Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supplementary Information

Rhodium(III)-catalyzed redox-neutral C−H [4+1] annulation of sulfoximines with α,α-difluoromethylene alkynes: Diastereoselective synthesis of *E*-monofluoroalkenyl benzoisothiazole 1-oxides

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1. General Remarks

Sulfoximines,[1] *α,α*-difluoromethylene alkynes,[2] and $Cu(1\text{-}AdCOO)_2$[3] were prepared according to previous synthetic procedures. Other chemicals were purchased from commercial suppliers, and were used without further purification. All the products obtained are analytically pure.

Nuclear magnetic resonance (NMR) spectra recorded on JEOL 400 MHz spectrometers at ambient temperature (25 °C) in either $CDCl_3$ or DMSO-d_6. Abbreviations for data quoted are s, singlet; brs, broad singlet; d, doublet; t, triplet; dd, doublet of doublets; m, multiplet. All NMR-data are reported in parts per million (ppm) relative to the solvent signal ($CDCl_3$: δ_H = 7.26 ppm, δ_C = 77.16 ppm; DMSO-d_6: δ_H = 2.50 ppm, δ_C = 39.52 ppm).

High-resolution mass spectrometry (HRMS) analyses were obtained on an agilent TOF-G6230B mass spectrometer and Thermo-DFS mass spectrometer with positive ion mode.

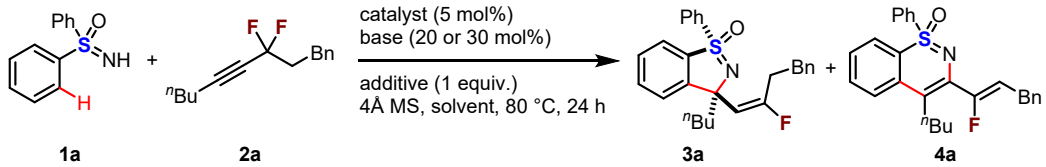
The enantiomeric ratio (e.r.) of the products was determined by high-performance liquid chromatography (HPLC) with a chiral stationary phase in comparison with the authentic racemate sample. The chiral stationary phases Chiralpak IA-3 and IE-3 used in this study were purchased from Daicel Chirsal Technologies.

Thin layer chromatographies (TLC) were conducted on pre-coated silica gel 60 F254 plates (Merck). Silica gel 60H (200-300 mesh) and preparative TLC (200x200 mm, 0.2-0.25 mm in thickness) manufactured by Qingdao Haiyang Chemical Group Co. (China) were used for general chromatography.

Melting points were measured on a Mettler Hanon-MP450 and not corrected.

2. Reaction Optimization

Table S1. Detailed screening of reaction conditions.[a]

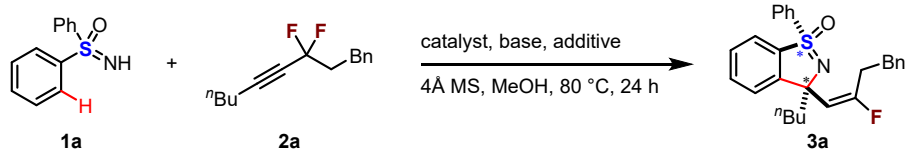


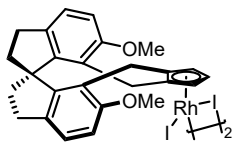
1a **2a** **3a** **4a**

entry	catalyst	base (mol%)	additive	solvent	yield (%)	
					3a (d.r.)	**4a**
1	$[Cp^*RhCl_2]_2$	$AgSbF_6$ (20)	PivOH	MeOH	34 (>20:1)	14
2	$[Cp^*RhCl_2]_2$	$AgSbF_6$ (20)	PivOH	TFE	20 (>20:1)	11
3	$[Cp^*RhCl_2]_2$	$AgSbF_6$ (20)	PivOH	MeCN	23 (>20:1)	10
4	$[Cp^*RhCl_2]_2$	$AgSbF_6$ (20)	PivOH	1,4-dioxane	<1	<1
5	$[Cp^*RhCl_2]_2$	$AgSbF_6$ (20)	PivOH	THF	<1	<1
6	$[Cp^*RhCl_2]_2$	$AgSbF_6$ (20)	PivOH	toluene	24 (>20:1)	13
7	$[Cp^*RhCl_2]_2$	$AgSbF_6$ (20)	PivOH	1,2-DCE	24 (>20:1)	10
8	$[Cp^*RhCl_2]_2$	$AgSbF_6$ (20)	PivOH	DMF	20 (>20:1)	15
9	$[Cp^*RhCl_2]_2$	$AgSbF_6$ (20)	PivOH	DCM	15 (>20:1)	9
10	$[Cp^*RhCl_2]_2$	$AgSbF_6$ (20)	PivOH	acetone	16 (>20:1)	12
11	$[Cp^*RhCl_2]_2$	$AgSbF_6$ (20)	PivOH	HFIP	28 (>20:1)	20
12	$[Cp^*RhCl_2]_2$	$AgSbF_6$ (20)	CsOPiv	MeOH	32 (>20:1)	20
13	$[Cp^*RhCl_2]_2$	$AgSbF_6$ (20)	K_2CO_3	MeOH	<1	<1
14	$[Cp^*RhCl_2]_2$	$AgSbF_6$ (20)	TsOH	MeOH	<1	<1
15	$[Cp^*RhCl_2]_2$	$AgSbF_6$ (20)	HOAc	MeOH	28 (>20:1)	37
16	$[Cp^*RhCl_2]_2$	$AgSbF_6$ (20)	1-AdCOOH	MeOH	35 (>20:1)	26
17	$[Cp^*RhCl_2]_2$	$Cu(AdCOO)_2$ (20)	1-AdCOOH	MeOH	68 (>20:1)	21
18	$[Cp^*RhCl_2]_2$	$Cu(OAc)_2$ (20)	1-AdCOOH	MeOH	53 (>20:1)	15
19	**$[Cp^*RhCl_2]_2$**	**$Cu(1\text{-}AdCOO)_2$ (30)**	**1-AdCOOH**	**MeOH**	**75 (>20:1)**	**22**
further variation from the optimal condition (entry 19)						
20	$[Cp^*IrCl_2]_2$	$Cu(1\text{-}AdCOO)_2$ (30)	1-AdCOOH	MeOH	<1	<1
21	$[Ru(p\text{-cymene})Cl_2]_2$	$Cu(1\text{-}AdCOO)_2$ (30)	1-AdCOOH	MeOH	<1	<1
22	$Pd(OAc)_2$	$Cu(1\text{-}AdCOO)_2$ (30)	1-AdCOOH	MeOH	<1	<1
23	-	$Cu(1\text{-}AdCOO)_2$ (30)	1-AdCOOH	MeOH	<1	<1
24	$[Cp^*RhCl_2]_2$	-	1-AdCOOH	MeOH	35 (>20:1)	26
25	$[Cp^*RhCl_2]_2$	$Cu(1\text{-}AdCOO)_2$ (30)	-	MeOH	53 (>20:1)	28
26[b]	$[Cp^*RhCl_2]_2$	$Cu(1\text{-}AdCOO)_2$ (30)	1-AdCOOH	MeOH	50 (>20:1)	12

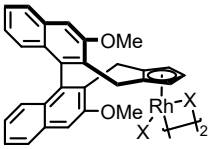
[a]Reaction conditions: **1a** (0.1 mmol), **2a** (1.5 equiv.), catalyst (5 mol%), base, additive (1 equiv.), 4Å MS (100 mg), solvent (1 mL), 80 °C, 24 h, under air; Isolated yields were given and diastereroselective ratios (d.r.) were determined by ^{1}H NMR analysis. [b]No 4Å MS.

Table S2. Preliminary screening of enantioselective reaction.[a]

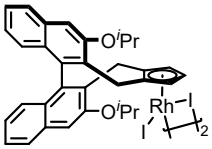




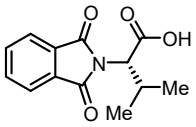
(*R*)-**SCpRh**



X = Cl, (*R*)-**Rh1**
X = I, (*R*)-**Rh2**



(*R*)-**Rh3**



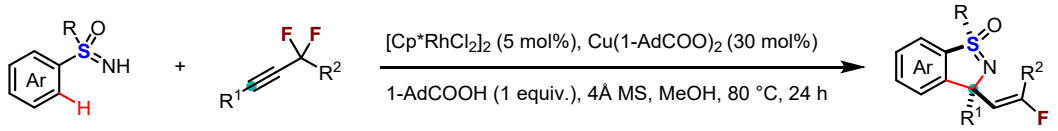
(*S*)-**AA**

entry	catalyst	base	additive (equiv.)	**3a**		
				yield (%)[a]	e.r.[a]	d.r.[a]
1	(*R*)-**SCpRh**	$Cu(1\text{-}AdCOO)_2$	1-AdCOOH (1)	<5	-	-
2	(*R*)-**SCpRh**	$AgSbF_6$	1-AdCOOH (1)	10	72:28	>20:1
3	(*R*)-**SCpRh**	$AgSbF_6$	PivOH (1)	25	81:19	>20:1
4	(*R*)-**SCpRh**	$AgSbF_6$	HOAc (1)	15	58:42	>20:1
5	(*R*)-**SCpRh**	$AgNTf_2$	PivOH (1)	<5	-	-
6	(*R*)-**SCpRh**	$AgSbF_6$	(*R*)-**AA** (0.2)	<5	-	-
7	(*R*)-**SCpRh**	$AgSbF_6$	(*S*)-**AA** (0.2)	15	72:28	>20:1
8	$[Cp^*RhCl_2]_2$	$AgSbF_6$	(*S*)-**AA** (0.2)	20	53:47	>20:1
9	(*R*)-**Rh1**	$AgSbF_6$	PivOH (1)	<5	-	-
10	(*R*)-**Rh2**	$AgSbF_6$	PivOH (1)	<5	-	-
11	(*R*)-**Rh3**	$AgSbF_6$	PivOH (1)	<5	-	-

[a]Reaction conditions: **1a** (0.1 mmol), **2a** (1.5 equiv.), catalyst (5 mol%), base (30 mol%), additive, 4Å MS (100 mg), MeOH (1 mL), 80 °C, 24 h, under air; [b]Isolated yields. [c]Determined by HPLC with a chiral stationary phase. [d]determined by ^1H NMR analysis.

3. General Procedure

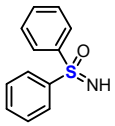
General procedure for rhodium(III)-catalyzed redox-neutral C−H [4+1] annulation of sulfoximines with α,α-difluoromethylene alkynes



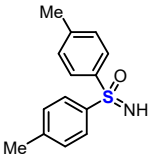
1 **2** **3**

A dry 5 mL vial equipped with a Teflon™-coated stirring bar, was charged with a solution of sulfoximines **1** (0.2 mmol, 1.0 equiv.), *α,α*-difluoromethylene alkynes **2** (0.3 mmol, 1.5 equiv.), $[Cp^*RhCl_2]_2$ (3.1 mg, 0.01 mmol, 0.05 equiv.), $Cu(1\text{-}AdCOO)_2$ (12.7 mg, 0.06 mmol, 0.3 equiv.), 1-AdCOOH (18 mg, 0.1 mmol, 1.0 equiv.) and 4Å MS (100 mg) in dry methanol (1.0 mL). The vial was closed with a screw cap and stirred at 80 °C (oil bath) for 24 h under air. Once completed, the mixture was diluted with EtOAc (2×2 mL) and filtered through a short silica gel column (200-300 mesh). The volatiles in the filtrate were removed by a rotary evaporator under reduced pressure and the residue was purified by preparative TLC (eluent: petroleum ether/dichloromethane) to yield products **3**.

4. Substrate List



1a



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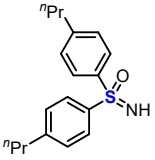

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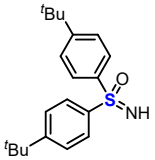
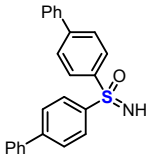
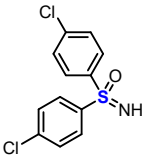


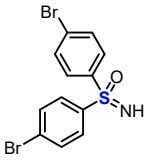
1d



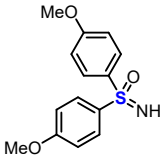
1e



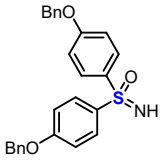
1f



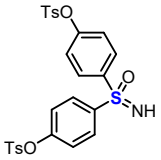
1g



1h



1i



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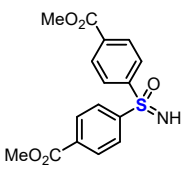

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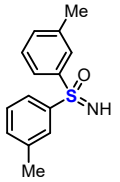
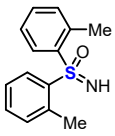
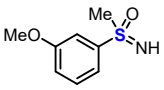


1l



1m

1n



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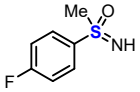

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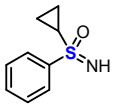
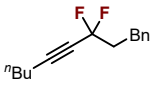


1q

1r



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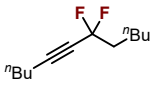

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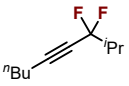

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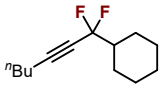

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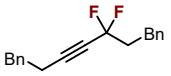
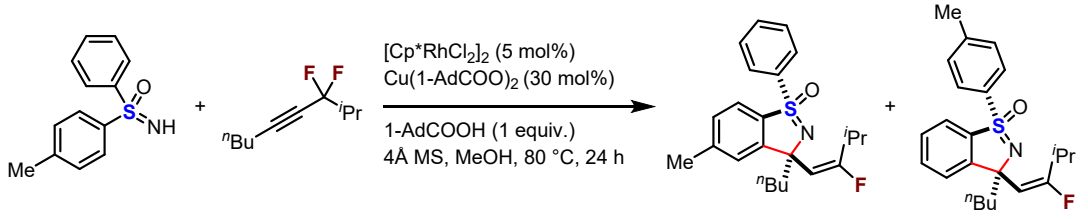


2e

5. Attempt of Unsymmetric Biaryl Sulfoximines



1r **2c** *an inseperable regioselctive mixture of 1:1*

A dry 5 mL vial equipped with a Teflon™-coated stirring bar, was charged with a solution of sulfoximine **1r** (46.2 mg, 0.2 mmol, 1.0 equiv.), *α,α*-difluoromethylene alkyne **2c** (52.2 mg, 0.3 mmol, 1.5 equiv.), $[Cp^*RhCl_2]_2$ (3.1 mg, 0.01 mmol, 0.05 equiv.), $Cu(1\text{-}AdCOO)_2$ (12.7 mg, 0.06 mmol, 0.3 equiv.), 1-AdCOOH (18 mg, 0.1 mmol, 1.0 equiv.) and 4Å MS (100 mg) in dry methanol (1.0 mL). The vial was closed with a screw cap and stirred at 80 °C (oil bath) for 24 h under air. Once completed, the mixture was diluted with EtOAc (2×2 mL) and filtered through a short silica gel column (200-300 mesh). The volatiles in the filtrate were removed by a rotary evaporator under reduced pressure and the residue was purified by preparative TLC (eluent: petroleum ether/dichloromethane) to give an inseparable regioselective mixture of 1:1 in a total yield of xx (10.8 mg, 0.025 mmol).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (d, *J* = 7.8 Hz, 2H), 7.86 (d, *J* = 8.2 Hz, 2H), 7.59–7.45 (m, 9H), 7.21 (d, *J* = 7.9 Hz, 1H), 5.43 (d, *J* = 5.5 Hz, 1H), 5.36 (d, *J* = 5.6 Hz, 1H), 3.82–3.59 (m, 2H), 2.45 (d, *J* = 11.0 Hz, 6H), 2.13–2.05 (m, 2H), 1.72–1.61 (m, 6H), 1.43–1.38 (m, 4H), 1.12 (d, *J* = 6.9 Hz, 6H), 1.01–0.92 (m, 12H) ppm.

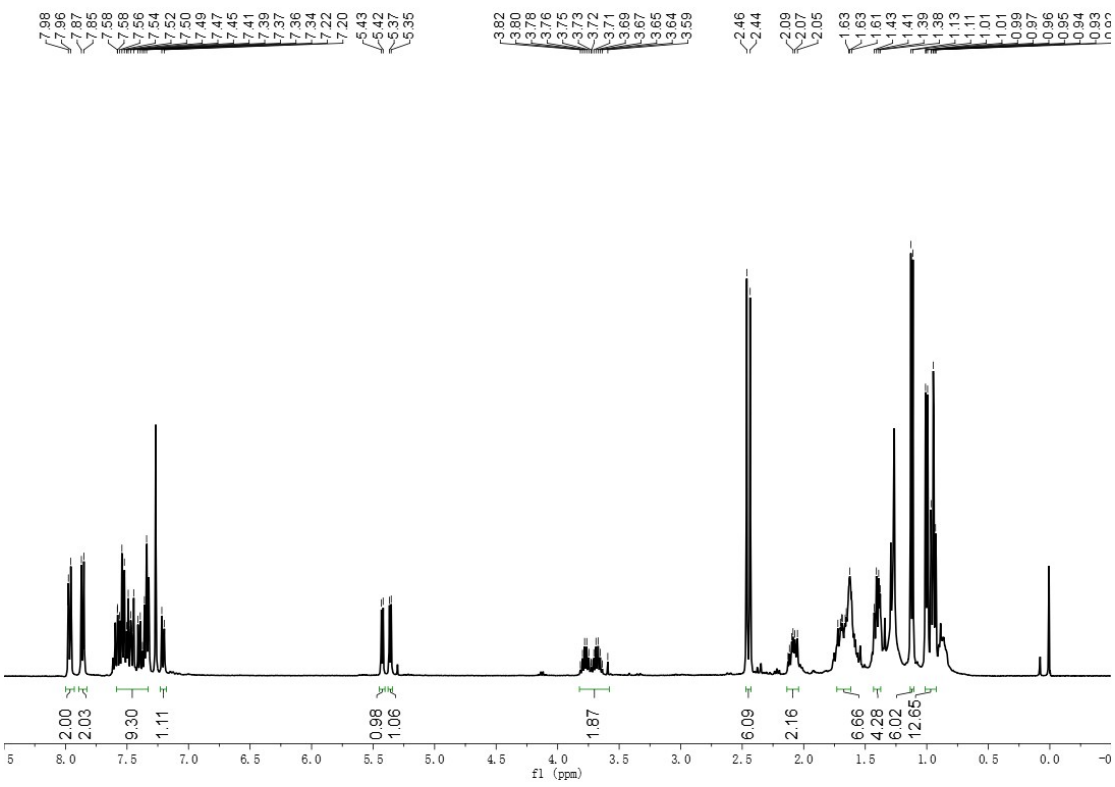
^{13}C NMR (100 MHz, $CDCl_3$): δ 167.71, 167.67, 165.18, 165.15, 153.43, 153.41, 152.61, 152.59, 144.46, 143.79, 140.56, 138.31, 137.05, 135.37, 133.26, 132.56, 130.15, 129.99, 129.87, 129.61, 129.23, 129.00, 123.73, 123.37, 122.42, 122.25, 110.02, 109.96, 109.76, 109.71, 74.41, 74.28, 74.25, 74.12, 44.35, 44.33, 29.84, 27.55, 27.53, 27.38, 27.37, 27.28, 23.20, 23.19, 21.90, 21.67, 19.17, 19.14, 18.72, 18.69, 14.21 ppm (the split and coupling constant are difficult to distinguish).

^{19}F NMR (376 MHz, $CDCl_3$): δ -113.54 – -113.36 (m) ppm.

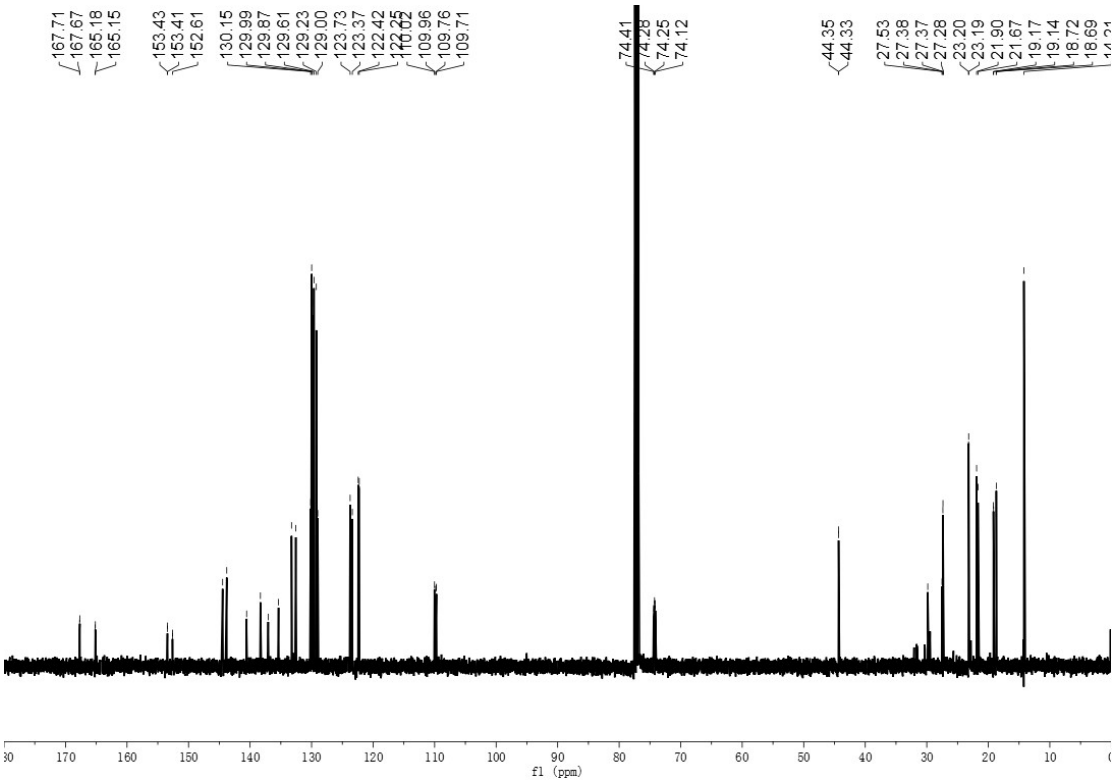
HRMS (ESI) *m*/*z*: $[M+Na]^+$ Calcd for $C_{23}H_{28}FNOSNa$: 408.1773; Found: 408.1756.

The copies of NMR and HRMS spectra are listed below.

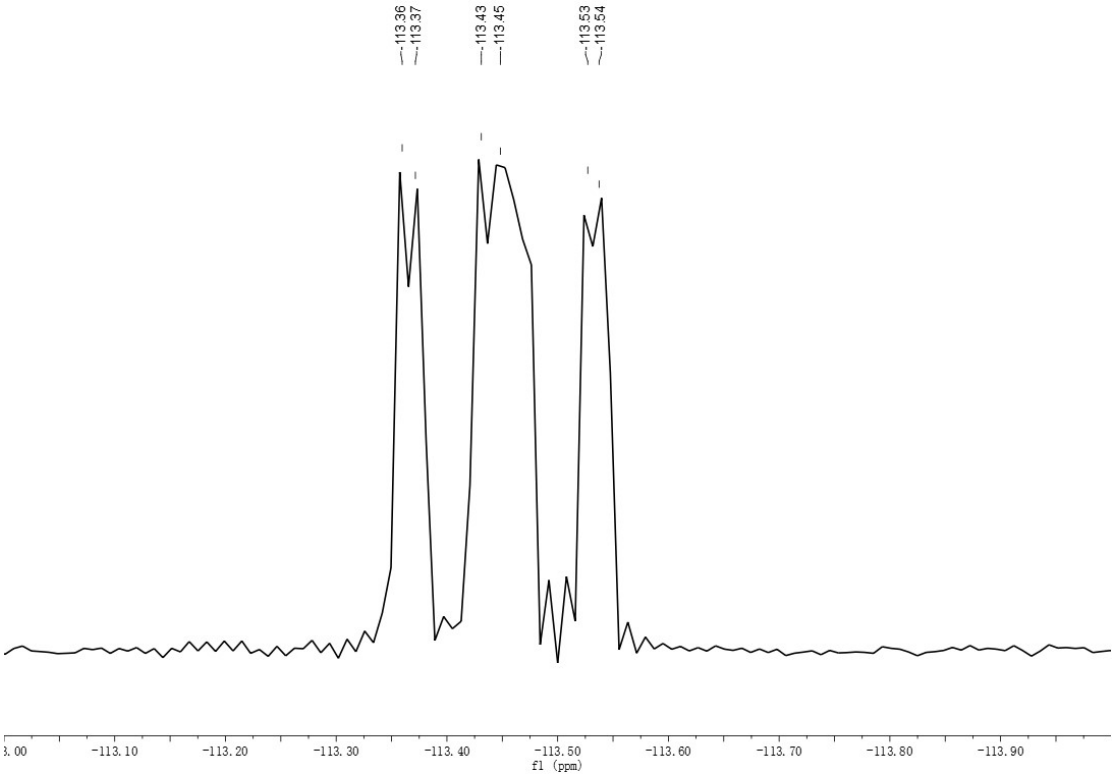
^{1}H NMR (400 MHz, $CDCl_3$)



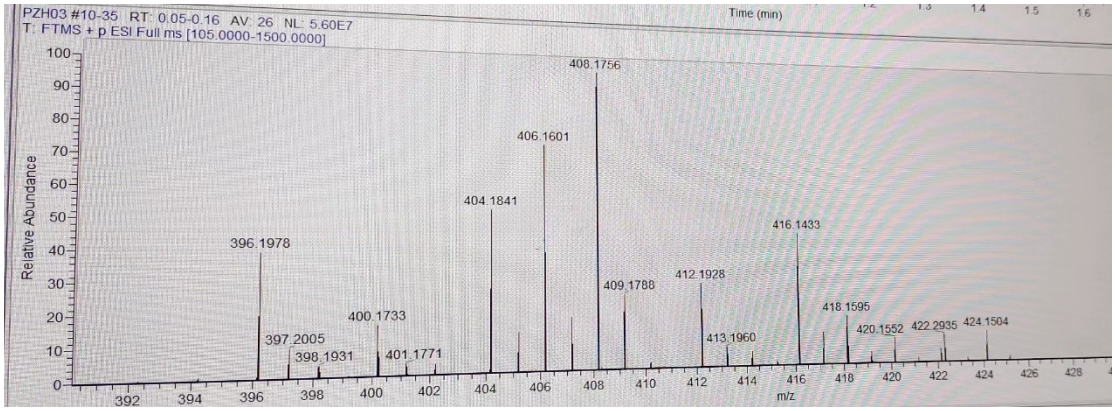
^{13}C NMR (100 MHz, $CDCl_3$)



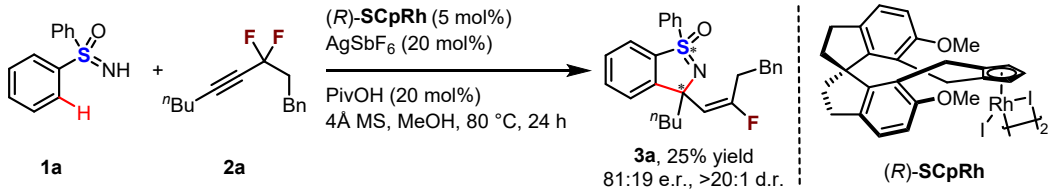
^{19}F NMR (376 MHz, $CDCl_3$)



HRMS spectrum

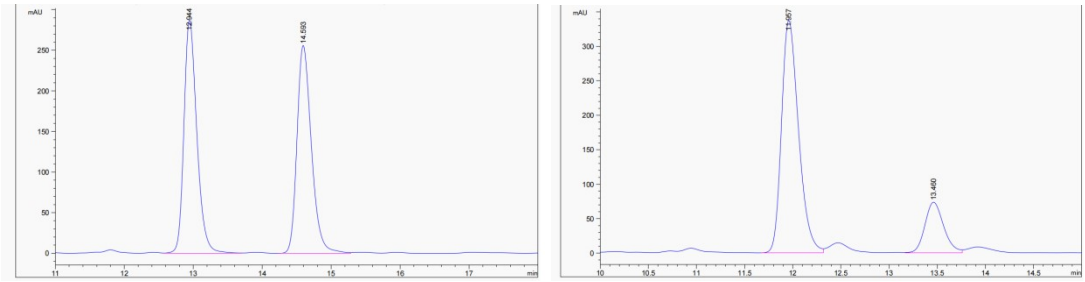


6. Preliminary Asymmetric Attempt



A dry 5 mL vial equipped with a Teflon™-coated stirring bar, was charged with a solution of **1a** (21.7 mg, 0.1 mmol, 1 equiv.) and **2a** (35.4 mg, 0.15 mmol, 1.5 equiv.), (*R*)-**SCpRh** (3.8 mg, 0.005 mmol, 0.05 equiv.), $AgSbF_6$ (6.9 mg, 0.02 mmol, 0.2 equiv.), PivOH (10.2 mg, 0.1 mmol, 1 equiv.) and 4Å MS (100 mg) in dry methanol (1 mL) The reaction mixture was stirred at 80 °C for 24 h under air. Once completed, the mixture was diluted with EtOAc (2×2 mL) and filtered through a short silica gel column (200-300 mesh). The volatiles in the filtrate were removed by a rotary evaporator under reduced pressure and the residue was purified by preparative TLC (eluent: petroleum ether/dichloromethane) to obtain the product **3a** in 25% yield (10.8 mg, 0.025 mmol) with 81:19 enantioselective ratio.

HPLC conditions: Daicel Chiralpak IE-3 column (90:10 hexane: 2-propanol, 1.0 mL/min, 30 °C, 254 nm); t_R (major) = 11.9 min, t_R (minor) = 13.4 min, 81:19 e.r..

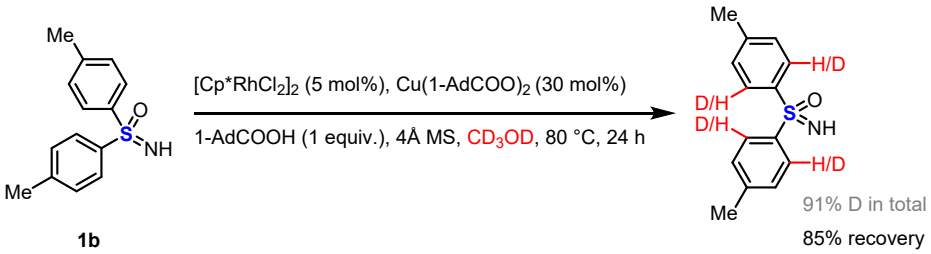


No.	Time	Area	Area (%)
1	12.944	3743.82568	50.1518
2	14.593	3721.16357	49.8482

No.	Time	Area	Area (%)
1	11.957	4163.96826	80.6668
2	13.460	997.96509	19.3332

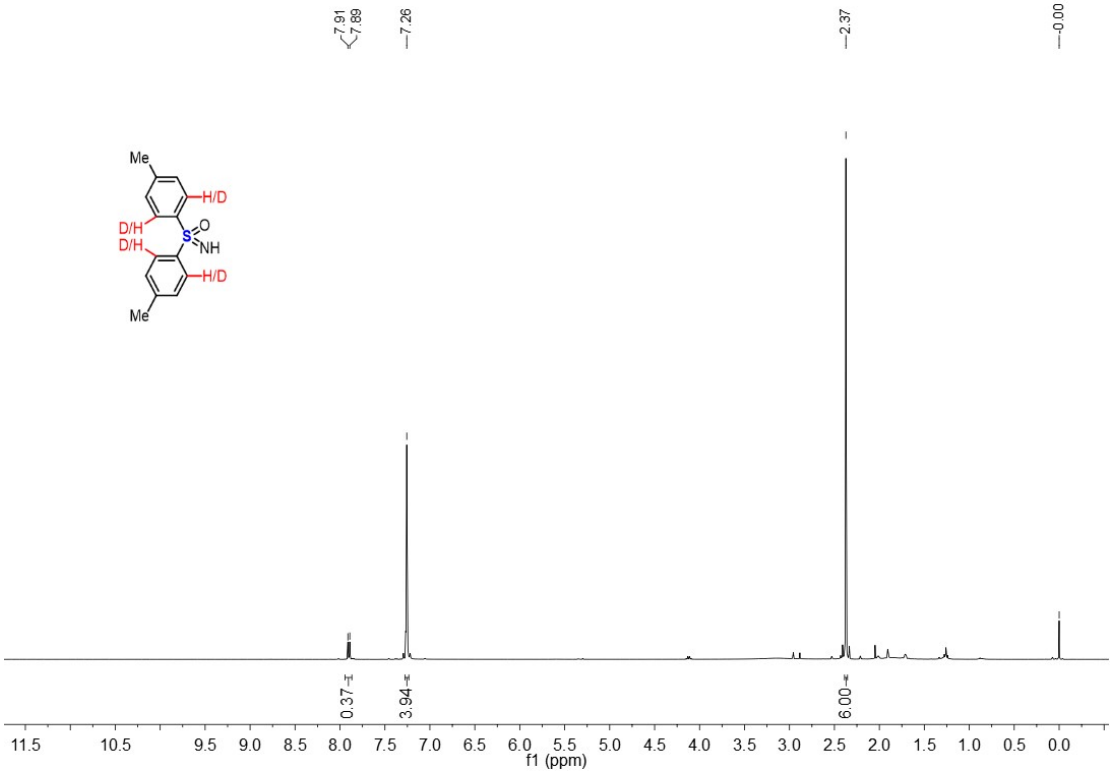
7. Mechanistic Investigation

Reversibility of C−H activation:

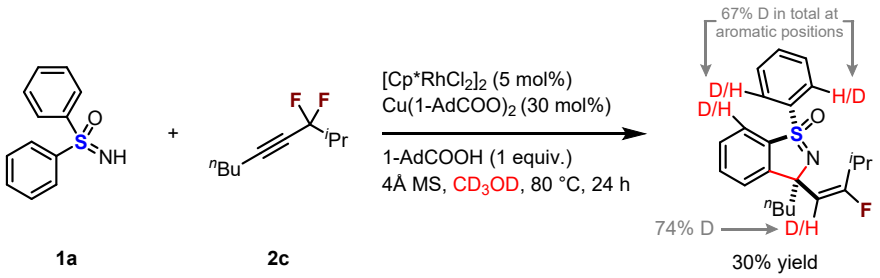


1b

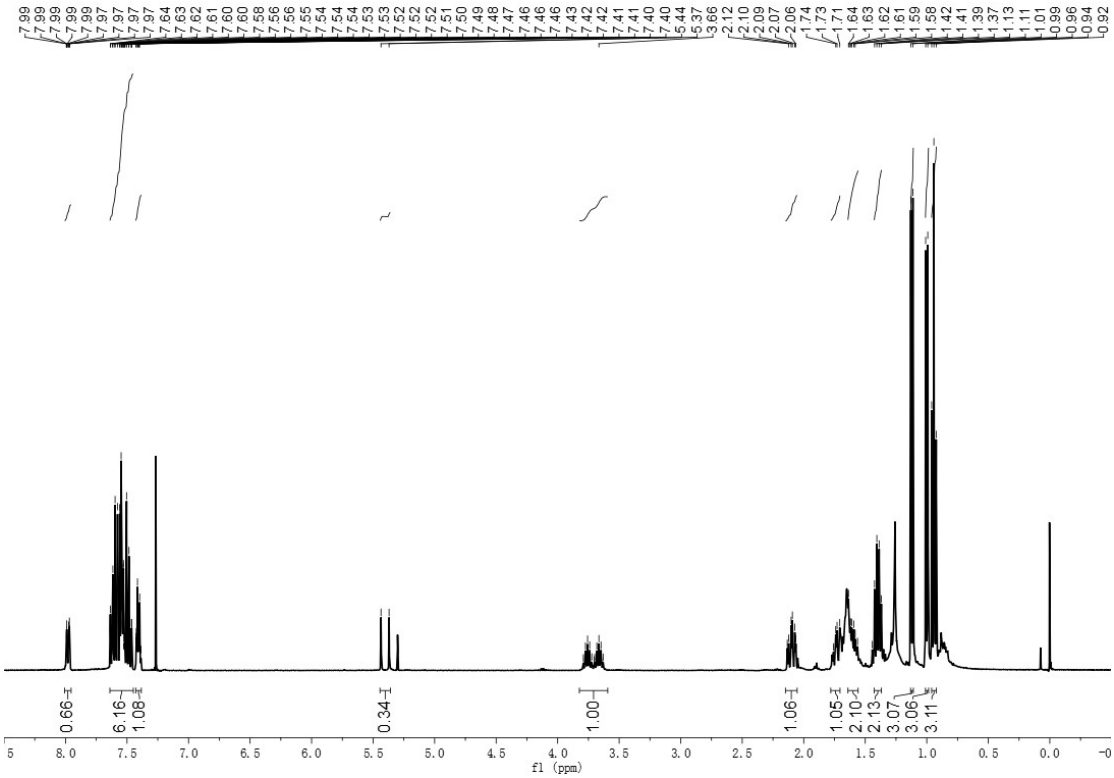
A dry 5 mL vial equipped with a Teflon™-coated stirring bar, was charged with a solution of sulfoximine **1b** (24.5 mg, 0.1 mmol, 1.0 equiv.), $[Cp^*RhCl_2]_2$ (3.1 mg, 0.005 mol, 0.05 equiv.), $Cu(1\text{-}AdCOO)_2$ (12.7 mg, 0.03 mol, 0.3 equiv.), 1-AdCOOH (18.0 mg, 0.1 mmol, 1.0 equiv.) and 4Å MS (50 mg) in CD_3OD (0.5 mL). The vial was closed with a screw cap and stirred at 80 °C for 24 h under air. Once completed, the mixture was diluted with EtOAc (2×2 mL) and filtered through a short silica gel column (200-300 mesh). The volatiles in the filtrate were removed by a rotary evaporator under reduced pressure and the residue was purified by preparative TLC (eluent: petroleum ether/dichloromethane) to yield the product, which was analyzed via ^1H NMR spectroscopy (in $CDCl_3$). We observed a total 91% deuterium at the *ortho*-positions.



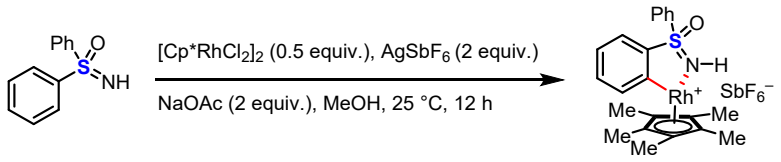
Involvement of protonolysis step:



A dry 5 mL vial equipped with a Teflon™-coated stirring bar, was charged with a solution of sulfoximines **1a** (43.4 mg, 0.2 mmol, 1.0 equiv.), *α,α*-difluoromethylene alkynes **2c** (52.2 mg, 0.3 mmol, 1.5 equiv.), $[Cp^*RhCl_2]_2$ (6.2 mg, 0.01 mol, 0.05 equiv.), $Cu(1\text{-}AdCOO)_2$ (25.4 mg, 0.06 mol, 0.3 equiv.), 1-AdCOOH (36.0 mg. 0.2 mmol, 1.0 equiv.) and 4Å MS (100 mg) in CD_3OD (1.0 mL), and the resulting mixture was stirred at 80 °C (oil bath) for 24 h under air. Once completed, the mixture was diluted with EtOAc (2×2 mL) and filtered through a short silica gel column (200-300 mesh). The volatiles in the filtrate were removed by a rotary evaporator under reduced pressure and the residue was purified by preparative TLC (eluent: petroleum ether/dichloromethane) to give the product (22.3 mg, 0.06 mmol, 30% yield), which was analyzed by ^1H NMR spectroscopy (in $CDCl_3$). We observed a 66% deuterium at the vinylic position and a total 67% deuterium at the aromatic *ortho*-positions.

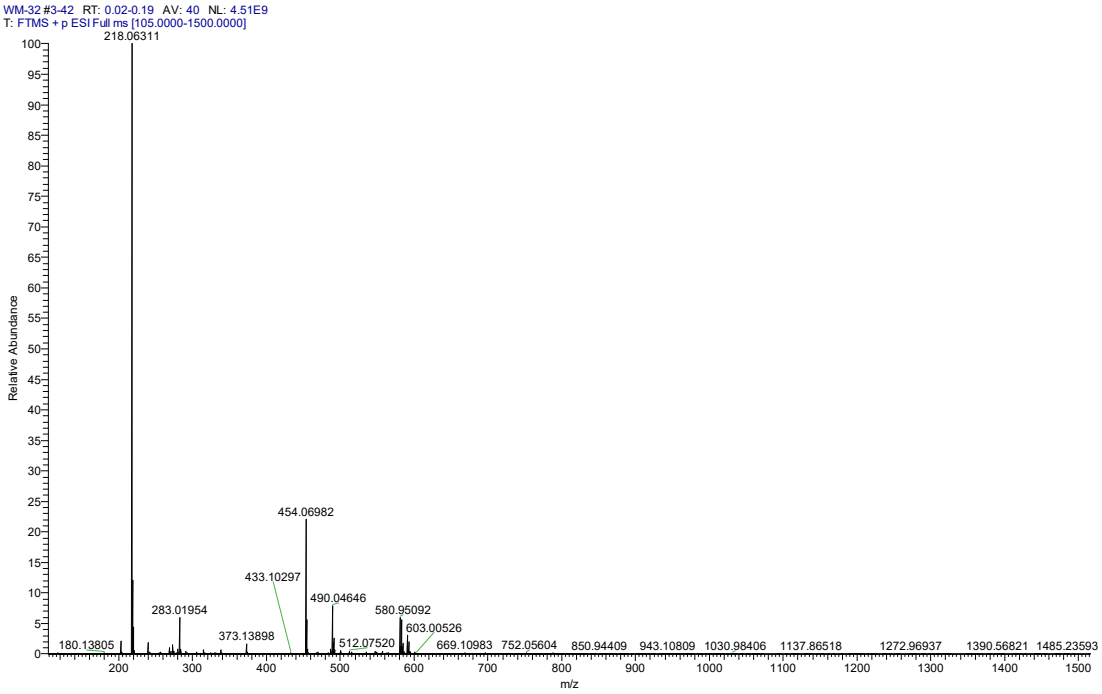


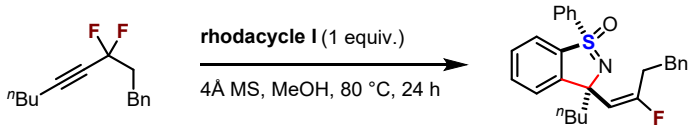
Identification of rhodacycle I as a catalytically active intermediate:



1a **rhodacycle I**

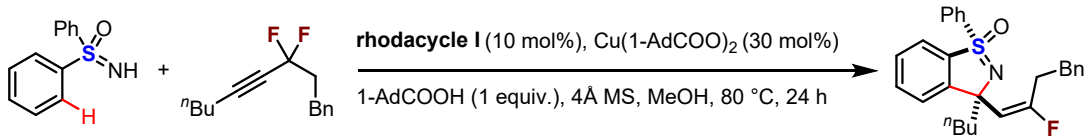
Synthesis of **rhodacyclic I** complex:[4] A dry 5 mL vial equipped with a Teflon™-coated stirring bar, was charged with a solution of **1a** (21.7 mg, 0.2 mmol), $[Cp^*RhCl_2]_2$ (3.1 mg, 0.1 mmol, 0.5 equiv.), $AgSbF_6$ (137.4 mg, 0.4 mmol, 2 equiv.), NaOAc (32.8 mg, 0.4 mmol, 2 equiv.) in dry methanol (4 mL) The reaction mixture was stirred at 25°C for 12 h under air. Once completed, the mixture was diluted with EtOAc (2×2 mL) and filtered through a short column of celite. The volatiles in the filtrate were removed by a rotary evaporator under reduced pressure. The **rhodacycle I** complex was obtained and used for the next catalytic setup without further purification. The HRMS analysis of the obtained residue indicates this rhodacycle intermediate: **HRMS (ESI)** calcd. for $C_{22}H_{25}NORhS^+$ $[M–SbF_6]^+$ 454.0706; found 454.0698.





2a **3a**, 45%, >20:1 d.r.

A dry 5 mL vial equipped with a Teflon™-coated stirring bar, was charged with a solution of the above obtained **rhodacycle I** (18.0 mg, 0.05 mmol, 1 equiv.), **2a** (14.1 mg, 0.075 mmol, 1.5 equiv.) and 4Å MS (50 mg) in dry methanol (0.5 mL) The reaction mixture was stirred at 80 °C for 24 h under air. Once completed, the mixture was diluted with EtOAc (2×2 mL) and filtered through a short silica gel column (200-300 mesh). The volatiles in the filtrate were removed by a rotary evaporator under reduced pressure and the residue was purified by preparative TLC (eluent: petroleum ether/dichloromethane) to give the product **3a** in 45% yield (9.7 mg, 0.023 mmol). This result supports the intermediacy of a rhodacycle in this conversion.



1a **2a** **3a**
60%, >20:1 d.r.

A dry 5 mL vial equipped with a Teflon™-coated stirring bar, was charged with a solution of the above obtained **rhodacycle I** (6.9 mg, 0.01 mol, 0.1 equiv.), **1a** (21.7 mg, 0.1 mmol, 1 equiv.) and **2a** (35.4 mg, 0.15 mmol, 1.5 equiv.), $Cu(1\text{-}AdCOO)_2$ (12.7 mg, 0.03 mol, 0.3 equiv.), 1-AdCOOH (18.0 mg, 0.1 mmol, 1 equiv.) and 4Å MS (100 mg) in dry methanol (1 mL) The reaction mixture was stirred at 80 °C for 24 h under air. Once completed, the mixture was diluted with EtOAc (2×2 mL) and filtered through a short silica gel column (200-300 mesh). The volatiles in the filtrate were removed by a rotary evaporator under reduced pressure and the residue was purified by preparative TLC (eluent: petroleum ether/dichloromethane) to give the product **3a** in 60% yield (26.0 mg, 0.06 mmol). This result supports the intermediacy of a rhodacycle in this conversion.

8. DFT Calculations

Computational details:

Density functional theory (DFT) calculations were carried out using Gaussian 09 program[5]. Geometry optimizations and frequency analyses were performed at the level of the B3LYP functional[6] with a standard 6-31G(d) basis set (lanl2dz basis set[7] for Rh). Single point energies were further refined at the TPSS[8] functional with a standard 6-311++G(d,p) basis set (SDD basis set for Rh) level using SMD[9] solvation model (solvent =MeOH). Throughout the paper, the energies presented are the TPSS-calculated Gibbs free energies in MeOH solvent with B3LYP-calculated thermodynamic corrections. And the calculated NPA charge distribution for **INT-1** follows the above method.

Various energy values for all of the relevant species [optimized at the level of B3LYP/6-31G(d) (lanl2dz for Rh) as well as the single-point results at the level of TPSS/6-311++G(d,p) (SDD for Rh) with SMD atomic radii for experimental solvent MeOH]:

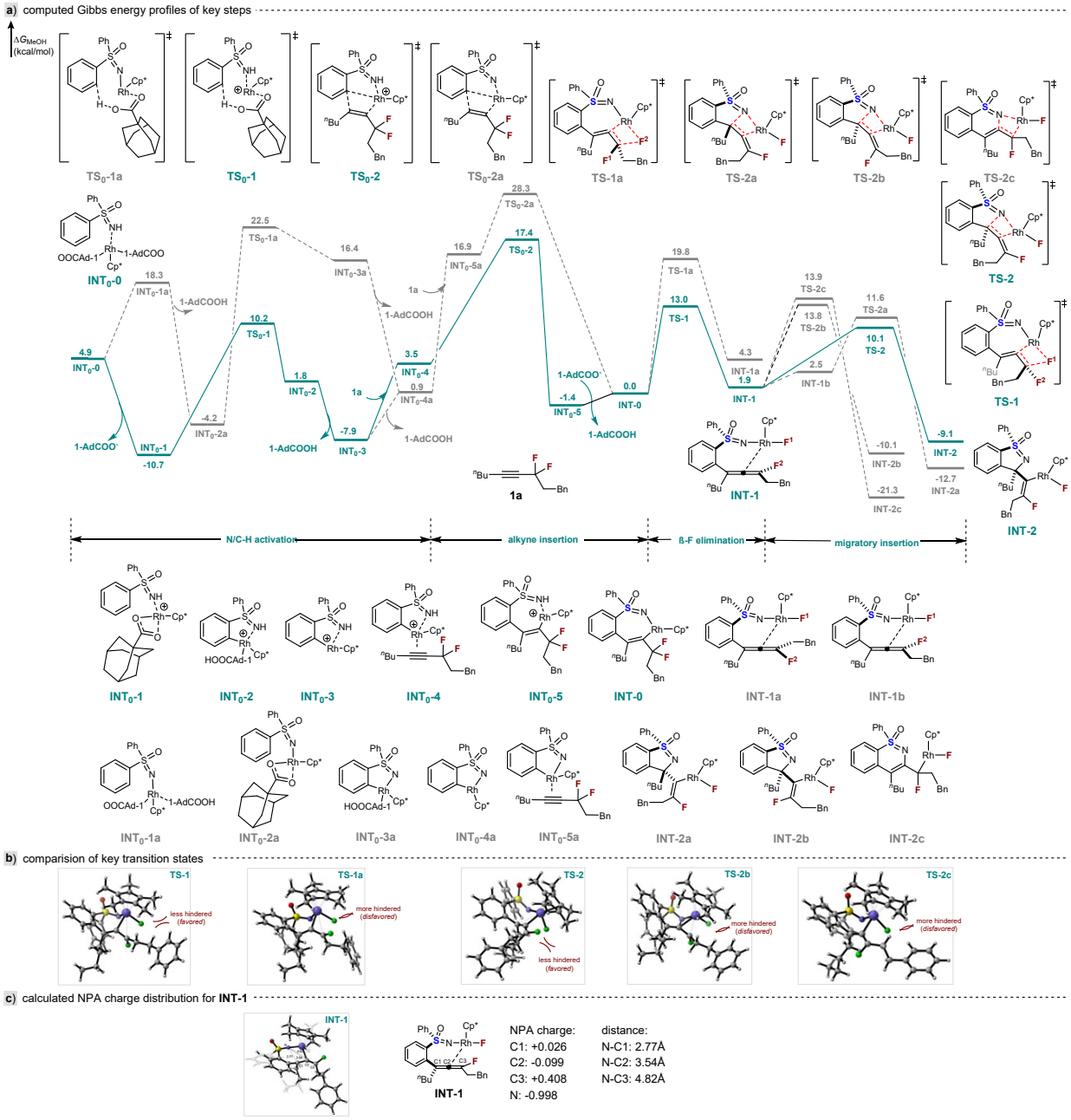
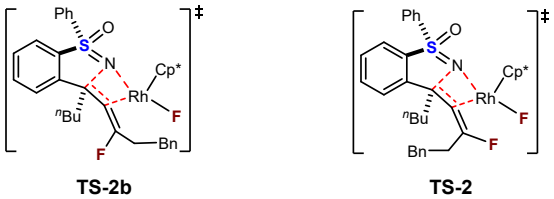


Figure S1. Detailed computational mechanistic investigations.

Table S3. Compared the key structures and the reaction barriers using different basis-sets.



