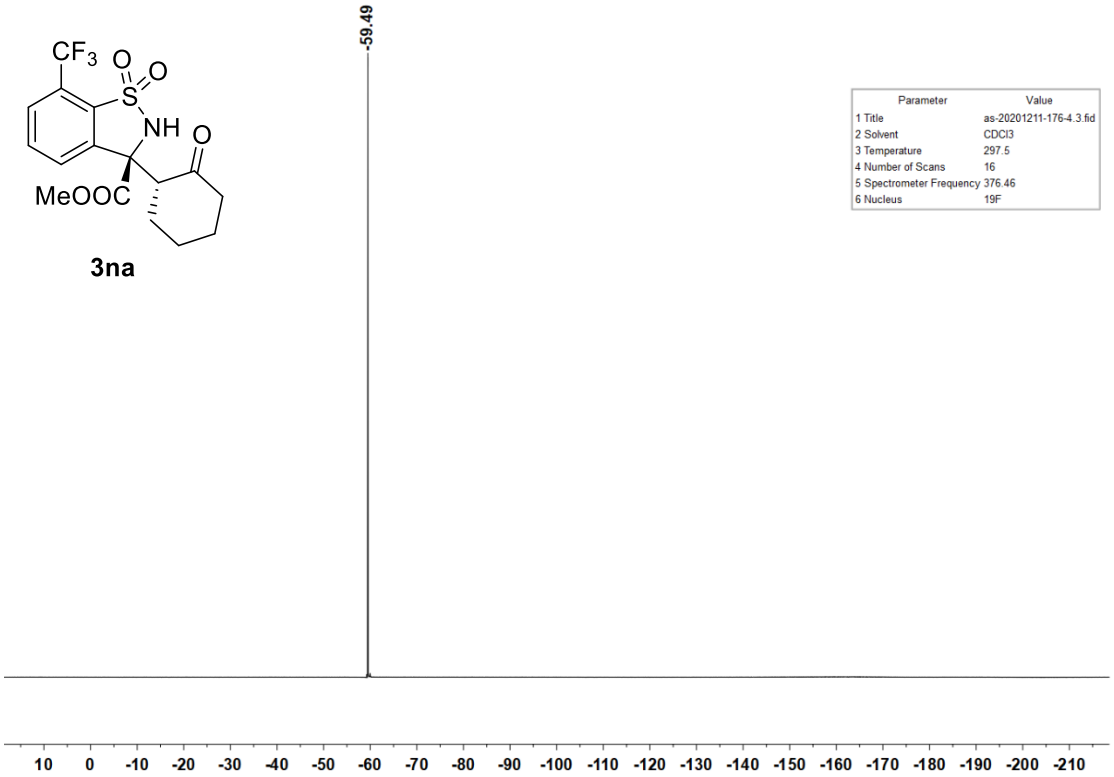
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2 Solvent CDCl3
3 Temperature 297.5
4 Number of Scans 16
5 Spectrometer Frequency 376.46
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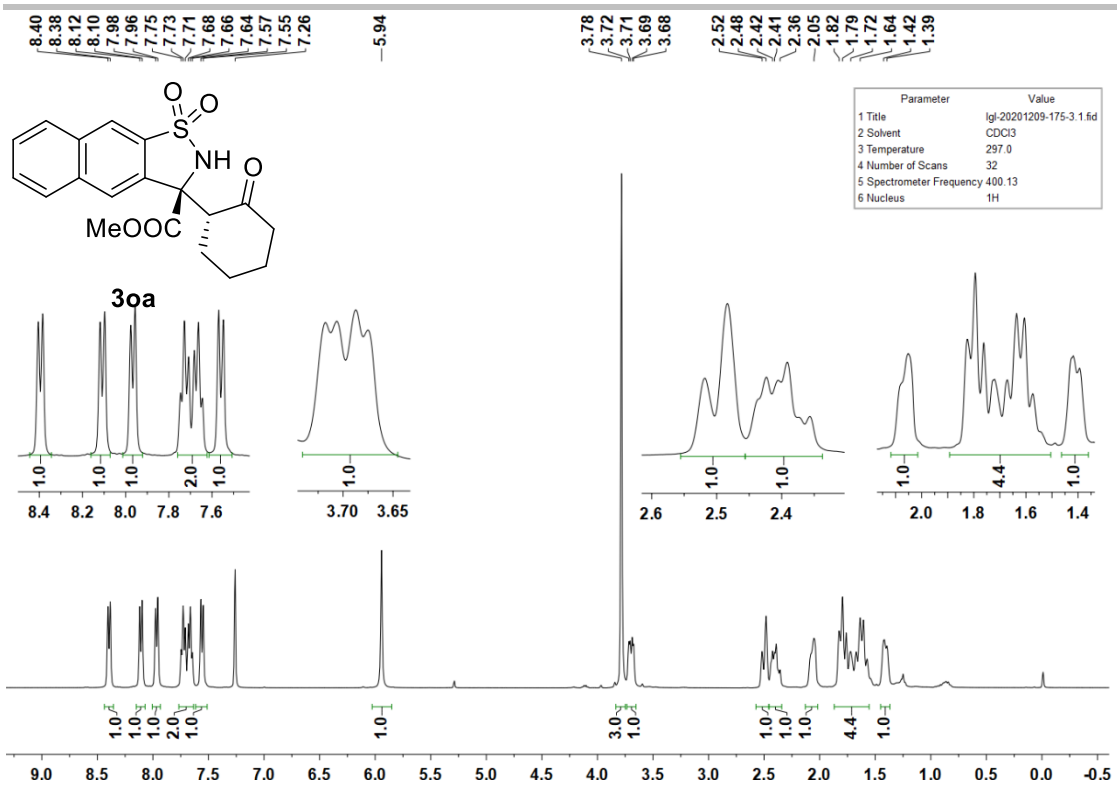
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5.94
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2.52 2.48 2.42 2.41 2.36 2.05 1.82 1.79 1.72 1.64 1.42 1.39
Parameter Value
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3 Temperature 297.0
4 Number of Scans 32
5 Spectrometer Frequency 400.13
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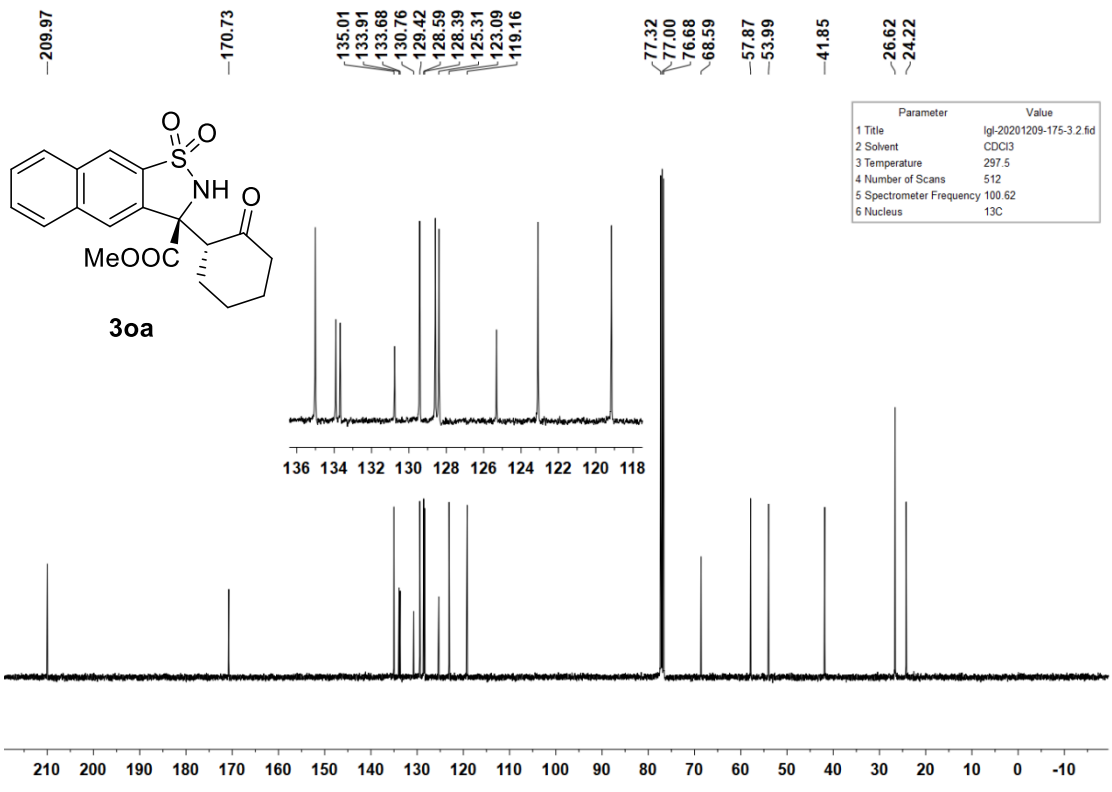
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41.85
26.62 24.22
Parameter Value
1 Title lgl-20201209-175-3.2.fid
2 Solvent CDCl3
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6 Nucleus 13C
MeOOC
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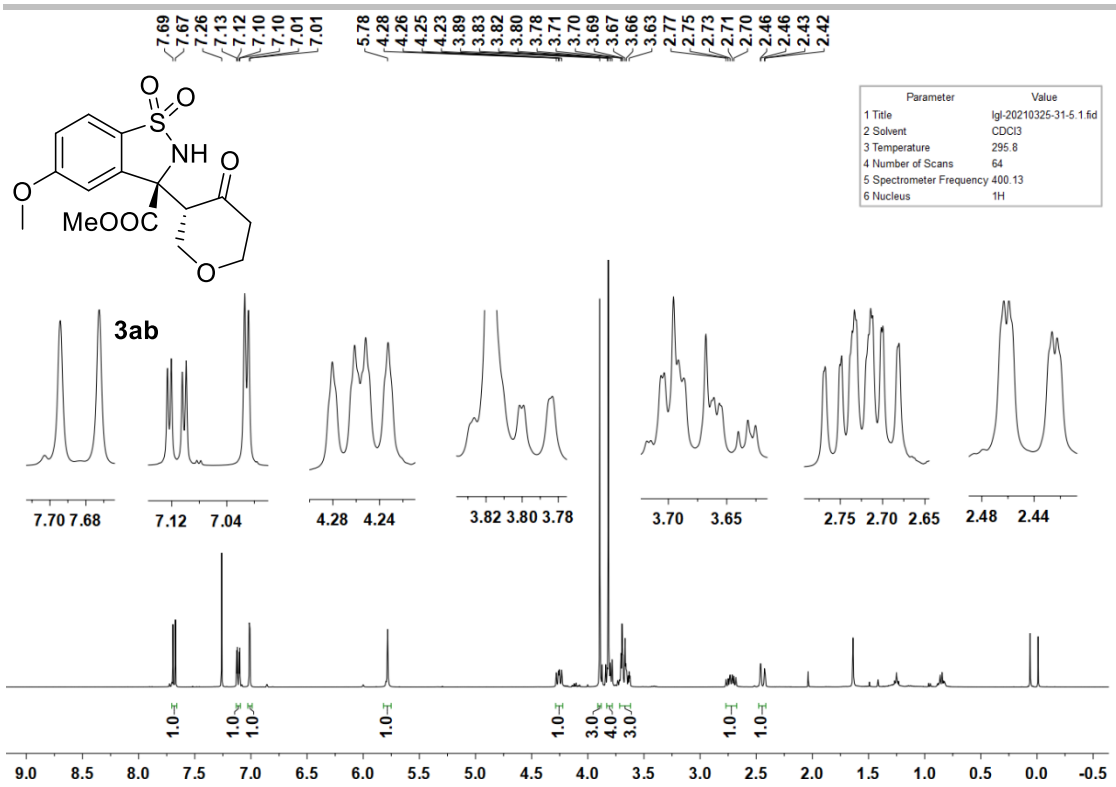
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2.77 2.75 2.73 2.71 2.70 2.46 2.46 2.43 2.42
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3 Temperature 295.8
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5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
S
NH
O
O
MeOOC
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7.12 7.04
4.28 4.24
3.82 3.80 3.78
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2.75 2.70 2.65
2.48 2.44
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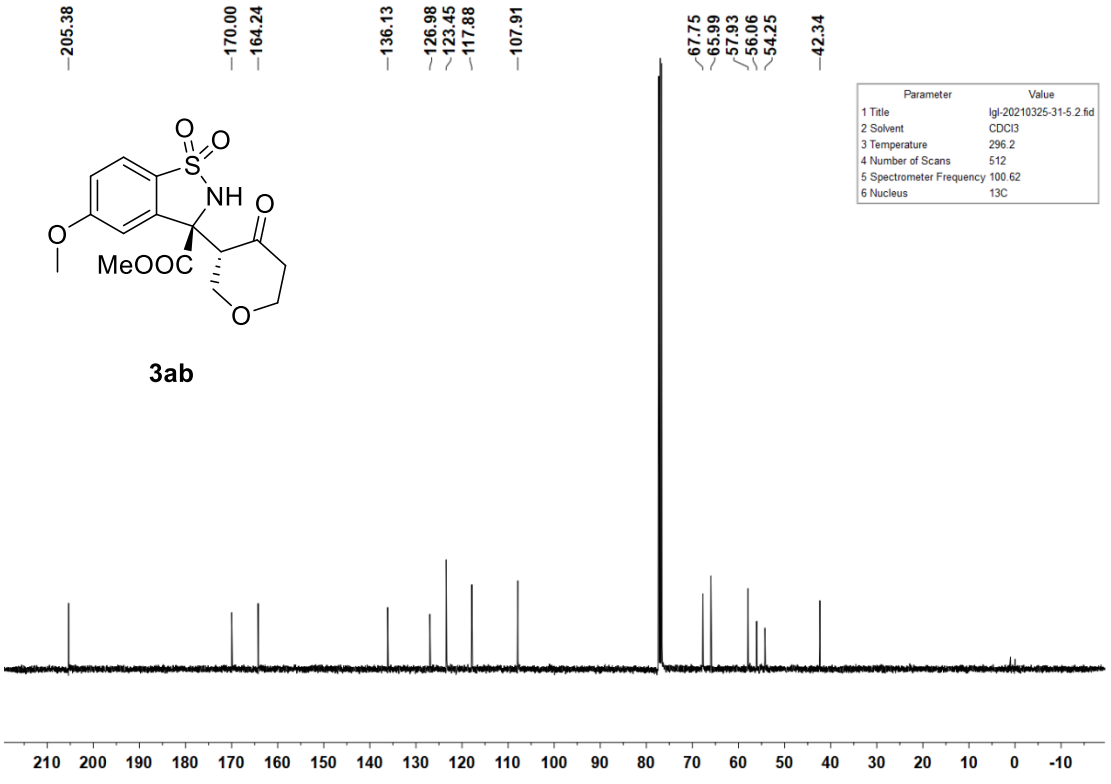
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2 Solvent CDCl3
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4 Number of Scans 512
5 Spectrometer Frequency 100.62
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O
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MeOOC
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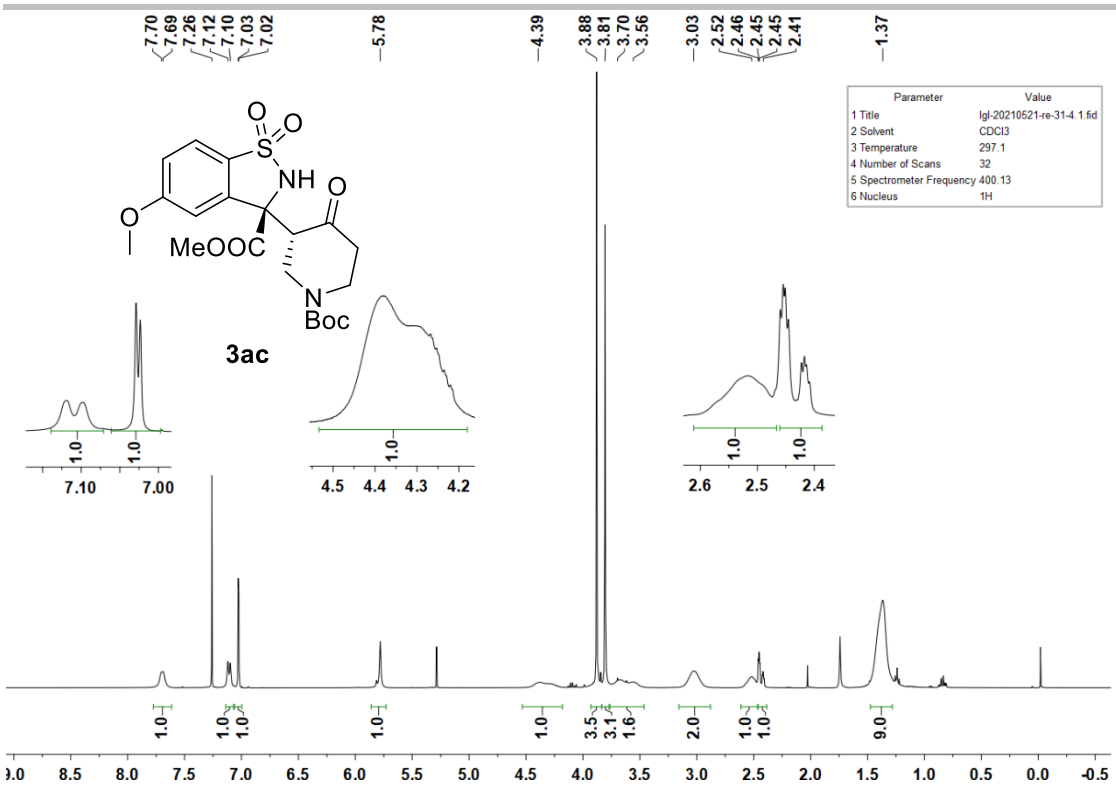
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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3.56
3.03
2.52
2.46
2.45
2.45
2.41
1.37
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2 Solvent CDCl3
3 Temperature 297.1
4 Number of Scans 32
5 Spectrometer Frequency 400.13
6 Nucleus 1H
MeOOC
Boc
3ac
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1.0
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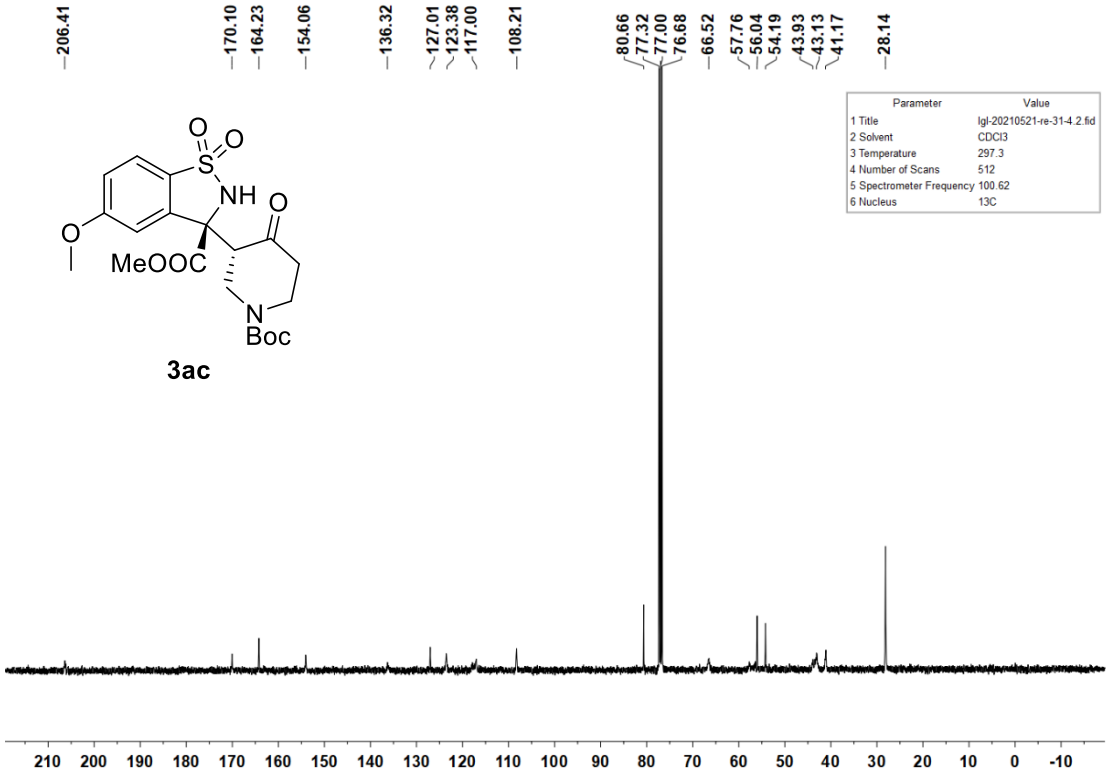
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77.00
76.68
66.52
57.76
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54.19
43.93
43.13
41.17
28.14
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MeOOC
Boc
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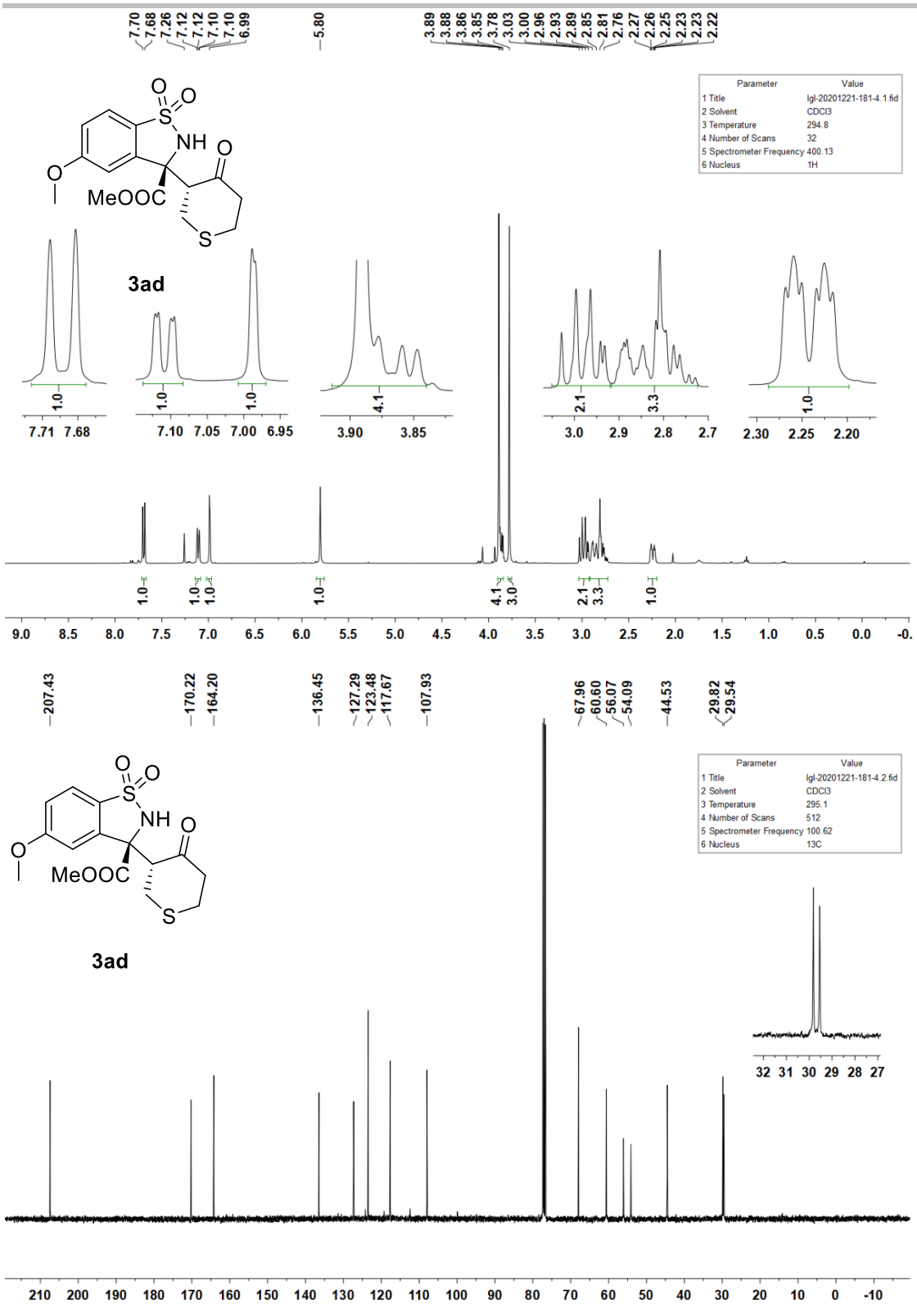
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Parameter Value
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2 Solvent CDCl3
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4 Number of Scans 32
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O
O
MeOOC
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3.3
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2.30 2.25 2.20
