

Stereoselective β -F Elimination Enabled Redox-Neutral [4+1] Annulation via Rh(III)-Catalyzed C–H Activation: Access to Z-Monofluoroalkenyl Dihydrobenzo[*d*]isoxazole Framework

Hui Gao,^{†,§} Ming Sun,^{†,§} Haiman Zhang,^{†,§} Mengyao Bian,[†] Min Wu,[†] Guoxun Zhu,[‡] Zhi Zhou^{†,*} and Wei Yi^{†,*}

[†]Key Laboratory of Molecular Target & Clinical Pharmacology and State Key Laboratory of Respiratory Disease, School of Pharmaceutical Sciences & the Fifth Affiliated Hospital, Guangzhou Medical University, Guangzhou, Guangdong 511436, China

[‡]School of Chemical Engineering and Technology, Sun Yat-sen University, Guangzhou, Guangdong 510275, China

[§]These authors contributed equally.

*E-mail: yiwei@gzmu.edu.cn and zhoushi@gzmu.edu.cn

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I. General

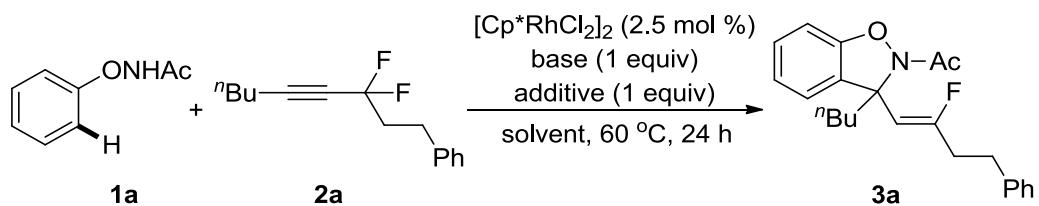
NMR spectra were recorded on JEOL 400 NMR (^1H 400 MHz; ^{13}C 100 MHz) in either CDCl_3 or $\text{DMSO}-d_6$. Abbreviations for data quoted are s, singlet; brs, broad singlet; d, doublet; t, triplet; dd, doublet of doublets; m, multiplet. The residual solvent signals were used as references and the chemical shifts converted to the TMS scale (CDCl_3 : $\delta_{\text{H}} = 7.26$ ppm, $\delta_{\text{C}} = 77.16$ ppm; $d_6\text{-DMSO}$: $\delta_{\text{H}} = 2.50$ ppm, $\delta_{\text{C}} = 39.52$ ppm). Mass spectra and high-resolution mass spectra were measured on an agilent TOF-G6230B mass spectrometer and Thermo-DFS mass spectrometer. Thin-layer chromatographies were done 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. $[\text{Cp}^*\text{IrCl}_2]_2$, $[\text{Cp}^*\text{RhCl}_2]_2$, $[\text{Ru}(\text{p-cymene})\text{Cl}_2]_2$ and CsOAc were purchased from Aldrich and used without further purification. Substrates *N*-phenoxy amides^{S1} and α,α -difluoromethylene alkynes^{S2} were synthesized according to published procedures. Other chemicals were purchased from commercial suppliers and were dried and purified when necessary. No attempts were made to optimize yields for substrate synthesis.

II. Experimental Information and Characterization Data

Optimization studies:

The mixture of *N*-phenoxyacetamide **1a** (0.1 mmol, 1.0 equiv), α,α -difluoromethylene alkynes **2a** (0.1 mmol, 1.0 equiv), $[\text{Cp}^*\text{RhCl}_2]_2$ (2.5 mol %), base (1.0 equiv) and additive (1.0 equiv) in the solvent was stirred at 60 °C for 24 h without exclusion of air or moisture. Afterwards, it was diluted with EtOAc and filtered through a short silica gel column to remove the metal residues. Then, the reaction mixture was concentrated and purified by preparative TLC (eluent: PE/EA = 10/1) to give the corresponding monofluoroalkenyl dihydrobenzo[*d*]isoxazole derivative **3a**.

Table S1. Conditions Screening for the Synthesis of **3a**.^a

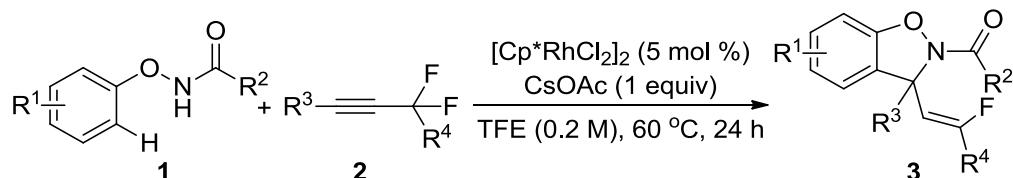


Entry	Base (1 equiv)	Additive (1 equiv)	Solvent	Yield (%) ^b
1 ^c	NaOAc	-	MeOH	10
2 ^c	NaOAc	-	CH ₃ CN	trace
3	NaOAc	-	DCE	trace
4	NaOAc	-	DCM	trace
5	NaOAc	-	TFE	45
6	NaOAc	-	toluene	trace
7 ^c	NaOAc	-	THF	19
8	NaOAc	-	DMF	8
9	NaOAc	-	DMSO	n.d.
10	NaOAc	-	dioxane	12
11	NaOAc	-	acetone	trace (23) ^d
12	NaOAc	-	DMA	trace
13	NaOAc	-	HFIP	11
14 ^e	NaOAc	-	TFE	n.d.
15 ^f	NaOAc	-	TFE	n.d.
16 ^g	NaOAc	-	TFE	n.d.
17	CsOAc	-	TFE	56
18	K ₃ PO ₄	-	TFE	trace
19	KOAc	-	TFE	15
20	K ₂ CO ₃	-	TFE	trace
21	KOPiv	-	TFE	37
22 ^h	CsOAc	-	TFE	29
23 ⁱ	CsOAc	-	TFE	51
24 ^j	CsOAc	-	TFE	46
25 ^k	CsOAc	-	TFE	47
26	CsOAc	HOAc	TFE	50
27	CsOAc	HOPiv	TFE	36
28	CsOAc	Zn(OAc) ₂	TFE	55
29	CsOAc	K ₂ CO ₃	TFE	5
30	CsOAc	4 Å MS	TFE	9
31 ^l	CsOAc	-	TFE	60
32 ^m	CsOAc	-	TFE	57
33 ^{l,n}	CsOAc	-	TFE	75

^aReaction Conditions: **1a** (0.1 mmol), **2a** (0.1 mmol), [Cp*RhCl₂]₂ (2.5 mol %), base (1.0 equiv) and additive (1.0 equiv) in solvent (0.2 M) at 60 °C for 24 h under air. ^bIsolated yield. ^cThe C-N

reductive elimination product was obtained as the main side product.^d *ortho*-Alkenylation product was obtained, the isolated yield of this side product was given in the parentheses. ^e5 mol % of Cp^{*}Co(CO)I₂ was used as the catalyst. ^f2.5 mol % Cp^{*}IrCl₂ was used as the catalyst. ^g2.5 mol % [Ru(*p*-cymene)Cl₂]₂ was used as the catalyst. ^hThe reaction was conducted at room temperature. ⁱThe reaction was conducted at 80 °C. ^jTFE (0.4 M). ^kTFE (0.1 M). ^l**2a** (1.4 equiv). ^m**2a** (2.0 equiv). ⁿ5 mol % of [Cp^{*}RhCl₂]₂ was used.

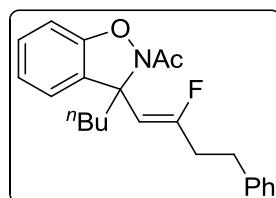
General procedure for C-H annulations:



The mixture of *N*-phenoxy amides **1** (0.2 mmol, 1.0 equiv), α,α -difluoromethylene alkynes **2** (0.28 mmol, 1.4 equiv), [Cp^{*}RhCl₂]₂ (5 mol %), and CsOAc (1 equiv) in TFE (1 mL) was stirred at 60 °C for 24 h without exclusion of air or moisture. Afterwards, it was diluted with EtOAc and filtered through a short silica gel column to remove the metal residues. Then, the reaction mixture was concentrated and purified by preparative TLC to give the desired monofluoroalkenyl dihydrobenzo[*d*]isoxazole derivative **3**.

Characterization of products:

(Z)-1-(3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)benzo[*d*]isoxazol-2(3*H*)-yl)ethanone (3a)



This compound was obtained in 75% yield (55.1 mg) as light yellow oil. Eluent: PE/EA = 10/1, R_f = 0.5.

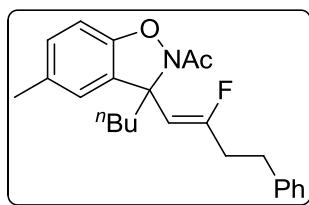
¹H NMR (400 MHz, CDCl₃): δ 7.32-7.28 (m, 1H), 7.22-7.12 (m, 3H), 7.07-7.04 (m, 2H), 6.87 (d, *J* = 8.2 Hz, 1H), 6.83 (d, *J* = 6.9 Hz, 2H), 5.72 (d, *J* = 22.1 Hz, 1H), 2.66-2.53 (m, 2H), 2.31-2.23 (m, 1H), 2.18 (s, 3H), 2.09-1.98 (m, 2H), 1.88-1.79 (m, 1H), 1.29-1.06 (m, 4H), 0.79 (t, *J* = 7.2 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 165.6, 163.6 (d, *J* = 253.8 Hz), 152.9, 140.7, 129.6, 129.3, 128.5, 128.3, 126.2, 123.2, 123.1, 111.8 (d, *J* = 27.1 Hz), 107.1, 69.0 (d, *J* = 13.6 Hz), 39.9, 31.8, 31.4 (d, *J* = 25.5 Hz), 25.5, 22.3, 21.8, 14.1.

¹⁹F NMR (376 MHz, CDCl₃): δ -96.58 - -96.77 (m).

HRMS (ESI) calculated for C₂₄H₂₇FNO₂ ([M+H]⁺): 368.2026; found: 368.2014.

(Z)-1-(3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-5-methylbenzo[*d*]isoxazol-2(3*H*)-yl)ethanone (3b)



This compound was obtained in 72% yield (54.9 mg) as light yellow oil. Eluent: PE/EA/Et₃N = 20/1/0.1, R_f = 0.7.

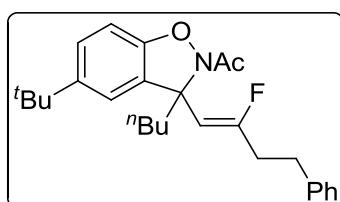
¹H NMR (400 MHz, CDCl₃): δ 7.20 (t, *J* = 7.2 Hz, 2H), 7.15 (d, *J* = 7.1 Hz, 1H), 7.08 (d, *J* = 8.2 Hz, 1H), 6.87-6.82 (m, 3H), 6.75 (d, *J* = 8.3 Hz, 1H), 5.70 (d, *J* = 22.1 Hz, 1H), 2.67-2.53 (m, 2H), 2.33 (s, 3H), 2.30-2.24 (m, 1H), 2.17 (s, 3H), 2.10-1.99 (m, 2H), 1.85-1.75 (m, 1H), 1.28-1.05 (m, 4H), 0.79 (t, *J* = 7.3 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 165.5, 163.6 (d, *J* = 253.8 Hz), 151.0, 140.7, 132.8, 129.8, 129.6, 128.5, 128.3, 126.2, 123.3, 111.8 (d, *J* = 26.9 Hz), 106.6, 69.0 (d, *J* = 13.9 Hz), 39.8, 31.8, 31.4 (d, *J* = 26.2 Hz), 25.5, 22.4, 21.8, 21.1, 14.1.

¹⁹F NMR (376 MHz, CDCl₃): δ -96.75 - -96.94 (m).

HRMS (ESI) calculated for C₂₄H₂₉FNO₂ ([M+H]⁺): 382.2182; found: 382.2172.

(Z)-1-(5-(tert-butyl)-3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)benzo[*d*]isoxazol-2(3*H*)-yl)ethanone (3c)



This compound was obtained in 62% yield (52.5 mg) as yellow solid. Eluent: PE/EA/Et₃N = 20/1/0.1, R_f = 0.7.

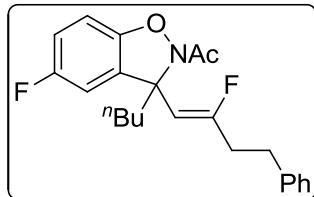
¹H NMR (400 MHz, CDCl₃): δ 7.35 (dd, *J* = 8.6, 2.0 Hz, 1H), 7.21-7.16 (m, 2H), 7.15-7.11 (m, 2H), 6.82-6.76 (m, 3H), 5.73 (d, *J* = 21.9 Hz, 1H), 2.65-2.53 (m, 2H), 2.19-2.11 (m, 4H), 2.10-1.96 (m, 2H), 1.86 (td, *J* = 13.6, 4.1 Hz, 1H), 1.30 (s, 9H), 1.27-1.08 (m, 4H), 0.79 (t, *J* = 7.2 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 165.6, 163.8 (d, *J* = 253.8 Hz), 150.9, 146.6, 140.7, 129.4, 128.4, 128.3, 126.23, 126.18, 111.8 (d, *J* = 26.7 Hz), 111.7, 106.3, 69.2 (d, *J* = 14.1 Hz), 39.8, 34.8, 31.8, 31.7, 31.5, 25.5, 22.3, 21.8, 14.0.

¹⁹F NMR (376 MHz, CDCl₃): δ -96.60 - -96.78 (m).

HRMS (ESI) calculated for C₂₇H₃₅FNO₂ ([M+H]⁺): 424.2652; found: 424.2639.

(Z)-1-(3-butyl-5-fluoro-3-(2-fluoro-4-phenylbut-1-en-1-yl)benzo[d]isoxazol-2(3H)-yl)ethanone (3d)



This compound was obtained in 83% yield (63.9 mg) as light yellow oil. Eluent: PE/EA/Et₃N = 20/1/0.1, R_f = 0.7.

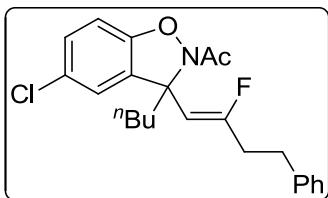
¹H NMR (400 MHz, CDCl₃): δ 7.24-7.12 (m, 3H), 6.98 (td, *J* = 8.7, 2.6 Hz, 1H), 6.88 (d, *J* = 6.9 Hz, 2H), 6.79 (dd, *J* = 8.6, 3.8 Hz, 1H), 6.71 (dd, *J* = 7.5, 2.5 Hz, 1H), 5.66 (d, *J* = 21.9 Hz, 1H), 2.66-2.57 (m, 2H), 2.43-2.35 (m, 1H), 2.20-1.99 (m, 5H), 1.83-1.74 (m, 1H), 1.34-1.05 (m, 4H), 0.80 (t, *J* = 7.3 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 165.7, 163.7 (d, *J* = 254.8 Hz), 158.9 (d, *J* = 240.1 Hz), 148.9, 140.4, 131.0 (d, *J* = 8.1 Hz), 128.5, 128.3, 126.3, 116.1 (d, *J* = 24.6 Hz), 111.4 (d, *J* = 27.7 Hz), 110.2 (d, *J* = 25.2 Hz), 107.8 (d, *J* = 8.4 Hz), 69.4 (d, *J* = 13.1 Hz), 39.7, 31.7, 31.5, 31.2, 25.5, 22.3, 21.8, 14.0.

¹⁹F NMR (376 MHz, CDCl₃): δ -96.12 - -96.31 (m), -119.51 (s).

HRMS (ESI) calculated for C₂₃H₂₅F₂NNaO₂ ([M+H]⁺): 408.1751; found: 408.1736.

(Z)-1-(3-butyl-5-chloro-3-(2-fluoro-4-phenylbut-1-en-1-yl)benzo[d]isoxazol-2(3H)-yl)ethanone (3e)



This compound was obtained in 70% yield (58.9 mg) as light yellow oil. Eluent: PE/EA = 10/1, R_f = 0.6.

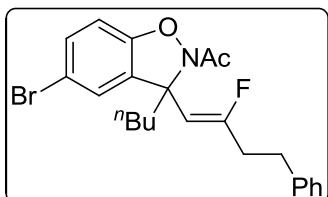
^1H NMR (400 MHz, CDCl_3): δ 7.26-7.14 (m, 4H), 7.01 (d, J = 1.9 Hz, 1H), 6.88 (d, J = 6.9 Hz, 2H), 6.79 (d, J = 8.6 Hz, 1H), 5.66 (d, J = 21.8 Hz, 1H), 2.67-2.59 (m, 2H), 2.41-2.33 (m, 1H), 2.19-2.00 (m, 5H), 1.78 (td, J = 13.6, 4.1 Hz, 1H), 1.31-1.04 (m, 4H), 0.80 (t, J = 7.3 Hz, 3H).

^{13}C NMR (100 MHz, CDCl_3): δ 165.7, 163.7 (d, J = 254.8 Hz), 151.4, 140.4, 131.5, 129.4, 128.5, 128.2, 126.3, 123.2, 111.4 (d, J = 27.7 Hz), 108.3, 69.2 (d, J = 14.3 Hz), 39.7, 31.7, 31.6, 31.3, 25.5, 22.3, 21.8, 14.1.

^{19}F NMR (376 MHz, CDCl_3): δ -95.94 - -96.11 (m).

HRMS (ESI) calculated for $\text{C}_{23}\text{H}_{25}\text{ClFNaNO}_2$ ($[\text{M}+\text{Na}]^+$): 424.1450; found: 424.1443.

(Z)-1-(5-bromo-3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)benzo[d]isoxazol-2(3H)-yl)ethanone (3f)



This compound was obtained in 82% yield (72.9 mg) as light yellow oil. Eluent: PE/EA/ Et_3N = 20/1/0.1, R_f = 0.7.

^1H NMR (400 MHz, CDCl_3): δ 7.39 (dd, J = 8.6, 2.0 Hz, 1H), 7.25-7.13 (m, 4H), 6.89 (d, J = 6.9 Hz, 2H), 6.75 (d, J = 8.5 Hz, 1H), 5.66 (d, J = 21.8 Hz, 1H), 2.67-2.59

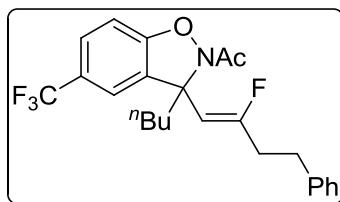
(m, 2H), 2.40-2.33 (m, 1H), 2.16 (s, 3H), 2.13-1.98 (m, 2H), 1.82-1.73 (m, 1H), 1.32-1.04 (m, 4H), 0.81 (t, $J = 7.3$ Hz, 3H).