TS-2b **TS-2**

	△*G*(**TS-2b**)-△*G*(**TS-2**) (kcal/mol)
OPT: **B3LYP**/6-31G(d)+ SDD for Rh SP: SMD(MeOH) TPSSTPSS /6-311++G(d,p)+SDD for Rh	3.8

OPT: **B3LYP-D3**/6-31G(d)+ SDD for Rh SP: SMD(MeOH) TPSSTPSS /6-311++G(d,p)+SDD for Rh	1.9
OPT: **M11L**/6-31G(d)+ SDD for Rh SP: SMD(MeOH) TPSSTPSS /6-311++G(d,p)+SDD for Rh	2.8
OPT: **M062X**/6-31G(d)+ SDD for Rh SP: SMD(MeOH) TPSSTPSS /6-311++G(d,p)+SDD for Rh	3.3

INT_0-0

Zero-point correction= 0.925544 (Hartree/Particle)
Thermal correction to Energy= 0.975469
Thermal correction to Enthalpy= 0.976413
Thermal correction to Gibbs Free Energy= 0.839767
Sum of electronic and zero-point Energies= -2648.057673
Sum of electronic and thermal Energies= -2648.007748
Sum of electronic and thermal Enthalpies= -2648.006804
Sum of electronic and thermal Free Energies= -2648.143450
SCF Done: E(RTPSS-TPSS) = -2651.08300468 A.U. after 35 cycles
NFock= 35 Conv=0.31D-08 -V/T= 2.0309
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.41
(included in total energy above)

INT_0-1

Zero-point correction= 0.678128 (Hartree/Particle)
Thermal correction to Energy= 0.716783
Thermal correction to Enthalpy= 0.717727
Thermal correction to Gibbs Free Energy= 0.605765
Sum of electronic and zero-point Energies= -2069.445823
Sum of electronic and thermal Energies= -2069.407168
Sum of electronic and thermal Enthalpies= -2069.406224
Sum of electronic and thermal Free Energies= -2069.518186
SCF Done: E(RTPSS-TPSS) = -2071.99215118 A.U. after 18 cycles
NFock= 18 Conv=0.58D-08 -V/T= 2.0387
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.75
(included in total energy above)

TS_0-1

Zero-point correction= 0.672456 (Hartree/Particle)
Thermal correction to Energy= 0.710643
Thermal correction to Enthalpy= 0.711587
Thermal correction to Gibbs Free Energy= 0.601750

Sum of electronic and zero-point Energies= -2069.407330
Sum of electronic and thermal Energies= -2069.369142
Sum of electronic and thermal Enthalpies= -2069.368198
Sum of electronic and thermal Free Energies= -2069.478035
SCF Done: E(RTPSS-TPSS) = -2071.95493492 A.U. after 19 cycles
NFock= 19 Conv=0.25D-08 -V/T= 2.0387
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.14
(included in total energy above)

INT_0-2

Zero-point correction= 0.677930 (Hartree/Particle)
Thermal correction to Energy= 0.716572
Thermal correction to Enthalpy= 0.717516
Thermal correction to Gibbs Free Energy= 0.606337
Sum of electronic and zero-point Energies= -2069.430475
Sum of electronic and thermal Energies= -2069.391833
Sum of electronic and thermal Enthalpies= -2069.390889
Sum of electronic and thermal Free Energies= -2069.502068
SCF Done: E(RTPSS-TPSS) = -2071.97279125 A.U. after 19 cycles
NFock= 19 Conv=0.23D-08 -V/T= 2.0387
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.22
(included in total energy above)

INT_0-3

Zero-point correction= 0.417255 (Hartree/Particle)
Thermal correction to Energy= 0.444345
Thermal correction to Enthalpy= 0.445289
Thermal correction to Gibbs Free Energy= 0.359307
Sum of electronic and zero-point Energies= -1490.385541
Sum of electronic and thermal Energies= -1490.358450
Sum of electronic and thermal Enthalpies= -1490.357506
Sum of electronic and thermal Free Energies= -1490.443488
SCF Done: E(RTPSS-TPSS) = -1492.40908729 A.U. after 18 cycles
NFock= 18 Conv=0.23D-08 -V/T= 2.0527
SMD-CDS (non-electrostatic) energy (kcal/mol) = 0.03
(included in total energy above)

INT_0-4

Zero-point correction= 0.714063 (Hartree/Particle)
Thermal correction to Energy= 0.759862
Thermal correction to Enthalpy= 0.760806
Thermal correction to Gibbs Free Energy= 0.631216
Sum of electronic and zero-point Energies= -2272.168237
Sum of electronic and thermal Energies= -2272.122439

Sum of electronic and thermal Enthalpies= -2272.121494
Sum of electronic and thermal Free Energies= -2272.251085
SCF Done: E(RTPSS-TPSS) = -2274.83704415 A.U. after 19 cycles
NFock= 19 Conv=0.43D-08 -V/T= 2.0354
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.96
(included in total energy above)

TS_0-2

Zero-point correction= 0.712990 (Hartree/Particle)
Thermal correction to Energy= 0.758030
Thermal correction to Enthalpy= 0.758974
Thermal correction to Gibbs Free Energy= 0.631429
Sum of electronic and zero-point Energies= -2272.142722
Sum of electronic and thermal Energies= -2272.097682
Sum of electronic and thermal Enthalpies= -2272.096737
Sum of electronic and thermal Free Energies= -2272.224283
SCF Done: E(RTPSS-TPSS) = -2274.81511988 A.U. after 19 cycles
NFock= 19 Conv=0.59D-08 -V/T= 2.0354
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.79
(included in total energy above)

INT_0-5

Zero-point correction= 0.715398 (Hartree/Particle)
Thermal correction to Energy= 0.760582
Thermal correction to Enthalpy= 0.761526
Thermal correction to Gibbs Free Energy= 0.633961
Sum of electronic and zero-point Energies= -2272.183780
Sum of electronic and thermal Energies= -2272.138596
Sum of electronic and thermal Enthalpies= -2272.137652
Sum of electronic and thermal Free Energies= -2272.265217
SCF Done: E(RTPSS-TPSS) = -2274.84767709 A.U. after 19 cycles
NFock= 19 Conv=0.49D-08 -V/T= 2.0354
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.86
(included in total energy above)

INT0-1a

Zero-point correction= 0.925239 (Hartree/Particle)
Thermal correction to Energy= 0.975679
Thermal correction to Enthalpy= 0.976623
Thermal correction to Gibbs Free Energy= 0.837630
Sum of electronic and zero-point Energies= -2648.024745
Sum of electronic and thermal Energies= -2647.974305
Sum of electronic and thermal Enthalpies= -2647.973361
Sum of electronic and thermal Free Energies= -2648.112354

SCF Done: E(RTPSS-TPSS) = -2651.05948078 A.U. after 19 cycles
NFock= 19 Conv=0.41D-08 -V/T= 2.0309
SMD-CDS (non-electrostatic) energy (kcal/mol) = -5.08
(included in total energy above)

INT_0-2a

Zero-point correction= 0.664606 (Hartree/Particle)
Thermal correction to Energy= 0.703401
Thermal correction to Enthalpy= 0.704346
Thermal correction to Gibbs Free Energy= 0.590106
Sum of electronic and zero-point Energies= -2069.015744
Sum of electronic and thermal Energies= -2068.976949
Sum of electronic and thermal Enthalpies= -2068.976004
Sum of electronic and thermal Free Energies= -2069.090244
SCF Done: E(RTPSS-TPSS) = -2071.51572388 A.U. after 19 cycles
NFock= 19 Conv=0.32D-08 -V/T= 2.0386
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.32
(included in total energy above)

TS_0-1a

Zero-point correction= 0.660141 (Hartree/Particle)
Thermal correction to Energy= 0.697742
Thermal correction to Enthalpy= 0.698686
Thermal correction to Gibbs Free Energy= 0.590503
Sum of electronic and zero-point Energies= -2068.973809
Sum of electronic and thermal Energies= -2068.936208
Sum of electronic and thermal Enthalpies= -2068.935264
Sum of electronic and thermal Free Energies= -2069.043447
SCF Done: E(RTPSS-TPSS) = -2071.47357757 A.U. after 19 cycles
NFock= 19 Conv=0.21D-08 -V/T= 2.0386
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.19
(included in total energy above)

INT_0-3a

Zero-point correction= 0.665396 (Hartree/Particle)
Thermal correction to Energy= 0.703592
Thermal correction to Enthalpy= 0.704537
Thermal correction to Gibbs Free Energy= 0.594870
Sum of electronic and zero-point Energies= -2068.992579
Sum of electronic and thermal Energies= -2068.954383
Sum of electronic and thermal Enthalpies= -2068.953439
Sum of electronic and thermal Free Energies= -2069.063105
SCF Done: E(RTPSS-TPSS) = -2071.48760273 A.U. after 19 cycles
NFock= 19 Conv=0.39D-08 -V/T= 2.0386

SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.12
(included in total energy above)

INT_0-4a

Zero-point correction= 0.404485 (Hartree/Particle)
Thermal correction to Energy= 0.431386
Thermal correction to Enthalpy= 0.432330
Thermal correction to Gibbs Free Energy= 0.346171
Sum of electronic and zero-point Energies= -1489.959097
Sum of electronic and thermal Energies= -1489.932197
Sum of electronic and thermal Enthalpies= -1489.931252
Sum of electronic and thermal Free Energies= -1490.017411
SCF Done: E(RTPSS-TPSS) = -1491.93160720 A.U. after 19 cycles
NFock= 19 Conv=0.33D-08 -V/T= 2.0527
SMD-CDS (non-electrostatic) energy (kcal/mol) = 0.18
(included in total energy above)

TS_0-2a

Zero-point correction= 0.699946 (Hartree/Particle)
Thermal correction to Energy= 0.744884
Thermal correction to Enthalpy= 0.745828
Thermal correction to Gibbs Free Energy= 0.617827
Sum of electronic and zero-point Energies= -2271.707328
Sum of electronic and thermal Energies= -2271.662390
Sum of electronic and thermal Enthalpies= -2271.661445
Sum of electronic and thermal Free Energies= -2271.789446
SCF Done: E(RTPSS-TPSS) = -2274.33373937 A.U. after 19 cycles
NFock= 19 Conv=0.35D-08 -V/T= 2.0354
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.63
(included in total energy above)

INT-0

Zero-point correction= 0.703730 (Hartree/Particle)
Thermal correction to Energy= 0.748316
Thermal correction to Enthalpy= 0.749260
Thermal correction to Gibbs Free Energy= 0.622973
Sum of electronic and zero-point Energies= -2271.759736
Sum of electronic and thermal Energies= -2271.715151
Sum of electronic and thermal Enthalpies= -2271.714207
Sum of electronic and thermal Free Energies= -2271.840493
SCF Done: E(RTPSS-TPSS) = -2274.37365987 A.U. after 18 cycles
NFock= 18 Conv=0.56D-08 -V/T= 2.0354
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.36
(included in total energy above)

TS-1

Zero-point correction= 0.701620 (Hartree/Particle)
Thermal correction to Energy= 0.745915
Thermal correction to Enthalpy= 0.746859
Thermal correction to Gibbs Free Energy= 0.622370
Sum of electronic and zero-point Energies= -2271.718500
Sum of electronic and thermal Energies= -2271.674206
Sum of electronic and thermal Enthalpies= -2271.673262
Sum of electronic and thermal Free Energies= -2271.797750
SCF Done: E(RTPSS-TPSS) = -2274.35238688 A.U. after 22 cycles
NFock= 22 Conv=0.57D-08 -V/T= 2.0354
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.54
(included in total energy above)

INT-1

Zero-point correction= 0.702135 (Hartree/Particle)
Thermal correction to Energy= 0.747296
Thermal correction to Enthalpy= 0.748240
Thermal correction to Gibbs Free Energy= 0.621457
Sum of electronic and zero-point Energies= -2271.730742
Sum of electronic and thermal Energies= -2271.685582
Sum of electronic and thermal Enthalpies= -2271.684638
Sum of electronic and thermal Free Energies= -2271.811421
SCF Done: E(RTPSS-TPSS) = -2274.36915653 A.U. after 19 cycles
NFock= 19 Conv=0.61D-08 -V/T= 2.0354
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.71
(included in total energy above)

TS-1a

Zero-point correction= 0.701814 (Hartree/Particle)
Thermal correction to Energy= 0.745984
Thermal correction to Enthalpy= 0.746928
Thermal correction to Gibbs Free Energy= 0.623181
Sum of electronic and zero-point Energies= -2271.722930
Sum of electronic and thermal Energies= -2271.678760
Sum of electronic and thermal Enthalpies= -2271.677816
Sum of electronic and thermal Free Energies= -2271.801563
SCF Done: E(RTPSS-TPSS) = -2274.34937497 A.U. after 19 cycles
NFock= 19 Conv=0.49D-08 -V/T= 2.0354
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.64
(included in total energy above)

INT-1a

Zero-point correction= 0.703140 (Hartree/Particle)

Thermal correction to Energy= 0.747551
Thermal correction to Enthalpy= 0.748495
Thermal correction to Gibbs Free Energy= 0.625071
Sum of electronic and zero-point Energies= -2271.734712
Sum of electronic and thermal Energies= -2271.690301
Sum of electronic and thermal Enthalpies= -2271.689357
Sum of electronic and thermal Free Energies= -2271.812781
SCF Done: E(RTPSS-TPSS) = -2274.36893324 A.U. after 19 cycles
NFock= 19 Conv=0.53D-08 -V/T= 2.0354
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.77
(included in total energy above)

INT-1b

Zero-point correction= 0.700272 (Hartree/Particle)
Thermal correction to Energy= 0.745823
Thermal correction to Enthalpy= 0.746767
Thermal correction to Gibbs Free Energy= 0.618179
Sum of electronic and zero-point Energies= -2271.709120
Sum of electronic and thermal Energies= -2271.663569
Sum of electronic and thermal Enthalpies= -2271.662625
Sum of electronic and thermal Free Energies= -2271.791213
SCF Done: E(RTPSS-TPSS) = -2274.33708289 A.U. after 18 cycles
NFock= 18 Conv=0.97D-08 -V/T= 2.0354
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.47
(included in total energy above)

TS-2

Zero-point correction= 0.701120 (Hartree/Particle)
Thermal correction to Energy= 0.745929
Thermal correction to Enthalpy= 0.746873
Thermal correction to Gibbs Free Energy= 0.620404
Sum of electronic and zero-point Energies= -2271.723118
Sum of electronic and thermal Energies= -2271.678309
Sum of electronic and thermal Enthalpies= -2271.677365
Sum of electronic and thermal Free Energies= -2271.803834
SCF Done: E(RTPSS-TPSS) = -2274.35506790 A.U. after 19 cycles
NFock= 19 Conv=0.38D-08 -V/T= 2.0354
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.77
(included in total energy above)

INT-2

Zero-point correction= 0.703421 (Hartree/Particle)
Thermal correction to Energy= 0.747980
Thermal correction to Enthalpy= 0.748924

Thermal correction to Gibbs Free Energy= 0.623188
Sum of electronic and zero-point Energies= -2271.763410
Sum of electronic and thermal Energies= -2271.718851
Sum of electronic and thermal Enthalpies= -2271.717907
Sum of electronic and thermal Free Energies= -2271.843643
SCF Done: E(RTPSS-TPSS) = -2274.38845394 A.U. after 20 cycles
NFock= 20 Conv=0.21D-08 -V/T= 2.0353
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.87
(included in total energy above)

TS-2b

Zero-point correction= 0.701098 (Hartree/Particle)
Thermal correction to Energy= 0.745787
Thermal correction to Enthalpy= 0.746731
Thermal correction to Gibbs Free Energy= 0.621378
Sum of electronic and zero-point Energies= -2271.723113
Sum of electronic and thermal Energies= -2271.678423
Sum of electronic and thermal Enthalpies= -2271.677479
Sum of electronic and thermal Free Energies= -2271.802832
SCF Done: E(RTPSS-TPSS) = -2274.35356078 A.U. after 19 cycles
NFock= 19 Conv=0.72D-08 -V/T= 2.0354
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.68
(included in total energy above)

INT-2b

Zero-point correction= 0.703992 (Hartree/Particle)
Thermal correction to Energy= 0.748275
Thermal correction to Enthalpy= 0.749219
Thermal correction to Gibbs Free Energy= 0.625506
Sum of electronic and zero-point Energies= -2271.774764
Sum of electronic and thermal Energies= -2271.730481
Sum of electronic and thermal Enthalpies= -2271.729537
Sum of electronic and thermal Free Energies= -2271.853250
SCF Done: E(RTPSS-TPSS) = -2274.39637654 A.U. after 18 cycles
NFock= 18 Conv=0.63D-08 -V/T= 2.0354
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.86
(included in total energy above)

TS-2c

Zero-point correction= 0.701591 (Hartree/Particle)
Thermal correction to Energy= 0.745655
Thermal correction to Enthalpy= 0.746599
Thermal correction to Gibbs Free Energy= 0.622914
Sum of electronic and zero-point Energies= -2271.709774

Sum of electronic and thermal Energies= -2271.665710
Sum of electronic and thermal Enthalpies= -2271.664766
Sum of electronic and thermal Free Energies= -2271.788451
SCF Done: E(RTPSS-TPSS) = -2274.35138915 A.U. after 38 cycles
NFock= 38 Conv=0.43D-09 -V/T= 2.0354
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.47
(included in total energy above)

INT-2c

Zero-point correction= 0.703571 (Hartree/Particle)
Thermal correction to Energy= 0.748105
Thermal correction to Enthalpy= 0.749049
Thermal correction to Gibbs Free Energy= 0.623898
Sum of electronic and zero-point Energies= -2271.768283
Sum of electronic and thermal Energies= -2271.723750
Sum of electronic and thermal Enthalpies= -2271.722806
Sum of electronic and thermal Free Energies= -2271.847957
SCF Done: E(RTPSS-TPSS) = -2274.39073112 A.U. after 19 cycles
NFock= 19 Conv=0.23D-08 -V/T= 2.0353
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.75
(included in total energy above)

TS-2d

Zero-point correction= 0.702074 (Hartree/Particle)
Thermal correction to Energy= 0.746545
Thermal correction to Enthalpy= 0.747489
Thermal correction to Gibbs Free Energy= 0.623422
Sum of electronic and zero-point Energies= -2271.720128
Sum of electronic and thermal Energies= -2271.675657
Sum of electronic and thermal Enthalpies= -2271.674713
Sum of electronic and thermal Free Energies= -2271.798779
SCF Done: E(RTPSS-TPSS) = -2274.35207212 A.U. after 28 cycles
NFock= 28 Conv=0.54D-08 -V/T= 2.0354
SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.57
(included in total energy above)

INT-2d

Zero-point correction= 0.704272 (Hartree/Particle)
Thermal correction to Energy= 0.748378
Thermal correction to Enthalpy= 0.749322
Thermal correction to Gibbs Free Energy= 0.625654
Sum of electronic and zero-point Energies= -2271.755638
Sum of electronic and thermal Energies= -2271.711532
Sum of electronic and thermal Enthalpies= -2271.710588

Sum of electronic and thermal Free Energies= -2271.834256

SCF Done: E(RTPSS-TPSS) = -2274.41039416 A.U. after 18 cycles

NFock= 18 Conv=0.69D-08 -V/T= 2.0353

SMD-CDS (non-electrostatic) energy (kcal/mol) = -2.72

(included in total energy above)

INT_0-0

0 1

C	5.37764100	5.52589200	-4.57882800
C	6.61143900	6.17784000	-4.51422800
C	7.54559600	5.75743600	-3.56587900
C	7.27402600	4.71217700	-2.67736500
C	6.03520100	4.07480300	-2.75465000
C	5.08863900	4.48013700	-3.70026100
H	4.64196700	5.84422000	-5.31181900
H	6.83025100	6.99816600	-5.18833700
H	8.03048000	4.40266700	-1.96267000
H	5.80991700	3.26394300	-2.06784500
H	4.12343000	3.98362400	-3.74915600
S	9.12784800	6.58895600	-3.34195800
C	9.03899200	8.09692200	-4.34520000
C	8.64637100	9.28069600	-3.71543500
C	9.39432800	8.06878100	-5.69586100
C	8.59881800	10.45763100	-4.46341800
H	8.40439500	9.27203600	-2.65822000
C	9.34228800	9.25344000	-6.43222200
H	9.71893900	7.13730900	-6.14734700
C	8.94305800	10.44328900	-5.81770900
H	8.30054100	11.38647800	-3.98602700
H	9.62057200	9.24778200	-7.48218000
H	8.90767000	11.36347500	-6.39417400
O	9.24230500	7.04412700	-1.93922500
N	10.18716600	5.63474700	-4.02887600
H	11.12516100	6.01892600	-3.84914900
Rh	10.80270000	3.50109800	-3.56871900
C	10.91475200	2.82623000	-5.67005800
C	11.92170500	2.13830000	-4.93072600
C	11.27692800	1.37850600	-3.87834500
C	9.84121900	1.52056700	-4.05666300
C	9.61856400	2.42816900	-5.13160500
C	8.79206700	0.78663700	-3.27965800
H	8.68320600	-0.23242700	-3.67689500
H	9.07301100	0.73438000	-2.22665200
H	7.81911500	1.27985600	-3.35733700

C	8.30073000	2.82774200	-5.72080900
H	8.08818400	2.21638300	-6.60929400
H	7.47846800	2.69087300	-5.01596000
H	8.30409100	3.87526000	-6.03371200
C	11.97573400	0.44932000	-2.93631200
H	11.34896000	0.23354200	-2.07189800
H	12.22932000	-0.48944100	-3.45084300
H	12.89126700	0.91687300	-2.56764000
C	13.39570400	2.17310900	-5.18810200
H	13.95271700	2.14191600	-4.25043100
H	13.68049600	1.30384800	-5.79738700
H	13.68989300	3.07417100	-5.73306200
C	11.11330400	3.70802500	-6.86585900
H	12.13685000	4.08803100	-6.91843600
H	10.91372100	3.15514400	-7.79422000
H	10.43761000	4.56809300	-6.83686400
C	11.38211100	4.62149700	0.96425700
H	11.39087200	5.37670400	0.17058800
H	12.29550700	4.02196800	0.85106700
C	10.14018800	3.70884200	0.78026000
C	11.35212400	5.29034900	2.35382800
H	12.24029700	5.92748800	2.46799300
C	10.07831500	6.15165900	2.48038300
H	10.07884600	6.93895900	1.71440000
H	10.05439600	6.65140300	3.45957200
C	8.87012500	4.58821700	0.92178600
H	7.97196300	3.96607000	0.78565200
H	8.86563200	5.35338300	0.13831500
C	8.83333200	5.25531000	2.31315300
H	7.92477400	5.86822300	2.39575700
C	8.83077800	4.17092100	3.40989500
H	8.78621600	4.63856900	4.40412900
H	7.93674900	3.53821200	3.31350400
C	10.13550000	2.63748500	1.89361900
H	11.02334400	2.00261800	1.79391100
H	9.26830400	1.97727700	1.76741200
C	11.34789500	4.20535100	3.45053200
H	12.26070100	3.59730400	3.38237700
H	11.34697700	4.67269600	4.44599200
C	10.10355900	3.30901100	3.28195800
H	10.10160100	2.53310500	4.06003900
C	10.20014500	3.03935900	-0.61396800
O	10.25551500	1.81224300	-0.71847400
O	10.18535500	3.89779500	-1.59764100

C	15.84586200	5.03345800	-3.05494000
H	15.56234100	5.08674500	-4.11671900
H	16.17527400	4.00637700	-2.85833100
C	14.60899700	5.34695700	-2.16862300
C	16.98241100	6.03521000	-2.76579500
H	17.84449400	5.79958800	-3.40530200
C	16.49306600	7.46826700	-3.06138600
H	16.21746200	7.56162500	-4.12168800
H	17.30221500	8.18915300	-2.87650200
C	14.14058700	6.78885000	-2.46444700
H	13.25701800	7.02455600	-1.85776200
H	13.83520300	6.87211900	-3.51545700
C	15.27754100	7.79155100	-2.16781400
H	14.92562600	8.81048400	-2.38092200
C	15.69036400	7.68709100	-0.68506000
H	16.48488400	8.41348800	-0.46191500
H	14.83742000	7.93604300	-0.03848600
C	15.04190200	5.25491800	-0.68221900
H	15.35477900	4.22775900	-0.46642500
H	14.17979200	5.46872200	-0.03615700
C	17.39321800	5.93085300	-1.28251600
H	17.76303100	4.91945700	-1.06439600
H	18.21721400	6.62689300	-1.06975800
C	16.17863900	6.25411100	-0.38824200
H	16.46726000	6.17339600	0.66861000
C	13.53587600	4.26465300	-2.44603300
O	13.76105500	3.09531900	-2.12142700
O	12.47071600	4.69872400	-3.05401700

INT_0-1

1 1

C	6.08106000	5.49765800	-5.75526700
C	7.27285000	5.97730400	-5.21184200
C	7.48589600	5.83748300	-3.83722400
C	6.54211600	5.24498200	-2.99658800
C	5.35804200	4.76312000	-3.55943000
C	5.12706600	4.89100500	-4.93058900
H	5.89108400	5.61171600	-6.81832300
H	8.00508600	6.46872600	-5.84310800
H	6.73882400	5.16104000	-1.93405100
H	4.61267000	4.29958600	-2.92043000
H	4.19700300	4.52887700	-5.35879500
S	8.97188000	6.47754400	-3.05748300
C	9.31338000	8.09278400	-3.77466600

C	8.83345600	9.20970900	-3.08372400
C	10.03905700	8.21458200	-4.96457800
C	9.08204700	10.47776500	-3.60880100
H	8.29582400	9.08296200	-2.15053300
C	10.28055800	9.49110500	-5.47302000
H	10.41901000	7.33257100	-5.46860300
C	9.80037100	10.61746600	-4.79920200
H	8.71985000	11.35579000	-3.08312800
H	10.84744900	9.60525400	-6.39195200
H	9.99239700	11.60805200	-5.20047800
O	8.70774400	6.67707100	-1.61744400
N	10.14226100	5.50795400	-3.57203000
H	11.02943000	5.90348700	-3.24458100
Rh	10.24588800	3.37226400	-3.17743900
C	10.27936600	2.72573600	-5.31317900
C	11.57379200	2.53305400	-4.70311400
C	11.41886500	1.55396400	-3.64028300
C	10.03361900	1.21040600	-3.54917200
C	9.32010400	1.94886800	-4.58688900
C	9.40220500	0.23536200	-2.60389000
H	9.17322400	-0.70270200	-3.12597600
H	10.06150200	-0.00031600	-1.76575800
H	8.46729400	0.62825500	-2.19393000
C	7.85911000	1.81492100	-4.88465400
H	7.68969000	0.97207500	-5.56851900
H	7.28464400	1.62241700	-3.97480800
H	7.45434400	2.71478700	-5.35317600
C	12.53589700	1.04006800	-2.78738600
H	12.16753000	0.51299800	-1.90532700
H	13.15223000	0.34001200	-3.36638800
H	13.18347600	1.85397000	-2.44835700
C	12.87594000	3.10384200	-5.17693400
H	13.57870400	3.23678800	-4.34961500
H	13.34653900	2.43095300	-5.90637400
H	12.73742600	4.07274800	-5.66393600
C	10.00819600	3.58406200	-6.50793300
H	10.61678900	4.49211500	-6.49328000
H	10.25677400	3.02984300	-7.42257400
H	8.95788400	3.87647900	-6.56791100
C	10.83731500	5.45655800	1.13365000
H	10.44022000	6.32666800	0.59569400
H	11.86902500	5.30594800	0.79528300
C	9.98543400	4.20560400	0.78442900
C	10.79925900	5.70432000	2.65596100

H	11.40073000	6.59331600	2.88475600
C	9.34128800	5.93154000	3.10544500
H	8.92321600	6.81411400	2.60240100
H	9.30686900	6.13194300	4.18445700
C	8.52732000	4.42977100	1.25038600
H	7.91752200	3.55320000	0.99967300
H	8.10075900	5.28483900	0.71235700
C	8.49975900	4.68213700	2.77269600
H	7.46049400	4.84196900	3.08697600
C	9.08093800	3.45752300	3.50912600
H	9.04324800	3.61674800	4.59472600
H	8.47581600	2.56510700	3.29714100
C	10.57669900	2.97472600	1.54012700
H	11.60714600	2.80043400	1.20584500
H	9.99293800	2.07643300	1.29465600
C	11.38122900	4.48026600	3.39231900
H	12.42760500	4.32179100	3.09736700
H	11.37895700	4.65601300	4.47605200
C	10.53917600	3.23105100	3.06078600
H	10.95499400	2.35561600	3.57591700
C	10.05773300	3.91406100	-0.69722100
O	11.17779500	3.94496600	-1.32289000
O	9.02907200	3.58524600	-1.38147300

TS_0-1

1 1

C	6.19548900	6.73687700	-5.74153200
C	7.48688100	7.17169500	-5.42383400
C	8.16076800	6.52922300	-4.39102000
C	7.62077000	5.46784000	-3.63341500
C	6.31174800	5.08086200	-3.97651400
C	5.60900600	5.69908900	-5.01457100
H	5.64840400	7.22087100	-6.54478500
H	7.94426400	7.98602400	-5.97635200
H	7.76398400	5.46846700	-2.34263800
H	5.81972100	4.31177500	-3.38702900
H	4.59602700	5.38303900	-5.24736600
S	9.77152200	7.09352300	-3.84093200
C	10.53543200	8.01205400	-5.18108200
C	10.59226400	9.40438900	-5.06636500
C	11.05654100	7.33595800	-6.28935600
C	11.18348300	10.13461600	-6.09857100
H	10.19578300	9.89327600	-4.18319900
C	11.64134900	8.08203700	-7.31123000

H	11.01538600	6.25336100	-6.33934400
C	11.70277800	9.47625600	-7.21583200
H	11.24130900	11.21614000	-6.02527100
H	12.05544900	7.57642400	-8.17825300
H	12.16286900	10.05051300	-8.01447300
O	9.67580200	7.99697800	-2.67567100
N	10.52098200	5.68108800	-3.69266600
H	11.36037900	5.81474200	-3.12274700
Rh	9.31936700	3.99882500	-3.08462200
C	8.79962500	2.38622100	-4.58517800
C	10.21202700	2.57684800	-4.57924900
C	10.70148900	2.30638100	-3.23696900
C	9.57658200	1.87113200	-2.44224700
C	8.39626600	1.96502100	-3.24594800
C	9.65533900	1.42907400	-1.01604500
H	10.26461800	2.11713000	-0.42351600
H	8.66760700	1.36720100	-0.55479900
H	10.11689800	0.43458000	-0.96224000
C	7.02201300	1.52197200	-2.84207700
H	6.92808100	0.43405400	-2.95988000
H	6.80807900	1.76057800	-1.79669100
H	6.24941000	1.98301700	-3.46099600
C	12.13695500	2.29135700	-2.80703600
H	12.23704800	2.50714600	-1.74008500
H	12.57923700	1.30253900	-2.98963900
H	12.73240500	3.02291000	-3.36047700
C	11.07299500	2.96011400	-5.74125100
H	11.83872500	3.68311600	-5.44669000
H	11.58468300	2.07185600	-6.13449400
H	10.48731600	3.39427400	-6.55475700
C	7.89844400	2.45712500	-5.77978800
H	8.30029600	3.11346000	-6.55545100
H	7.78442200	1.45603900	-6.21670500
H	6.90290400	2.82093200	-5.51700100
C	10.38413400	6.59049100	0.99329500
H	10.26441000	7.48989700	0.37494400
H	11.20013100	6.00144200	0.55726500
C	9.06885700	5.75970800	0.96185400
C	10.71980200	6.97687400	2.44916000
H	11.64724300	7.56382500	2.45348300
C	9.56876900	7.81434600	3.04236900
H	9.43666300	8.73961000	2.46531900
H	9.81225300	8.11166500	4.07087900
C	7.92281000	6.60262300	1.56872500

H	6.98564800	6.03374400	1.53597200
H	7.76576200	7.50215400	0.96231500
C	8.26803800	6.98591700	3.02288800
H	7.44466600	7.58110400	3.43711000
C	8.45715300	5.70628300	3.86324900
H	8.68113600	5.96757300	4.90580600
H	7.52831400	5.11949900	3.87463700
C	9.26996500	4.47871200	1.81772900
H	10.07833700	3.87323000	1.39011700
H	8.35500400	3.86971600	1.79566600
C	10.91074000	5.69601200	3.28841300
H	11.74375800	5.10101000	2.88855200
H	11.17416500	5.95935400	4.32105000
C	9.60897800	4.86872400	3.27165200
H	9.74421100	3.95303200	3.86156100
C	8.76361400	5.37197100	-0.48644200
O	9.64386900	4.67204600	-1.10452500
O	7.68560700	5.75016800	-1.02410300

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C	6.39849800	7.36836300	-5.23477700
C	7.73574500	7.62514200	-4.93840000
C	8.50085300	6.60073300	-4.37611700
C	8.01474000	5.31268400	-4.07462200
C	6.65265100	5.11048700	-4.36393600
C	5.86047900	6.11494900	-4.93464500
H	5.78150300	8.14168900	-5.68108100
H	8.17035700	8.60012100	-5.14007200
H	7.34017200	5.69927100	-2.05341000
H	6.18954600	4.15475700	-4.13964900
H	4.81316200	5.91404100	-5.14362700
S	10.14448300	6.96329300	-3.79173700
C	11.01535800	7.89717800	-5.05357500
C	11.31561700	9.23692100	-4.79316300
C	11.37020300	7.27670900	-6.25625000
C	11.98800300	9.97238200	-5.77088800
H	11.03722900	9.67916800	-3.84290100
C	12.03850400	8.02696200	-7.22180000
H	11.13337000	6.23152700	-6.42511000
C	12.34534600	9.37024200	-6.97920900
H	12.23378500	11.01334200	-5.58500900
H	12.32377200	7.56403500	-8.16155600
H	12.86824100	9.94783700	-7.73571300

O	10.12458400	7.79398800	-2.56540800
N	10.73460700	5.47652300	-3.74302000
H	11.62764000	5.47354200	-3.24684400
Rh	9.33445300	3.91742500	-3.29959000
C	8.53694700	2.08646900	-4.33164200
C	9.86126000	2.43817400	-4.79426600
C	10.80079300	2.18291000	-3.69388700
C	10.05202100	1.83413000	-2.55850700
C	8.62884100	1.83050500	-2.93124700
C	10.55432000	1.52982500	-1.18100600
H	11.63218800	1.68598300	-1.09705200
H	10.06358800	2.16296800	-0.43439400
H	10.34571600	0.48457300	-0.91968200
C	7.52153100	1.40923000	-2.01210100
H	7.50350900	0.31595800	-1.90820600
H	7.65577700	1.83147000	-1.01180700
H	6.54204500	1.72260500	-2.38262000
C	12.29059200	2.30011700	-3.80996800
H	12.77443800	2.35571800	-2.83173400
H	12.69943600	1.42594800	-4.33333200
H	12.57971000	3.18500700	-4.38567000
C	10.25682900	2.70035300	-6.21588000
H	11.12624400	3.36124400	-6.27055400
H	10.52249500	1.76045400	-6.71890900
H	9.44273200	3.16178100	-6.78105200
C	7.32904300	1.92818600	-5.20221000
H	7.27238000	2.69790900	-5.97580600
H	7.37832200	0.95421000	-5.70735200
H	6.39976300	1.94626200	-4.62772700
C	9.75590900	6.95748600	0.88255900
H	9.37034300	7.81052600	0.31138600
H	10.66303700	6.61223200	0.37204600
C	8.69572800	5.80782500	0.89414700
C	10.07516800	7.37300200	2.33317800
H	10.81730200	8.18082900	2.30718600
C	8.78942100	7.86713600	3.02673900
H	8.38547500	8.74112500	2.49813200
H	9.01652800	8.19023200	4.05080200
C	7.41309300	6.31386100	1.60108300
H	6.65061600	5.52365700	1.60097800
H	6.99253000	7.16290400	1.05170400
C	7.74722900	6.73029400	3.04901300
H	6.82782900	7.08041300	3.53406100
C	8.31497500	5.52113200	3.81948600

H	8.53214900	5.80353100	4.85766100
H	7.57227100	4.71240700	3.85780200
C	9.27916800	4.60355600	1.67953500
H	10.18401300	4.24098000	1.17884100
H	8.55258600	3.77863000	1.68311800
C	10.64562900	6.16473300	3.10361500
H	11.57475500	5.81720400	2.63108200
H	10.90131300	6.46008500	4.12936600
C	9.60185500	5.02920900	3.12638700
H	10.00730800	4.16415100	3.66606000
C	8.44750300	5.41996300	-0.54962500
O	9.22311000	4.68514600	-1.18048500
O	7.36449500	5.94419900	-1.10107800

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C	6.55066200	7.15555400	-6.02482600
C	7.64808100	7.49695600	-5.23569500
C	8.46089600	6.46573700	-4.76314200
C	8.24364700	5.09820700	-5.00463500
C	7.13525100	4.80308800	-5.81301200
C	6.30576900	5.81131900	-6.31691100
H	5.89777900	7.93156300	-6.41148800
H	7.86293400	8.53620000	-5.00347100
H	6.90835700	3.77326100	-6.06792300
H	5.45852900	5.54376500	-6.94248500
S	9.84564300	6.86270800	-3.71797200
C	10.82601600	8.12865800	-4.52419600
C	10.91868900	9.37715000	-3.90381400
C	11.46663900	7.84809300	-5.73667700
C	11.67796000	10.37239200	-4.52214700
H	10.41719600	9.55317900	-2.95836100
C	12.21663000	8.85535200	-6.33962200
H	11.38408800	6.86646000	-6.19157100
C	12.32105300	10.11265900	-5.73409200
H	11.76603400	11.34773900	-4.05382900
H	12.72270400	8.65909000	-7.27981500
H	12.90935500	10.89150300	-6.21001200
O	9.47008900	7.35673700	-2.37862500
N	10.65250900	5.46214100	-3.81754400
H	11.46088000	5.48070300	-3.19448600
Rh	9.59110600	3.75295000	-4.22205000
C	8.37567700	1.89645700	-4.02612700
C	9.47083300	1.63456400	-4.89192600

C	10.72140300	1.74237700	-4.11050800
C	10.39228500	2.13328000	-2.80458700
C	8.93724000	2.32659700	-2.75819200
C	11.31671700	2.34667600	-1.64424600
H	12.35571600	2.45620800	-1.96483600
H	11.04214300	3.23476000	-1.06645500
H	11.27165500	1.48903700	-0.96046800
C	8.15627100	2.67146500	-1.53104700
H	7.98730700	1.76192300	-0.93673700
H	8.68997800	3.38495800	-0.89778200
H	7.17988300	3.09462600	-1.77827600
C	12.08235000	1.45451300	-4.66376600
H	12.87544400	1.83739400	-4.01756000
H	12.22746800	0.37042000	-4.76310800
H	12.21454400	1.88989200	-5.65938400
C	9.40679000	1.16468100	-6.31163800
H	10.21722900	1.58746700	-6.91253500
H	9.50649000	0.07121200	-6.34997300
H	8.45928800	1.42959900	-6.78609300
C	6.91735500	1.69131700	-4.30343500
H	6.70996200	1.62507700	-5.37402100
H	6.58917400	0.74694900	-3.84987800
H	6.30154600	2.49141900	-3.88433100

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1 1

C	7.57678300	8.25580600	-5.74973300
C	8.48388300	8.12575400	-4.70321800
C	8.94489100	6.84540500	-4.37710000
C	8.54172300	5.66789900	-5.02689800
C	7.61026300	5.84178400	-6.06234700
C	7.14131000	7.10923900	-6.42181200
H	7.20844400	9.23623700	-6.03421100
H	8.82993400	8.99790900	-4.15570600
H	7.22917200	4.97872400	-6.59888200
H	6.42402700	7.20135200	-7.23322000
S	9.98026500	6.62404000	-2.95359000
C	11.28235900	7.86055500	-2.99478900
C	11.29838400	8.83430600	-1.99307300
C	12.23997200	7.82791800	-4.01413900
C	12.30489000	9.80179100	-2.01891200
H	10.54492200	8.82131800	-1.21326900
C	13.23495900	8.80314600	-4.02602300
H	12.20724500	7.05539500	-4.77499800

C	13.26668800	9.78641500	-3.03106900
H	12.33573000	10.56418400	-1.24668100
H	13.98795200	8.79487700	-4.80818500
H	14.04668800	10.54185100	-3.04564100
O	9.25427500	6.79627900	-1.67355000
N	10.61653100	5.19665300	-3.31842800
H	11.02277600	4.78043200	-2.47854100
Rh	9.37022800	3.86234300	-4.43726100
C	8.97904200	2.08450500	-5.80242700
C	9.70891500	3.05736600	-6.56139400
C	10.95594800	3.28637100	-5.88638700
C	11.05931300	2.32352700	-4.78849000
C	9.85649400	1.58673800	-4.74411900
C	12.26124600	2.13424700	-3.91228400
H	12.82138900	3.06631200	-3.79576400
H	11.98198900	1.78015300	-2.91710000
H	12.94340000	1.39611600	-4.35432300
C	9.53881800	0.42819700	-3.84902600
H	9.74894700	-0.51073400	-4.37906300
H	10.13417100	0.43848100	-2.93483000
H	8.48541700	0.41330200	-3.55916100
C	12.06458900	4.17677000	-6.35823600
H	12.60621400	4.61424500	-5.51510800
H	12.78591800	3.60496700	-6.95723300
H	11.68609900	4.99124700	-6.98159500
C	9.31265300	3.64888200	-7.87960300
H	9.57628500	4.70656400	-7.95680900
H	9.83712500	3.11587500	-8.68391100
H	8.24211700	3.54860200	-8.07191900
C	7.65645100	1.47682100	-6.16525500
H	7.03857800	2.16270500	-6.75122700
H	7.80336000	0.57003100	-6.76736600
H	7.09285200	1.18705900	-5.27396100
C	2.46118000	3.78238400	-1.93347600
C	3.50628800	4.02750700	-3.02678900
H	1.45091100	3.98344800	-2.30468900
H	2.48744400	2.74351200	-1.58396500
H	2.63344400	4.43124500	-1.06674600
C	4.93796400	3.75487600	-2.54542700
H	3.28750900	3.39048100	-3.89528100
H	3.43480600	5.06572000	-3.37940600
C	5.97988400	4.01437800	-3.65929200
H	5.16890600	4.39457100	-1.68425000
H	5.02414100	2.71598700	-2.20196800

H	5.75983600	3.38184300	-4.52969500
H	5.90753500	5.05183000	-4.00485400
C	7.34823000	3.75226600	-3.19321800
C	8.34061200	3.46797400	-2.50219900
C	8.95622800	3.01764300	-1.22256300
C	8.43488100	3.75175000	0.00415900
H	7.34991900	3.60271300	0.03858300
H	8.60943700	4.82236600	-0.14334300
F	10.33855000	3.14343500	-1.28761800
F	8.73020400	1.66493800	-1.09691200
C	9.08091700	3.26272900	1.31829500
H	10.16008300	3.44582400	1.27433300
H	8.94200500	2.17969500	1.40350700
C	8.48178000	3.96021000	2.52218500
C	8.98952800	5.18903800	2.96484400
C	7.38727900	3.40473600	3.19795300
C	8.41829200	5.84741700	4.05477800
H	9.84471000	5.62980800	2.45624100
C	6.81284700	4.05980000	4.28847100
H	6.98787100	2.44563600	2.87419600
C	7.32680900	5.28439100	4.71934600
H	8.82956900	6.79603500	4.38924000
H	5.96957900	3.61030700	4.80575100
H	6.88443400	5.79305100	5.57125000

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C	7.52244900	7.99478400	-5.78905900
C	8.50074700	7.97265200	-4.79331600
C	8.84292300	6.75162700	-4.21523300
C	8.22858400	5.52692700	-4.55757200
C	7.24774100	5.59283600	-5.56480800
C	6.91002200	6.80057900	-6.17852400
H	7.24662900	8.93430400	-6.25695200
H	9.00124100	8.88796600	-4.49296900
H	6.72573200	4.68790600	-5.86006300
H	6.15527500	6.81049200	-6.96004400
S	10.09486500	6.66841700	-2.94405000
C	11.27892000	7.98516100	-3.25074600
C	11.32752700	9.04950100	-2.34624100
C	12.12805400	7.91282300	-4.36011700
C	12.25364900	10.07037400	-2.56742900
H	10.66378200	9.06255600	-1.48878000
C	13.04401600	8.94268900	-4.56669500

H	12.07556400	7.06679900	-5.03704600
C	13.10577800	10.01719800	-3.67286700
H	12.30968600	10.90326200	-1.87340300
H	13.71348700	8.90482000	-5.42061800
H	13.82462300	10.81419700	-3.83829500
O	9.55735200	6.87644500	-1.57979000
N	10.75357300	5.26633800	-3.34852100
H	11.36896500	4.94733300	-2.59643400
Rh	9.44679000	3.76261800	-4.22395200
C	8.91205400	2.02577600	-5.55190700
C	9.69167300	2.93147300	-6.38593700
C	10.96297800	3.07579000	-5.78927900
C	11.01010300	2.21185400	-4.59824000
C	9.77205600	1.51482700	-4.50952800
C	12.22606000	1.97592800	-3.75274300
H	12.86416100	2.86358700	-3.70961800
H	11.95537600	1.70030800	-2.73082800
H	12.83116000	1.16178400	-4.17401700
C	9.43422400	0.41220700	-3.55235700
H	9.69530200	-0.55561400	-4.00123000
H	9.98188100	0.50788700	-2.61363400
H	8.36923700	0.39272000	-3.31248500
C	12.11785200	3.88882000	-6.28806100
H	12.59924900	4.43413800	-5.47042600
H	12.87569900	3.23802100	-6.74372700
H	11.80640500	4.61424600	-7.04399800
C	9.22283500	3.54714300	-7.66941800
H	9.78975100	4.44685800	-7.92109800
H	9.34363100	2.83465900	-8.49606800
H	8.16509500	3.82121400	-7.62924500
C	7.54562900	1.50058100	-5.88035600
H	6.95005100	2.23090900	-6.43482800
H	7.62734400	0.60447000	-6.51074200
H	6.99165900	1.21964100	-4.98083200
C	2.70329100	3.10829800	-3.45012500
C	3.69150600	4.18564400	-2.99133700
H	1.67038600	3.41173200	-3.25067200
H	2.79191400	2.91826000	-4.52677200
H	2.87820600	2.16004100	-2.92810600
C	5.15358500	3.79950900	-3.25408200
H	3.46900200	5.13290000	-3.50190000
H	3.55504300	4.37664800	-1.91804700
C	6.13909700	4.88670200	-2.77890000
H	5.39121300	2.85887200	-2.74043800

H	5.29593300	3.61448700	-4.32717100
H	5.92010100	5.84305100	-3.26111800
H	6.00705600	5.04037000	-1.69790300
C	7.57899700	4.51103700	-2.94182000
C	8.48807700	3.78245200	-2.40579600
C	8.81545400	3.10087000	-1.12054600
C	8.45956100	3.88804500	0.13198400
H	7.37828100	4.06702100	0.11673900
H	8.94548200	4.86709600	0.06895500
F	10.16996600	2.80536500	-1.10919300
F	8.17413900	1.87662000	-1.10510500
C	8.85062100	3.16015600	1.43576500
H	9.93487600	3.00465800	1.44410200
H	8.38441400	2.16915700	1.44355400
C	8.42641800	3.94626700	2.65915800
C	9.25401400	4.94508900	3.18969600
C	7.18491400	3.71339800	3.26562000
C	8.85212000	5.69349700	4.29684100
H	10.22594000	5.13190900	2.73712000
C	6.77886100	4.45941900	4.37347400
H	6.53491900	2.93352300	2.87369700
C	7.61164700	5.45305400	4.89151500
H	9.51015100	6.45877000	4.69966000
H	5.81613000	4.25931800	4.83598900
H	7.29947900	6.03093600	5.75686200

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C	7.94574900	7.17662500	-6.76523800
C	8.89753300	7.32688400	-5.75927100
C	8.77870000	6.58094100	-4.58129400
C	7.70751300	5.67873000	-4.36247000
C	6.76369800	5.56276100	-5.40255600
C	6.87719000	6.29297000	-6.58251900
H	8.03022400	7.75829000	-7.67787600
H	9.71692800	8.02452600	-5.88725000
H	5.92248300	4.89112100	-5.26050200
H	6.12408900	6.18408500	-7.35761500
S	9.98898700	6.80408100	-3.24871600
C	11.02345300	8.21293900	-3.67198500
C	10.71478200	9.44553300	-3.08701300
C	12.11794200	8.05014800	-4.52763600
C	11.52338900	10.54336100	-3.38111500
H	9.87589300	9.53079100	-2.40510600

C	12.91518700	9.15949100	-4.80987300
H	12.34060100	7.07483100	-4.94699900
C	12.61664200	10.40085800	-4.24015700
H	11.30313500	11.50704200	-2.93252500
H	13.77265000	9.05313600	-5.46732300
H	13.24364500	11.25951600	-4.46115900
O	9.33892700	7.11863100	-1.96056100
N	10.85590000	5.47425300	-3.45080300
H	11.47720400	5.32756600	-2.65208700
Rh	9.78373600	3.80164000	-4.29830400
C	9.29939200	2.24289600	-5.81098600
C	10.41349700	3.00803400	-6.41588200
C	11.52606100	2.89997000	-5.58017400
C	11.12226200	2.10740800	-4.40782100
C	9.77981400	1.59578600	-4.64214500
C	12.06352000	1.63854800	-3.34423400
H	12.83137000	2.38679600	-3.12751000
H	11.53885000	1.40001800	-2.41901100
H	12.57972300	0.73112800	-3.68953800
C	9.09981600	0.51589800	-3.86009800
H	9.39618500	-0.46087600	-4.26647500
H	9.37300200	0.54388000	-2.80556400
H	8.01269100	0.59180200	-3.92339700
C	12.88553000	3.50466500	-5.75739500
H	13.17089000	4.10528900	-4.88647900
H	13.64396900	2.72115300	-5.87780600
H	12.93098500	4.14861600	-6.63892100
C	10.29310000	3.76465100	-7.70226400
H	11.19429500	4.34091200	-7.92334200
H	10.12291200	3.07330700	-8.53764600
H	9.44430300	4.45833900	-7.68059200
C	7.97203100	2.02618200	-6.47116100
H	7.61049200	2.93740100	-6.95642800
H	8.05758800	1.25260200	-7.24675000
H	7.21625100	1.69608900	-5.75438700
C	2.81953500	3.60387900	-1.41090200
C	3.91498600	4.67484000	-1.44366300
H	1.96028900	3.93504000	-0.81811200
H	2.45768800	3.37319500	-2.42037500
H	3.18953100	2.67059700	-0.96955300
C	5.14327100	4.24702200	-2.25749100
H	3.50680300	5.60633900	-1.86050000
H	4.22743600	4.91272700	-0.41705900
C	6.23786800	5.33369800	-2.29956300

H	5.56150700	3.32144200	-1.84505800
H	4.83148100	4.00316000	-3.28392800
H	5.82404400	6.23788900	-2.76221300
H	6.51078800	5.62752400	-1.28089500
C	7.50013700	4.93685200	-3.06566600
C	8.42436600	4.00629500	-2.76777100
C	8.51150400	3.17383200	-1.51043300
C	8.21911000	3.82590500	-0.16268000
H	7.15451600	4.06358800	-0.12004000
H	8.76490100	4.77392400	-0.10371900
F	9.80499900	2.65462400	-1.44098100
F	7.69228300	2.05879700	-1.65042700
C	8.57066300	2.91751800	1.03705900
H	9.65153900	2.74653300	1.05857000
H	8.09419700	1.94193300	0.88955200
C	8.11146700	3.52554700	2.34584600
C	8.94536700	4.38940200	3.06825500
C	6.82837300	3.26265800	2.84509200
C	8.50953200	4.97760100	4.25671100
H	9.94880000	4.59643800	2.70121600
C	6.38812000	3.84811700	4.03310200
H	6.17217900	2.58381500	2.30365100
C	7.22811900	4.70923800	4.74213800
H	9.17280600	5.63970300	4.80684800
H	5.39299500	3.62558800	4.40877700
H	6.88932100	5.16199900	5.66974600

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C	5.53378400	5.22843600	-4.99860400
C	6.85380400	5.68254400	-4.98836000
C	7.48597400	5.94723700	-3.76959700
C	6.81182300	5.75210700	-2.56415200
C	5.49574100	5.28172200	-2.57997000
C	4.85518200	5.02159100	-3.79338200
H	5.03387000	5.03977800	-5.94546500
H	7.38238900	5.85080400	-5.92248400
H	7.32205500	5.97346700	-1.63364900
H	4.96785700	5.12783100	-1.64212500
H	3.82820300	4.66576500	-3.80233400
S	9.26058600	6.44655000	-3.73297100
C	9.26388800	7.83238900	-4.91938300
C	8.79476100	9.07375900	-4.48488000
C	9.75963300	7.66109700	-6.21183800