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9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
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127.29
123.48
117.67
107.93
67.96
60.60
56.07
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44.53
29.82
29.54
Parameter Value
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3 Temperature 295.1
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5 Spectrometer Frequency 100.62
6 Nucleus 13C
O
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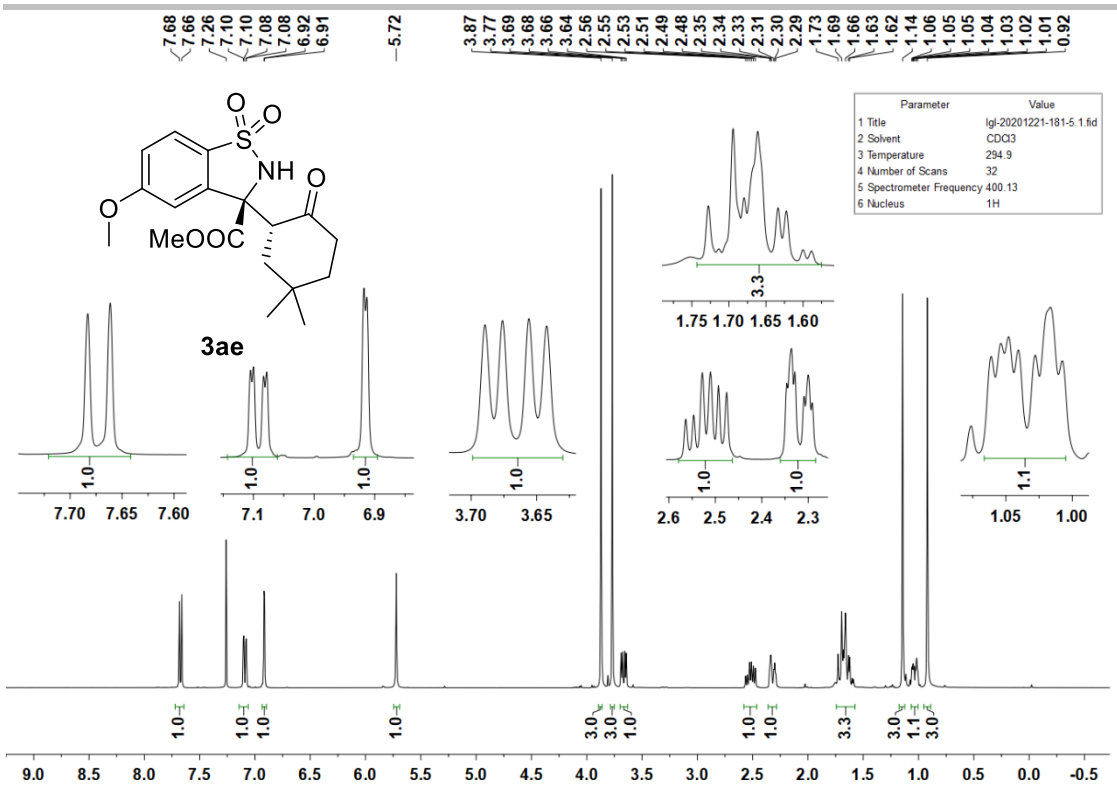
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Parameter Value
1 Title lgl-20201221-181-5.1.fid
2 Solvent CDCl3
3 Temperature 294.9
4 Number of Scans 32
5 Spectrometer Frequency 400.13
6 Nucleus 1H
MeOOC
3ae
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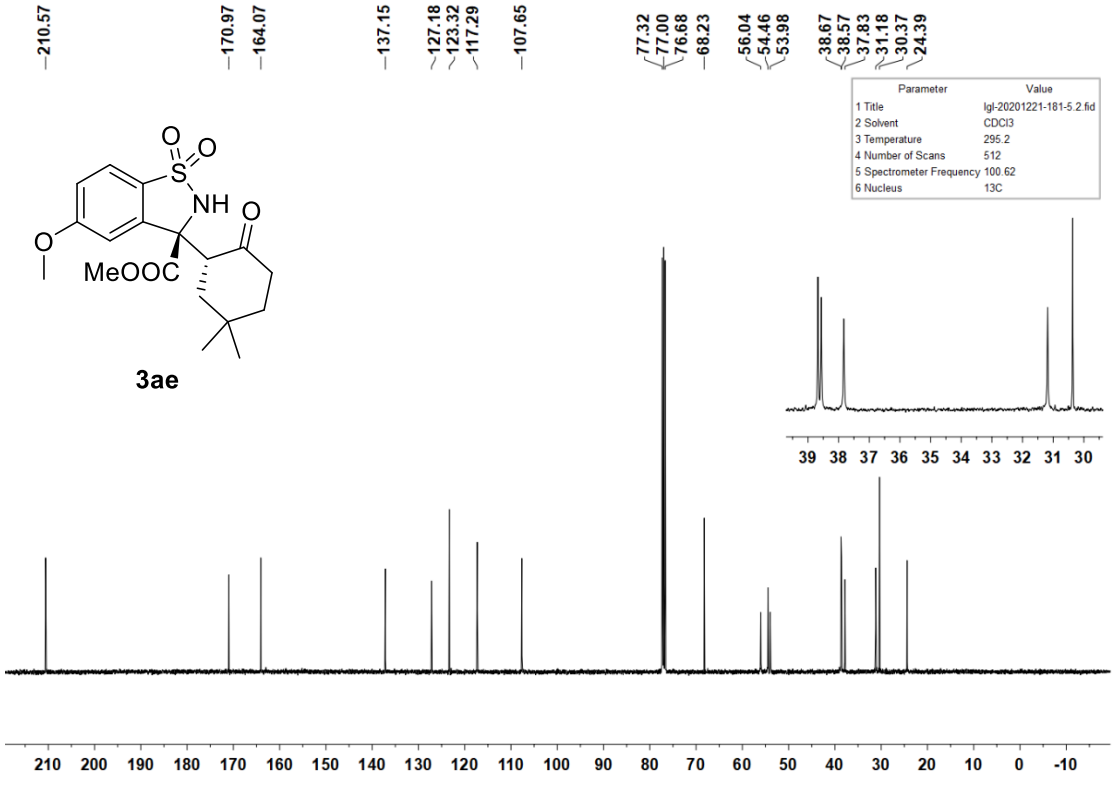
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Parameter Value
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2 Solvent CDCl3
3 Temperature 295.2
4 Number of Scans 512
5 Spectrometer Frequency 100.62
6 Nucleus 13C
MeOOC
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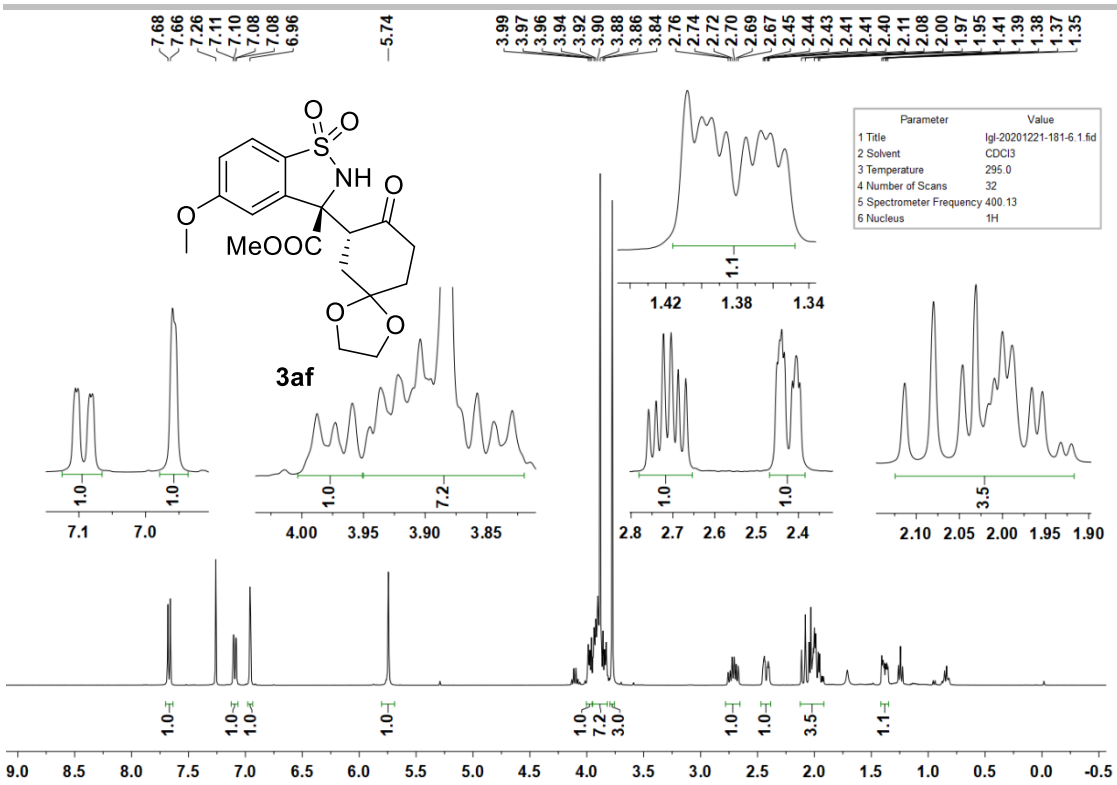
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3.99 3.97 3.96 3.94 3.92 3.90 3.88 3.86 3.84 2.76 2.74 2.72 2.70 2.69 2.67 2.45 2.44 2.43 2.41 2.41 2.40 2.11 2.08 2.00 1.97 1.95 1.41 1.39 1.38 1.37 1.35
Parameter Value
1 Title lgl-20201221-181-6.1.fid
2 Solvent CDCl3
3 Temperature 295.0
4 Number of Scans 32
5 Spectrometer Frequency 400.13
6 Nucleus 1H
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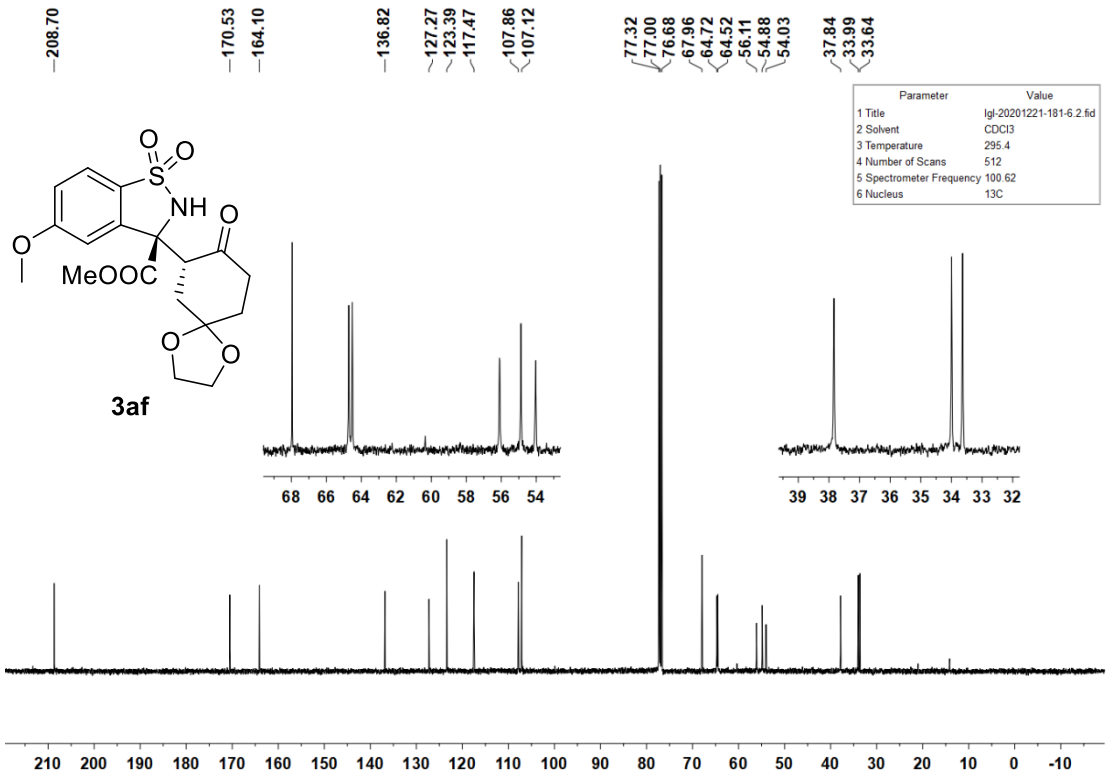
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Parameter Value
1 Title lgl-20201221-181-6.2.fid
2 Solvent CDCl3
3 Temperature 295.4
4 Number of Scans 512
5 Spectrometer Frequency 100.62
6 Nucleus 13C
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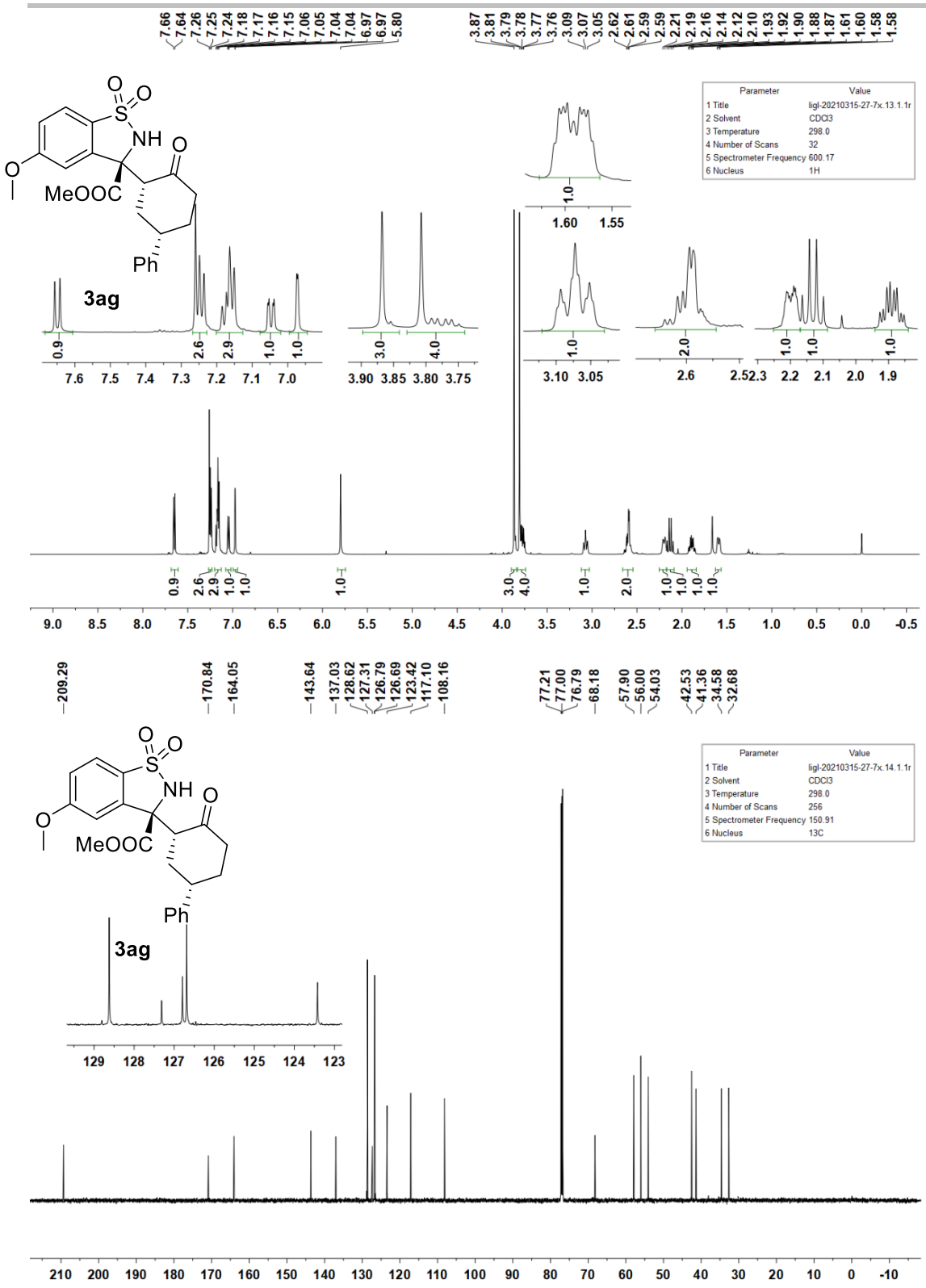
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3.87 3.81 3.79 3.78 3.77 3.76 3.09 3.07 3.05 2.62 2.61 2.59 2.59 2.21 2.19 2.16 2.14 2.12 2.10 1.93 1.92 1.90 1.88 1.87 1.61 1.60 1.58 1.58
Parameter Value
1 Title ligl-20210315-27-7x.13.1.1r
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 32
5 Spectrometer Frequency 600.17
6 Nucleus 1H
MeOOC
Ph
3ag
0.9 2.6 2.9 1.0 1.0 3.0 4.0 1.0 1.0 2.0 1.0 1.0 1.0
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
209.29 170.84 164.05 143.64 137.03 128.62 127.31 126.79 126.69 123.42 117.10 108.16 77.21 77.00 76.79 68.18 57.90 56.00 54.03 42.53 41.36 34.58 32.68
Parameter Value
1 Title ligl-20210315-27-7x.14.1.1r
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 256
5 Spectrometer Frequency 150.91
6 Nucleus 13C
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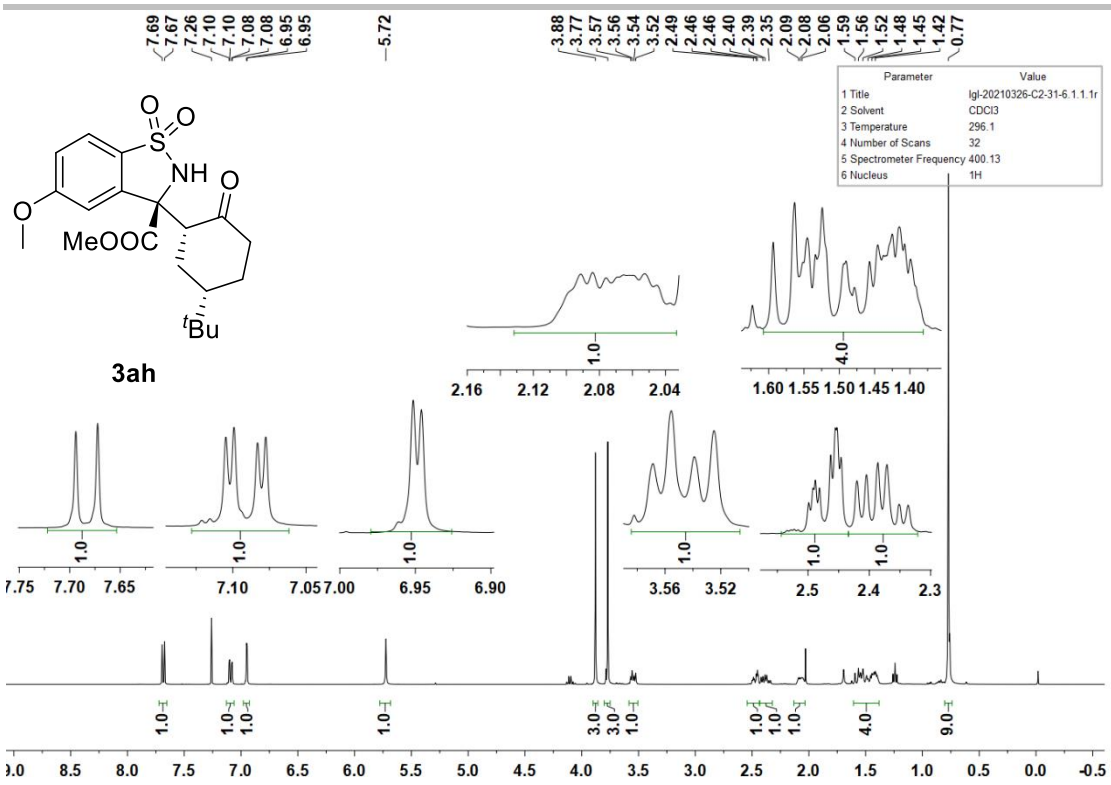
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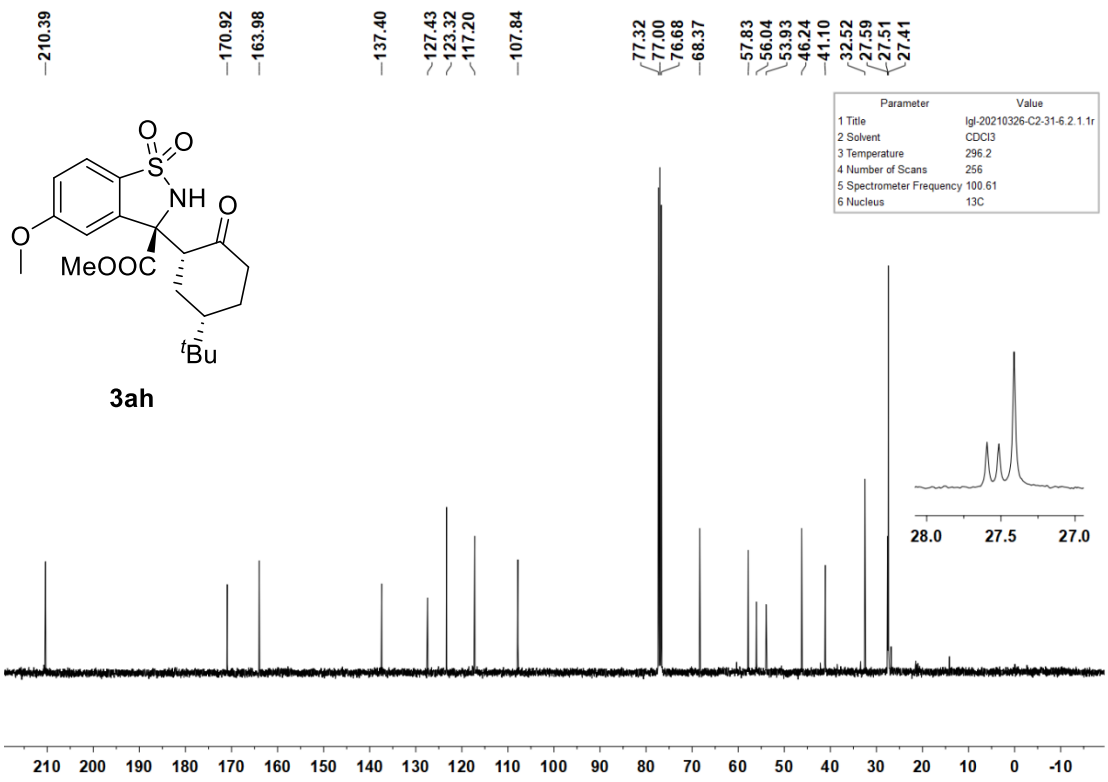
5.72
3.88 3.77 3.57 3.56 3.54 3.52 2.49 2.46 2.46 2.40 2.39 2.35 2.09 2.08 2.06 1.59 1.56 1.52 1.48 1.45 1.42 0.77
Parameter Value
1 Title Igl-20210326-C2-31-6.1.1.1r
2 Solvent CDCl3
3 Temperature 296.1
4 Number of Scans 32
5 Spectrometer Frequency 400.13
6 Nucleus 1H
MeOOC
tBu