^{13}C NMR (100 MHz, CDCl_3): δ 165.7, 163.8 (d, $J = 254.6$ Hz), 151.9, 140.4, 132.3, 132.0, 128.6, 128.2, 126.3, 126.0, 115.2, 111.4 (d, $J = 27.8$ Hz), 108.8, 69.1 (d, $J = 14.2$ Hz), 39.8, 31.6 (d, $J = 5.9$ Hz), 31.3, 25.5, 22.3, 21.8, 14.1.

^{19}F NMR (376 MHz, CDCl_3): δ -95.88 - -96.06 (m).

HRMS (ESI) calculated for $\text{C}_{23}\text{H}_{25}\text{BrNaFO}_2$ ($[\text{M}+\text{Na}]^+$): 468.0950; found: 468.0941.

(Z)-1-(3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-5-(trifluoromethyl)benzo[d]isoxazol-2(3H)-yl)ethanone (3g)



This compound was obtained in 52% yield (45.2 mg) as light yellow oil. Eluent: PE/EA/Et₃N = 20/1/0.1, $R_f = 0.7$.

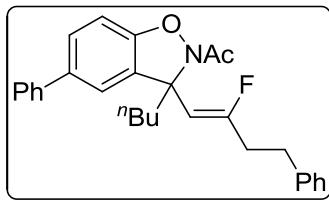
^1H NMR (400 MHz, CDCl_3): δ 7.59 (dd, $J = 8.5, 1.0$ Hz, 1H), 7.34 (s, 1H), 7.22-7.12 (m, 3H), 6.95 (d, $J = 8.4$ Hz, 1H), 6.84 (d, $J = 6.9$ Hz, 2H), 5.70 (d, $J = 21.6$ Hz, 1H), 2.67-2.58 (m, 2H), 2.34-2.26 (m, 1H), 2.19 (s, 3H), 2.13-1.99 (m, 2H), 1.83 (td, $J = 13.6, 4.1$ Hz, 1H), 1.33-1.00 (m, 4H), 0.80 (t, $J = 7.3$ Hz, 3H).

^{13}C NMR (100 MHz, CDCl_3): δ 165.9, 163.9 (d, $J = 255.5$ Hz), 155.1, 140.3, 130.9, 128.6, 128.2, 127.22, 127.20, 126.4, 126.1, 125.8, 125.3, 122.6, 120.6, 111.4 (d, $J = 27.9$ Hz), 107.5, 69.1 (d, $J = 14.1$ Hz), 39.8, 31.63, 31.56, 31.4, 25.5, 22.2, 21.8, 14.0.

^{19}F NMR (376 MHz, CDCl_3): δ -61.23 (s), -95.61 - -95.80 (m).

HRMS (ESI) calculated for $\text{C}_{24}\text{H}_{25}\text{F}_4\text{NNaO}_2$ ($[\text{M}+\text{Na}]^+$): 458.1719; found: 458.1709.

(Z)-1-(3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-5-phenylbenzo[d]isoxazol-2(3H)-yl)ethanone (3h)



This compound was obtained in 58% yield (51.4 mg) as light yellow solid. Eluent: PE/EA = 10/1, R_f = 0.6.

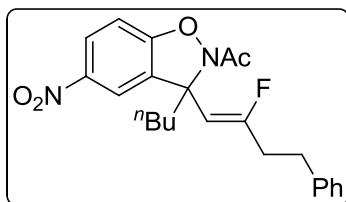
^1H NMR (400 MHz, CDCl_3): δ 7.57-7.51 (m, 3H), 7.44 (t, J = 7.6 Hz, 2H), 7.35 (t, J = 7.3 Hz, 1H), 7.31 (s, 1H), 7.18-7.08 (m, 3H), 6.94 (d, J = 8.4 Hz, 1H), 6.82 (d, J = 7.2 Hz, 2H), 5.75 (d, J = 21.9 Hz, 1H), 2.67-2.58 (m, 2H), 2.35-2.25 (m, 1H), 2.21 (s, 3H), 2.17-2.03 (m, 2H), 1.94-1.82 (m, 1H), 1.31-1.13 (m, 3H), 0.94-0.85 (m, 1H), 0.80 (t, J = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, CDCl_3): δ 165.7, 163.7 (d, J = 254.6 Hz), 152.5, 140.6, 140.2, 136.89, 130.5, 129.1, 128.5, 128.32, 128.26, 127.5, 127.0, 126.2, 121.6, 111.8 (d, J = 27.2 Hz), 107.3, 69.2 (d, J = 14.0 Hz), 39.9, 31.8, 31.6 (d, J = 26.5 Hz), 25.6, 22.3, 21.8, 14.1.

^{19}F NMR (376 MHz, CDCl_3): δ -96.36 - -96.55 (m).

HRMS (ESI) calculated for $\text{C}_{29}\text{H}_{31}\text{FNO}_2$ ($[\text{M}+\text{H}]^+$): 444.2339; found: 444.2328.

(Z)-1-(3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-5-nitrobenzo[d]isoxazol-2(3H)-yl)ethanone (3i)



This compound was obtained in 48% yield (39.6 mg) as orange solid. Eluent: PE/EA = 10/1, R_f = 0.3.

^1H NMR (400 MHz, CDCl_3): δ 8.20 (dd, J = 8.9, 2.3 Hz, 1H), 7.82 (d, J = 2.2 Hz, 1H), 7.18-7.08 (m, 3H), 6.94 (d, J = 8.9 Hz, 1H), 6.82 (d, J = 6.8 Hz, 2H), 5.69 (d, J = 21.4 Hz, 1H), 2.68-2.56 (m, 2H), 2.52-2.43 (m, 1H), 2.26-2.13 (m, 4H), 2.11-1.96 (m,

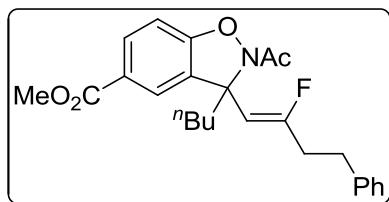
1H), 1.81 (td, $J = 13.7, 4.1$ Hz, 1H), 1.30-1.14 (m, 3H), 1.11-1.00 (m, 1H), 0.79 (t, $J = 7.3$ Hz, 3H).

^{13}C NMR (100 MHz, CDCl_3): δ 166.0, 156.8, 144.1, 140.0, 131.4, 128.5, 128.1, 126.4, 126.3, 119.5, 111.4 (d, $J = 28.5$ Hz), 107.4, 69.1 (d, $J = 14.2$ Hz), 39.9, 31.5, 31.3, 25.4, 22.2, 21.8, 14.0.

^{19}F NMR (376 MHz, CDCl_3): δ -95.75 - -95.91 (m).

HRMS (ESI) calculated for $\text{C}_{23}\text{H}_{26}\text{FN}_2\text{O}_4$ ($[\text{M}+\text{H}]^+$): 413.1876; found: 413.1864.

(Z)-methyl 2-acetyl-3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-2,3-dihydrobenzo[*d*]isoxazole-5-carboxylate (3j)



This compound was obtained in 56% yield (47.6 mg) as white solid. Eluent: PE/EA = 5/1, $R_f = 0.5$.

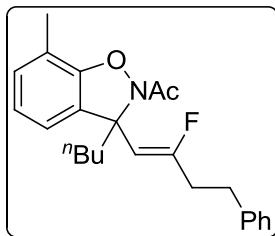
^1H NMR (400 MHz, CDCl_3): δ 8.04 (dd, $J = 8.6, 1.7$ Hz, 1H), 7.76 (d, $J = 0.9$ Hz, 1H), 7.21-7.09 (m, 3H), 6.91 (d, $J = 8.5$ Hz, 1H), 6.82 (d, $J = 7.0$ Hz, 2H), 5.71 (d, $J = 21.7$ Hz, 1H), 3.92 (s, 3H), 2.69-2.54 (m, 2H), 2.36-2.28 (m, 1H), 2.19 (s, 3H), 2.12-1.95 (m, 2H), 1.90-1.78 (m, 1H), 1.29-1.16 (m, 2H), 1.12-1.01 (m, 1H), 0.82-0.72 (m, 4H).

^{13}C NMR (100 MHz, CDCl_3): δ 166.0, 165.8, 163.7 (d, $J = 255.3$ Hz), 156.1, 140.4, 131.8, 130.4, 128.5, 128.2, 126.2, 125.7, 125.0, 111.6 (d, $J = 27.7$ Hz), 106.9, 68.9 (d, $J = 14.2$ Hz), 52.4, 39.9, 31.6, 31.3, 25.5, 22.2, 21.8, 14.0.

^{19}F NMR (376 MHz, CDCl_3): δ -96.12 - -96.31 (m).

HRMS (ESI) calculated for $\text{C}_{25}\text{H}_{29}\text{FNO}_2$ ($[\text{M}+\text{H}]^+$): 426.2080; found: 426.2066.

(Z)-1-(3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-7-methylbenzo[*d*]isoxazol-2(3*H*)-yl)ethanone (3k)



This compound was obtained in 39% yield (29.7 mg) as light yellow oil. Eluent: PE/EA = 10/1, R_f = 0.6.

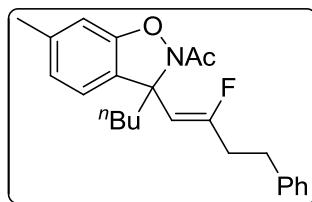
^1H NMR (400 MHz, CDCl_3): δ 7.22-7.14 (m, 3H), 7.10 (d, J = 7.3 Hz, 1H), 6.97 (t, J = 7.5 Hz, 1H), 6.89 (d, J = 7.5 Hz, 1H), 6.82 (d, J = 7.1 Hz, 2H), 5.72 (d, J = 22.0 Hz, 1H), 2.67-2.51 (m, 2H), 2.27 (s, 3H), 2.26-2.21 (m, 1H), 2.20 (s, 3H), 2.07-1.96 (m, 2H), 1.84 (td, J = 13.3, 4.1 Hz, 1H), 1.28-1.20 (m, 2H), 1.16-1.04 (m, 1H), 0.85-0.77 (m, 4H).

^{13}C NMR (100 MHz, CDCl_3): δ 165.5, 163.7 (d, J = 254.1 Hz), 151.4, 140.8, 130.5, 129.0, 128.5, 128.3, 126.2, 123.3, 120.5, 117.7, 111.9 (d, J = 26.8 Hz), 69.5 (d, J = 14.6 Hz), 39.9, 31.9, 31.5 (d, J = 27.2 Hz), 25.6, 22.4, 21.8, 15.0, 14.1.

^{19}F NMR (376 MHz, CDCl_3): δ -96.69 - -96.88 (m).

HRMS (ESI) calculated for $\text{C}_{24}\text{H}_{29}\text{FNO}_2$ ($[\text{M}+\text{H}]^+$): 382.2182; found: 382.2171.

(Z)-1-(3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-6-methylbenzo[d]isoxazol-2(3H)-yl)ethanone (3l)



This compound was obtained in 66% yield (50.3 mg) as light yellow oil. Eluent: PE/EA = 10/1, R_f = 0.6.

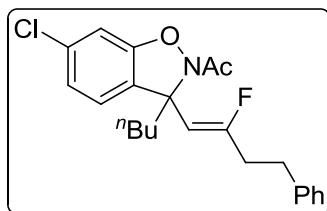
^1H NMR (400 MHz, CDCl_3): δ 7.22-7.12 (m, 3H), 6.93 (d, J = 7.7 Hz, 1H), 6.87 (d, J = 7.8 Hz, 1H), 6.82 (d, J = 6.9 Hz, 2H), 6.68 (s, 1H), 5.70 (d, J = 22.2 Hz, 1H), 2.62-2.54 (m, 2H), 2.39 (s, 3H), 2.31-2.24 (m, 1H), 2.16 (s, 3H), 2.09-1.96 (m, 2H), 1.82 (td, J = 13.2, 4.2 Hz, 1H), 1.29-1.03 (m, 4H), 0.79 (t, J = 7.2 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 165.6, 163.6 (d, *J* = 253.6 Hz), 153.1, 140.8, 139.8, 128.43, 128.35, 126.7, 126.2, 124.1, 122.7, 111.8 (d, *J* = 26.8 Hz), 107.5, 68.9 (d, *J* = 14.2 Hz), 39.8, 31.8, 31.5 (d, *J* = 26.5 Hz), 25.5, 22.4, 21.8, 21.7, 14.1.

¹⁹F NMR (376 MHz, CDCl₃): δ -96.79 - -96.97 (m).

HRMS (ESI) calculated for C₂₄H₂₈FNaNO₂ ([M+Na]⁺): 404.2002; found: 404.1989.

(Z)-1-(3-butyl-6-chloro-3-(2-fluoro-4-phenylbut-1-en-1-yl)benzo[d]isoxazol-2(3H)-yl)ethanone (3m)



This compound was obtained in 67% yield (53.7 mg) as light yellow oil. Eluent: PE/EA = 10/1, R_f = 0.5.

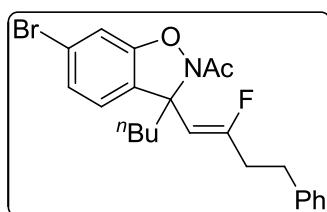
¹H NMR (400 MHz, CDCl₃): δ 7.22 (t, *J* = 7.3 Hz, 2H), 7.18-7.14 (m, 1H), 7.01 (dd, *J* = 8.1, 1.6 Hz, 1H), 6.91 (d, *J* = 8.1 Hz, 1H), 6.88-6.83 (m, 3H), 5.68 (d, *J* = 21.9 Hz, 1H), 2.65-2.57 (m, 2H), 2.37-2.31 (m, 1H), 2.18-1.97 (m, 5H), 1.79 (td, *J* = 13.4, 4.1 Hz, 1H), 1.31-1.02 (m, 4H), 0.79 (t, *J* = 7.3 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃): δ 165.8, 163.6 (d, *J* = 254.9 Hz), 153.4, 140.4, 134.9, 128.6, 128.4, 128.3, 126.3, 123.8, 123.6, 111.5 (d, *J* = 27.6 Hz), 107.9, 69.0 (d, *J* = 13.6 Hz), 39.7, 31.63, 31.60, 31.3, 25.4, 22.3, 21.7, 14.0.

¹⁹F NMR (376 MHz, CDCl₃): δ -96.30 - -96.48 (m).

HRMS (ESI) calculated for C₂₃H₂₆ClFNO₂ ([M+H]⁺): 402.1636; found: 402.1629.

(Z)-1-(6-bromo-3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)benzo[d]isoxazol-2(3H)-yl)ethanone (3n)



This compound was obtained in 80% yield (71.2 mg) as light yellow oil. Eluent: PE/EA = 10/1, R_f = 0.5.

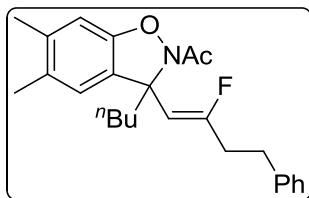
$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.26-7.21 (m, 2H), 7.18-7.14 (m, 2H), 7.03 (s, 1H), 6.85 (t, J = 8.8 Hz, 3H), 5.67 (d, J = 21.9 Hz, 1H), 2.65-2.57 (m, 2H), 2.39-2.29 (m, 1H), 2.15 (s, 3H), 2.12-1.91 (m, 2H), 1.79 (td, J = 13.5, 3.9 Hz, 1H), 1.31-1.00 (m, 4H), 0.79 (t, J = 7.3 Hz, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 165.8, 163.7 (d, J = 254.6 Hz), 153.5, 140.4, 129.0, 128.6, 128.3, 126.5, 126.3, 124.2, 122.4, 111.5 (d, J = 27.4 Hz), 110.7, 69.0 (d, J = 14.2 Hz), 39.7, 31.7, 31.4, 25.5, 22.3, 21.8, 14.0.

$^{19}\text{F NMR}$ (376 MHz, CDCl_3): δ -96.29 - -96.47 (m).

HRMS (ESI) calculated for $\text{C}_{23}\text{H}_{25}\text{BrNaFNO}_2$ ($[\text{M}+\text{H}]^+$): 468.0950; found: 468.0937.

(Z)-1-(3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-5,6-dimethylbenzo[*d*]isoxazol-2(3*H*)-yl)ethanone (3o)



This compound was obtained in 75% yield (59.3 mg) as light yellow oil. Eluent: PE/EA = 10/1, R_f = 0.7.

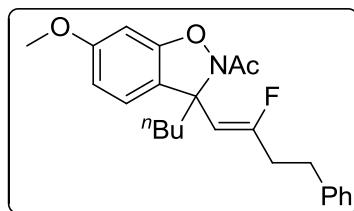
$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.21-7.11 (m, 3H), 6.84-6.78 (m, 3H), 6.65 (s, 1H), 5.69 (d, J = 22.3 Hz, 1H), 2.67-2.53 (m, 2H), 2.33-2.25 (m, 4H), 2.22 (s, 3H), 2.16 (s, 3H), 2.09-1.97 (m, 2H), 1.81 (td, J = 13.0, 4.1 Hz, 1H), 1.29-1.05 (m, 4H), 0.80 (t, J = 7.3 Hz, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 165.5, 163.5 (d, J = 253.7 Hz), 151.3, 140.8, 138.1, 131.4, 128.4, 128.3, 126.7, 126.1, 123.6, 111.8 (d, J = 26.4 Hz), 107.9, 69.0 (d, J = 14.1 Hz), 39.8, 31.9, 31.5, 31.3, 25.6, 22.4, 21.8, 20.4, 19.7, 14.1.

$^{19}\text{F NMR}$ (376 MHz, CDCl_3): δ -96.96 - -97.15 (m).

HRMS (ESI) calculated for $\text{C}_{25}\text{H}_{30}\text{FNaNO}_2$ ($[\text{M}+\text{Na}]^+$): 418.2153; found: 418.2148.