C	8.80699900	10.15470000	-5.36795300
H	8.44352100	9.18452700	-3.46425500
C	9.77271200	8.74942200	-7.08711400
H	10.14383500	6.68789700	-6.49840100
C	9.29324600	9.99307100	-6.66809200
H	8.44442200	11.12495600	-5.03851700
H	10.16070900	8.62694700	-8.09519900
H	9.30426600	10.83783100	-7.35207500
O	9.41216300	7.08449600	-2.39146800
N	10.16073900	5.39386900	-4.37209500
H	12.94471600	6.80132400	-1.51078700
Rh	10.76445400	3.58794400	-3.59901900
C	10.14107200	2.40273600	-5.37649300
C	11.51956600	2.15073500	-5.13911600
C	11.65729100	1.51988200	-3.82247900
C	10.36904800	1.42442700	-3.24954700
C	9.41378600	2.03834400	-4.16822100
C	10.03492500	0.83174200	-1.91554100
H	9.77251300	-0.22972700	-2.02462300
H	10.87994500	0.91517300	-1.22902200
H	9.18315300	1.34334800	-1.45952900
C	7.92452200	2.03536600	-4.00320400
H	7.50659100	1.06947000	-4.32267600
H	7.64141200	2.19350900	-2.95921500
H	7.45173500	2.82186900	-4.59574400
C	12.93591900	1.05983900	-3.19007100
H	12.99020400	1.41403000	-2.15658200
H	13.00338800	-0.03667100	-3.19409800
H	13.80423800	1.44950900	-3.72693800
C	12.66549400	2.42095800	-6.06582500
H	13.48254900	2.91456500	-5.53117700
H	13.05181800	1.48328400	-6.48758100
H	12.36895600	3.06809300	-6.89472500
C	9.52102400	2.98162200	-6.60977700
H	10.27207900	3.43278300	-7.26257500
H	9.00038900	2.20037600	-7.17979700
H	8.79844500	3.75911000	-6.34992100
C	11.49275200	5.49122000	1.22858500
H	11.51135000	6.33741200	0.52739700
H	12.49885600	5.05408800	1.25334700
C	10.48946200	4.42485900	0.70970100
C	11.08033300	5.98426600	2.63004500
H	11.80175500	6.73745300	2.97741000
C	9.67205500	6.60973200	2.55747200

H	9.67743100	7.47169100	1.87630600
H	9.37335300	6.98339800	3.54748700
C	9.08359300	5.06106800	0.65665000
H	8.36017400	4.32308700	0.28588200
H	9.08739200	5.88869700	-0.06061700
C	8.66633600	5.55072700	2.06048500
H	7.66340000	5.99628200	2.00591300
C	8.64999100	4.36199300	3.04397800
H	8.33352100	4.69721700	4.04217200
H	7.91975600	3.60968900	2.71321900
C	10.47550300	3.24409300	1.71551400
H	11.46956100	2.78340700	1.74254700
H	9.77329600	2.47287400	1.36600600
C	11.06523600	4.79312200	3.61013500
H	12.06924800	4.35188700	3.68432600
H	10.79077700	5.13638400	4.61779700
C	10.05757000	3.73414500	3.11664900
H	10.04795400	2.88284500	3.81155500
C	10.99162400	3.91072000	-0.66152800
O	12.08526200	3.32211700	-0.71567900
O	10.20154900	4.15046500	-1.65692900
C	15.72167800	5.61763500	-3.52835700
H	15.43793000	6.55391000	-4.02898400
H	15.50206200	4.80178000	-4.22571600
C	14.86930200	5.42775800	-2.24266000
C	17.22097700	5.63986600	-3.16911800
H	17.80550800	5.77337500	-4.08882200
C	17.50023300	6.80916800	-2.20280400
H	17.24623400	7.76554000	-2.68078300
H	18.56997400	6.84914900	-1.95692800
C	15.16936600	6.59603300	-1.27047500
H	14.58711000	6.48031900	-0.34375000
H	14.89103800	7.55721100	-1.72876300
C	16.67256700	6.62140300	-0.91529900
H	16.85995200	7.45637300	-0.22813600
C	17.05912100	5.29052300	-0.23895000
H	18.12194100	5.30776900	0.03825100
H	16.48788100	5.15838100	0.69005500
C	15.27991800	4.09085100	-1.56277600
H	15.06497600	3.26596600	-2.25015900
H	14.65957400	3.92359900	-0.67492900
C	17.61083600	4.30936100	-2.49188400
H	17.43599800	3.47053400	-3.17935800
H	18.68321300	4.30975300	-2.25282400

C	16.77880100	4.12220900	-1.20573700
H	17.04919300	3.17307800	-0.72504000
C	13.39424800	5.33024800	-2.64776400
O	13.00320700	4.47464100	-3.42973000
O	12.52196900	6.20752300	-2.15186400

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C	7.33050900	5.95646100	-5.45440400
C	8.41939800	6.06282600	-4.58771300
C	8.24045400	6.62546800	-3.32055200
C	6.98403700	7.06825700	-2.90861800
C	5.89479800	6.94524000	-3.77550100
C	6.06588300	6.39336100	-5.04653900
H	7.46834600	5.53753100	-6.44815500
H	9.40419600	5.72578400	-4.89864600
H	6.87515900	7.50008700	-1.92040500
H	4.91314600	7.28764000	-3.45821100
H	5.21836600	6.30781800	-5.72164900
S	9.65034200	6.68817400	-2.13996500
C	10.88790000	7.61076800	-3.10466600
C	10.72479800	8.99229700	-3.22903900
C	11.98083400	6.95960000	-3.67483600
C	11.66262600	9.72606200	-3.95651300
H	9.88341700	9.47861600	-2.74669600
C	12.91807300	7.70296100	-4.39543800
H	12.09104300	5.89134100	-3.52474700
C	12.75659000	9.08272400	-4.54163900
H	11.54392800	10.80144300	-4.05882500
H	13.77613900	7.20463300	-4.83906300
H	13.48677900	9.65820500	-5.10456900
O	9.18011000	7.64312800	-1.08864500
N	10.27457800	5.31542900	-1.89183300
Rh	9.33456700	3.76063300	-0.91670200
C	9.87211600	2.29925900	-2.49884400
C	10.59389200	2.02444400	-1.28653400
C	9.62395900	1.63105000	-0.26574000
C	8.32647300	1.75491700	-0.82138700
C	8.47085600	2.21660200	-2.20266500
C	7.01304000	1.48347500	-0.15090900
H	6.55306900	0.57050700	-0.55201000
H	7.13078800	1.35193500	0.92752500
H	6.31221200	2.30923600	-0.30931600
C	7.33764700	2.41248700	-3.16407500

H	7.08991800	1.46644300	-3.66604800
H	6.43807800	2.75939600	-2.64796600
H	7.58190800	3.15191400	-3.93068700
C	9.98534300	1.21873500	1.12881000
H	9.11120100	1.19596500	1.78385200
H	10.43502200	0.21677700	1.12990300
H	10.70999000	1.91208200	1.56692800
C	12.08498800	1.99062500	-1.13896700
H	12.38860300	2.22925100	-0.11562900
H	12.48130300	0.99467800	-1.38277200
H	12.56030000	2.71695000	-1.80362500
C	10.49851000	2.66881800	-3.80743600
H	11.11419200	1.84212800	-4.18358200
H	9.74252000	2.89821300	-4.56210300
H	11.13333600	3.55275400	-3.68831100
C	7.72770600	5.51058300	3.27265900
H	8.60869400	4.93620400	3.58553200
H	6.92890900	4.78918400	3.04801500
C	8.07088900	6.32740100	1.99248100
C	7.27688800	6.46372500	4.39886200
H	7.03628600	5.87326300	5.29375500
C	8.41508100	7.45497800	4.72022600
H	9.30343300	6.90910100	5.06752000
H	8.11007400	8.12392600	5.53750500
C	9.21163400	7.32360800	2.33340900
H	9.47823200	7.88301700	1.43016500
H	10.10248500	6.76365300	2.64033800
C	8.75676800	8.27452700	3.45846800
H	9.57019000	8.97685700	3.68529000
C	7.50820800	9.05768100	3.00296900
H	7.19038100	9.75529000	3.79118500
H	7.74533700	9.66034900	2.11586000
C	6.81851200	7.11728100	1.55015000
H	6.01045700	6.42073900	1.29488700
H	7.05648300	7.68318600	0.64269600
C	6.02901100	7.24675900	3.94122300
H	5.20442000	6.55189700	3.72756200
H	5.68616600	7.91190500	4.74632100
C	6.36984900	8.06756400	2.67998000
H	5.48046300	8.62257800	2.35160300
C	8.53191000	5.36065600	0.91428800
O	9.66788000	4.79331900	1.00272900
O	7.78748600	5.06528600	-0.08191300

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C	7.00785200	6.88404300	-5.03818000
C	8.20070800	7.21803800	-4.38534600
C	8.50489800	6.58673500	-3.18470300
C	7.66037500	5.62950800	-2.58107000
C	6.46085000	5.34065700	-3.25672200
C	6.13850100	5.94814100	-4.47445000
H	6.75689900	7.36456400	-5.98043400
H	8.87673300	7.95002000	-4.81709500
H	7.41549600	5.75121200	-1.28154700
H	5.74903000	4.65584500	-2.80119200
H	5.20491000	5.70423400	-4.97544700
S	10.04643900	6.81900600	-2.25669200
C	11.24265100	7.47882600	-3.45290300
C	11.54687000	8.84051400	-3.41694500
C	11.85130700	6.62488300	-4.37480600
C	12.47066900	9.35537100	-4.32969400
H	11.06828000	9.46749100	-2.67227100
C	12.77086600	7.14836500	-5.28393700
H	11.61078700	5.56734800	-4.36005300
C	13.07883000	8.51209000	-5.26224000
H	12.71801900	10.41328300	-4.30823600
H	13.25236000	6.49276100	-6.00467100
H	13.79796300	8.91591100	-5.97009600
O	9.80847300	7.93359100	-1.29044500
N	10.50879800	5.40260600	-1.87556600
Rh	8.93524300	4.10409900	-1.43902700
C	10.17907900	2.39562600	-2.22811800
C	9.95215600	2.26208700	-0.81487100
C	8.52689900	2.02582500	-0.61197400
C	7.88203500	2.10902100	-1.86870500
C	8.90172900	2.39907100	-2.87884400
C	6.43381800	1.83499400	-2.15040800
H	6.27303100	0.76050300	-2.31636600
H	5.79098300	2.14022800	-1.31941200
H	6.09292400	2.35624800	-3.04811000
C	8.65601300	2.46986100	-4.35737100
H	8.58319800	1.46302300	-4.79184900
H	7.72637800	3.00013300	-4.58098300
H	9.46406400	2.99956600	-4.86825800
C	7.89592800	1.76521300	0.72260100
H	6.80497000	1.74180600	0.65678500
H	8.22963400	0.80045800	1.12669200

H	8.17603300	2.54376500	1.44036800
C	11.00465900	2.22072100	0.25160200
H	10.63840800	2.67036900	1.17889200
H	11.30577900	1.18639300	0.47119900
H	11.89360500	2.77753900	-0.05585900
C	11.51996900	2.60035000	-2.86205100
H	12.22944800	1.84079800	-2.51381600
H	11.46231900	2.53284900	-3.95184800
H	11.90566100	3.59305000	-2.59624300
C	8.91815800	5.96706400	3.07724500
H	9.90855900	6.11542400	2.63206900
H	8.79052800	4.88422200	3.20810500
C	7.83280500	6.51204600	2.12343200
C	8.82466300	6.68124700	4.44232600
H	9.60046900	6.28277800	5.10996600
C	9.03828800	8.19650200	4.24662500
H	10.03487200	8.38544300	3.82478200
H	8.99725700	8.71167800	5.21687700
C	8.04035200	8.04293400	1.93684100
H	7.27690900	8.42753800	1.25169100
H	9.01195500	8.22666800	1.46229000
C	7.95120500	8.75137800	3.30359500
H	8.10359300	9.82907700	3.15730800
C	6.55932500	8.50368500	3.92133300
H	6.47429800	9.02426600	4.88566800
H	5.77806900	8.91301200	3.26613300
C	6.43398400	6.27576700	2.75323900
H	6.26213800	5.19700200	2.88171800
H	5.66054000	6.64710700	2.07174800
C	7.43309700	6.43460300	5.06122400
H	7.27834900	5.35870100	5.22575900
H	7.36458300	6.92099900	6.04435300
C	6.34455300	6.98845900	4.11867400
H	5.35166700	6.80883700	4.55300400
C	7.89039400	5.85537800	0.74326000
O	8.81298600	5.02034700	0.49714500
O	7.00649000	6.19635000	-0.10558400

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C	6.33124700	7.21232300	-4.24451100
C	7.62165900	7.47654100	-3.77836000
C	8.28312900	6.49710500	-3.04163700
C	7.71862100	5.24683500	-2.71010500

C	6.40199000	5.03650600	-3.16048600
C	5.72305100	5.99735900	-3.92433000
H	5.80159900	7.95396900	-4.83645300
H	8.10343200	8.42844900	-3.98578800
H	6.78112600	5.92209600	-0.89047800
H	5.88723300	4.11107300	-2.91531500
H	4.71040600	5.79319700	-4.26509100
S	9.89736200	6.72780400	-2.26912500
C	10.96777800	7.47745500	-3.53148200
C	11.23683100	8.84629800	-3.47902200
C	11.52001400	6.67085300	-4.52803100
C	12.06268400	9.41624300	-4.45082300
H	10.81128300	9.43607100	-2.67421700
C	12.34211200	7.24832900	-5.49594400
H	11.31231300	5.60593200	-4.52330700
C	12.61144000	8.61974700	-5.45845500
H	12.28184400	10.48019100	-4.41676300
H	12.77854100	6.62896700	-6.27514800
H	13.25495300	9.06604300	-6.21221300
O	9.72995300	7.80960100	-1.24340600
N	10.40585400	5.30920300	-1.97194100
Rh	8.88249100	3.94668100	-1.59888000
C	10.41328500	2.22116900	-1.71685400
C	9.62683700	1.97380600	-0.57834300
C	8.23039600	1.81641300	-1.00204800
C	8.17693800	1.94986800	-2.40985700
C	9.50922700	2.32525700	-2.86358800
C	7.00989100	1.66018900	-3.30512900
H	7.08213300	0.63590300	-3.69707600
H	6.05650600	1.73924200	-2.77419900
H	6.97554600	2.33840500	-4.16209200
C	9.95199300	2.43892900	-4.29251800
H	10.23722000	1.45623600	-4.69566600
H	9.15752400	2.84252400	-4.92681100
H	10.81874500	3.09980500	-4.37902900
C	7.11033500	1.43570600	-0.07860500
H	6.13089900	1.61669000	-0.53061000
H	7.16203000	0.36943100	0.18377900
H	7.15713300	2.00336700	0.85643500
C	10.08064600	1.88265700	0.84862200
H	9.54334200	2.60168900	1.47722700
H	9.89783500	0.88005900	1.25785300
H	11.14763400	2.09781400	0.94422900
C	11.88679000	2.48293500	-1.78130500

H	12.37931000	2.24324300	-0.83499600
H	12.35656500	1.87953700	-2.56763800
H	12.06384600	3.54439600	-1.99918000
C	8.99450500	5.98907500	2.91737900
H	9.93001800	6.01583300	2.34783000
H	8.77040700	4.93132900	3.10933800
C	7.85985400	6.61895800	2.07871700
C	9.14821100	6.75066800	4.24921600
H	9.95577300	6.28908000	4.83252900
C	9.49415200	8.22587700	3.95991600
H	10.44262500	8.28930100	3.40992500
H	9.63068200	8.77366500	4.90272800
C	8.20097000	8.11438400	1.79705400
H	7.39861700	8.56367300	1.20087700
H	9.11341800	8.17503700	1.19393300
C	8.36034000	8.86577400	3.13306000
H	8.60480300	9.91467700	2.92004500
C	7.03941900	8.79139000	3.92690900
H	7.13214500	9.34576800	4.87117000
H	6.22858000	9.26453000	3.35601200
C	6.53076800	6.55387300	2.88243400
H	6.26616800	5.50521900	3.07961000
H	5.71660000	6.98832900	2.29134700
C	7.82729400	6.67568600	5.04271800
H	7.58312000	5.62904400	5.27339300
H	7.93230700	7.19797000	6.00373800
C	6.69357700	7.31546500	4.21525900
H	5.74930400	7.25827800	4.77296900
C	7.72290000	5.90454500	0.74753500
O	8.47889000	5.00028000	0.38829500
O	6.71911900	6.34680300	-0.00361300

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C	6.10646600	7.31383100	-3.88587600
C	7.31258500	7.63495800	-3.26340900
C	8.13542100	6.59083600	-2.84715700
C	7.83932800	5.22364400	-2.98768200
C	6.62005000	4.94596800	-3.63018800
C	5.77219200	5.96865700	-4.07062700
H	5.43462700	8.10000600	-4.21939500
H	7.60365700	8.66858000	-3.09545600
H	6.31108600	3.91852200	-3.79515700
H	4.83411000	5.71207300	-4.55864600

S	9.70044500	6.85826300	-2.02256400
C	10.78313200	7.54589700	-3.31263300
C	11.21406300	8.86478000	-3.17304800
C	11.18493600	6.76098600	-4.39612600
C	12.05787800	9.41028800	-4.14400500
H	10.89359100	9.43796200	-2.30959300
C	12.02062600	7.31794700	-5.36327100
H	10.85144700	5.73094000	-4.47119200
C	12.45721100	8.64079600	-5.23782600
H	12.40229100	10.43593100	-4.04295100
H	12.33688800	6.71832600	-6.21264100
H	13.11181100	9.06869400	-5.99244800
O	9.58048000	7.91717700	-0.98876500
N	10.24823800	5.43960900	-1.62894600
Rh	9.20258100	3.88259000	-2.18206300
C	10.53690400	2.03401400	-1.86435900
C	9.73114300	2.21457700	-0.72623300
C	8.32580000	2.15111600	-1.15312700
C	8.29664500	1.82218700	-2.54787500
C	9.64681600	1.85407500	-3.01406000
C	7.09108900	1.44111400	-3.35463100
H	6.98550500	0.34785900	-3.39060000
H	6.17047200	1.84149100	-2.92180700
H	7.15957700	1.79695700	-4.38712300
C	10.10408300	1.56342200	-4.41172900
H	10.33810700	0.49498900	-4.52549400
H	9.33557900	1.81571700	-5.14746100
H	11.00890400	2.12451600	-4.66334300
C	7.14862800	2.20118100	-0.22645700
H	6.23737400	2.50063500	-0.75086300
H	6.96909900	1.21458300	0.22478900
H	7.31235800	2.91300300	0.58738200
C	10.18577900	2.45163600	0.68210100
H	9.54517800	3.17903300	1.18899100
H	10.15533800	1.51831500	1.26145400
H	11.20775100	2.83669500	0.71414500
C	12.03543900	2.03910000	-1.92632600
H	12.46810500	2.58595900	-1.08477500
H	12.43364000	1.01511300	-1.90493900
H	12.39597200	2.51349800	-2.84422400

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C	7.49338400	8.11417300	-5.64928000

C	8.41864700	8.02928500	-4.60380200
C	8.74452900	6.78103500	-4.08085200
C	8.14970200	5.58854100	-4.54532600
C	7.21669800	5.70552000	-5.59177900
C	6.90488700	6.94886500	-6.14762900
H	7.23768300	9.08225500	-6.07107500
H	8.89674200	8.92519000	-4.21803900
H	6.71618300	4.81569100	-5.96625200
H	6.19296800	7.00764100	-6.96741800
S	10.04226300	6.48744700	-2.85552000
C	11.25259200	7.81878900	-3.12010600
C	11.33041400	8.85755600	-2.19120200
C	12.10163500	7.77348200	-4.22756700
C	12.27189400	9.87195000	-2.38177500
H	10.66552900	8.84756400	-1.33427800
C	13.03623400	8.79256600	-4.41186400
H	12.03168000	6.94216900	-4.92090700
C	13.12102600	9.84061000	-3.49016800
H	12.34402300	10.68317400	-1.66226000
H	13.70279300	8.76639600	-5.26982500
H	13.85296800	10.63096600	-3.63480100
O	9.47108800	6.77306200	-1.50060500
N	10.68250600	5.16127200	-3.28406100
Rh	9.33217000	3.81109600	-4.20309200
C	8.91076000	2.09360800	-5.71394200
C	9.79528400	3.04056000	-6.36773000
C	10.99030400	3.11106600	-5.60992700
C	10.86333400	2.20007900	-4.47383500
C	9.60148400	1.53588200	-4.58697200
C	11.95789800	1.93026300	-3.48528900
H	12.37539800	2.87105300	-3.11327500
H	11.58946000	1.36892900	-2.62458800
H	12.76993500	1.35248600	-3.94903800
C	9.09117200	0.43052400	-3.70794600
H	9.35419200	-0.54864200	-4.13172000
H	9.51198400	0.48979500	-2.70293600
H	8.00225900	0.46465000	-3.60785700
C	12.21581300	3.92400900	-5.89128300
H	12.47729000	4.52256800	-5.01173000
H	13.06742000	3.27273900	-6.12920700
H	12.06736900	4.60170200	-6.73699000
C	9.49741000	3.75915300	-7.65111400
H	10.17133800	4.60675800	-7.80081700
H	9.60978200	3.08625000	-8.51237800

H	8.47489300	4.14972800	-7.67058600
C	7.58637900	1.62873500	-6.24753800
H	7.08639600	2.41135400	-6.82653000
H	7.71418100	0.76519900	-6.91608000
H	6.91215900	1.32070700	-5.44283800
C	2.71447300	2.67070200	-3.67572800
C	3.59064200	3.84672200	-3.23121600
H	1.65025900	2.89046600	-3.53401800
H	2.86862200	2.43997800	-4.73715800
H	2.94761000	1.76505400	-3.10262100
C	5.08984400	3.57571800	-3.41160000
H	3.31251400	4.74740200	-3.79662000
H	3.38909300	4.07521300	-2.17514400
C	5.96504500	4.75677500	-2.94792100
H	5.38227100	2.68422500	-2.84222100
H	5.29908000	3.35691600	-4.46789800
H	5.70098900	5.66689700	-3.49319700
H	5.76228000	4.95273300	-1.88469400
C	7.43312800	4.47385800	-3.03376700
C	8.32598800	3.77840500	-2.42758200
C	8.52615700	3.07995800	-1.13301200
C	8.43795200	3.98010000	0.09104100
H	7.42589000	4.40039600	0.11940500
H	9.12069200	4.82230400	-0.05702700
F	9.73675700	2.41847500	-1.13132600
F	7.56884000	2.06942000	-1.03356500
C	8.73851000	3.22649500	1.40258100
H	9.76088200	2.83529500	1.35558100
H	8.06969800	2.36218500	1.48081100
C	8.57945300	4.11276500	2.61992100
C	9.57488400	5.03807100	2.96602500
C	7.42783700	4.04682200	3.41486100
C	9.42373100	5.87253900	4.07352400
H	10.47589200	5.10376600	2.35994700
C	7.27186800	4.87949500	4.52511200
H	6.64763400	3.33117800	3.16324500
C	8.27038400	5.79593000	4.85820700
H	10.20833800	6.58138700	4.32580800
H	6.37197200	4.80871700	5.13105900
H	8.15284800	6.44352500	5.72314400

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Rh	1.25077200	0.31522100	-6.37626500
C	1.82751800	-1.27839100	-7.89877700

C	0.98880600	-0.31117600	-8.63459700
C	1.60901500	0.94128300	-8.59863000
C	2.80729600	0.80716500	-7.76346100
C	2.98037900	-0.60564300	-7.43792800
C	3.85596100	1.86553300	-7.62056200
H	4.47014900	1.71660500	-6.72991700
H	4.52098200	1.84482300	-8.49720400
H	3.41353700	2.86220000	-7.56199000
C	4.19281200	-1.19068700	-6.77621800
H	3.99596600	-2.19057700	-6.37989300
H	5.02009200	-1.27570200	-7.49416600
H	4.53317200	-0.56452500	-5.94658900
C	1.13199300	2.23547800	-9.18795100
H	1.00063100	3.00055500	-8.41423500
H	1.85202500	2.61577200	-9.92443200
H	0.17068100	2.11402500	-9.69337300
C	-0.31312300	-0.67321400	-9.28336600
H	-0.86800800	0.21291700	-9.59969100
H	-0.14556400	-1.30291800	-10.16791800
H	-0.95344400	-1.24024500	-8.59836300
C	1.51957900	-2.74226600	-7.79497400
H	0.48659300	-2.91229300	-7.47446100
H	1.64999700	-3.23903400	-8.76643900
H	2.17621100	-3.24091000	-7.07715900
C	-1.46066400	2.70780900	-1.57777500
C	-0.77434800	2.42574300	-2.76135400
C	-0.31993100	3.48437900	-3.54876300
C	-0.55443900	4.81257600	-3.18372100
C	-1.24098000	5.08228700	-1.99926900
C	-1.69098700	4.03123500	-1.19544200
H	-1.82242300	1.89040100	-0.95966100
H	-0.60261300	1.40354600	-3.07682000
H	-1.43169100	6.11197800	-1.70846800
H	-2.22829800	4.24455000	-0.27491600
C	0.89853500	-1.22379300	-3.94220000
F	0.03747000	-0.92720400	-2.88912000
F	0.01597800	-1.58664700	-4.97629800
C	1.70235000	-2.46694500	-3.57726000
C	0.82791500	-3.67824800	-3.19023200
H	2.37496900	-2.21100600	-2.75299800
H	2.33801500	-2.71697300	-4.43344700
H	0.20698000	-3.40274200	-2.33105500
H	0.14578600	-3.90179600	-4.01698800
C	1.66390800	-4.89706500	-2.86370600

C	1.99073300	-5.83056000	-3.85705100
C	2.16008800	-5.10394500	-1.56889200
C	2.79222600	-6.93646600	-3.56865100
H	1.60473900	-5.69234500	-4.86527100
C	2.96199200	-6.20774300	-1.27477900
H	1.90955500	-4.39476100	-0.78236600
C	3.28195900	-7.12802800	-2.27524500
H	3.02905000	-7.65144600	-4.35254300
H	3.33233200	-6.35194100	-0.26303600
H	3.90298000	-7.99023500	-2.04741800
C	2.35599100	0.79206600	-3.54667100
C	2.44605500	0.57904900	-2.02716700
H	1.63664700	-0.08435300	-1.71855000
C	1.68130800	-0.00686200	-4.39838900
C	2.35627700	3.14323500	-4.61192800
C	3.04222500	4.31398700	-4.95251000
C	3.02958600	2.04287200	-4.03488000
C	4.41568200	4.42425900	-4.74041800
H	2.47945700	5.12409000	-5.40201700
C	4.42137100	2.17719400	-3.86160300
H	-0.21790600	5.61114800	-3.83553100
C	5.10924300	3.34110400	-4.20448300
H	4.93552400	5.34099800	-5.00509600
H	4.97780100	1.33720900	-3.46134200
H	6.18442000	3.39487800	-4.05315400
S	0.56907400	3.13642200	-5.09893400
O	0.42582500	4.39762500	-5.89204500
N	0.11225200	1.80198300	-5.66837800
C	3.76906800	0.01121500	-1.46105200
H	4.56124500	0.76782800	-1.50636400
H	4.10346800	-0.82685200	-2.08798800
C	3.64425400	-0.47437800	-0.00560700
H	2.86339500	-1.24661000	0.05316300
H	4.58342000	-0.96844300	0.27843000
C	3.33903400	0.63661500	1.00667100
H	4.10448200	1.42212400	0.97086500
H	2.36979500	1.10978000	0.81440300
H	3.31564700	0.24152000	2.02884900
H	2.24086000	1.54407500	-1.54593100

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Rh	1.23321300	0.14256100	-6.08901100
C	2.35408900	-1.18759800	-7.54007600
C	1.13074800	-0.72728300	-8.15828500

C	1.17685000	0.70038300	-8.25503200
C	2.44641200	1.13915800	-7.70676000
C	3.16081700	-0.03003000	-7.26934400
C	3.00417800	2.52445000	-7.84000800
H	3.82133200	2.70590900	-7.13797400
H	3.40247100	2.66196600	-8.85597500
H	2.23677100	3.28381400	-7.67254400
C	4.54988700	-0.03306100	-6.70348000
H	4.72766500	-0.90918000	-6.07345500
H	5.29286100	-0.04975900	-7.51267600
H	4.73460400	0.85895400	-6.09885100
C	0.14306400	1.60037700	-8.86355000
H	0.04028400	2.52435100	-8.28767600
H	0.42368500	1.86362500	-9.89332300
H	-0.83704500	1.11777200	-8.89286700
C	-0.03112800	-1.60946300	-8.49613200
H	-0.73727400	-1.11025300	-9.16424600
H	0.30255000	-2.53530800	-8.97803100
H	-0.55580200	-1.86448100	-7.56332100
C	2.74511400	-2.62534500	-7.36486500
H	1.90085100	-3.23361800	-7.02734900
H	3.10089800	-3.05412800	-8.31248200
H	3.55414900	-2.74132100	-6.63708100
C	-1.63741800	3.40493100	-1.65373600
C	-0.91141300	2.87604200	-2.72249400
C	-0.48026600	3.73255000	-3.73686600
C	-0.77485900	5.09675400	-3.71052500
C	-1.49980500	5.61484700	-2.63599300
C	-1.92711800	4.77114700	-1.60742500
H	-1.98519900	2.74740400	-0.86130500
H	-0.69784800	1.81523500	-2.79823700
H	-1.73894300	6.67464500	-2.60698600
H	-2.49460100	5.17733900	-0.77408400
C	1.20025800	-0.98601500	-3.64439500
F	0.12178200	-0.79235800	-2.88252800
F	-0.27854700	-1.14329000	-5.48907400
C	1.57585500	-2.42768900	-3.77312700
C	0.40346400	-3.42987000	-3.86960700
H	2.16244000	-2.65273500	-2.86600800
H	2.26206000	-2.53869300	-4.61399400
H	-0.25142800	-3.28649000	-3.00258800
H	-0.17377100	-3.16734600	-4.75617100
C	0.88956400	-4.86207500	-3.92480400
C	0.84079800	-5.58811400	-5.12227800

C	1.41091500	-5.49598300	-2.78682000
C	1.30436000	-6.90415600	-5.18661300
H	0.42022900	-5.11961000	-6.00937900
C	1.87646600	-6.80984600	-2.84488500
H	1.44278100	-4.95722100	-1.84140400
C	1.82663200	-7.51880700	-4.04778000
H	1.25190400	-7.44978100	-6.12533900
H	2.27194600	-7.28323400	-1.94974600
H	2.18577000	-8.54344000	-4.09403100
C	2.52610700	1.08999500	-3.32435400
C	2.83951200	0.81601100	-1.84610300
H	1.93611100	0.39350800	-1.38732900
C	1.90156300	0.13828700	-4.03988700
C	2.22717500	3.32531100	-4.59441200
C	2.77165500	4.55616700	-4.97922900
C	3.00349700	2.39911400	-3.86129000
C	4.08330400	4.89928900	-4.66002900
H	2.14865200	5.23229400	-5.55308200
C	4.32816700	2.77585900	-3.55146200
H	-0.45680800	5.72776000	-4.53332900
C	4.86947700	3.99544900	-3.94654900
H	4.48488800	5.86070100	-4.96855600
H	4.95026000	2.08445300	-2.99303900
H	5.89827000	4.23675300	-3.69267500
S	0.45973600	3.04797200	-5.13399500
O	0.31964800	4.06402300	-6.23435400
N	0.03504300	1.59593000	-5.24745000
C	4.00635700	-0.16038800	-1.58128200
H	4.94355900	0.24605400	-1.98544900
H	3.81792900	-1.08700800	-2.13799200
C	4.20528800	-0.49806400	-0.09366700
H	3.26751800	-0.90409200	0.31228800
H	4.94469300	-1.30663200	-0.01838300
C	4.66826900	0.68091100	0.77126900
H	5.60873700	1.10177900	0.39353600
H	3.92849900	1.48878400	0.79455200
H	4.83926200	0.36369400	1.80612800
H	3.02919400	1.76789700	-1.34019700

INT-1

Rh	1.63320000	-0.38589400	-5.49593800
C	1.59921900	-2.04265200	-7.05022700
C	0.39394700	-1.25214800	-7.17070300
C	0.75806800	0.06795400	-7.57097500

C	2.20556000	0.13119100	-7.65498300
C	2.70874800	-1.18795500	-7.37747800
C	3.00932700	1.28780800	-8.17425700
H	4.03235100	1.26693100	-7.78663500
H	3.07095500	1.25199200	-9.27135000
H	2.56272100	2.24246900	-7.88672100
C	4.14131700	-1.60303100	-7.52949600
H	4.36572200	-2.49578800	-6.94636100
H	4.35196800	-1.81871500	-8.58605200
H	4.82318200	-0.80758400	-7.21599500
C	-0.20546300	1.16908700	-7.88167600
H	0.27202500	2.14880300	-7.85232800
H	-0.63411500	1.00731300	-8.88101600
H	-1.02149700	1.18580900	-7.15464100
C	-0.97895300	-1.76156700	-6.85630400
H	-1.74823000	-1.02516600	-7.10024700
H	-1.19302800	-2.68200900	-7.41301600
H	-1.03439500	-1.98066600	-5.78179400
C	1.58820300	-3.52382100	-6.81466900
H	1.08243900	-3.76309200	-5.87368000
H	1.04076000	-4.02373900	-7.62517900
H	2.59290700	-3.94326300	-6.77444400
C	-0.76971700	4.14041200	-1.83926300
C	-0.15932800	3.29448500	-2.76841700
C	0.60954100	3.85097800	-3.79145300
C	0.74923000	5.23512300	-3.91936100
C	0.14502800	6.07062000	-2.97893900
C	-0.60893700	5.52435800	-1.93687500
H	-1.37756500	3.71629100	-1.04469900
H	-0.29287800	2.21883000	-2.73694200
H	0.25193500	7.14831500	-3.06849000
H	-1.08299600	6.17869300	-1.21011900
C	3.94995200	-2.05481500	-4.06218700
F	3.68929600	-3.15868200	-4.83390300
F	0.47103700	-1.30381700	-4.13014700
C	5.08556800	-2.33338100	-3.11906100
C	6.39181000	-2.72977400	-3.85322100
H	4.79448000	-3.15664900	-2.45162400
H	5.26184500	-1.45976900	-2.48618500
H	6.18094600	-3.59476900	-4.49144900
H	6.68788900	-1.90812600	-4.51763400
C	7.51604300	-3.05124900	-2.89270600
C	8.43643600	-2.06766000	-2.50644400
C	7.63996900	-4.33295300	-2.33770800

C	9.45145900	-2.35268500	-1.59141700
H	8.36096700	-1.06917800	-2.93291100
C	8.65204000	-4.62306800	-1.42176700
H	6.93921600	-5.11204800	-2.63112300
C	9.56154900	-3.63253400	-1.04475800
H	10.15795300	-1.57641400	-1.30896700
H	8.73327600	-5.62414500	-1.00621600
H	10.35217100	-3.85778900	-0.33411900
C	2.97316800	0.31506600	-3.73167000
C	2.16429000	0.43395900	-2.43815000
H	1.27804700	-0.19690400	-2.53960600
C	3.26692600	-0.93806500	-4.22804900
C	3.16618000	2.71017800	-4.61479000
C	3.94681300	3.82174300	-4.93704700
C	3.75921400	1.52477900	-4.14616300
C	5.32971000	3.78934700	-4.75811400
H	3.47034600	4.69664400	-5.36461300
C	5.15666500	1.50077300	-4.00524400
H	1.29619700	5.64832800	-4.75937400
C	5.93500500	2.62119500	-4.29475600
H	5.92939000	4.66179600	-5.00212100
H	5.63159500	0.58934100	-3.65585200
H	7.01325800	2.57596000	-4.16704900
S	1.36950200	2.75663600	-5.03466900
O	1.37217900	3.58554000	-6.28853700
N	0.68992400	1.40101800	-4.85773500
C	2.98682600	0.00987700	-1.20437600
H	3.93820900	0.56226500	-1.16908700
H	3.23894100	-1.05302700	-1.29845100
C	2.23538600	0.22039300	0.12287200
H	1.25591900	-0.27386300	0.06085700
H	2.78891500	-0.29689300	0.91833500
C	2.04943000	1.68851900	0.52589600
H	3.01723300	2.19997200	0.60455900
H	1.44083300	2.24292900	-0.19679600
H	1.55320600	1.76609400	1.50042300
H	1.83869400	1.46892200	-2.32386200

TS-1a

Rh	0.42479600	-1.56764700	-0.35636600
C	0.87520400	-3.67914900	0.21919700
C	0.61271400	-3.62753800	-1.21362800
C	1.60668500	-2.81558600	-1.82964100
C	2.48141800	-2.31853800	-0.78128800

C	2.04147900	-2.89782800	0.47152000
C	3.77747300	-1.60272300	-1.01633800
H	4.09662300	-1.03766100	-0.13693700
H	4.56901600	-2.32918300	-1.25254100
H	3.69615700	-0.90614500	-1.85380600
C	2.73181300	-2.71979000	1.79071800
H	2.04812600	-2.87844200	2.62894100
H	3.55486300	-3.44085600	1.88919600
H	3.15633100	-1.71652100	1.88591000
C	1.76230900	-2.52224000	-3.29168600
H	1.96680000	-1.46113100	-3.46135400
H	2.59536600	-3.10637800	-3.70765100
H	0.85931300	-2.78290700	-3.84950100
C	-0.59214700	-4.24583300	-1.85071400
H	-0.57376500	-4.14957100	-2.93872800
H	-0.66723400	-5.31091500	-1.59950400
H	-1.49005000	-3.73821800	-1.47096800
C	0.04569300	-4.45285300	1.20015500
H	-1.01719900	-4.23930600	1.04670700
H	0.19689400	-5.53450500	1.08290100
H	0.29349900	-4.19119200	2.23240500
C	-1.23206000	4.41494100	-1.58551200
C	-0.67913100	3.15770500	-1.33921200
C	0.42550400	2.74000000	-2.08277800
C	0.97454600	3.55209600	-3.07627600
C	0.41384700	4.80809900	-3.31712700
C	-0.68457700	5.24098800	-2.57088200
H	-2.09591600	4.74555600	-1.01497900
H	-1.10497100	2.49097900	-0.59799500
H	0.83122000	5.44489200	-4.09263400
H	-1.11959900	6.21840900	-2.76228600
C	-1.17793800	-0.58263400	1.57870200
F	-1.66956700	-1.82749300	-0.18224300
F	-1.30535300	-1.63022300	2.39466300
C	-2.44451400	0.14607600	1.27823800
C	-3.73735000	-0.69023200	1.42581600
H	-2.33363800	0.52971600	0.26132200
H	-2.47940800	1.02425200	1.94236000
H	-3.48778100	-1.72712600	1.19453200
H	-4.09233000	-0.65324400	2.46197200
C	-4.82133100	-0.21899500	0.47922700
C	-5.98842400	0.39995900	0.93869800
C	-4.65181100	-0.40692000	-0.90223900
C	-6.97200200	0.82513500	0.04085300

H	-6.13305600	0.54720000	2.00736300
C	-5.63077800	0.01905000	-1.79848800
H	-3.74250300	-0.88981600	-1.25350900
C	-6.79489500	0.63657900	-1.33005100
H	-7.87458400	1.30263000	0.41434500
H	-5.48665500	-0.13316900	-2.86515100
H	-7.55822700	0.96677500	-2.02998500
C	0.83453800	0.89016400	1.60389800
C	0.39116300	1.72737200	2.81342700
H	-0.65196100	2.03661800	2.66355600
C	0.10928100	-0.17742100	1.22814600
C	2.37386400	1.46368700	-0.40734600
C	3.61843100	1.92589700	-0.85335400
C	2.12799900	1.29971700	0.97542900
C	4.64511800	2.22397700	0.03874200
H	3.77349500	2.02599100	-1.92105600
C	3.19071100	1.60496600	1.85427600
H	1.81313300	3.18552000	-3.65813900
C	4.43013800	2.04983300	1.40530600
H	5.60224900	2.58037000	-0.33209800
H	3.03682100	1.47736600	2.92122900
H	5.21935600	2.26227100	2.12165400
S	1.15278200	1.10094100	-1.77794200
O	2.07760100	0.87242500	-2.94197700
N	0.00514900	0.17789800	-1.40553700
C	0.48232000	0.99846200	4.17136900
H	1.51730700	0.67428500	4.35135000
H	-0.11291800	0.07873000	4.11334300
C	-0.00111700	1.83828800	5.36584100
H	-1.03257000	2.17129600	5.18037500
H	-0.04705800	1.18764400	6.24926700
C	0.87831300	3.05284000	5.68786900
H	1.91422500	2.74803700	5.88368600
H	0.89504200	3.77765400	4.86633300
H	0.51321000	3.57649400	6.57854600
H	0.97455600	2.65212000	2.84268900

INT-1a

Rh	1.43595000	-0.16347600	-6.11453300
C	2.32614400	-0.94139900	-8.06706200
C	0.95207300	-0.61997600	-8.35940500
C	0.74694800	0.77812100	-8.12635400
C	2.01342400	1.35072200	-7.73739000
C	2.98571800	0.28247800	-7.69771100

C	2.30620700	2.81792300	-7.65012200
H	3.17336500	3.02637200	-7.01919300
H	2.52380700	3.20560600	-8.65603000
H	1.45303500	3.36984800	-7.25068100
C	4.45736100	0.43663200	-7.45399200
H	4.86115400	-0.42791800	-6.92137500
H	4.99077700	0.52473800	-8.41029400
H	4.67629500	1.33021200	-6.86420700
C	-0.52952300	1.53497800	-8.34560200
H	-0.65683600	2.31835300	-7.59434600
H	-0.53289800	2.00091900	-9.34136200
H	-1.39586500	0.87169300	-8.28212200
C	-0.10252300	-1.61983200	-8.69778000
H	-0.95386700	-1.15680500	-9.20283900
H	0.29142400	-2.41739300	-9.33537300
H	-0.44993100	-2.05847800	-7.74832600
C	2.97237300	-2.28043400	-8.27094200
H	2.25762000	-3.09194300	-8.10944000
H	3.36027400	-2.37340100	-9.29492000
H	3.80399800	-2.43204000	-7.58033400
C	-0.90042700	2.03324800	-0.65125400
C	-0.26898300	1.78561800	-1.87017600
C	-0.50484500	2.64704300	-2.94305100
C	-1.36905700	3.73568200	-2.82526000
C	-1.99906800	3.97174500	-1.60139300
C	-1.76194300	3.12575000	-0.51586600
H	-0.72748800	1.36767600	0.19006700
H	0.37980900	0.92729200	-2.00540400
H	-2.67899100	4.81321600	-1.49892900
H	-2.25441700	3.31255900	0.43474800
C	2.62100800	-1.33320200	-4.62026700
F	0.01889700	-1.59243800	-5.79527800
F	3.67748700	-1.99596000	-5.22790700
C	1.78893700	-2.24483700	-3.76331800
C	1.52528000	-3.63538800	-4.38170100
H	0.84413500	-1.73663200	-3.56651000
H	2.31229700	-2.36566800	-2.80069400
H	1.18349600	-3.47387800	-5.40613900
H	2.45729600	-4.21067500	-4.41183500
C	0.46441200	-4.39178900	-3.61091900
C	0.78632300	-5.46879400	-2.77701300
C	-0.87981800	-3.99873600	-3.71678800
C	-0.20751400	-6.14341500	-2.06232800
H	1.82379200	-5.78629200	-2.68934900

C	-1.87240400	-4.67057100	-3.00428300
H	-1.12503300	-3.16048700	-4.36462300
C	-1.54021600	-5.74556000	-2.17398900
H	0.06059800	-6.97996900	-1.42143000
H	-2.90904200	-4.35635200	-3.09875900
H	-2.31545800	-6.26978500	-1.62072100
C	3.29767700	0.97874600	-3.72568100
C	4.18216900	0.50520100	-2.56089700
H	3.64116100	-0.27765700	-2.01382500
C	2.74999000	0.03540100	-4.49034500
C	1.97602700	3.13259300	-4.28114100
C	1.97975100	4.52600400	-4.42851300
C	3.15832200	2.44797500	-3.92461900
C	3.13917700	5.27036000	-4.23348500
H	1.05786900	5.01558400	-4.71924300
C	4.31742700	3.23149600	-3.72794600
H	-1.55004000	4.36691400	-3.68844000
C	4.31886400	4.61298500	-3.88333700
H	3.12056000	6.34958000	-4.35725500
H	5.24437900	2.73471300	-3.46134500
H	5.23866100	5.17145900	-3.73163100
S	0.30620900	2.34246900	-4.53771400
O	-0.32803800	3.30516900	-5.50200700
N	0.28081600	0.82544300	-4.69063500
C	5.55159600	-0.06716400	-2.98528800
H	6.12068500	0.69286000	-3.54027400
H	5.37552700	-0.88820800	-3.68953800
C	6.40111700	-0.57919000	-1.81008100
H	5.82502900	-1.32860900	-1.24857300
H	7.27130700	-1.11018900	-2.21838100
C	6.89072200	0.51341600	-0.85125700
H	7.48597500	1.26683100	-1.38283900
H	6.05977300	1.03254900	-0.36001800
H	7.52243200	0.08927700	-0.06256500
H	4.31480500	1.33297000	-1.85704400

INT-1b

Rh	1.54381400	-0.14250900	-5.46975300
C	1.73659600	-1.78195700	-7.11619900
C	0.42030500	-1.75596000	-6.60130000
C	-0.12077600	-0.41511400	-6.81205200
C	0.85267400	0.33681800	-7.56203600
C	2.02413200	-0.47205600	-7.70007900
C	0.64364300	1.72444000	-8.08085200

H	1.57652000	2.17507600	-8.42583900
H	-0.06163700	1.70907300	-8.92272400
H	0.23017200	2.36571100	-7.29676800
C	3.20526900	-0.15132800	-8.56656200
H	4.09633600	-0.69295100	-8.25008100
H	2.98929300	-0.43308200	-9.60740000
H	3.43821100	0.91566200	-8.55225600
C	-1.49708800	0.02875700	-6.42276000
H	-2.24484800	-0.32957700	-7.14442900
H	-1.75120300	-0.36051400	-5.43331800
H	-1.55836600	1.11861100	-6.37489300
C	-0.30868000	-2.83787900	-5.86891400
H	-1.29014100	-3.02098700	-6.32278100
H	0.24765700	-3.77875100	-5.86720800
H	-0.45866400	-2.51158800	-4.83212700
C	2.63457200	-2.98187400	-7.19042000
H	2.33092800	-3.75319200	-6.47799600
H	2.59185300	-3.42382900	-8.19582300
H	3.67184400	-2.71860400	-6.98378600
C	3.58079400	4.97501600	-7.88646800
C	2.84929100	4.60719100	-6.75510600
C	3.20967000	3.45915100	-6.04473100
C	4.29431500	2.68097800	-6.45323800
C	5.03140500	3.06382800	-7.57686700
C	4.67361800	4.20707100	-8.29685400
H	3.30462800	5.86904600	-8.43960700
H	2.01453300	5.20362800	-6.40200200
H	5.88533900	2.46795500	-7.88903400
H	5.24895500	4.50160300	-9.17059100
C	4.66745600	-0.70883300	-4.77225400
F	4.79957100	-1.02923900	-6.10340200
F	0.39487100	-0.75178000	-3.86918800
C	5.95978400	-0.98084100	-4.05680300
C	6.35031300	-2.48149700	-4.05371500
H	5.89529600	-0.61150100	-3.02955300
H	6.76142800	-0.41397600	-4.55084500
H	5.56061300	-3.04994900	-3.54715800
H	6.38338900	-2.83392700	-5.09069500
C	7.68281000	-2.72353100	-3.37882600
C	8.87938000	-2.64126300	-4.10484800
C	7.75502700	-2.99482500	-2.00560400
C	10.11300100	-2.82154300	-3.47768800
H	8.84245500	-2.43900800	-5.17348600
C	8.98621600	-3.17665400	-1.37348000

H	6.83597000	-3.07140700	-1.42786400
C	10.17029100	-3.08912900	-2.10827200
H	11.02903600	-2.75812200	-4.05938300
H	9.02013000	-3.39169700	-0.30854100
H	11.12972000	-3.23340100	-1.61884700
C	3.19595700	0.22720000	-3.03035500
C	2.41568400	-0.57903900	-2.05312200
H	2.86463300	-1.58284900	-1.98661000
C	3.51209700	-0.27140900	-4.28974900
C	3.46803400	2.78581600	-3.32702200
C	4.10801500	3.95969800	-2.91777700
C	3.71411500	1.57497900	-2.66121400
C	5.03337900	3.94278700	-1.87766700
H	3.85651600	4.89037800	-3.41519700
C	4.62551500	1.58275600	-1.58224900
H	4.56434900	1.78688700	-5.90110900
C	5.29406100	2.74444800	-1.21007600
H	5.53184300	4.86002400	-1.57709300
H	4.82415000	0.65889300	-1.04845100
H	6.00490800	2.71420900	-0.38908800
S	2.15010700	2.98339000	-4.61367400
O	1.49878300	4.26585700	-4.23085300
N	1.24034600	1.78921900	-4.80185300
C	2.08065400	-0.00988700	-0.66620800
H	1.85308400	1.05997600	-0.74870100
H	2.94453700	-0.09090800	0.00608600
C	0.87567100	-0.72736900	-0.02604700
H	1.01377400	-1.81532700	-0.11222400
H	0.86875100	-0.50816900	1.05016300
C	-0.47418200	-0.32239000	-0.63464000
H	-0.67697100	0.73938800	-0.44675200
H	-0.49581800	-0.47317600	-1.71856600
H	-1.29241200	-0.90129500	-0.18960000
H	1.46855100	-0.76429400	-2.62054600

TS-2

Rh	0.42479600	-1.56764700	-0.35636600
C	0.87520400	-3.67914900	0.21919700
C	0.61271400	-3.62753800	-1.21362800
C	1.60668500	-2.81558600	-1.82964100
C	2.48141800	-2.31853800	-0.78128800
C	2.04147900	-2.89782800	0.47152000
C	3.77747300	-1.60272300	-1.01633800
H	4.09662300	-1.03766100	-0.13693700

H	4.56901600	-2.32918300	-1.25254100
H	3.69615700	-0.90614500	-1.85380600
C	2.73181300	-2.71979000	1.79071800
H	2.04812600	-2.87844200	2.62894100
H	3.55486300	-3.44085600	1.88919600
H	3.15633100	-1.71652100	1.88591000
C	1.76230900	-2.52224000	-3.29168600
H	1.96680000	-1.46113100	-3.46135400
H	2.59536600	-3.10637800	-3.70765100
H	0.85931300	-2.78290700	-3.84950100
C	-0.59214700	-4.24583300	-1.85071400
H	-0.57376500	-4.14957100	-2.93872800
H	-0.66723400	-5.31091500	-1.59950400
H	-1.49005000	-3.73821800	-1.47096800
C	0.04569300	-4.45285300	1.20015500
H	-1.01719900	-4.23930600	1.04670700
H	0.19689400	-5.53450500	1.08290100
H	0.29349900	-4.19119200	2.23240500
C	-1.23206000	4.41494100	-1.58551200
C	-0.67913100	3.15770500	-1.33921200
C	0.42550400	2.74000000	-2.08277800
C	0.97454600	3.55209600	-3.07627600
C	0.41384700	4.80809900	-3.31712700
C	-0.68457700	5.24098800	-2.57088200
H	-2.09591600	4.74555600	-1.01497900
H	-1.10497100	2.49097900	-0.59799500
H	0.83122000	5.44489200	-4.09263400
H	-1.11959900	6.21840900	-2.76228600
C	-1.17793800	-0.58263400	1.57870200
F	-1.66956700	-1.82749300	-0.18224300
F	-1.30535300	-1.63022300	2.39466300
C	-2.44451400	0.14607600	1.27823800
C	-3.73735000	-0.69023200	1.42581600
H	-2.33363800	0.52971600	0.26132200
H	-2.47940800	1.02425200	1.94236000
H	-3.48778100	-1.72712600	1.19453200
H	-4.09233000	-0.65324400	2.46197200
C	-4.82133100	-0.21899500	0.47922700
C	-5.98842400	0.39995900	0.93869800
C	-4.65181100	-0.40692000	-0.90223900
C	-6.97200200	0.82513500	0.04085300
H	-6.13305600	0.54720000	2.00736300
C	-5.63077800	0.01905000	-1.79848800
H	-3.74250300	-0.88981600	-1.25350900

C	-6.79489500	0.63657900	-1.33005100
H	-7.87458400	1.30263000	0.41434500
H	-5.48665500	-0.13316900	-2.86515100
H	-7.55822700	0.96677500	-2.02998500
C	0.83453800	0.89016400	1.60389800
C	0.39116300	1.72737200	2.81342700
H	-0.65196100	2.03661800	2.66355600
C	0.10928100	-0.17742100	1.22814600
C	2.37386400	1.46368700	-0.40734600
C	3.61843100	1.92589700	-0.85335400
C	2.12799900	1.29971700	0.97542900
C	4.64511800	2.22397700	0.03874200
H	3.77349500	2.02599100	-1.92105600
C	3.19071100	1.60496600	1.85427600
H	1.81313300	3.18552000	-3.65813900
C	4.43013800	2.04983300	1.40530600
H	5.60224900	2.58037000	-0.33209800
H	3.03682100	1.47736600	2.92122900
H	5.21935600	2.26227100	2.12165400
S	1.15278200	1.10094100	-1.77794200
O	2.07760100	0.87242500	-2.94197700
N	0.00514900	0.17789800	-1.40553700
C	0.48232000	0.99846200	4.17136900
H	1.51730700	0.67428500	4.35135000
H	-0.11291800	0.07873000	4.11334300
C	-0.00111700	1.83828800	5.36584100
H	-1.03257000	2.17129600	5.18037500
H	-0.04705800	1.18764400	6.24926700
C	0.87831300	3.05284000	5.68786900
H	1.91422500	2.74803700	5.88368600
H	0.89504200	3.77765400	4.86633300
H	0.51321000	3.57649400	6.57854600
H	0.97455600	2.65212000	2.84268900