3ah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Parameter Value
1 Title Igl-20210326-C2-31-6.2.1.1r
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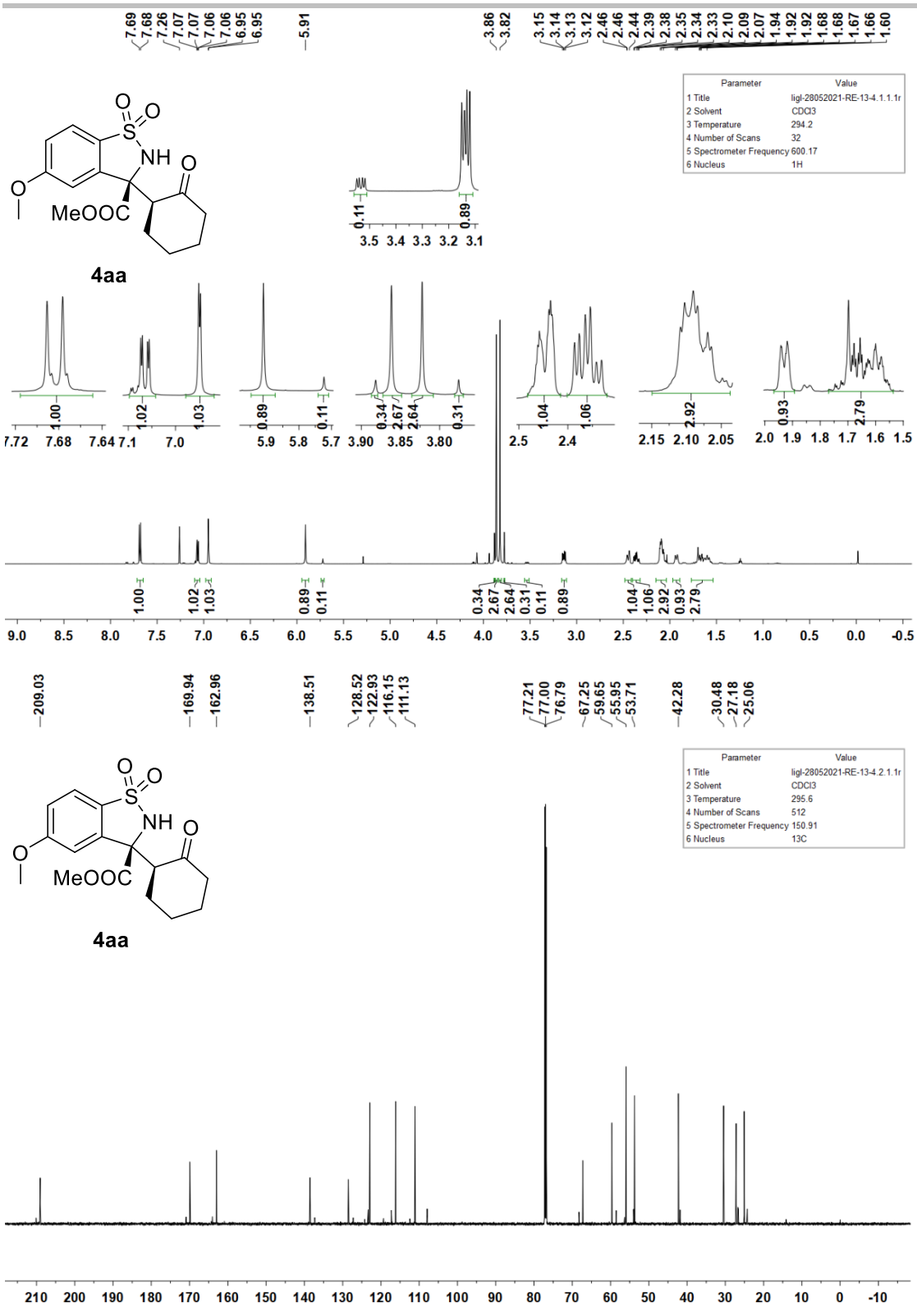
3 Temperature 296.2
4 Number of Scans 256
5 Spectrometer Frequency 100.61
6 Nucleus 13C
MeOOC
tBu
3ah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5.91
3.86 3.82
3.15 3.14 3.13 3.12 2.46 2.46 2.44 2.39 2.38 2.35 2.34 2.33 2.10 2.09 2.07 1.94 1.92 1.92 1.68 1.68 1.67 1.66 1.60
Parameter Value
1 Title ligl-28052021-RE-13-4.1.1.1r
2 Solvent CDCl3
3 Temperature 294.2
4 Number of Scans 32
5 Spectrometer Frequency 600.17
6 Nucleus 1H
MeOOC
4aa
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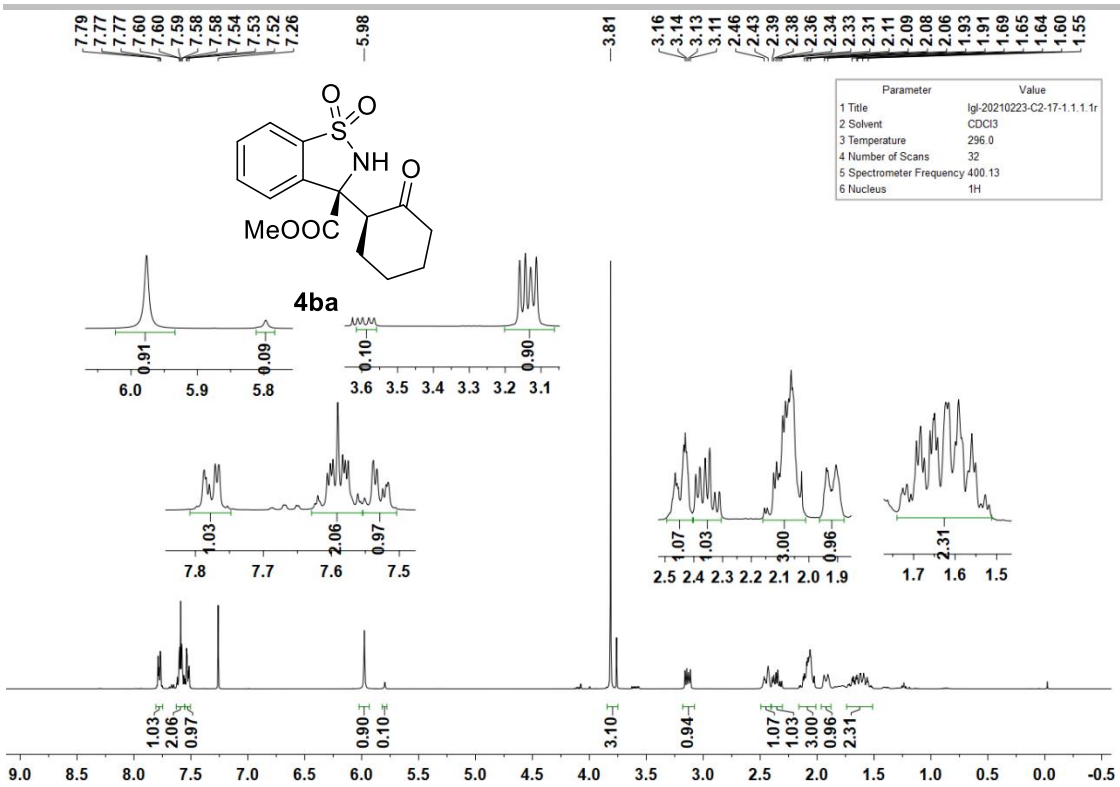
Parameter Value
1 Title ligl-28052021-RE-13-4.2.1.1r
2 Solvent CDCl3
3 Temperature 295.6
4 Number of Scans 512
5 Spectrometer Frequency 150.91
6 Nucleus 13C
MeOOC
4aa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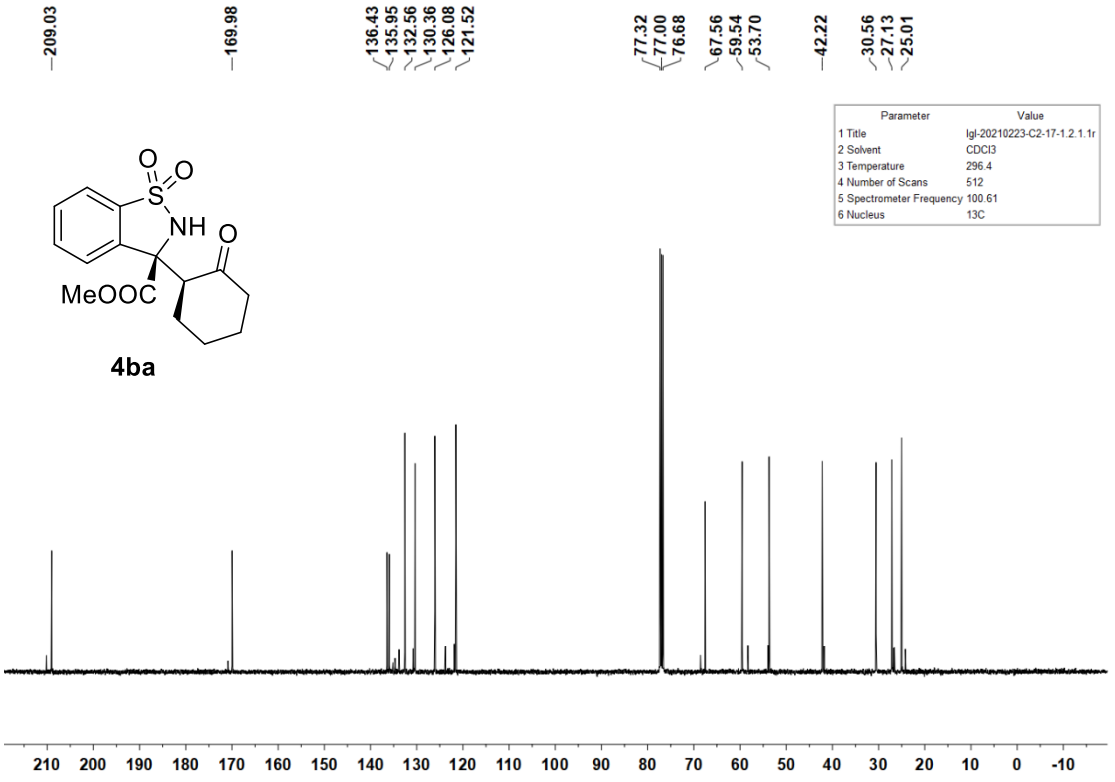
5.98
3.81
3.16 3.14 3.13 3.11 2.46 2.43 2.39 2.38 2.36 2.34 2.33 2.31 2.11 2.09 2.08 2.06 1.93 1.91 1.69 1.65 1.64 1.60 1.55
Parameter Value
1 Title lgl-20210223-C2-17-1.1.1.1r
2 Solvent CDCl3
3 Temperature 296.0
4 Number of Scans 32
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
O
S
NH
O
MeOOC
4ba
0.91 0.09
6.0 5.9 5.8
0.10 0.90
3.6 3.5 3.4 3.3 3.2 3.1
1.03 2.06 0.97
7.8 7.7 7.6 7.5
1.07 1.03 3.00 0.96
2.5 2.4 2.3 2.2 2.1 2.0 1.9
2.31
1.7 1.6 1.5
1.03 2.06 0.97 0.90 0.10 3.10 0.94 1.07 1.03 3.00 0.96 2.31
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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77.32 77.00 76.68
67.56 59.54 53.70
42.22
30.56 27.13 25.01
Parameter Value
1 Title lgl-20210223-C2-17-1.2.1.1r
2 Solvent CDCl3
3 Temperature 296.4
4 Number of Scans 512
5 Spectrometer Frequency 100.61
6 Nucleus 13C
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O
S
NH
O
MeOOC
4ba
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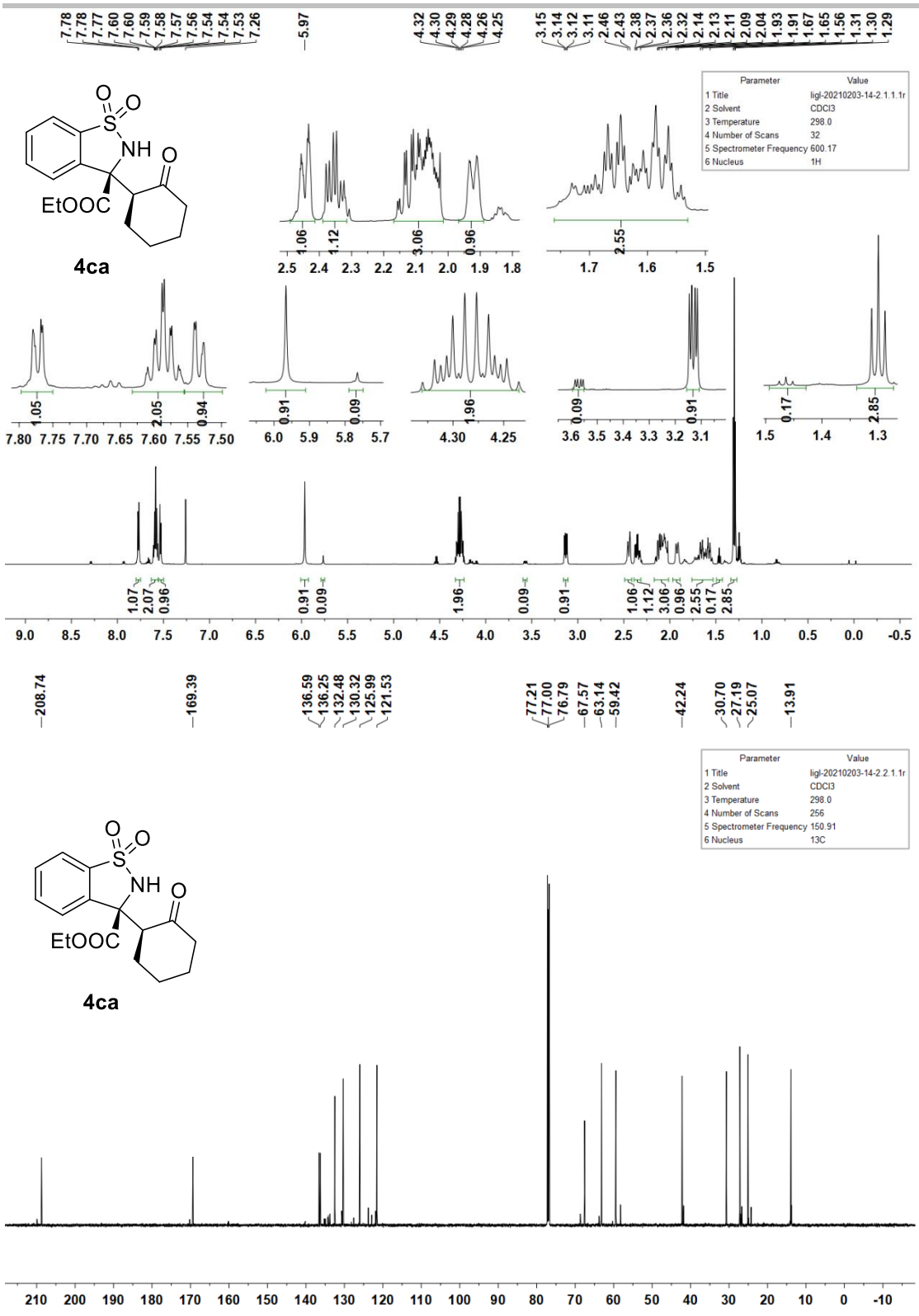
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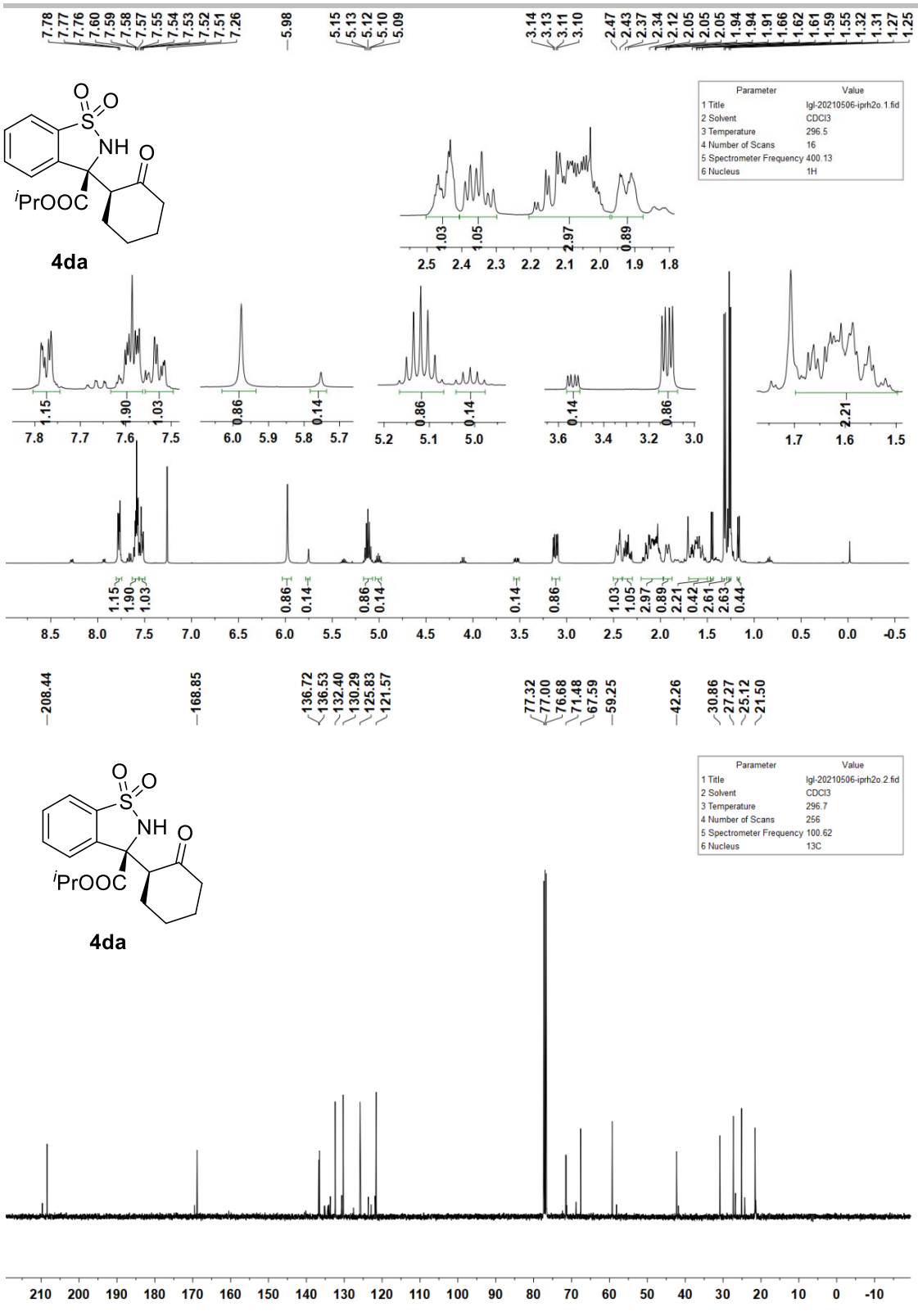
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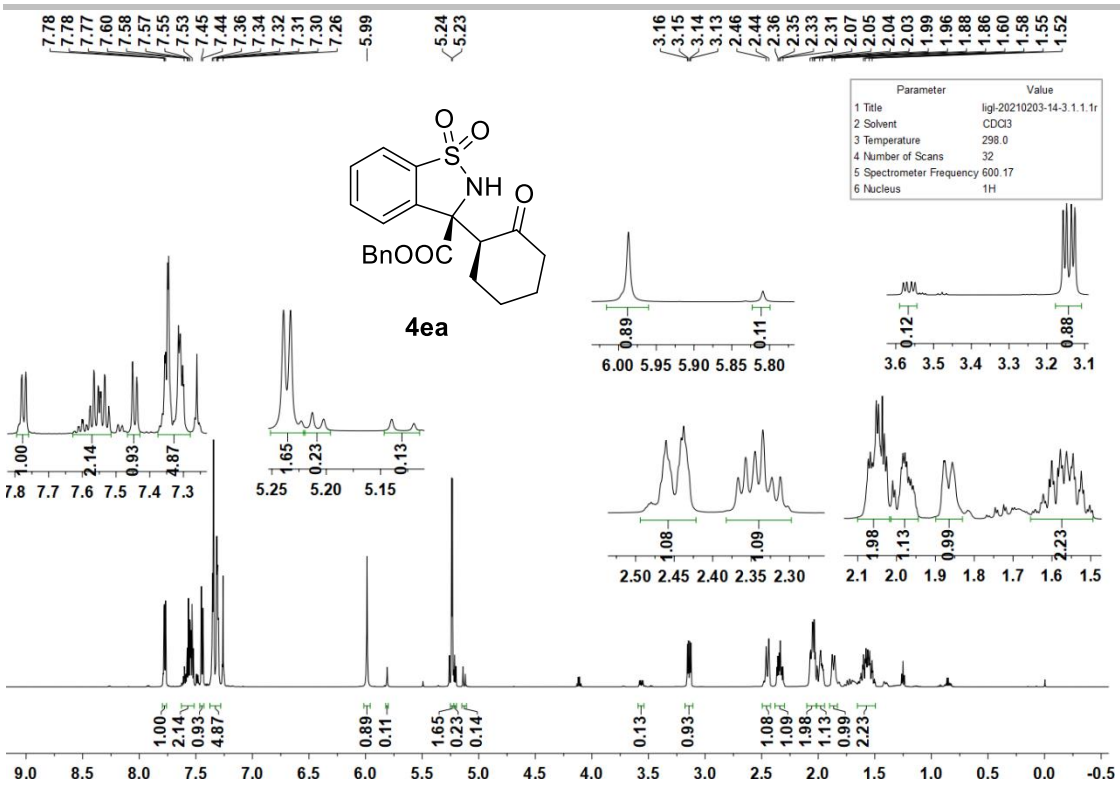
2 Solvent CDCl3
3 Temperature 296.5
4 Number of Scans 16
5 Spectrometer Frequency 400.13
6 Nucleus 1H
4da
Parameter Value
1 Title lgl-20210506-iprh2o.2.fid
2 Solvent CDCl3
3 Temperature 296.7
4 Number of Scans 256
5 Spectrometer Frequency 100.62
6 Nucleus 13C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Parameter Value
1 Title ligl-20210203-14-3.1.1.1r
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 32
5 Spectrometer Frequency 600.17
6 Nucleus 1H
BnOOC
4ea
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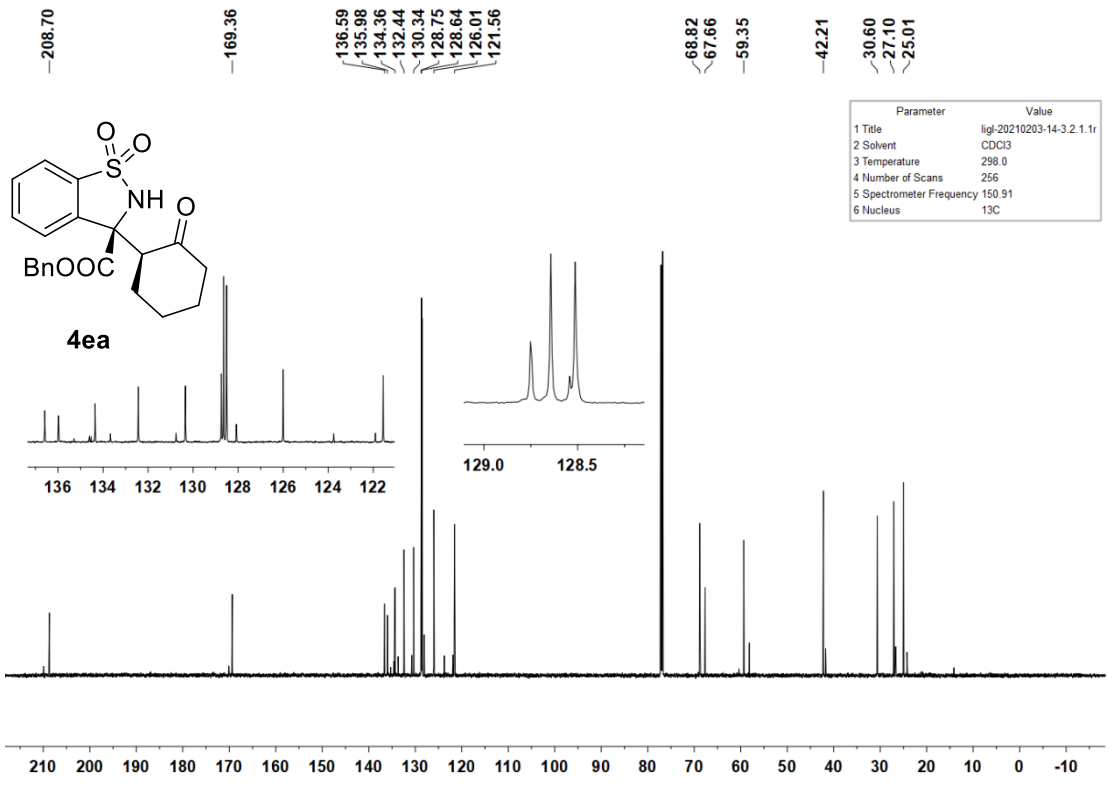
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Parameter Value
1 Title ligl-20210203-14-3.2.1.1r
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 256
5 Spectrometer Frequency 150.91
6 Nucleus 13C
BnOOC
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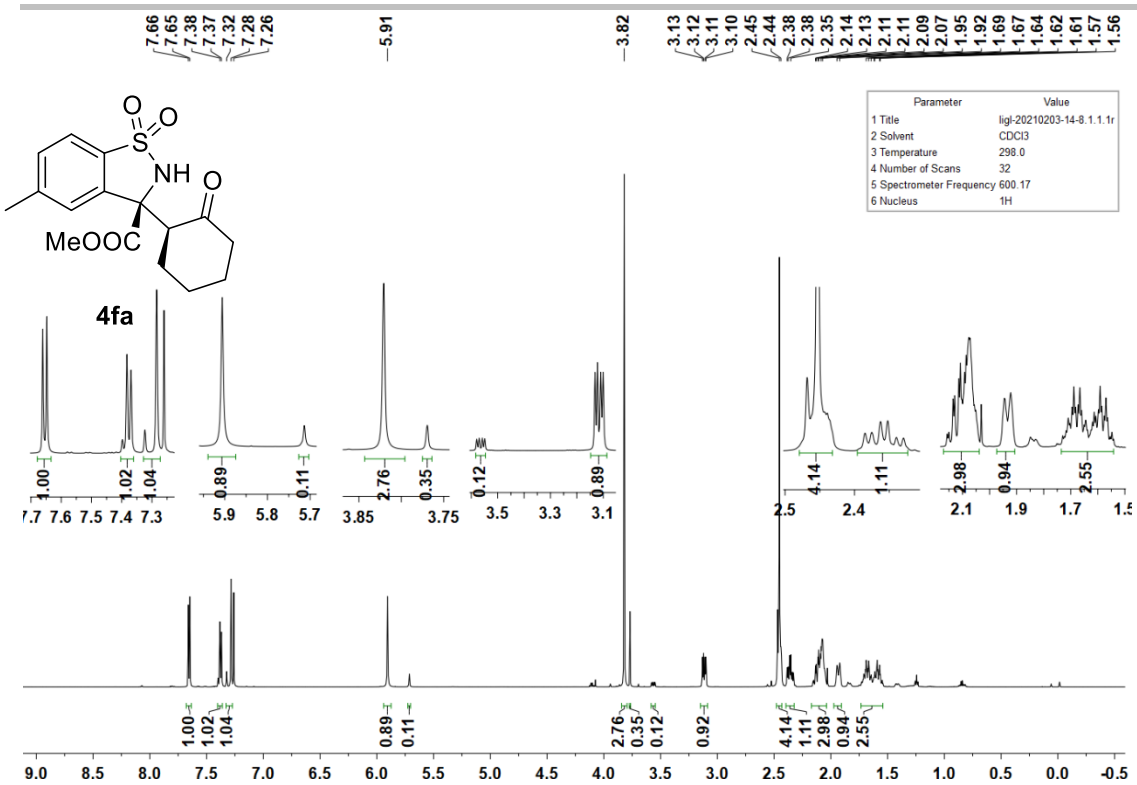
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7.37
7.32
7.28
7.26
5.91
3.82
3.13
3.12
3.11