(Z)-1-(3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-6-methoxybenzo[d]isoxazol-2(3H)-yl)ethanone (3p)



This compound was obtained in 18% yield (14.3 mg) as light yellow oil. Eluent: PE/EA = 10/1, R_f = 0.4.

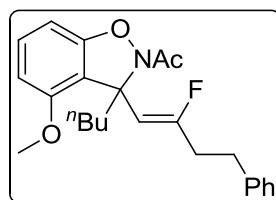
^1H NMR (400 MHz, CDCl_3): δ 7.23-7.14 (m, 3H), 6.91 (d, J = 8.4 Hz, 1H), 6.87 (d, J = 7.1 Hz, 2H), 6.60 (dd, J = 8.4, 2.1 Hz, 1H), 6.41 (d, J = 1.7 Hz, 1H), 5.70 (d, J = 22.3 Hz, 1H), 3.82 (s, 3H), 2.63-2.57 (m, 2H), 2.37-2.28 (m, 1H), 2.16 (s, 3H), 2.12-1.99 (m, 2H), 1.81 (td, J = 13.4, 4.1 Hz, 1H), 1.32-1.02 (m, 4H), 0.80 (t, J = 7.3 Hz, 3H).

^{13}C NMR (100 MHz, CDCl_3): δ 165.5, 163.5 (d, J = 253.4 Hz), 161.0, 154.0, 140.7, 128.4, 128.3, 126.2, 123.4, 121.4, 111.8 (d, J = 26.7 Hz), 109.5, 93.2, 68.9 (d, J = 14.8 Hz), 55.8, 39.9, 31.8, 31.4 (d, J = 27.0 Hz), 25.5, 22.3, 21.8, 14.1.

^{19}F NMR (376 MHz, CDCl_3): δ -96.80 - -96.99 (m).

HRMS (ESI) calculated for $\text{C}_{24}\text{H}_{29}\text{FNO}_3$ ($[\text{M}+\text{H}]^+$): 398.2131; found: 398.2115.

(Z)-1-(3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-4-methoxybenzo[d]isoxazol-2(3H)-yl)ethanone (3p')



This compound was obtained in 37% yield (29.4 mg) as light yellow oil. Eluent: PE/EA = 10/1, R_f = 0.3.

^1H NMR (400 MHz, CDCl_3): δ 7.25 (t, J = 8.2 Hz, 1H), 7.21-7.13 (m, 3H), 6.86 (d, J = 6.9 Hz, 2H), 6.55-6.48 (m, 2H), 5.69 (d, J = 22.6 Hz, 1H), 3.80 (s, 3H), 2.65-2.54

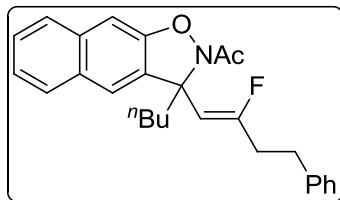
(m, 2H), 2.31-2.22 (m, 1H), 2.20-2.08 (m, 6H), 1.31-1.02 (m, 4H), 0.79 (t, J = 7.3 Hz, 3H).

^{13}C NMR (100 MHz, CDCl_3): δ 165.3, 162.1 (d, J = 251.5 Hz), 155.2, 153.7, 140.9, 130.6, 128.4, 128.3, 126.1, 115.5, 111.0 (d, J = 27.2 Hz), 105.3, 100.0, 69.5 (d, J = 14.6 Hz), 55.8, 36.3, 32.0, 31.2 (d, J = 25.9 Hz), 26.0, 22.2, 21.9, 14.1.

^{19}F NMR (376 MHz, CDCl_3): δ -98.48 - -98.64 (m).

HRMS (ESI) calculated for $\text{C}_{24}\text{H}_{29}\text{FNO}_3$ ($[\text{M}+\text{H}]^+$): 398.2131; found: 398.2112.

(Z)-1-(3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)naphtho[2,3-d]isoxazol-2(3H)-yl)ethanone (3q)



This compound was obtained in 46% yield (38.4 mg) as light yellow oil. Two inseparable regioisomers were observed, the ratio was determined to be 97:3 by $^1\text{H-NMR}$ analysis. Eluent: PE/EA = 10/1, R_f = 0.6.

^1H NMR (400 MHz, CDCl_3): δ 7.79 (d, J = 8.8 Hz, 2H), 7.53-7.48 (m, 2H), 7.47-7.34 (m, 1H), 7.19 (s, 1H), 7.03-6.95 (m, 3H), 6.56-6.48 (m, 2H), 5.81 (d, J = 21.8 Hz, 1H), 2.70 (t, J = 11.5 Hz, 1H), 2.58-2.51 (m, 1H), 2.24-2.15 (m, 4H), 2.13-2.02 (m, 1H), 2.01-1.88 (m, 2H), 1.28-1.13 (m, 3H), 0.89-0.79 (m, 1H), 0.76 (t, J = 7.2 Hz, 3H).

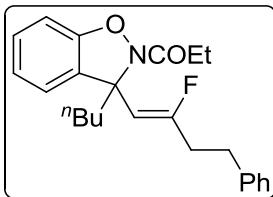
^{13}C NMR (100 MHz, CDCl_3): δ 165.7, 163.7 (d, J = 253.9 Hz), 151.6, 140.3, 134.3, 132.5, 130.4, 128.4, 128.3, 128.1, 127.4, 127.2, 126.1, 124.8, 122.2, 112.1 (d, J = 27.7 Hz), 101.8, 68.5 (d, J = 13.9 Hz), 40.4, 31.9, 31.6, 25.5, 22.4, 21.9, 14.0.

^{19}F NMR (376 MHz, CDCl_3): δ -96.19 - -96.30 (m, minor); -97.29 - -97.47 (m, major).

HRMS (ESI) calculated for $\text{C}_{27}\text{H}_{28}\text{FNaNO}_2$ ($[\text{M}+\text{Na}]^+$): 440.2002; found: 440.1991.

(Z)-1-(3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)benzo[d]isoxazol-2(3H)-yl)propa

n-1-one (3r)



This compound was obtained in 61% yield (46.5 mg) as light yellow oil. Eluent: PE/EA = 10/1, R_f = 0.6.

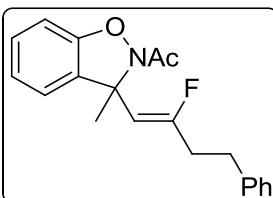
$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.33-7.26 (m, 1H), 7.21-7.11 (m, 3H), 7.07-7.04 (m, 2H), 6.87 (d, J = 8.1 Hz, 1H), 6.82 (d, J = 6.8 Hz, 2H), 5.72 (d, J = 22.1 Hz, 1H), 2.66-2.42 (m, 4H), 2.31-2.20 (m, 1H), 2.08-1.97 (m, 2H), 1.88-1.80 (m, 1H), 1.28-1.07 (m, 6H), 0.78 (t, J = 7.2 Hz, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 169.2, 163.6 (d, J = 254.2 Hz), 153.0, 140.7, 129.6, 129.3, 128.4, 128.3, 126.2, 123.2, 123.1, 111.9 (d, J = 27.2 Hz), 107.1, 69.0 (d, J = 14.8 Hz), 39.8, 31.7, 31.4 (d, J = 25.7 Hz), 27.2, 25.5, 22.3, 14.1, 8.4.

$^{19}\text{F NMR}$ (376 MHz, CDCl_3): δ -96.58 - -96.77 (m).

HRMS (ESI) calculated for $\text{C}_{24}\text{H}_{29}\text{FNO}_2$ ($[\text{M}+\text{H}]^+$): 382.2182; found: 382.2173.

(Z)-1-(3-(2-fluoro-4-phenylbut-1-en-1-yl)-3-methylbenzo[d]isoxazol-2(3H)-yl)ethanone (3s)



This compound was obtained in 55% yield (35.8 mg) as light yellow oil. Eluent: PE/EA = 10/1, R_f = 0.5.

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.31-7.26 (m, 1H), 7.22-7.12 (m, 3H), 7.09-7.03 (m, 2H), 6.89-6.84 (m, 3H), 5.73 (d, J = 22.1 Hz, 1H), 2.63-2.55 (m, 1H), 2.37-2.27 (m, 1H), 2.16 (s, 3H), 2.13-2.01 (m, 2H), 1.85 (s, 3H).

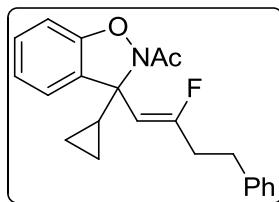
$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 166.0, 163.5 (d, J = 254.7 Hz), 152.4, 140.6, 131.6, 129.3, 128.5, 128.3, 126.2, 123.3, 122.9, 111.5 (d, J = 27.6 Hz), 107.3, 65.4 (d, J =

14.1 Hz), 31.7, 31.2 (d, J = 25.7 Hz), 28.8, 22.0.

^{19}F NMR (376 MHz, CDCl_3): δ -96.45 - -96.64 (m).

HRMS (ESI) calculated for $\text{C}_{20}\text{H}_{21}\text{FNO}_2$ ($[\text{M}+\text{H}]^+$): 326.1556; found: 326.1541.

(Z)-1-(3-cyclopropyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)benzo[d]isoxazol-2(3H)-yl)ethanone (3t)



This compound was obtained in 68% yield (47.7 mg) as light yellow oil. Eluent: PE/EA = 10/1, R_f = 0.5.

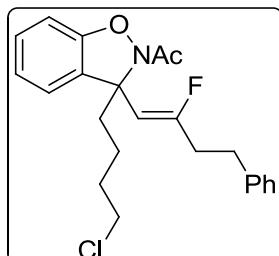
^1H NMR (400 MHz, CDCl_3): δ 7.31-7.27 (m, 1H), 7.22-7.14 (m, 3H), 7.02-6.94 (m, 2H), 6.88-6.82 (m, 3H), 5.85 (d, J = 21.9 Hz, 1H), 2.67-2.53 (m, 1H), 2.38-2.33 (m, 1H), 2.19 (s, 3H), 2.16-2.01 (m, 3H), 0.60-0.52 (m, 1H), 0.46-0.37 (m, 2H), -0.03--0.11 (m, 1H).

^{13}C NMR (100 MHz, CDCl_3): δ 166.4, 163.3 (d, J = 250.6 Hz), 153.3, 140.7, 129.6, 128.5, 128.3, 127.0, 126.2, 124.4, 122.6, 110.9 (d, J = 28.3 Hz), 107.2, 69.7 (d, J = 15.0 Hz), 31.8, 31.7, 31.5, 22.1, 19.8, 2.4, 1.2.

^{19}F NMR (376 MHz, CDCl_3): δ -97.29 - -97.47 (m).

HRMS (ESI) calculated for $\text{C}_{22}\text{H}_{22}\text{FNaNO}_2$ ($[\text{M}+\text{H}]^+$): 374.1532; found: 374.1520.

(Z)-1-(3-(4-chlorobutyl)-3-(2-fluoro-4-phenylbut-1-en-1-yl)benzo[d]isoxazol-2(3H)-yl)ethanone (3u)



This compound was obtained in 65% yield (52.3 mg) as light yellow oil. Eluent:

PE/EA = 10/1, R_f = 0.5.

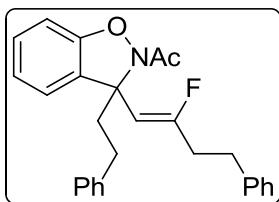
$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.34-7.29 (m, 1H), 7.22-7.12 (m, 3H), 7.08-7.05 (m, 2H), 6.88 (d, J = 8.2 Hz, 1H), 6.85-6.81 (m, 2H), 5.71 (d, J = 22.0 Hz, 1H), 3.42 (t, J = 6.6 Hz, 2H), 2.65 (td, J = 13.2, 4.3 Hz, 1H), 2.60-2.52 (m, 1H), 2.32-2.23 (m, 1H), 2.18 (s, 3H), 2.09-1.97 (m, 2H), 1.87 (td, J = 13.3, 4.5 Hz, 1H), 1.74-1.62 (m, 2H), 1.32-1.22 (m, 1H), 1.06-0.94 (m, 1H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 165.8, 163.8 (d, J = 254.0 Hz), 152.9, 140.6, 129.5, 129.1, 128.5, 128.3, 126.2, 123.4, 123.1, 111.5 (d, J = 27.4 Hz), 107.2, 68.8 (d, J = 14.7 Hz), 44.6, 39.1, 32.0, 31.7, 31.4 (d, J = 26.3 Hz), 21.8, 20.8.

$^{19}\text{F NMR}$ (376 MHz, CDCl_3): δ -96.04 - -96.23 (m).

HRMS (ESI) calculated for $\text{C}_{23}\text{H}_{25}\text{FClNaNO}_2$ ($[\text{M}+\text{Na}]^+$): 424.1456; found: 424.1441.

(Z)-1-(3-(2-fluoro-4-phenylbut-1-en-1-yl)-3-phenethylbenzo[d]isoxazol-2(3H)-yl)ethanone (3v)



This compound was obtained in 79% yield (65.6 mg) as light yellow oil. Eluent: PE/EA = 10/1, R_f = 0.5.

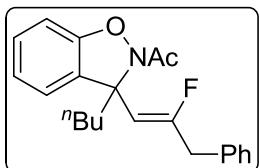
$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.37-7.31 (m, 1H), 7.23-7.18 (m, 4H), 7.17-7.12 (m, 2H), 7.12-7.09 (m, 2H), 7.02 (d, J = 7.1 Hz, 2H), 6.91 (d, J = 8.2 Hz, 1H), 6.84 (d, J = 6.8 Hz, 2H), 5.73 (d, J = 22.0 Hz, 1H), 3.09-2.96 (m, 1H), 2.62-2.54 (m, 1H), 2.42 (td, J = 13.5, 5.3 Hz, 1H), 2.33-2.23 (m, 1H), 2.20-2.00 (m, 7H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 165.7, 163.8 (d, J = 254.6 Hz), 153.0, 140.7, 140.6, 129.6, 129.1, 128.5, 128.3, 126.2, 126.1, 123.5, 123.1, 111.6 (d, J = 27.5 Hz), 107.2, 68.8 (d, J = 14.8 Hz), 41.6, 31.7, 31.4 (d, J = 25.8 Hz), 30.0, 21.8.

$^{19}\text{F NMR}$ (376 MHz, CDCl_3): δ -95.96 - -96.14 (m).

HRMS (ESI) calculated for $\text{C}_{27}\text{H}_{27}\text{FNO}_2$ ($[\text{M}+\text{H}]^+$): 416.2026; found: 416.2014.

(Z)-1-(3-butyl-3-(2-fluoro-3-phenylprop-1-en-1-yl)benzo[d]isoxazol-2(3H)-yl)ethanone (3w)



This compound was obtained in 59% yield (41.7 mg) as light yellow oil. Eluent: PE/EA = 10/1, R_f = 0.6.

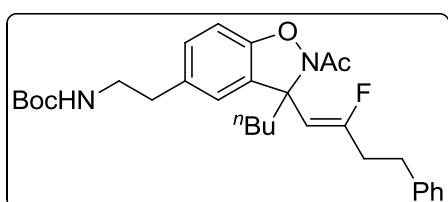
^1H NMR (400 MHz, CDCl_3): δ 7.30-7.26 (m, 1H), 7.20-7.13 (m, 3H), 7.10-7.02 (m, 2H), 6.87 (d, J = 8.1 Hz, 1H), 6.83 (d, J = 6.7 Hz, 2H), 5.82 (d, J = 21.6 Hz, 1H), 3.11 (d, J = 23.9 Hz, 2H), 2.67 (td, J = 13.1, 4.0 Hz, 1H), 2.08 (s, 3H), 1.88 (td, J = 13.8, 4.2 Hz, 1H), 1.34-1.05 (m, 4H), 0.79 (t, J = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, CDCl_3): δ 165.6, 162.1 (d, J = 254.1 Hz), 153.0, 135.2, 129.4, 128.50, 128.47, 126.7, 123.3, 123.2, 112.7 (d, J = 26.8 Hz), 107.1, 68.9 (d, J = 14.1 Hz), 39.9, 35.0 (d, J = 27.5 Hz), 25.5, 22.3, 21.6, 14.1.

^{19}F NMR (376 MHz, CDCl_3): δ -93.39 - -93.58 (m).

HRMS (ESI) calculated for $\text{C}_{22}\text{H}_{25}\text{FNO}_2$ ($[\text{M}+\text{H}]^+$): 354.1869; found: 354.1863.

(Z)-*tert*-butyl (2-(2-acetyl-3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-2,3-dihydrobenzo[d]isoxazol-5-yl)ethyl)carbamate (4)



This compound was obtained in 55% yield (56.1 mg) as white solid. Eluent: PE/EA = 5/1, R_f = 0.5.

^1H NMR (400 MHz, CDCl_3): δ 7.22-7.18 (m, 2H), 7.16-7.11 (m, 2H), 6.91 (s, 1H), 6.84-6.80 (m, 3H), 5.69 (d, J = 21.9 Hz, 1H), 4.48 (s, 1H), 3.32-3.27 (m, 2H), 2.81-2.75 (m, 2H), 2.67-2.54 (m, 2H), 2.29-2.21 (m, 1H), 2.17 (s, 3H), 2.11-2.00 (m,

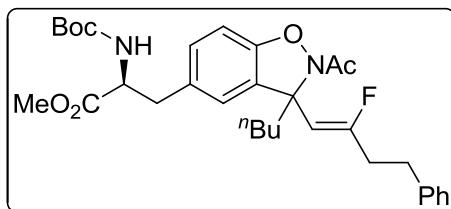
2H), 1.82 (td, $J = 13.5, 4.0$ Hz, 1H), 1.42 (s, 9H), 1.34-1.15 (m, 3H), 1.14-1.03 (m, 1H), 0.79 (t, $J = 7.3$ Hz, 3H).

^{13}C NMR (100 MHz, CDCl_3): δ 165.6, 163.6 (d, $J = 253.8$ Hz), 155.9, 151.7, 140.6, 134.2, 130.1, 129.6, 128.5, 128.3, 126.3, 123.3, 111.7 (d, $J = 27.0$ Hz), 107.1, 79.5, 69.1 (d, $J = 14.0$ Hz), 42.2, 39.8, 35.8, 31.8, 31.4 (d, $J = 26.5$ Hz), 28.5, 25.5, 22.3, 21.8, 14.1.

^{19}F NMR (376 MHz, CDCl_3): δ -96.45 - -96.64 (m).