INT-2

Rh	1.43595000	-0.16347600	-6.11453300
C	2.32614400	-0.94139900	-8.06706200
C	0.95207300	-0.61997600	-8.35940500
C	0.74694800	0.77812100	-8.12635400
C	2.01342400	1.35072200	-7.73739000
C	2.98571800	0.28247800	-7.69771100
C	2.30620700	2.81792300	-7.65012200
H	3.17336500	3.02637200	-7.01919300
H	2.52380700	3.20560600	-8.65603000

H	1.45303500	3.36984800	-7.25068100
C	4.45736100	0.43663200	-7.45399200
H	4.86115400	-0.42791800	-6.92137500
H	4.99077700	0.52473800	-8.41029400
H	4.67629500	1.33021200	-6.86420700
C	-0.52952300	1.53497800	-8.34560200
H	-0.65683600	2.31835300	-7.59434600
H	-0.53289800	2.00091900	-9.34136200
H	-1.39586500	0.87169300	-8.28212200
C	-0.10252300	-1.61983200	-8.69778000
H	-0.95386700	-1.15680500	-9.20283900
H	0.29142400	-2.41739300	-9.33537300
H	-0.44993100	-2.05847800	-7.74832600
C	2.97237300	-2.28043400	-8.27094200
H	2.25762000	-3.09194300	-8.10944000
H	3.36027400	-2.37340100	-9.29492000
H	3.80399800	-2.43204000	-7.58033400
C	-0.90042700	2.03324800	-0.65125400
C	-0.26898300	1.78561800	-1.87017600
C	-0.50484500	2.64704300	-2.94305100
C	-1.36905700	3.73568200	-2.82526000
C	-1.99906800	3.97174500	-1.60139300
C	-1.76194300	3.12575000	-0.51586600
H	-0.72748800	1.36767600	0.19006700
H	0.37980900	0.92729200	-2.00540400
H	-2.67899100	4.81321600	-1.49892900
H	-2.25441700	3.31255900	0.43474800
C	2.62100800	-1.33320200	-4.62026700
F	0.01889700	-1.59243800	-5.79527800
F	3.67748700	-1.99596000	-5.22790700
C	1.78893700	-2.24483700	-3.76331800
C	1.52528000	-3.63538800	-4.38170100
H	0.84413500	-1.73663200	-3.56651000
H	2.31229700	-2.36566800	-2.80069400
H	1.18349600	-3.47387800	-5.40613900
H	2.45729600	-4.21067500	-4.41183500
C	0.46441200	-4.39178900	-3.61091900
C	0.78632300	-5.46879400	-2.77701300
C	-0.87981800	-3.99873600	-3.71678800
C	-0.20751400	-6.14341500	-2.06232800
H	1.82379200	-5.78629200	-2.68934900
C	-1.87240400	-4.67057100	-3.00428300
H	-1.12503300	-3.16048700	-4.36462300
C	-1.54021600	-5.74556000	-2.17398900

H	0.06059800	-6.97996900	-1.42143000
H	-2.90904200	-4.35635200	-3.09875900
H	-2.31545800	-6.26978500	-1.62072100
C	3.29767700	0.97874600	-3.72568100
C	4.18216900	0.50520100	-2.56089700
H	3.64116100	-0.27765700	-2.01382500
C	2.74999000	0.03540100	-4.49034500
C	1.97602700	3.13259300	-4.28114100
C	1.97975100	4.52600400	-4.42851300
C	3.15832200	2.44797500	-3.92461900
C	3.13917700	5.27036000	-4.23348500
H	1.05786900	5.01558400	-4.71924300
C	4.31742700	3.23149600	-3.72794600
H	-1.55004000	4.36691400	-3.68844000
C	4.31886400	4.61298500	-3.88333700
H	3.12056000	6.34958000	-4.35725500
H	5.24437900	2.73471300	-3.46134500
H	5.23866100	5.17145900	-3.73163100
S	0.30620900	2.34246900	-4.53771400
O	-0.32803800	3.30516900	-5.50200700
N	0.28081600	0.82544300	-4.69063500
C	5.55159600	-0.06716400	-2.98528800
H	6.12068500	0.69286000	-3.54027400
H	5.37552700	-0.88820800	-3.68953800
C	6.40111700	-0.57919000	-1.81008100
H	5.82502900	-1.32860900	-1.24857300
H	7.27130700	-1.11018900	-2.21838100
C	6.89072200	0.51341600	-0.85125700
H	7.48597500	1.26683100	-1.38283900
H	6.05977300	1.03254900	-0.36001800
H	7.52243200	0.08927700	-0.06256500
H	4.31480500	1.33297000	-1.85704400

TS-2b

Rh	1.34246600	0.78856500	-1.20555500
C	0.52487100	0.87125500	0.87610300
C	-0.51783200	1.27460800	-0.05155500
C	-0.82064600	0.17261500	-0.90009900
C	0.06015400	-0.92459200	-0.53222500
C	0.84127000	-0.50586000	0.59554800
C	0.02951400	-2.27772800	-1.17661400
H	0.89855700	-2.87969900	-0.89570900
H	-0.86947200	-2.83439200	-0.87825900
H	0.02301200	-2.17913300	-2.26685500

C	1.76875200	-1.37618200	1.38940800
H	2.59140500	-0.79869900	1.81163400
H	1.22024700	-1.84845000	2.21588400
H	2.19214900	-2.17673400	0.77666700
C	-1.79599000	0.11508900	-2.03053700
H	-1.26133400	-0.10250000	-2.96477200
H	-2.53339000	-0.68113500	-1.86592100
H	-2.33343300	1.05814500	-2.15592100
C	-1.08433800	2.66002000	-0.11167100
H	-1.88923000	2.73739000	-0.84648600
H	-1.47832000	2.96439700	0.86552000
H	-0.28984500	3.35876500	-0.40126500
C	0.97834200	1.69922800	2.04187200
H	1.19338600	2.72711300	1.73373300
H	0.19355100	1.73823700	2.81085500
H	1.88119300	1.29485300	2.49953400
C	-1.01413000	4.33155000	-4.12191000
C	-0.03199800	3.36443300	-3.89539100
C	0.13568200	2.34822300	-4.84007800
C	-0.66071500	2.27520700	-5.98588100
C	-1.64570100	3.24394000	-6.19115800
C	-1.82041900	4.27258600	-5.26237400
H	-1.14983800	5.13464900	-3.40164600
H	0.59478900	3.37909000	-3.00352300
H	-2.27057300	3.19724300	-7.07931400
H	-2.58390200	5.02865600	-5.42806800
C	4.29345600	0.75140800	-0.13333000
F	3.80193500	1.05519900	1.11497100
F	1.71337400	2.73822900	-1.62192300
C	5.79148000	0.63859700	-0.08486700
C	6.28802400	-0.36880500	0.98323600
H	6.22465200	1.62462300	0.13683800
H	6.16851800	0.33736500	-1.06720300
H	5.89091500	-0.06700500	1.95785400
H	5.86720500	-1.35700300	0.75836500
C	7.79826300	-0.44681200	1.03587400
C	8.50050200	-1.35073200	0.22675600
C	8.53220200	0.41120700	1.86681300
C	9.89541500	-1.39708000	0.24510300
H	7.94775000	-2.02998900	-0.41946000
C	9.92714900	0.36930000	1.88869300
H	8.00409900	1.11519400	2.50684100
C	10.61390800	-0.53555800	1.07660600
H	10.42035500	-2.10920100	-0.38643100

H	10.47711800	1.04015700	2.54368700
H	11.69981800	-0.57217400	1.09488800
C	3.54456600	0.32255800	-2.51594100
C	3.79630200	-1.12169000	-2.94673200
H	2.93510100	-1.71748900	-2.63121100
C	3.47021500	0.60540100	-1.15655600
C	2.92997100	1.90058900	-4.45146600
C	3.26941900	2.90311900	-5.35548700
C	3.81946000	1.46021000	-3.46646900
C	4.52421800	3.50675600	-5.27669700
H	2.54760200	3.21815900	-6.10292300
C	5.07291800	2.08583100	-3.39404700
H	-0.49634200	1.47252900	-6.69612800
C	5.42330800	3.09411400	-4.29320000
H	4.79213000	4.29875200	-5.97009500
H	5.78023500	1.78692200	-2.62883100
H	6.39975800	3.56366700	-4.21362300
S	1.35497400	1.01041900	-4.55543800
O	1.35174300	0.25898600	-5.84484600
N	1.21168200	0.18107800	-3.27504600
C	4.09548300	-1.38439500	-4.42814900
H	4.96419200	-0.78946900	-4.74292500
H	3.24769800	-1.05887900	-5.03725900
C	4.37158800	-2.86992100	-4.72301100
H	3.51051300	-3.46972200	-4.39539800
H	4.42736700	-2.99389200	-5.81209300
C	5.65583300	-3.42873700	-4.09601500
H	6.53236200	-2.84676200	-4.40863800
H	5.62274300	-3.41519100	-2.99982800
H	5.82233100	-4.46818600	-4.40166500
H	4.64373600	-1.45674500	-2.32809900

INT-2b

Rh	1.22196600	0.93381600	-1.11763200
C	0.34304100	1.02833900	0.86833000
C	-0.73980000	1.44942000	-0.02578600
C	-1.04074400	0.38440200	-0.88903000
C	-0.15425900	-0.73341500	-0.54799500
C	0.61663000	-0.36266700	0.59732800
C	-0.21669700	-2.08803100	-1.19093400
H	0.68469500	-2.67171800	-0.98521900
H	-1.07813600	-2.65953800	-0.81759200
H	-0.31642700	-2.00803700	-2.27775500
C	1.50519600	-1.26276300	1.40444200

H	2.37953200	-0.72593600	1.77349700
H	0.95398100	-1.66116500	2.26765300
H	1.85654800	-2.11489600	0.81568500
C	-2.06566200	0.34558500	-1.98424500
H	-1.65835600	-0.09810900	-2.89853200
H	-2.93215200	-0.26104000	-1.68584400
H	-2.42776100	1.34536300	-2.23640800
C	-1.27291300	2.84989000	-0.06120800
H	-2.08385400	2.95842100	-0.78626900
H	-1.65140500	3.15495900	0.92199100
H	-0.46296700	3.53425800	-0.34518400
C	0.84092600	1.84091700	2.02655400
H	0.95267200	2.89154300	1.74215000
H	0.13589100	1.79220000	2.86940100
H	1.81415900	1.48887700	2.36997600
C	-1.01959200	3.98672900	-3.89790200
C	0.09260800	3.15648400	-3.73356000
C	0.26302200	2.10954100	-4.64169100
C	-0.63038300	1.87381000	-5.69257400
C	-1.73769100	2.71074000	-5.82919200
C	-1.92940800	3.76789000	-4.93536000
H	-1.17272000	4.80815500	-3.20331900
H	0.78396100	3.28140300	-2.89344000
H	-2.44390400	2.53949800	-6.63663200
H	-2.78932000	4.42281200	-5.05028600
C	4.14608900	0.71542400	-0.27388600
F	3.71602800	0.97996600	1.02210700
F	1.70845500	2.89555600	-1.44440200
C	5.64030200	0.55887100	-0.23646600
C	6.10607900	-0.55188700	0.74110700
H	6.09333500	1.51010100	0.07946000
H	6.03287500	0.33762900	-1.23129000
H	5.69163800	-0.33500500	1.73074100
H	5.67735200	-1.50837100	0.41682600
C	7.61328300	-0.65734900	0.81675000
C	8.31775300	-1.54738600	-0.00562100
C	8.34605700	0.16297500	1.68686400
C	9.71147600	-1.61718200	0.03706200
H	7.76694600	-2.19830000	-0.68217900
C	9.73929100	0.09810700	1.73330700
H	7.81673200	0.85560100	2.33821800
C	10.42773500	-0.79311400	0.90720700
H	10.23680600	-2.31857400	-0.60625400
H	10.28706300	0.73985400	2.41881700

H	11.51249200	-0.84788100	0.94469300
C	3.38820900	0.39746600	-2.72323500
C	4.08190900	-0.97163900	-2.98815500
H	3.49771200	-1.71651200	-2.43409300
C	3.22647800	0.65550600	-1.23132000
C	3.19665000	2.00000000	-4.57523700
C	3.56291600	2.98989400	-5.48240000
C	4.01235200	1.53822100	-3.54185900
C	4.81966000	3.57067000	-5.32385600
H	2.88913200	3.30334100	-6.27394000
C	5.27646000	2.12123700	-3.41522300
H	-0.44742600	1.05676600	-6.38067200
C	5.66431900	3.13355000	-4.29567800
H	5.14228000	4.36014700	-5.99608600
H	5.95324500	1.81161100	-2.62859100
H	6.64171300	3.59286300	-4.17614100
S	1.70560000	1.02874500	-4.56381500
O	1.60006800	0.15277500	-5.75768100
N	1.92039600	0.34767100	-3.13558600
C	4.23633000	-1.42424800	-4.44621800
H	4.86902700	-0.71211000	-4.99470500
H	3.25993000	-1.41468500	-4.93947300
C	4.84040100	-2.83433000	-4.58079700
H	4.21495300	-3.55011400	-4.02799500
H	4.78110500	-3.13324000	-5.63579600
C	6.29579700	-2.96083500	-4.11350000
H	6.94398300	-2.25407500	-4.64709900
H	6.40215000	-2.76181600	-3.04056200
H	6.68230800	-3.97004500	-4.29747600
H	5.06685900	-0.93240300	-2.51081800

TS-2c

Rh	0.98430100	0.08433900	-5.98521900
C	2.63255800	-1.09170200	-7.09723200
C	1.41765200	-1.13258500	-7.83112500
C	1.09401800	0.22996100	-8.25199400
C	2.14163700	1.08234400	-7.81859500
C	3.05090200	0.29332900	-7.02132800
C	2.31515100	2.52387800	-8.18702900
H	2.93360700	3.05776700	-7.46299900
H	2.81226900	2.58934600	-9.16540200
H	1.36123300	3.04921700	-8.24360300
C	4.36132800	0.75109200	-6.45281700
H	4.55622400	0.29638900	-5.47664000

H	5.18784000	0.46950800	-7.12036600
H	4.39139900	1.83435300	-6.32233700
C	-0.13834500	0.59409800	-9.02136600
H	-0.24004600	1.67710400	-9.12550000
H	-0.12879900	0.15158700	-10.02648000
H	-1.01650200	0.21648900	-8.48454400
C	0.57117900	-2.31750200	-8.16768700
H	0.41537600	-2.38864600	-9.25122000
H	1.02303700	-3.25247800	-7.82693600
H	-0.40421500	-2.18660000	-7.68089500
C	3.44138800	-2.25861500	-6.61357100
H	2.82951600	-3.14827700	-6.44413600
H	4.20603300	-2.52114100	-7.35830200
H	3.97023700	-2.02849200	-5.68316100
C	-1.56318200	3.78207000	-1.55358400
C	-0.86130400	3.13990000	-2.57534700
C	-0.35891700	3.90548500	-3.62924100
C	-0.55773900	5.28642700	-3.69034300
C	-1.25665800	5.91525100	-2.65964500
C	-1.75467600	5.16524300	-1.59077900
H	-1.96865600	3.19751500	-0.73236000
H	-0.73214000	2.06342100	-2.58928700
H	-1.42136000	6.98860100	-2.69725500
H	-2.30238600	5.65854800	-0.79223900
C	0.78481900	-0.72199400	-3.92257000
F	-0.49993700	-0.61396100	-3.47688700
F	-0.87322300	-0.70106500	-6.17018900
C	1.28303100	-2.13178800	-3.72421400
C	0.22338400	-3.18365000	-4.13384400
H	1.52686600	-2.26620900	-2.65890700
H	2.21289100	-2.28095500	-4.27505300
H	-0.61533800	-3.10888800	-3.43269100
H	-0.18241600	-2.91210200	-5.11280500
C	0.77138800	-4.59492500	-4.13618500
C	0.83963900	-5.33964900	-5.32157900
C	1.22522100	-5.19772000	-2.95224800
C	1.35372500	-6.63887900	-5.33113300
H	0.46672200	-4.90097000	-6.24396900
C	1.74164000	-6.49348200	-2.95589100
H	1.16561800	-4.64912800	-2.01446200
C	1.81091900	-7.21945800	-4.14783000
H	1.39108300	-7.19730600	-6.26315000
H	2.08444800	-6.94037100	-2.02598300
H	2.21025000	-8.23018000	-4.15104700

C	2.47451000	1.12244900	-3.24164400
C	2.90427300	0.54419900	-1.89147400
H	2.04916200	0.01462700	-1.45249400
C	1.51777500	0.46783700	-3.93346500
C	2.31208600	3.32881500	-4.49525700
C	2.87151400	4.55570100	-4.87541400
C	3.02135200	2.41565500	-3.67359600
C	4.14665200	4.91640500	-4.45249600
H	2.29550400	5.21280500	-5.51765100
C	4.29588200	2.83769100	-3.22684300
H	-0.19182000	5.84847900	-4.54273000
C	4.85198200	4.05129400	-3.61001900
H	4.58106300	5.86043900	-4.76848200
H	4.86981600	2.18033800	-2.58357300
H	5.84346600	4.32110600	-3.25577900
S	0.55996900	3.09311600	-4.96246800
O	0.36877000	3.93935000	-6.17593500
N	0.10438200	1.61594600	-4.85687200
C	4.09664500	-0.43703500	-1.93866500
H	4.98745300	0.06414000	-2.34258600
H	3.85723400	-1.23977300	-2.64715800
C	4.44293000	-1.06003100	-0.57502400
H	3.54890300	-1.55408600	-0.16786000
H	5.18316700	-1.85563700	-0.73350300
C	4.99276100	-0.06833400	0.45823400
H	5.89543600	0.43105200	0.08359000
H	4.26281100	0.70895500	0.71017300
H	5.26043400	-0.58017400	1.38957800
H	3.13030300	1.37184700	-1.20834500

INT-2c

Rh	1.70027100	-0.37362600	-5.21681800
C	1.44263400	-2.11117400	-6.50222300
C	0.27867800	-1.26085200	-6.77077500
C	0.74275900	-0.05209800	-7.31649300
C	2.20256700	-0.12537500	-7.42150500
C	2.60719500	-1.42984400	-7.00657300
C	3.08178000	0.87377700	-8.11547900
H	4.12557800	0.75917300	-7.80764500
H	3.04035400	0.73257800	-9.20570600
H	2.78232400	1.89820000	-7.88954900
C	3.99035000	-1.98800900	-7.18182200
H	4.09241400	-2.97956500	-6.73675300
H	4.21616200	-2.08442700	-8.25237500

H	4.75268500	-1.33873000	-6.74066600
C	-0.07904700	1.13151700	-7.73665400
H	0.42688800	2.06999400	-7.49422800
H	-0.24598000	1.11681200	-8.82293800
H	-1.05847700	1.13596600	-7.25024300
C	-1.11292900	-1.61474000	-6.34187000
H	-1.83964900	-0.86215500	-6.66009500
H	-1.42429100	-2.58183900	-6.75589100
H	-1.13324600	-1.67935800	-5.24517700
C	1.33216600	-3.52239800	-6.00634200
H	0.71709900	-3.55627500	-5.10098000
H	0.85921200	-4.16548300	-6.76193100
H	2.30664000	-3.95641500	-5.76766600
C	-1.43124900	4.40299000	-2.94990800
C	-0.35502200	3.58171600	-3.29189200
C	0.56898700	4.04272200	-4.23007800
C	0.43470700	5.29234000	-4.84376100
C	-0.63880900	6.10597400	-4.48317300
C	-1.56769300	5.66289600	-3.53666500
H	-2.16470400	4.05352600	-2.22916200
H	-0.23773400	2.59008800	-2.86890400
H	-0.75626500	7.08012600	-4.94916800
H	-2.40560000	6.29865900	-3.26428400
C	4.13596100	-1.05676400	-3.37288400
F	4.98746100	-0.66984500	-2.32965700
F	0.48141400	-1.02600700	-3.72715200
C	4.46959300	-2.45397600	-3.78163000
C	4.35809500	-3.45406500	-2.60043100
H	5.48979400	-2.50730500	-4.18922500
H	3.78100600	-2.75428500	-4.57015700
H	5.05593400	-3.14679600	-1.81391500
H	3.34754900	-3.38116600	-2.18116300
C	4.64177700	-4.87765800	-3.02583100
C	3.59805100	-5.74165300	-3.38748200
C	5.95712800	-5.35791900	-3.10518700
C	3.85851400	-7.04375100	-3.81933700
H	2.57076600	-5.38955100	-3.32064100
C	6.22316800	-6.65826200	-3.53670700
H	6.78019900	-4.70560600	-2.82000300
C	5.17353800	-7.50650900	-3.89676600
H	3.03336700	-7.69814300	-4.08928900
H	7.25025500	-7.01136700	-3.58652200
H	5.37875300	-8.52073400	-4.22920900
C	2.74428900	1.07401000	-3.12651700

C	1.93592900	0.85332400	-1.80446700
H	1.12128200	0.18283300	-2.09776200
C	3.16799900	-0.24055100	-3.77551800
C	3.37507700	3.37613400	-3.65733900
C	4.08871100	4.57238400	-3.62989400
C	3.75228500	2.21401100	-2.98138100
C	5.25019700	4.60527400	-2.86259200
H	3.75694300	5.43974000	-4.19239500
C	4.93460300	2.26631600	-2.23070900
H	1.14289000	5.60474000	-5.60378700
C	5.66456700	3.45487300	-2.17732200
H	5.83963500	5.51572000	-2.80750400
H	5.28626800	1.38300800	-1.71675200
H	6.58058300	3.48474300	-1.59342700
S	1.96981400	2.99840200	-4.67951300
O	2.22053000	3.29380200	-6.11232700
N	1.70063000	1.54557700	-4.13029400
C	2.66597100	0.28024200	-0.58427000
H	3.46956600	0.95484800	-0.25707100
H	3.14263400	-0.66607200	-0.85261500
C	1.71757100	0.02901600	0.60391700
H	0.90560100	-0.63637400	0.27958500
H	2.27241900	-0.51943200	1.37732800
C	1.12195800	1.29566500	1.23147600
H	1.91277700	1.98437100	1.55648600
H	0.47857700	1.83850400	0.52959600
H	0.51323100	1.05105800	2.10999900
H	1.50041400	1.82708300	-1.54341400

TS-2d

Rh	-0.56006900	-1.12627000	-0.19405200
C	-2.18137800	-2.58412800	0.28380000
C	-1.66866200	-2.88919700	-1.04113400
C	-0.30450700	-3.27606700	-0.92009000
C	0.05848400	-3.19668600	0.48723500
C	-1.11174900	-2.79858000	1.21797000
C	1.34198000	-3.69157400	1.08691100
H	1.55742900	-3.20034000	2.04046700
H	1.27301100	-4.77199000	1.27998500
H	2.18679200	-3.51591400	0.41821900
C	-1.21219000	-2.68534300	2.70994700
H	-1.97625100	-1.96224100	3.00729100
H	-1.47919100	-3.65601400	3.15000700
H	-0.26249500	-2.37008600	3.15080500

C	0.59295700	-3.72944200	-2.03058900
H	1.61764400	-3.38151200	-1.88268000
H	0.60421700	-4.82783000	-2.07970600
H	0.24693500	-3.35419700	-2.99716000
C	-2.45831000	-2.71734800	-2.30226100
H	-1.92987900	-3.12073400	-3.16931900
H	-3.43091900	-3.21819900	-2.22955800
H	-2.62451500	-1.64441700	-2.46526500
C	-3.63066700	-2.36192500	0.60096200
H	-4.11549500	-1.71963000	-0.13989300
H	-4.16512700	-3.32287000	0.60264200
H	-3.77227400	-1.90858100	1.58532200
C	4.00504600	2.39280900	-3.11203500
C	3.16453900	1.52711100	-2.40775000
C	3.72824400	0.50317600	-1.64594700
C	5.11177800	0.31491100	-1.59793600
C	5.94281500	1.19391100	-2.29326600
C	5.39116100	2.23343300	-3.04723400
H	3.57443000	3.18676200	-3.71606800
H	2.08355400	1.61124700	-2.45242900
H	7.02040100	1.05918000	-2.25618900
H	6.04202700	2.91114100	-3.59306000
C	-1.62909600	1.15743700	1.61166200
F	-1.48784400	2.12725100	2.58320700
F	-1.63435400	0.14460400	-1.36263200
C	-3.05129100	0.99611100	1.20981500
C	-3.56395800	2.27405100	0.48937000
H	-3.69182600	0.77905100	2.07545500
H	-3.10321400	0.17353600	0.50360700
H	-3.66987200	3.09294100	1.20921800
H	-2.79936100	2.56546700	-0.23924600
C	-4.86727000	2.01800200	-0.23521400
C	-4.86329300	1.21878200	-1.39082400
C	-6.08251700	2.54124300	0.21941500
C	-6.05192700	0.95391300	-2.07063800
H	-3.91501100	0.81065900	-1.73660200
C	-7.27403300	2.27650000	-0.46197300
H	-6.09728200	3.16487600	1.11115200
C	-7.26184900	1.48208100	-1.60885200
H	-6.03447100	0.33960700	-2.96775300
H	-8.20940100	2.69379000	-0.09706000
H	-8.18694900	1.27769800	-2.14190300
C	0.79735200	0.94041000	1.01927400
C	1.14070200	2.30088200	0.43999000

H	0.37619600	2.56927100	-0.29380200
C	-0.53278800	0.55959800	1.14767800
C	2.93768000	-0.42407000	1.00945800
C	4.00568100	-1.02007500	1.67648500
C	1.91139900	0.22144700	1.70751500
C	4.07565500	-0.94391700	3.06905100
H	4.74519700	-1.57711200	1.11036100
C	1.97150300	0.25950900	3.10925500
H	5.53173100	-0.51813100	-1.04468200
C	3.05537400	-0.30876400	3.78165400
H	4.90637800	-1.40400700	3.59685000
H	1.17165600	0.74506300	3.66084900
H	3.09461600	-0.26576500	4.86659300
S	2.62792300	-0.66195900	-0.78147800
O	3.23672800	-2.00587200	-1.05644100
N	1.19874200	-0.21592100	-1.07636700
C	1.23242800	3.39589600	1.53567600
H	1.99743800	3.11427200	2.27215300
H	0.28108600	3.45092300	2.06933600
C	1.57340800	4.78102400	0.95694900
H	0.83167200	5.04471200	0.19009500
H	1.45307800	5.51913300	1.76145100
C	2.98623200	4.90757700	0.37496300
H	3.74510900	4.65195500	1.12537900
H	3.14128300	4.25201100	-0.48917900
H	3.18002600	5.93456300	0.04426000
H	2.09912600	2.24075500	-0.07877400

INT-2d

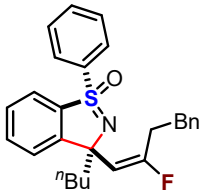
Rh	0.35092200	0.12972200	-5.67778100
C	0.21761200	-1.37717000	-7.36158400
C	-1.07671600	-0.95066400	-6.89351900
C	-1.25763900	0.44563100	-7.30784200
C	-0.05724900	0.89090300	-7.87909600
C	0.89772300	-0.22221000	-7.85098300
C	0.23973000	2.24713600	-8.44912100
H	1.25121900	2.58073800	-8.19705900
H	0.17031400	2.22840800	-9.54606500
H	-0.45791300	3.00422600	-8.08324400
C	2.26504300	-0.19168700	-8.47073200
H	2.89186600	-1.00786800	-8.09981700
H	2.20333900	-0.29162100	-9.56400400
H	2.78414300	0.74748500	-8.25511700
C	-2.47843400	1.24779100	-6.97319100

H	-2.44439400	2.24547400	-7.41926600
H	-3.39041900	0.74975800	-7.32409100
H	-2.53945600	1.35411500	-5.88141200
C	-2.17103300	-1.81351700	-6.33653700
H	-2.87287700	-2.12502200	-7.12365100
H	-1.77093800	-2.71638500	-5.86647700
H	-2.73661000	-1.27167700	-5.57274100
C	0.71483500	-2.78798100	-7.44628700
H	0.15775300	-3.45189100	-6.78123600
H	0.58444900	-3.16576600	-8.47025800
H	1.77748100	-2.87540700	-7.20192700
C	-0.99757100	4.61917300	-5.33151500
C	-0.08049100	3.66111400	-4.89004300
C	1.27008300	3.87248100	-5.18090100
C	1.72077100	4.98503700	-5.89833800
C	0.78648600	5.92975600	-6.32353200
C	-0.56923900	5.74858700	-6.03441500
H	-2.05438000	4.47288100	-5.12693400
H	-0.41552100	2.74285100	-4.39953600
H	1.11649100	6.80070000	-6.88260000
H	-1.29430500	6.48736100	-6.36571300
C	1.26457100	-0.86808600	-4.06028200
F	0.32662300	-1.43348700	-3.19214800
F	-0.89534900	0.88999000	-4.25623800
C	2.35718500	-1.92153600	-4.36446200
C	1.91738100	-3.38246700	-4.12217100
H	3.23182600	-1.72767500	-3.72800600
H	2.71349200	-1.79744900	-5.39218600
H	1.58954600	-3.47751900	-3.08175600
H	1.04417300	-3.61973300	-4.73680000
C	3.03067600	-4.37469500	-4.39448500
C	3.00300800	-5.21891400	-5.51262900
C	4.12710000	-4.47263800	-3.52320100
C	4.03739400	-6.12482900	-5.76064200
H	2.15507900	-5.17680400	-6.19207600
C	5.16310200	-5.37419300	-3.76554700
H	4.16464600	-3.83982800	-2.63865900
C	5.12351100	-6.20417800	-4.88883700
H	3.98997400	-6.77133200	-6.63344400
H	5.99974100	-5.43336600	-3.07385100
H	5.92881700	-6.90902300	-5.07798300
C	2.21965600	0.70384700	-2.19533700
C	2.19982500	-0.35693000	-1.10908400
H	1.59378300	-1.19649900	-1.45258900

C	1.83807900	0.40881100	-3.47570700
C	2.75723300	3.08416700	-2.85479400
C	3.13802000	4.39877800	-2.53955400
C	2.63540800	2.05867300	-1.87860900
C	3.40650500	4.74375100	-1.22638200
H	3.22218000	5.13928900	-3.32895700
C	2.92675100	2.46324300	-0.54743900
H	2.77612000	5.09110900	-6.12618200
C	3.29697700	3.75870400	-0.23127500
H	3.70055500	5.75778300	-0.97438100
H	2.84736300	1.73381600	0.24905600
H	3.50253800	4.01399500	0.80490300
S	2.50255300	2.71767300	-4.56187100
O	3.72338300	2.91879000	-5.37437000
N	1.82681300	1.27805800	-4.56225000
C	3.59778400	-0.87595400	-0.70691700
H	4.22602900	-0.04655900	-0.35399300
H	4.09546200	-1.26183200	-1.60651700
C	3.56833100	-1.98073000	0.36345400
H	2.92389700	-2.80197100	0.01791800
H	4.57776600	-2.40380300	0.45731300
C	3.09839200	-1.51303100	1.74681600
H	3.73302200	-0.70051000	2.12388500
H	2.06520100	-1.14816000	1.72766800
H	3.14201900	-2.33118100	2.47494400
H	1.67815600	0.03276100	-0.22537100

9. Synthesis and Characterization of Products

(*E*)-3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-1-phenyl-3*H*-benzo[*d*]isothiazole 1-oxide **(3a)**



This compound was obtained following the General Procedure in 75% yield (65.0 mg, 0.15 mmol, >20:1 dr) as a white solid. m.p.: 110–111 °C. Eluent: PE/DCM = 1/1. R_f = 0.60.

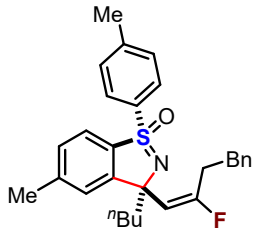
^{1}H NMR (400 MHz, CDCl$_3$): δ 7.99 (d, *J* = 7.5 Hz, 2H), 7.62 (t, *J* = 7.3 Hz, 1H), 7.55 (q, *J* = 6.6 Hz, 3H), 7.50–7.38 (m, 3H), 7.24–7.18 (m, 4H), 7.12 (t, *J* = 6.2 Hz, 1H), 5.56 (d, *J* = 26.0 Hz, 1H), 3.14 (ddd, *J* = 23.4, 17.1, 8.4 Hz, 1H), 2.83 (d, *J* = 8.0 Hz, 2H), 2.07–1.99 (m, 1H), 1.69–1.52 (m, 4H), 1.35 (dd, *J* = 14.5, 7.2 Hz, 2H), 0.91 (t, *J* = 7.3 Hz, 3H) ppm.

^{13}C NMR (100 MHz, CDCl$_3$): δ 161.9 (d, $J_{C–F}$ = 248.6 Hz), 152.6, 141.8, 140.4, 137.9, 133.4, 132.8, 129.6, 129.3, 129.1, 128.8, 128.3, 125.8, 123.4, 122.6, 112.0 (d, $J_{C–F}$ = 25.1 Hz), 74.4 (d, $J_{C–F}$ = 13.0 Hz), 44.4, 32.5, 31.2 (d, $J_{C–F}$ = 25.5 Hz), 27.2, 23.1, 14.2 ppm.

^{19}F NMR (376 MHz, CDCl$_3$): δ -96.20 – -96.45 (m) ppm.

HRMS (ESI) *m*/*z*: [M+H]$^+$ Calcd for $C_{27}H_{29}FNOS$: 434.1948; Found: 434.1949.

(*E*)-3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-5-methyl-1-(*p*-tolyl)-3*H*-benzo[*d*]isothiazole 1-oxide **(3b)**



This compound was obtained following the General Procedure in 64% yield (59.0 mg, 0.128 mmol, >20:1 dr) as a white solid. m.p.: 114–115 °C. Eluent: PE/DCM = 1/1. R_f = 0.50.

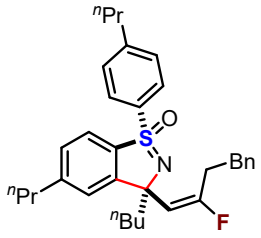
^{1}H NMR (400 MHz, CDCl$_3$): δ 7.84 (d, *J* = 7.9 Hz, 2H), 7.37-7.29 (m, 3H), 7.27-7.17 (m, 6H), 7.15-7.08 (m, 1H), 5.53 (d, *J* = 26.2 Hz, 1H), 3.24-3.05 (m, 1H), 2.90-2.75 (m, 2H), 2.44 (d, *J* = 5.0 Hz, 6H), 2.06-1.94 (m, 1H), 1.68-1.52 (m, 4H), 1.40-1.30 (m, 2H), 0.91 (t, *J* = 7.3 Hz, 3H) ppm.

^{13}C NMR (100 MHz, CDCl$_3$): δ 161.8 (d, $J_{C–F}$ = 248.0 Hz), 153.1, 144.2, 143.6, 141.9, 137.7, 135.6, 130.1, 129.9, 129.5, 128.8, 128.2, 125.7, 123.7, 122.2, 112.1 (d, $J_{C–F}$ = 24.8 Hz), 73.9 (d, $J_{C–F}$ = 12.9 Hz), 44.5, 32.5, 31.1 (d, $J_{C–F}$ = 25.5 Hz), 27.2, 23.2, 21.9, 21.7, 14.2 ppm.

^{19}F NMR (376 MHz, CDCl$_3$): δ -96.35 – -96.63 (m) ppm.

HRMS (ESI) *m*/*z*: [M+H]$^+$ Calcd for $C_{29}H_{33}FNOS$: 462.2261; Found: 462.2263.

(*E*)-3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-5-propyl-1-(4-propylphenyl)-3*H*-benzo[*d*]isothiazole 1-oxide **(3c)**



This compound was obtained following the General Procedure in 53% yield (54.8 mg, 0.106 mmol, >20:1 dr) as a white solid. m.p.: 116–117 °C. Eluent: PE/DCM = 1/1. R_f = 0.50.

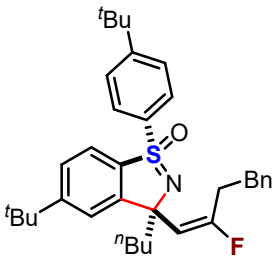
^{1}H NMR (400 MHz, CDCl$_3$): δ 7.84 (d, *J* = 7.9 Hz, 2H), 7.33 (t, *J* = 9.8 Hz, 3H), 7.22 (d, *J* = 6.9 Hz, 6H), 7.13 (d, *J* = 6.4 Hz, 1H), 5.53 (d, *J* = 26.2 Hz, 1H), 3.15 (dt, *J* = 24.9, 9.6 Hz, 1H), 2.82 (d, *J* = 7.6 Hz, 2H), 2.44 (d, *J* = 5.0 Hz, 6H), 2.01 (t, *J* = 11.0 Hz, 1H), 1.63 (d, *J* = 15.5 Hz, 4H), 1.40–1.32 (m, 2H), 0.91 (t, *J* = 7.3 Hz, 3H) ppm.

^{13}C NMR (100 MHz, CDCl$_3$): δ 161.8 (d, $J_{C–F}$ = 248.0 Hz), 153.02, 153.01, 148.8, 148.4, 141.9, 137.8, 135.8, 129.6, 129.4, 128.8, 128.2, 125.7, 123.1, 122.2, 112.1 (d, $J_{C–F}$ = 24.8 Hz), 73.9 (d, $J_{C–F}$ = 12.9 Hz), 44.4, 38.3, 38.0, 32.5, 31.1 (d, $J_{C–F}$ = 25.5 Hz), 27.2, 24.7, 24.4, 23.2, 14.3, 13.94, 13.89 ppm.

^{19}F NMR (376 MHz, CDCl$_3$): δ -96.44 – -96.72 (m) ppm.

HRMS (ESI) *m*/*z*: [M+H]$^+$ Calcd for $C_{33}H_{41}FNOS$: 518.2887; Found: 518.2885.

(*E*)-5-(tert-butyl)-3-butyl-1-(4-(tert-butyl)phenyl)-3-(2-fluoro-4-phenylbut-1-en-1-yl)-3*H*-benzo[*d*]isothiazole 1-oxide **(3d)**



This compound was obtained following the General Procedure in 50% yield (54.6 mg, 0.1 mmol, >20:1 dr) as a yellowish sticky oil. Eluent: PE/DCM = 1/1. R_f = 0.50.

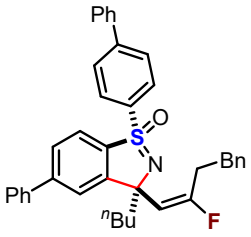
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.90 (d, *J* = 8.0 Hz, 2H), 7.54 (d, *J* = 8.1 Hz, 2H), 7.42 (s, 3H), 7.23 (s, 4H), 7.12 (s, 1H), 5.56 (d, *J* = 26.1 Hz, 1H), 3.26–3.08 (m, 1H), 2.82 (d, *J* = 6.7 Hz, 2H), 2.05–1.98 (m, 1H), 1.59 (d, *J* = 13.7 Hz, 4H), 1.34 (s, 18H), 1.27 (d, *J* = 10.9 Hz, 2H), 0.93 (t, *J* = 7.0 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ 161.9 (d, $J_{C–F}$ = 247.9 Hz), 157.1, 156.9, 152.8, 141.9, 137.5, 135.4, 129.4, 128.8, 128.2, 126.9, 126.3, 125.7, 121.9, 119.8, 112.2 (d, $J_{C–F}$ = 24.7 Hz), 74.1 (d, $J_{C–F}$ = 12.8 Hz), 44.4, 35.6, 35.3, 32.5, 31.5, 31.23, 31.21 (d, $J_{C–F}$ = 25.4 Hz), 27.3, 23.2, 14.3 ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ -96.45 – -96.70 (m) ppm.

HRMS (ESI) *m*/*z*: $[M+H]^+$ Calcd for $C_{35}H_{45}FNOS$: 546.3200; Found: 546.3202.

(*E*)-1-([1,1'-biphenyl]-4-yl)-3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-5-phenyl-3*H*-benzo[*d*]isothiazole 1-oxide **(3e)**



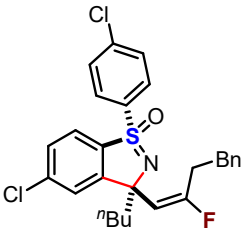
This compound was obtained following the General Procedure in 45% yield (53.4 mg, 0.09 mmol, >20:1 dr) as a yellowish sticky oil. Eluent: PE/DCM = 1/1. R_f = 0.80.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.07 (d, *J* = 8.2 Hz, 2H), 7.76 (d, *J* = 8.2 Hz, 2H), 7.64–7.56 (m, 7H), 7.51–7.41 (m, 6H), 7.26–7.19 (m, 4H), 7.12 (d, *J* = 6.7 Hz, 1H), 5.62 (d, *J* = 25.9 Hz, 1H), 3.20 (dt, *J* = 22.2, 8.9 Hz, 1H), 2.86 (s, 2H), 2.09 (dd, *J* = 17.1, 11.7 Hz, 1H), 1.77–1.70 (m, 1H), 1.61 (s, 3H), 1.42–1.34 (m, 2H), 0.94 (t, *J* = 7.1 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ 162.0 (d, $J_{C–F}$ = 249.3 Hz), 153.6, 146.4, 146.3, 141.8, 139.8, 139.4, 139.0, 136.7, 130.1, 129.2, 128.8, 128.7, 128.61, 128.55, 128.2, 128.0, 127.7, 127.5, 125.8, 122.8, 121.9, 112.0 (d, $J_{C–F}$ = 24.6 Hz), 74.3 (d, $J_{C–F}$ = 12.8 Hz), 44.5, 32.5, 31.2 (d, $J_{C–F}$ = 25.3 Hz), 27.2, 23.1, 14.2 ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ -95.90 – -96.20 (m) ppm.

HRMS (ESI) *m*/*z*: $[M+H]^+$ Calcd for $C_{39}H_{37}FNOS$: 586.2574; Found: 586.2573.



(*E*)-3-butyl-5-chloro-1-(4-chlorophenyl)-3-(2-fluoro-4-phenylbut-1-en-1-yl)-3*H*-benzo[*d*]isothiazole 1-oxide **(3f)**

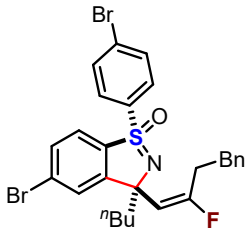
This compound was obtained following the General Procedure in 45% yield (45.2 mg, 0.09 mmol, >20:1 dr) as a yellowish sticky oil. Eluent: PE/DCM = 1/1. R_f = 0.50.

^{1}H NMR (400 MHz, $CDCl_3$): δ7.89 (d, *J* = 7.2 Hz, 2H), 7.52 (d, *J* = 7.0 Hz, 2H), 7.40 (d, *J* = 12.6 Hz, 3H), 7.22 (d, *J* = 2.0 Hz, 4H), 7.13 (s, 1H), 5.48 (d, *J* = 25.5 Hz, 1H), 3.18–3.03 (m, 1H), 2.83 (s, 3H), 1.98 (s, 1H), 1.56 (s, 3H), 1.35 (d, *J* = 5.5 Hz, 2H), 0.93 (d, *J* = 6.5 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ 162.3 (d, $J_{C–F}$ = 249.0 Hz), 154.9, 141.6, 140.5, 139.8, 138.5, 136.0, 131.0, 129.7, 128.8, 128.3, 125.9, 123.8, 123.5, 111.2 (d, $J_{C–F}$ = 26.3 Hz), 74.2 (d, $J_{C–F}$ = 12.8 Hz), 44.2, 32.4, 31.2 (d, $J_{C–F}$ = 25.1 Hz), 27.1, 23.0, 14.2 ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ -96.25 – -96.50 (m) ppm.

HRMS (ESI) *m*/*z*: $[M+H]^+$ Calcd for $C_{27}H_{27}Cl_2FNOS$: 502.1169; Found: 502.1167.



(*E*)-5-bromo-1-(4-bromophenyl)-3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-3*H*-benzo[*d*]isothiazole 1-oxide **(3g)**

This compound was obtained following the General Procedure in 40% yield (47.4 mg, 0.08 mmol, >20:1 dr) as a yellowish sticky oil. Eluent: PE/DCM = 1/1. R_f = 0.70.

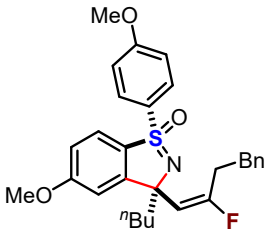
^{1}H NMR (400 MHz, CDCl$_3$): δ 7.80 (d, *J* = 8.3 Hz, 2H), 7.69 (d, *J* = 8.5 Hz, 2H), 7.59 (s, 1H), 7.54 (d, *J* = 8.3 Hz, 1H), 7.32 (d, *J* = 8.2 Hz, 1H), 7.22 (d, *J* = 4.1 Hz, 4H), 7.13 (s, 1H), 5.47 (d, *J* = 25.5 Hz, 1H), 3.17–3.04 (m, 1H), 2.83 (d, *J* = 5.1 Hz, 2H), 1.98 (s, 1H), 1.35 (d, *J* = 8.7 Hz, 2H), 1.25 (s, 4H), 0.92 (t, *J* = 7.3 Hz, 3H) ppm.

^{13}C NMR (100 MHz, CDCl$_3$): δ 162.3 (d, $J_{C–F}$ = 250.3 Hz), 154.99, 154.96, 141.6, 139.0, 136.4, 132.7, 132.6, 131.1, 129.2, 128.8, 128.3, 126.9, 125.9, 123.7, 111.2 (d, $J_{C–F}$ = 26.3 Hz), 74.3 (d, $J_{C–F}$ = 13.0 Hz), 44.3, 32.4, 31.2 (d, $J_{C–F}$ = 25.3 Hz), 27.1, 23.1, 14.2 ppm.

^{19}F NMR (376 MHz, CDCl$_3$): δ -94.98 – -95.23 (m) ppm.

HRMS (ESI) *m*/*z*: [M+H]$^+$ Calcd for $C_{27}H_{27}Br_2FNOS$: 590.0159; Found: 590.0159.

(*E*)-3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-5-methoxy-1-(4-methoxyphenyl)-3*H*-benzo[*d*]isothiazole 1-oxide **(3h)**



This compound was obtained following the General Procedure in 53% yield (52.4 mg, 0.106 mmol, >20:1 dr) as a yellowish sticky oil. Eluent: PE/DCM = 1/1. R_f = 0.30.

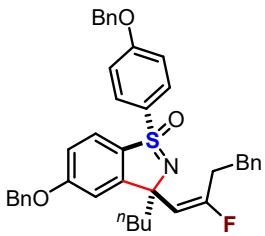
^{1}H NMR (400 MHz, CDCl$_3$): δ 7.89 (d, *J* = 8.4 Hz, 2H), 7.35 (d, *J* = 8.4 Hz, 1H), 7.22 (s, 4H), 7.11 (s, 1H), 6.98 (d, *J* = 8.4 Hz, 2H), 6.89 (d, *J* = 7.5 Hz, 1H), 6.83 (s, 1H), 5.52 (d, *J* = 26.1 Hz, 1H), 3.85 (s, 6H), 3.22–3.05 (m, 1H), 2.85 (d, *J* = 12.9 Hz, 2H), 1.98 (s, 1H), 1.92–1.50 (m, 4H), 1.36 (d, *J* = 6.3 Hz, 2H), 0.93 (d, *J* = 6.9 Hz, 3H) ppm.

^{13}C NMR (100 MHz, CDCl$_3$): δ 163.6, 163.5, 161.9 (d, $J_{C–F}$ = 248.6 Hz), 155.3, 141.8, 132.0, 131.6, 130.5, 128.8, 128.2, 125.7, 123.5, 116.1, 114.4, 112.1 (d, $J_{C–F}$ = 24.8 Hz), 107.2, 73.4 (d, $J_{C–F}$ = 12.9 Hz), 56.0, 55.8, 44.5, 32.4, 31.1 (d, $J_{C–F}$ = 25.5 Hz), 27.1, 23.1, 14.2 ppm.

^{19}F NMR (376 MHz, CDCl$_3$): δ -96.25 – -96.50 (m) ppm.

HRMS (ESI) *m*/*z*: [M+H]$^+$ Calcd for $C_{29}H_{33}FNO_3S$: 499.2160; Found: 499.2158.

(*E*)-5-(benzyloxy)-1-(4-(benzyloxy)phenyl)-3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-3*H*-benzo[*d*]isothiazole 1-oxide **(3i)**



This compound was obtained following the General Procedure in 57% yield (73.6 mg, 0.114 mmol, >20:1 dr) as a yellowish sticky oil. Eluent: PE/DCM = 1/1. R_f = 0.30.

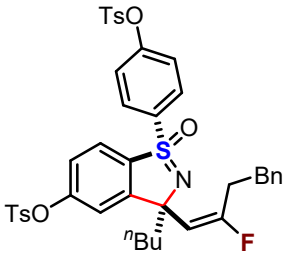
^{1}H NMR (400 MHz, CDCl$_3$): δ 7.88 (d, *J* = 8.4 Hz, 2H), 7.39 (dd, *J* = 8.6, 4.3 Hz, 8H), 7.37–7.33 (m, 3H), 7.20 (dd, *J* = 12.7, 4.5 Hz, 4H), 7.13–7.08 (m, 1H), 7.05 (d, *J* = 8.1 Hz, 2H), 6.97–6.90 (m, 2H), 5.50 (d, *J* = 26.1 Hz, 1H), 5.09 (d, *J* = 9.6 Hz, 4H), 3.26–3.03 (m, 1H), 2.89–2.77 (m, 3H), 1.99 (ddd, *J* = 15.0, 9.7, 4.0 Hz, 1H), 1.65–1.50 (m, 3H), 1.36–1.26 (m, 2H), 0.91 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, CDCl$_3$): δ 162.7, 162.5, 161.9 (d, $J_{C–F}$ = 248.5 Hz), 155.2, 141.8, 135.9, 135.8, 132.2, 131.6, 130.6, 128.82, 128.77, 128.5, 128.4, 128.2, 127.7, 127.5, 125.7, 123.6, 116.6, 115.3, 112.1 (d, $J_{C–F}$ = 24.9 Hz), 108.3, 73.4 (d, $J_{C–F}$ = 12.8 Hz), 70.7, 70.4, 44.5, 32.4, 31.11 (d, $J_{C–F}$ = 25.6 Hz), 27.1, 23.1, 14.2 ppm.

^{19}F NMR (376 MHz, CDCl$_3$): δ -96.24 – -96.50 (m) ppm.

HRMS (ESI) *m*/*z*: [M+H]$^+$ Calcd for $C_{41}H_{41}FNO_3S$: 646.2786; Found: 646.2788.

(*E*)-3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-1-oxido-1-(4-(tosyloxy)phenyl)-3*H*-1λ^4-benzo[*d*]isothiazol-5-yl 4-methylbenzenesulfonate **(3j)**



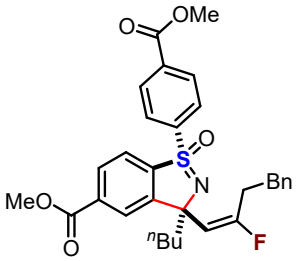
This compound was obtained following the General Procedure in 50% yield (77.3 mg, 0.1 mmol, >20:1 dr) as a white solid. m.p.: 114–115 °C. Eluent: PE/DCM = 1/1. R_f = 0.80.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91–7.88 (m, 2H), 7.75–7.72 (m, 2H), 7.69–7.66 (m, 2H), 7.41 (d, *J* = 8.4 Hz, 1H), 7.32 (d, *J* = 8.7 Hz, 4H), 7.22 (d, *J* = 4.4 Hz, 4H), 7.19 (d, *J* = 1.8 Hz, 1H), 7.17–7.13 (m, 2H), 6.85 (d, *J* = 2.0 Hz, 1H), 5.22 (d, *J* = 25.5 Hz, 1H), 3.15–2.95 (m, 1H), 2.88–2.76 (m, 3H), 2.45 (s, 6H), 1.86–1.75 (m, 1H), 1.52–1.40 (m, 3H), 1.34–1.27 (m, 2H), 0.89 (t, *J* = 7.3 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ 162.1 (d, $J_{C–F}$ = 249.9 Hz), 155.0, 153.5, 153.0, 146.3, 146.2, 141.5, 138.3, 135.6, 131.9, 131.5, 130.2, 130.1, 130.0, 128.7, 128.5, 128.3, 127.2, 125.9, 124.1, 123.8, 123.3, 117.6, 111.0 (d, $J_{C–F}$ = 26.1 Hz), 74.0 (d, $J_{C–F}$ = 13.1 Hz), 43.9, 32.3, 31.0 (d, $J_{C–F}$ = 25.6 Hz), 27.0, 22.9, 21.82, 21.77, 14.1 ppm.