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2.45
2.44
2.38
2.38
2.35
2.14
2.13
2.11
2.11
2.09
2.07
1.95
1.92
1.69
1.67
1.64
1.62
1.61
1.57
1.56
Parameter Value
1 Title ligl-20210203-14-8.1.1.1r
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 32
5 Spectrometer Frequency 600.17
6 Nucleus 1H
O
O
S
NH
O
MeOOC
4fa
1.00
1.02
1.04
0.89
0.11
2.76
0.35
0.12
0.89
4.14
1.11
2.98
0.94
2.55
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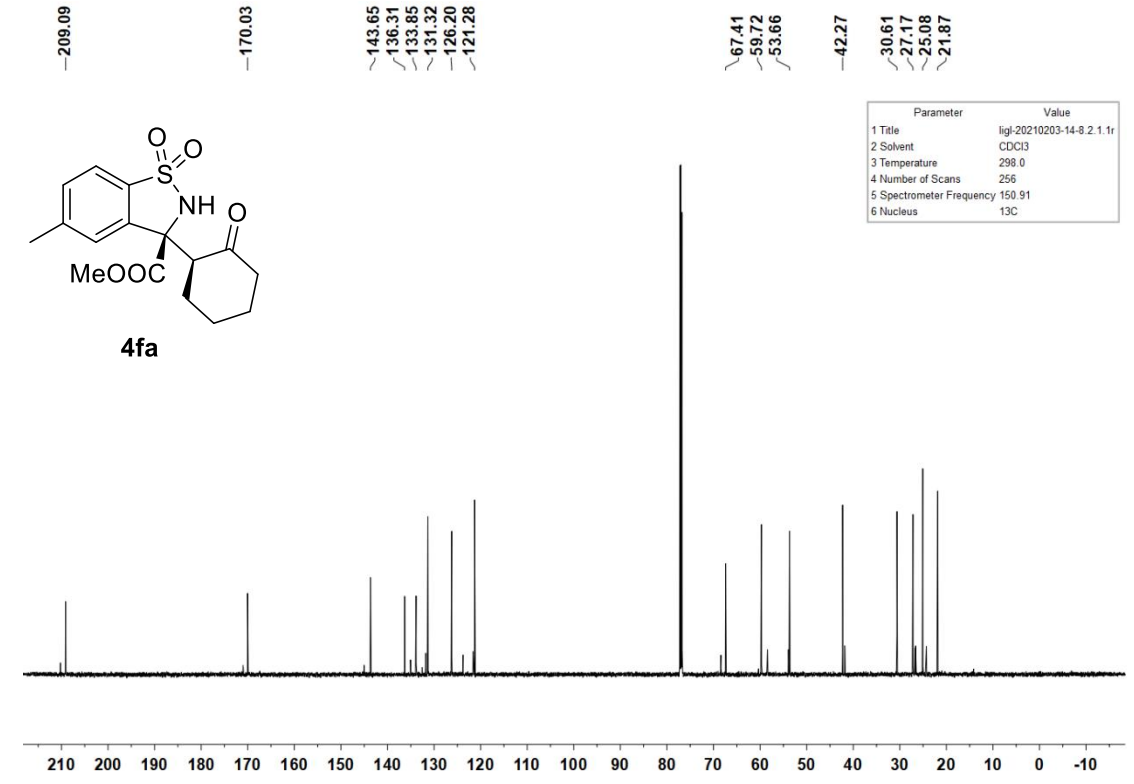
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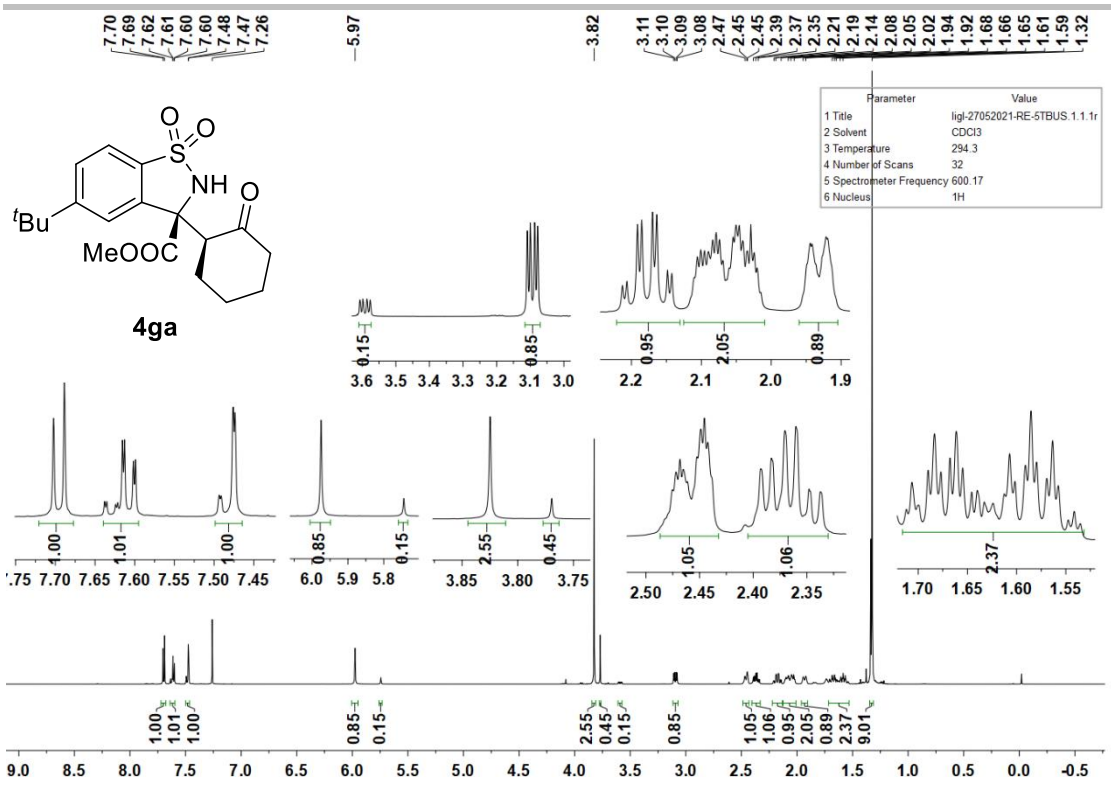
121.28
67.41
59.72
53.66
42.27
30.61
27.17
25.08
21.87
Parameter Value
1 Title ligl-20210203-14-8.2.1.1r
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 256
5 Spectrometer Frequency 150.91
6 Nucleus 13C
O
O
S
NH
O
MeOOC
4fa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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3.82
3.11 3.10 3.09 3.08 2.47 2.45 2.45 2.39 2.37 2.35 2.21 2.19 2.14 2.08 2.05 2.02 1.94 1.92 1.68 1.66 1.65 1.61 1.59 1.32
Parameter Value
1 Title ligl-27052021-RE-5TBUS.1.1.1r
2 Solvent CDCl3
3 Temperature 294.3
4 Number of Scans 32
5 Spectrometer Frequency 600.17
6 Nucleus 1H
tBu
MeOOC
NH
4ga
1.00 1.01 1.00
0.85 0.15
2.55 0.45
1.05 1.06
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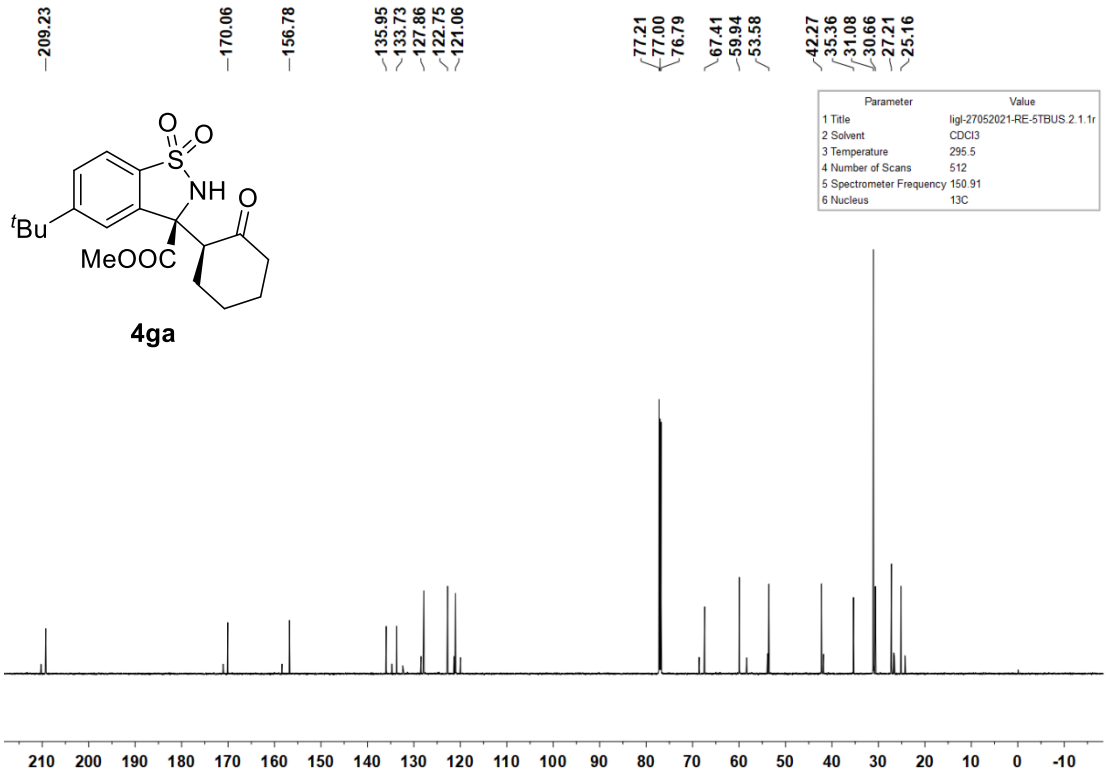
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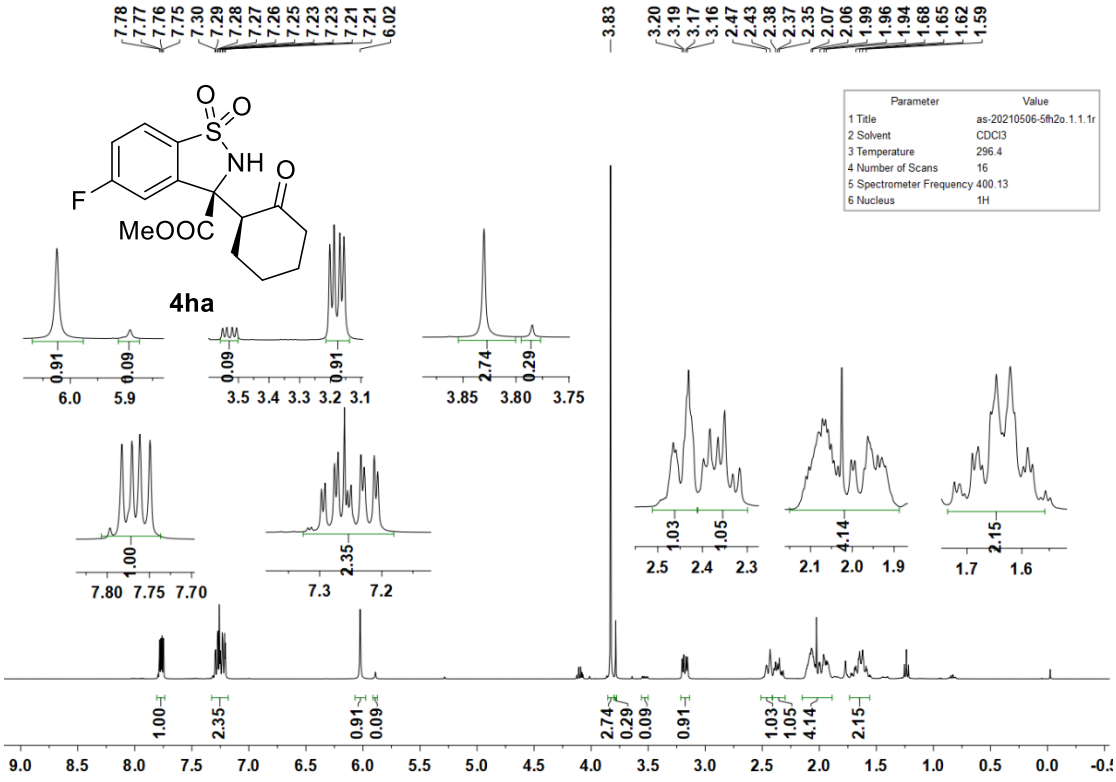
156.78
135.95 133.73 127.86 122.75 121.06
77.21 77.00 76.79
67.41
59.94
53.58
42.27 35.36 31.08 30.66 27.21 25.16
Parameter Value
1 Title ligl-27052021-RE-5TBUS.2.1.1r
2 Solvent CDCl3
3 Temperature 295.5
4 Number of Scans 512
5 Spectrometer Frequency 150.91
6 Nucleus 13C
tBu
MeOOC
NH
4ga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3.83
3.20 3.19 3.17 3.16 2.47 2.43 2.38 2.37 2.35 2.07 2.06 1.99 1.96 1.94 1.68 1.65 1.62 1.59
Parameter Value
1 Title as-20210506-5fh2o.1.1.1r
2 Solvent CDCl3
3 Temperature 296.4
4 Number of Scans 16
5 Spectrometer Frequency 400.13
6 Nucleus 1H
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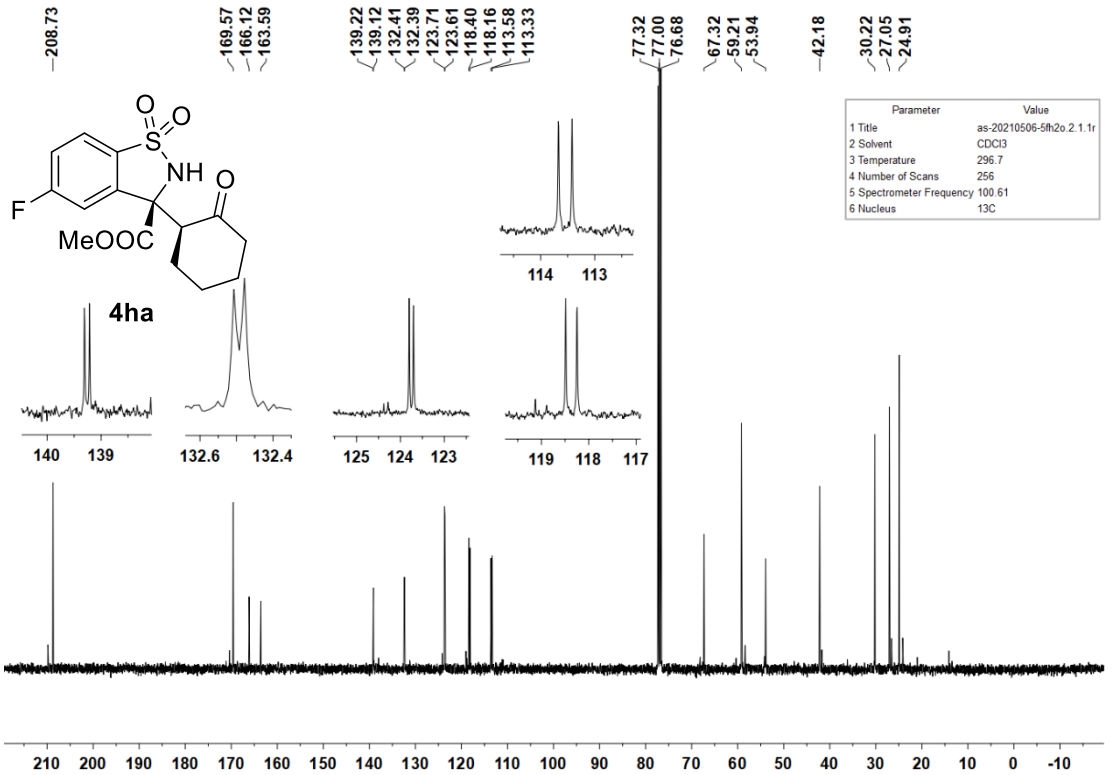
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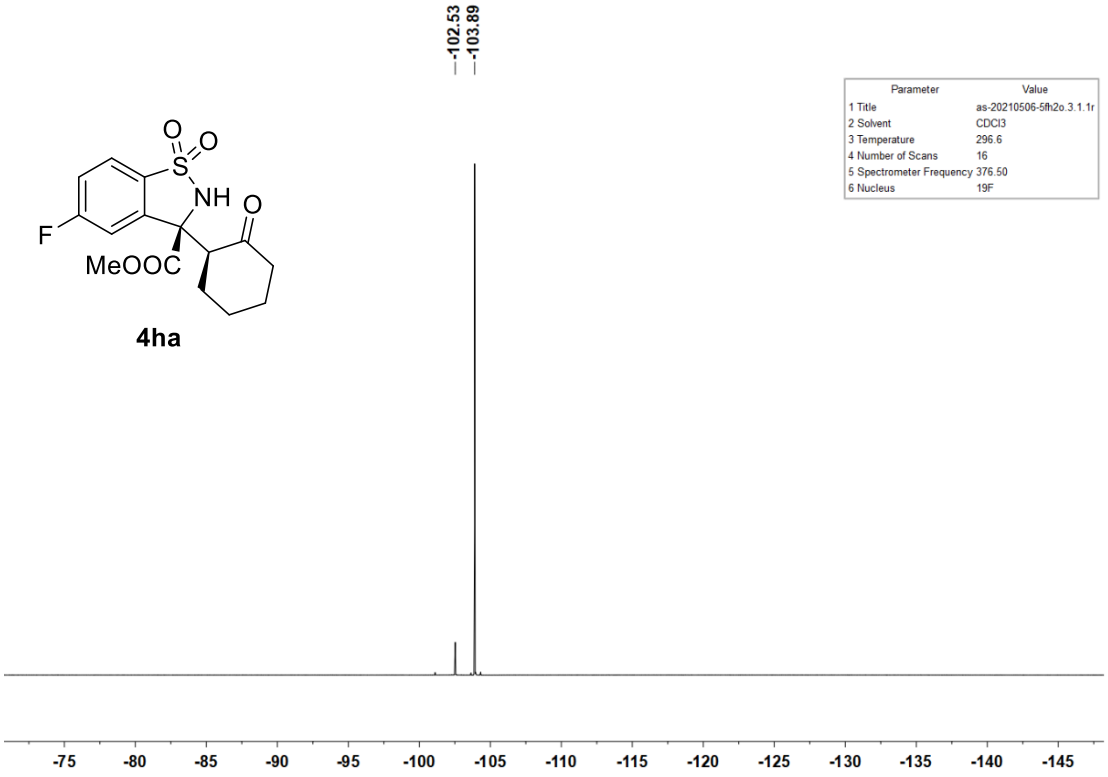
139.22 139.12 132.41 132.39 123.71 123.61 118.40 118.16 113.58 113.33
77.32 77.00 76.68
67.32 59.21 53.94
42.18
30.22 27.05 24.91
Parameter Value
1 Title as-20210506-5fh2o.2.1.1r
2 Solvent CDCl3
3 Temperature 296.7
4 Number of Scans 256
5 Spectrometer Frequency 100.61
6 Nucleus 13C
4ha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2 Solvent CDCl3
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4 Number of Scans 16
5 Spectrometer Frequency 376.50
6 Nucleus 19F
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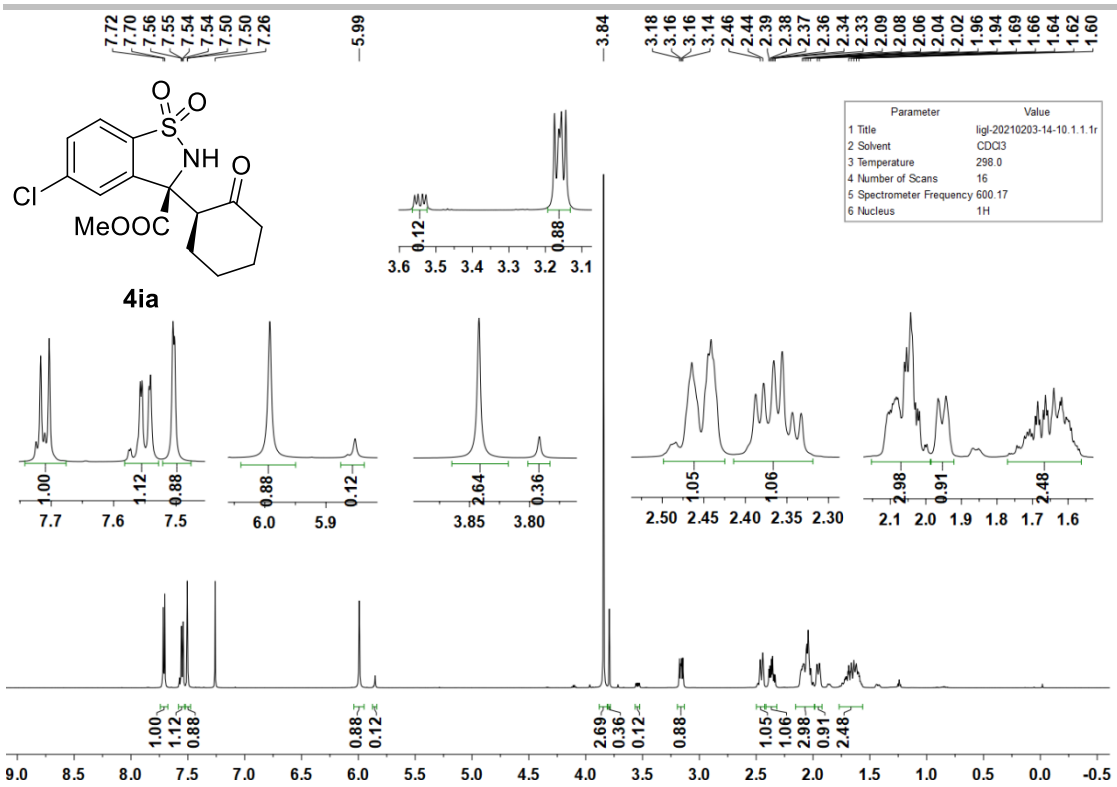
NH
O
F
MeOOC
-75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145

4ha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7.50
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5.99
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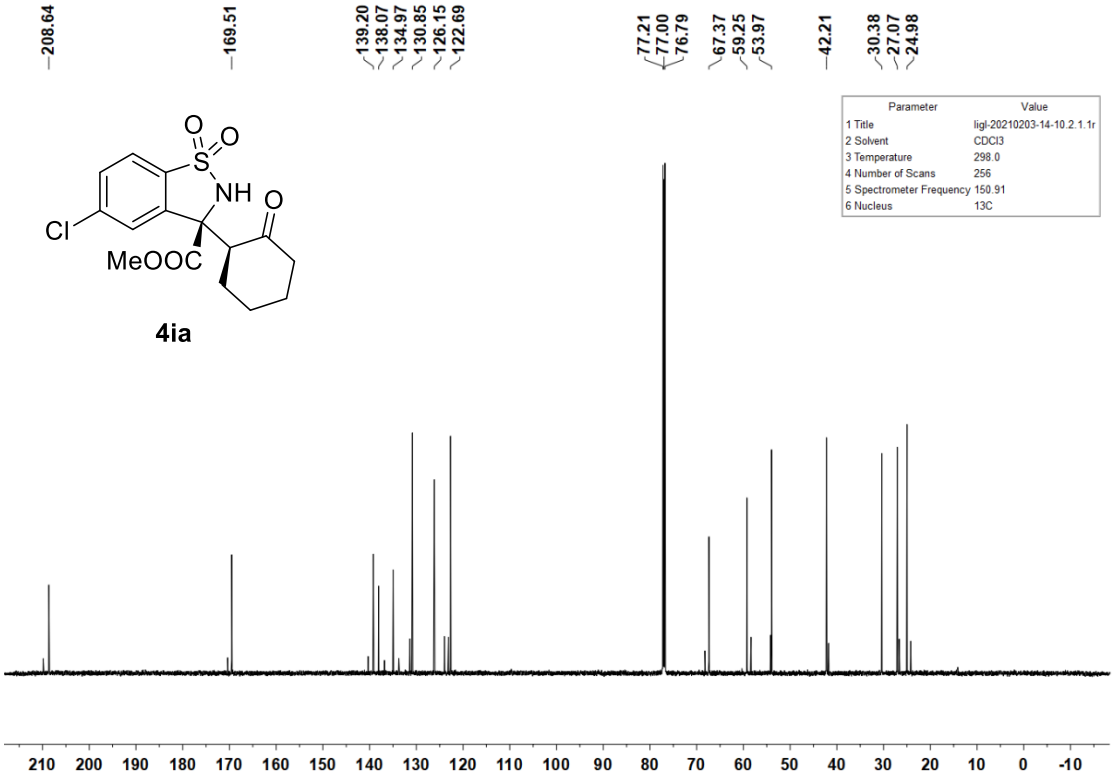
3.18
3.16
3.16
3.14
2.46
2.44
2.39
2.38
2.37
2.36
2.34
2.33
2.09
2.08
2.06
2.04
2.02
1.96