HRMS (ESI) calculated for $\text{C}_{30}\text{H}_{39}\text{FNaN}_2\text{O}_4 ([\text{M}+\text{H}]^+)$: 533.2792; found: 533.2779.

(2S)-methyl 3-(2-acetyl-3-butyl-3-((Z)-2-fluoro-4-phenylbut-1-en-1-yl)-2,3-di hydrobenzo[*d*]isoxazol-5-yl)-2-((tert-butoxycarbonyl)amino)propanoate (5)



This compound was obtained in 43% yield (48.8 mg) as colorless oil. Eluent: PE/EA = 5/1, $R_f = 0.4$. An inseparable diastereoisomers were contained for this compound, the ratio was determined as 1:1 by ^1H -NMR analysis.

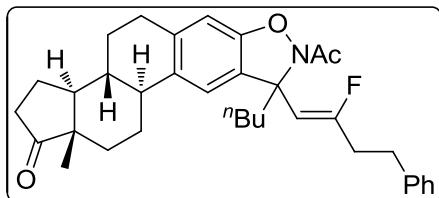
^1H NMR (400 MHz, CDCl_3): δ 7.20 (td, $J = 7.2, 1.6$ Hz, 2H), 7.14 (t, $J = 7.2$ Hz, 1H), 7.03 (d, $J = 8.2$ Hz, 1H), 6.87 (t, $J = 7.0$ Hz, 2H), 6.80 (t, $J = 9.3$ Hz, 2H), 5.68 (d, $J = 21.7$ Hz, 1H), 4.97-4.93 (m, 1H), 4.58-4.45 (m, 1H), 3.65 (s, 1.5H), 3.63 (s, 1.5H), 3.17-2.99 (m, 2H), 2.69-2.54 (m, 2H), 2.36-2.25 (m, 1H), 2.16 (s, 3H), 2.11-1.98 (m, 2H), 1.84-1.74 (m, 1H), 1.43-1.40 (m, 9H), 1.33-1.01 (m, 4H), 0.80 (t, $J = 7.3$ Hz, 3H).

^{13}C NMR (100 MHz, CDCl_3): δ 172.13, 172.06, 165.6, 155.1, 152.1, 140.7, 140.6, 131.3, 131.2, 130.2, 130.1, 128.5, 128.3, 126.2, 123.9, 111.7 (d, $J = 27.2$ Hz), 107.0, 80.3, 69.0 (d, $J = 14.1$ Hz), 54.8, 54.7, 52.3, 39.8, 37.9, 37.7, 31.8, 31.52, 31.50, 31.3, 31.2, 28.41, 28.39, 25.5, 22.4, 22.3, 21.8, 14.1.

^{19}F NMR (376 MHz, CDCl_3): δ -96.25 - -96.59 (m).

HRMS (ESI) calculated for $\text{C}_{32}\text{H}_{42}\text{FN}_2\text{O}_6 ([\text{M}+\text{H}]^+)$: 569.3027; found: 569.3021.

(3a*S*,3b*R*,10b*S*,12a*S*)-8-acetyl-9-butyl-9-((*Z*)-2-fluoro-4-phenylbut-1-en-1-yl)-12a-methyl-2,3,3a,3b,4,5,8,9,10b,11,12,12a-dodecahydro-1*H*-cyclopenta[7,8]phenanthro[3,2-*d*]isoxazol-1-one (6)



This compound was obtained in 32% yield (34.8 mg) as light yellow oil. Eluent: PE/EA = 10/1, R_f = 0.3. An inseparable diastereoisomers were contained for this compound, the ratio was determined as 1:1 by ^1H -NMR analysis.

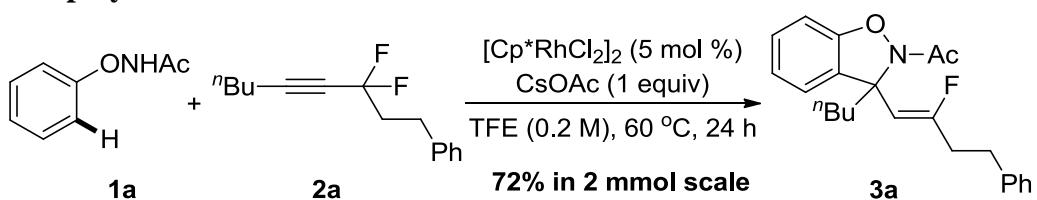
^1H NMR (400 MHz, CDCl_3): δ 7.21-7.12 (m, 3H), 7.04 (s, 0.5H), 7.00 (s, 0.5H), 6.83-6.77 (m, 2H), 6.61 (s, 0.5H), 6.59 (s, 0.5H), 5.71 (d, J = 22.2 Hz, 0.5H), 5.70 (d, J = 22.2 Hz, 0.5H), 2.98-2.94 (m, 2H), 2.64-2.45 (m, 3H), 2.41-2.35 (m, 1H), 2.31-1.92 (m, 13H), 1.85-1.77 (m, 1H), 1.67 (s, 3H), 1.65-1.58 (m, 1H), 1.53-1.41 (m, 3H), 1.29-1.05 (m, 4H), 0.81 (t, J = 7.3 Hz, 1.5H), 0.80 (t, J = 7.3 Hz, 1.5H).

^{13}C NMR (100 MHz, CDCl_3): δ 220.7, 165.58, 165.55, 163.6 (d, J = 253.1 Hz), 151.4, 151.3, 140.83, 140.77, 138.3, 138.2, 134.9, 128.44, 128.42, 128.3, 128.2, 127.5, 127.3, 126.2, 119.9, 119.8, 111.83 (d, J = 26.7 Hz), 111.76 (d, J = 26.7 Hz), 106.8, 69.2 (d, J = 14.0 Hz), 69.1 (d, J = 14.1 Hz), 50.49, 50.47, 48.1, 48.0, 44.4, 44.3, 39.9, 39.8, 38.32, 38.27, 36.0, 35.9, 32.0, 31.9, 31.60, 31.55, 31.48, 31.3, 31.2, 30.1, 26.5, 26.4, 26.3, 26.2, 25.5, 22.4, 22.3, 21.8, 21.7, 14.10, 14.07, 14.05, 13.8.

^{19}F NMR (376 MHz, CDCl_3): δ -96.62 - -96.92 (m).

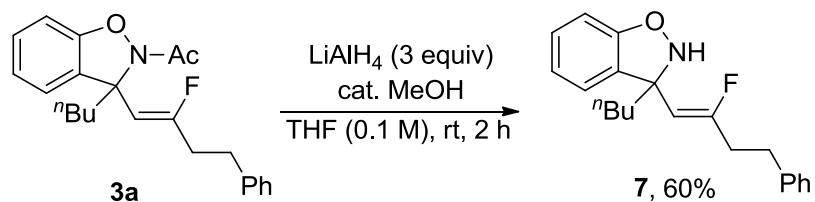
HRMS (ESI) calculated for $\text{C}_{35}\text{H}_{43}\text{FNO}_3$ ($[\text{M}+\text{H}]^+$): 544.3227; found: 544.3223.

Scale-up Synthesis of 3a:



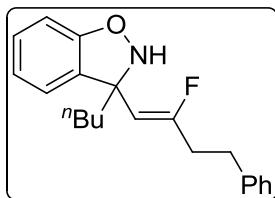
The mixture of *N*-phenoxyacetamide **1a** (2 mmol, 1.0 equiv), α,α -difluoromethylene alkyne **2a** (2.8 mmol, 1.4 equiv), $[\text{Cp}^*\text{RhCl}_2]_2$ (5 mol %) and CsOAc (1 equiv) in TFE (10 mL) was stirred at 60 °C without exclusion of air or moisture. The reaction was monitored by TLC. After completion, it was diluted with EtOAc and filtered through a short silica gel column to remove the metal residues. Then, the reaction mixture was concentrated and purified by silica gel column chromatography to give the desired monofluoroalkenyl dihydrobenzo[*d*]isoxazole derivative **3a** (0.5285 g, 72%).

Deacetylation of 3a:



Dihydrobenzo[*d*]isoxazole **3a** (0.1 mmol, 1.0 equiv) and LiAlH₄ (0.3 mmol, 3.0 equiv) was dissolved in THF (1 mL), 1 drop of MeOH was added, the resulted mixture was stirred at room temperature for 2 h without exclusion of air or moisture. Afterwards, the reaction was quenched with MeOH and diluted with EtOAc. Then, the reaction mixture was concentrated and purified by preparative TLC (eluent: PE/EA = 10/1) to give the desired deacetylated derivative **7** in 60% isolated yield (19.6 mg) as light yellow oil.

(Z)-3-butyl-3-(2-fluoro-4-phenylbut-1-en-1-yl)-2,3-dihydrobenzo[*d*]isoxazole (7)



¹H NMR (400 MHz, DMSO-*d*₆): δ 7.90 (s, 1H), 7.30-7.24 (m, 2H), 7.22-7.12 (m, 5H), 6.94 (t, *J* = 7.3 Hz, 1H), 6.85 (d, *J* = 8.0 Hz, 1H), 5.40 (d, *J* = 23.3 Hz, 1H), 2.77-2.53 (m, 4H), 1.72-1.62 (m, 2H), 1.24-1.13 (m, 3H), 1.12-1.03 (m, 1H), 0.80 (t, *J* = 7.1 Hz, 3H).

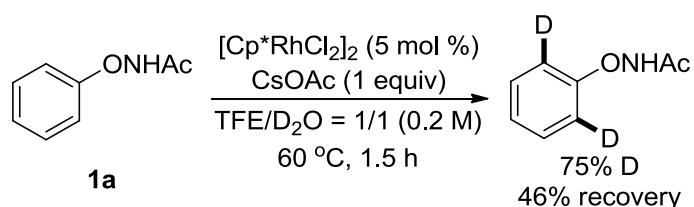
¹³C NMR (100 MHz, DMSO-*d*₆): δ 158.6, 140.6, 133.4, 128.32, 128.26, 128.21, 126.1, 122.5, 121.2, 109.8 (d, *J* = 23.9 Hz), 107.3, 66.3 (d, *J* = 12.7 Hz), 31.8, 31.4 (d, *J* = 23.3 Hz), 25.6, 22.4, 13.9.

¹⁹F NMR (376 MHz, DMSO-*d*₆): δ -96.99 (s).

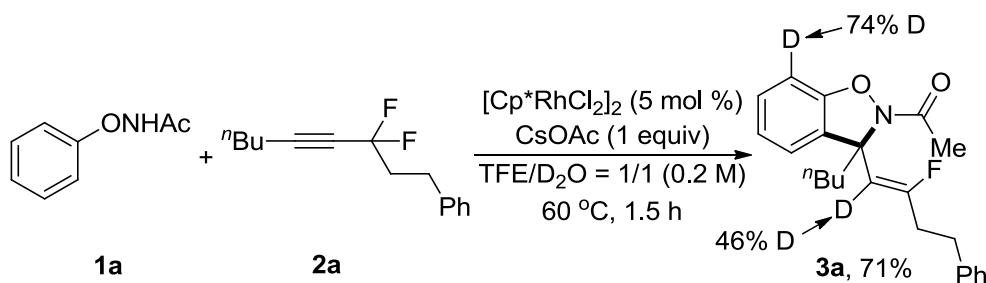
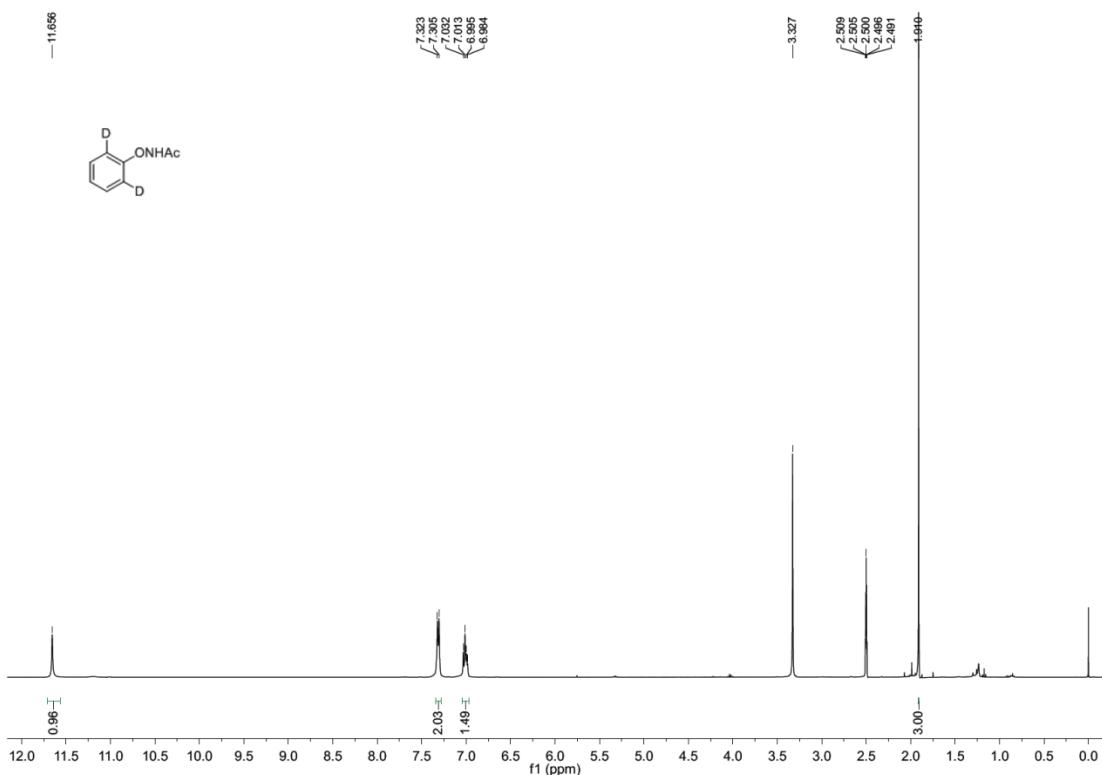
HRMS (ESI) calculated for C₂₁H₂₅FNO ([M+H]⁺): 326.1920; found: 326.1906.

III. Experimental Mechanistic Studies

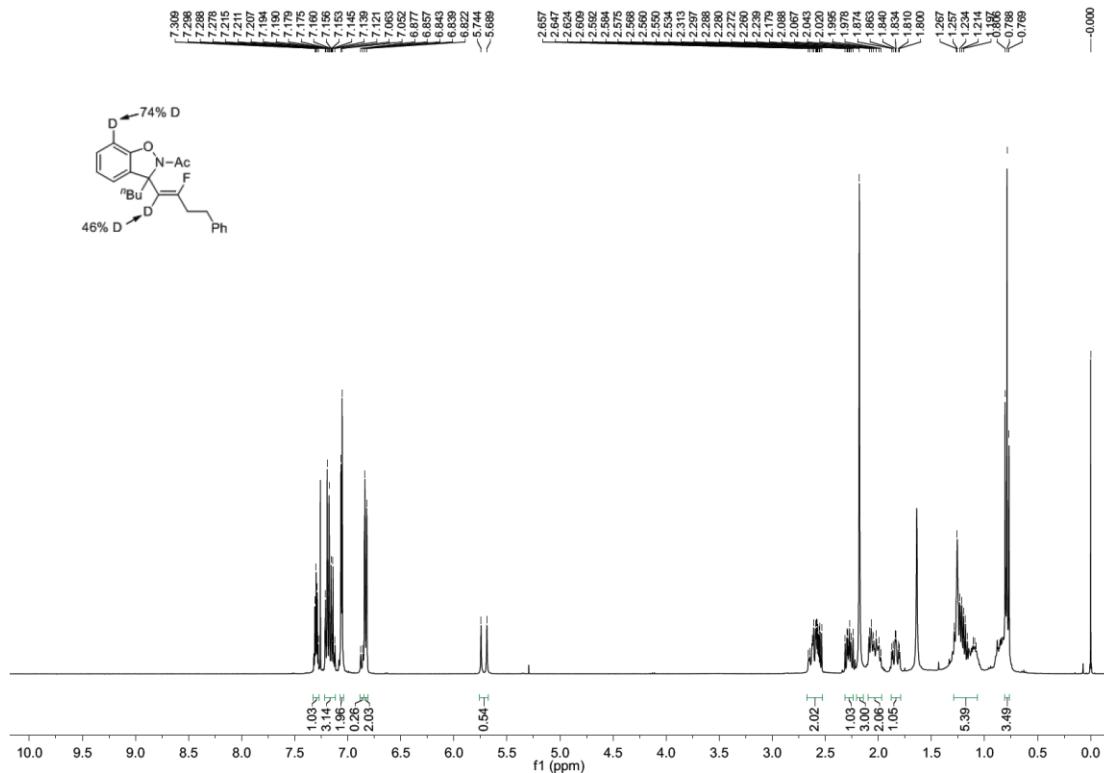
Deuterium-labeling experiment:



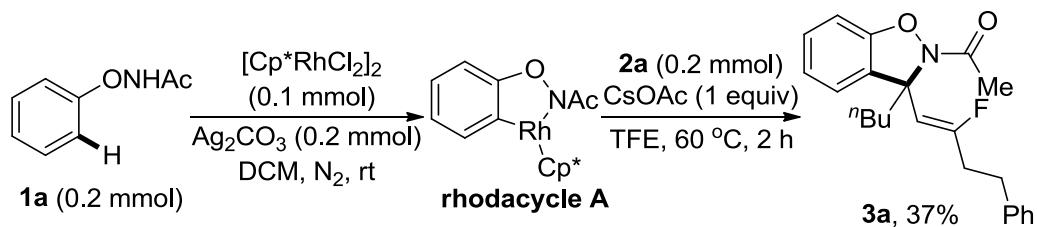
1a (0.2 mmol, 1.0 equiv) was dissolved in the mixed solvent of TFE/D₂O (1/1, 1.0 mL) in the presence of [Cp*RhCl₂]₂ (5 mol %) and CsOAc (0.2 mmol, 1 equiv). The mixture was stirred at 60 °C for 1.5 h. Afterwards, the mixture was diluted with EtOAc and transferred to a round bottom flask. Silica gel was added to the flask and volatiles were evaporated under reduced pressure. After purification by flash column chromatography, **1a** was recovered and the deuterium incorporation was analyzed by ¹H-NMR.