HRMS (ESI) *m*/*z*: [M+H]$^+$ Calcd for $C_{40}H_{41}FNO_7S_3$: 774.2024; Found: 774.2025.

(*E*)-3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-1-(4-(methoxycarbonyl)phenyl)-3*H*-1λ^4-benzo[*d*]isothiazole-5-carboxylate 1-oxide **(3k)**



This compound was obtained following the General Procedure in 45% yield (49.4 mg, 0.09 mmol, >20:1 dr) as a yellowish solid. m.p.: 112–113 °C. Eluent: PE/DCM = 1/1. R_f = 0.6.

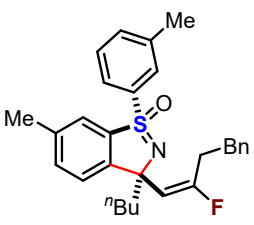
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (d, *J* = 8.5 Hz, 2H), 8.13 (d, *J* = 0.7 Hz, 1H), 8.11–8.07 (m, 1H), 8.05 (d, *J* = 8.6 Hz, 2H), 7.54 (d, *J* = 8.1 Hz, 1H), 7.24–7.19 (m, 4H), 7.13 (dd, *J* = 5.9, 2.9 Hz, 1H), 5.58 (d, *J* = 25.5 Hz, 1H), 3.98–3.95 (m, 6H), 3.22–3.02 (m, 1H), 2.84 (d, *J* = 6.5 Hz, 3H), 2.15–1.97 (m, 1H), 1.74–1.56 (m, 3H), 1.36 (dd, *J* = 14.6, 7.3 Hz, 2H), 0.91 (d, *J* = 7.3 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ 165.7, 162.2 (d, $J_{C–F}$ = 249.9 Hz), 160.9, 153.4, 143.9, 141.6, 140.7, 134.8, 134.6, 130.7, 129.6, 128.7, 128.3, 125.8, 124.8, 122.6, 111.3 (d, $J_{C–F}$ = 26.0 Hz), 74.8 (d, $J_{C–F}$ = 12.8 Hz), 52.91, 52.85, 44.2, 32.4, 31.2 (d, $J_{C–F}$ = 25.7 Hz), 27.2, 23.0, 14.2 ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ -95.18 – -95.45 (m) ppm.

HRMS (ESI) *m*/*z*: [M+H]$^+$ Calcd for $C_{31}H_{33}FNO_5S$: 550.2058; Found: 550.2046.

(*E*)-3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-6-methyl-1-(*m*-tolyl)-3*H*-benzo[*d*]isothiazole 1-oxide **(3l)**



This compound was obtained following the General Procedure in 64% yield (59.0 mg, 0.128 mmol, >20:1 dr) as a white solid. m.p.: 110–111 °C. Eluent: PE/DCM = 1/1. R_f = 0.50.

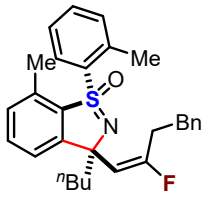
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79 (d, *J* = 8.7 Hz, 2H), 7.45–7.40 (m, 2H), 7.33 (dd, *J* = 17.8, 7.9 Hz, 2H), 7.25 (d, *J* = 17.1 Hz, 5H), 7.13 (d, *J* = 5.7 Hz, 1H), 5.54 (d, *J* = 26.1 Hz, 1H), 3.12 (ddd, *J* = 25.4, 13.9, 6.8 Hz, 1H), 2.83 (t, *J* = 10.1 Hz, 2H), 2.42 (s, 3H), 2.37 (s, 3H), 2.05–1.97 (m, 1H), 1.70–1.53 (m, 4H), 1.34 (dd, *J* = 11.8, 4.7 Hz, 2H), 0.91 (t, *J* = 7.3 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ 161.7 (d, $J_{C–F}$ = 248.2 Hz), 149.9, 141.9, 140.3, 139.5, 139.5, 138.2, 134.2, 133.9, 129.9, 129.1, 128.8, 128.2, 126.8, 125.7, 123.0, 122.4, 112.4 (d, $J_{C–F}$ = 24.8 Hz), 74.0 (d, $J_{C–F}$ = 12.8 Hz), 44.4, 32.5, 31.2 (d, $J_{C–F}$ = 25.7 Hz), 27.3, 23.2, 21.5, 21.2, 14.3 ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ -96.70 – -97.00 (m) ppm.

HRMS (ESI) *m*/*z*: $[M+H]^+$ Calcd for $C_{29}H_{33}FNOS$: 462.2261; Found: 462.2257.

(*E*)-3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-7-methyl-1-(*o*-tolyl)-3*H*-benzo[*d*]isothiazole 1-oxide **(3m)**



This compound was obtained following the General Procedure in 50% yield (46.2 mg, 0.1 mmol, >20:1 dr) as a yellowish sticky oil. Eluent: PE/DCM = 1/1. R_f = 0.80.

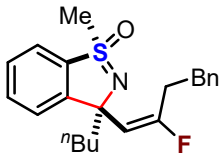
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76 (d, *J* = 6.5 Hz, 1H), 7.48 (d, *J* = 28.0 Hz, 2H), 7.27 (t, *J* = 20.4 Hz, 8H), 7.15 (s, 1H), 5.48 (d, *J* = 25.7 Hz, 1H), 3.28–3.11 (m, 1H), 2.93–2.73 (m, 3H), 2.45 (s, 3H), 2.24 (s, 3H), 1.96 (s, 1H), 1.72 (s, 1H), 1.25 (s, 4H), 0.79 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ 161.5 (d, $J_{C–F}$ = 248.5 Hz), 153.4, 142.1, 138.7, 138.3, 135.9, 134.5, 133.5, 133.2, 132.7, 130.5, 129.3, 128.8, 128.3, 126.6, 125.8, 121.2, 113.0 (d, $J_{C–F}$ = 24.6 Hz), 74.5 (d, $J_{C–F}$ = 12.7 Hz), 42.7, 32.4, 31.4 (d, $J_{C–F}$ = 25.5 Hz), 26.9, 23.0, 20.9, 17.6, 14.1 ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ -97.24 – -97.51 (m) ppm.

HRMS (ESI) *m*/*z*: $[M+H]^+$ Calcd for $C_{29}H_{33}FNOS$: 462.2261; Found: 462.2262.

(*E*)-3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-1-methyl-3*H*-1λ^4-benzo[*d*]isothiazole 1-oxide **(3n)**



This compound was obtained following the General Procedure in 59% yield (43.8 mg, 0.118 mmol, >20:1 dr) as a yellowish solid. m.p.: 108–109 °C. Eluent: PE/DCM = 3/1. R_f = 0.40.

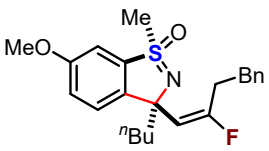
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, *J* = 7.5 Hz, 2H), 7.62–7.51 (m, 4H), 7.48 (d, *J* = 5.3 Hz, 2H), 7.41 (t, *J* = 7.2 Hz, 1H), 5.43 (d, *J* = 26.5 Hz, 1H), 3.19 (dt, *J* = 36.2, 11.4 Hz, 1H), 2.08 (t, *J* = 10.3 Hz, 1H), 1.79 (s, 1H), 1.72–1.60 (m, 5H), 1.41–1.29 (m, 3H), 1.23–1.05 (m, 2H), 0.94 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ 166.2 (d, $J_{C–F}$ = 252.3 Hz), 152.8, 140.4, 137.9, 133.4, 132.7, 129.6, 129.3, 129.0, 123.5, 122.5, 110.0 (d, $J_{C–F}$ = 26.2 Hz), 74.4 (d, $J_{C–F}$ = 13.4 Hz), 44.6, 36.9 (d, $J_{C–F}$ = 24.5 Hz), 28.8, 28.7, 27.3, 26.0, 25.9, 23.2, 14.2 ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ -108.30 – -108.55 (m) ppm.

HRMS (ESI) *m*/*z*: $[M+H]^+$ Calcd for $C_{22}H_{27}FNOS$: 372.1792; Found: 372.1783.

(*E*)-3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-1,6-dimethyl-3*H*-1λ^4-benzo[*d*]isothiazole 1-oxide **(3o)**



This compound was obtained following the General Procedure in 38% yield (29.2 mg, 0.076 mmol, >20:1 dr) as a yellowish sticky oil. Eluent: PE/DCM = 1/1. R_f = 0.50.

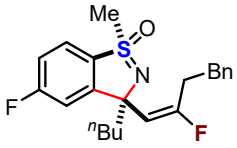
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.25-7.18 (m, 6H), 7.15-7.11 (m, 2H), 5.49 (d, *J* = 25.7 Hz, 1H), 3.85 (s, 3H), 3.35 (s, 3H), 2.98-2.83 (m, 1H), 2.78-2.68 (m, 3H), 1.93-1.85 (m, 1H), 1.69-1.62 (m, 1H), 1.25-1.16 (m, 3H), 0.83-0.79 (m, 4H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ 161.3 (d, $J_{C–F}$ = 248.7 Hz), 160.4, 144.9, 141.6, 137.6, 128.7, 128.2, 125.8, 124.2, 121.4, 112.9 (d, $J_{C–F}$ = 24.3 Hz), 104.5, 73.9 (d, $J_{C–F}$ = 13.2 Hz), 56.0, 44.7, 44.2, 32.4, 30.9 (d, $J_{C–F}$ = 26.0 Hz), 26.6, 22.7, 14.1 ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ -96.64 – -96.92 (m) ppm.

HRM (EI) *m*/*z*: $[M+H]^+$ Calcd for $C_{23}H_{29}FNO_2$: 402.1898; Found: 402.1901.

(*E*)-3-butyl-5-fluoro-3-(2-fluoro-4-phenylbut-1-en-1-yl)-1-methyl-3*H*-1λ^4-benzo[*d*]isothiazole 1-oxide **(3p)**



This compound was obtained following the General Procedure in 61% yield (32.0 mg, 0.122 mmol, >20:1 dr) as a yellowish sticky oil. Eluent: PE/DCM = 1/1. R_f = 0.50.

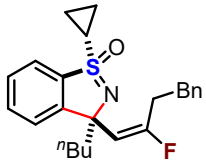
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (dd, *J* = 8.5, 4.6 Hz, 1H), 7.23 (s, 1H), 7.21–7.09 (m, 5H), 7.01 (dd, *J* = 8.3, 2.2 Hz, 1H), 5.45 (d, *J* = 25.3 Hz, 1H), 3.34 (d, *J* = 0.5 Hz, 3H), 3.02–2.86 (m, 1H), 2.82–2.67 (m, 3H), 1.88 (s, 3H), 1.27–1.16 (m, 3H), 0.82 (dd, *J* = 9.7, 4.7 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ 165.9 (d, $J_{C–F}$ = 255.7 Hz), 161.9 (d, $J_{C–F}$ = 249.9 Hz), 156.6 (dd, $J_{C–F}$ = 7.8, 1.3 Hz), 141.4, 132.4, 128.7, 128.2, 125.9, 123.9 (d, $J_{C–F}$ = 10.4 Hz), 117.1 (d, $J_{C–F}$ = 24.8 Hz), 112.2 (d, $J_{C–F}$ = 25.3 Hz), 110.7 (d, $J_{C–F}$ = 23.5 Hz), 74.1 (d, $J_{C–F}$ = 12.2 Hz), 45.0, 44.2, 32.3, 30.9 (d, $J_{C–F}$ = 25.8 Hz), 26.5, 22.7, 14.1 ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ -95.87 – -96.13 (m), -104.48 (d, *J* = 4.0 Hz) ppm.

HRMS (ESI) *m*/*z*: [M+H]$^+$ Calcd for $C_{22}H_{29}F_2NOS$: 390.1698; Found: 390.1696.

(*E*)-3-butyl-1-cyclopropyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-3*H*-benzo[*d*]isothiazole 1-oxide **(3q)**



This compound was obtained following the General Procedure in 56% yield (43.4 mg, 0.112 mmol, >20:1 dr) as a yellowish sticky oil. Eluent: PE/DCM = 1/1. R_f = 0.30.

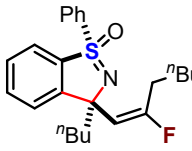
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (d, *J* = 7.5 Hz, 1H), 7.58 (t, *J* = 7.3 Hz, 1H), 7.49 (t, *J* = 7.3 Hz, 1H), 7.38 (d, *J* = 7.7 Hz, 1H), 7.27–7.18 (m, 4H), 7.14 (d, *J* = 6.7 Hz, 1H), 5.51 (d, *J* = 25.8 Hz, 1H), 2.95 (ddd, *J* = 19.2, 16.0, 8.2 Hz, 1H), 2.78–2.61 (m, 3H), 2.52–2.43 (m, 1H), 1.94 (td, *J* = 12.9, 3.2 Hz, 1H), 1.60 (t, *J* = 9.8 Hz, 2H), 1.24 (dd, *J* = 20.3, 8.4 Hz, 4H), 1.19–1.11 (m, 2H), 1.05–0.96 (m, 1H), 0.82 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ 161.6 (d, $J_{C–F}$ = 248.8 Hz), 153.1, 141.8, 136.9, 133.0, 128.9, 128.8, 128.2, 125.8, 123.5, 122.3, 112.7 (d, $J_{C–F}$ = 24.6 Hz), 73.7 (d, $J_{C–F}$ = 13.1 Hz), 44.5, 32.5, 31.3, 31.1 (d, $J_{C–F}$ = 25.9 Hz), 26.7, 22.9, 14.2, 6.6, 5.1 ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ -96.78 – -97.07 (m) ppm.

HRMS (ESI) *m*/*z*: [M+H]$^+$ Calcd for $C_{24}H_{29}FNOS$: 398.1948; Found: 398.1948.

(*E*)-3-butyl-3-(2-fluorohept-1-en-1-yl)-1-phenyl-3*H*-benzo[*d*]isothiazole 1-oxide **(3r)**



This compound was obtained following the General Procedure in 53% yield (40.8 mg, 0.106 mmol, >20:1 dr) as a yellowish sticky oil. Eluent: PE/DCM = 1/1. R_f = 0.60.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00–7.96 (m, 2H), 7.64–7.59 (m, 1H), 7.58–7.52 (m, 3H), 7.48 (dd, *J* = 4.1, 3.5 Hz, 2H), 7.43–7.39 (m, 1H), 5.52 (d, *J* = 26.3 Hz, 1H), 2.70–2.57 (m, 2H), 2.08 (dt, *J* = 12.7, 4.5 Hz, 1H), 1.71–1.59 (m, 3H), 1.51–1.37 (m, 4H), 1.25 (dd, *J* = 6.6, 3.4 Hz, 4H), 0.94 (dd, *J* = 8.1, 6.5 Hz, 3H), 0.85–0.80 (m, 3H) ppm.

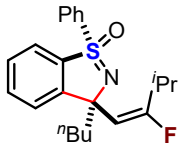
^{13}C NMR (100 MHz, $CDCl_3$): δ 163.1 (d, $J_{C–F}$ = 248.6 Hz), 152.8, 140.4, 137.7, 133.4, 132.7, 129.5, 129.3, 129.0, 123.5, 122.5, 111.2 (d, $J_{C–F}$ = 25.9 Hz), 74.4 (d, $J_{C–F}$ = 13.3 Hz), 44.6, 31.6, 28.9 (d, $J_{C–F}$ = 25.8 Hz), 27.3, 26.0, 23.2, 22.6, 14.2, 14.1 ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ -95.38 – -95.62 (m) ppm.

HRMS (ESI) *m*/*z*: [M+H]$^+$ Calcd for $C_{24}H_{31}FNOS$: 400.2105; Found: 400.2100.

(*E*)-3-butyl-3-(2-fluoro-3-methylbut-1-en-1-yl)-1-phenyl-3H-benzo[d]isothiazole 1-oxide **(3s)**

This compound was obtained following the General Procedure in 62% yield (46.0 mg, 0.124 mmol, >20:1 dr) as a white solid. m.p.: 111–112 °C. Eluent: PE/DCM = 1/1. R_f = 0.40.



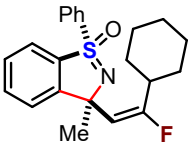
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, *J* = 7.5 Hz, 2H), 7.63–7.46 (m, 6H), 7.41 (t, *J* = 7.3 Hz, 1H), 5.40 (d, *J* = 26.2 Hz, 1H), 3.73 (ddt, *J* = 36.9, 13.6, 6.8 Hz, 1H), 2.11 (dd, *J* = 18.2, 6.4 Hz, 1H), 1.74–1.69 (m, 1H), 1.63 (s, 2H), 1.40 (dd, *J* = 14.5, 7.3 Hz, 2H), 1.12 (d, *J* = 6.9 Hz, 3H), 1.01 (d, *J* = 6.8 Hz, 3H), 0.94 (t, *J* = 7.3 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ 166.3 (d, $J_{C–F}$ = 253.6 Hz), 152.5, 139.8, 137.7, 133.4, 132.6, 129.6, 129.2, 128.9, 123.2, 122.4, 109.6 (d, $J_{C–F}$ = 26.0 Hz), 74.3 (d, $J_{C–F}$ = 13.3 Hz), 44.1, 27.3 (d, $J_{C–F}$ = 25.4 Hz), 27.2, 23.0, 19.0, 18.5, 14.1 ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ -113.28 – -113.50 (m) ppm.

HRMS (ESI) *m*/*z*: $[M+H]^+$ Calcd for $C_{22}H_{27}FNOS$: 372.1792; Found: 372.1782.

(*E*)-3-(2-cyclohexyl-2-fluorovinyl)-3-methyl-1-phenyl-3*H*-benzo[*d*]isothiazole 1-oxide **(3t)**



This compound was obtained following the General Procedure in 51% yield (37.6 mg, 0.102 mmol, >20:1 dr) as a white solid. m.p.: 106–107 °C. Eluent: PE/DCM = 1/1. R_f = 0.30.

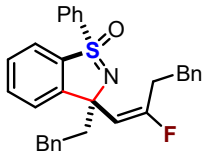
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, *J* = 7.4 Hz, 2H), 7.60 (dd, *J* = 12.1, 6.1 Hz, 2H), 7.51 (dd, *J* = 14.7, 7.6 Hz, 4H), 7.42 (t, *J* = 6.7 Hz, 1H), 5.54 (d, *J* = 25.6 Hz, 1H), 2.86 (dt, *J* = 22.6, 11.1 Hz, 1H), 1.81 (s, 3H), 1.68 (s, 2H), 1.58 (s, 2H), 1.40 (d, *J* = 7.3 Hz, 2H), 1.26 (s, 2H), 1.06 (s, 2H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ 166.0 (d, $J_{C–F}$ = 253.8 Hz), 153.1, 140.2, 137.9, 133.4, 132.8, 129.6, 129.3, 129.1, 123.5, 122.5, 111.3 (d, $J_{C–F}$ = 26.3 Hz), 71.0 (d, $J_{C–F}$ = 14.0 Hz), 37.1 (d, $J_{C–F}$ = 24.6 Hz), 32.8, 28.7 (d, $J_{C–F}$ = 11.6 Hz), 25.9, 25.8 ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ -109.10 – -109.36 (m) ppm.

HRMS (ESI) *m*/*z*: $[M+H]^+$ Calcd for $C_{22}H_{25}FNOS$: 370.1635; Found: 370.1631.

(*E*)-3-(2-fluoro-4-phenylbut-1-en-1-yl)-3-phenethyl-1-phenyl-3H-benzo[d]isothiazole 1-oxide **(3u)**



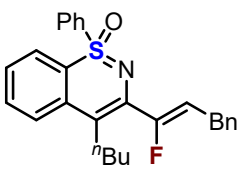
This compound was obtained following the General Procedure in 40% yield (38.5 mg, 0.08 mmol, >20:1 dr) as a yellowish sticky oil. Eluent: PE/DCM = 1/1. R_f = 0.50.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02 (d, *J* = 7.3 Hz, 2H), 7.63 (t, *J* = 7.3 Hz, 1H), 7.56 (t, *J* = 7.4 Hz, 3H), 7.49 (dd, *J* = 17.6, 7.6 Hz, 2H), 7.41 (t, *J* = 7.4 Hz, 1H), 7.29–7.25 (m, 4H), 7.20 (t, *J* = 6.5 Hz, 5H), 7.11 (t, *J* = 7.0 Hz, 1H), 5.62 (d, *J* = 25.8 Hz, 1H), 3.21 (tdd, *J* = 14.8, 11.7, 6.4 Hz, 1H), 2.89 (d, *J* = 8.7 Hz, 3H), 2.36 (dt, *J* = 13.5, 7.6 Hz, 1H), 1.93–1.86 (m, 1H), 1.31 (d, *J* = 20.7 Hz, 1H), 0.88 (t, *J* = 6.6 Hz, 1H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ 162.2 (d, $J_{C–F}$ = 249.3 Hz), 152.3, 142.4, 141.7, 140.3, 137.9, 133.5, 132.9, 129.6, 129.4, 129.3, 128.8, 128.6, 128.5, 128.3, 126.0, 125.9, 123.3, 122.6, 111.6 (d, $J_{C–F}$ = 25.4 Hz), 74.2 (d, $J_{C–F}$ = 13.1 Hz), 46.6, 32.5, 31.6, 31.2 (d, $J_{C–F}$ = 25.4 Hz) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ -95.29 – -95.53 (m) ppm.

HRMS (ESI) *m*/*z*: $[M+H]^+$ Calcd for $C_{30}H_{27}FNOS$: 482.1949; Found: 482.1951.



(*Z*)-4-butyl-3-(1-fluoro-3-phenylprop-1-en-1-yl)-1-phenylbenzo[e][1,2]thiazine 1-oxide **(4a)**

This compound was obtained following the General Procedure as a light yellow soild. m.p.: 120–121 °C. Eluent: PE/DCM = 1/1. R_f = 0.60.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01–7.97 (m, 2H), 7.71 (d, *J* = 8.4 Hz, 1H), 7.65 (t, *J* = 7.4 Hz, 1H), 7.57 (t, *J* = 7.6 Hz, 3H), 7.28 (d, *J* = 6.3 Hz, 5H), 7.20 (ddd, *J* = 12.3, 6.9, 2.2 Hz, 2H), 5.75 (dt, *J* = 34.8, 7.8 Hz, 1H), 3.67 (dd, *J* = 15.5, 8.2 Hz, 1H), 3.57 (dd, *J* =

15.6, 7.4 Hz, 1H), 2.83 (t, *J* = 7.6 Hz, 2H), 1.69–1.60 (m, 2H), 1.45 (dd, *J* = 14.7, 7.4 Hz, 2H), 0.96 (t, *J* = 7.3 Hz, 3H) ppm.

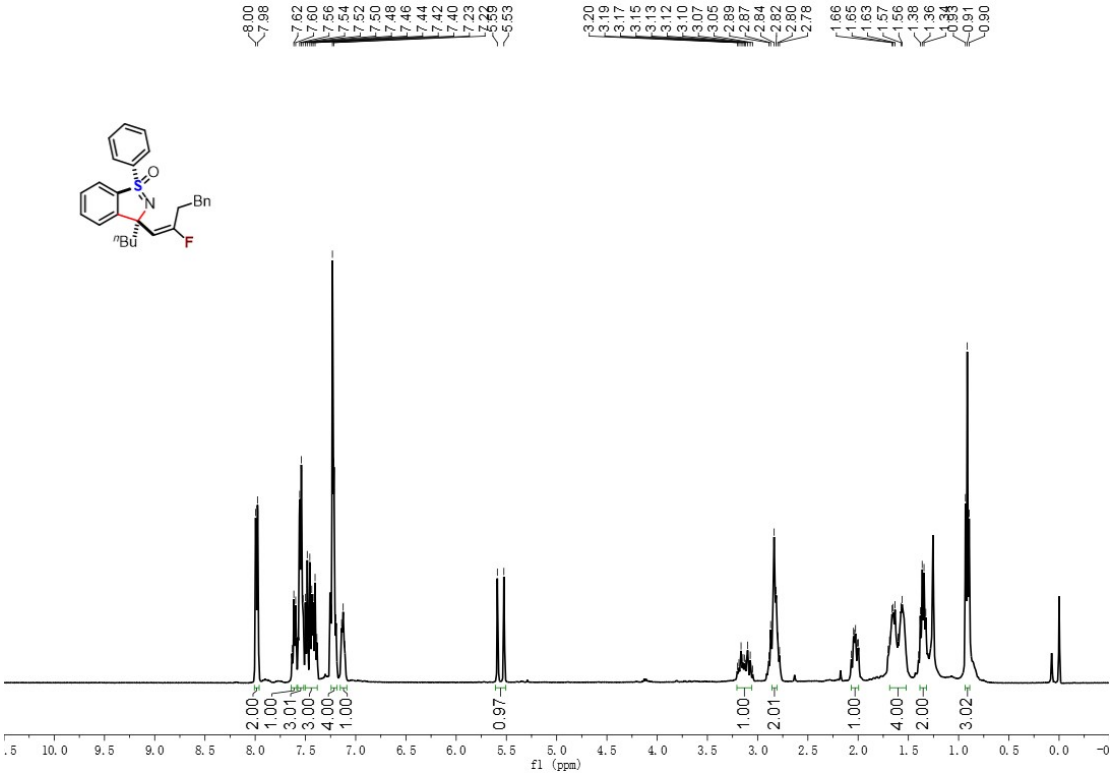
^{13}C NMR (100 MHz, $CDCl_3$): δ 157.5 (d, $J_{C\text{-}F}$ = 253.5 Hz), 140.2, 139.0, 136.5 (d, $J_{C\text{-}F}$ = 29.6 Hz), 135.8, 133.7, 132.0, 130.0, 129.1, 128.7, 128.6, 126.7, 126.2, 125.1, 124.3, 122.4, 112.1 (d, $J_{C\text{-}F}$ = 23.4 Hz), 111.8, 32.98, 30.8 (d, $J_{C\text{-}F}$ = 4.7 Hz), 28.3 (d, $J_{C\text{-}F}$ = 6.7 Hz), 23.1, 14.1 ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ -110.6 – -110.7 (m) ppm.

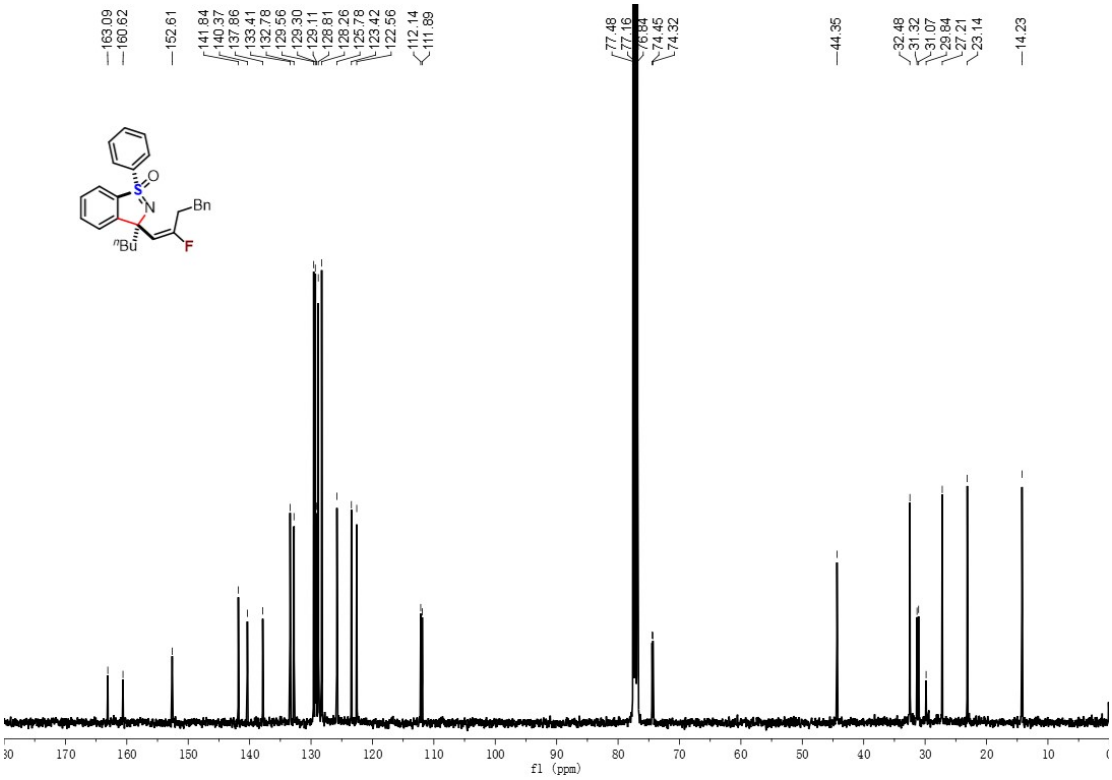
HRMS (ESI) *m*/*z*: $[M+H]^+$ Calcd for $C_{27}H_{27}FNOS$: 432.1792; Found: 432.1785.

10. Copies of NMR Spectra

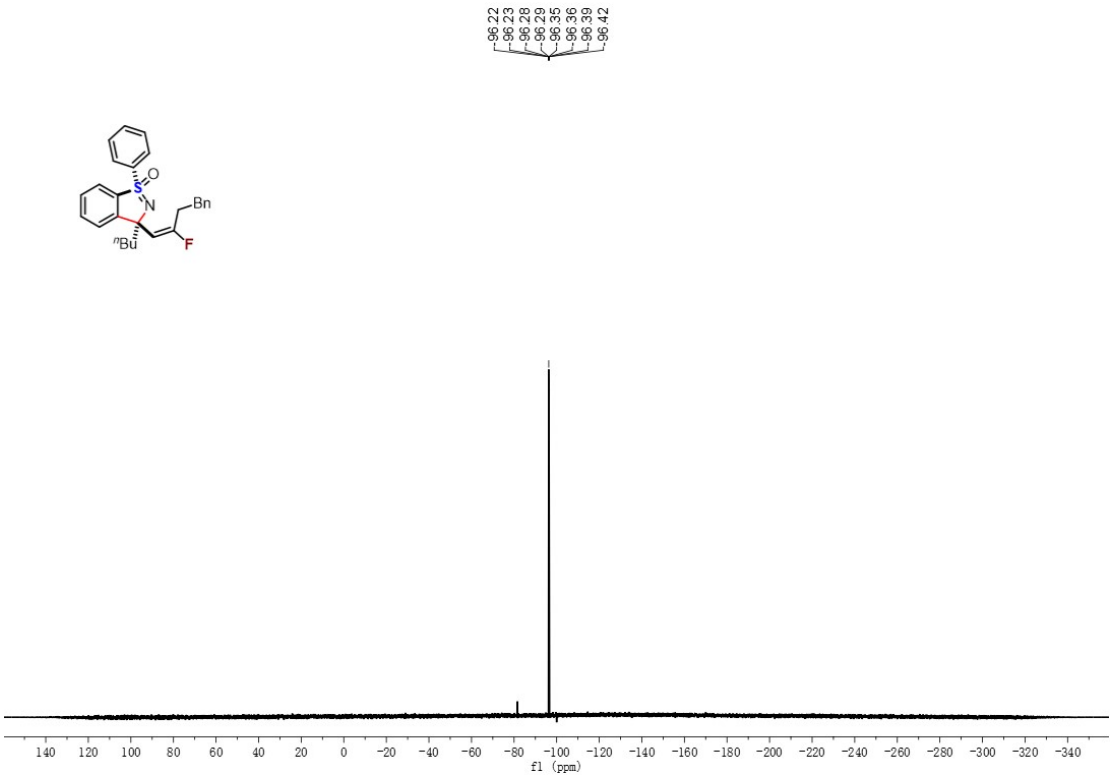
3a-^{1}H NMR (400 MHz, $CDCl_3$)



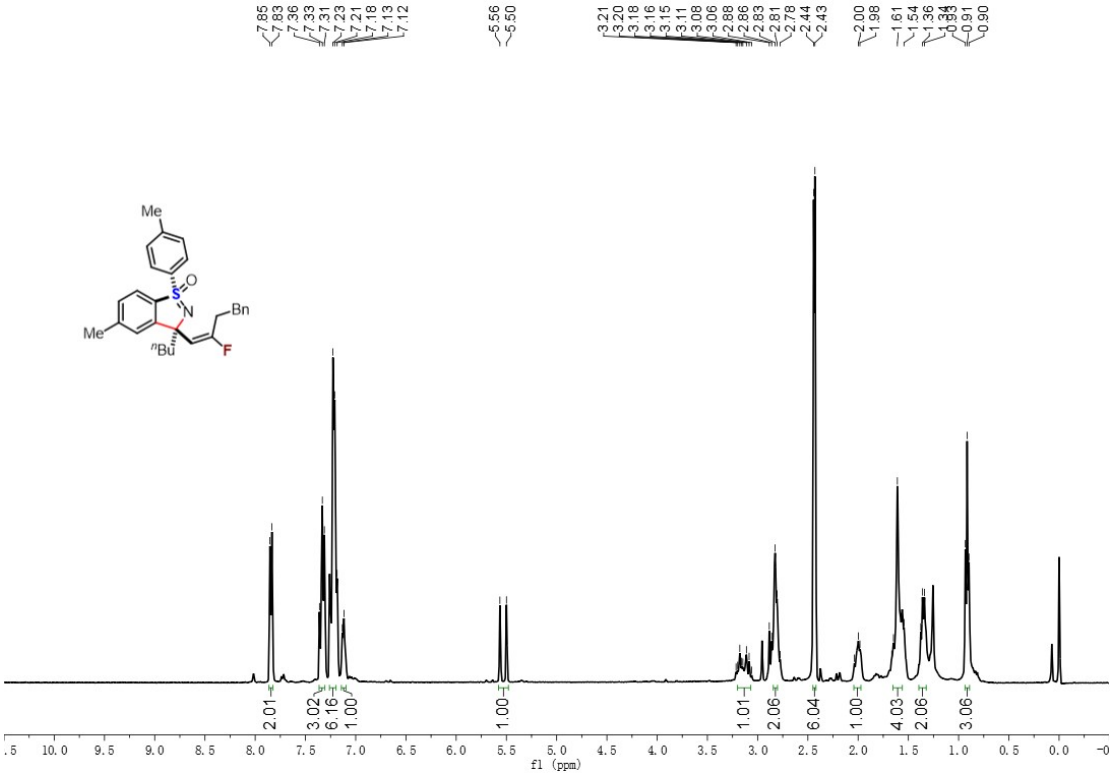
3a-^{13}C NMR (100 MHz, $CDCl_3$)



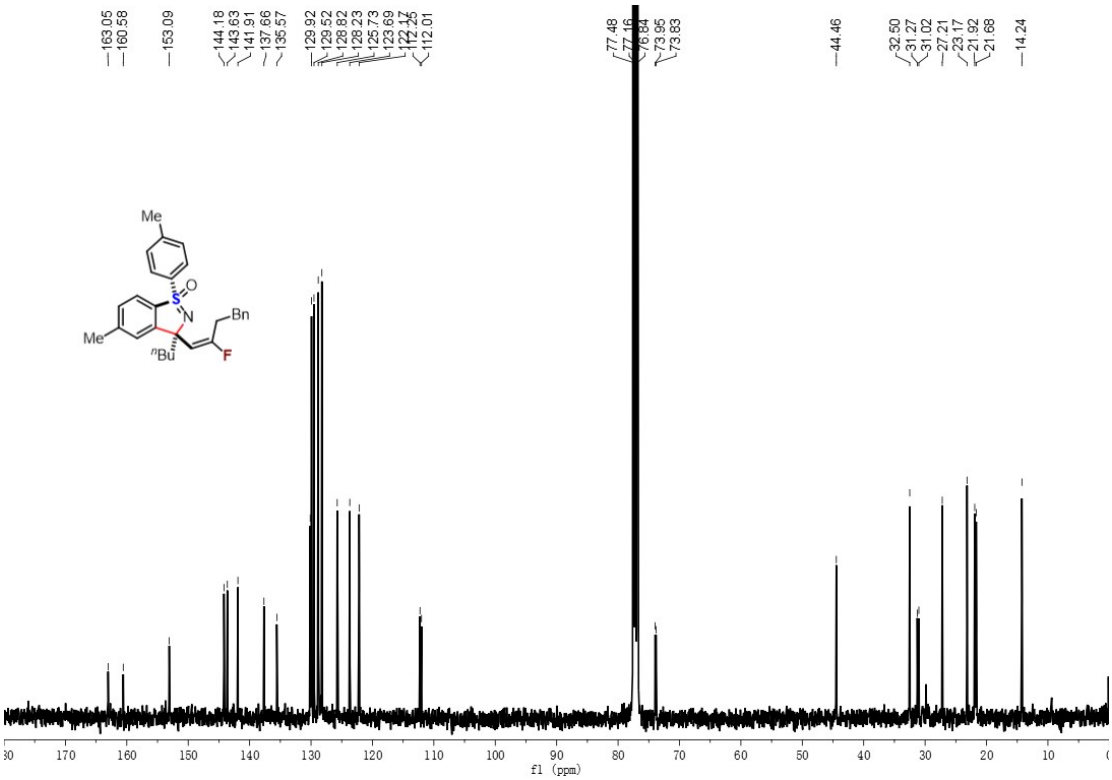
3a-^{19}F NMR (376 MHz, $CDCl_3$)



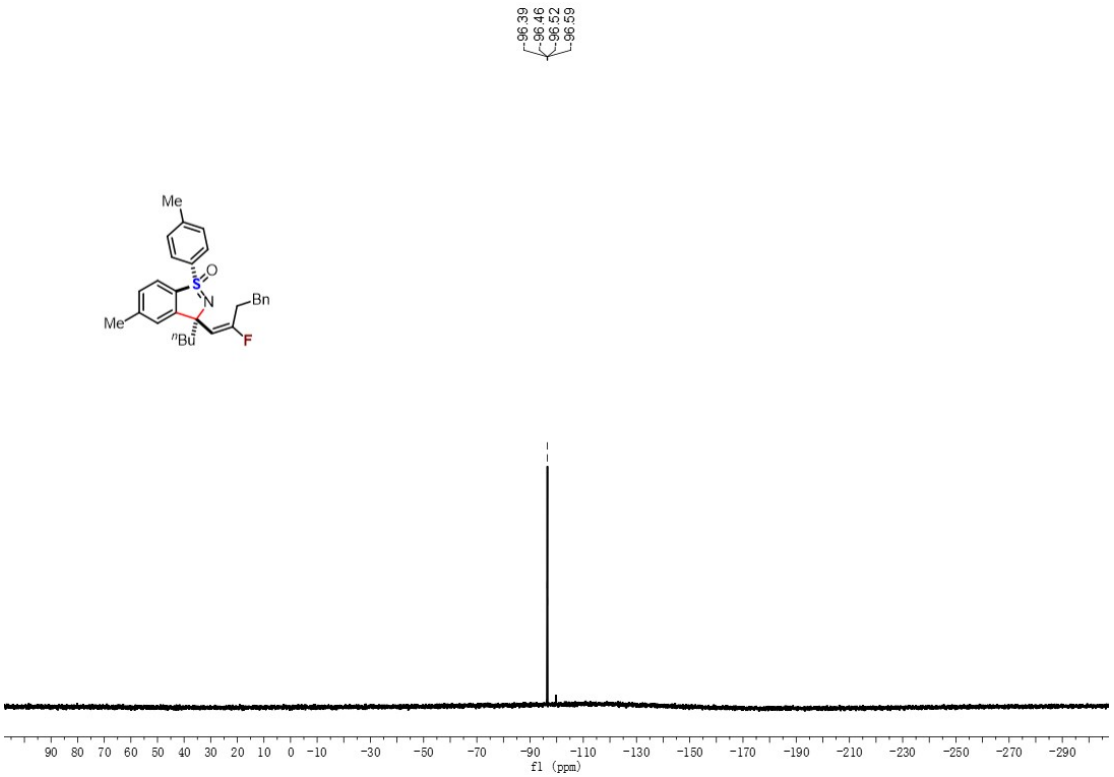
3b-^{1}H NMR (400 MHz, $CDCl_3$)



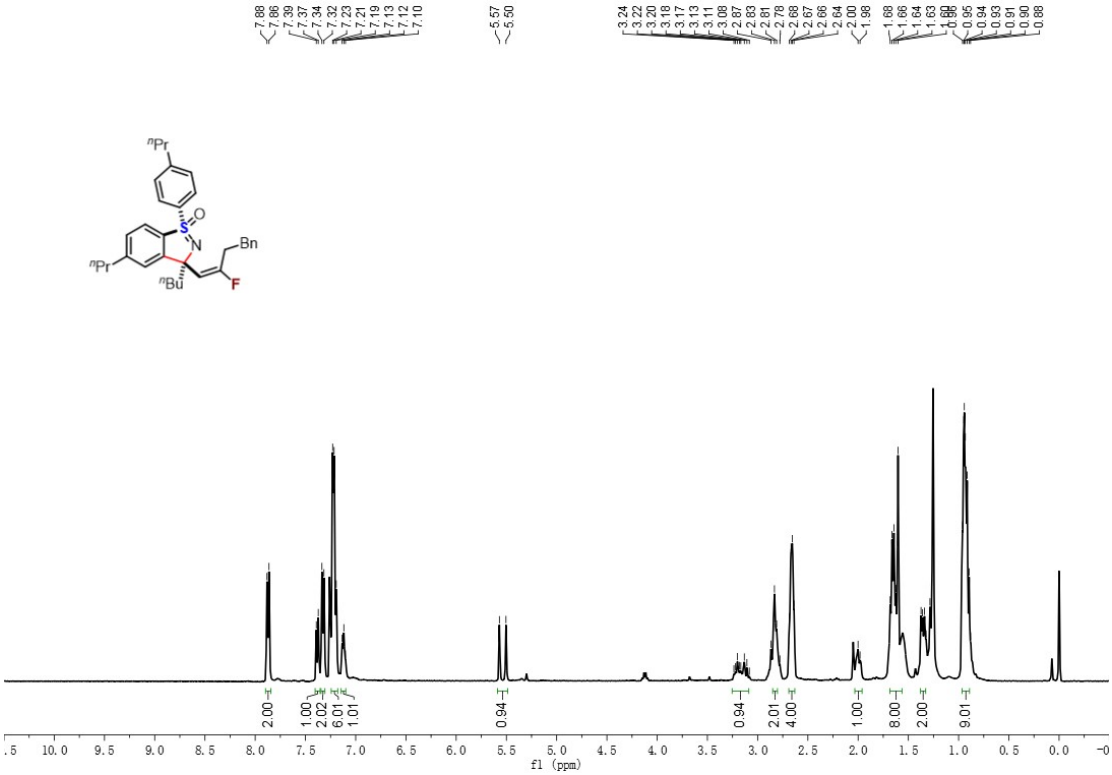
3b-^{13}C NMR (100 MHz, $CDCl_3$)



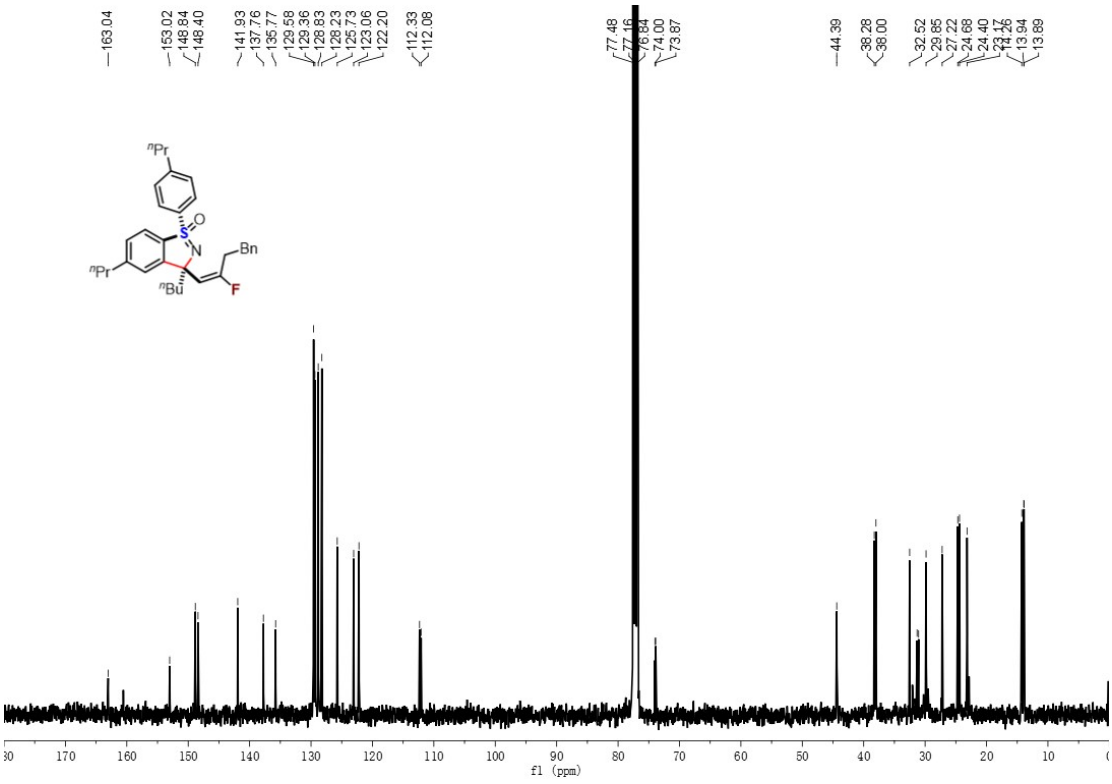
3b-^{19}F NMR (376 MHz, $CDCl_3$)



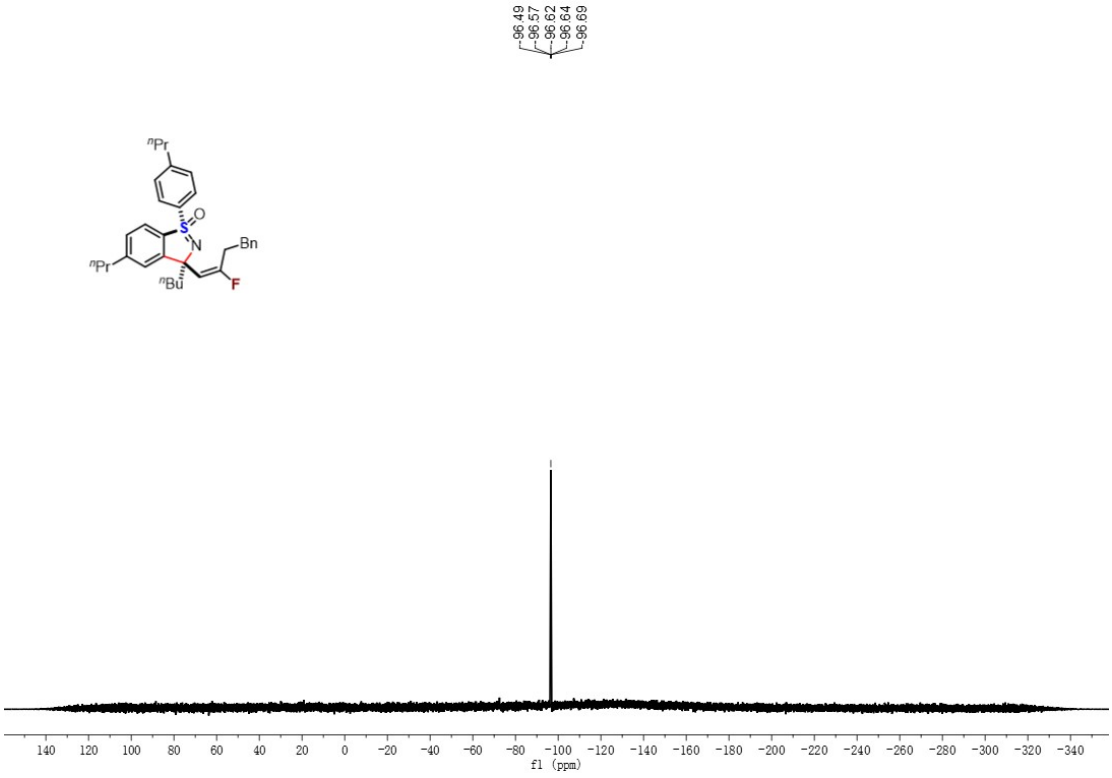
3c-^{1}H NMR (400 MHz, $CDCl_3$)



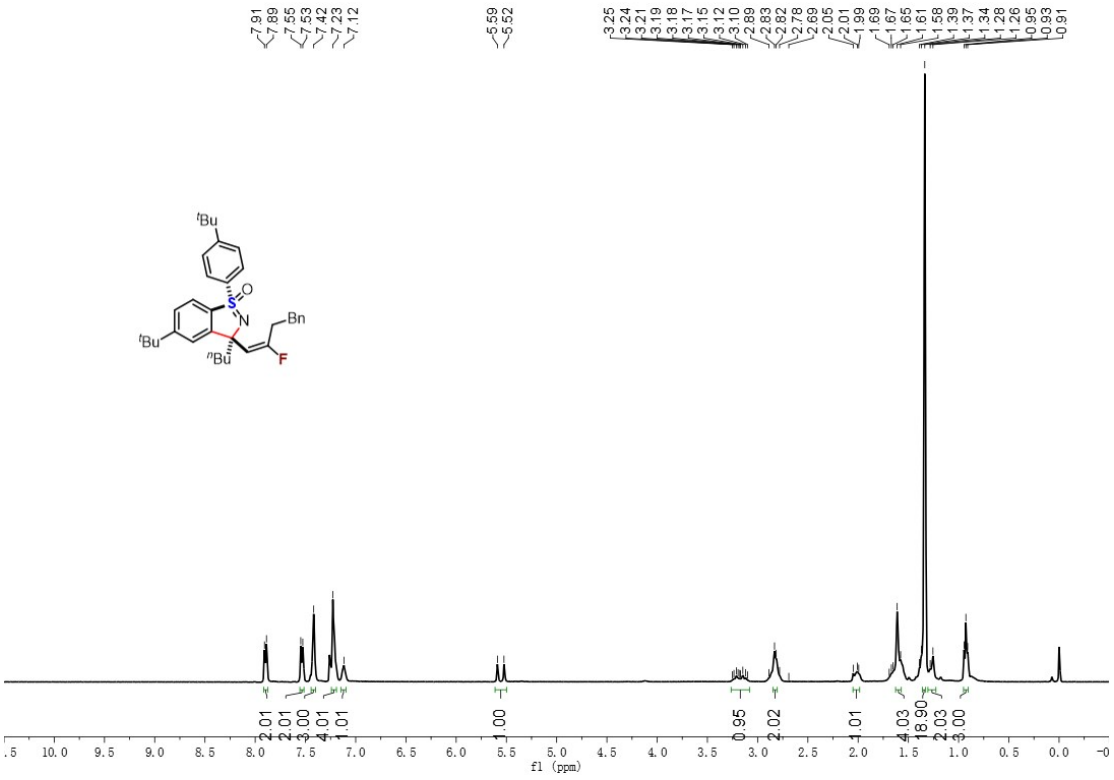
3c-^{13}C NMR (100 MHz, $CDCl_3$)