1.94
1.69
1.66
1.64
1.62
1.60
Cl
NH
O
MeOOC
4ia
Parameter Value
1 Title ligl-20210203-14-10.1.1.1r
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 16
5 Spectrometer Frequency 600.17
6 Nucleus 1H
1.00 1.12 0.88 0.88 0.12 2.64 0.36 1.05 1.06 2.98 0.91 2.48
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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77.00
76.79
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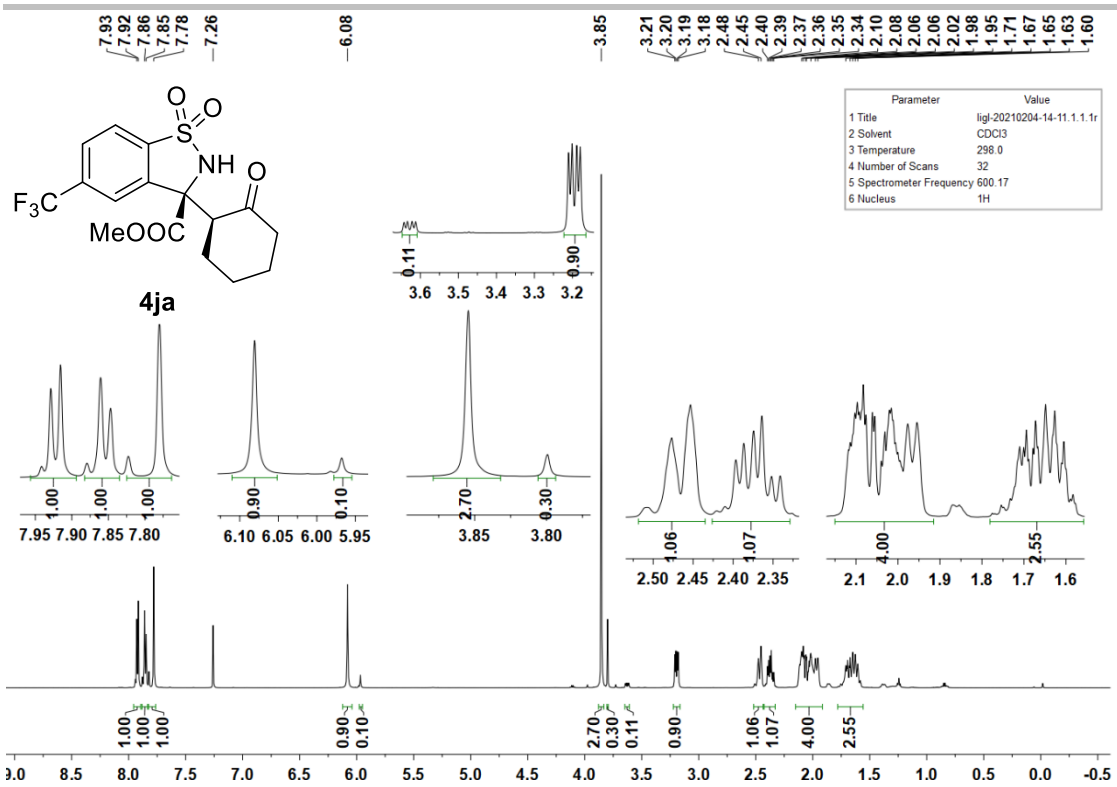
53.97
42.21
30.38
27.07
24.98
Cl
NH
O
MeOOC
4ia
Parameter Value
1 Title ligl-20210203-14-10.2.1.1r
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 256
5 Spectrometer Frequency 150.91
6 Nucleus 13C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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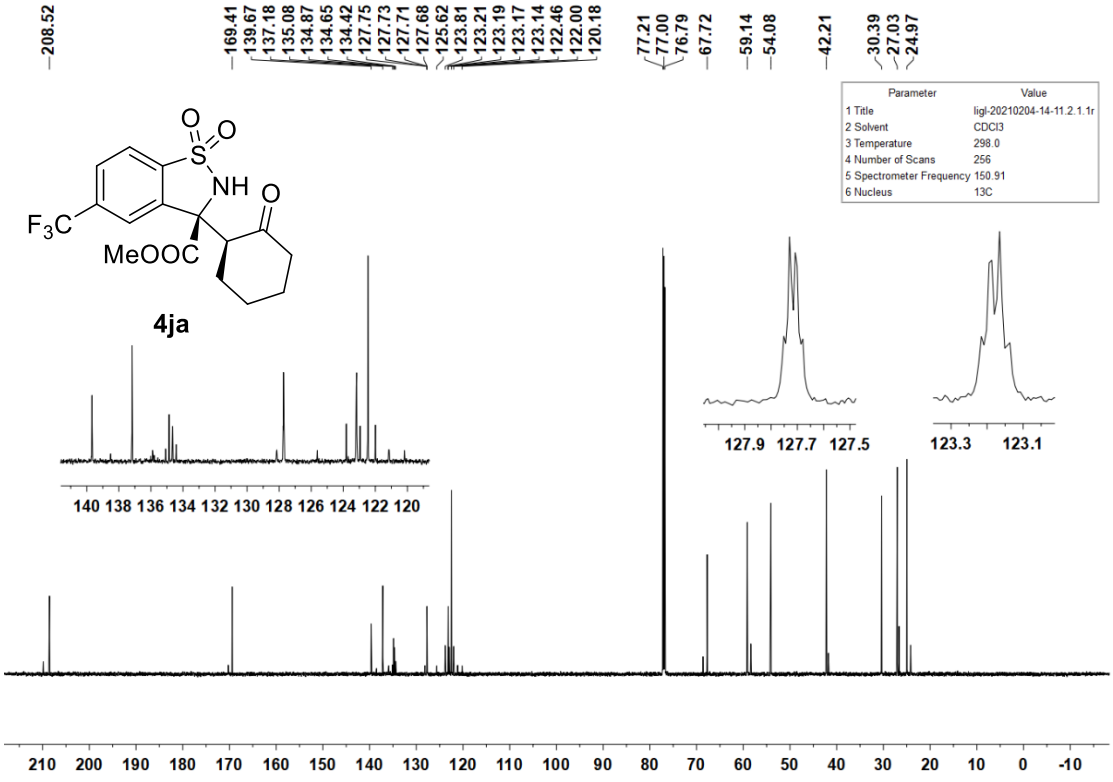
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 32
5 Spectrometer Frequency 600.17
6 Nucleus 1H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Parameter Value
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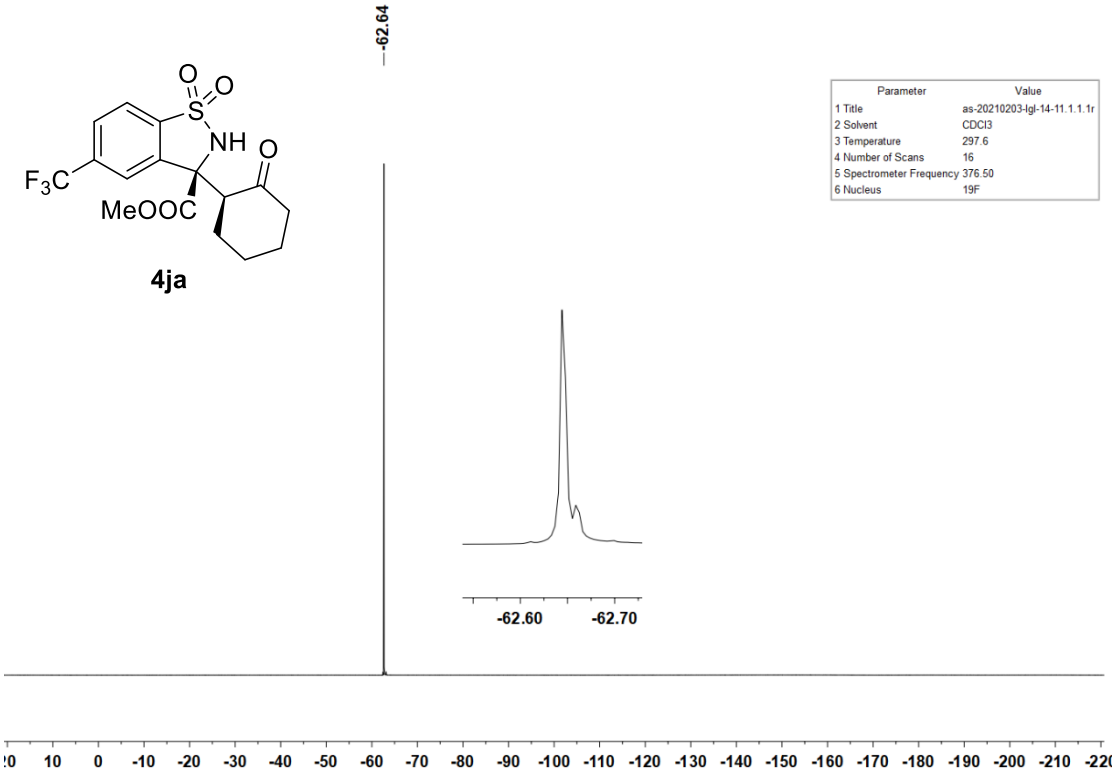
3 Temperature 298.0
4 Number of Scans 256
5 Spectrometer Frequency 150.91
6 Nucleus 13C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O
O
S
NH
O
F3C
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4ja
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2 Solvent CDCl3
3 Temperature 297.6
4 Number of Scans 16
5 Spectrometer Frequency 376.50
6 Nucleus 19F
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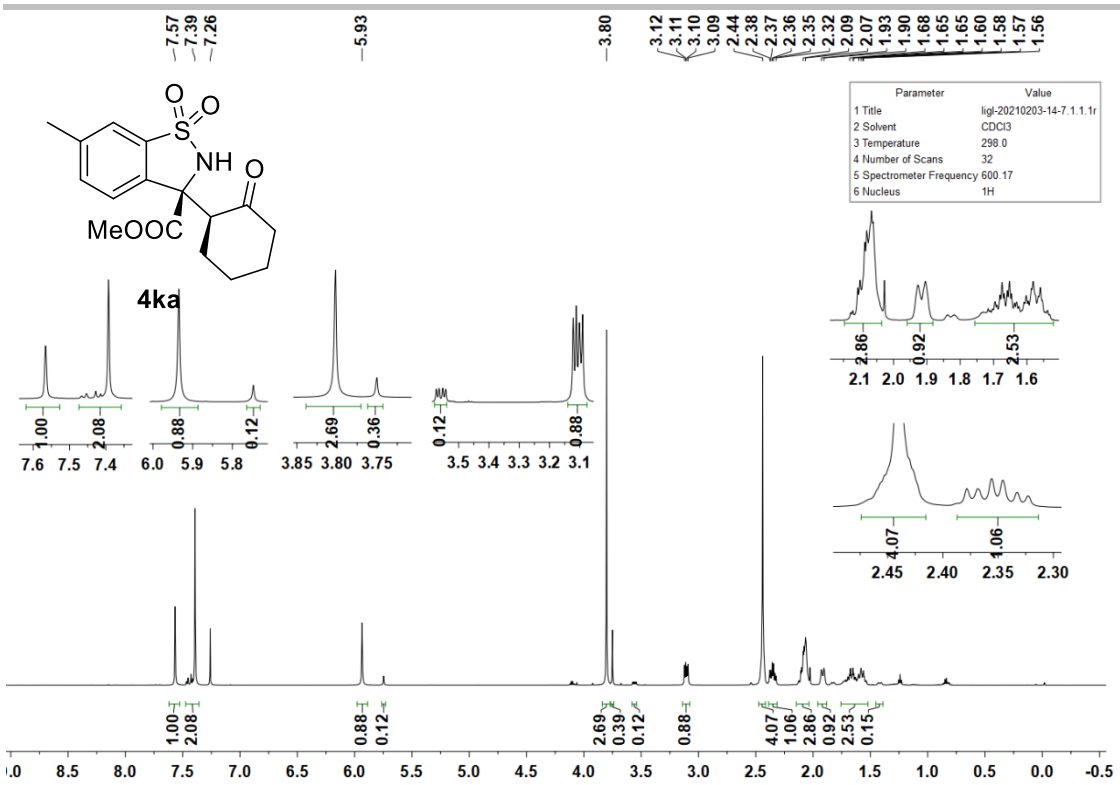
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2.07
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1.56
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1 Title ligl-20210203-14-7.1.1.1r
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 32
5 Spectrometer Frequency 600.17
6 Nucleus 1H
MeOOC
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2.86 0.92 2.53
2.1 2.0 1.9 1.8 1.7 1.6
4.07 1.06
2.45 2.40 2.35 2.30
1.00 2.08 0.88 0.12 2.69 0.39 0.12 0.88 4.07 1.06 2.86 0.92 2.53 0.15
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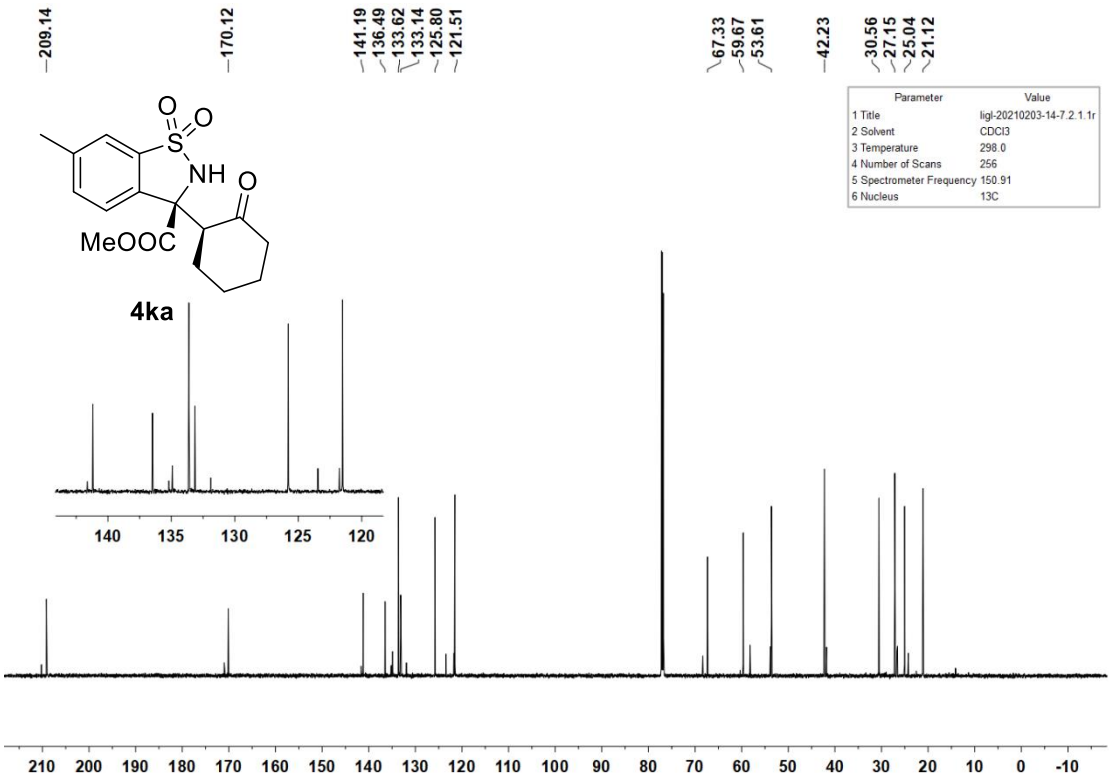
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121.51
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53.61
42.23
30.56
27.15
25.04
21.12
Parameter Value
1 Title ligl-20210203-14-7.2.1.1r
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 256
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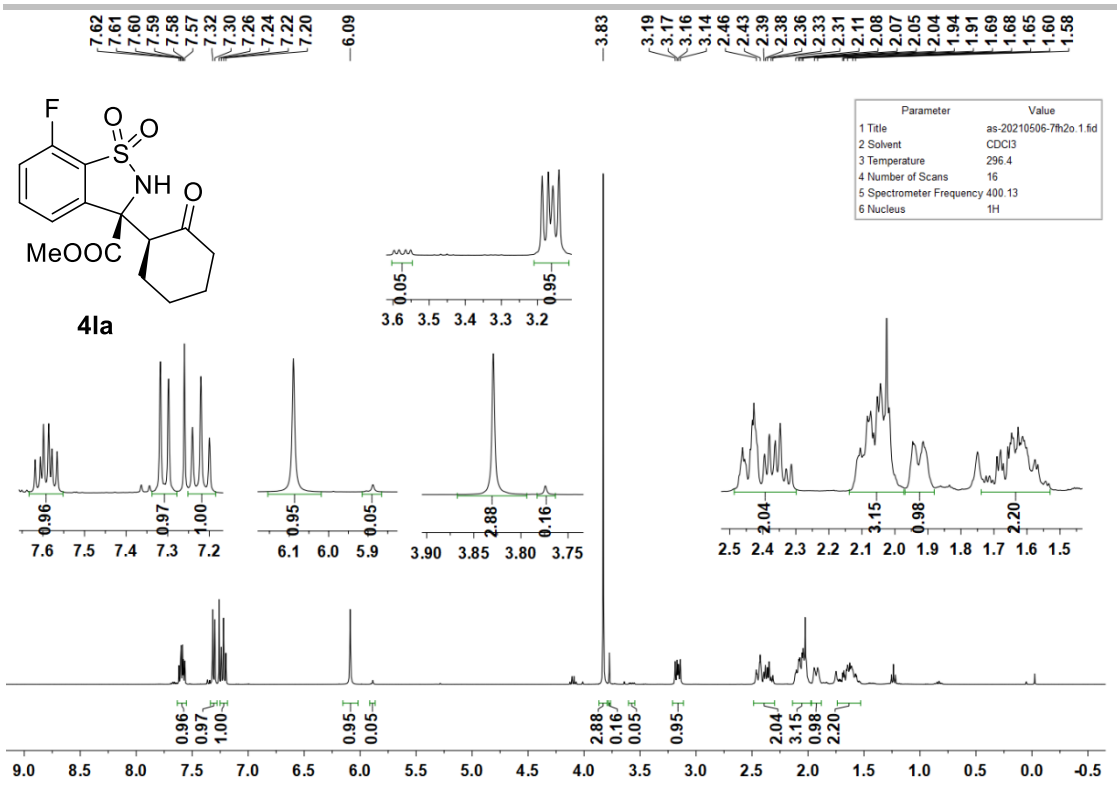
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F
O
O
S
NH
O
MeOOC
4la
Parameter Value
1 Title as-20210506-7fh2o.1.fid
2 Solvent CDCl3
3 Temperature 296.4
4 Number of Scans 16
5 Spectrometer Frequency 400.13
6 Nucleus 1H
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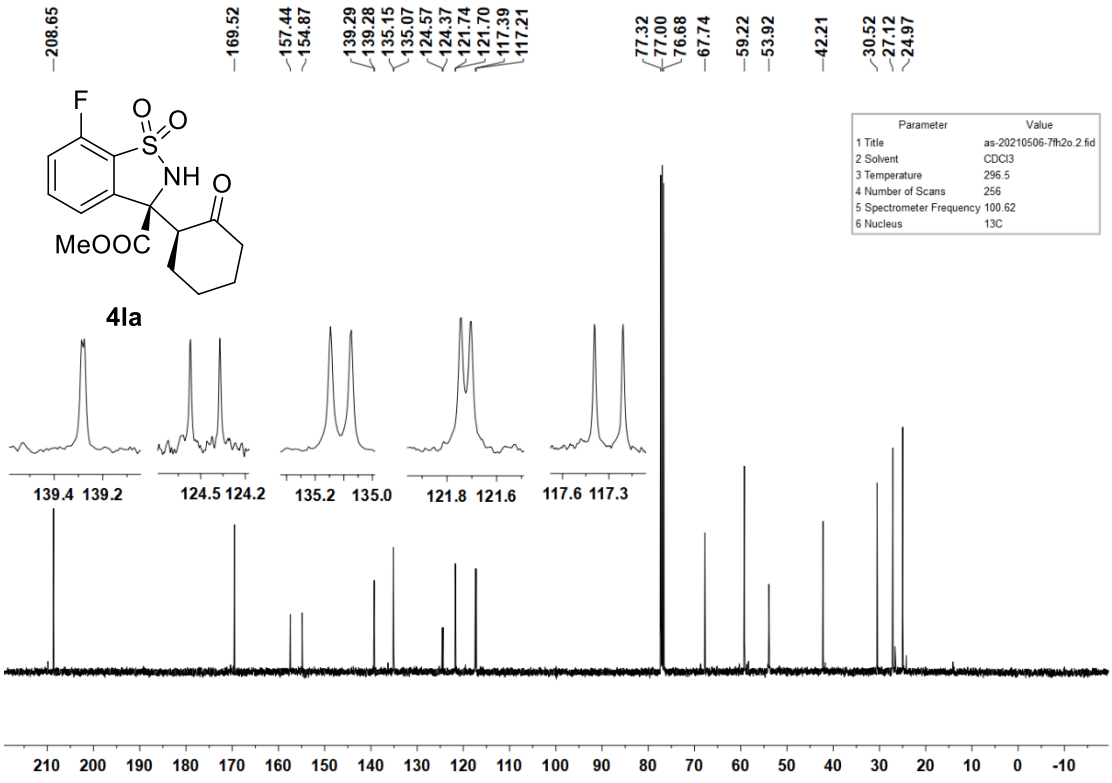
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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F
O
O
S
NH
O
MeOOC
4la
Parameter Value
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2 Solvent CDCl3
3 Temperature 296.5
4 Number of Scans 256
5 Spectrometer Frequency 100.62
6 Nucleus 13C