The mixture of *N*-phenoxyacetamide **1a** (0.2 mmol, 1.0 equiv), α,α -difluoromethylene alkyne **2a** (0.28 mmol, 1.4 equiv), $[\text{Cp}^*\text{RhCl}_2]_2$ (5 mol %) and CsOAc (0.2 mmol, 1.0 equiv) in TFE/D₂O (1/1, 1.0 mL) was stirred at 60 °C for 1.5 h without exclusion of air or moisture. Afterwards, the solvent was removed under reduce pressure, and the resulted mixture was purified by preparative TLC to afford the corresponding product **3a**. The deuterium incorporation was analyzed by ¹H-NMR.



Defining rhodacycle A as the active intermediate:



The mixture of $[\text{Cp}^*\text{RhCl}_2]_2$ (0.1 mmol, 1.0 equiv), Ag_2CO_3 (0.2 mmol, 2.0 equiv) and *N*-phenoxyacetamide **1a** (0.2 mmol, 2.0 equiv) in DCM (2.0 mL) was stirred for 12 h at room temperature. Afterwards, the filtration was conducted to remove any precipitate with celite. The solvent was removed under reduced pressure to afford the analytically pure rhodacycle complex in 85% yield. The rhodacycle complex is a known compound and all data were in agreement with those reported.^[S3]

The mixture of the above obtained rhodacycle complex, **2a** (0.2 mmol, 2.0 equiv), CsOAc (0.2 mmol, 2.0 equiv) and TFE (1.0 mL) was stirred at 60 °C for 2 h under nitrogen. Afterwards, the solvent was removed under reduced pressure, purified by preparative TLC (eluent: PE/EA = 10/1) directly to give the compound **3a** in 37% yield.

IV. DFT Studies

Computational Details:

Gaussian 09 program^{S4} has been used to perform all the theoretical calculations. Geometry optimizations and frequency analyses were calculated using the the B3LYP functional^{S5} with a standard 6-31G(d) basis set (lanl2dz basis set for Rh) in gas phase. Single point energies were further calculated at the M06 functional^{S6} with a standard 6-311++G(d,p) basis set (SDD^{S7} basis set for Rh) level using SMD solvation model^{S8} (solvent = TFE). Throughout the paper, the energies presented are the M06-calculated Gibbs free energies in a TFE solvent with B3LYP-calculated thermodynamic corrections.

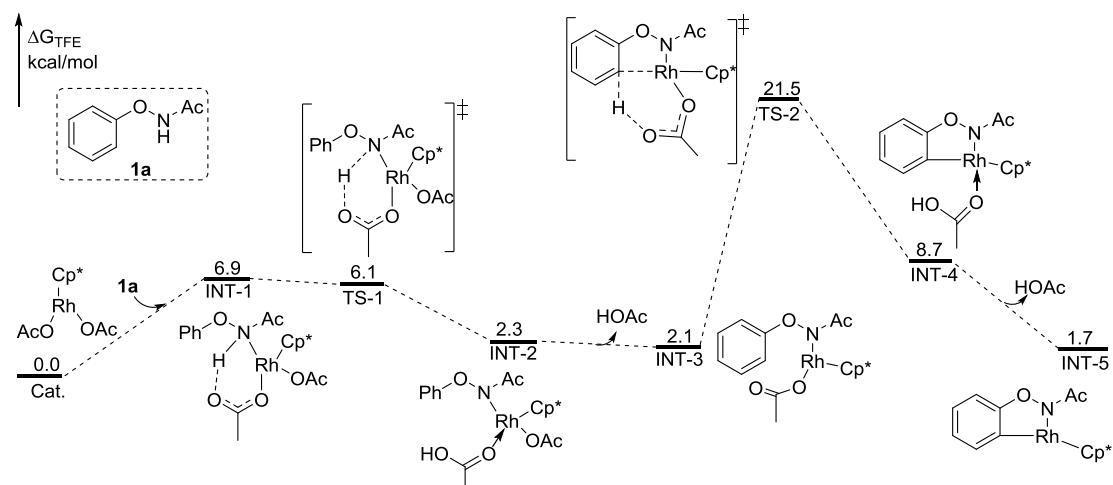


Figure S1. Free energy profiles for N-H deprotonation, C-H activation. (Some hydrogen atoms are omitted for clarity. The distances are in Å.)

Various Energy Values for All of the Relevant Species[gas phase results optimized at the level of B3LYP/6-31G(d) (lanl2dz for Rh)] as well as the single-point results with SMD atomic radii for experimental solvent TFE at the M06/6-311++G(d,p)(SDD for Rh)(SMDTFE)//B3LYP/6-31G(d)(lanl2dz for Rh).]:

N-phenoxycetamide (1a)

Zero-point correction=	0.159084 (Hartree/Particle)
Thermal correction to Energy=	0.169319
Thermal correction to Enthalpy=	0.170264

Thermal correction to Gibbs Free Energy=	0.121442
Sum of electronic and zero-point Energies=	-515.247907
Sum of electronic and thermal Energies=	-515.237672
Sum of electronic and thermal Enthalpies=	-515.236728
Sum of electronic and thermal Free Energies=	-515.285549

SCF Done: E(RM06) = -515.226843991 A.U. after 15 cycles
 NFock= 15 Conv=0.46D-08 -V/T= 2.0039
 SMD-CDS (non-electrostatic) energy (kcal/mol) = 4.49
 (included in total energy above)

a,a-difluoromethylene alkyne (2a)

Zero-point correction=	0.294413 (Hartree/Particle)
Thermal correction to Energy=	0.312121
Thermal correction to Enthalpy=	0.313065
Thermal correction to Gibbs Free Energy=	0.243173
Sum of electronic and zero-point Energies=	-781.762265
Sum of electronic and thermal Energies=	-781.744557
Sum of electronic and thermal Enthalpies=	-781.743613
Sum of electronic and thermal Free Energies=	-781.813505

SCF Done: E(RM06) = -781.767887337 A.U. after 14 cycles
 NFock= 14 Conv=0.77D-08 -V/T= 2.0042
 SMD-CDS (non-electrostatic) energy (kcal/mol) = -0.93
 (included in total energy above)

Cp*Rh(OAc)₂

Zero-point correction=	0.327107 (Hartree/Particle)
Thermal correction to Energy=	0.351405
Thermal correction to Enthalpy=	0.352349
Thermal correction to Gibbs Free Energy=	0.272878
Sum of electronic and zero-point Energies=	-956.300285
Sum of electronic and thermal Energies=	-956.275988
Sum of electronic and thermal Enthalpies=	-956.275043
Sum of electronic and thermal Free Energies=	-956.354515

SCF Done: E(RM06) = -957.389900151 A.U. after 17 cycles
 NFock= 17 Conv=0.99D-08 -V/T= 2.0831
 SMD-CDS (non-electrostatic) energy (kcal/mol) = 7.03
 (included in total energy above)

CH₃COOH

Zero-point correction=	0.062054 (Hartree/Particle)
Thermal correction to Energy=	0.066606

Thermal correction to Enthalpy=	0.067550
Thermal correction to Gibbs Free Energy=	0.034882
Sum of electronic and zero-point Energies=	-229.015555
Sum of electronic and thermal Energies=	-229.011003
Sum of electronic and thermal Enthalpies=	-229.010059
Sum of electronic and thermal Free Energies=	-229.042727

SCF Done: E(RM06) = -229.038254863 A.U. after 11 cycles
 NFock= 11 Conv=0.68D-08 -V/T= 2.0034
 SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.22
 (included in total energy above)

HF

Zero-point correction=	0.009004 (Hartree/Particle)
Thermal correction to Energy=	0.011364
Thermal correction to Enthalpy=	0.012309
Thermal correction to Gibbs Free Energy=	-0.007428
Sum of electronic and zero-point Energies=	-100.409173
Sum of electronic and thermal Energies=	-100.406813
Sum of electronic and thermal Enthalpies=	-100.405868
Sum of electronic and thermal Free Energies=	-100.425605

SCF Done: E(RM06) = -100.456497009 A.U. after 8 cycles
 NFock= 8 Conv=0.20D-08 -V/T= 2.0024
 SMD-CDS (non-electrostatic) energy (kcal/mol) = 0.64
 (included in total energy above)

3a

Zero-point correction=	0.443436 (Hartree/Particle)
Thermal correction to Energy=	0.469656
Thermal correction to Enthalpy=	0.470600
Thermal correction to Gibbs Free Energy=	0.382988
Sum of electronic and zero-point Energies=	-1196.625337
Sum of electronic and thermal Energies=	-1196.599117
Sum of electronic and thermal Enthalpies=	-1196.598173
Sum of electronic and thermal Free Energies=	-1196.685785

SCF Done: E(RM06) = -1196.58679404 A.U. after 15 cycles
 NFock= 15 Conv=0.59D-08 -V/T= 2.0042
 SMD-CDS (non-electrostatic) energy (kcal/mol) = 1.69
 (included in total energy above)

3a'

Zero-point correction=	0.443312 (Hartree/Particle)
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Thermal correction to Energy=	0.469595
Thermal correction to Enthalpy=	0.470539
Thermal correction to Gibbs Free Energy=	0.383598
Sum of electronic and zero-point Energies=	-1196.623647
Sum of electronic and thermal Energies=	-1196.597364
Sum of electronic and thermal Enthalpies=	-1196.596419
Sum of electronic and thermal Free Energies=	-1196.683361
 SCF Done: E(RM06) = -1196.58527564	A.U. after 15 cycles
NFock= 15 Conv=0.80D-08	-V/T= 2.0042
SMD-CDS (non-electrostatic) energy (kcal/mol) = 1.22	
(included in total energy above)	

3a"

Zero-point correction=	0.427015 (Hartree/Particle)
Thermal correction to Energy=	0.452540
Thermal correction to Enthalpy=	0.453484
Thermal correction to Gibbs Free Energy=	0.365994
Sum of electronic and zero-point Energies=	-1096.157656
Sum of electronic and thermal Energies=	-1096.132132
Sum of electronic and thermal Enthalpies=	-1096.131187
Sum of electronic and thermal Free Energies=	-1096.218678
 SCF Done: E(RM06) = -1096.10026872	A.U. after 16 cycles
NFock= 16 Conv=0.74D-08	-V/T= 2.0044
SMD-CDS (non-electrostatic) energy (kcal/mol) = 2.01	
(included in total energy above)	

INT-1

Zero-point correction=	0.488086 (Hartree/Particle)
Thermal correction to Energy=	0.523585
Thermal correction to Enthalpy=	0.524530
Thermal correction to Gibbs Free Energy=	0.418912
Sum of electronic and zero-point Energies=	-1471.558003
Sum of electronic and thermal Energies=	-1471.522504
Sum of electronic and thermal Enthalpies=	-1471.521560
Sum of electronic and thermal Free Energies=	-1471.627178
 SCF Done: E(RM06) = -1472.63030490	A.U. after 18 cycles
NFock= 18 Conv=0.44D-08	-V/T= 2.0540
SMD-CDS (non-electrostatic) energy (kcal/mol) = 7.42	
(included in total energy above)	

TS-1

Zero-point correction=	0.483454 (Hartree/Particle)
Thermal correction to Energy=	0.518499
Thermal correction to Enthalpy=	0.519443
Thermal correction to Gibbs Free Energy=	0.415182
Sum of electronic and zero-point Energies=	-1471.555350
Sum of electronic and thermal Energies=	-1471.520306
Sum of electronic and thermal Enthalpies=	-1471.519361
Sum of electronic and thermal Free Energies=	-1471.623622

SCF Done: E(RM06) = -1472.62789144 A.U. after 18 cycles
 NFock= 18 Conv=0.53D-08 -V/T= 2.0540
 SMD-CDS (non-electrostatic) energy (kcal/mol) = 7.30
 (included in total energy above)

INT-2

Zero-point correction=	0.486754 (Hartree/Particle)
Thermal correction to Energy=	0.522526
Thermal correction to Enthalpy=	0.523470
Thermal correction to Gibbs Free Energy=	0.416385
Sum of electronic and zero-point Energies=	-1471.553391
Sum of electronic and thermal Energies=	-1471.517619
Sum of electronic and thermal Enthalpies=	-1471.516674
Sum of electronic and thermal Free Energies=	-1471.623759

SCF Done: E(RM06) = -1472.63509515 A.U. after 18 cycles
 NFock= 18 Conv=0.56D-08 -V/T= 2.0541
 SMD-CDS (non-electrostatic) energy (kcal/mol) = 7.18
 (included in total energy above)

INT-3

Zero-point correction=	0.423858 (Hartree/Particle)
Thermal correction to Energy=	0.453637
Thermal correction to Enthalpy=	0.454581
Thermal correction to Gibbs Free Energy=	0.362958
Sum of electronic and zero-point Energies=	-1242.530592
Sum of electronic and thermal Energies=	-1242.500814
Sum of electronic and thermal Enthalpies=	-1242.499870
Sum of electronic and thermal Free Energies=	-1242.591493

SCF Done: E(RM06) = -1243.57867486 A.U. after 18 cycles
 NFock= 18 Conv=0.59D-08 -V/T= 2.0639
 SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.87
 (included in total energy above)

TS-2

Zero-point correction=	0.418543 (Hartree/Particle)
Thermal correction to Energy=	0.447872
Thermal correction to Enthalpy=	0.448817
Thermal correction to Gibbs Free Energy=	0.359252
Sum of electronic and zero-point Energies=	-1242.504292
Sum of electronic and thermal Energies=	-1242.474963
Sum of electronic and thermal Enthalpies=	-1242.474019
Sum of electronic and thermal Free Energies=	-1242.563583
SCF Done: E(RM06) = -1243.54410209	A.U. after 18 cycles
NFock= 18 Conv=0.51D-08	-V/T= 2.0639
SMD-CDS (non-electrostatic) energy (included in total energy above)	(kcal/mol) = 6.05

INT-4

Zero-point correction=	0.423183 (Hartree/Particle)
Thermal correction to Energy=	0.452797
Thermal correction to Enthalpy=	0.453741
Thermal correction to Gibbs Free Energy=	0.362978
Sum of electronic and zero-point Energies=	-1242.527259
Sum of electronic and thermal Energies=	-1242.497645
Sum of electronic and thermal Enthalpies=	-1242.496701
Sum of electronic and thermal Free Energies=	-1242.587464
SCF Done: E(RM06) = -1243.56817098	A.U. after 18 cycles
NFock= 18 Conv=0.69D-08	-V/T= 2.0639
SMD-CDS (non-electrostatic) energy (included in total energy above)	(kcal/mol) = 6.37

INT-5

Zero-point correction=	0.360841 (Hartree/Particle)
Thermal correction to Energy=	0.384584
Thermal correction to Enthalpy=	0.385529
Thermal correction to Gibbs Free Energy=	0.308860
Sum of electronic and zero-point Energies=	-1013.500253
Sum of electronic and thermal Energies=	-1013.476509
Sum of electronic and thermal Enthalpies=	-1013.475565
Sum of electronic and thermal Free Energies=	-1013.552233
SCF Done: E(RM06) = -1014.52184887	A.U. after 18 cycles
NFock= 18 Conv=0.22D-08	-V/T= 2.0786
SMD-CDS (non-electrostatic) energy (included in total energy above)	(kcal/mol) = 3.20

INT-6

Zero-point correction=	0.656707 (Hartree/Particle)
Thermal correction to Energy=	0.699504
Thermal correction to Enthalpy=	0.700448
Thermal correction to Gibbs Free Energy=	0.578789
Sum of electronic and zero-point Energies=	-1795.253810
Sum of electronic and thermal Energies=	-1795.211013
Sum of electronic and thermal Enthalpies=	-1795.210069
Sum of electronic and thermal Free Energies=	-1795.331728

SCF Done: E(RM06) = -1796.29922279 A.U. after 19 cycles
NFock= 19 Conv=0.33D-08 -V/T= 2.0450
SMD-CDS (non-electrostatic) energy (kcal/mol) = 1.03
(included in total energy above)

INT-6'

Zero-point correction=	0.717052 (Hartree/Particle)
Thermal correction to Energy=	0.764471
Thermal correction to Enthalpy=	0.765415
Thermal correction to Gibbs Free Energy=	0.633361
Sum of electronic and zero-point Energies=	-2024.278925
Sum of electronic and thermal Energies=	-2024.231506
Sum of electronic and thermal Enthalpies=	-2024.230562
Sum of electronic and thermal Free Energies=	-2024.362616

SCF Done: E(RM06) = -1796.29183672 A.U. after 18 cycles
NFock= 18 Conv=0.67D-08 -V/T= 2.0449
SMD-CDS (non-electrostatic) energy (kcal/mol) = 1.64
(included in total energy above)

TS-3

Zero-point correction=	0.656219 (Hartree/Particle)
Thermal correction to Energy=	0.698174
Thermal correction to Enthalpy=	0.699118
Thermal correction to Gibbs Free Energy=	0.580032
Sum of electronic and zero-point Energies=	-1795.238069
Sum of electronic and thermal Energies=	-1795.196115
Sum of electronic and thermal Enthalpies=	-1795.195171
Sum of electronic and thermal Free Energies=	-1795.314257

SCF Done: E(RM06) = -1796.28114907 A.U. after 18 cycles
NFock= 18 Conv=0.53D-08 -V/T= 2.0450
SMD-CDS (non-electrostatic) energy (kcal/mol) = 1.24

(included in total energy above)

TS-3'

Zero-point correction=	0.655379 (Hartree/Particle)
Thermal correction to Energy=	0.697551
Thermal correction to Enthalpy=	0.698495
Thermal correction to Gibbs Free Energy=	0.577447
Sum of electronic and zero-point Energies=	-1795.233452
Sum of electronic and thermal Energies=	-1795.191280
Sum of electronic and thermal Enthalpies=	-1795.190336
Sum of electronic and thermal Free Energies=	-1795.311383

SCF Done: E(RM06) = -1796.27536028 A.U. after 18 cycles
NFock= 18 Conv=0.69D-08 -V/T= 2.0450

SMD-CDS (non-electrostatic) energy (kcal/mol) = 1.13

(included in total energy above)

INT-7

Zero-point correction=	0.657990 (Hartree/Particle)
Thermal correction to Energy=	0.700126
Thermal correction to Enthalpy=	0.701070
Thermal correction to Gibbs Free Energy=	0.580140
Sum of electronic and zero-point Energies=	-1795.283937
Sum of electronic and thermal Energies=	-1795.241801
Sum of electronic and thermal Enthalpies=	-1795.240857
Sum of electronic and thermal Free Energies=	-1795.361787