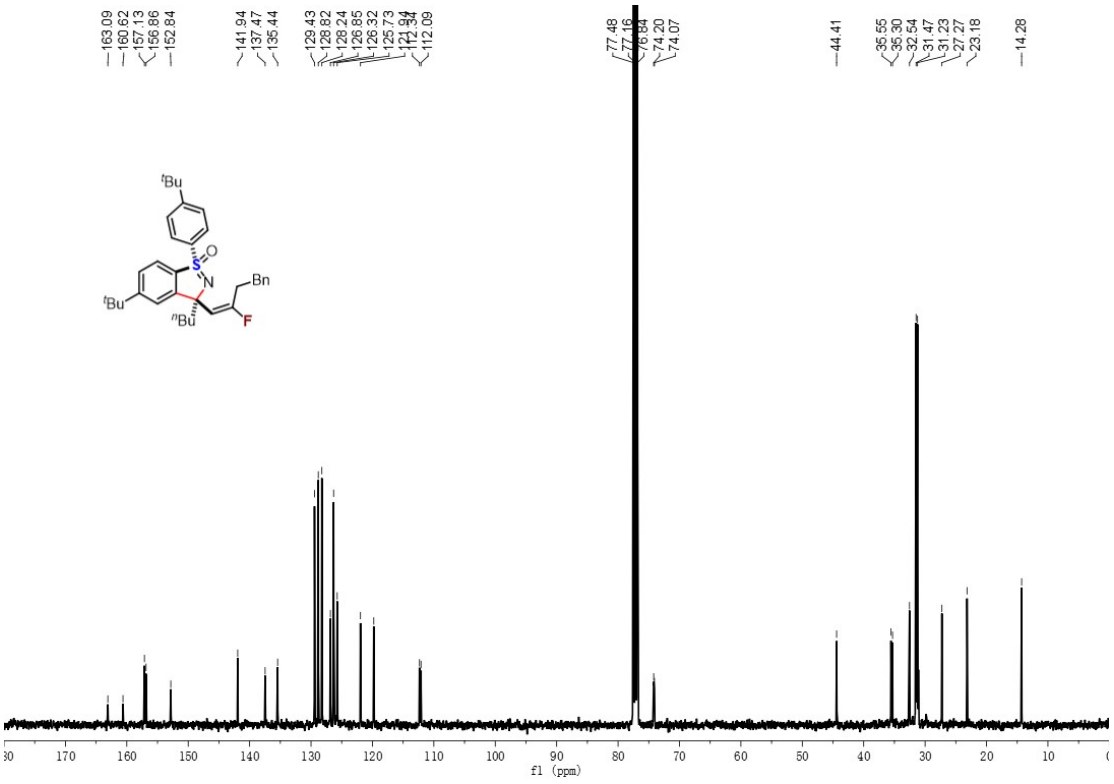
3c-^{19}F NMR (376 MHz, $CDCl_3$)



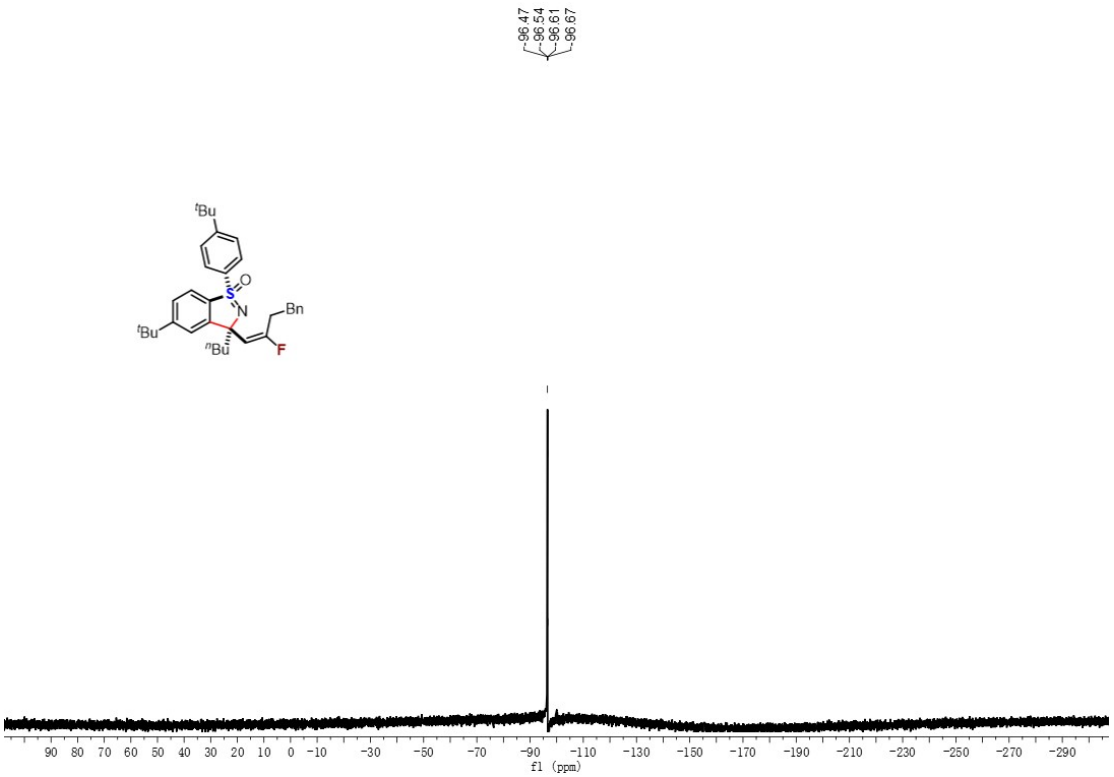
3d-^{1}H NMR (400 MHz, $CDCl_3$)



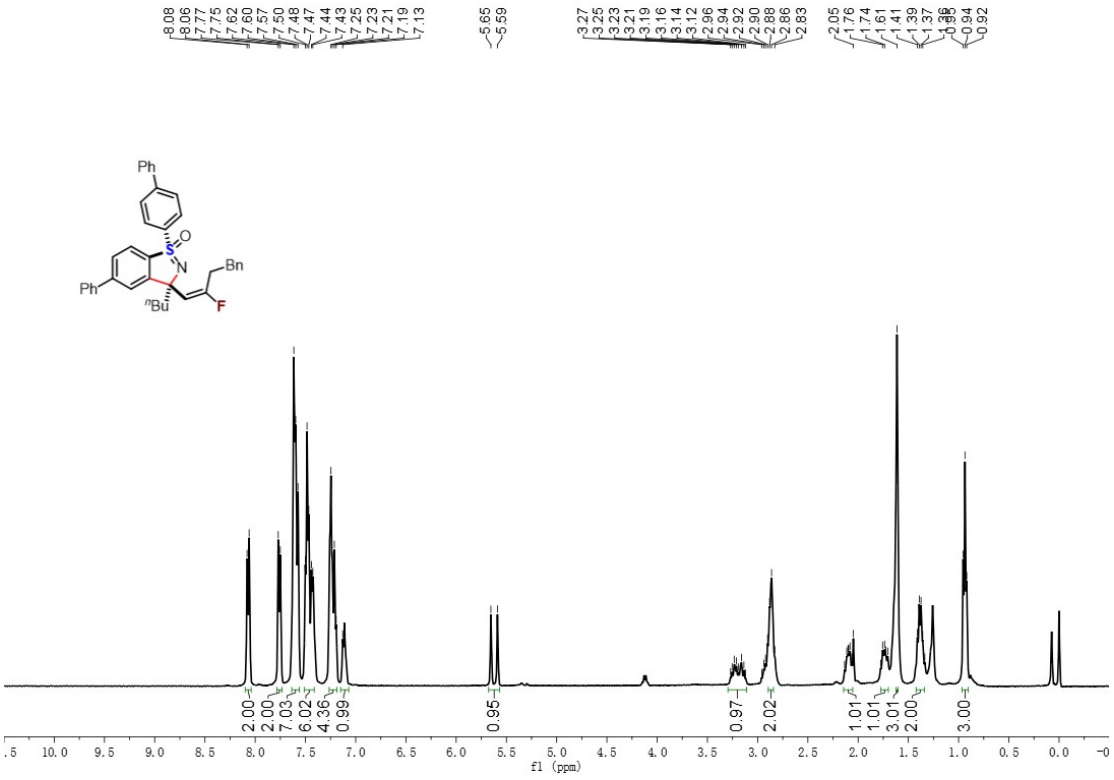
3d-^{13}C NMR (100 MHz, $CDCl_3$)



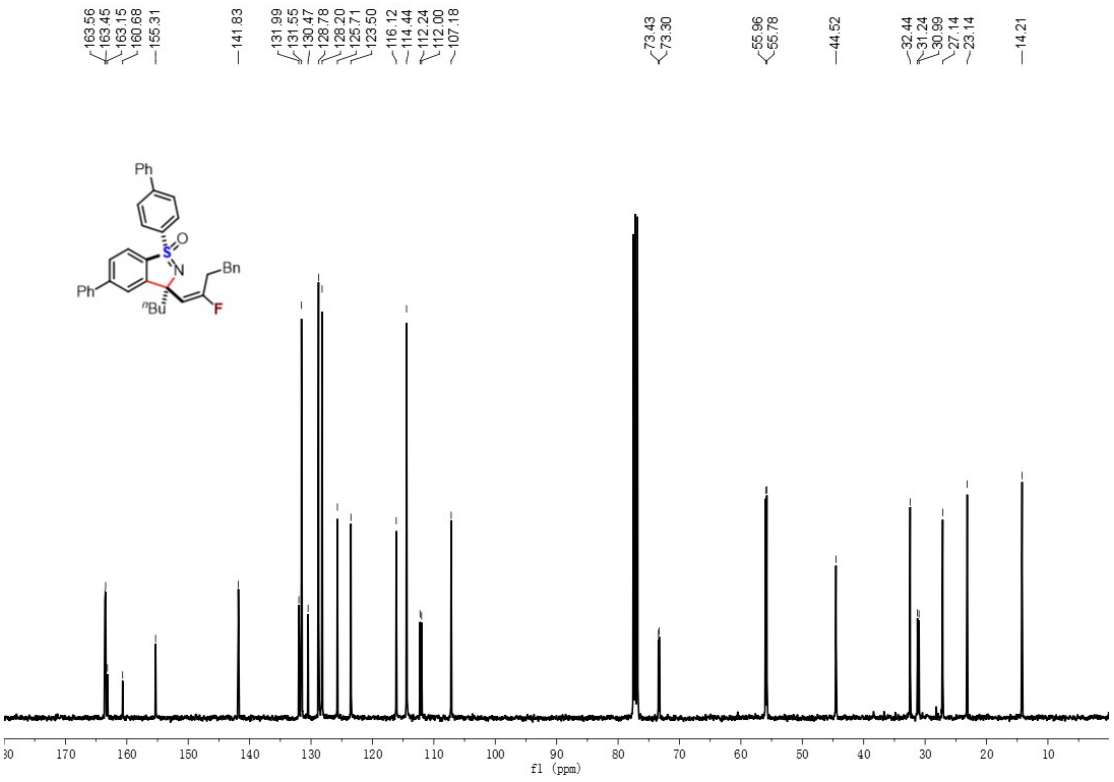
3d-^{19}F NMR (376 MHz, $CDCl_3$)



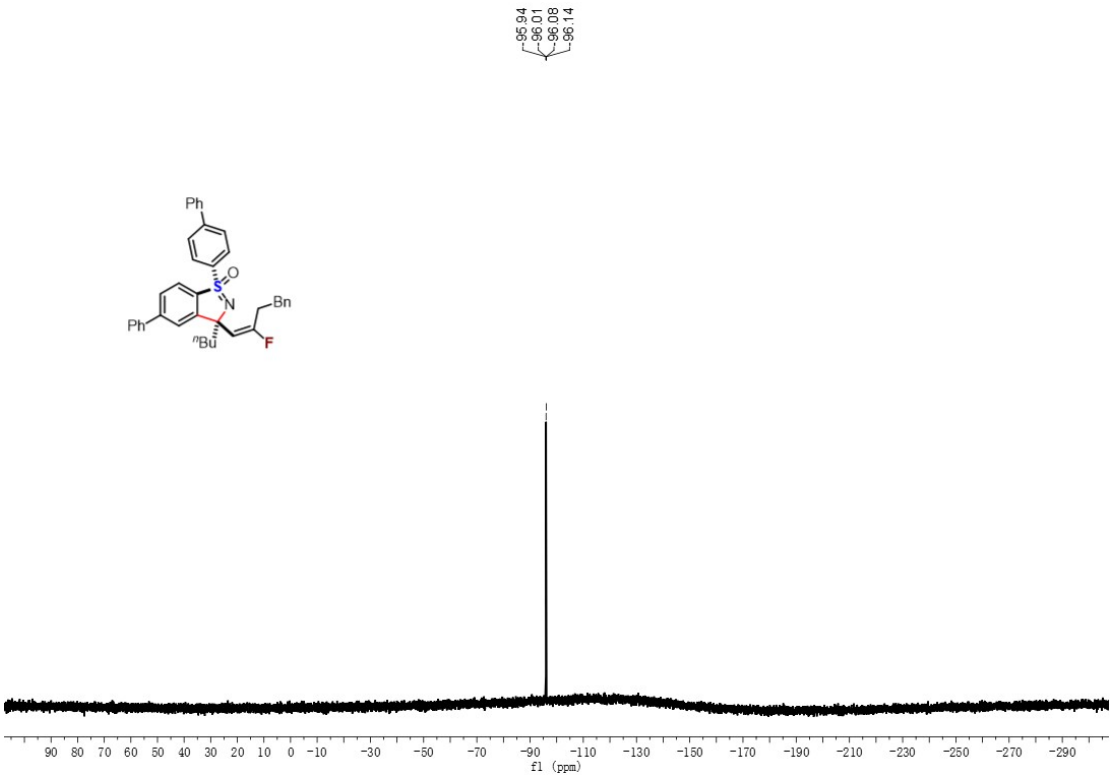
3e-^{1}H NMR (400 MHz, $CDCl_3$)



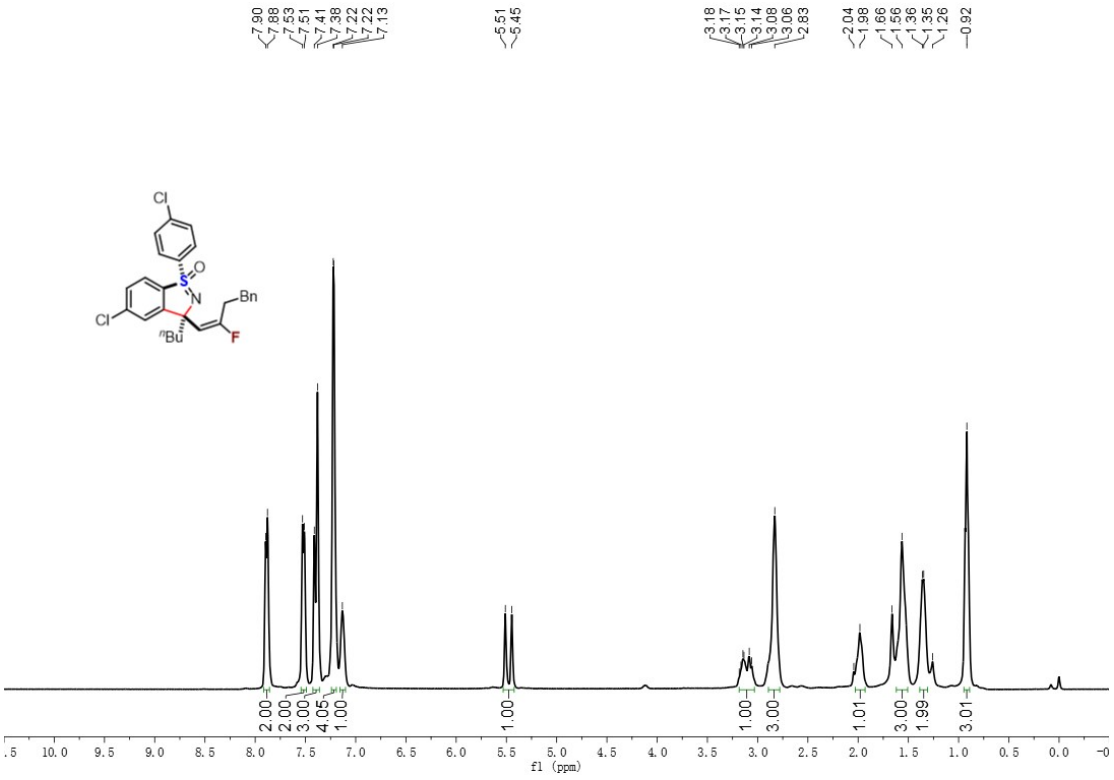
3e-^{13}C NMR (100 MHz, $CDCl_3$)



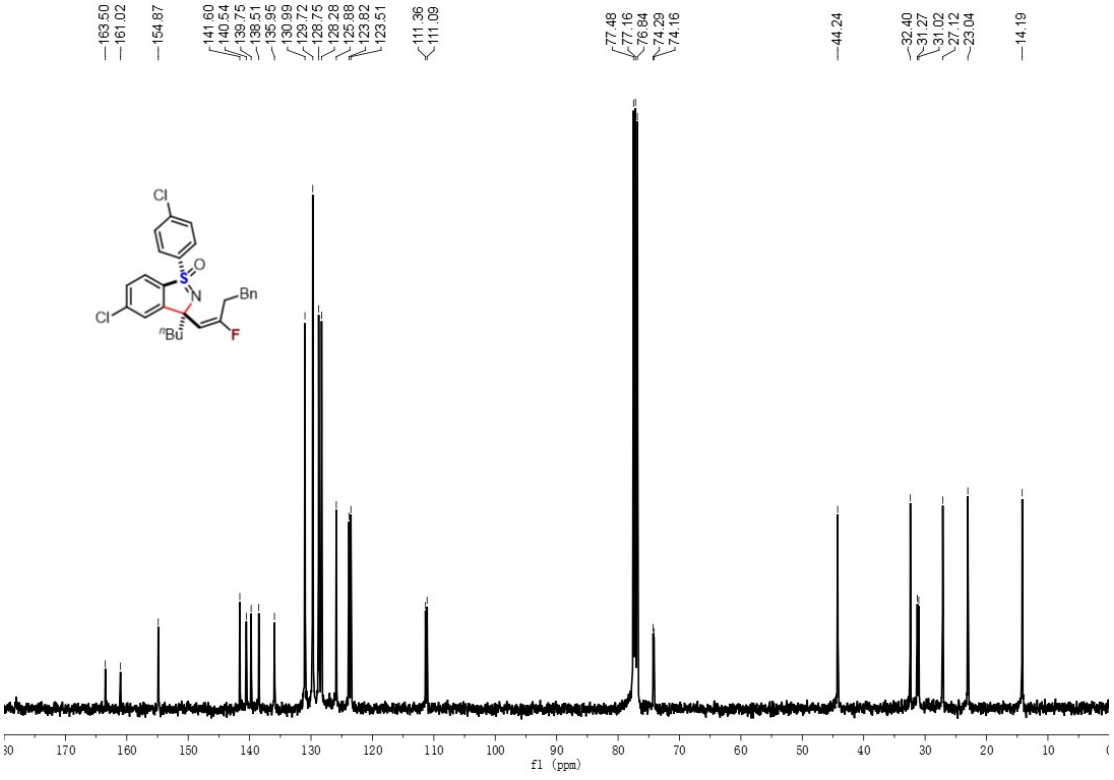
3e-^{19}F NMR (376 MHz, $CDCl_3$)



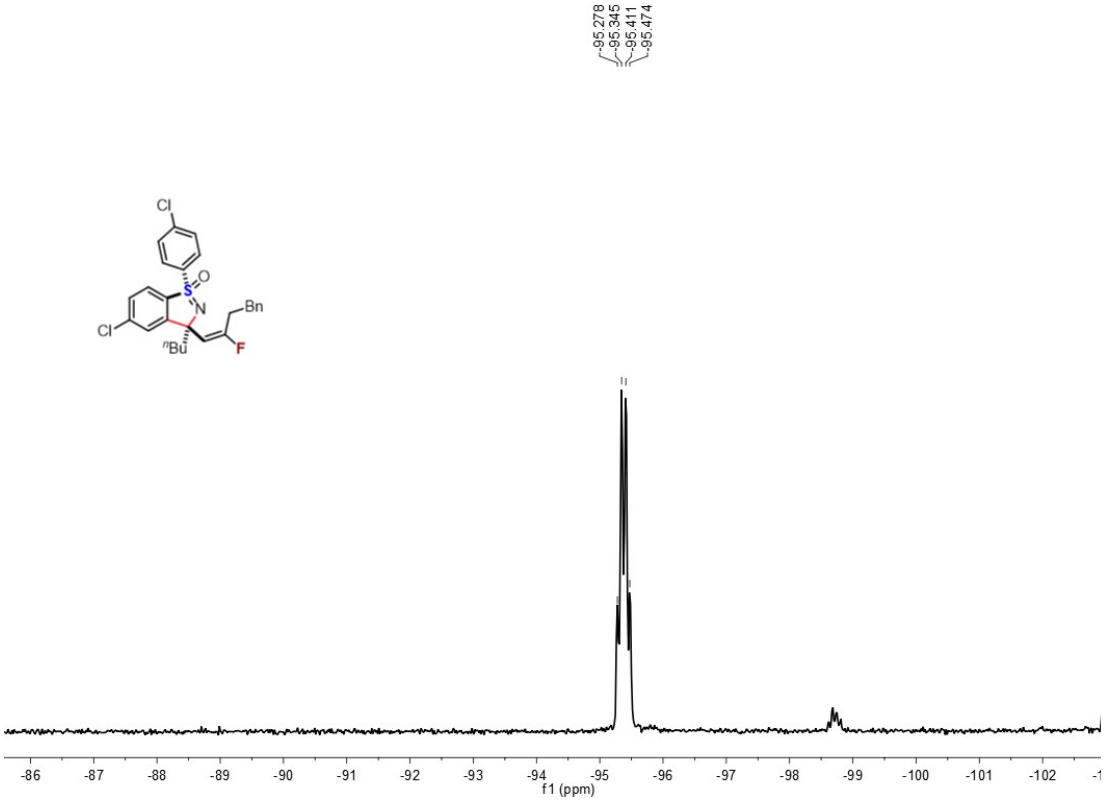
3f-^{1}H NMR (400 MHz, $CDCl_3$)



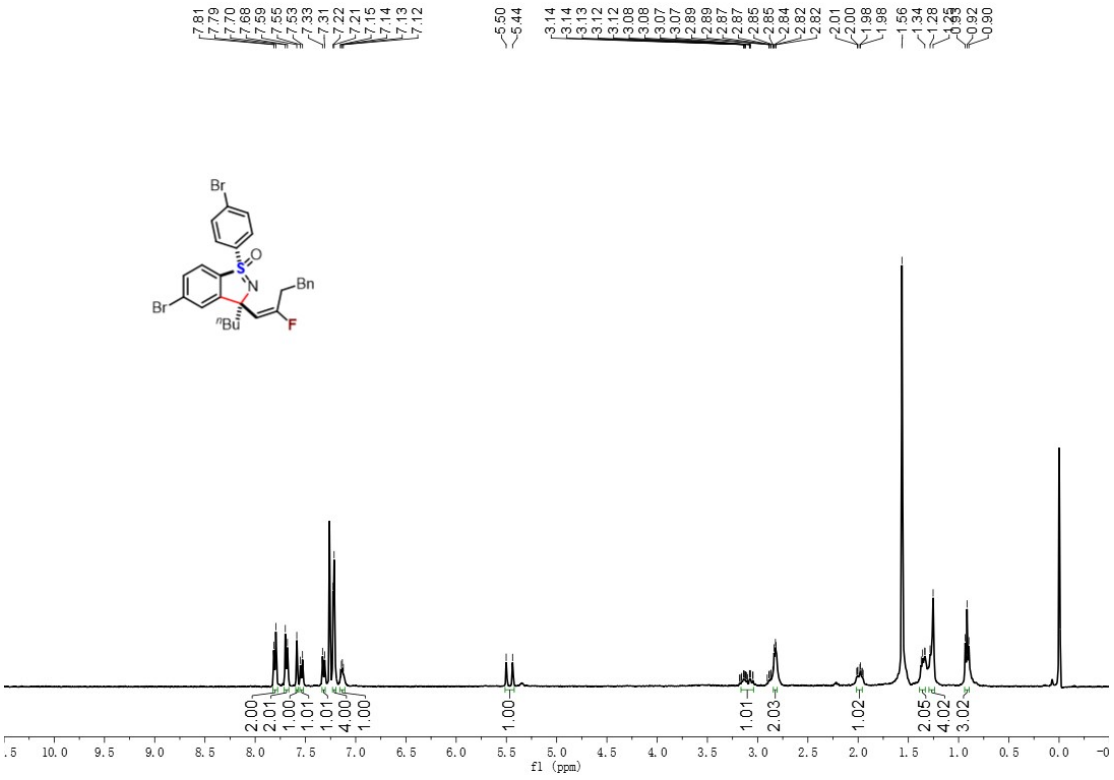
3f-^{13}C NMR (100 MHz, $CDCl_3$)



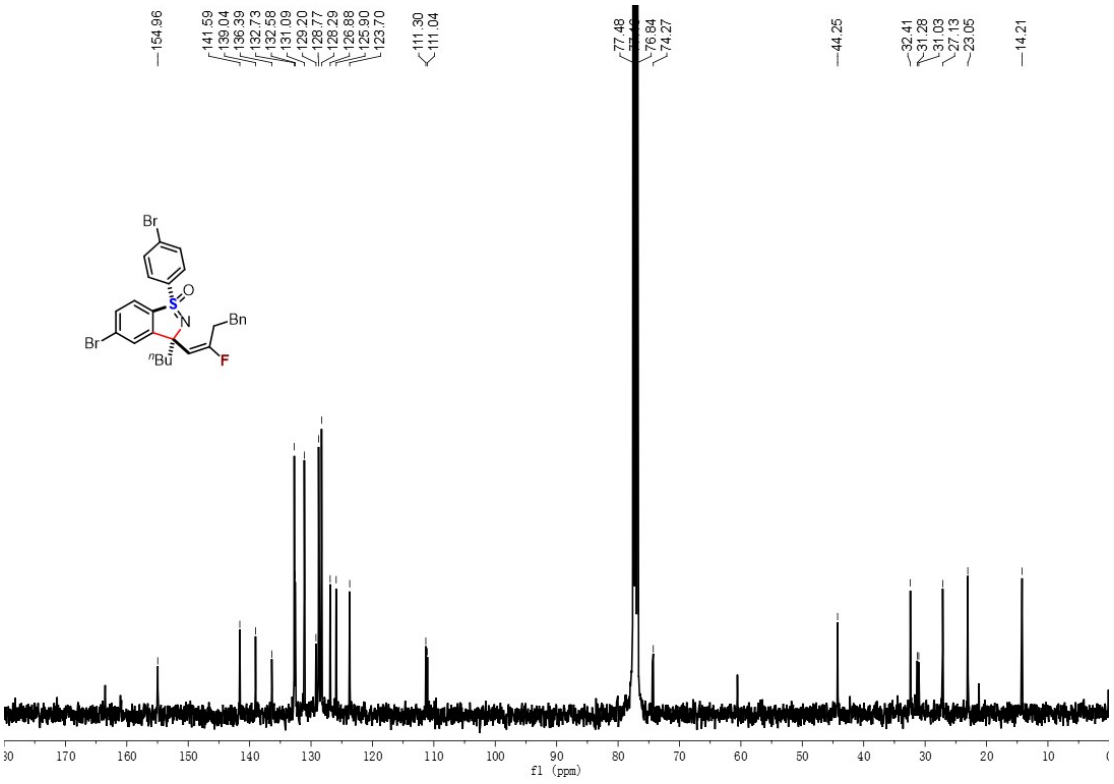
3f-^{19}F NMR (376 MHz, $CDCl_3$)



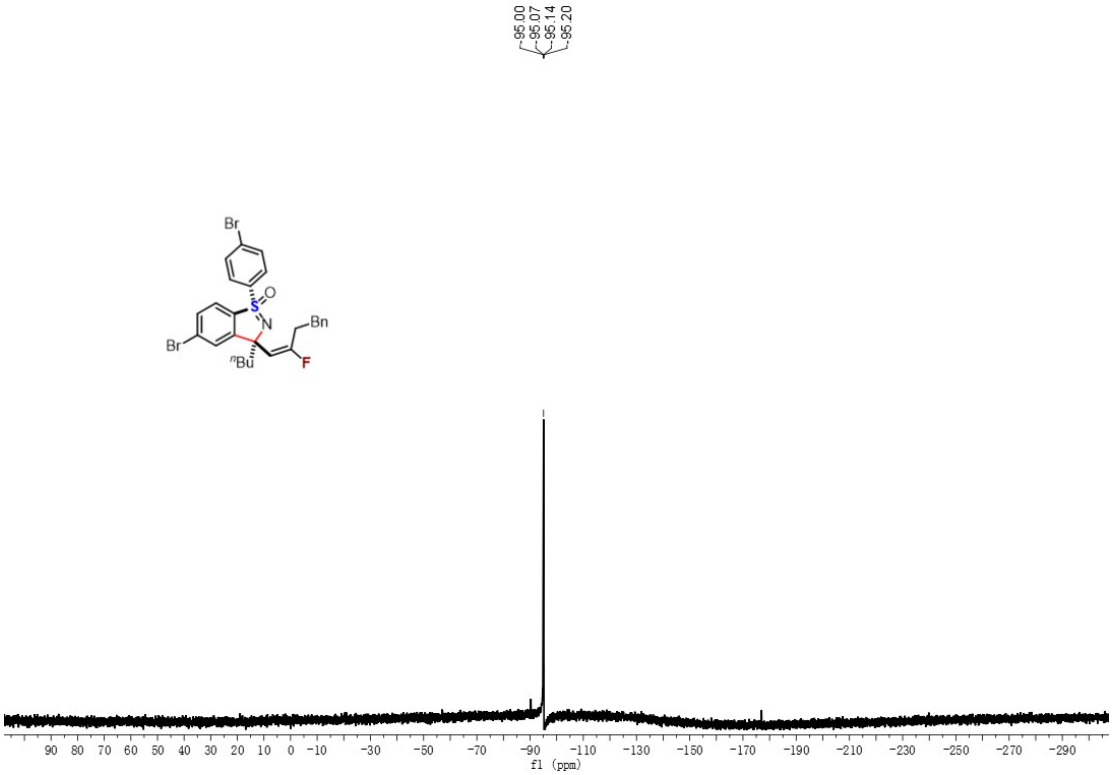
3g-^{1}H NMR (400 MHz, $CDCl_3$)



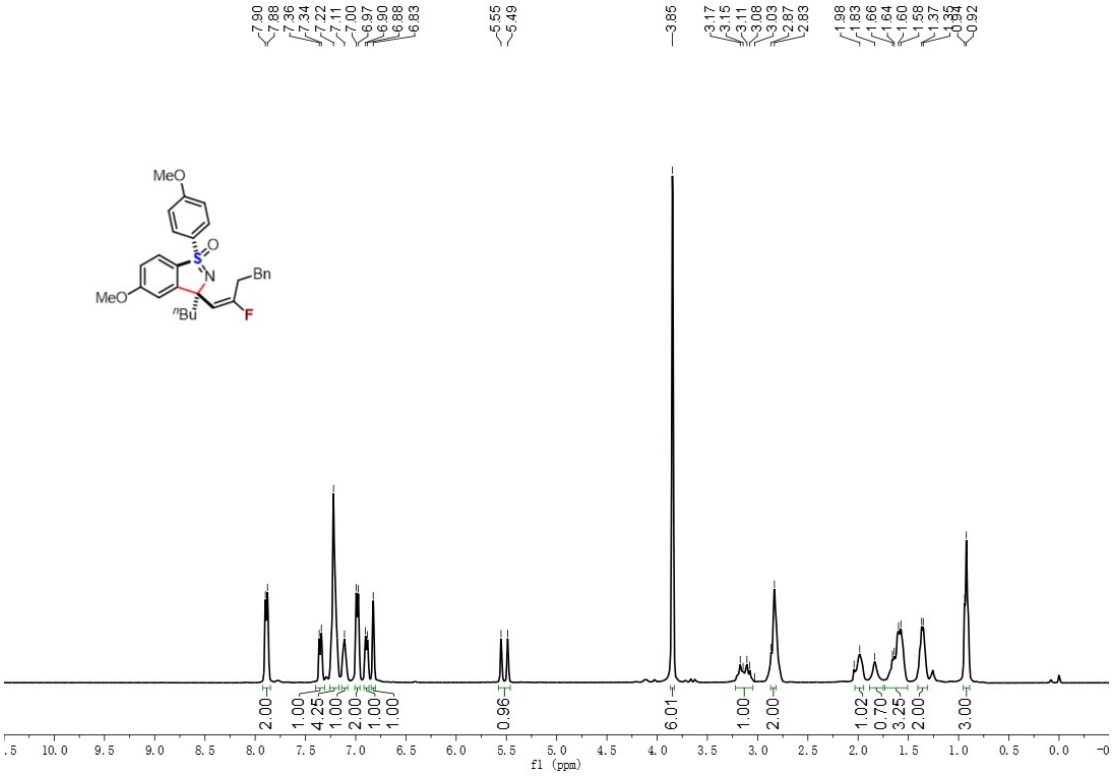
3g-^{13}C NMR (100 MHz, $CDCl_3$)



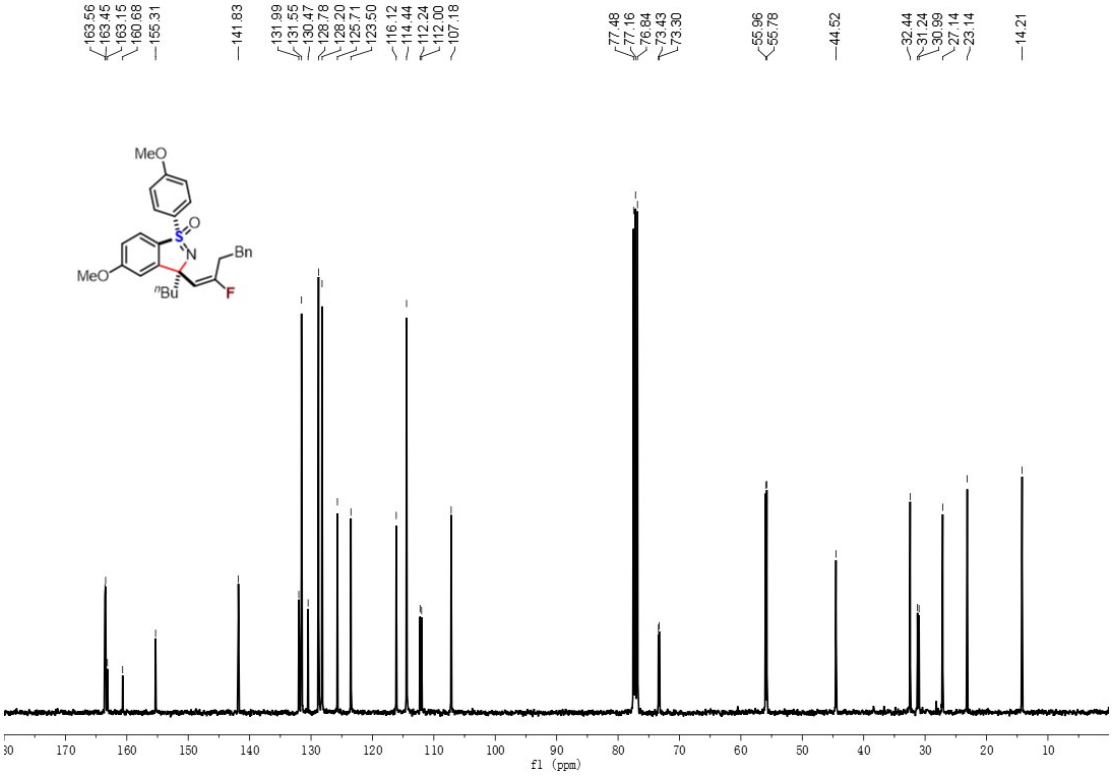
3g-^{19}F NMR (376 MHz, $CDCl_3$)



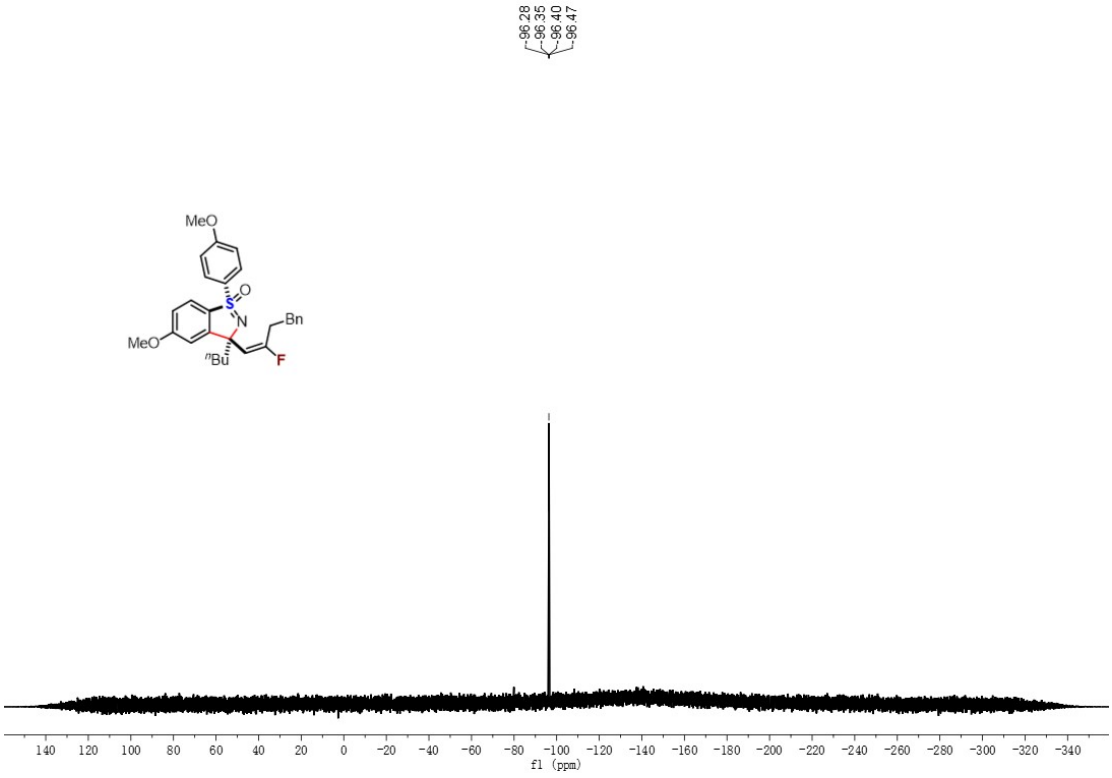
3h-^{1}H NMR (400 MHz, $CDCl_3$)



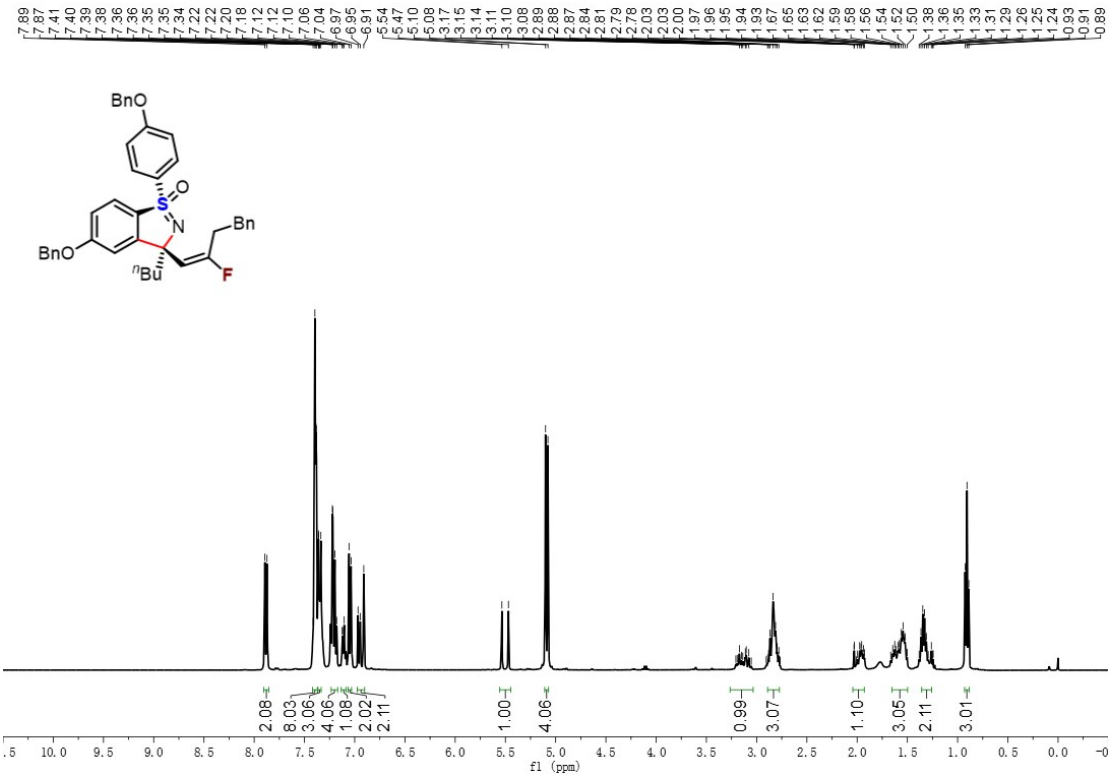
3h-^{13}C NMR (100 MHz, $CDCl_3$)



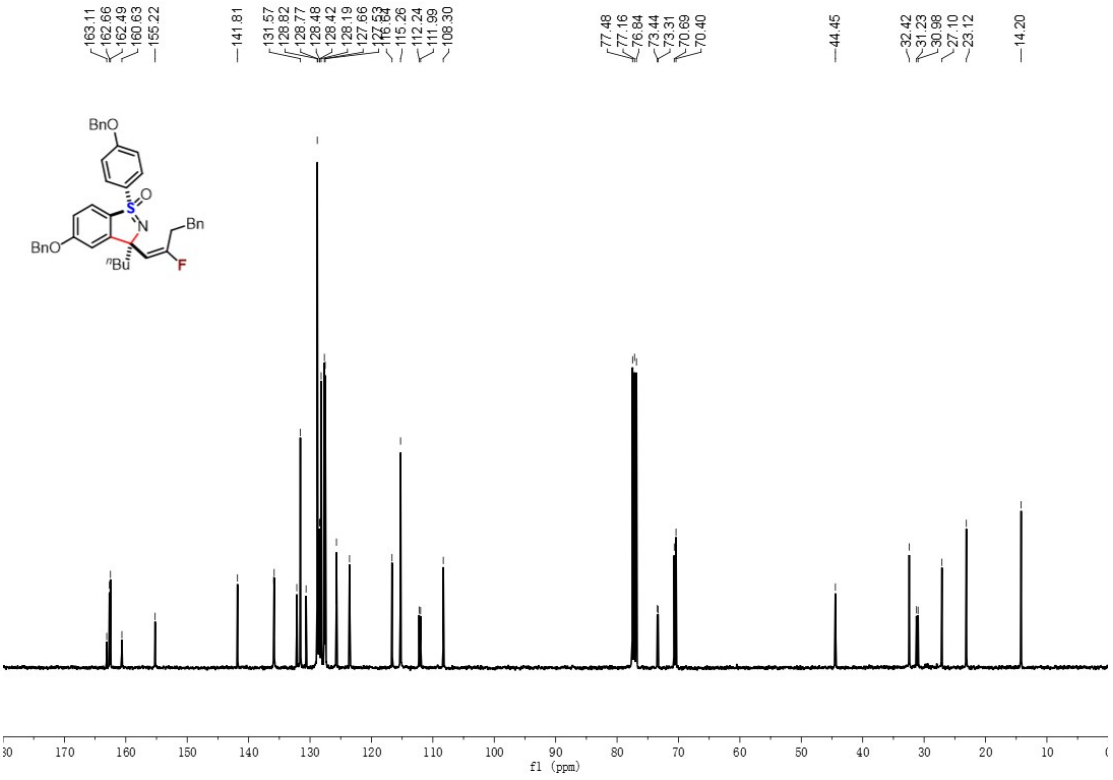
3h-^{19}F NMR (376 MHz, $CDCl_3$)



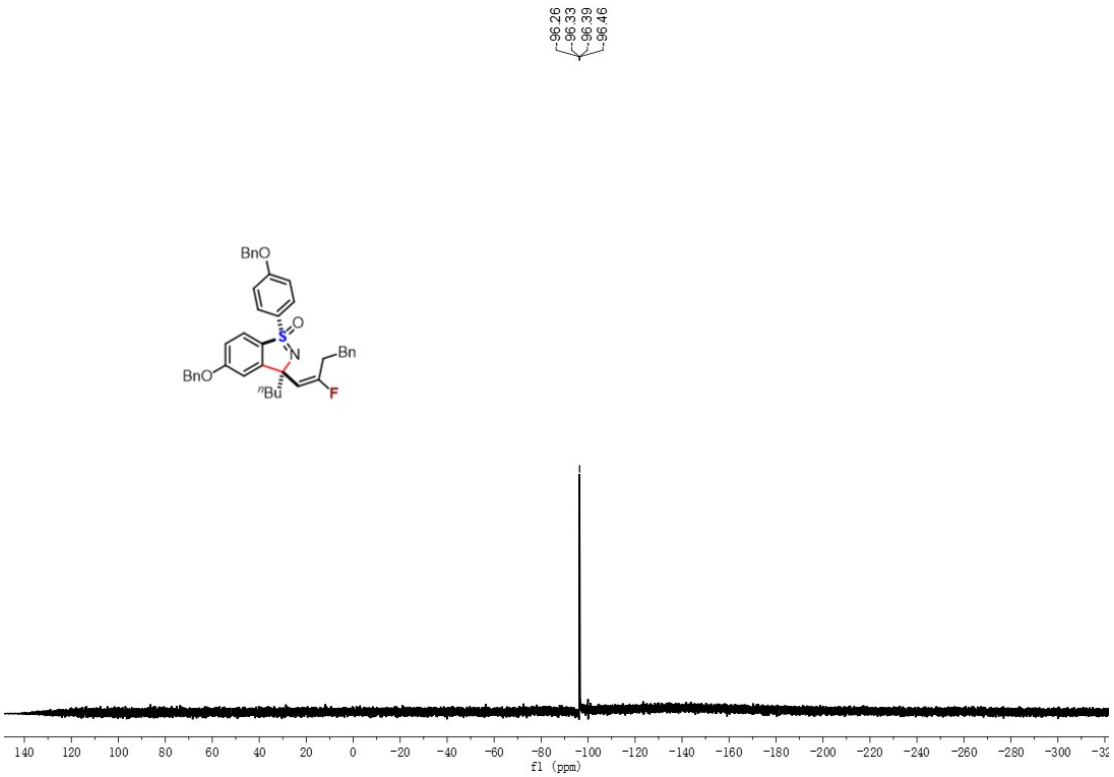
3i-^{1}H NMR (400 MHz, $CDCl_3$)



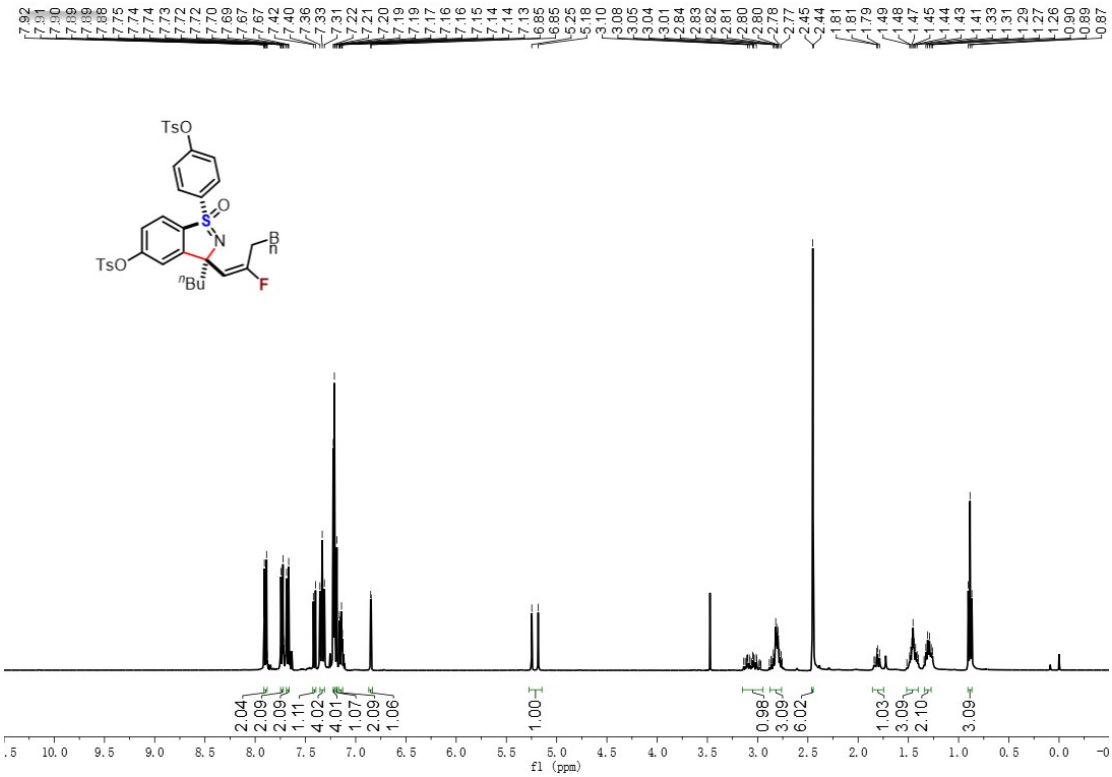
3i-^{13}C NMR (100 MHz, $CDCl_3$)



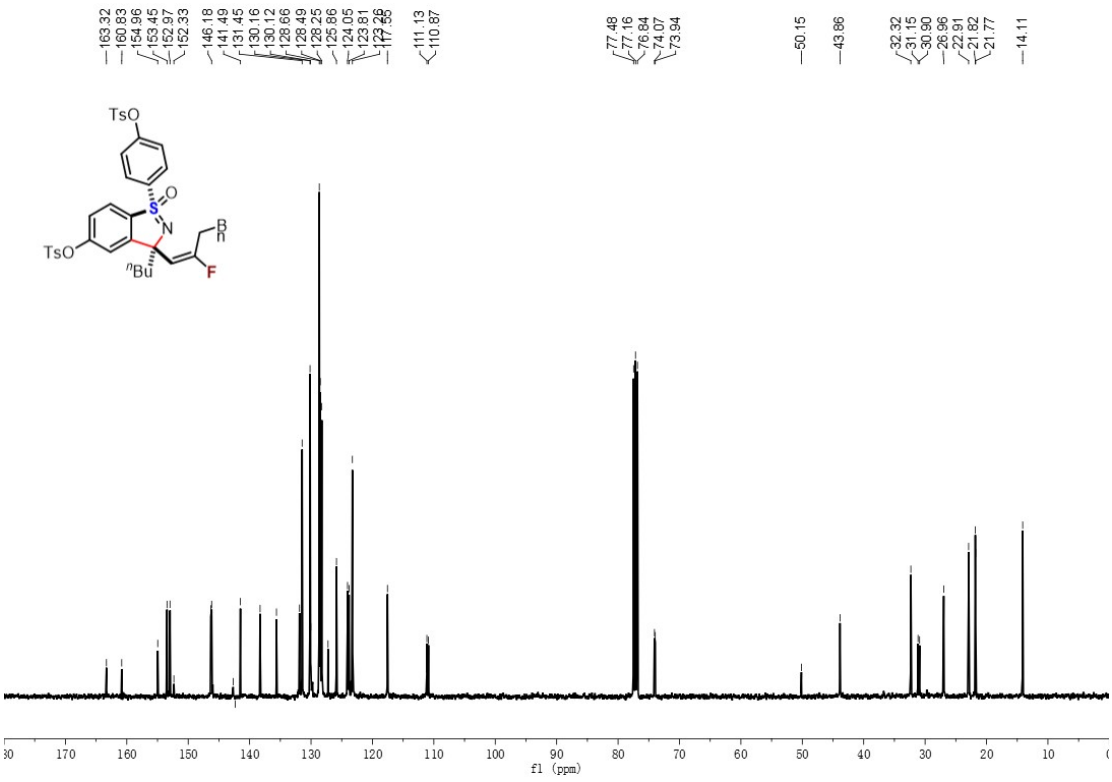
3i-^{19}F NMR (376 MHz, $CDCl_3$)