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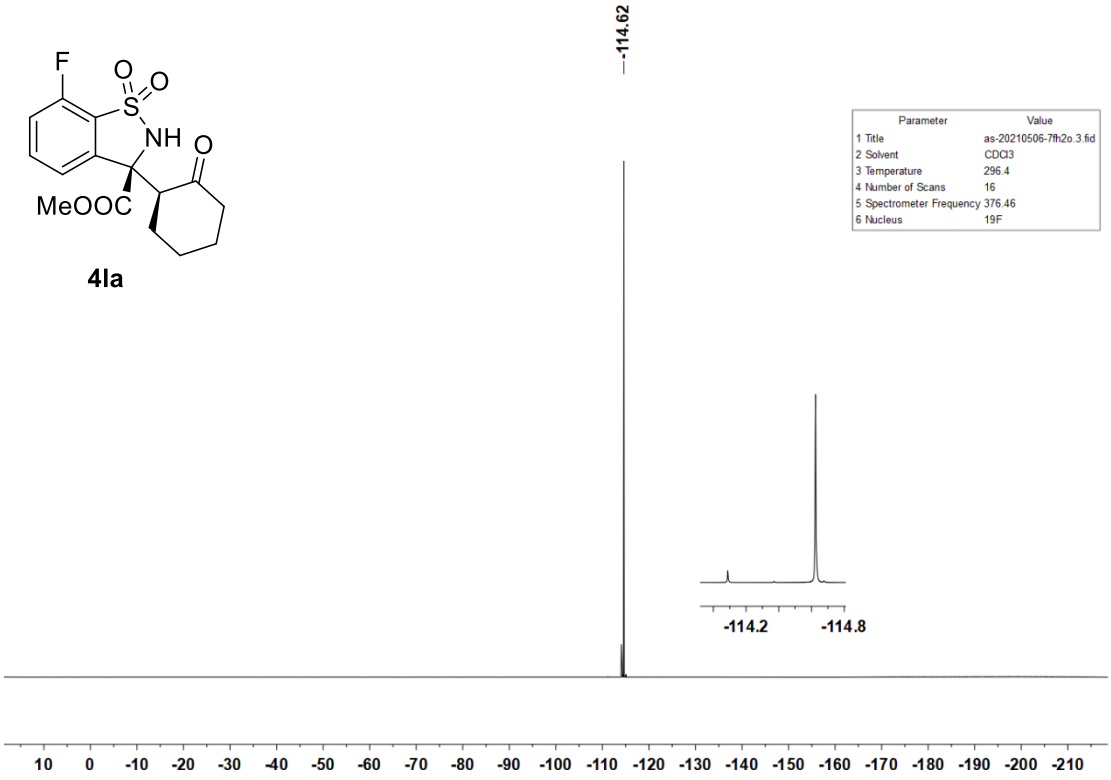
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4 Number of Scans 16
5 Spectrometer Frequency 376.46
6 Nucleus 19F
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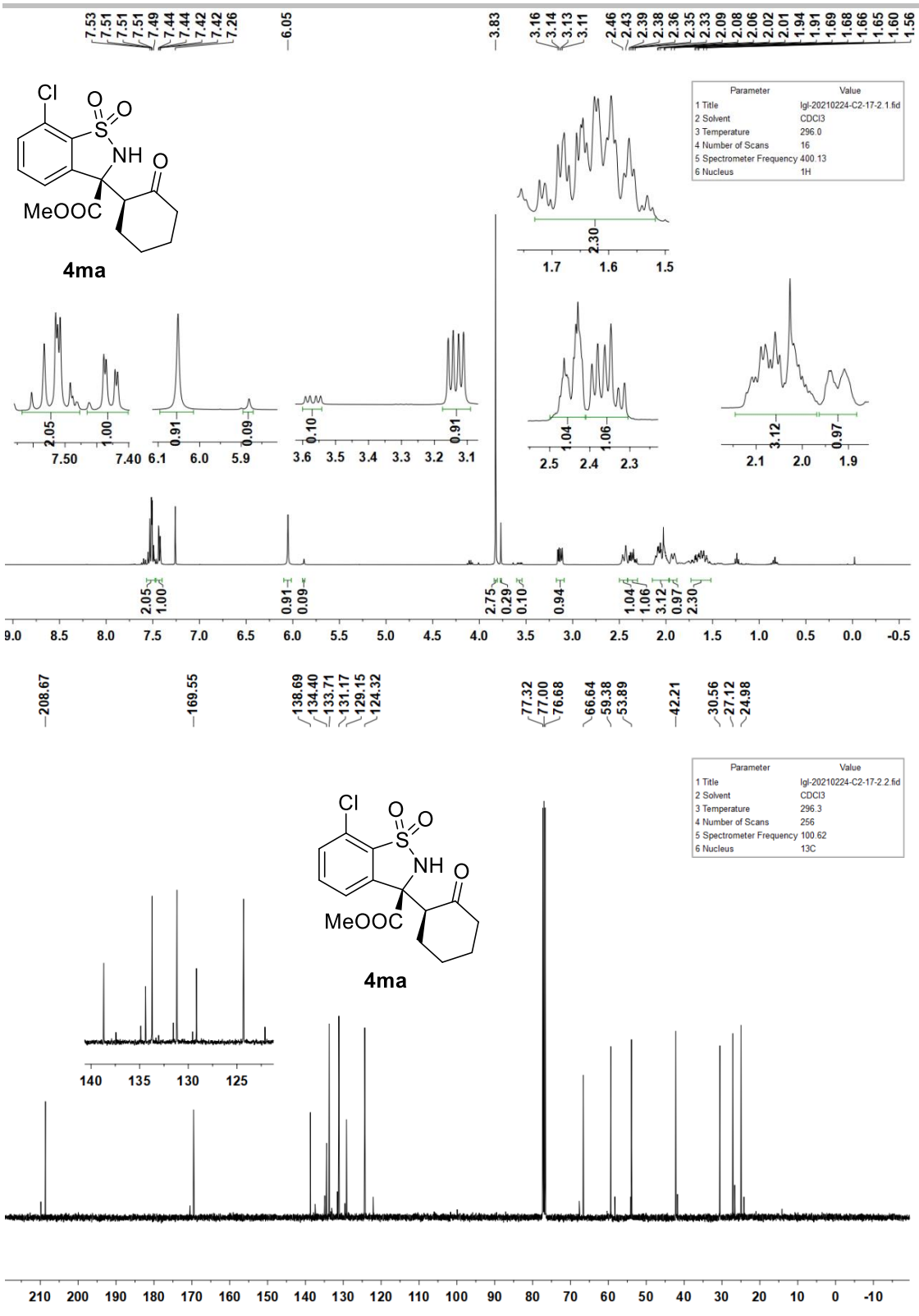
4la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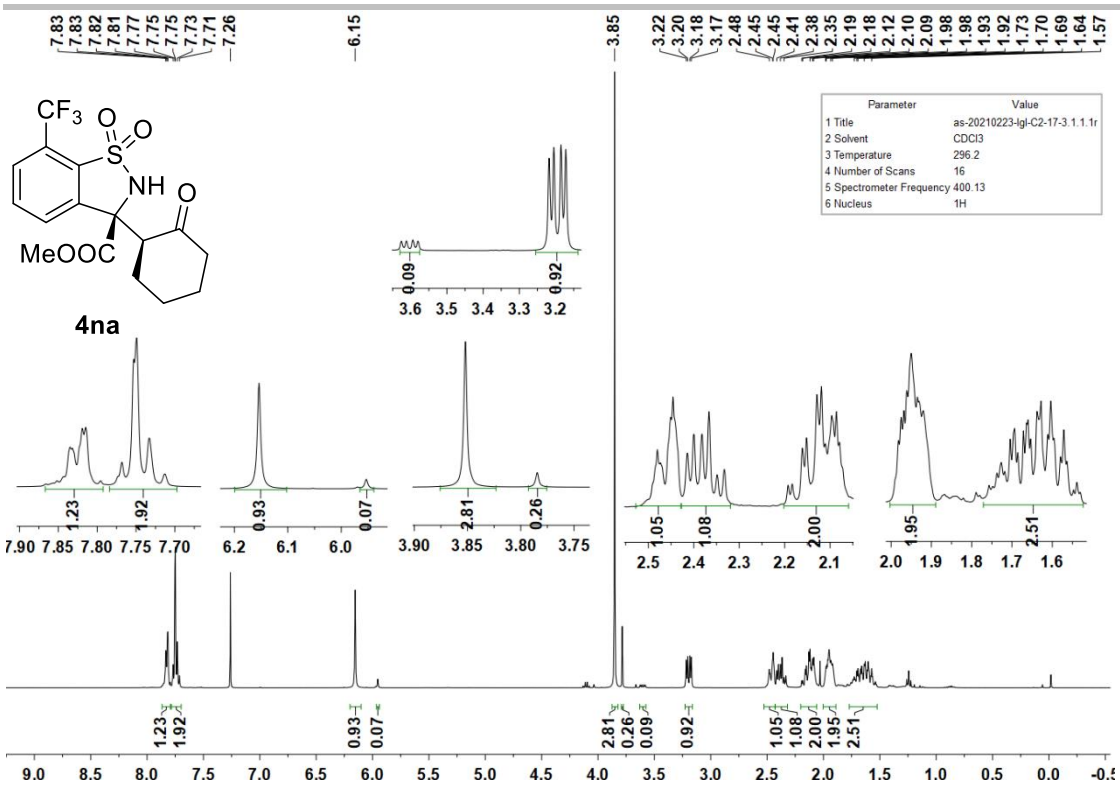
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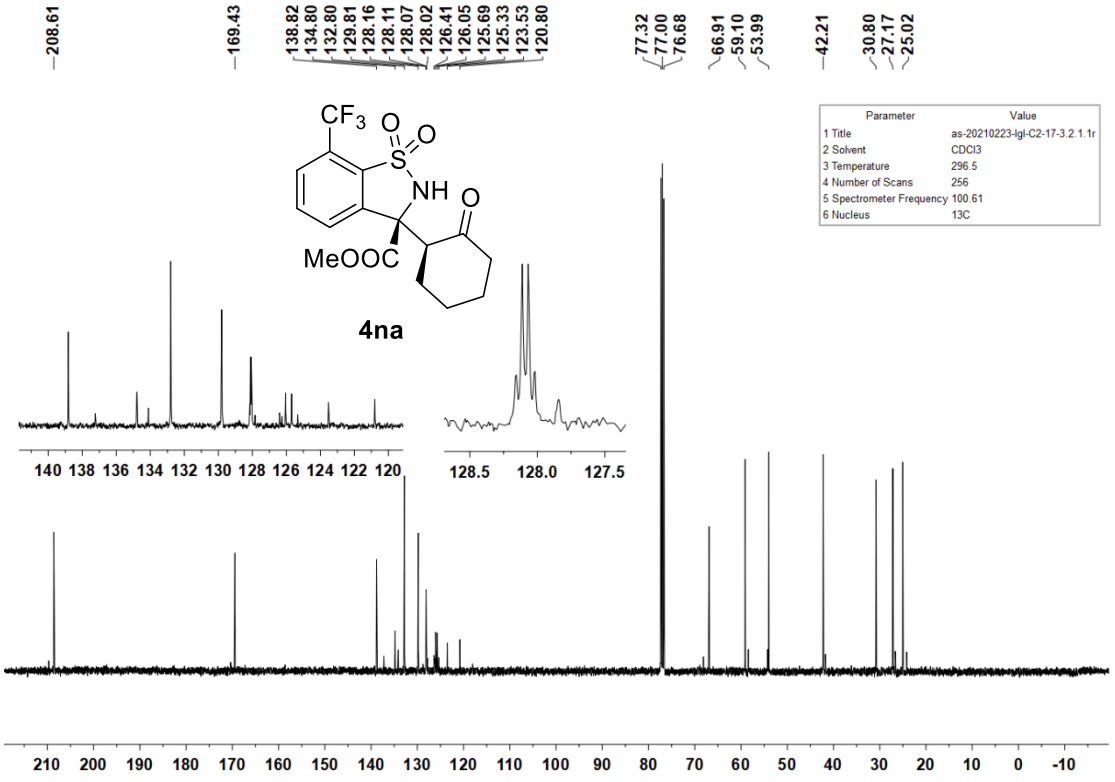
4 Number of Scans 16
5 Spectrometer Frequency 400.13
6 Nucleus 1H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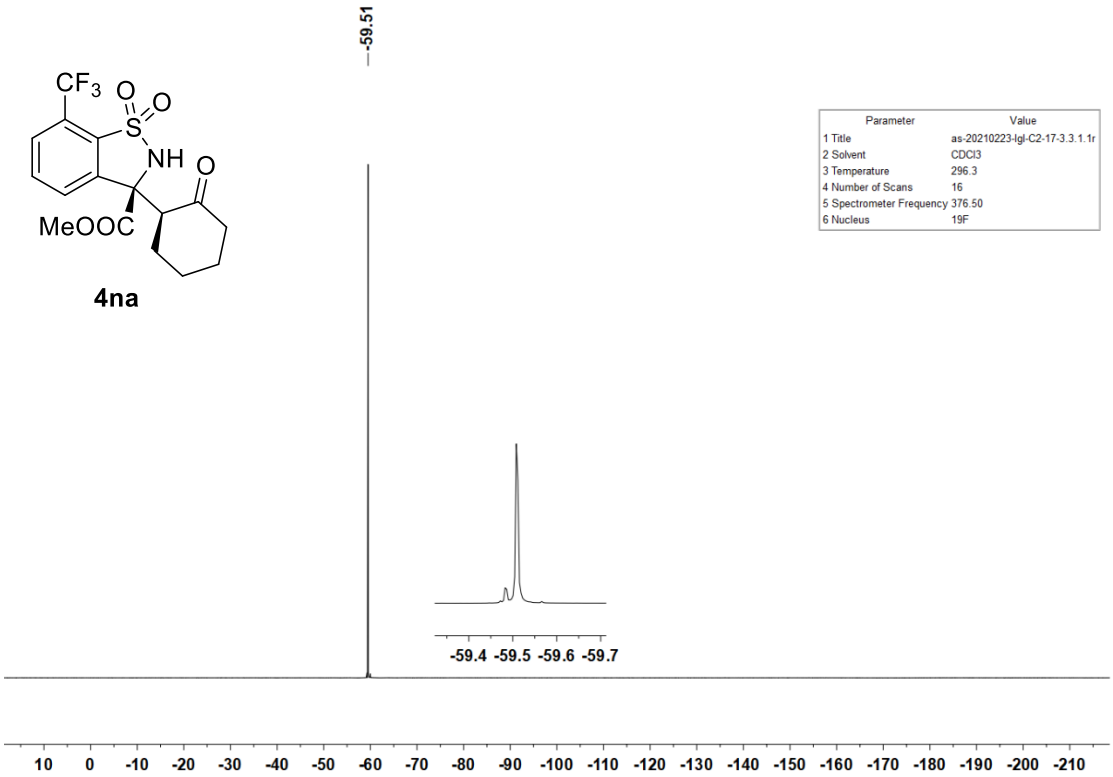
5 Spectrometer Frequency 100.61
6 Nucleus 13C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CDCl3
3 Temperature
296.3
4 Number of Scans
16
5 Spectrometer Frequency
376.50
6 Nucleus
19F
-59.4 -59.5 -59.6 -59.7
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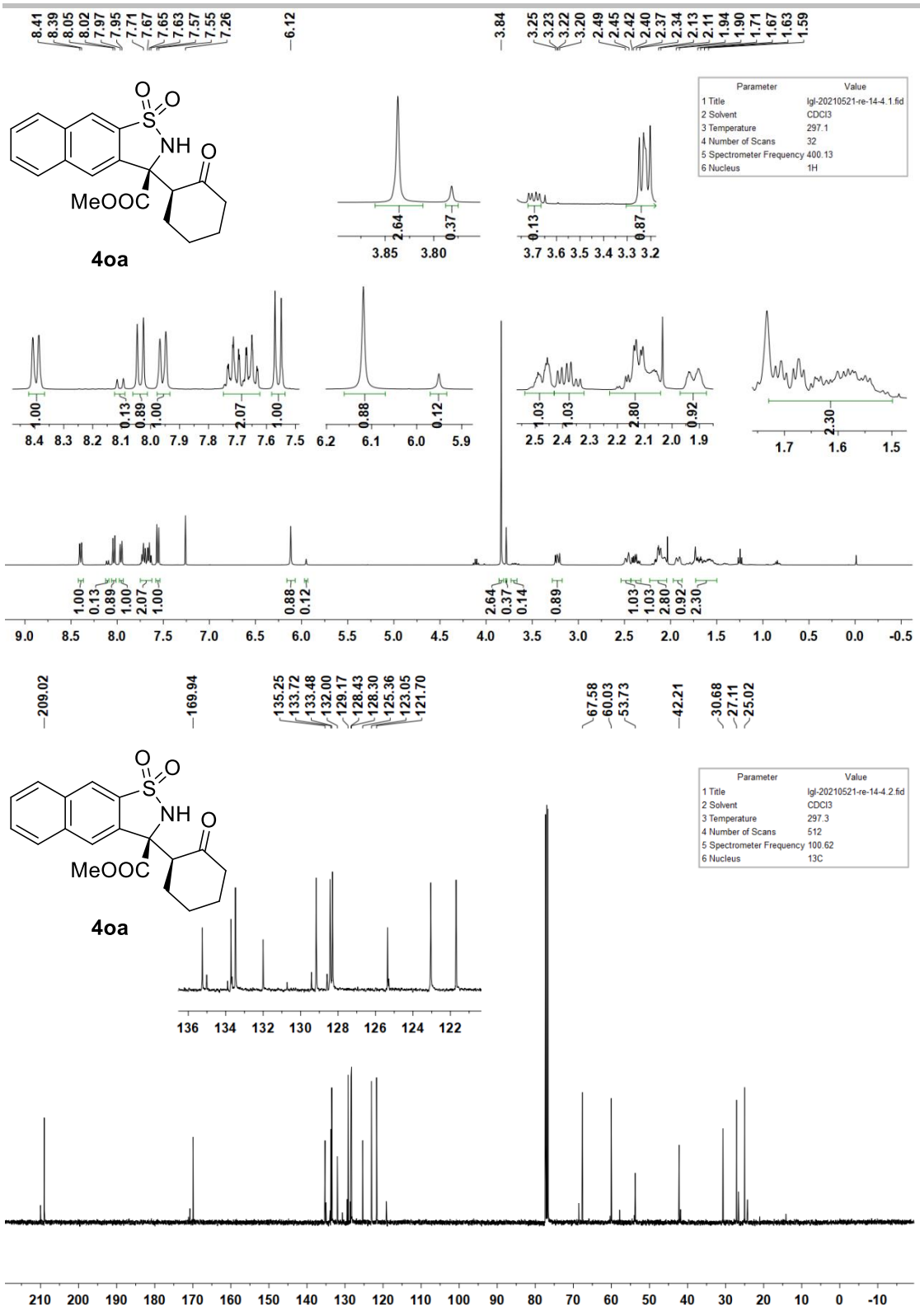
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6.12
3.84
3.25 3.23 3.22 3.20 2.49 2.45 2.42 2.40 2.37 2.34 2.13 2.11 1.94 1.90 1.71 1.67 1.63 1.59
O
O
S
NH
O
MeOOC
4oa
Parameter Value
1 Title lgl-20210521-re-14-4.1.fid
2 Solvent CDCl3
3 Temperature 297.1
4 Number of Scans 32
5 Spectrometer Frequency 400.13
6 Nucleus 1H
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3.85 3.80
0.13 0.87
3.7 3.6 3.5 3.4 3.3 3.2
1.00 0.13 0.89 1.00 2.07 1.00
8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5
0.88 0.12
6.2 6.1 6.0 5.9
1.03 1.03 2.80 0.92
2.5 2.4 2.3 2.2 2.1 2.0 1.9
2.30
1.7 1.6 1.5
1.00 0.13 0.89 1.00 2.07 1.00 0.88 0.12 2.64 0.37 0.14 0.89 1.03 1.03 2.80 0.92 2.30
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
209.02
169.94
135.25 133.72 133.48 132.00 129.17 128.43 128.30 125.36 123.05 121.70
67.58 60.03 53.73
42.21
30.68 27.11 25.02
O
O
S
NH
O
MeOOC
4oa
Parameter Value
1 Title lgl-20210521-re-14-4.2.fid
2 Solvent CDCl3
3 Temperature 297.3
4 Number of Scans 512
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6 Nucleus 13C
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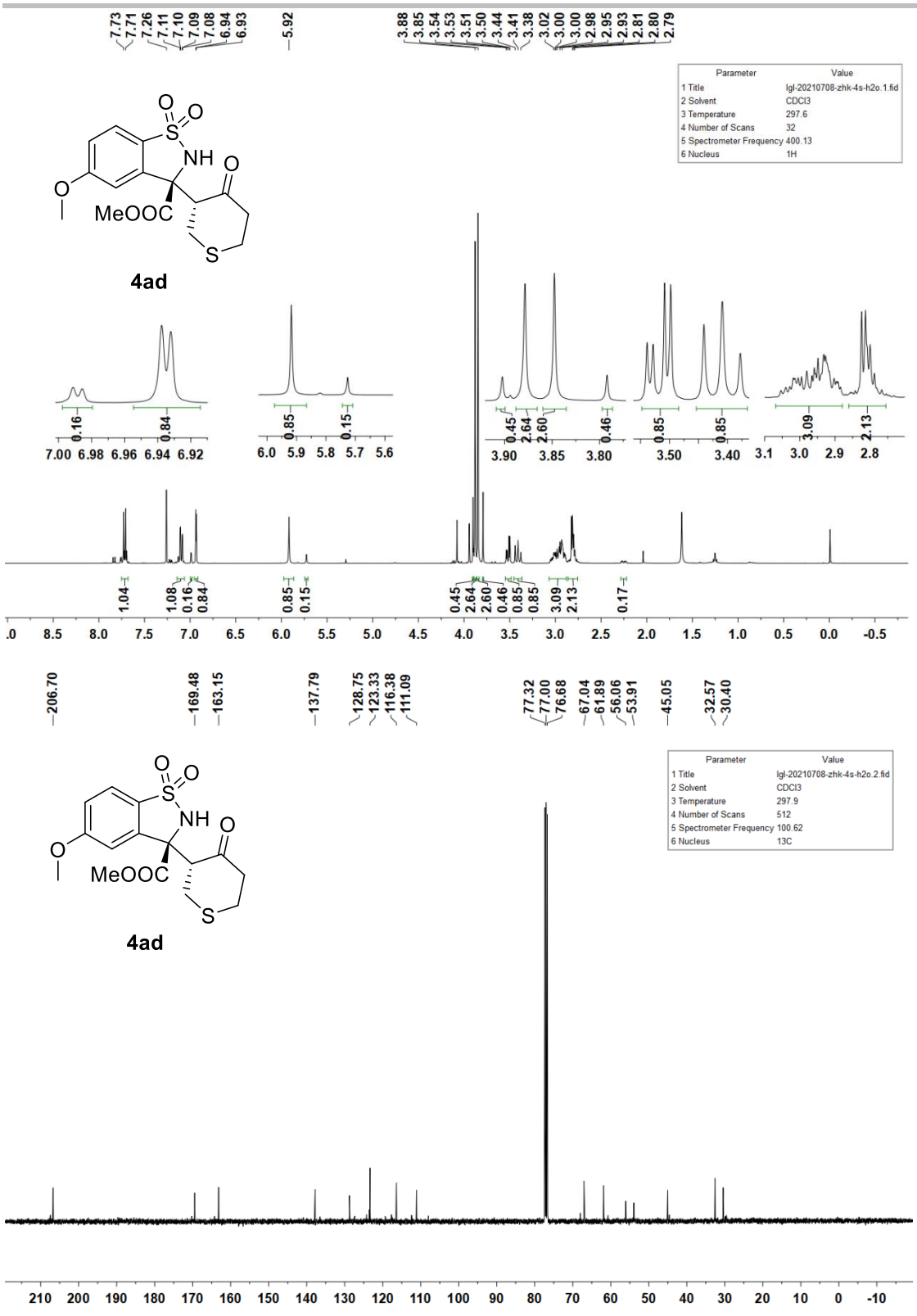
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5.92
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3.54
3.53
3.51
3.50
3.44
3.41
3.38
3.02
3.00
3.00
2.98
2.95
2.93
2.81
2.80
2.79
Parameter Value
1 Title lgl-20210708-zhk-4s-h2o.1.fid
2 Solvent CDCl3
3 Temperature 297.6
4 Number of Scans 32
5 Spectrometer Frequency 400.13
6 Nucleus 1H
4ad
1.04
1.08
0.16
0.84
0.85
0.15
0.45
2.64
2.60
0.46
0.85
0.85
3.09
2.13
0.17
206.70
169.48
163.15
137.79
128.75
123.33
116.38
111.09
77.32
77.00
76.68
67.04
61.89
56.06
53.91
45.05
32.57
30.40
Parameter Value
1 Title lgl-20210708-zhk-4s-h2o.2.fid
2 Solvent CDCl3
3 Temperature 297.9
4 Number of Scans 512
5 Spectrometer Frequency 100.62
6 Nucleus 13C
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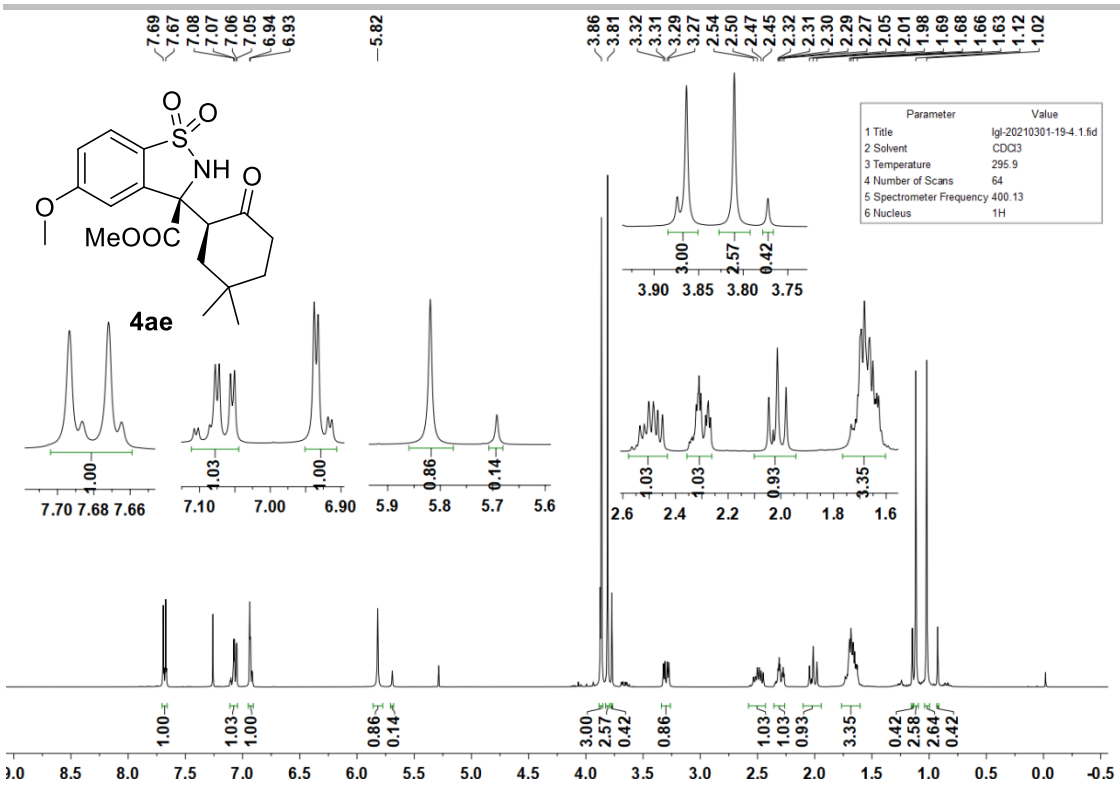
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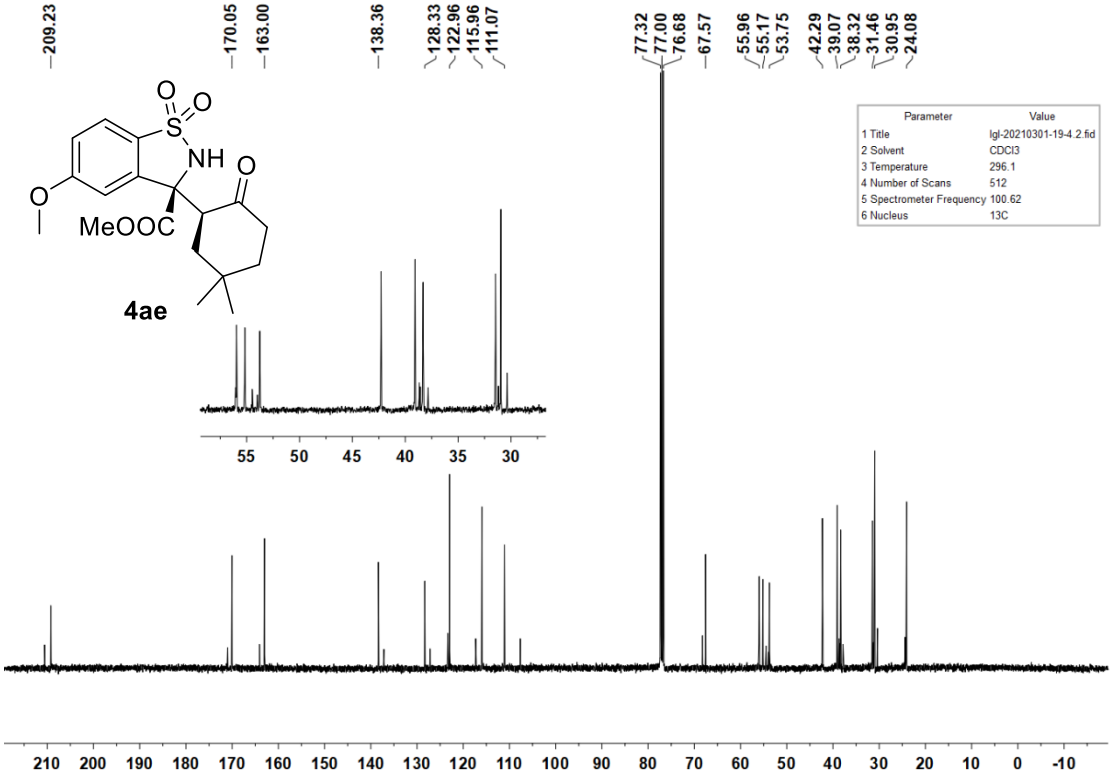
3 Temperature 295.9
4 Number of Scans 64
5 Spectrometer Frequency 400.13
6 Nucleus 1H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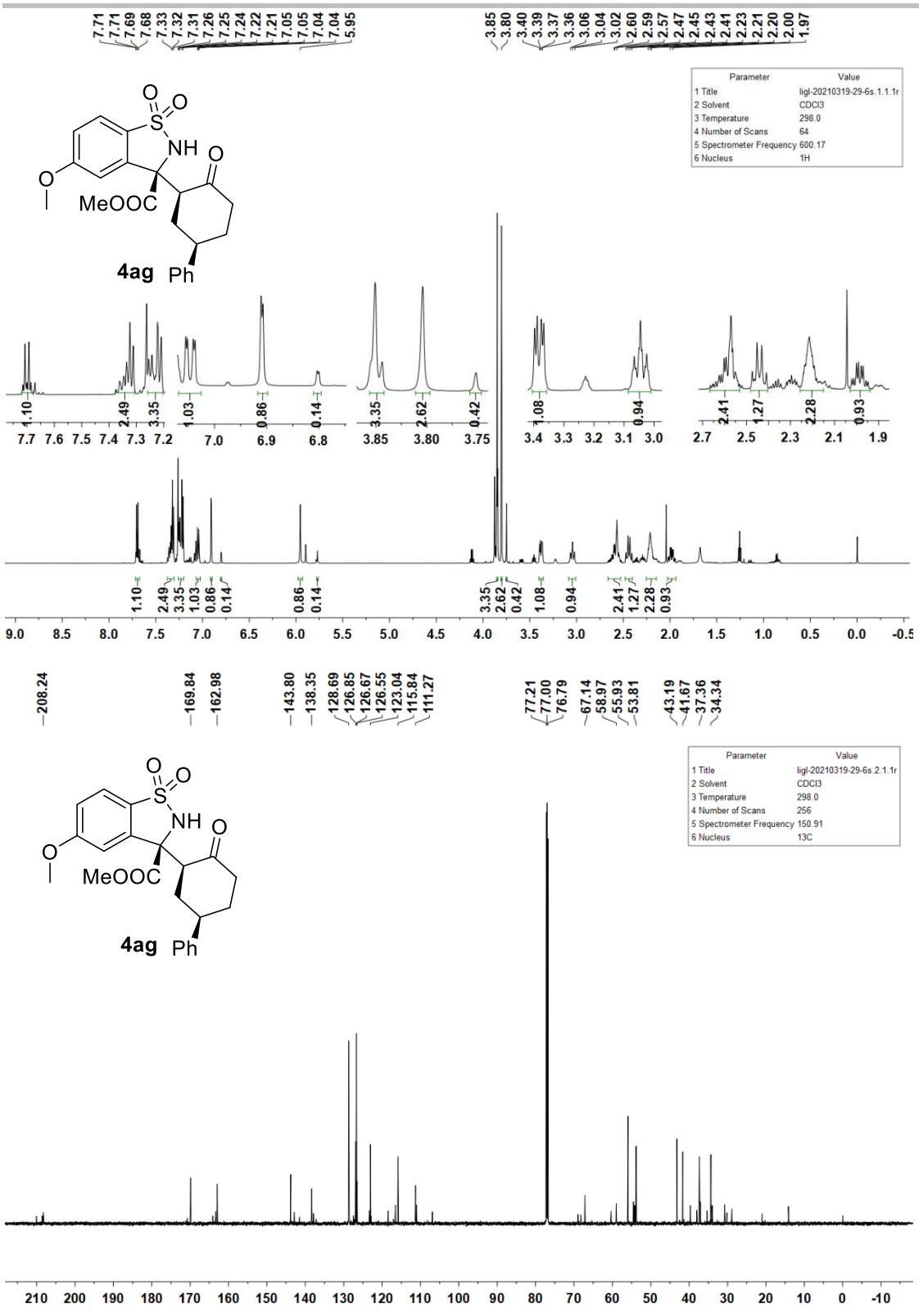
4 Number of Scans 512