SCF Done: E(RM06) = -1796.32643626 A.U. after 19 cycles
NFock= 19 Conv=0.43D-08 -V/T= 2.0449

SMD-CDS (non-electrostatic) energy (kcal/mol) = 1.41

(included in total energy above)

INT-7'

Zero-point correction=	0.658090 (Hartree/Particle)
Thermal correction to Energy=	0.700071
Thermal correction to Enthalpy=	0.701015
Thermal correction to Gibbs Free Energy=	0.580609
Sum of electronic and zero-point Energies=	-1795.276525
Sum of electronic and thermal Energies=	-1795.234544
Sum of electronic and thermal Enthalpies=	-1795.233600
Sum of electronic and thermal Free Energies=	-1795.354006

SCF Done: E(RM06) = -1796.32297162 A.U. after 18 cycles
NFock= 18 Conv=0.62D-08 -V/T= 2.0449

SMD-CDS (non-electrostatic) energy (kcal/mol) = 1.21
 (included in total energy above)

TS-4

Zero-point correction=	0.655353 (Hartree/Particle)
Thermal correction to Energy=	0.697620
Thermal correction to Enthalpy=	0.698564
Thermal correction to Gibbs Free Energy=	0.578041
Sum of electronic and zero-point Energies=	-1795.252152
Sum of electronic and thermal Energies=	-1795.209885
Sum of electronic and thermal Enthalpies=	-1795.208941
Sum of electronic and thermal Free Energies=	-1795.329465

SCF Done: E(RM06) = -1796.30041390 A.U. after 18 cycles
 NFock= 18 Conv=0.49D-08 -V/T= 2.0449

SMD-CDS (non-electrostatic) energy (kcal/mol) = 0.86
 (included in total energy above)

TS-4'

Zero-point correction=	0.655795 (Hartree/Particle)
Thermal correction to Energy=	0.697874
Thermal correction to Enthalpy=	0.698818
Thermal correction to Gibbs Free Energy=	0.579531
Sum of electronic and zero-point Energies=	-1795.246512
Sum of electronic and thermal Energies=	-1795.204433
Sum of electronic and thermal Enthalpies=	-1795.203489
Sum of electronic and thermal Free Energies=	-1795.322776

SCF Done: E(RM06) = -1796.29961862 A.U. after 18 cycles
 NFock= 18 Conv=0.82D-08 -V/T= 2.0449

SMD-CDS (non-electrostatic) energy (kcal/mol) = 1.10
 (included in total energy above)

TS-4''

Zero-point correction=	0.655357 (Hartree/Particle)
Thermal correction to Energy=	0.697465
Thermal correction to Enthalpy=	0.698409
Thermal correction to Gibbs Free Energy=	0.579090
Sum of electronic and zero-point Energies=	-1795.240386
Sum of electronic and thermal Energies=	-1795.198279
Sum of electronic and thermal Enthalpies=	-1795.197334
Sum of electronic and thermal Free Energies=	-1795.316654

SCF Done: E(RM06) = -1796.28114294 A.U. after 25 cycles

NFock= 25 Conv=0.37D-08 -V/T= 2.0450
 SMD-CDS (non-electrostatic) energy (kcal/mol) = 1.36
 (included in total energy above)

INT-8

Zero-point correction=	0.656909 (Hartree/Particle)
Thermal correction to Energy=	0.699162
Thermal correction to Enthalpy=	0.700106
Thermal correction to Gibbs Free Energy=	0.581689
Sum of electronic and zero-point Energies=	-1795.260197
Sum of electronic and thermal Energies=	-1795.217944
Sum of electronic and thermal Enthalpies=	-1795.217000
Sum of electronic and thermal Free Energies=	-1795.335417

SCF Done: E(RM06) = -1796.30731334 A.U. after 19 cycles
 NFock= 19 Conv=0.35D-08 -V/T= 2.0450
 SMD-CDS (non-electrostatic) energy (kcal/mol) = 0.63
 (included in total energy above)

INT-8'

Zero-point correction=	0.656773 (Hartree/Particle)
Thermal correction to Energy=	0.699335
Thermal correction to Enthalpy=	0.700279
Thermal correction to Gibbs Free Energy=	0.580242
Sum of electronic and zero-point Energies=	-1795.249568
Sum of electronic and thermal Energies=	-1795.207005
Sum of electronic and thermal Enthalpies=	-1795.206061
Sum of electronic and thermal Free Energies=	-1795.326098

SCF Done: E(RM06) = -1796.29786258 A.U. after 19 cycles
 NFock= 19 Conv=0.42D-08 -V/T= 2.0449
 SMD-CDS (non-electrostatic) energy (kcal/mol) = 1.18
 (included in total energy above)

INT-8''

Zero-point correction=	0.658839 (Hartree/Particle)
Thermal correction to Energy=	0.700677
Thermal correction to Enthalpy=	0.701621
Thermal correction to Gibbs Free Energy=	0.583752
Sum of electronic and zero-point Energies=	-1795.284768
Sum of electronic and thermal Energies=	-1795.242931
Sum of electronic and thermal Enthalpies=	-1795.241987
Sum of electronic and thermal Free Energies=	-1795.359856

SCF Done: E(RM06) = -1796.32772562 A.U. after 22 cycles
 NFock= 22 Conv=0.29D-08 -V/T= 2.0449
 SMD-CDS (non-electrostatic) energy (kcal/mol) = 0.58
 (included in total energy above)

INT-9

Zero-point correction=	0.656597 (Hartree/Particle)
Thermal correction to Energy=	0.699342
Thermal correction to Enthalpy=	0.700286
Thermal correction to Gibbs Free Energy=	0.579370
Sum of electronic and zero-point Energies=	-1795.243789
Sum of electronic and thermal Energies=	-1795.201044
Sum of electronic and thermal Enthalpies=	-1795.200099
Sum of electronic and thermal Free Energies=	-1795.321015

SCF Done: E(RM06) = -1796.30874054 A.U. after 19 cycles
 NFock= 19 Conv=0.36D-08 -V/T= 2.0450
 SMD-CDS (non-electrostatic) energy (kcal/mol) = 0.84
 (included in total energy above)

INT-9'

Zero-point correction=	0.656395 (Hartree/Particle)
Thermal correction to Energy=	0.699217
Thermal correction to Enthalpy=	0.700161
Thermal correction to Gibbs Free Energy=	0.578753
Sum of electronic and zero-point Energies=	-1795.251830
Sum of electronic and thermal Energies=	-1795.209008
Sum of electronic and thermal Enthalpies=	-1795.208064
Sum of electronic and thermal Free Energies=	-1795.329472

SCF Done: E(RM06) = -1796.31172543 A.U. after 21 cycles
 NFock= 21 Conv=0.36D-08 -V/T= 2.0450
 SMD-CDS (non-electrostatic) energy (kcal/mol) = 0.57
 (included in total energy above)

TS-5

Zero-point correction=	0.655488 (Hartree/Particle)
Thermal correction to Energy=	0.697588
Thermal correction to Enthalpy=	0.698533
Thermal correction to Gibbs Free Energy=	0.578938
Sum of electronic and zero-point Energies=	-1795.239461
Sum of electronic and thermal Energies=	-1795.197360
Sum of electronic and thermal Enthalpies=	-1795.196416
Sum of electronic and thermal Free Energies=	-1795.316011

SCF Done: E(RM06) = -1796.29812775 A.U. after 18 cycles
 NFock= 18 Conv=0.54D-08 -V/T= 2.0449
 SMD-CDS (non-electrostatic) energy (kcal/mol) = 0.92
 (included in total energy above)

TS-5'

Zero-point correction=	0.654864 (Hartree/Particle)
Thermal correction to Energy=	0.697257
Thermal correction to Enthalpy=	0.698201
Thermal correction to Gibbs Free Energy=	0.576472
Sum of electronic and zero-point Energies=	-1795.245438
Sum of electronic and thermal Energies=	-1795.203046
Sum of electronic and thermal Enthalpies=	-1795.202102
Sum of electronic and thermal Free Energies=	-1795.323830

SCF Done: E(RM06) = -1796.29626636 A.U. after 18 cycles
 NFock= 18 Conv=0.55D-08 -V/T= 2.0449
 SMD-CDS (non-electrostatic) energy (kcal/mol) = 1.04
 (included in total energy above)

INT-10

Zero-point correction=	0.658345 (Hartree/Particle)
Thermal correction to Energy=	0.700271
Thermal correction to Enthalpy=	0.701215
Thermal correction to Gibbs Free Energy=	0.581448
Sum of electronic and zero-point Energies=	-1795.269664
Sum of electronic and thermal Energies=	-1795.227738
Sum of electronic and thermal Enthalpies=	-1795.226794
Sum of electronic and thermal Free Energies=	-1795.346561

SCF Done: E(RM06) = -1796.32448802 A.U. after 18 cycles
 NFock= 18 Conv=0.50D-08 -V/T= 2.0449
 SMD-CDS (non-electrostatic) energy (kcal/mol) = 1.15
 (included in total energy above)

INT-10'

Zero-point correction=	0.658215 (Hartree/Particle)
Thermal correction to Energy=	0.700280
Thermal correction to Enthalpy=	0.701224
Thermal correction to Gibbs Free Energy=	0.581244
Sum of electronic and zero-point Energies=	-1795.270477
Sum of electronic and thermal Energies=	-1795.228411
Sum of electronic and thermal Enthalpies=	-1795.227467

Sum of electronic and thermal Free Energies= -1795.347447
 SCF Done: E(RM06) = -1796.32059776 A.U. after 21 cycles
 NFock= 21 Conv=0.42D-08 -V/T= 2.0449
 SMD-CDS (non-electrostatic) energy (kcal/mol) = 1.20
 (included in total energy above)

INT-11

Zero-point correction=	0.721371 (Hartree/Particle)
Thermal correction to Energy=	0.768976
Thermal correction to Enthalpy=	0.769920
Thermal correction to Gibbs Free Energy=	0.637412
Sum of electronic and zero-point Energies=	-2024.314794
Sum of electronic and thermal Energies=	-2024.267189
Sum of electronic and thermal Enthalpies=	-2024.266245
Sum of electronic and thermal Free Energies=	-2024.398752
SCF Done: E(RM06) = -2025.38037726 A.U. after 21 cycles	
NFock= 21 Conv=0.40D-08 -V/T= 2.0401	
SMD-CDS (non-electrostatic) energy (kcal/mol) = 3.79	
(included in total energy above)	

INT-11'

Zero-point correction=	0.722247 (Hartree/Particle)
Thermal correction to Energy=	0.769376
Thermal correction to Enthalpy=	0.770321
Thermal correction to Gibbs Free Energy=	0.639797
Sum of electronic and zero-point Energies=	-2024.318689
Sum of electronic and thermal Energies=	-2024.271559
Sum of electronic and thermal Enthalpies=	-2024.270615
Sum of electronic and thermal Free Energies=	-2024.401138

SCF Done: E(RM06) = -2025.38307775 A.U. after 18 cycles
 NFock= 18 Conv=0.65D-08 -V/T= 2.0401
 SMD-CDS (non-electrostatic) energy (kcal/mol) = 2.75
 (included in total energy above)

INT-11''

Zero-point correction=	0.656343 (Hartree/Particle)
Thermal correction to Energy=	0.699328
Thermal correction to Enthalpy=	0.700272
Thermal correction to Gibbs Free Energy=	0.578394
Sum of electronic and zero-point Energies=	-1795.253377
Sum of electronic and thermal Energies=	-1795.210392

Sum of electronic and thermal Enthalpies=	-1795.209448
Sum of electronic and thermal Free Energies=	-1795.331326
SCF Done: E(RM06) = -1796.31490977	A.U. after 18 cycles
NFock= 18 Conv=0.51D-08	-V/T= 2.0449
SMD-CDS (non-electrostatic) energy (included in total energy above)	(kcal/mol) = 1.18

TS-6

Zero-point correction=	0.716876 (Hartree/Particle)
Thermal correction to Energy=	0.764325
Thermal correction to Enthalpy=	0.765270
Thermal correction to Gibbs Free Energy=	0.633480
Sum of electronic and zero-point Energies=	-2024.281482
Sum of electronic and thermal Energies=	-2024.234033
Sum of electronic and thermal Enthalpies=	-2024.233089
Sum of electronic and thermal Free Energies=	-2024.364878
SCF Done: E(RM06) = -2025.35398684	A.U. after 18 cycles
NFock= 18 Conv=0.70D-08	-V/T= 2.0401
SMD-CDS (non-electrostatic) energy (included in total energy above)	(kcal/mol) = 3.26

TS-6'

Zero-point correction=	0.717052 (Hartree/Particle)
Thermal correction to Energy=	0.764471
Thermal correction to Enthalpy=	0.765415
Thermal correction to Gibbs Free Energy=	0.633361
Sum of electronic and zero-point Energies=	-2024.278925
Sum of electronic and thermal Energies=	-2024.231506
Sum of electronic and thermal Enthalpies=	-2024.230562
Sum of electronic and thermal Free Energies=	-2024.362616
SCF Done: E(RM06) = -2025.35054927	A.U. after 19 cycles
NFock= 19 Conv=0.27D-08	-V/T= 2.0401
SMD-CDS (non-electrostatic) energy (included in total energy above)	(kcal/mol) = 3.58

TS-6''

Zero-point correction=	0.655319 (Hartree/Particle)
Thermal correction to Energy=	0.697787
Thermal correction to Enthalpy=	0.698731
Thermal correction to Gibbs Free Energy=	0.575786
Sum of electronic and zero-point Energies=	-1795.227593

Sum of electronic and thermal Energies=	-1795.185125
Sum of electronic and thermal Enthalpies=	-1795.184181
Sum of electronic and thermal Free Energies=	-1795.307126
 SCF Done: E(RM06) = -1796.29183672	A.U. after 18 cycles
NFock= 18 Conv=0.67D-08	-V/T= 2.0449
SMD-CDS (non-electrostatic) energy (included in total energy above)	(kcal/mol) = 1.64

Cp***RhF**₂

Zero-point correction=	0.227106 (Hartree/Particle)
Thermal correction to Energy=	0.244163
Thermal correction to Enthalpy=	0.245107
Thermal correction to Gibbs Free Energy=	0.180876
Sum of electronic and zero-point Energies=	-699.081416
Sum of electronic and thermal Energies=	-699.064358
Sum of electronic and thermal Enthalpies=	-699.063414
Sum of electronic and thermal Free Energies=	-699.127645
 SCF Done: E(RM06) = -700.207371817	A.U. after 22 cycles
NFock= 22 Conv=0.64D-08	-V/T= 2.1152
SMD-CDS (non-electrostatic) energy (included in total energy above)	(kcal/mol) = 0.60

Cp***RhF(OAc)**

Zero-point correction=	0.277497 (Hartree/Particle)
Thermal correction to Energy=	0.297774
Thermal correction to Enthalpy=	0.298718
Thermal correction to Gibbs Free Energy=	0.229062
Sum of electronic and zero-point Energies=	-827.698008
Sum of electronic and thermal Energies=	-827.677732
Sum of electronic and thermal Enthalpies=	-827.676787
Sum of electronic and thermal Free Energies=	-827.746444
 SCF Done: E(RM06) = -828.798209910	A.U. after 17 cycles
NFock= 17 Conv=0.93D-08	-V/T= 2.0964
SMD-CDS (non-electrostatic) energy (included in total energy above)	(kcal/mol) = 4.34

Cartesian Coordinates for All of the Species [gas phase results optimized at the level of B3LYP/6-31G(d) (lanl2dz for Rh)]:

N-phenoxyacetamide (**1a**)

C	2.23935900	1.48982600	-0.07974900
C	0.95228000	1.02185400	0.20030300
C	0.74041700	-0.35259000	0.28436400
C	1.78873900	-1.25646900	0.09198300
C	3.06469200	-0.77251500	-0.18601100
C	3.29848000	0.60325200	-0.27290100
H	2.40704400	2.56149300	-0.14813800
H	0.12808300	1.70897800	0.34713400
H	1.58632900	-2.32074000	0.15901800
H	3.87908800	-1.47586300	-0.33738900
H	4.29433300	0.97742600	-0.49150600
O	-0.48176900	-0.94764800	0.57075500
N	-1.53803600	-0.04693500	0.74610700
H	-1.88010200	-0.12321300	1.69934400
C	-2.48947100	-0.03263900	-0.27804100
O	-2.26096700	-0.43186000	-1.39896600
C	-3.80576500	0.59867100	0.15091800
H	-3.74547400	1.12888200	1.10675200
H	-4.12610900	1.29662600	-0.62635600
H	-4.56742900	-0.18532200	0.22888400

α,α -difluoromethylene alkyne (2a)

C	0.80712600	1.40408800	-1.47012900
C	0.26976600	2.31785500	-0.88862300
C	1.48976900	0.29704000	-2.14507100
C	2.74502100	-0.21061400	-1.44380400
H	3.09344200	-1.07837300	-2.01573200
H	2.45778300	-0.56685800	-0.44858400
C	3.85969300	0.84637300	-1.34065300
H	4.09974500	1.19899500	-2.34973400
H	3.48041400	1.71098000	-0.78279800
C	5.10346700	0.30300300	-0.66896400
C	5.25346300	0.36607500	0.72316600
C	6.11869700	-0.30367300	-1.42101200
C	6.38363000	-0.16342300	1.34806200
H	4.47848000	0.84004700	1.32234500
C	7.25097000	-0.83478900	-0.80116300
H	6.02228500	-0.35520800	-2.50360600
C	7.38674400	-0.76689800	0.58687200
H	6.48267000	-0.10043400	2.42872500
H	8.02889300	-1.29748100	-1.40306000
H	8.26902600	-1.17691600	1.07103800
F	0.61398300	-0.75841800	-2.28226100
F	1.82334700	0.68539900	-3.42766400

C	-0.41592000	3.41915700	-0.21361200
C	-1.82926000	3.68975200	-0.77424700
H	0.19348200	4.32993900	-0.29997000
H	-0.48338700	3.19940900	0.86135800
C	-2.53185600	4.84739100	-0.05492800
H	-1.75154800	3.90757000	-1.84706300
H	-2.42926700	2.77503400	-0.68595900
C	-3.93565700	5.12426700	-0.60309600
H	-2.59496000	4.62298500	1.01945500
H	-1.91811500	5.75533400	-0.14189200
H	-4.41333300	5.95484600	-0.07148000
H	-3.90094700	5.38512200	-1.66780500
H	-4.58246700	4.24473600	-0.49853100