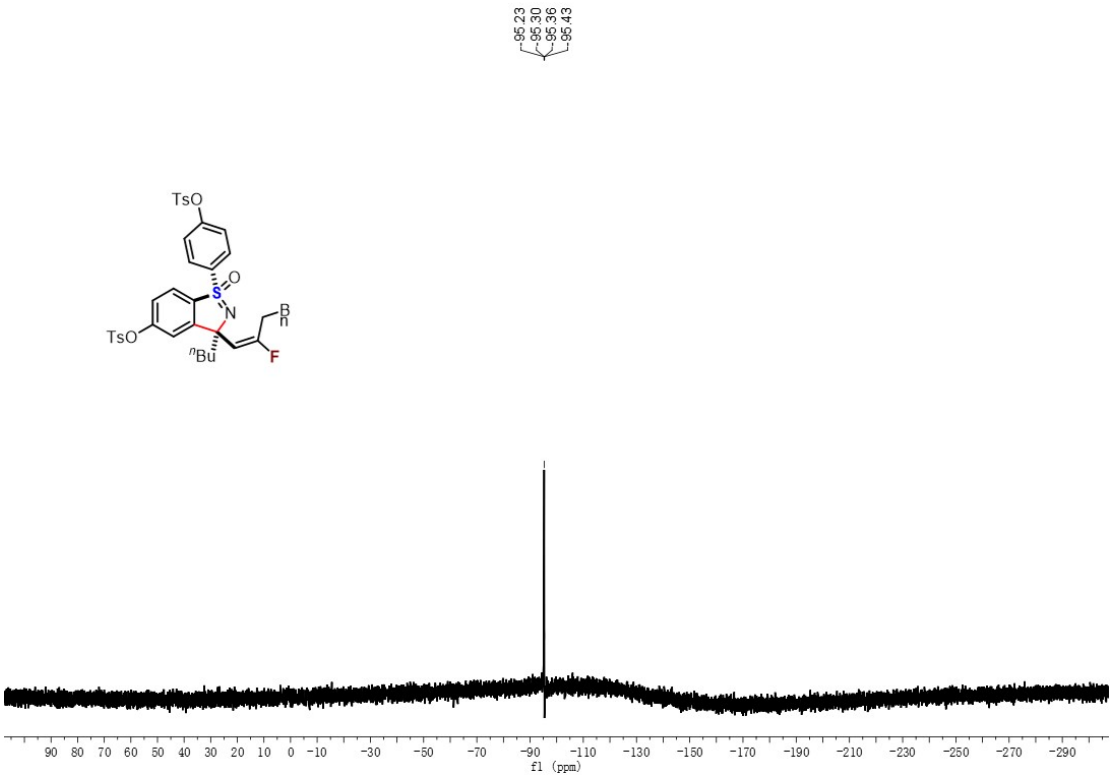
3j-^{1}H NMR (400 MHz, $CDCl_3$)



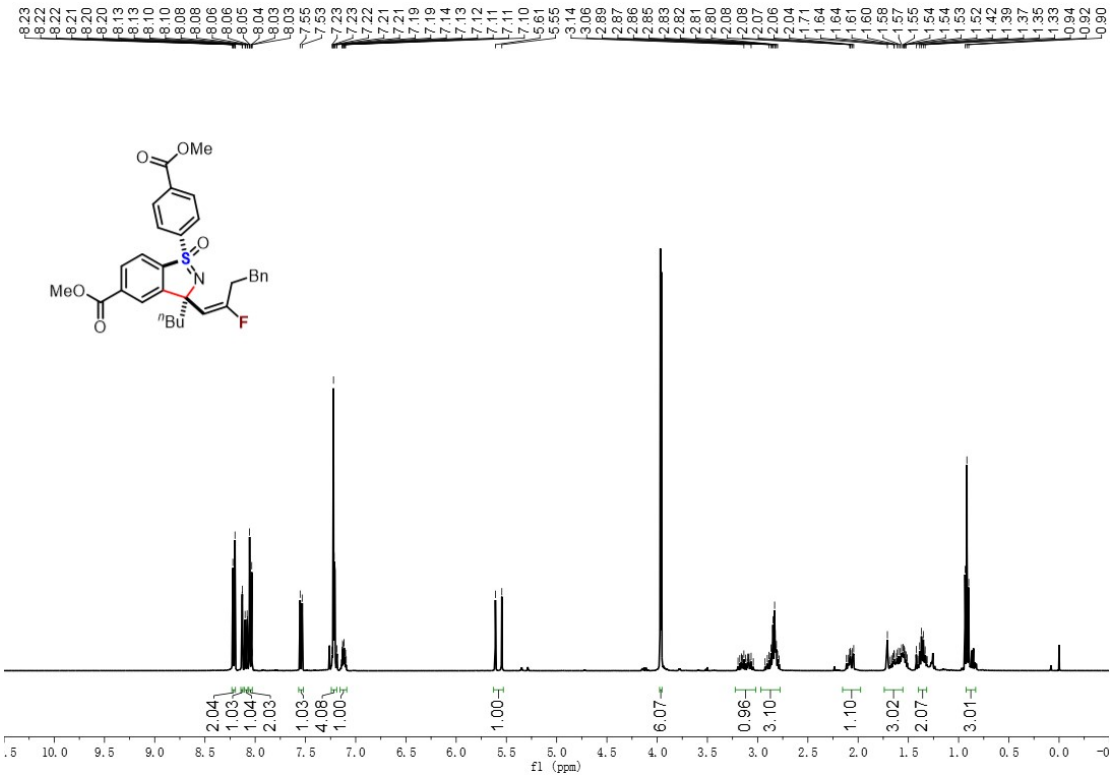
3j-^{13}C NMR (100 MHz, $CDCl_3$)



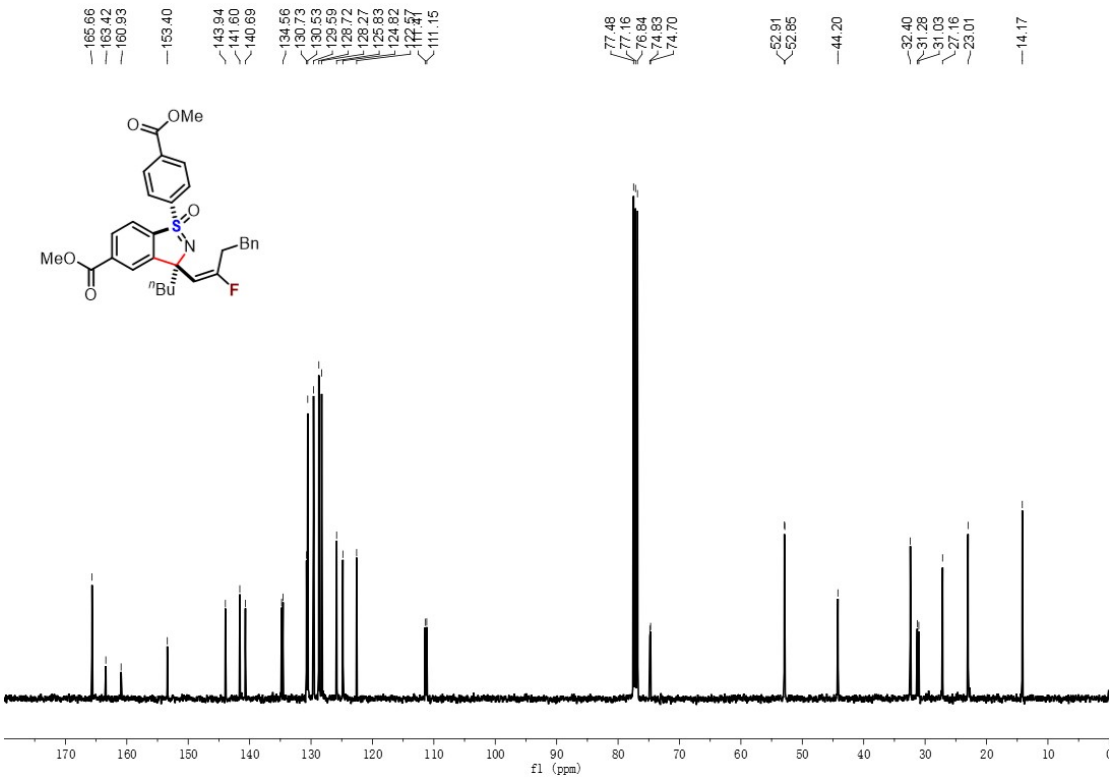
3j-^{19}F NMR (376 MHz, $CDCl_3$)



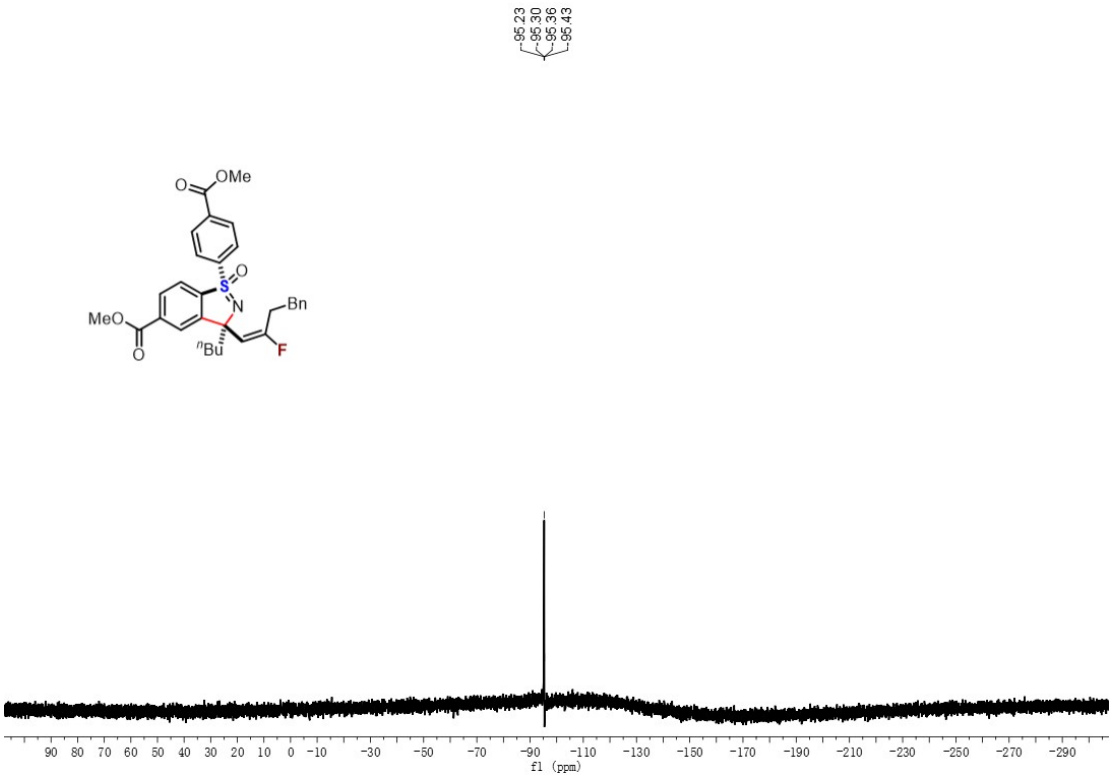
3k-^{1}H NMR (400 MHz, $CDCl_3$)



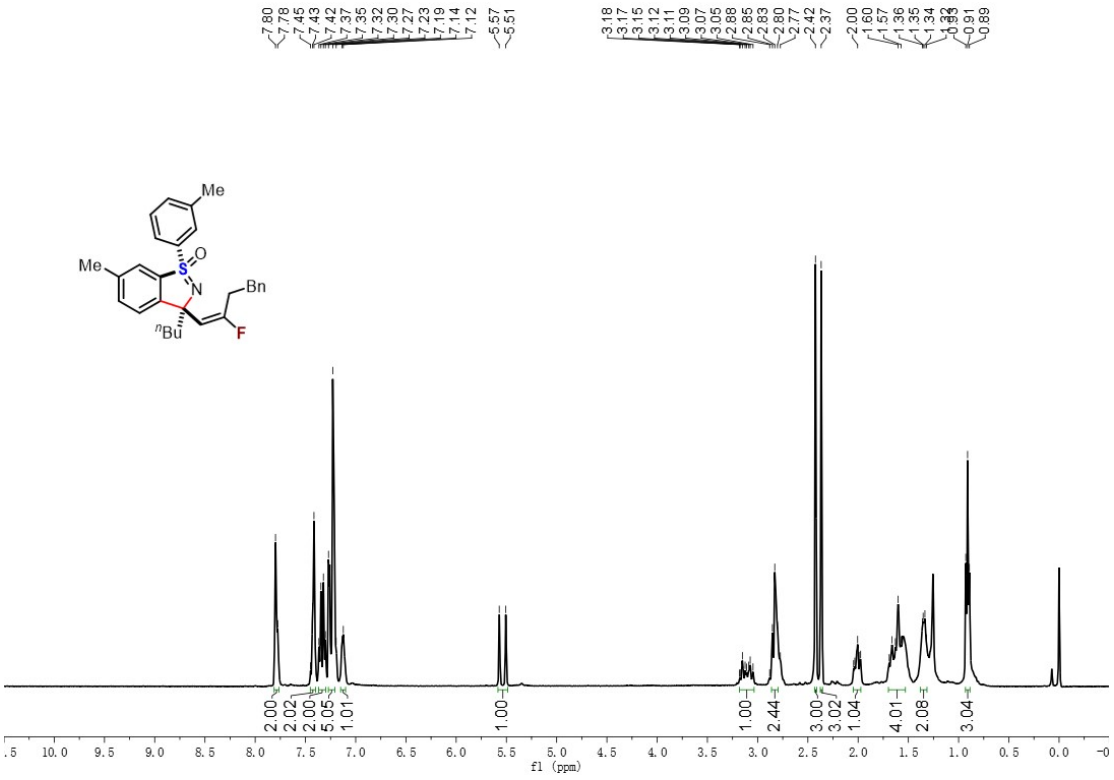
3k-^{13}C NMR (100 MHz, $CDCl_3$)



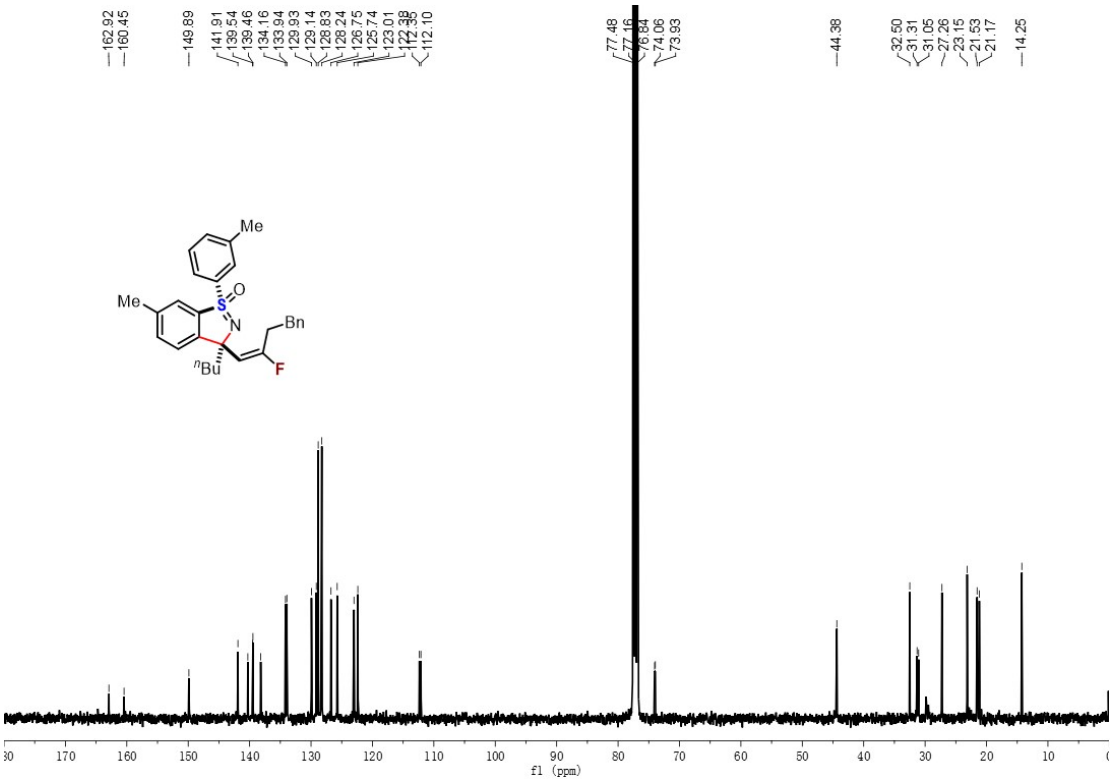
3k-^{19}F NMR (376 MHz, $CDCl_3$)



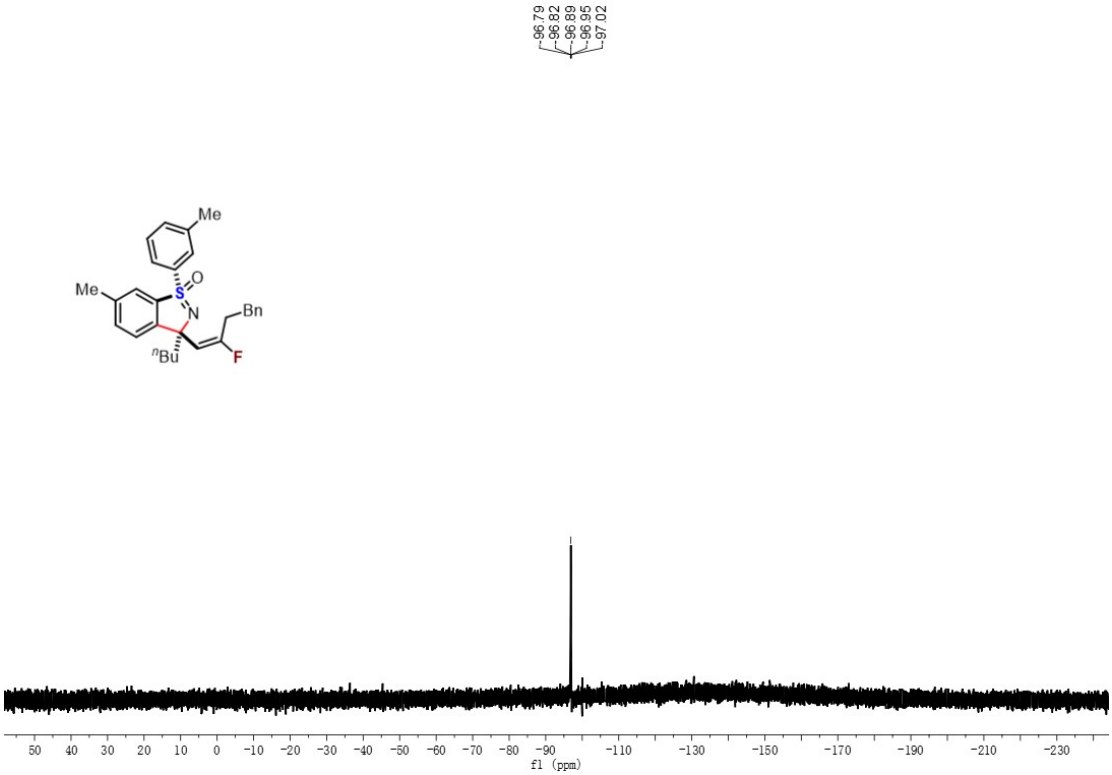
3l-^{1}H NMR (400 MHz, $CDCl_3$)



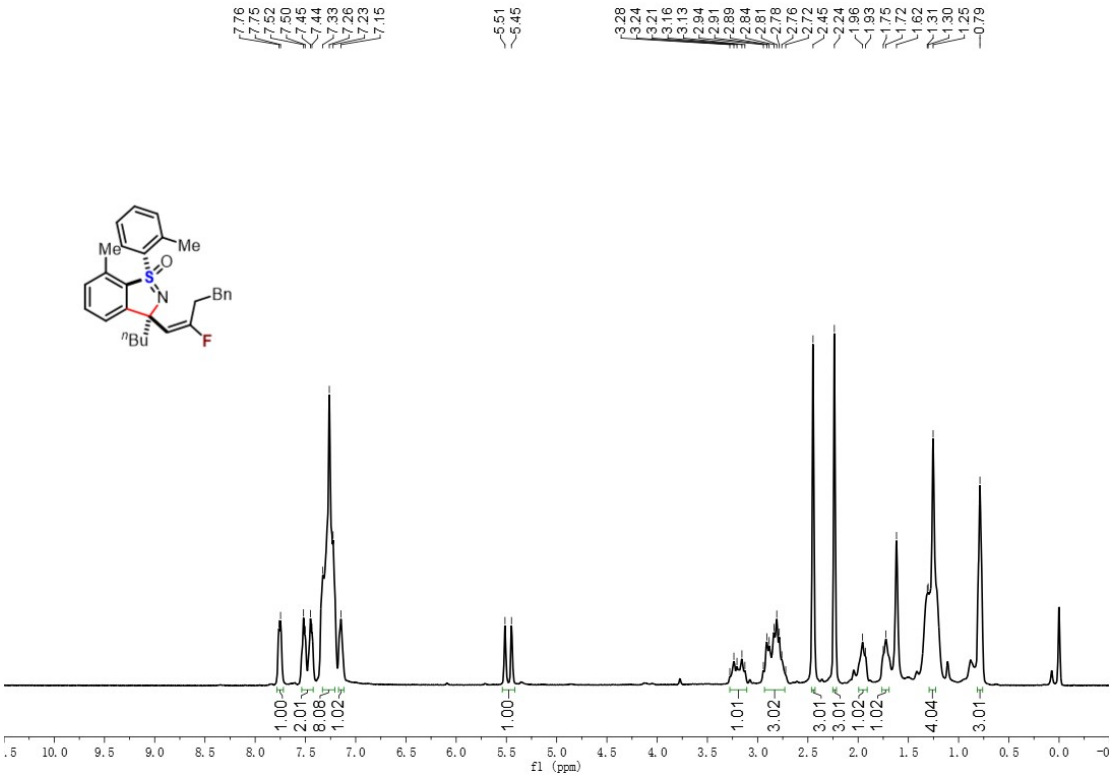
3l-^{13}C NMR (100 MHz, $CDCl_3$)



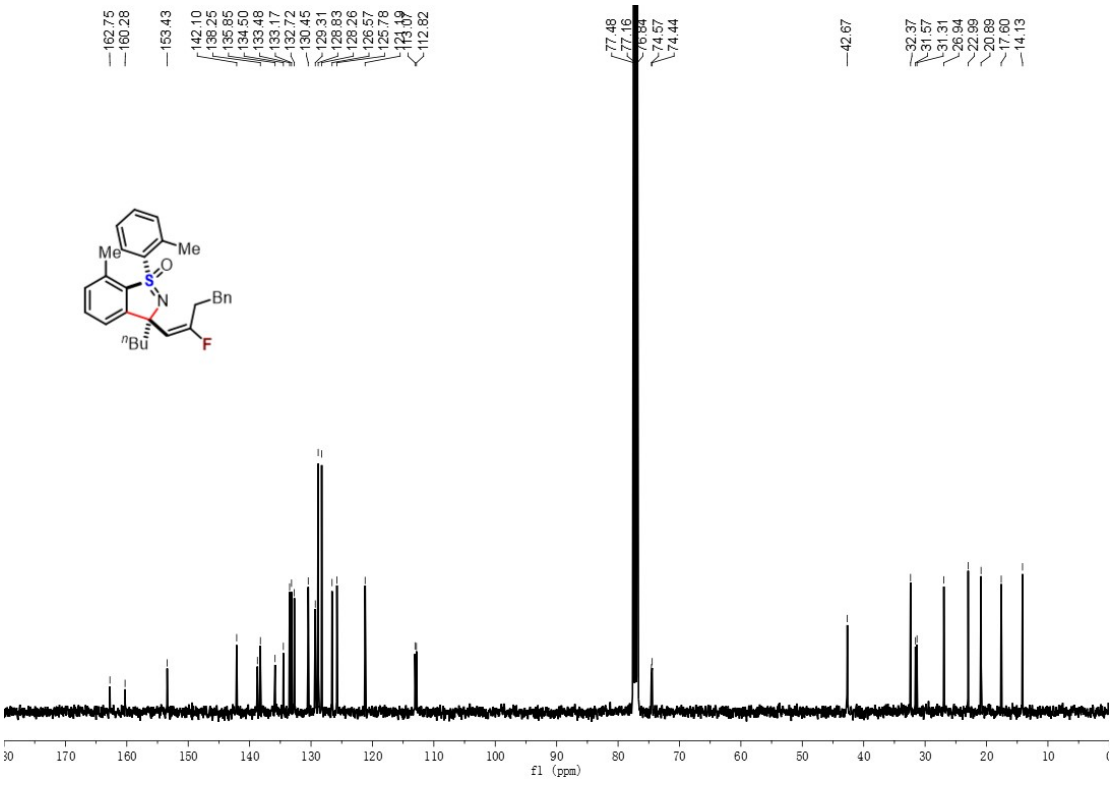
3l-^{19}F NMR (376 MHz, $CDCl_3$)



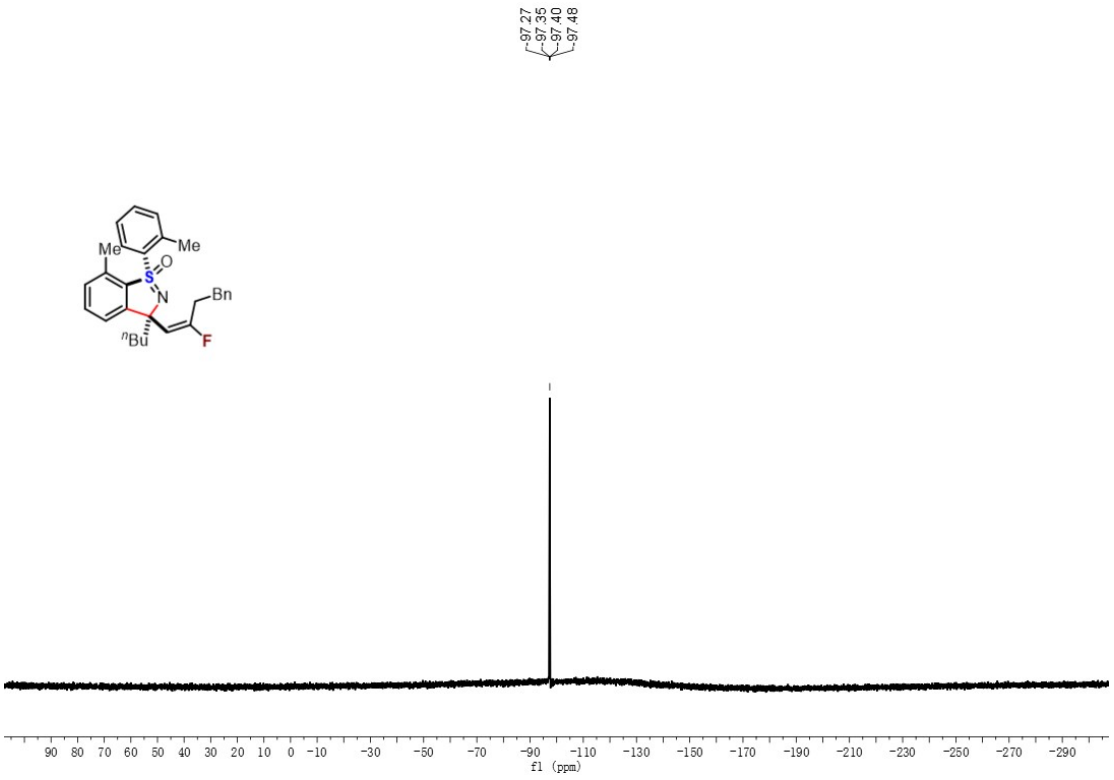
3m-^{1}H NMR (400 MHz, $CDCl_3$)



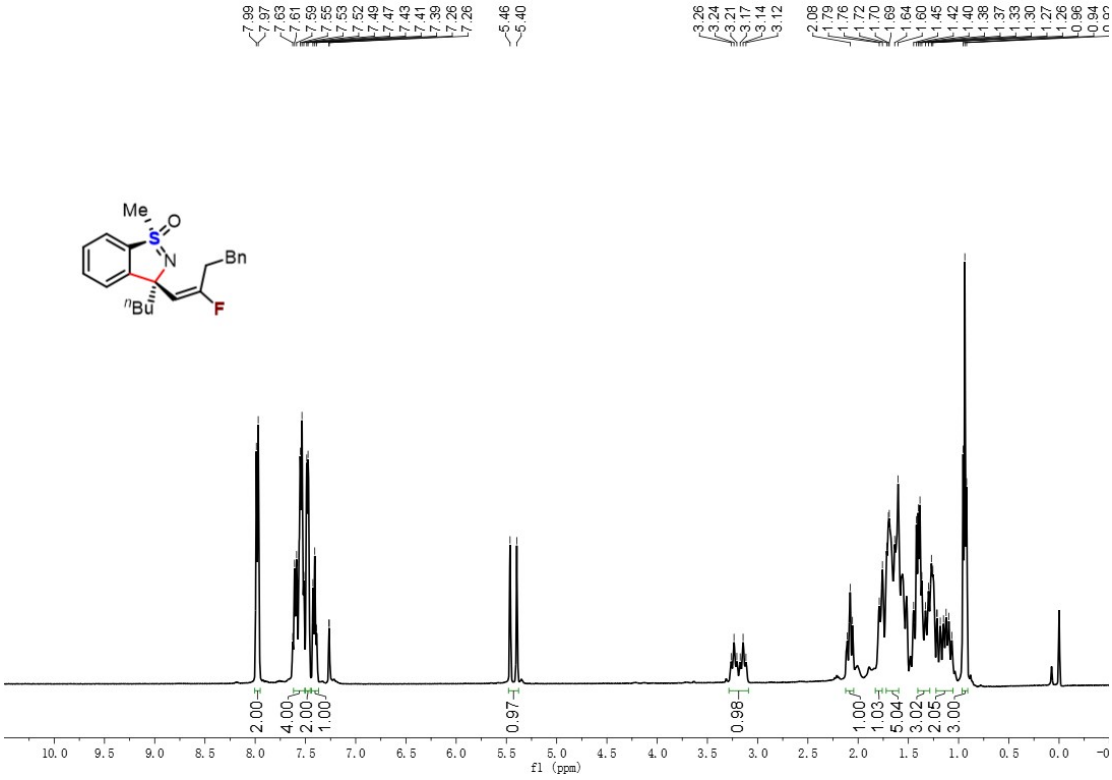
3m-^{13}C NMR (100 MHz, $CDCl_3$)



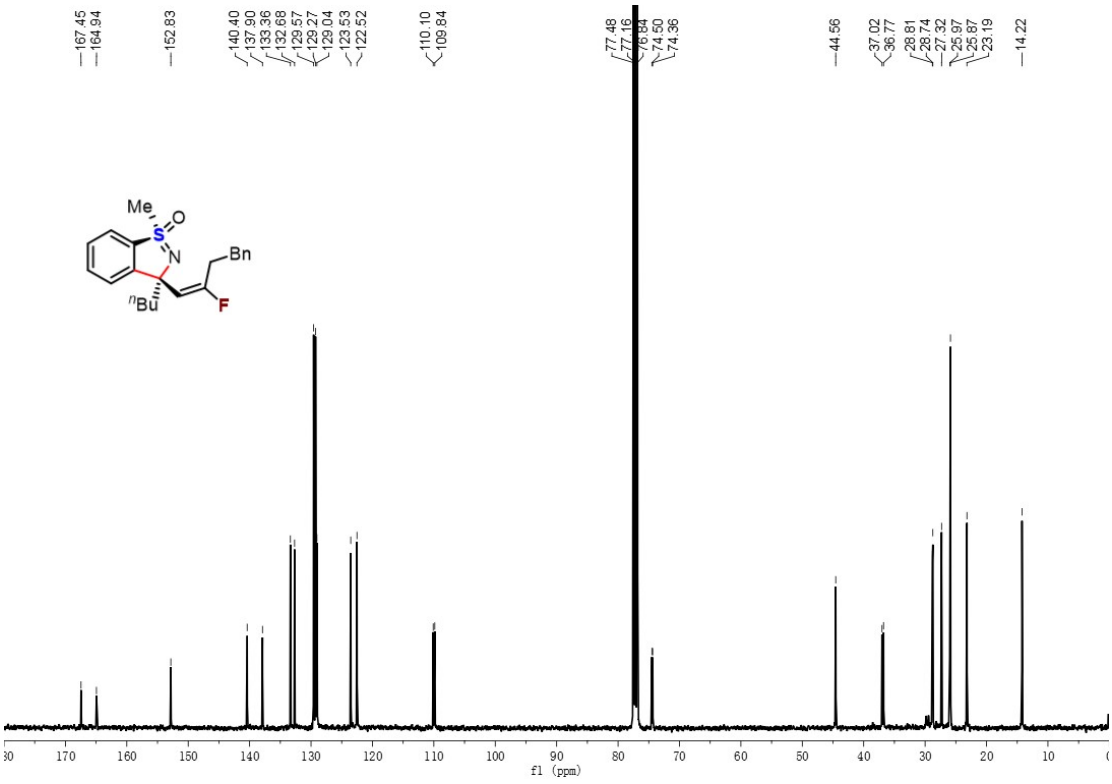
3m-^{19}F NMR (376 MHz, $CDCl_3$)



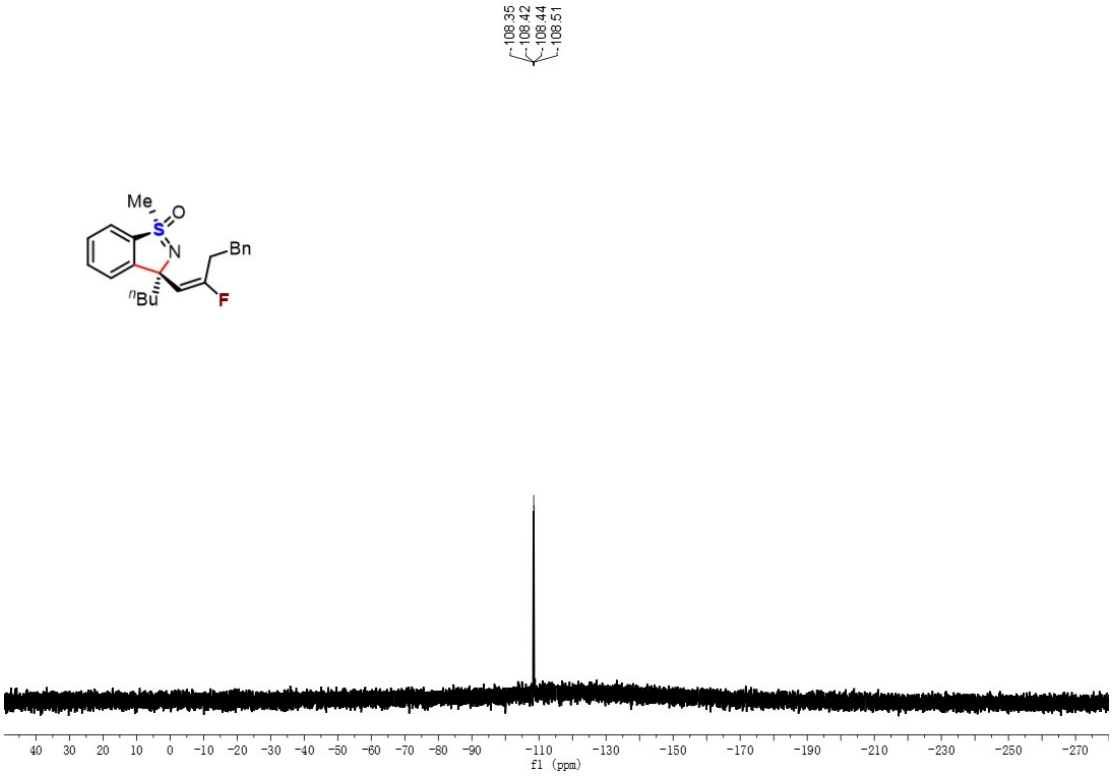
3n-^{1}H NMR (400 MHz, $CDCl_3$)



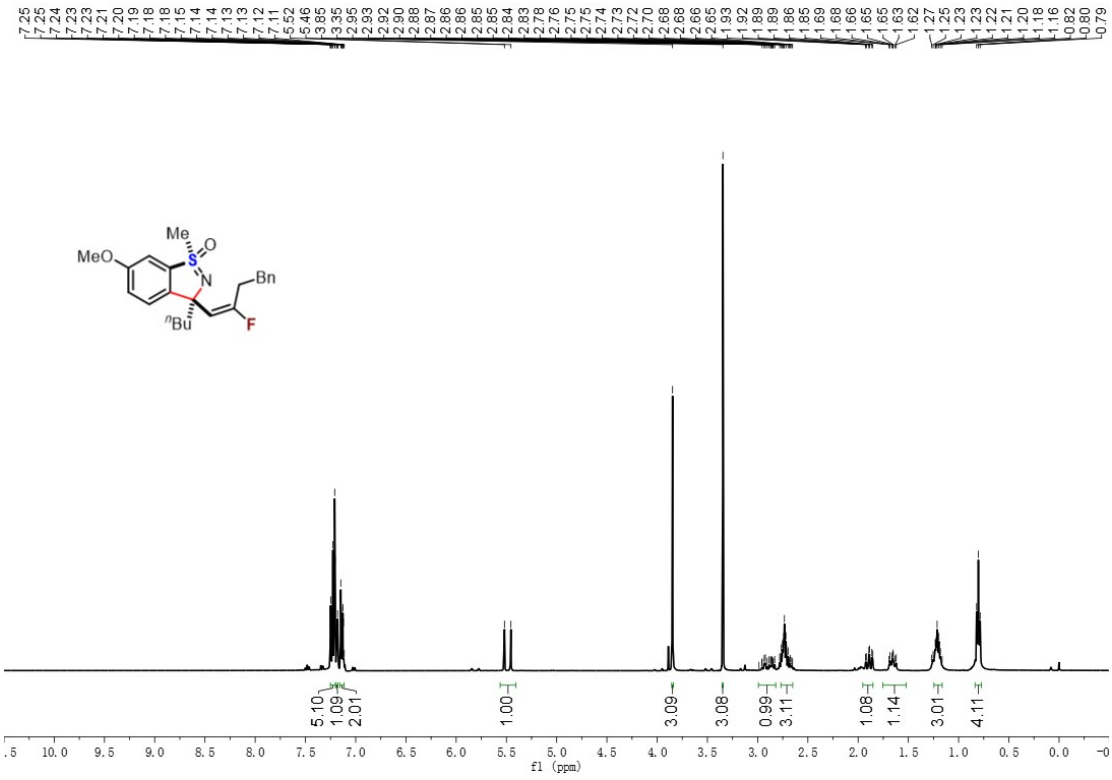
3n-^{13}C NMR (100 MHz, $CDCl_3$)



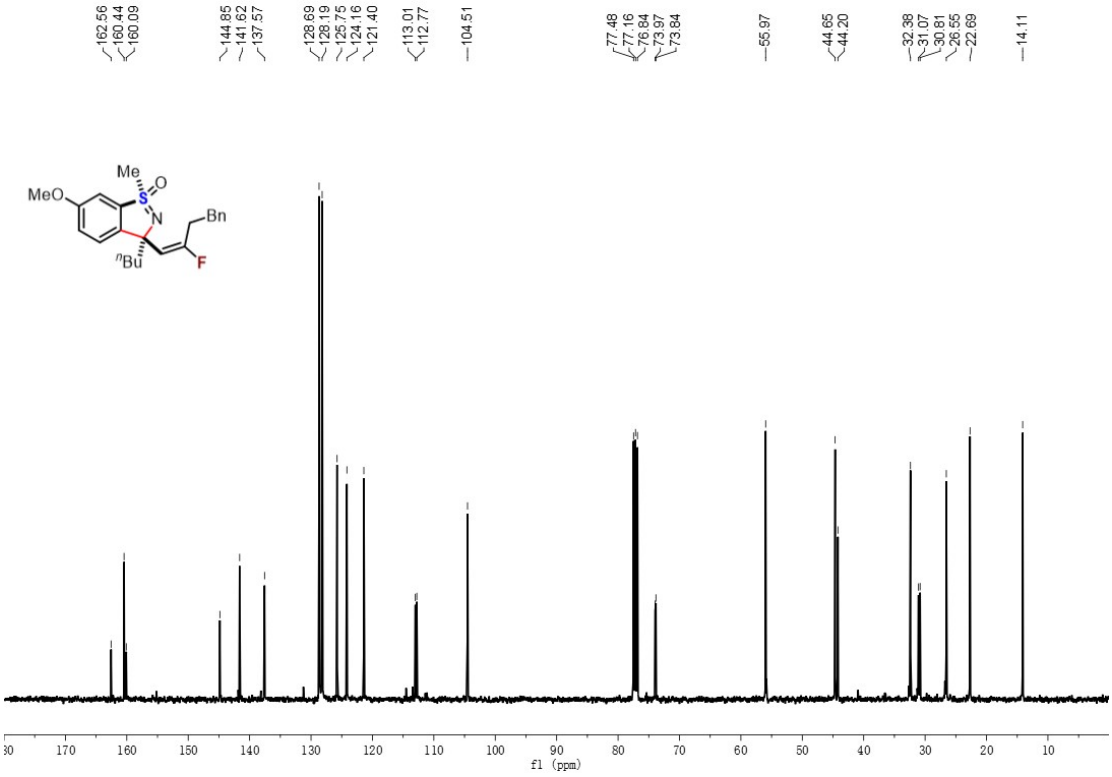
3n-^{19}F NMR (376 MHz, $CDCl_3$)



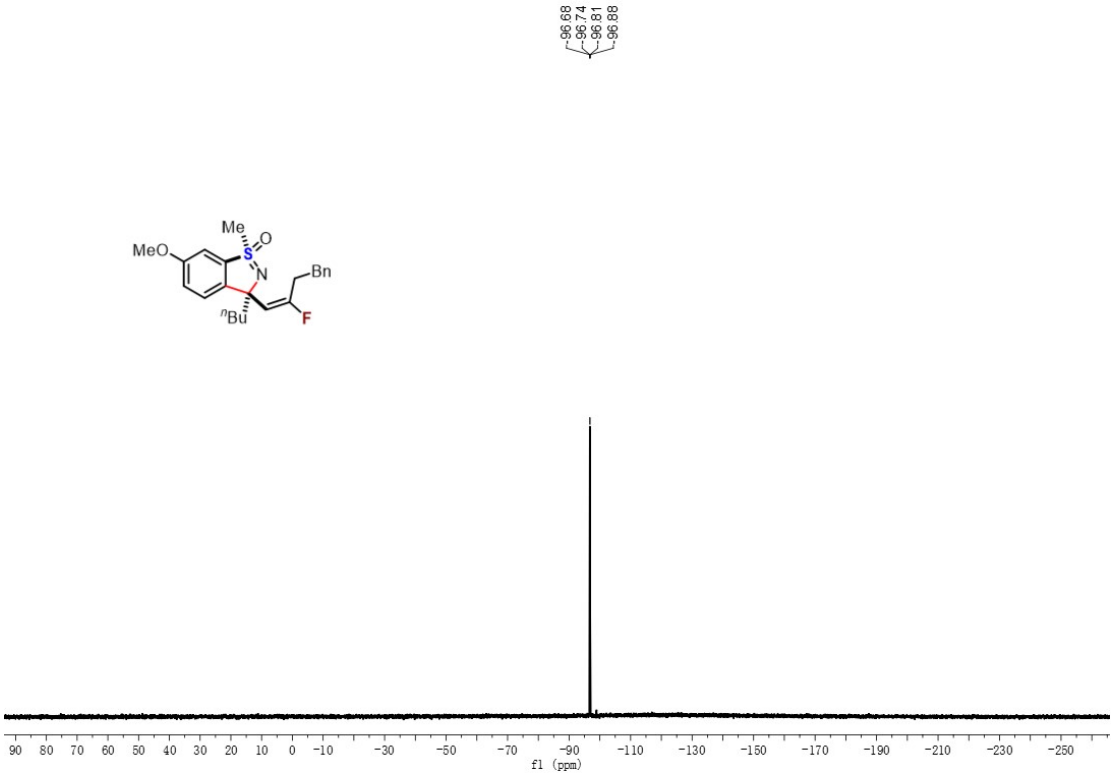
3o-^{1}H NMR (400 MHz, $CDCl_3$)



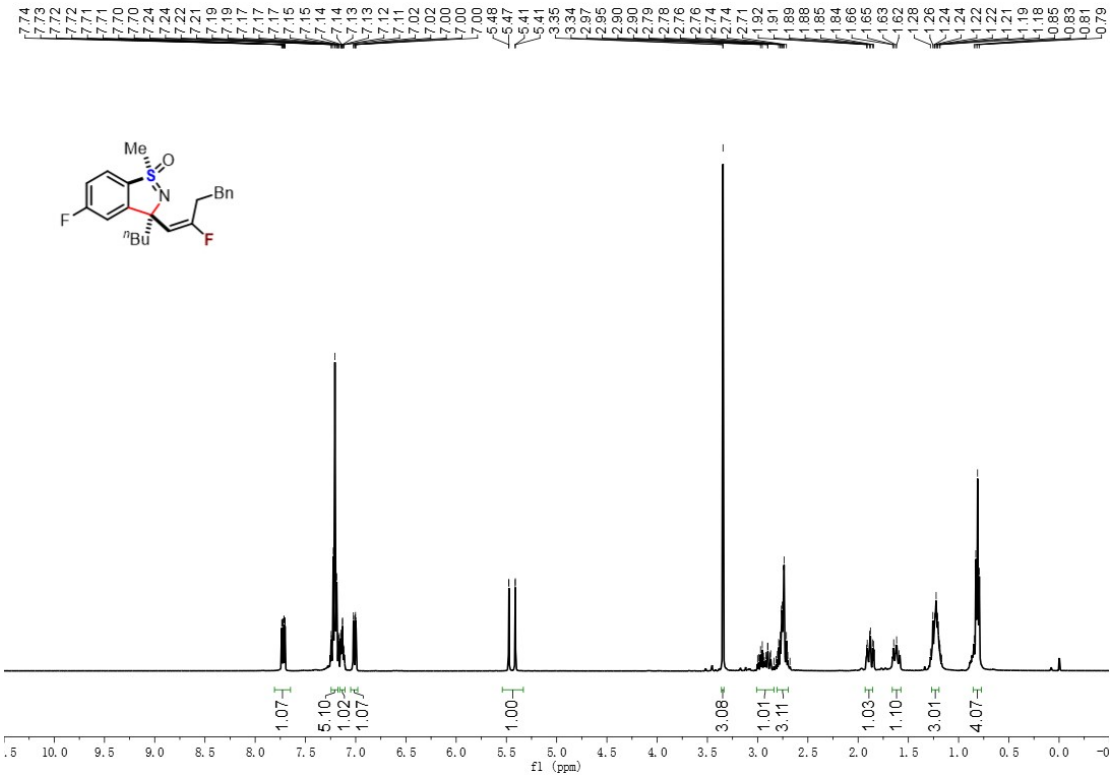
3o-^{13}C NMR (100 MHz, $CDCl_3$)



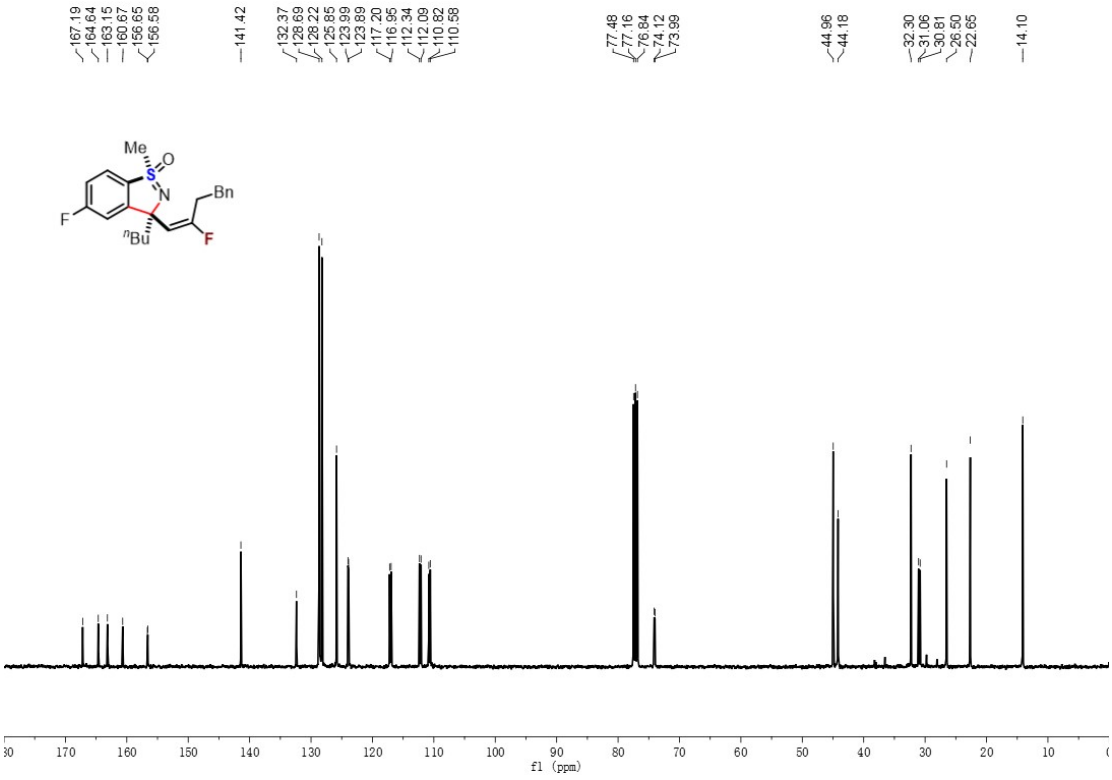
3o-^{19}F NMR (376 MHz, $CDCl_3$)



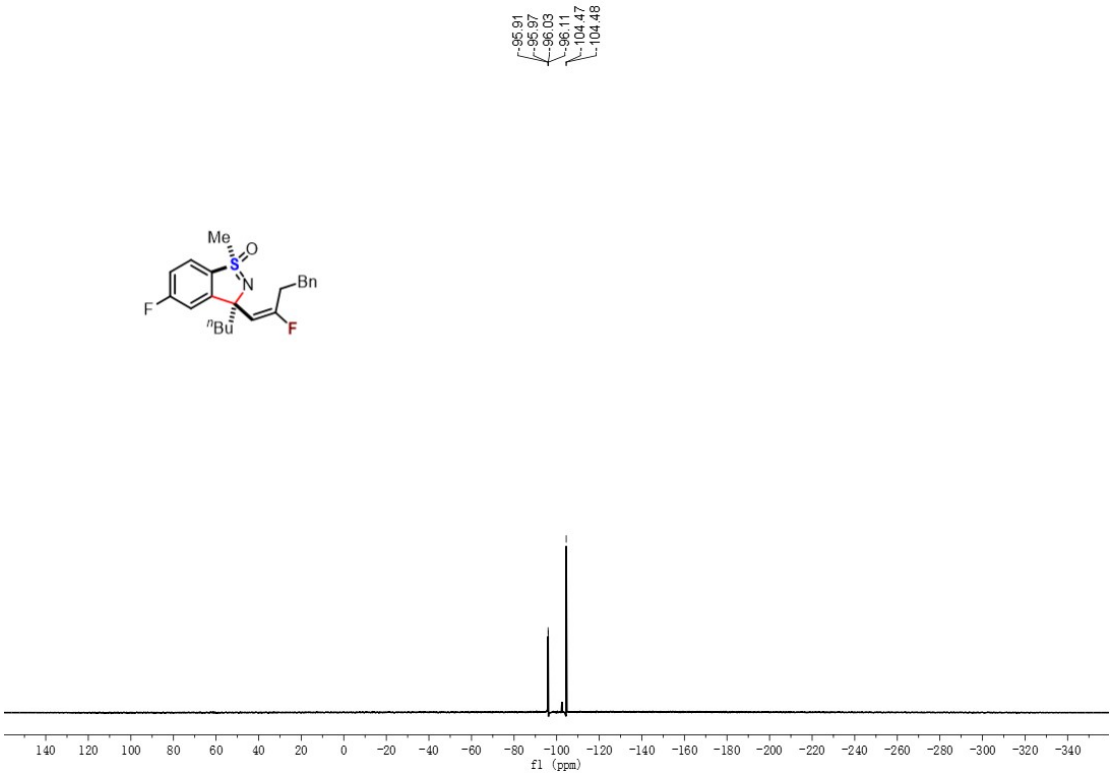
3p-^{1}H NMR (400 MHz, $CDCl_3$)