5 Spectrometer Frequency 100.62
6 Nucleus 13C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3.85 3.80 3.40 3.39 3.37 3.36 3.06 3.04 3.02 2.60 2.59 2.57 2.47 2.45 2.43 2.41 2.23 2.21 2.20 2.00 1.97
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3 Temperature 298.0
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5 Spectrometer Frequency 600.17
6 Nucleus 1H
MeOOC
4ag Ph
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208.24 169.84 162.98 143.80 138.35 128.69 126.85 126.67 126.55 123.04 115.84 111.27 77.21 77.00 76.79 67.14 58.97 55.93 53.81 43.19 41.67 37.36 34.34
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1 Title ligl-20210319-29-6s.2.1.1r
2 Solvent CDCl3
3 Temperature 298.0
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6 Nucleus 13C
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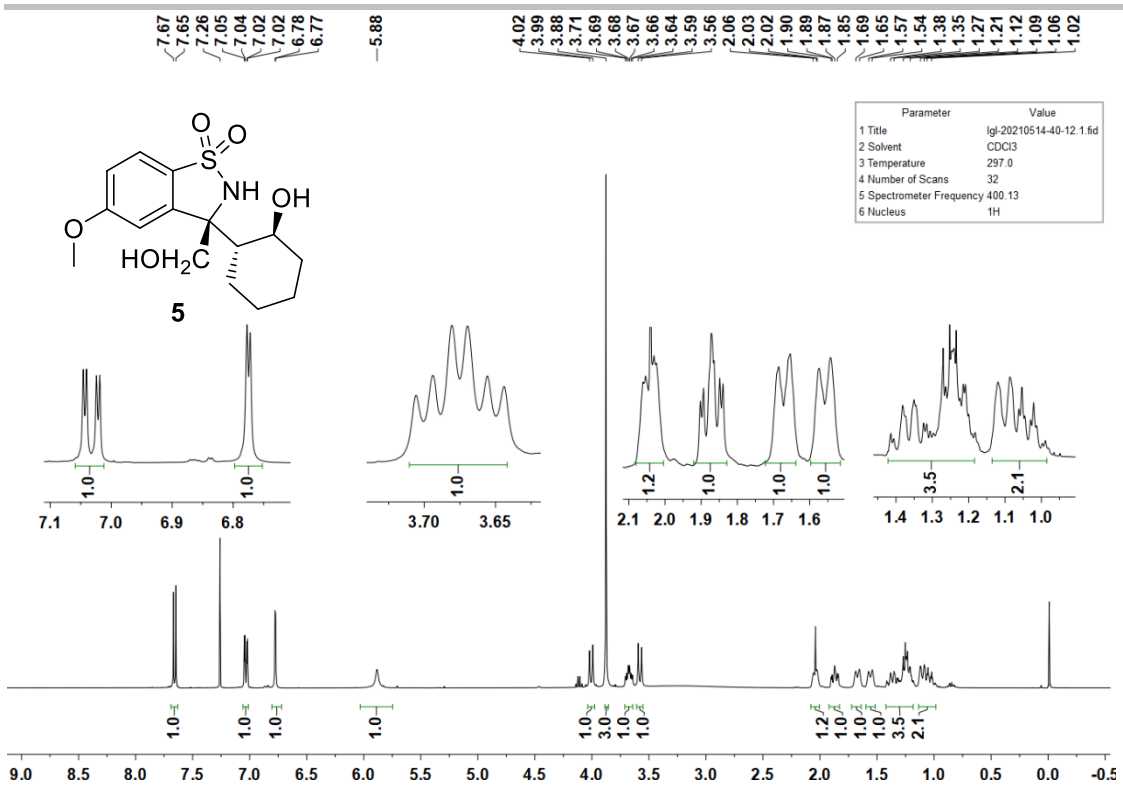
4ag Ph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Parameter Value
1 Title lgl-20210514-40-12.1.fid
2 Solvent CDCl3
3 Temperature 297.0
4 Number of Scans 32
5 Spectrometer Frequency 400.13
6 Nucleus 1H
O
O
S
NH
OH
O
HOH2C
5
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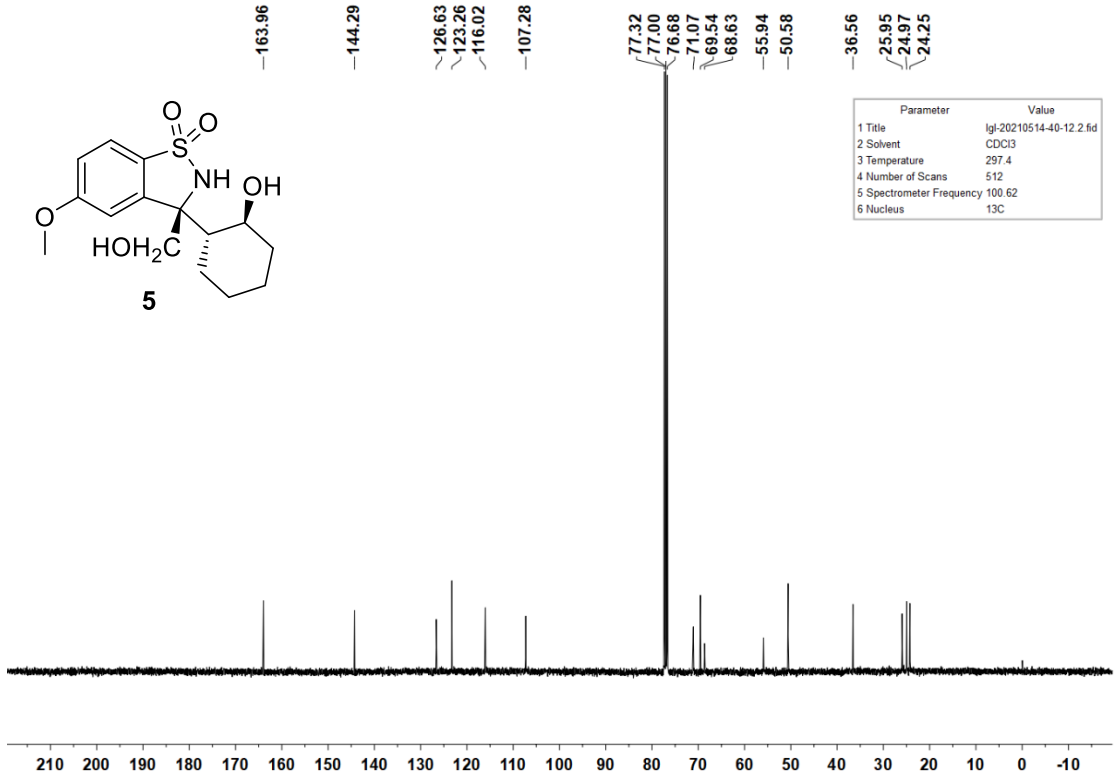
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1 Title lgl-20210514-40-12.2.fid
2 Solvent CDCl3
3 Temperature 297.4
4 Number of Scans 512
5 Spectrometer Frequency 100.62
6 Nucleus 13C
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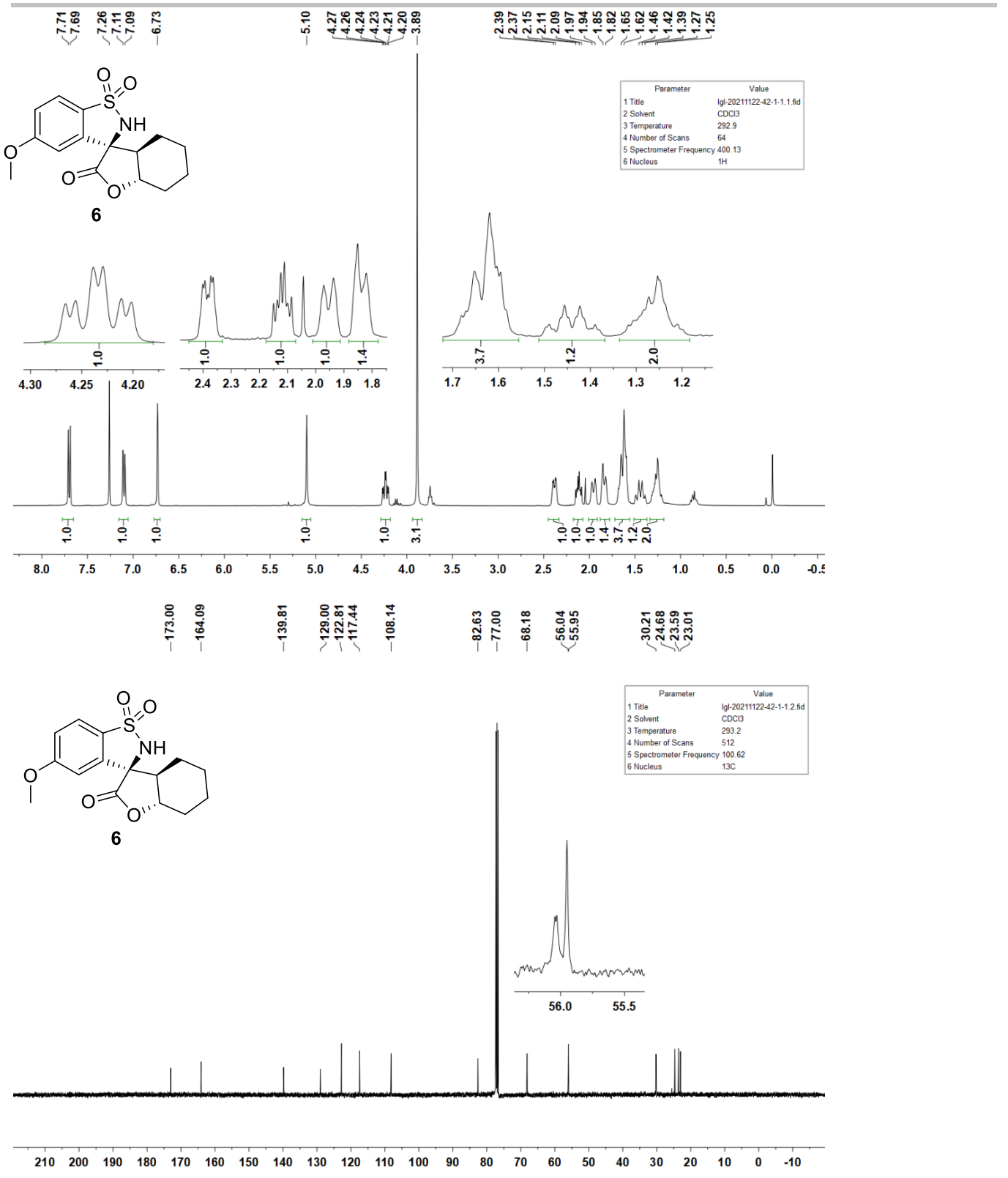
O
S
NH
OH
O
HOH2C
5
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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4.23
4.21
4.20
3.89
2.39
2.37
2.15
2.11
2.09
1.97
1.94
1.85
1.82
1.65
1.62
1.46
1.42
1.39
1.27
1.25
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1 Title lgl-20211122-42-1-1.1.fid
2 Solvent CDCl3
3 Temperature 292.9
4 Number of Scans 64
5 Spectrometer Frequency 400.13
6 Nucleus 1H
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1.0
4.30 4.25 4.20
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2.4 2.3 2.2 2.1 2.0 1.9 1.8
3.7 1.2 2.0
1.7 1.6 1.5 1.4 1.3 1.2
1.0 1.0 1.0 1.0 1.0 3.1 1.0 1.0 1.4 3.7 1.2 2.0
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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164.09
139.81
129.00
122.81
117.44
108.14
82.63
77.00
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55.95
30.21
24.68
23.59
23.01
Parameter Value
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3 Temperature 293.2
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6 Nucleus 13C
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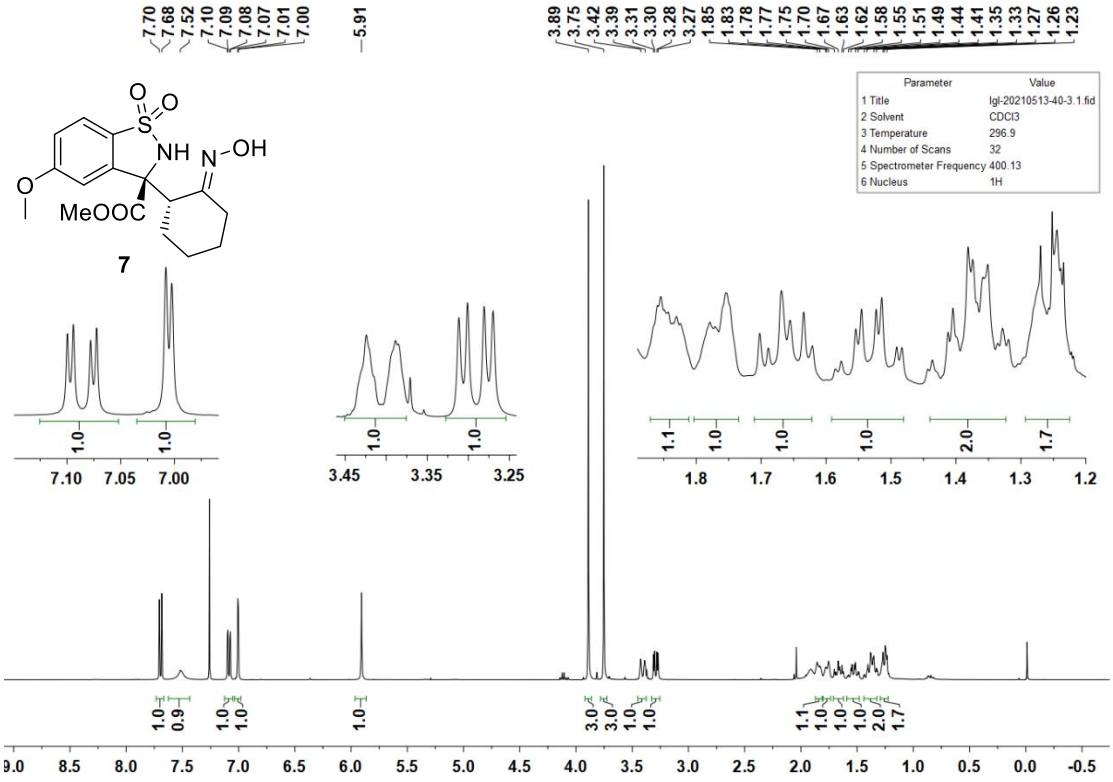
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1.63
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1.33
1.27
1.26
1.23
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1 Title lgl-20210513-40-3.1.fid
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3 Temperature 296.9
4 Number of Scans 32
5 Spectrometer Frequency 400.13
6 Nucleus 1H
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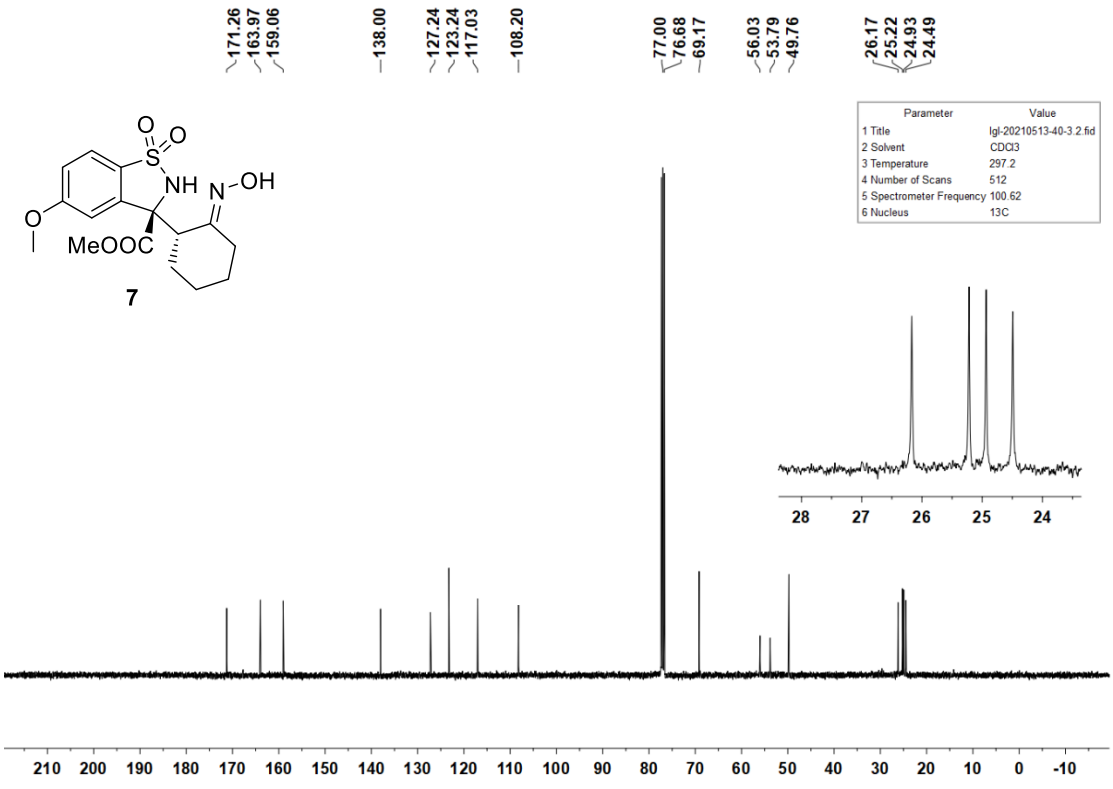
N-OH
O
MeOOC
7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108.20