Cp*Rh(OAc)₂

Rh	0.01248800	0.21555500	-0.09519100
C	1.26170300	-1.13344500	1.09663400
C	1.16844900	-1.67569900	-0.23078900
C	1.68335100	-0.69688400	-1.14902200
C	2.19283200	0.42736000	-0.36743500
C	1.93160300	0.16024700	1.00539000
C	-1.29942700	2.38848200	0.06421100
O	-0.69392600	2.08523200	-1.01283500
O	-1.13753700	1.65261200	1.09081800
C	-2.22697300	3.57520200	0.11408000
H	-3.23131100	3.24794700	-0.17942200
H	-2.28000300	3.97786000	1.12844000
H	-1.90013200	4.34595000	-0.58824700
O	-1.85433900	-0.44084600	-0.68700800
C	-2.48254400	-1.36823700	-0.01835800
O	-2.03490600	-2.02907800	0.92177700
C	-3.91401300	-1.57301400	-0.51196000
H	-4.53458900	-0.73561900	-0.17215200
H	-3.95192100	-1.58564400	-1.60533500
H	-4.31974900	-2.50249300	-0.10677300
C	2.84993100	1.64067000	-0.95245100
H	3.86510800	1.39894400	-1.29409300
H	2.28677200	2.01816100	-1.81132200
H	2.92434500	2.45076600	-0.22320700
C	2.25233700	1.03540800	2.17903300
H	3.08396700	0.61081100	2.75632000
H	2.53878900	2.04232800	1.86633700
H	1.39084100	1.12589800	2.84741900
C	1.80614000	-0.83890600	-2.63584000

H	1.70332500	0.12819900	-3.13648800
H	2.78769500	-1.25299200	-2.90542900
H	1.03883900	-1.50519700	-3.03794700
C	0.62317400	-3.02586500	-0.57979000
H	0.32149900	-3.07784300	-1.62916100
H	1.39618100	-3.78916900	-0.41492200
H	-0.24545300	-3.26021300	0.03846400
C	0.84145200	-1.82657400	2.35575200
H	-0.16307300	-2.23897900	2.23131000
H	1.53920700	-2.63981300	2.59892700
H	0.82527900	-1.13471400	3.20213700

CH₃COOH

C	-0.09247900	0.12588400	-0.00051300
O	-0.64583400	1.20200500	0.00013000
O	-0.77834800	-1.04695000	0.00005600
H	-1.72324000	-0.80312200	0.00038200
C	1.39740000	-0.10970100	0.00007600
H	1.68462900	-0.69081700	0.88265800
H	1.68510500	-0.69207000	-0.88150500
H	1.91743000	0.84846800	-0.00039900

HF

F	0.00000000	0.00000000	0.09347700
H	0.00000000	0.00000000	-0.84129300

3a

N	-1.82967300	-1.34507700	0.97406900
C	-3.44842300	-1.54255600	-0.53682600
C	-2.66594900	-0.47665700	-0.97035900
C	-4.49923500	-2.06366100	-1.28134500
C	-2.90952100	0.08633800	-2.21837500
C	-4.74748000	-1.47334700	-2.52539200
H	-5.08789900	-2.89675500	-0.91238000
C	-3.96057500	-0.41731100	-2.99589400
H	-2.29036700	0.89857400	-2.58711900
H	-5.55907900	-1.85512500	-3.13846600
H	-4.16263500	0.01398000	-3.97171300
C	-0.23424000	-0.16098400	-0.44152600
C	-1.64667800	-0.12964300	0.10988300
C	0.83807200	0.54985600	-0.08979600
C	2.23274600	0.38612100	-0.60698800
H	2.56958500	1.33289900	-1.05149300
H	2.24004400	-0.36520300	-1.40329100

C	3.22448700	-0.01981300	0.51459400
H	3.19054500	0.74278600	1.29999100
H	2.87461800	-0.95430600	0.96830800
C	4.63759200	-0.17917300	-0.00196000
C	5.09762600	-1.41926800	-0.46601300
C	5.50845000	0.91791000	-0.06174600
C	6.38885200	-1.56087100	-0.97700300
H	4.43851400	-2.28383000	-0.41878700
C	6.80030400	0.78207900	-0.57230400
H	5.17187000	1.88647500	0.30263500
C	7.24476700	-0.45906600	-1.03288300
H	6.72780700	-2.53276800	-1.32655000
H	7.46152700	1.64426300	-0.60500900
H	8.25164700	-0.56779300	-1.42708600
F	0.76739100	1.53373300	0.84147600
C	-2.05951800	1.13873500	0.90954500
C	-2.07885300	2.45555400	0.12316900
H	-1.38849100	1.22356200	1.76658900
H	-3.06612500	0.94298500	1.30217500
C	-2.43716200	3.65221700	1.01681300
H	-1.09915800	2.63552800	-0.33459600
H	-2.80656700	2.39220300	-0.69655600
C	-2.48919800	4.97784000	0.25012300
H	-3.40827300	3.46926700	1.49853100
H	-1.70136600	3.72598100	1.82926300
H	-2.74229900	5.81323000	0.91301500
H	-1.52209500	5.20386000	-0.21595900
H	-3.24163000	4.94602300	-0.54781700
O	-3.07101600	-2.02271800	0.68977400
C	-1.25909300	-1.60562300	2.19547700
O	-0.31032100	-0.93788900	2.59127400
C	-1.84657300	-2.77405000	2.96400900
H	-2.87494300	-2.55545300	3.27205800
H	-1.87776600	-3.68067900	2.35174500
H	-1.22622200	-2.93738900	3.84639100
H	-0.06174600	-0.93327100	-1.18525200

3a'

N	-1.43738900	-0.20248200	1.25060900
C	-3.55070700	-0.64449600	0.71033400
C	-2.88354800	-0.51284100	-0.50087400
C	-4.91690900	-0.88495400	0.79989100
C	-3.59113200	-0.63414700	-1.69156400
C	-5.61957600	-0.99529800	-0.40409900

H	-5.40679800	-0.98231400	1.76273300
C	-4.96973000	-0.87198500	-1.63740100
H	-3.08194600	-0.54967200	-2.64774700
H	-6.68944200	-1.18149000	-0.37570400
H	-5.53703600	-0.96476700	-2.55848500
C	-0.64995300	-1.54762800	-0.70737700
C	-1.39562800	-0.29618000	-0.25004600
C	0.62925400	-1.76366500	-1.03426600
C	1.86823200	-0.92954500	-1.05906000
H	1.64888300	0.08722300	-0.74376000
H	2.24864900	-0.89045600	-2.08945000
C	2.96943700	-1.51426400	-0.13515900
H	2.53998900	-1.62973900	0.86492700
H	3.24813400	-2.50961700	-0.49603600
C	4.18480600	-0.61545600	-0.06936700
C	5.30308600	-0.84415900	-0.88136200
C	4.19804400	0.48975600	0.79540200
C	6.40943800	0.00704600	-0.83450700
H	5.30976000	-1.70109300	-1.55222200
C	5.30216400	1.34147400	0.84448100
H	3.33413200	0.67205100	1.43056100
C	6.41187700	1.10355900	0.02925100
H	7.27001100	-0.18951900	-1.46917400
H	5.29866000	2.19036300	1.52386800
H	7.27305700	1.76553300	0.07013200
F	0.92216600	-3.04422400	-1.41286500
C	-0.88689300	1.04139000	-0.84984800
C	-1.74613200	2.27207300	-0.53242200
H	-0.81572300	0.90339200	-1.93664700
H	0.12426500	1.21879500	-0.48038500
C	-1.13108900	3.56659000	-1.08359800
H	-2.75556600	2.14669400	-0.94443000
H	-1.86455600	2.36363100	0.55576400
C	-1.97715800	4.80701700	-0.77776900
H	-0.12342200	3.69766000	-0.66513000
H	-0.99910400	3.47307400	-2.17111600
H	-1.51493100	5.71487400	-1.18181900
H	-2.98013800	4.72067100	-1.21371500
H	-2.09779800	4.94714500	0.30351300
O	-2.72594700	-0.52757800	1.79844800
C	-0.39546900	-0.14349000	2.12960200
O	0.74604300	0.06167500	1.71869100
C	-0.74159100	-0.30893800	3.59552800
H	-1.49127700	0.42327000	3.91179300

H	-1.15954000	-1.30341300	3.78522400
H	0.17515200	-0.17665900	4.17169000
H	-1.27689300	-2.43417700	-0.76459000

3a"

N	-1.98460900	-0.05365100	-1.34244300
C	-2.90807400	1.77332200	-0.45404400
C	-2.31228400	1.11230000	0.61315300
C	-3.67263700	2.92336000	-0.29470700
C	-2.46337900	1.60375100	1.90377100
C	-3.82451400	3.40635700	1.00900200
H	-4.12754600	3.41621400	-1.14718100
C	-3.23171600	2.75768600	2.09833600
H	-1.98845800	1.10617500	2.74471500
H	-4.41718500	4.30177000	1.17406300
H	-3.36527500	3.15351500	3.10053300
C	-0.06594800	0.19299800	0.18865200
C	-1.51270000	-0.07192000	0.08165600
C	1.11516300	0.42408900	0.31310900
C	2.55572500	0.65112300	0.42464800
H	2.80445200	0.98443100	1.44143500
H	2.85512900	1.47062800	-0.24269400
C	3.39037800	-0.61357200	0.08343900
H	3.09639500	-1.41900900	0.76601100
H	3.12331200	-0.94320800	-0.92662800
C	4.87821800	-0.35641100	0.18176800
C	5.60363700	0.09597700	-0.92923200
C	5.55867900	-0.52860400	1.39531200
C	6.96876300	0.37031300	-0.83190800
H	5.09368400	0.22695700	-1.88149600
C	6.92364400	-0.25577200	1.49821900
H	5.01360100	-0.88735400	2.26621000
C	7.63341400	0.19593700	0.38369600
H	7.51406900	0.71508100	-1.70675700
H	7.43361900	-0.40097600	2.44714600
H	8.69701100	0.40537600	0.46058800
C	-1.85390700	-1.43176200	0.75126800
C	-3.33061600	-1.83553400	0.69901500
H	-1.51792600	-1.36041800	1.79434800
H	-1.23308600	-2.19072400	0.26629300
C	-3.58754500	-3.18624000	1.38247300
H	-3.94813300	-1.06292300	1.17688000
H	-3.65635300	-1.88973900	-0.34751800
C	-5.05875900	-3.61161900	1.32993100

H	-2.96554800	-3.95727000	0.90685900
H	-3.25923400	-3.13371300	2.43053900
H	-5.21321500	-4.57763200	1.82419600
H	-5.70261200	-2.87549600	1.82710800
H	-5.40584200	-3.70779600	0.29382000
O	-2.65653700	1.18472100	-1.66369900
C	-1.35462300	-0.67997500	-2.39904600
O	-0.61148700	-1.62778700	-2.18570100
C	-1.69552600	-0.16210700	-3.78099200
H	-2.77783200	-0.13874700	-3.94207100
H	-1.32726900	0.86183700	-3.90755700
H	-1.22166200	-0.81906000	-4.51164400

INT-1

C	3.00090700	0.71246300	-0.66038900
C	2.22791100	0.32488300	-1.82568500
C	1.78829700	-1.02104100	-1.63472600
C	2.36954500	-1.51536600	-0.38521400
C	3.11385500	-0.45420900	0.19831800
C	2.28233000	-2.93215800	0.09546400
H	2.52650900	-3.01676200	1.15769900
H	1.28867800	-3.36042000	-0.05977500
H	2.99917500	-3.55326200	-0.45922300
C	3.84715000	-0.46623500	1.50455200
H	3.78354000	-1.43983100	1.99653300
H	4.90732000	-0.23144700	1.35178800
H	3.42365300	0.28597000	2.17961800
C	3.72930500	2.00647600	-0.47120600
H	4.03383500	2.13451000	0.57107800
H	4.63558600	2.02564300	-1.09324000
H	3.08264600	2.84303900	-0.74164100
C	1.95545600	1.20159800	-3.00800800
H	1.79455900	2.23349300	-2.68942000
H	2.81456300	1.17264700	-3.69279200
H	1.07445400	0.86742100	-3.56182100
C	0.96677200	-1.85233900	-2.57313100
H	1.61238600	-2.54069800	-3.13575900
H	0.22684900	-2.44708700	-2.02976400
H	0.43076600	-1.22861200	-3.29200500
Rh	0.99133200	0.22141200	0.01604000
C	-0.14603000	2.93020600	-0.68697200
O	0.96856400	3.43106400	-0.84864000
O	-0.41225100	1.68186400	-0.42424700
C	-0.08499200	1.34282600	2.65957600

O	-1.25889600	0.99497900	2.42254600
O	0.96648400	0.98220800	1.99837900
C	0.20244300	2.27576800	3.82790600
H	1.09351600	1.95054800	4.37276300
H	0.40530700	3.27946300	3.43619900
H	-0.65803500	2.32257200	4.49844000
C	-1.41648500	3.77345700	-0.78923500
H	-2.07841200	3.36644200	-1.56102400
H	-1.96263400	3.73168900	0.15904900
H	-1.16123000	4.80809000	-1.02732600
C	-5.22584600	-0.53096700	0.35510500
C	-3.82948800	-0.48270600	0.41696100
C	-3.09469200	-0.87663400	-0.70209200
C	-3.73486500	-1.30444300	-1.86845300
C	-5.12607200	-1.33693700	-1.91420000
C	-5.88024600	-0.95431100	-0.80079900
H	-5.79993700	-0.22321000	1.22490000
H	-3.34455900	-0.12054500	1.31661300
H	-3.13168600	-1.61052100	-2.71720100
H	-5.62167300	-1.67214500	-2.82136700
H	-6.96526500	-0.98602100	-0.83629800
O	-1.70704900	-0.83406800	-0.79187300
N	-1.01981500	-0.81030500	0.43710700
H	-1.31364500	-0.03518500	1.08947400
C	-0.90497800	-2.10582100	1.02942100
O	-1.06588400	-3.11552600	0.37532000
C	-0.53049500	-2.08764500	2.49530600
H	0.36888900	-1.48996700	2.66940800
H	-1.33432000	-1.62888900	3.08051700
H	-0.37368100	-3.11742500	2.82035400

TS-1

C	2.99004300	0.66106100	-0.68733400
C	2.18525400	0.25279700	-1.81164700
C	1.73722000	-1.09311600	-1.57708100
C	2.36137300	-1.56402700	-0.34392100
C	3.10397100	-0.48117700	0.20412100
C	2.31436400	-2.97656200	0.15305800
H	2.60832700	-3.04916200	1.20345300
H	1.32159800	-3.42154400	0.04474500
H	3.01669100	-3.58925100	-0.42899000
C	3.87804500	-0.47251000	1.48714700
H	3.70683900	-1.38027500	2.07054900
H	4.95387400	-0.39845400	1.28364600

H	3.59302400	0.38622200	2.10351200
C	3.72086000	1.96059400	-0.54483100
H	4.06274700	2.10829300	0.48332600
H	4.60520900	1.97421000	-1.19744500
H	3.06264600	2.79118000	-0.80645200
C	1.88243600	1.09451100	-3.01143400
H	1.76382100	2.14175400	-2.72738800
H	2.70857400	1.01392900	-3.73181000
H	0.96898900	0.76450900	-3.51243900
C	0.90362700	-1.94408000	-2.48626900
H	1.54642300	-2.61746800	-3.07019600
H	0.19454600	-2.55188300	-1.91725400
H	0.32933600	-1.33334800	-3.18639900
Rh	0.96518000	0.17217900	0.03795700
C	-0.19760700	2.82912600	-0.77463100
O	0.91878900	3.34139000	-0.87869800
O	-0.46575800	1.58779900	-0.48002700
C	-0.18923100	1.41025400	2.57782600
O	-1.33081300	0.89522400	2.30211700
O	0.88984200	1.13061800	1.98753200
C	-0.15796600	2.43431400	3.68786700
H	0.83768200	2.48761000	4.13243000
H	-0.39497400	3.41503900	3.25822000
H	-0.91121100	2.20396500	4.44475600
C	-1.46869700	3.64680700	-1.00554200
H	-2.03459500	3.22803700	-1.84468700
H	-2.11603600	3.59081200	-0.12428800
H	-1.21151600	4.68693500	-1.21624100
C	-5.15153900	-0.71088600	0.48284100
C	-3.76007200	-0.81513300	0.56957900
C	-3.00507600	-0.84503300	-0.60454500
C	-3.63738400	-0.77629300	-1.85298500
C	-5.02356200	-0.67806600	-1.92130400
C	-5.79220400	-0.64308900	-0.75314200
H	-5.73387700	-0.68550700	1.40032900
H	-3.28207900	-0.86525100	1.53996600
H	-3.02679100	-0.80237600	-2.75020400
H	-5.50583000	-0.62555200	-2.89404600
H	-6.87400900	-0.56395100	-0.80869700
O	-1.63397600	-0.95537000	-0.66692100
N	-0.94422200	-0.87663500	0.57534900
H	-1.24391600	0.10865700	1.43910200
C	-0.75165800	-2.16083900	1.11356100
O	-1.00782700	-3.19705700	0.52061300

C	-0.22443500	-2.14948000	2.54201900
H	0.50448500	-1.35576700	2.72169800
H	-1.06440700	-1.99458200	3.23002100
H	0.21837300	-3.12410400	2.75641900