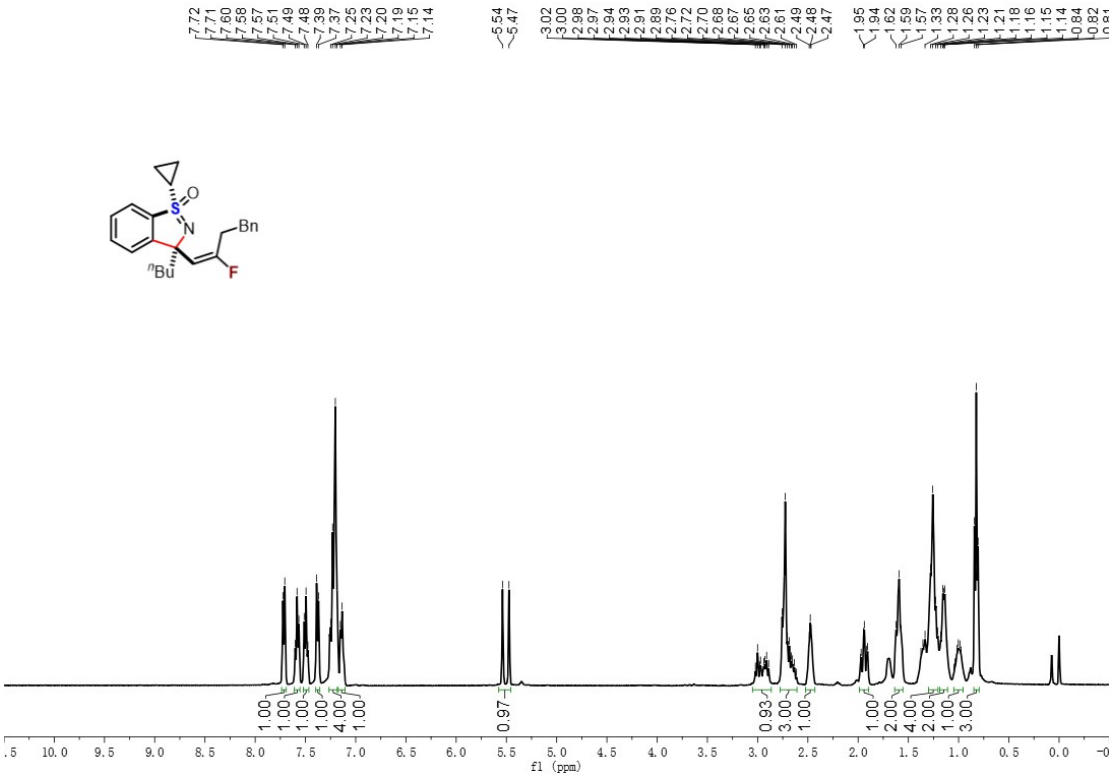
3p-^{13}C NMR (100 MHz, $CDCl_3$)



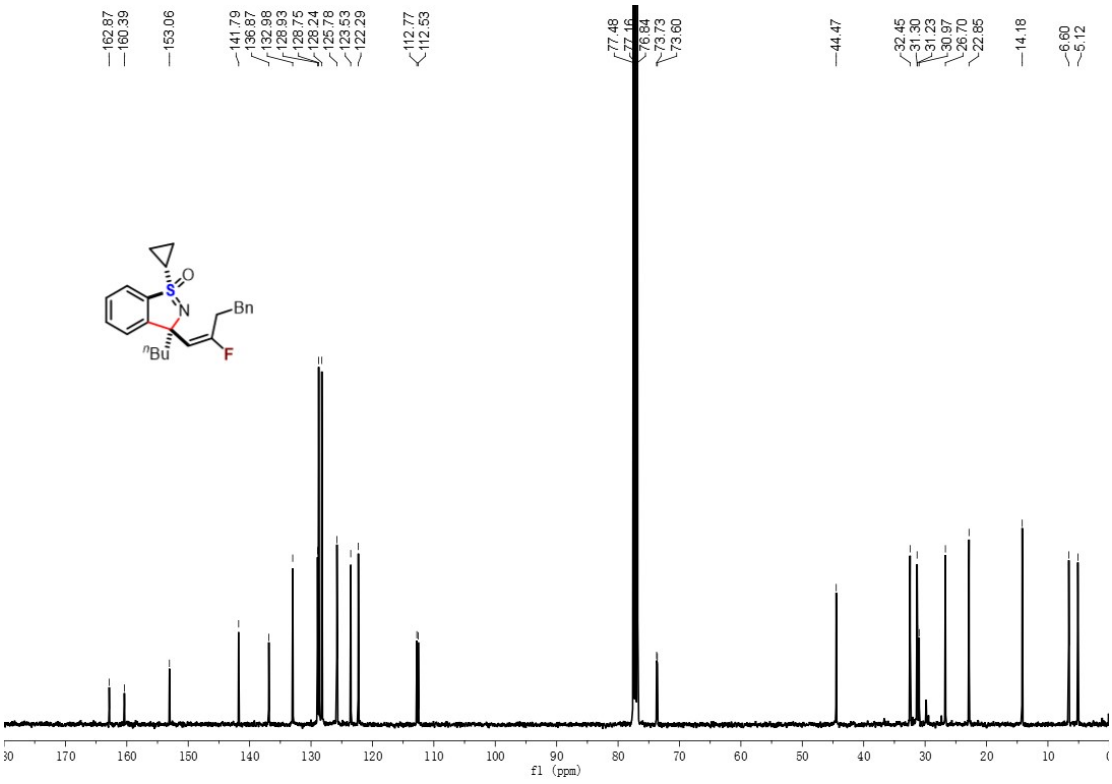
3p-^{19}F NMR (376 MHz, $CDCl_3$)



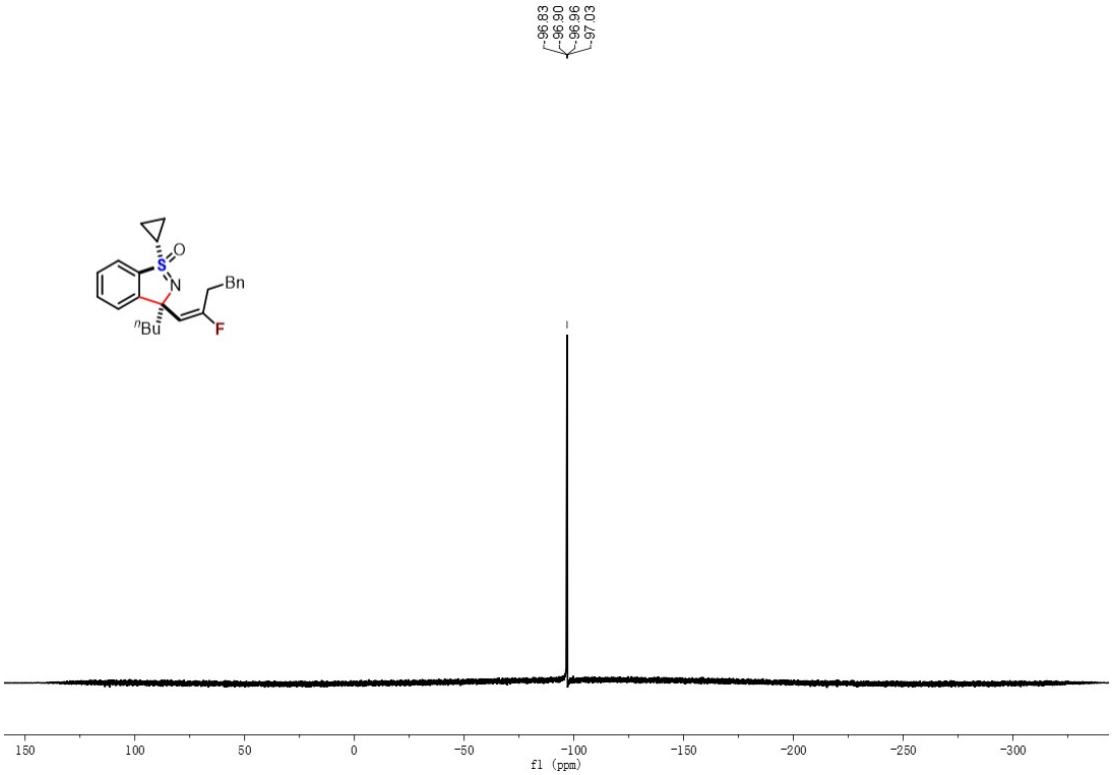
3q-^{1}H NMR (400 MHz, $CDCl_3$)



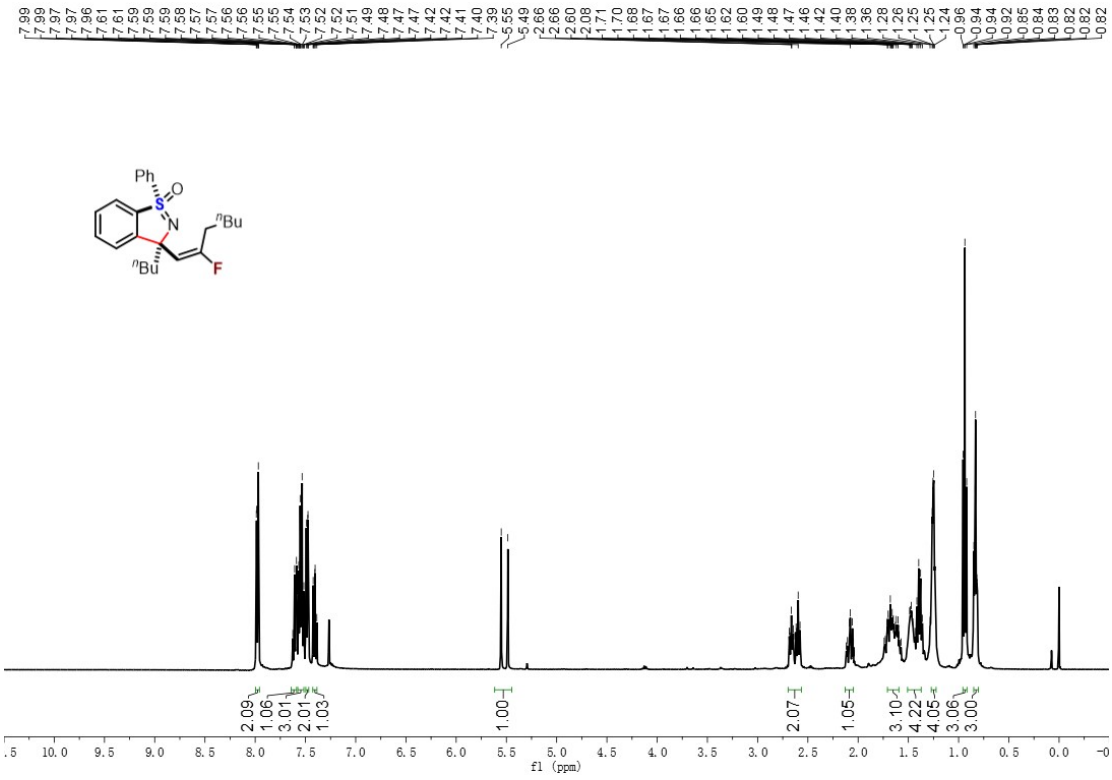
3q-^{13}C NMR (100 MHz, $CDCl_3$)



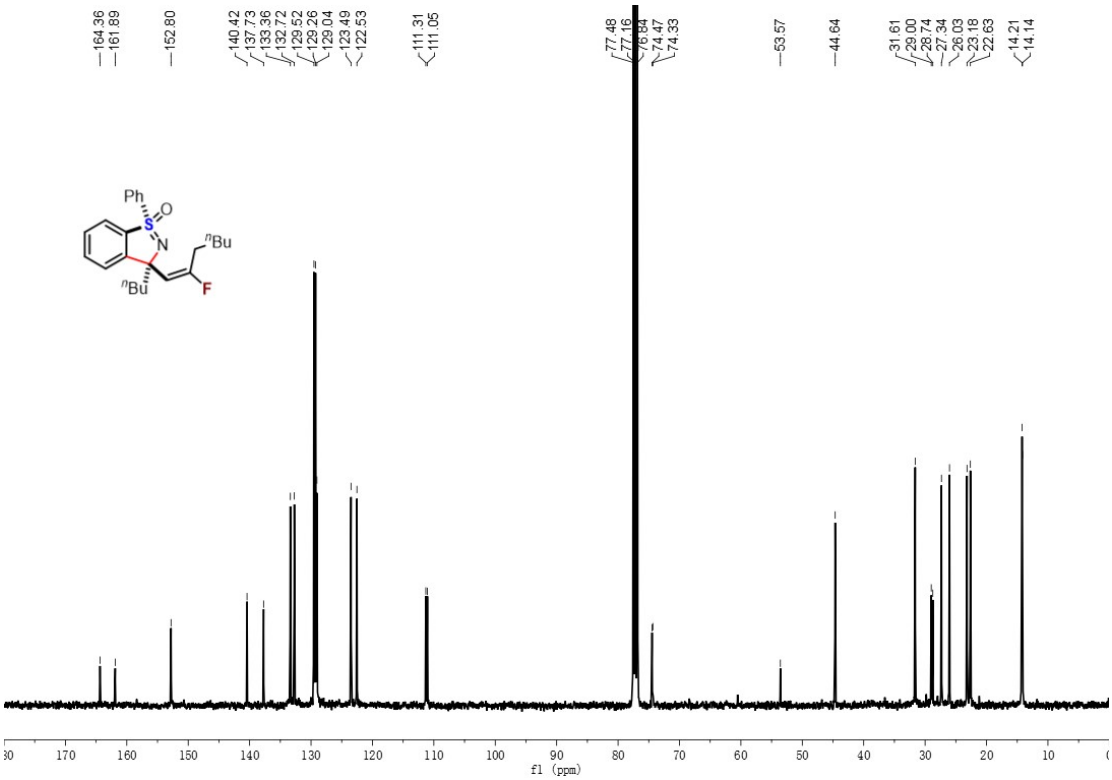
3q-^{19}F NMR (376 MHz, $CDCl_3$)



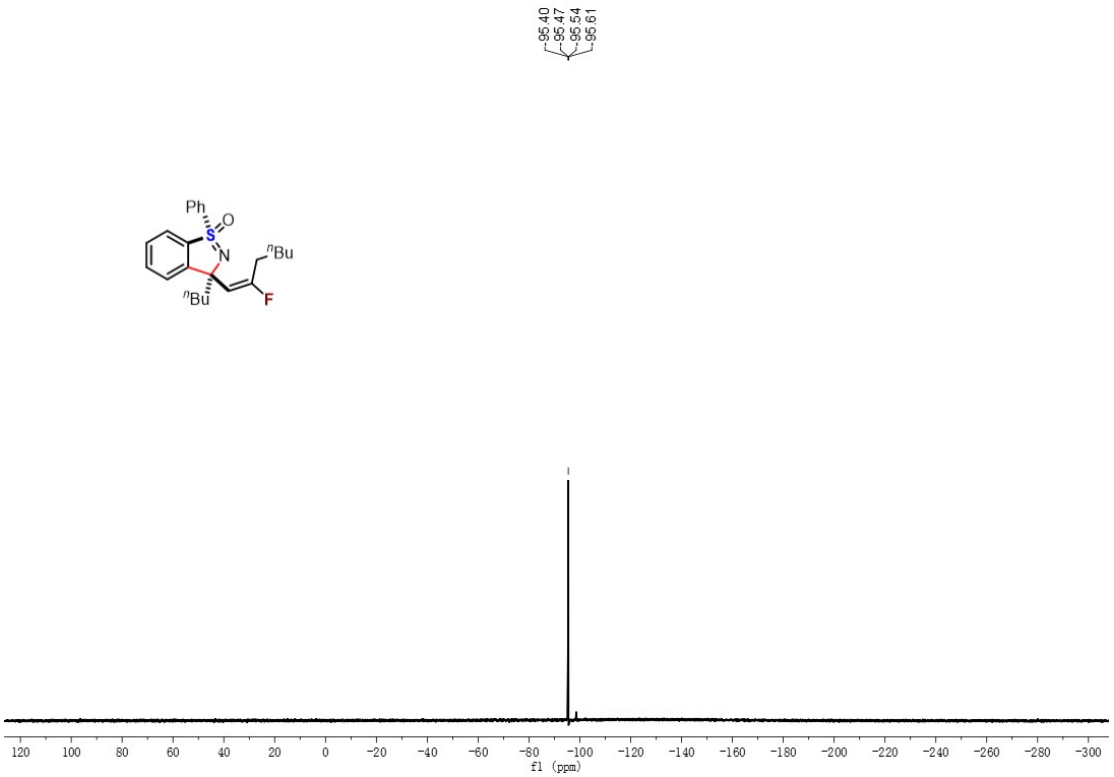
3r-^{1}H NMR (400 MHz, $CDCl_3$)



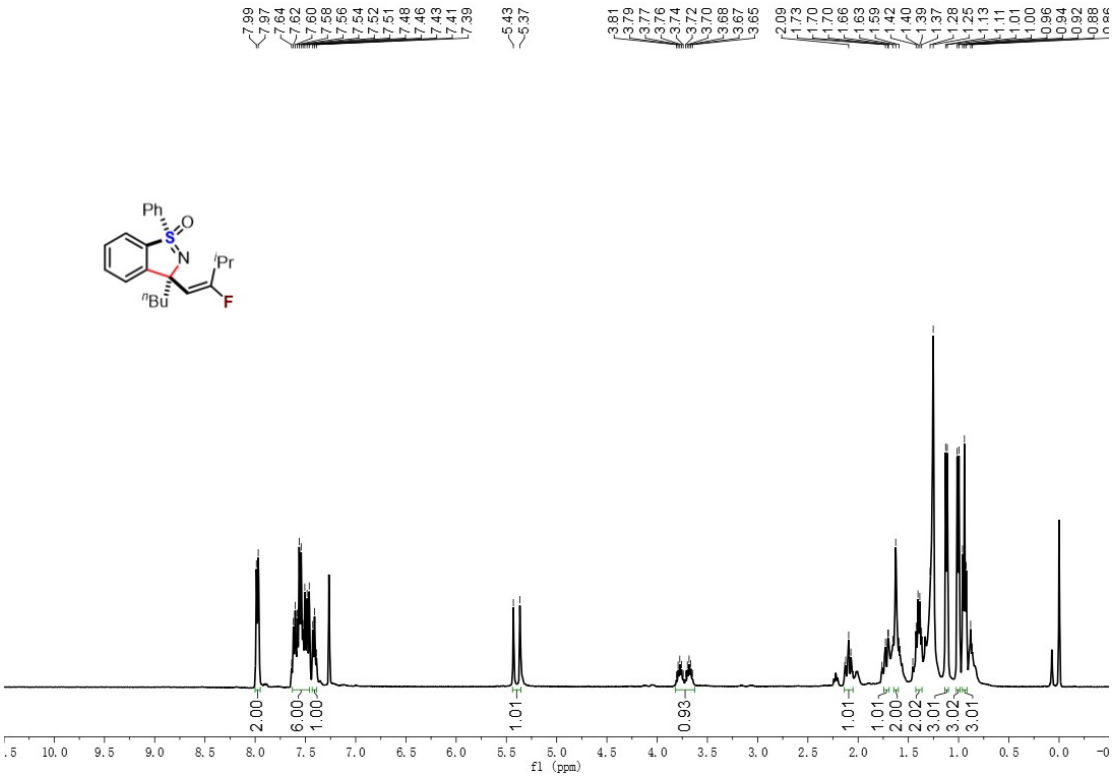
3r-^{13}C NMR (100 MHz, $CDCl_3$)



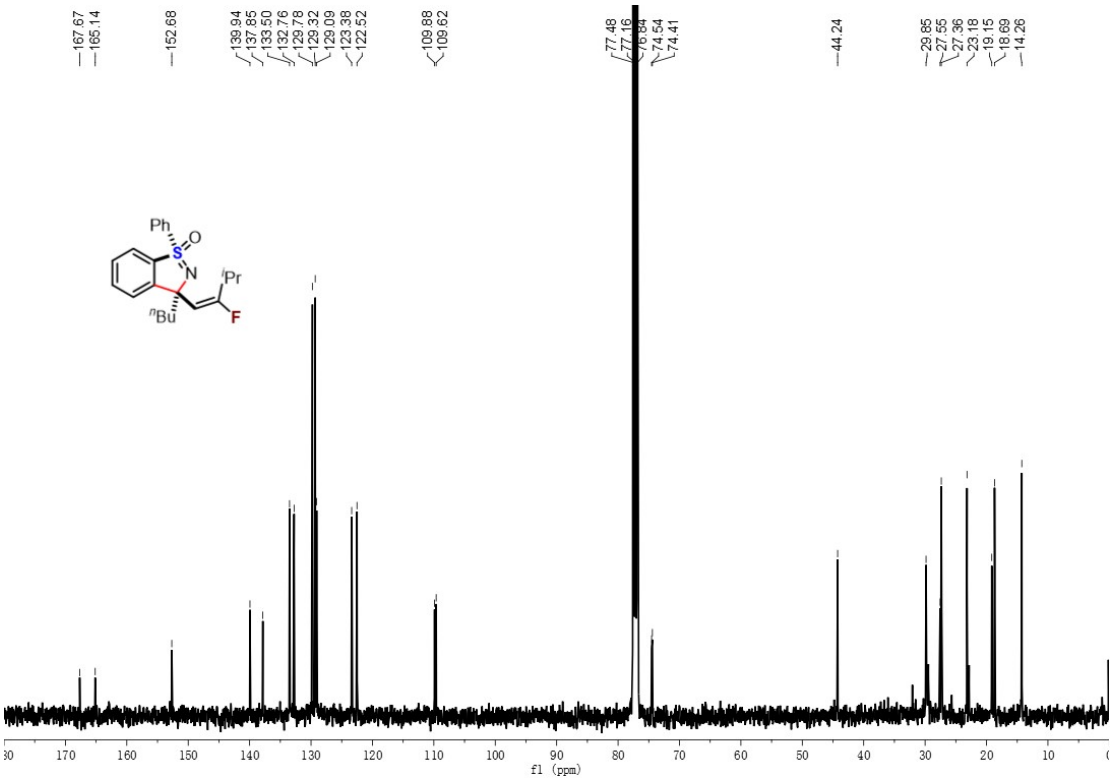
3r-^{19}F NMR (376 MHz, $CDCl_3$)



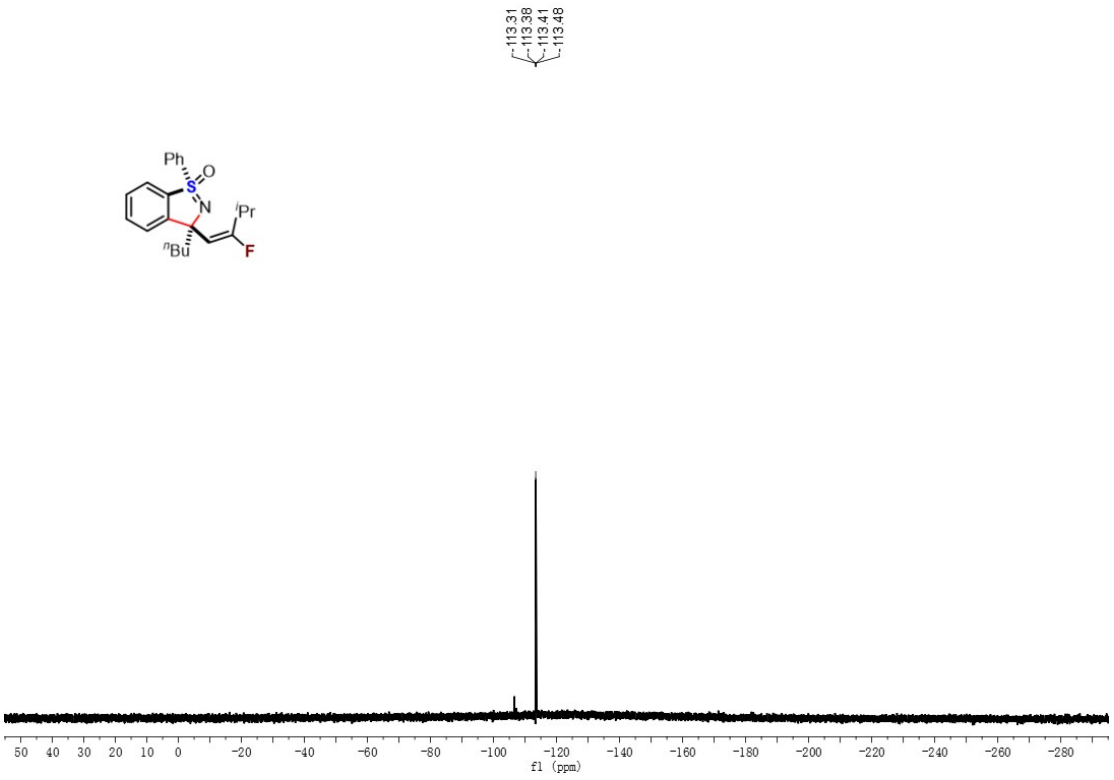
3s-^{1}H NMR (400 MHz, $CDCl_3$)



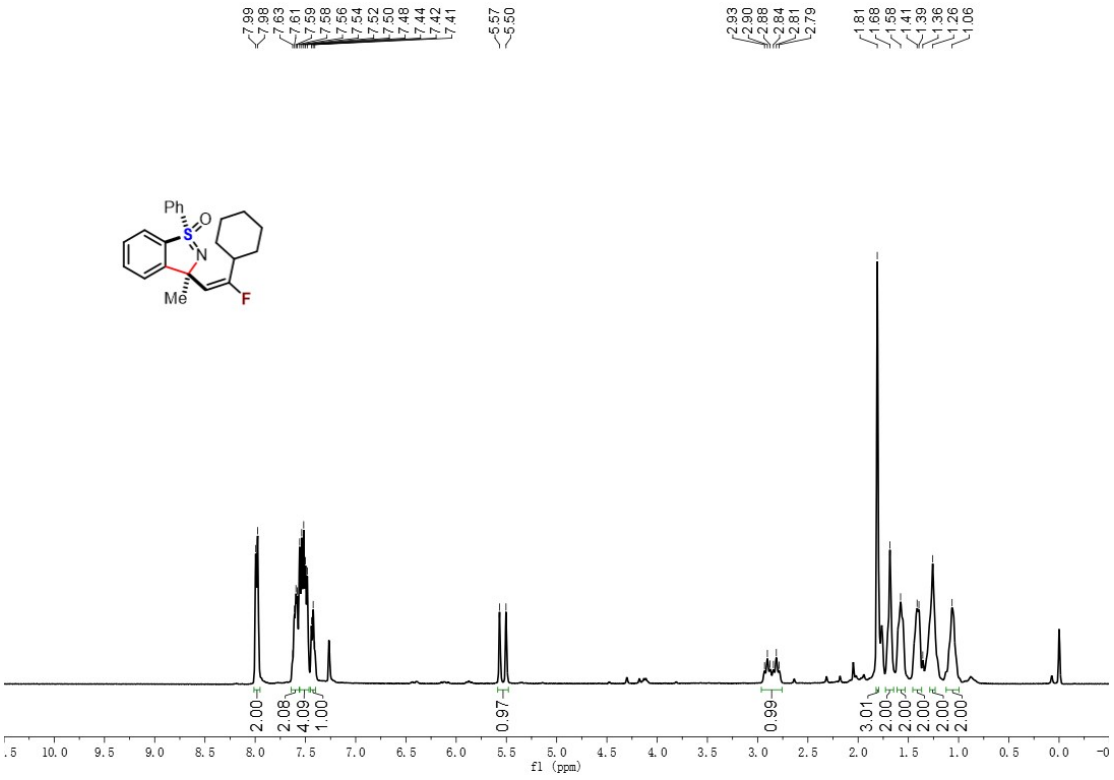
3s-^{13}C NMR (100 MHz, $CDCl_3$)



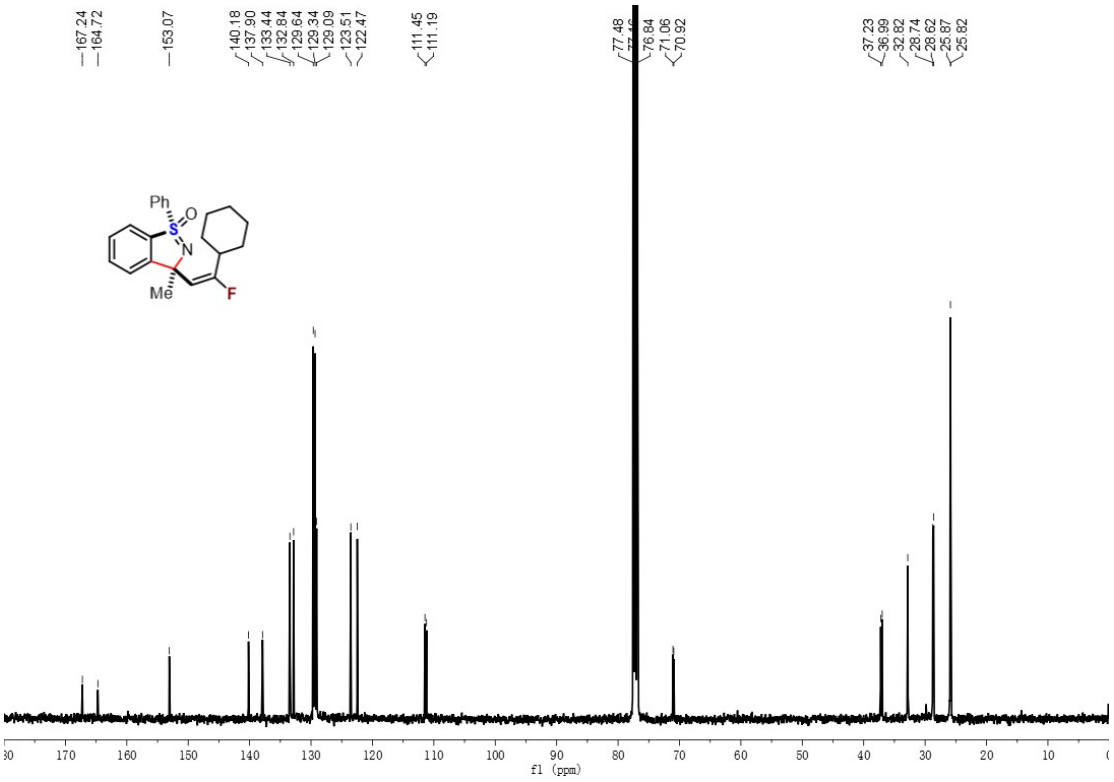
3s-^{19}F NMR (376 MHz, $CDCl_3$)



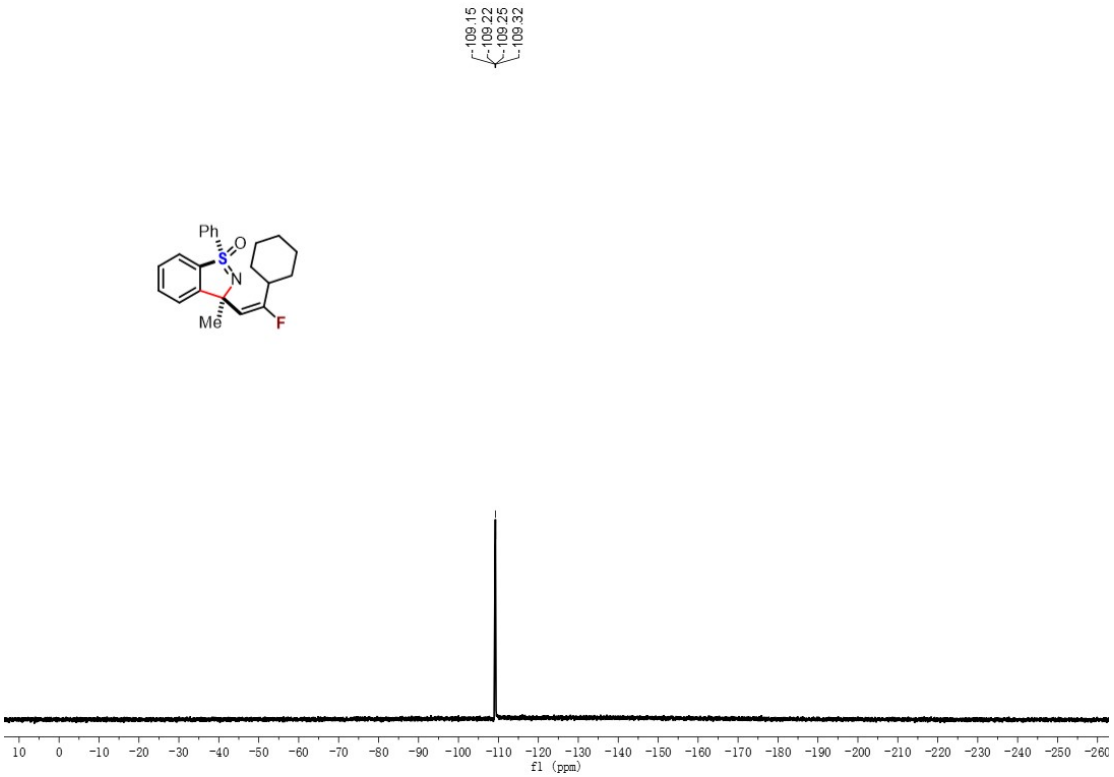
3t-^{1}H NMR (400 MHz, $CDCl_3$)



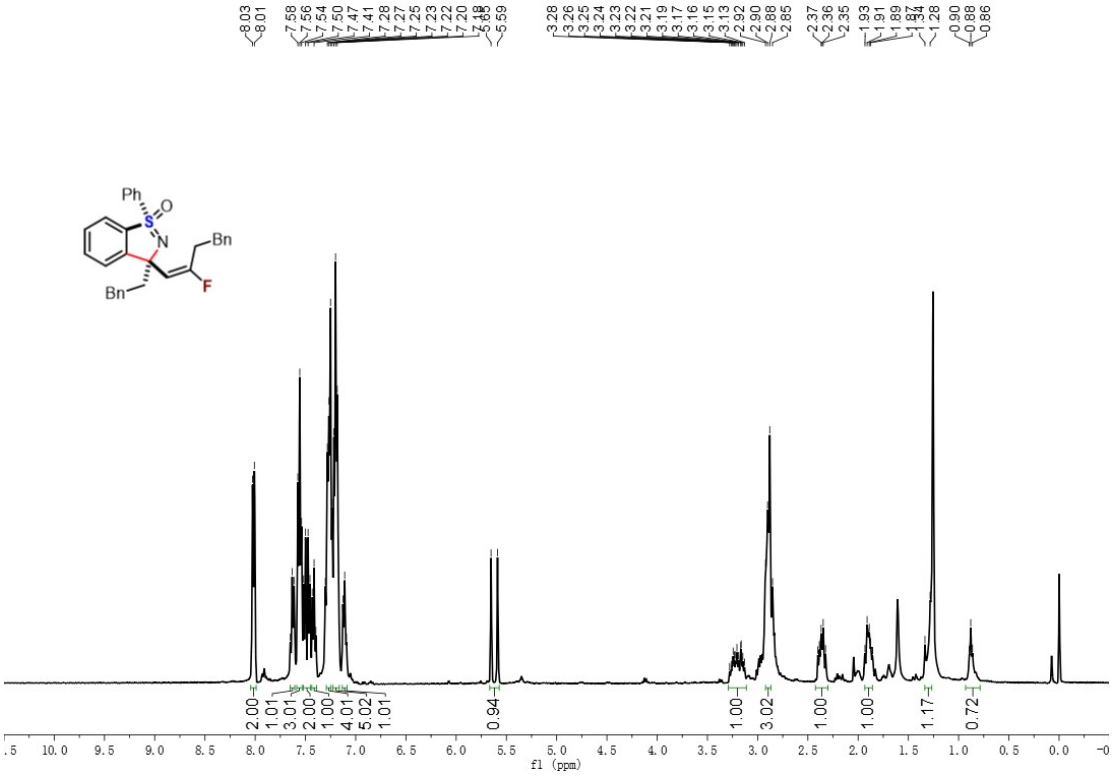
3t-^{13}C NMR (100 MHz, $CDCl_3$)



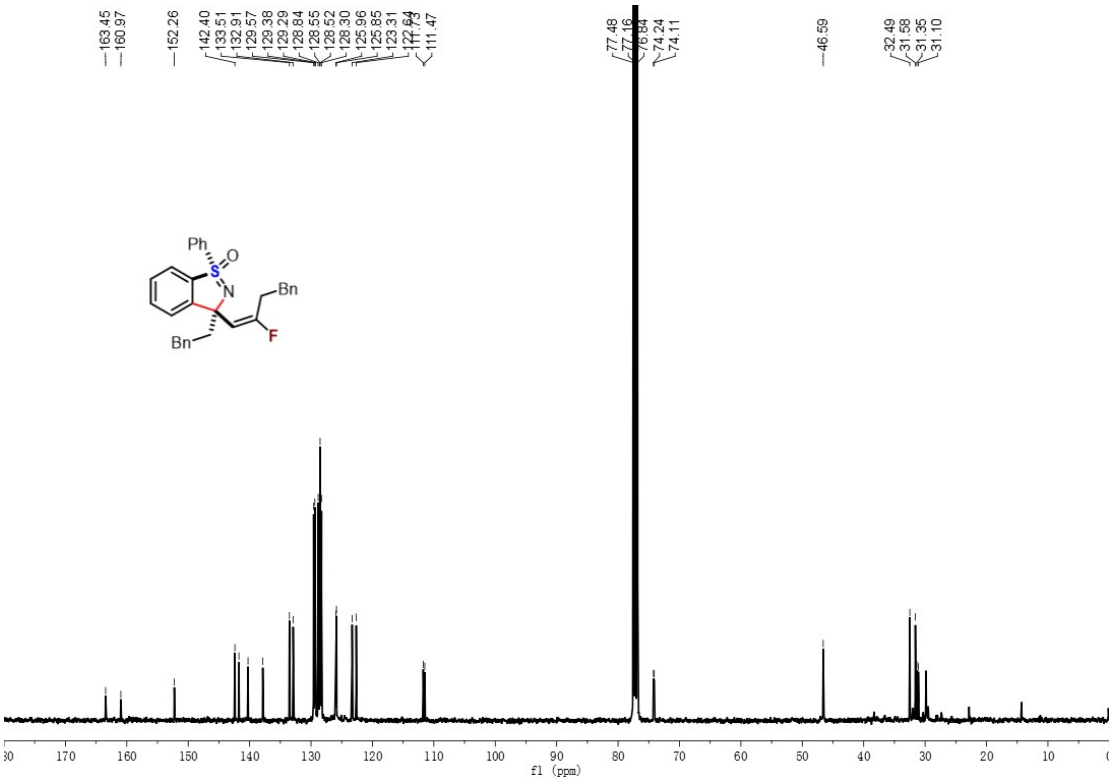
3t-^{19}F NMR (376 MHz, $CDCl_3$)



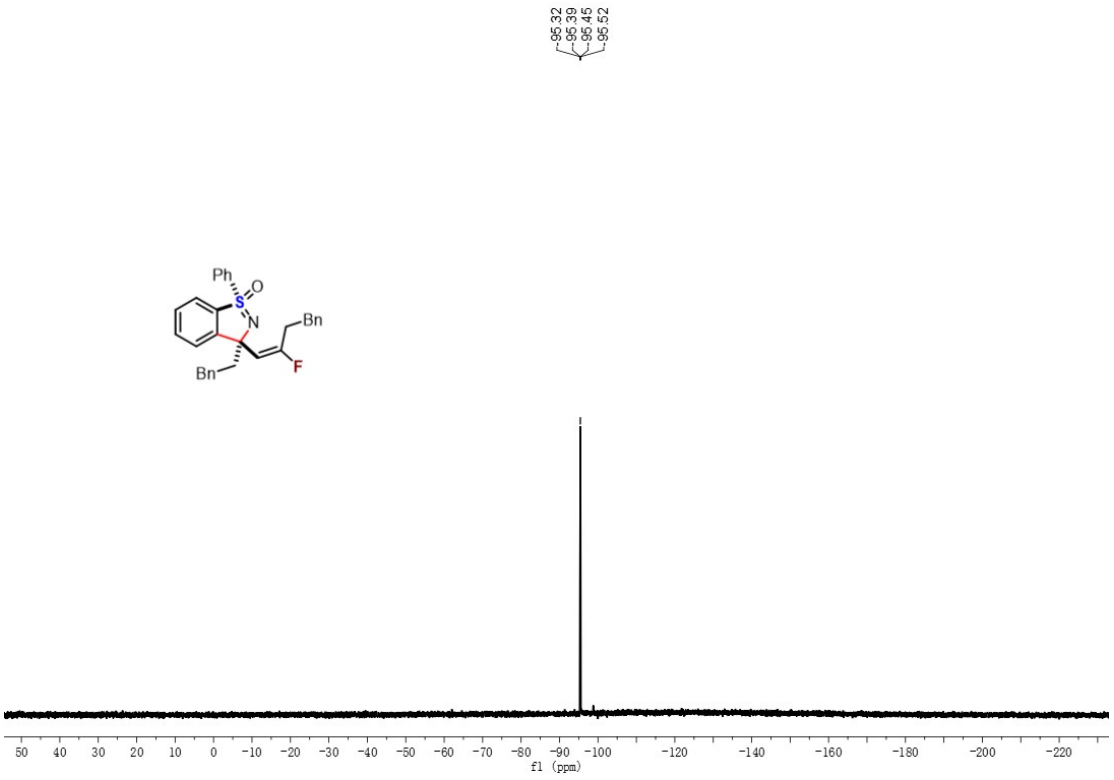
3u-^{1}H NMR (400 MHz, $CDCl_3$)



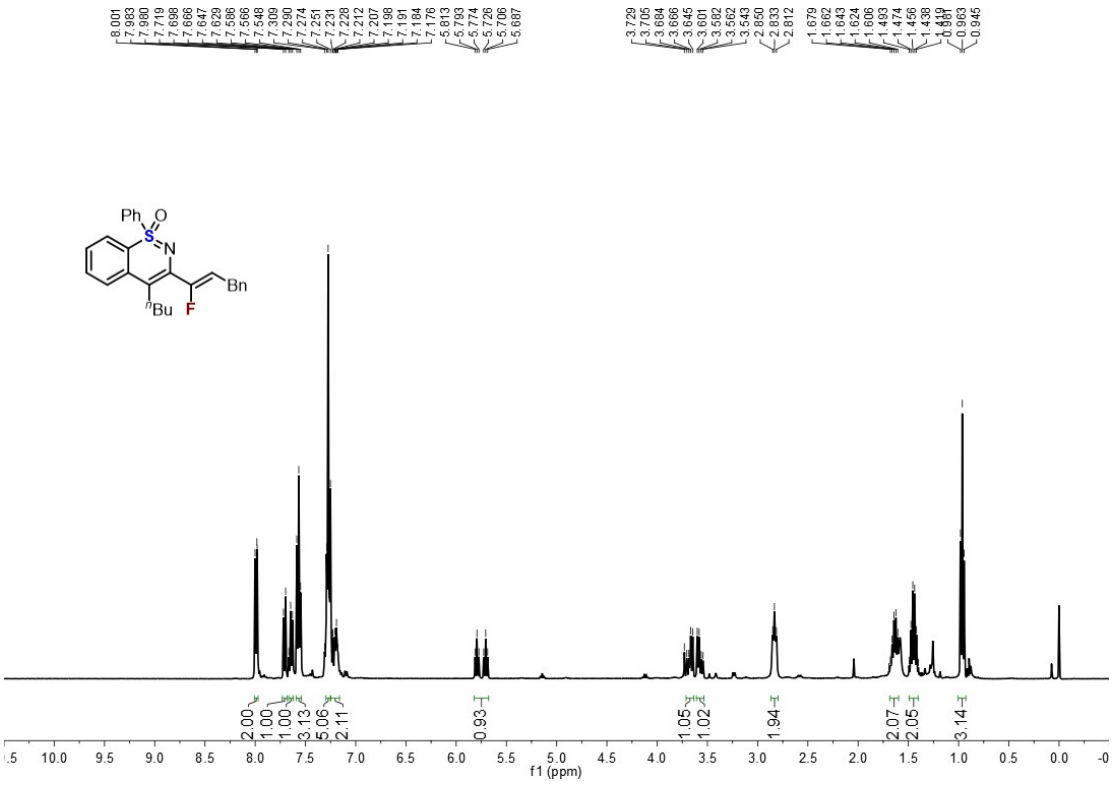
3u-^{13}C NMR (100 MHz, $CDCl_3$)



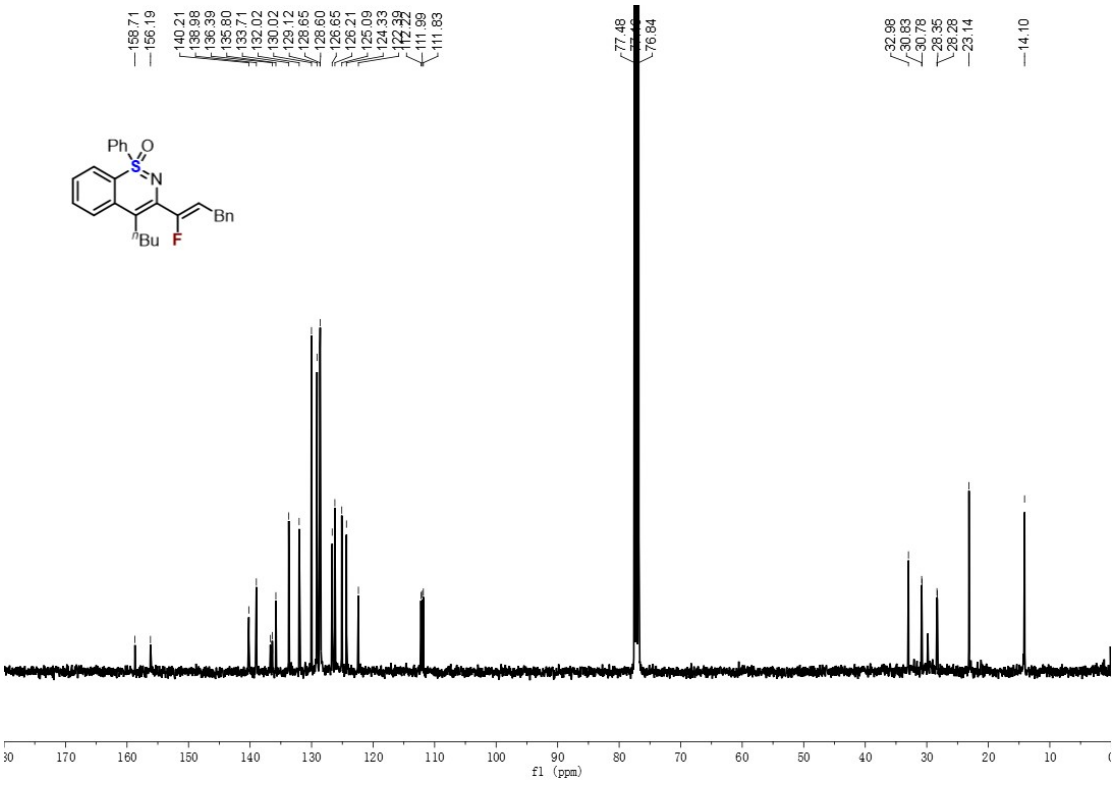
3u-^{19}F NMR (376 MHz, $CDCl_3$)



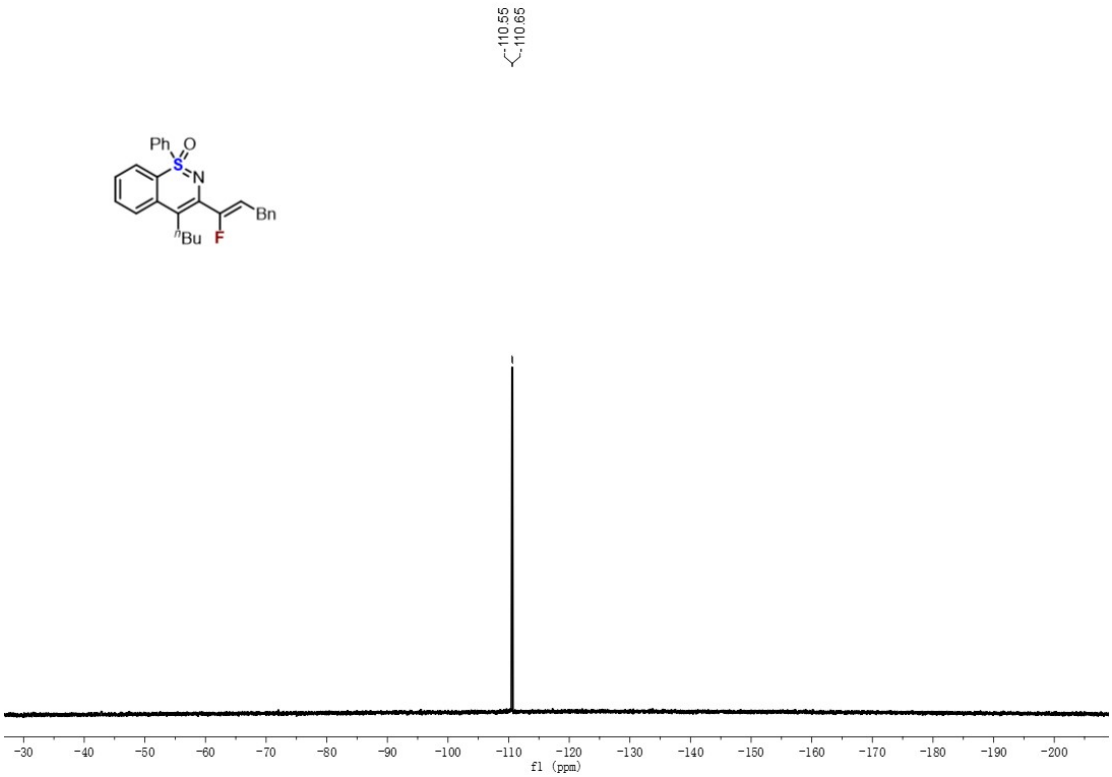
4a-^{1}H NMR (400 MHz, $CDCl_3$)



4a-^{13}C NMR (100 MHz, $CDCl_3$)



4a-^{19}F NMR (376 MHz, $CDCl_3$)



11. X-Ray Crystallographic Data

Single crystal growth of 3a: Compound **3a** was just dissolved in appropriate amount of EtOAc followed by the addition of petroleum ether to form a saturated solution. Then the solution was allowed to evaporate slowly at room temperature until the formation of a single crystal.

A suitable crystal was selected and measured on a XtaLAB Synergy R, DW system, HyPix diffractometer. The crystal was kept at 100.00(10) K during data collection. Using Olex2, the structure was solved with the ShelXT structure solution program using Intrinsic Phasing and refined with the ShelXL refinement package using Least Squares minimisation. The crystallographic data have already been deposited at the Cambridge Crystallographic Data Centre (CCDC: 2234183), which can be acquired from www.ccdc.cam.ac.uk/data_request/cif.

The ellipsoid contour percent probability level is 50% for the image of the structure.

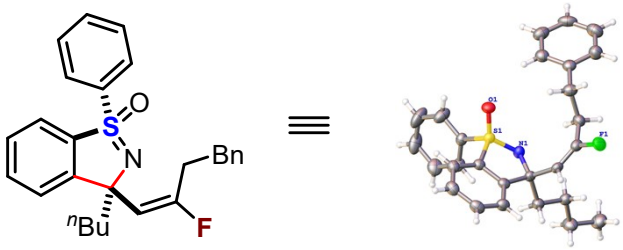


Table S3. Crystal data and structure refinement for **3a.**

Identification code	**3a**
Empirical formula	$C_{27}H_{28}FNOS$
Formula weight	433.56
Temperature/K	170.0(2)
Crystal system	monoclinic
Space group	$P2_1$-n
a/A	8.4633(6)
b/A	18.2176(15)
c/A	15.2067(10)
α/°	90
β/°	99.985(7)
γ/°	90
Volume/A^3	2309.1(3)
Z	4
$\rho_{calc}g/cm^3$	1.247
μ/mm^{-1}	0.167
F(000)	920.0
Crystal size/mm^3	0.15 × 0.12 × 0.1
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.472 to 49.998
Index ranges	-10 ≤ h ≤ 8, -21 ≤ k ≤ 14, -17 ≤ l ≤ 18

Reflections collected	10552
Independent reflections	4059 [R_{int} = 0.0391, R_{sigma} = 0.0457]
Data/restraints/parameters	4059/0/281
Goodness-of-fit on F^2	1.025
Final R indexes [I>=2σ (I)]	R_1 = 0.0485, wR_2 = 0.1129
Final R indexes [all data]	R_1 = 0.0642, wR_2 = 0.1245
Largest diff. peak/hole / e A^{-3}	0.36/-0.37

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