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69.17
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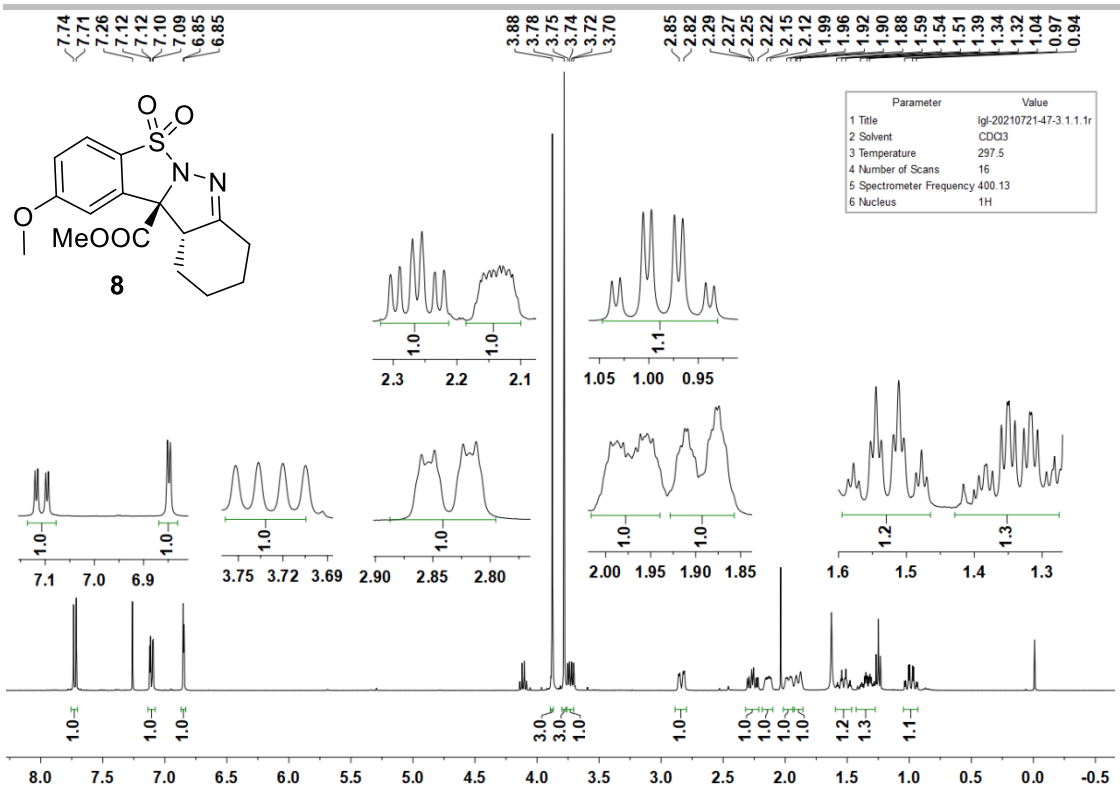
53.79
49.76
26.17
25.22
24.93
24.49
Parameter Value
1 Title lgl-20210513-40-3.2.fid
2 Solvent CDCl3
3 Temperature 297.2
4 Number of Scans 512
5 Spectrometer Frequency 100.62
6 Nucleus 13C
NH
N-OH
O
MeOOC
7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3.72
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2.82
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2.27
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2.22
2.15
2.12
1.99
1.96
1.92
1.90
1.88
1.59
1.54
1.51
1.39
1.34
1.32
1.04
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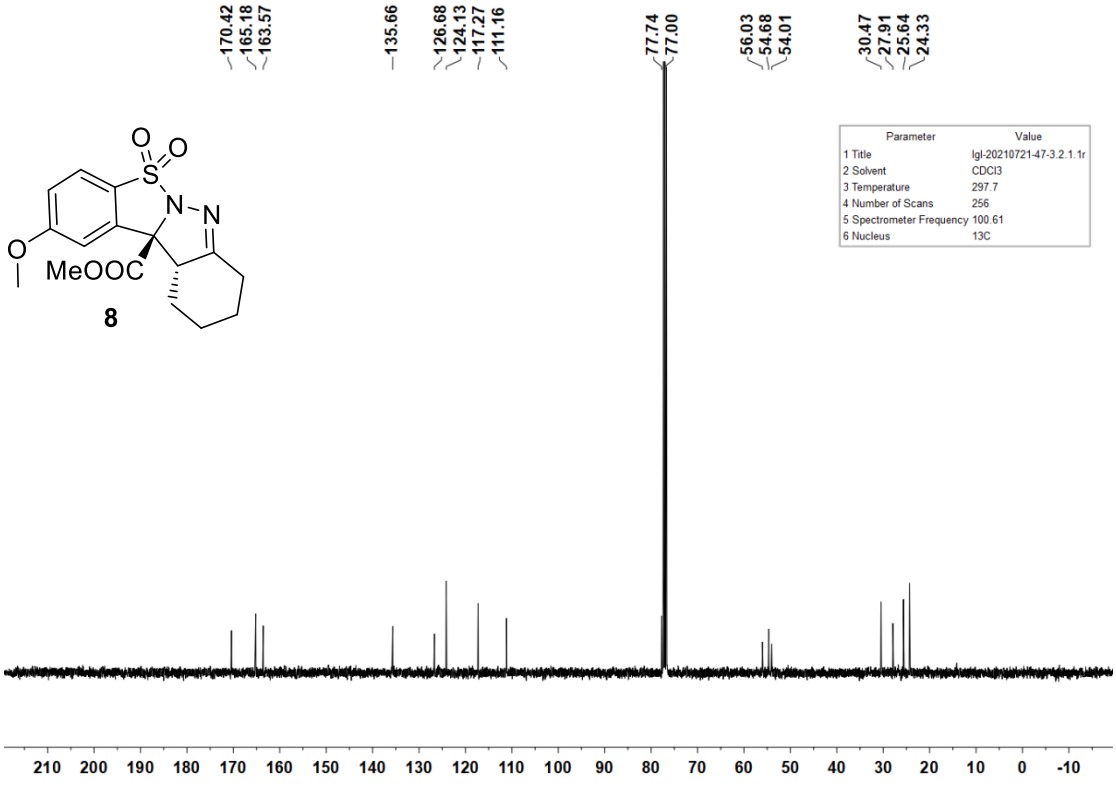
0.94
Parameter Value
1 Title lgl-20210721-47-3.1.1.1r
2 Solvent CDCl3
3 Temperature 297.5
4 Number of Scans 16
5 Spectrometer Frequency 400.13
6 Nucleus 1H
MeOOC
8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124.13
117.27
111.16
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77.00
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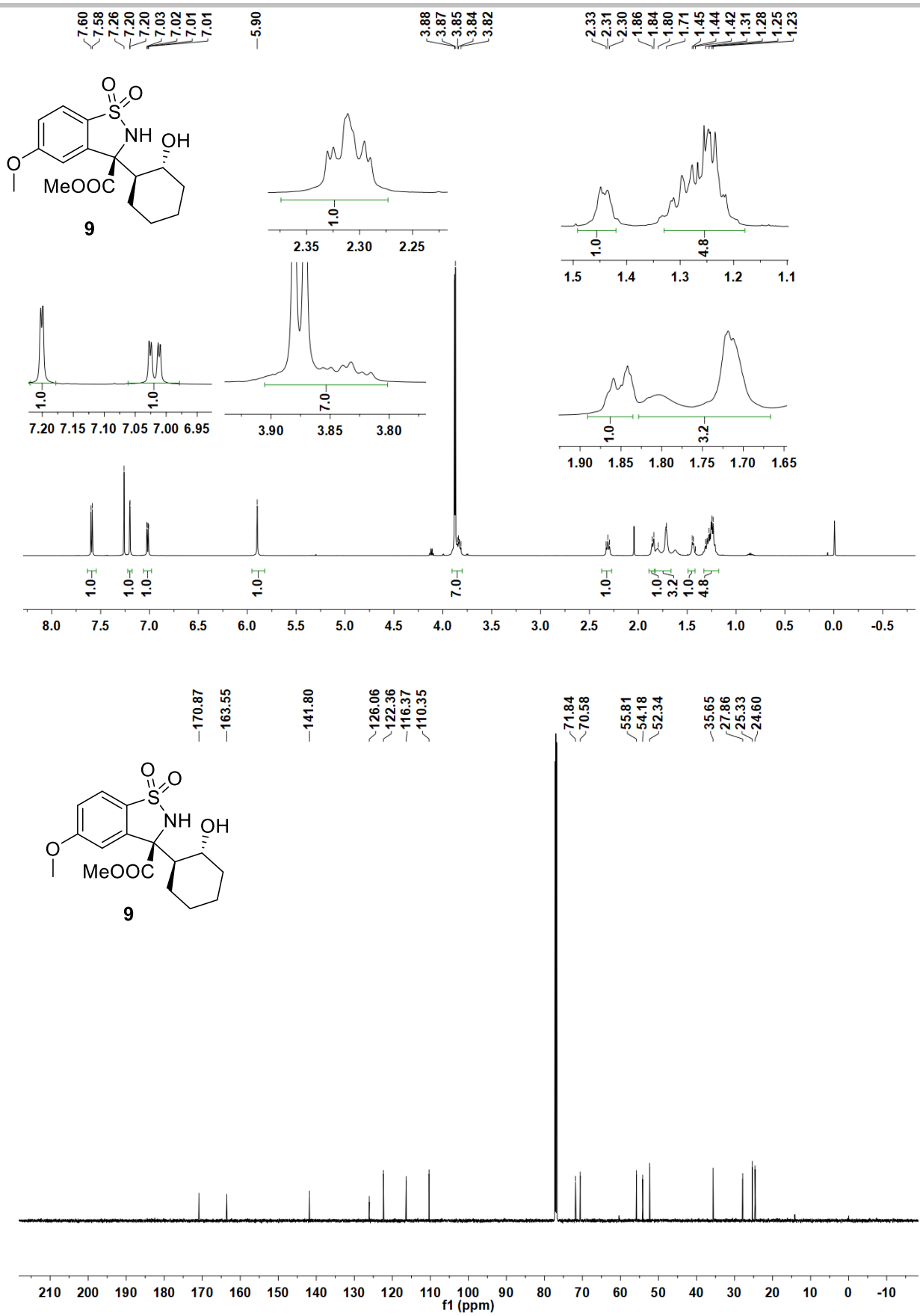
54.01
30.47
27.91
25.64
24.33
Parameter Value
1 Title lgl-20210721-47-3.2.1.1r
2 Solvent CDCl3
3 Temperature 297.7
4 Number of Scans 256
5 Spectrometer Frequency 100.61
6 Nucleus 13C
MeOOC
8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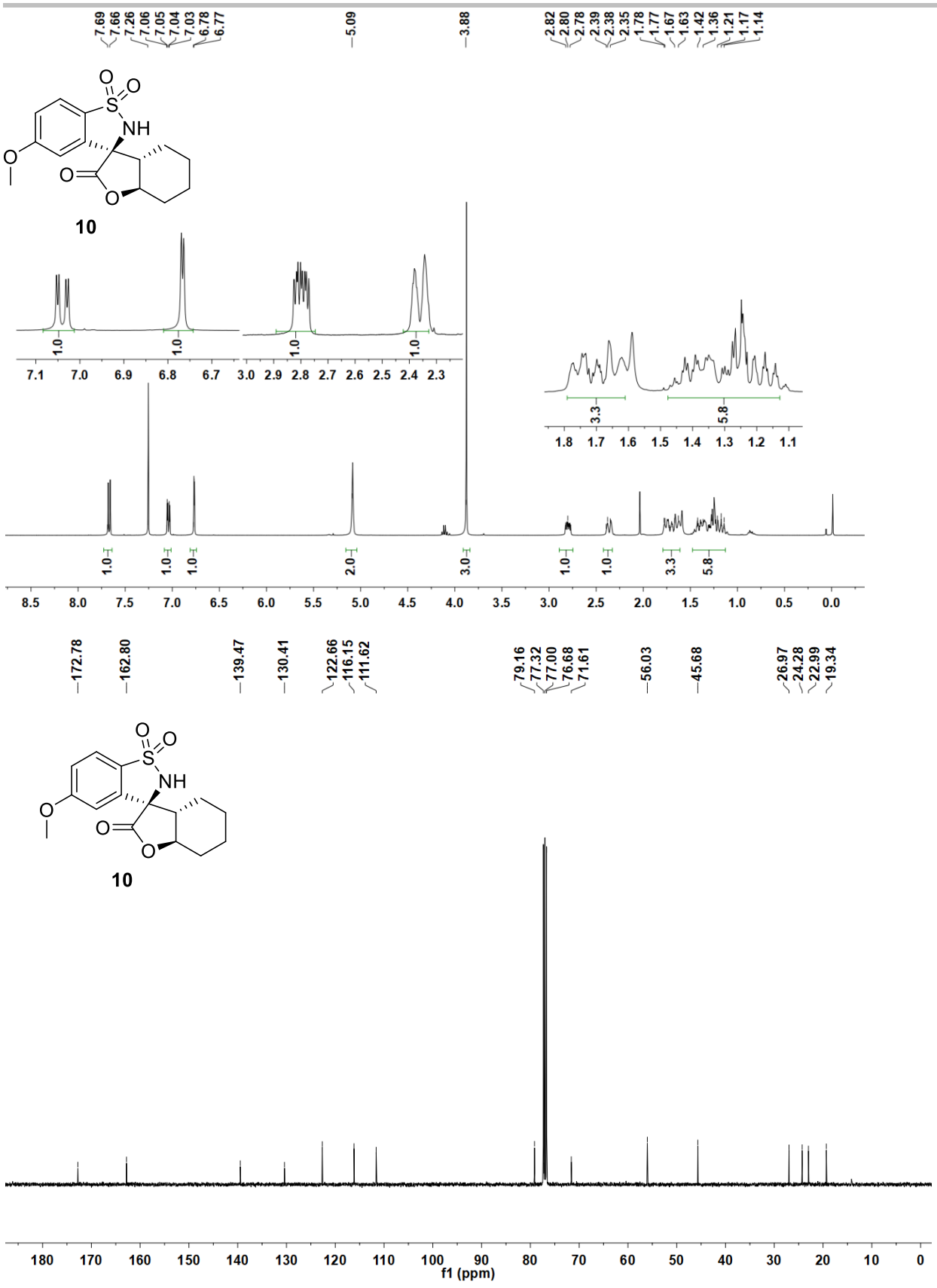
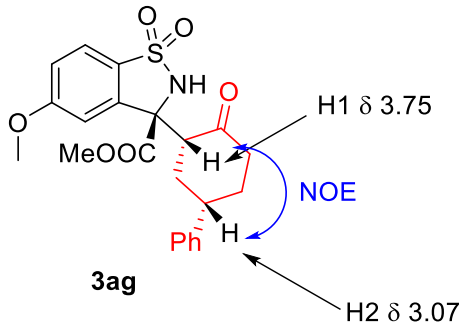
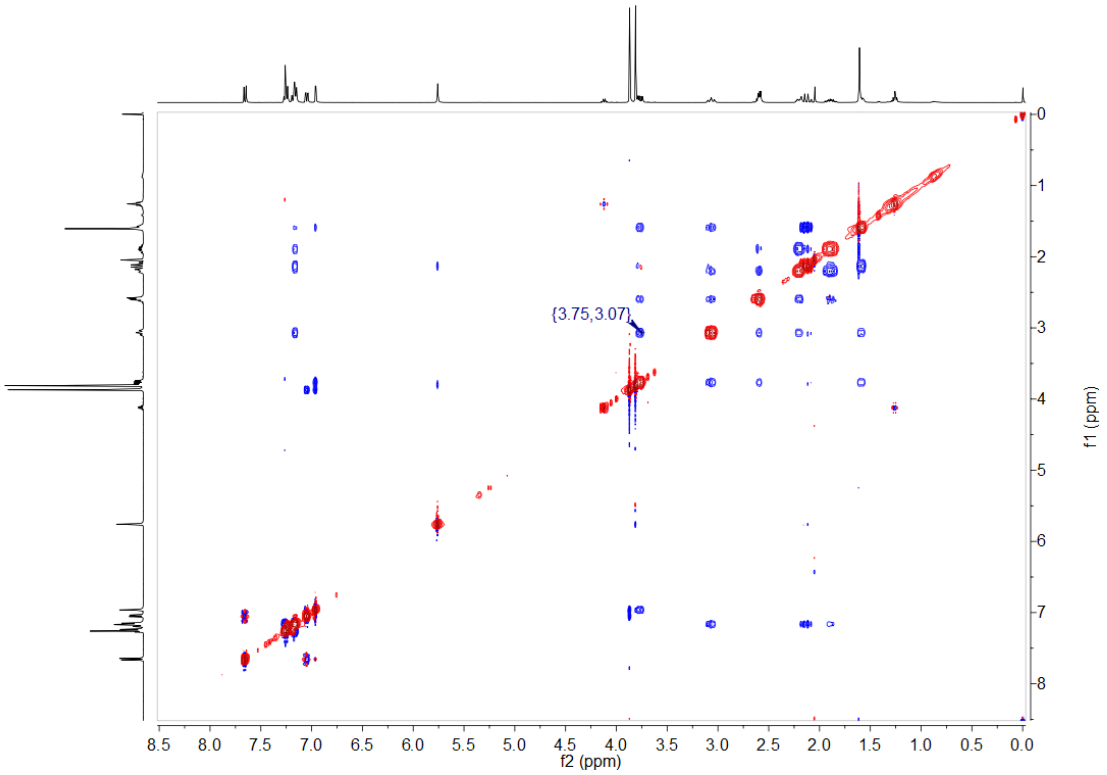
7.58
7.26
7.20
7.20
7.03
7.02
7.01
7.01
5.90
3.88
3.87
3.85
3.84
3.82
2.33
2.31
2.30
1.86
1.84
1.80
1.71
1.45
1.44
1.42
1.31
1.28
1.25
1.23
O
O
S
NH
OH
O
MeOOC
9
1.0
2.35 2.30 2.25
1.0
4.8
1.5 1.4 1.3 1.2 1.1
1.0
1.0
7.20 7.15 7.10 7.05 7.00 6.95
7.0
3.90 3.85 3.80
1.0
3.2
1.90 1.85 1.80 1.75 1.70 1.65
1.0 1.0 1.0 1.0 7.0 1.0 1.0 3.2 1.0 4.8
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
170.87
163.55
141.80
126.06
122.36
116.37
110.35
71.84
70.58
55.81
54.18
52.34
35.65
27.86
25.33
24.60
O
O
S
NH
OH
O
MeOOC
9
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

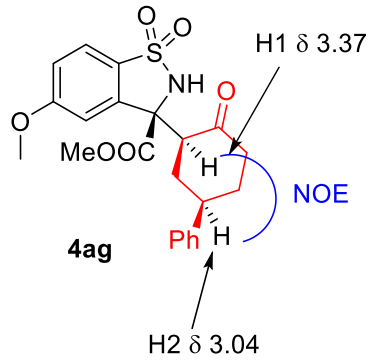

7.69
7.66
7.26
7.06
7.05
7.04
7.03
6.78
6.77
5.09
3.88
2.82
2.80
2.78
2.39
2.38
2.35
1.78
1.77
1.67
1.63
1.42
1.36
1.21
1.17
1.14
O
O
S
NH
O
O
O
10
1.0
1.0
1.0
1.0
7.1
7.0
6.9
6.8
6.7
3.0
2.9
2.8
2.7
2.6
2.5
2.4
2.3
3.3
5.8
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1.0
1.0
1.0
2.0
3.0
1.0
1.0
3.3
5.8
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
172.78
162.80
139.47
130.41
122.66
116.15
111.62
79.16
77.32
77.00
76.68
71.61
56.03
45.68
26.97
24.28
22.99
19.34
O
O
S
NH
O
O
O
10
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



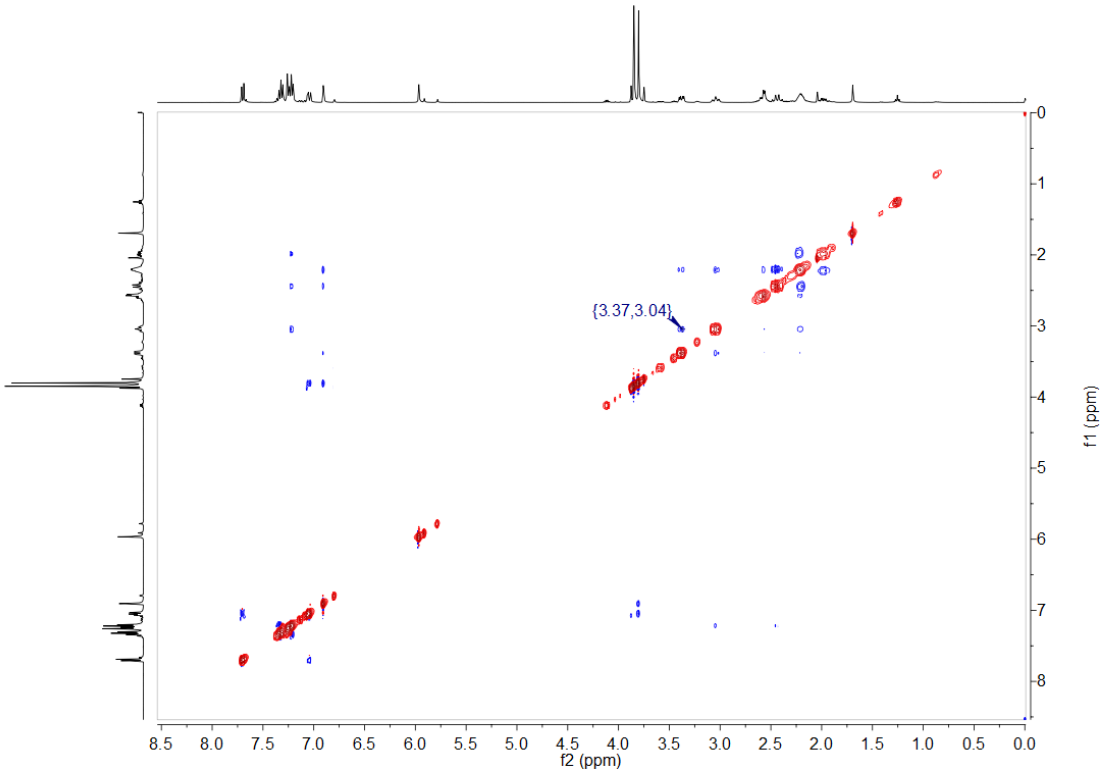
3ag

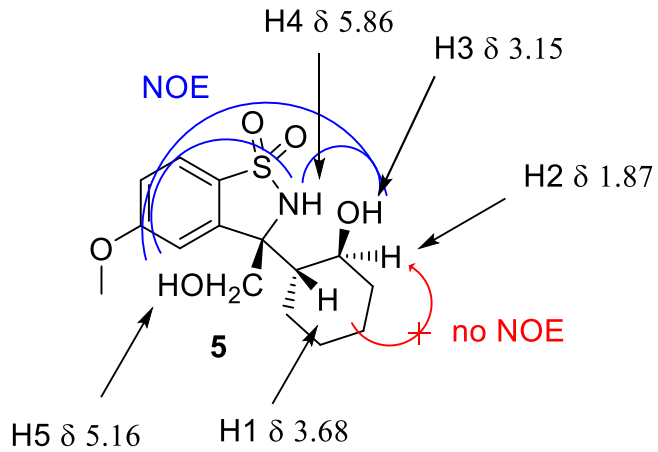
NOESY NMR of **3ag.**



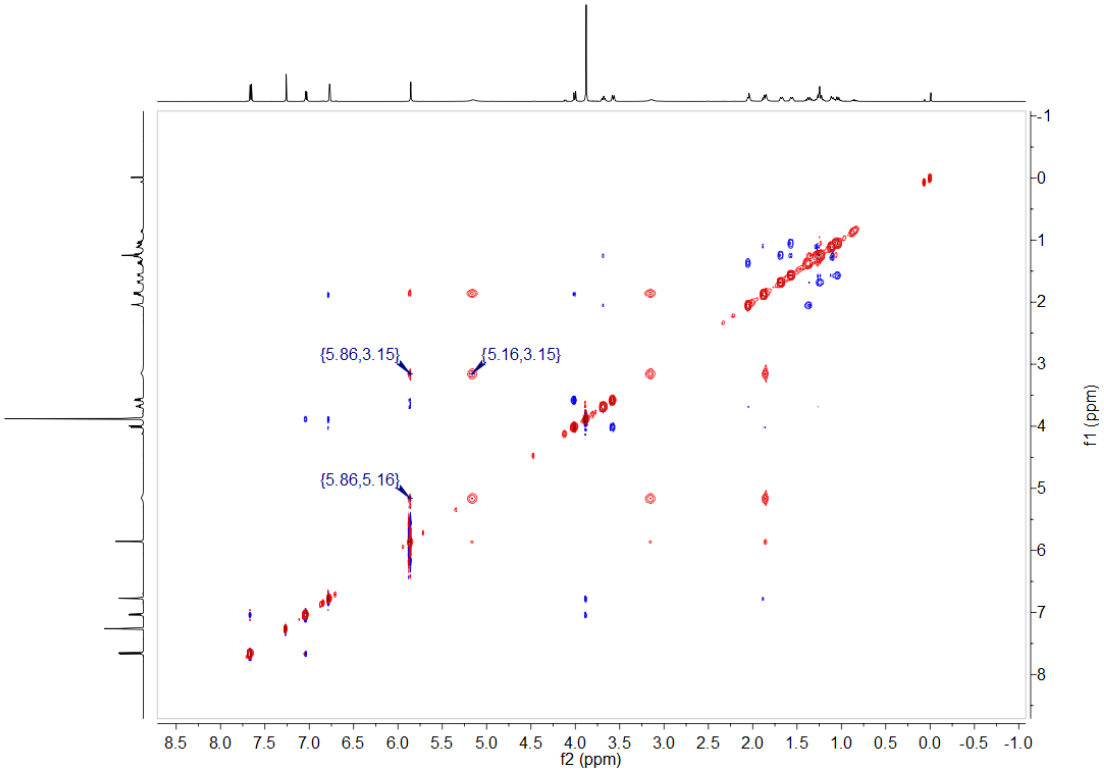


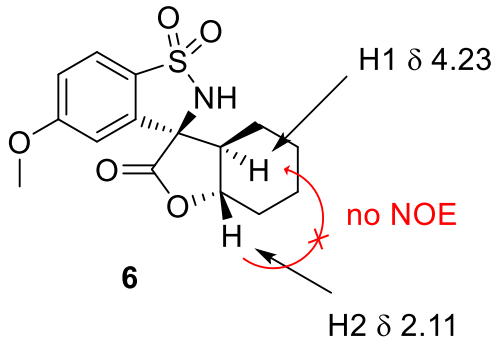
NOESY NMR of **3ag**





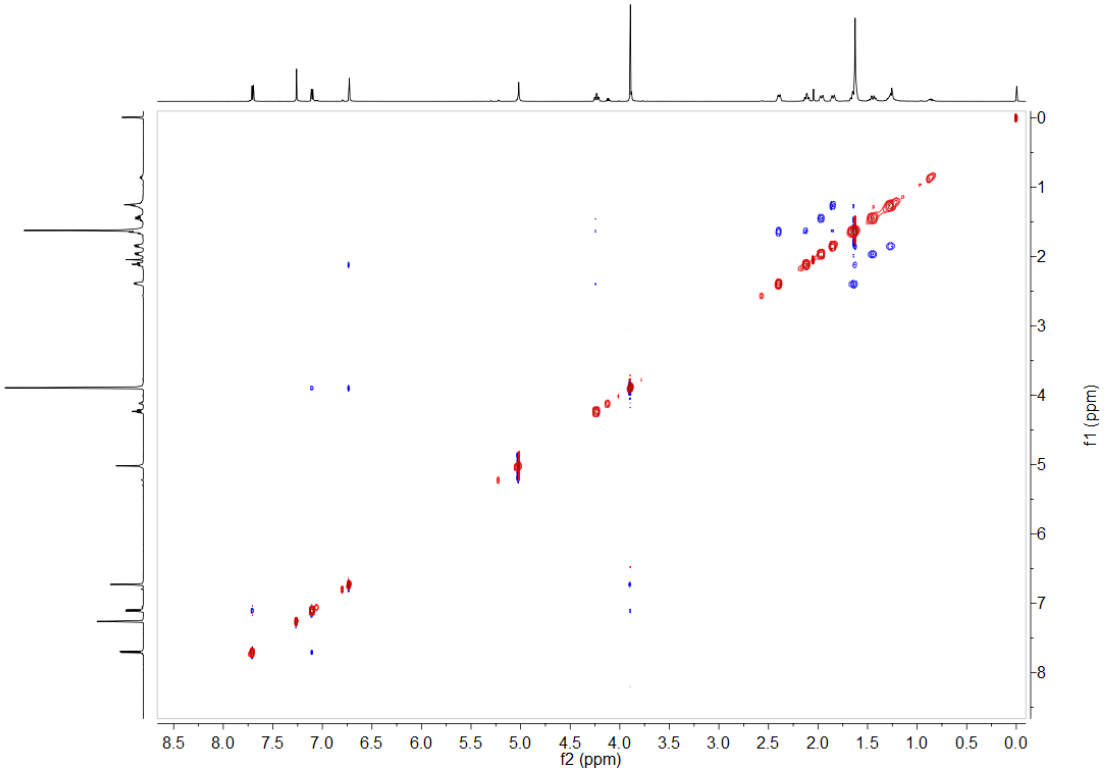
NOESY NMR of **5**

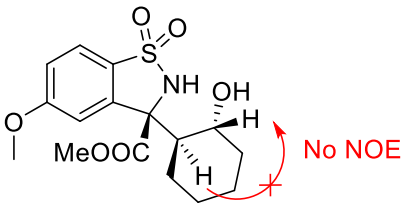




6

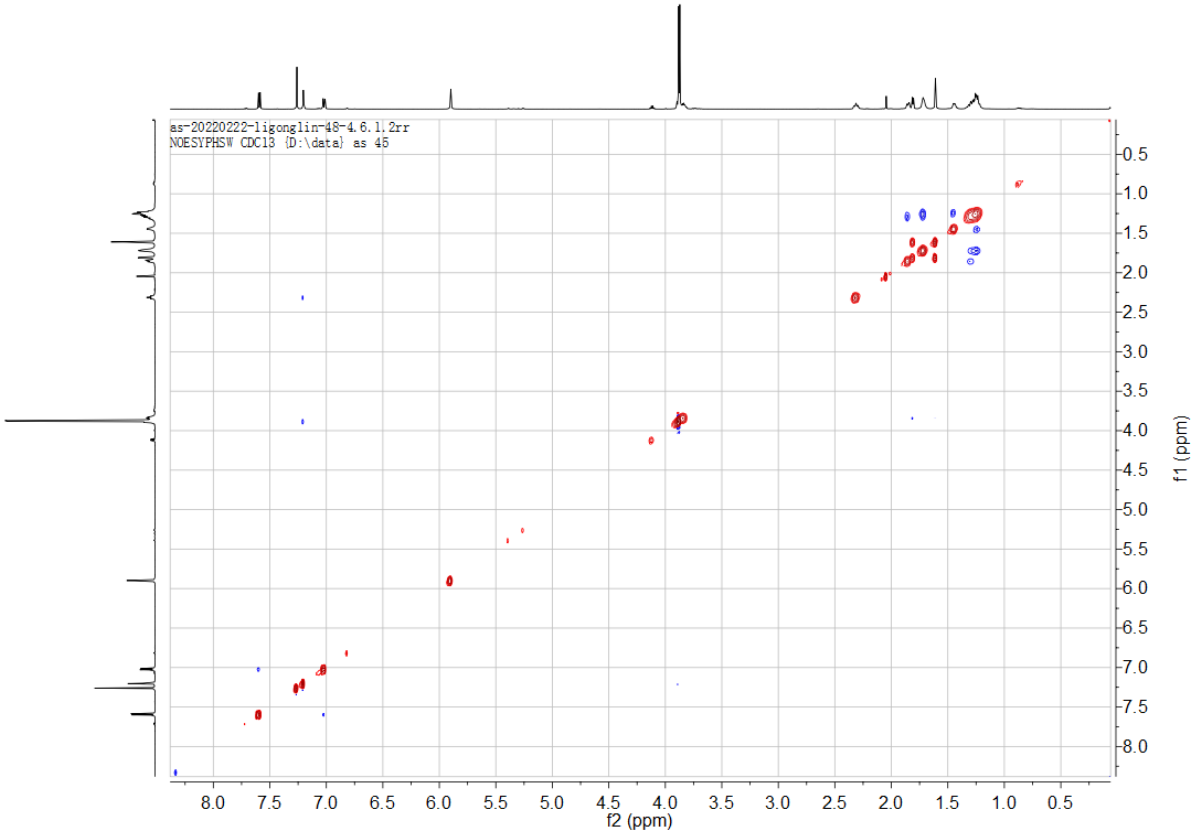
NOESY NMR of **6**





9

NOESY NMR of **9**



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