INT-2

C	2.97907200	0.62722500	-0.60304100
C	2.19616000	0.36116000	-1.76673100
C	1.68430400	-0.99082400	-1.66871700
C	2.27944600	-1.60320200	-0.48821300
C	3.02842500	-0.60002800	0.18765700
C	2.15773500	-3.05198500	-0.12890900
H	2.52424300	-3.25325600	0.88085100
H	1.12640600	-3.41190800	-0.18925700
H	2.76138400	-3.64943400	-0.82570100
C	3.78784500	-0.74743800	1.47142500
H	3.51647800	-1.66479800	1.99926900
H	4.86803700	-0.77607100	1.27711900
H	3.59240900	0.09721400	2.13947400
C	3.68411000	1.91182200	-0.28965900
H	4.01414500	1.93713000	0.75222600
H	4.57173500	2.03204400	-0.92566800
H	3.00891200	2.75603700	-0.45158800
C	1.93598100	1.32200400	-2.88410100
H	1.87813700	2.34628300	-2.51165500
H	2.74916100	1.25764700	-3.62045300
H	1.00016700	1.09068000	-3.39890900
C	0.86981000	-1.71977600	-2.69328500
H	1.52295700	-2.29813200	-3.36173000
H	0.16555800	-2.40618900	-2.21697200
H	0.28980600	-1.02537400	-3.30590400
Rh	0.90921400	0.11324400	0.02928200
C	-0.35256500	2.70489500	-0.71891000
O	0.73004700	3.27374700	-0.55530500
O	-0.58786800	1.42888500	-0.58135000
C	-0.17668900	1.60559300	2.50945800
O	-1.36255200	1.11288100	2.27284400
O	0.86624700	1.21718000	1.95272400
C	-0.13842800	2.72638400	3.51269700
H	0.82163300	2.73055000	4.03234600
H	-0.23215100	3.67255000	2.96625200
H	-0.96598600	2.64853500	4.22057600
C	-1.60578300	3.48125300	-1.12157900
H	-1.99044800	3.10348900	-2.07494500

H	-2.39445800	3.32969500	-0.37728300
H	-1.37560100	4.54496500	-1.21140000
C	-5.06873600	-0.73878400	0.49211400
C	-3.68965400	-0.93067300	0.61152400
C	-2.91180800	-1.04476200	-0.54366800
C	-3.51577500	-0.97946100	-1.80671200
C	-4.89178400	-0.79821200	-1.90863000
C	-5.67939900	-0.67210200	-0.75966100
H	-5.66744200	-0.64977800	1.39517200
H	-3.23263200	-0.99837400	1.59105600
H	-2.89085000	-1.07133500	-2.68970800
H	-5.35069700	-0.74851800	-2.89291300
H	-6.75264100	-0.52614100	-0.84159700
O	-1.55650600	-1.26120700	-0.56035000
N	-0.86994400	-0.99356100	0.66715000
H	-1.29634800	0.35799500	1.57514400
C	-0.65841700	-2.19299600	1.35069500
O	-1.01186300	-3.29527400	0.95450700
C	-0.00493400	-2.01618100	2.71779200
H	0.59592900	-1.10907100	2.80493000
H	-0.79414800	-1.98404600	3.47896900
H	0.61253200	-2.89419900	2.92415900

INT-3

C	2.86230900	6.59716700	-2.22986000
C	1.44913100	6.31921700	-2.48449100
C	1.08727200	5.15028400	-1.72669800
C	2.21134900	4.78612100	-0.91355200
C	3.32513000	5.66691900	-1.26584700
C	2.27495900	3.62458600	0.02978400
H	3.13269200	3.70958600	0.70257500
H	1.36795000	3.58917000	0.63800500
H	2.37563500	2.68186500	-0.52618900
C	4.69285800	5.58146900	-0.65902300
H	4.63481800	5.56637900	0.43394700
H	5.19904600	4.66256800	-0.98194400
H	5.31776400	6.42992400	-0.94781200
C	3.62829600	7.71705300	-2.86692700
H	4.62300500	7.82758000	-2.42883500
H	3.75079400	7.53404700	-3.94229000
H	3.10318300	8.66993100	-2.74436200
C	0.59965400	7.03327500	-3.49186100
H	0.86163300	8.09372700	-3.54871000
H	0.73590700	6.59974400	-4.49258000

H	-0.46118200	6.96639200	-3.23741300
C	-0.21662100	4.41816600	-1.78859900
H	-0.12015200	3.55736400	-2.46457700
H	-0.50679700	4.05563400	-0.80015300
H	-1.01785600	5.05469000	-2.17360300
Rh	1.63505400	6.84556200	-0.38591800
C	2.51276800	8.76882100	1.05208800
O	2.62304800	7.57250300	1.46468400
O	1.97475700	8.98136700	-0.08581100
C	2.98294000	9.92838200	1.89134000
H	3.49151900	10.66527500	1.26293100
H	2.10892600	10.41488200	2.33783800
H	3.64744600	9.58272200	2.68607400
C	-0.79041100	10.37662500	3.07041700
C	-0.62077400	9.22302400	2.29846500
C	-1.07844500	9.21533200	0.97758400
C	-1.69934500	10.34800200	0.43591300
C	-1.86135600	11.48756600	1.21954200
C	-1.40804300	11.51141700	2.54250700
H	-0.43832800	10.37808800	4.09932600
H	-0.13119800	8.34436500	2.70135400
H	-2.04619900	10.31482600	-0.59253000
H	-2.34293700	12.36352100	0.79231900
H	-1.53693100	12.40151900	3.15165400
O	-1.01463700	8.12437400	0.13859000
N	-0.19497200	7.04730300	0.59295900
C	-0.90924900	5.99939800	1.09096300
O	-0.36095800	4.91682200	1.34339500
C	-2.39655800	6.20190100	1.35771300
H	-2.57940600	7.05586600	2.01717900
H	-2.93674400	6.39329300	0.42411800
H	-2.77751600	5.29142600	1.82362400

TS-2

C	2.17666300	7.47696900	-2.09987500
C	0.82277500	6.95757900	-2.22828000
C	0.81237000	5.62851700	-1.66068300
C	2.10463600	5.36152900	-1.10823100
C	2.94765800	6.51035100	-1.39249200
C	2.52338800	4.10042100	-0.41357000
H	3.47378600	4.23750400	0.10897300
H	1.77018700	3.81279700	0.32524700
H	2.65111400	3.28047100	-1.13409600
C	4.38735500	6.62173800	-0.99095300

H	4.50046300	6.42975600	0.08086700
H	4.99610400	5.88776800	-1.53433700
H	4.79060200	7.61552000	-1.20188600
C	2.68164300	8.75103000	-2.71000300
H	3.50551600	9.18186200	-2.13371700
H	3.05319700	8.56104400	-3.72664100
H	1.89256500	9.50299900	-2.78220400
C	-0.28653200	7.60105400	-3.00755400
H	-0.28340300	8.68768500	-2.88414500
H	-0.18680600	7.38300000	-4.08004100
H	-1.26454000	7.23529700	-2.68394400
C	-0.34358300	4.67590600	-1.64612700
H	-0.22732600	3.94194600	-2.45567600
H	-0.39023300	4.14230100	-0.69384200
H	-1.29435100	5.19280400	-1.79961700
Rh	1.23629100	7.16831100	-0.07732800
C	2.49900400	7.96108400	2.58089400
O	2.50752200	7.07610900	1.67384900
O	1.80213600	9.01934900	2.55084000
C	3.36626300	7.71958500	3.80251000
H	2.75241500	7.24215500	4.57527500
H	4.19582100	7.05164000	3.56177800
H	3.73485200	8.66819000	4.20007600
C	0.67076200	10.35259800	-0.31094600
C	0.36260400	9.13101800	0.34420900
C	-1.00263800	8.92283300	0.68231100
C	-1.99028100	9.89202300	0.43915800
C	-1.62805600	11.07167400	-0.19585300
C	-0.29524900	11.30990700	-0.58265700
H	1.71053500	10.56027000	-0.55335100
H	1.10983500	9.00508200	1.38965500
H	-3.01856500	9.69377600	0.72512200
H	-2.38962200	11.82141000	-0.39563000
H	-0.02800500	12.24604800	-1.06486200
O	-1.39865800	7.77379500	1.24963200
N	-0.38865200	6.74462100	1.13335800
C	-0.75651000	5.58491000	1.72531000
O	-0.05522300	4.56688800	1.61505800
C	-2.05235100	5.56855400	2.52828400
H	-2.05457300	6.34442300	3.30029400
H	-2.91757000	5.75341700	1.88216600
H	-2.14410700	4.58351700	2.98897200

INT-4

C	1.61135900	7.28951400	-2.25664600
C	0.57612900	6.30829700	-2.02164300
C	1.19421000	5.13770800	-1.38634300
C	2.51243100	5.48290700	-1.06971200
C	2.77694000	6.84149900	-1.56477500
C	3.52612600	4.66258900	-0.33002200
H	3.90266500	5.20777300	0.54298900
H	3.10263200	3.71941900	0.02327300
H	4.38764300	4.43218400	-0.97089700
C	4.12406700	7.50209600	-1.53559300
H	4.59956200	7.38717700	-0.55641800
H	4.79619900	7.06107000	-2.28542900
H	4.05219700	8.57261600	-1.74775100
C	1.48067500	8.50903800	-3.11828800
H	2.15961600	9.30659900	-2.80841500
H	1.71761400	8.25248700	-4.16029300
H	0.46613200	8.91439100	-3.09410000
C	-0.80198900	6.31707800	-2.61604400
H	-1.19067200	7.33402400	-2.71693000
H	-0.79654700	5.85813100	-3.61507700
H	-1.50068700	5.74762500	-1.99639400
C	0.49738500	3.83269200	-1.15022700
H	0.08172300	3.44766800	-2.09069400
H	1.18804200	3.08016600	-0.75989500
H	-0.31628300	3.93664300	-0.42481300
Rh	1.13833700	7.16022200	-0.09190700
C	2.05025700	7.45184600	2.92016100
O	2.42412100	7.34084300	1.74085700
O	0.80127900	7.43809200	3.30071200
C	3.04276100	7.62345400	4.04174400
H	2.88983200	8.60094900	4.51185800
H	2.87126700	6.86076800	4.80776200
H	4.06181400	7.55409800	3.66000100
C	1.48083300	10.22462600	-0.18018700
C	0.66939400	9.12238700	0.10075500
C	-0.61719700	9.36978000	0.60446900
C	-1.10813200	10.66721100	0.77942400
C	-0.28794600	11.74915500	0.45790200
C	1.01055800	11.53336300	-0.00910900
H	2.49754300	10.07036900	-0.53444700
H	0.19232900	7.30065900	2.47330900
H	-2.11054800	10.81297400	1.17156900
H	-0.66077900	12.76133700	0.59158700
H	1.65751400	12.37645800	-0.23813700

O	-1.43408800	8.32495200	0.93176900
N	-0.63567900	7.11906800	1.10089100
C	-1.46034900	6.01760300	1.23184100
O	-0.95849800	4.90218700	1.37837700
C	-2.96385700	6.23150800	1.24577400
H	-3.25610500	6.91597500	2.04825600
H	-3.30124000	6.68450000	0.30748000
H	-3.44236200	5.26125700	1.38972500

INT-5

C	2.01707600	7.29989700	-2.41765900
C	0.88546500	6.47617500	-2.73460200
C	0.94145800	5.27534200	-1.90388400
C	2.04280100	5.40074100	-1.03496800
C	2.69027800	6.68140100	-1.31163600
C	2.46941200	4.39792000	-0.00513900
H	3.19292300	4.82464100	0.69526500
H	1.60626300	4.04712200	0.56754200
H	2.94565100	3.53106900	-0.48409800
C	3.94664200	7.17272800	-0.65886400
H	3.97224800	6.91565800	0.40383300
H	4.82894100	6.71791800	-1.13178100
H	4.04413200	8.25825400	-0.74258600
C	2.48042500	8.50594700	-3.17969300
H	3.03068200	9.20372500	-2.54224900
H	3.15278800	8.20661900	-3.99573900
H	1.64453300	9.05042900	-3.62787600
C	-0.09350300	6.71348700	-3.84420400
H	-0.18167700	7.77697600	-4.08090600
H	0.22612500	6.19076100	-4.75718900
H	-1.08983900	6.34498000	-3.58431400
C	-0.00791600	4.11606800	-1.95908300
H	0.47356800	3.24423000	-2.42337500
H	-0.33047100	3.83868500	-0.95152700
H	-0.89749700	4.35316700	-2.54943900
Rh	0.64310200	7.20713100	-0.66139900
C	0.48734700	10.32245900	-0.90126100
C	0.12328100	9.11421100	-0.27186400
C	-0.75764000	9.23011300	0.82527100
C	-1.25917900	10.45723500	1.28690500
C	-0.87083600	11.61730800	0.63335900
C	0.00489900	11.55222900	-0.46407200
H	1.16228600	10.30200900	-1.75119700
H	-1.93439600	10.47948700	2.13707800

H	-1.24735500	12.57815100	0.97430100
H	0.30479500	12.46600500	-0.97112600
O	-1.15433900	8.11389400	1.48331400
N	-0.56615200	6.96388900	0.90169800
C	-0.96416100	5.81995400	1.56487200
O	-0.54986000	4.72067900	1.19559100
C	-1.91231400	5.96144200	2.74279700
H	-1.47512800	6.59029300	3.52490700
H	-2.84986700	6.43643300	2.43670300
H	-2.11113500	4.96297300	3.13505900

INT-6

Rh	-1.11277700	-0.36613400	0.09153200
N	0.62529700	-1.06494600	1.03427900
C	-3.10283300	-1.36069400	0.62877300
C	-3.33856700	-0.40428400	-0.42284100
C	-2.64106300	-0.87146200	-1.59751600
C	-1.98732100	-2.10428100	-1.28595200
C	-2.25327700	-2.39204900	0.09782700
C	0.01244000	0.42726800	2.68437100
C	-1.08937900	0.70322000	1.86200300
C	0.17110200	1.03832900	3.93516300
C	-2.02791300	1.62849100	2.32591500
C	-0.78571600	1.95065500	4.37598300
H	1.03807300	0.79016800	4.54046900
C	-1.88882600	2.25048500	3.57446300
H	-2.87951500	1.89350400	1.70593100
H	-0.66585700	2.42604600	5.34590300
H	-2.63578200	2.96542100	3.90967700
C	0.23796000	0.64701800	-1.29006000
C	-0.25274100	1.61261200	-0.66784700
C	-1.82247200	-3.63642600	0.81232700
C	-1.27645700	-3.02481600	-2.23332300
C	-3.76624100	-1.37783400	1.97387900
C	-4.36548000	0.69060900	-0.39910700
C	-2.68210800	-0.21729000	-2.94652400
C	1.19110900	0.19760800	-2.33991100
H	-1.78817200	-3.48990100	1.89543400
H	-2.53696200	-4.44715900	0.61006700
H	-0.83413100	-3.95324200	0.47281300
H	-3.92979300	-0.36929500	2.36097000
H	-4.74229400	-1.87866000	1.90790300
H	-3.16511600	-1.91713700	2.71049300
H	-4.49837800	1.10744600	0.60258300

H	-4.10964700	1.50875900	-1.07732200
H	-5.34249000	0.29823100	-0.71576700
H	-2.85875900	0.85889500	-2.86622600
H	-1.74552900	-0.36572800	-3.48712100
H	-3.49630500	-0.64283100	-3.54916800
H	-0.29219600	-3.28688400	-1.83832000
H	-1.85947800	-3.94692900	-2.36557400
H	-1.14581700	-2.56761200	-3.21531300
C	2.54356400	-0.30723200	-1.86643900
H	3.09342200	-0.58393200	-2.77404000
H	2.37637700	-1.21959800	-1.28948800
C	3.32711500	0.74756200	-1.06329700
H	3.43289900	1.64794900	-1.68193700
H	2.74124100	1.03061900	-0.18223600
C	4.69364100	0.26617700	-0.62048400
C	4.96271400	0.02466700	0.73300800
C	5.72156800	0.05507100	-1.55102100
C	6.21982000	-0.42234700	1.14719800
H	4.17883400	0.19513500	1.46781700
C	6.97807100	-0.39256200	-1.14255300
H	5.53745300	0.24797300	-2.60603100
C	7.23160000	-0.63445300	0.20992100
H	6.40756000	-0.60179800	2.20279600
H	7.76137700	-0.54886700	-1.87998900
H	8.21061800	-0.98174600	0.52934800
F	0.60652100	-0.77149700	-3.12814300
F	1.38545800	1.28425100	-3.17904000
C	-0.45079100	3.02674700	-0.29741300
C	-1.71556800	3.67071600	-0.89801100
H	0.43621600	3.56895900	-0.65696300
H	-0.46871800	3.12775600	0.79219100
C	-1.82153300	5.16273700	-0.55770600
H	-1.70889500	3.53688500	-1.98798700
H	-2.60045700	3.14498900	-0.51936400
C	-3.07745500	5.82013100	-1.13913000
H	-1.81359100	5.28473800	0.53439500
H	-0.92869300	5.68381600	-0.93079300
H	-3.12508700	6.88393700	-0.88100800
H	-3.09652800	5.74150000	-2.23304500
H	-3.98859500	5.34386100	-0.75617700
O	0.97973600	-0.43309900	2.28140300
C	1.30181400	-2.21619200	0.84308600
O	1.15659700	-2.88264500	-0.19999800
C	2.28224200	-2.66947900	1.91848200

H	3.13453800	-1.98563500	1.98498500
H	1.81125500	-2.70134100	2.90548900
H	2.64115800	-3.66108000	1.63713100

INT-6'

Rh	-1.22825800	-0.49703700	-0.06989100
N	0.15382600	-1.30775000	1.25922500
C	-3.38888300	-1.21796900	0.20384500
C	-3.34676400	-0.31540900	-0.92171700
C	-2.53799400	-0.93326000	-1.93897000
C	-2.09136000	-2.21014800	-1.46252500
C	-2.61085500	-2.37839400	-0.13492500
C	-0.39421700	0.51060800	2.54824900
C	-1.32793100	0.79571300	1.54265000
C	-0.33648500	1.24900100	3.73471800
C	-2.20901900	1.85615600	1.75833600
C	-1.22633900	2.30572200	3.92268500
H	0.40099800	0.98806100	4.48800700
C	-2.16711100	2.61126500	2.93885200
H	-2.93987100	2.12115400	1.00049700
H	-1.18433600	2.88459800	4.84150700
H	-2.86422900	3.43343000	3.07986200
C	0.10937100	1.01949200	-0.89547500
C	0.60726900	-0.06357500	-1.27720200
C	-2.43425100	-3.60144800	0.71372600
C	-1.32615200	-3.25001400	-2.22742000
C	-4.23241200	-1.05265400	1.43323400
C	-4.21146300	0.89697500	-1.11600400
C	-2.30137800	-0.37048600	-3.30896300
C	0.25736300	2.49793000	-0.89197200
H	-2.53632600	-3.36930800	1.77722800
H	-3.20132600	-4.34740400	0.46151300
H	-1.44869700	-4.04336600	0.55469500
H	-4.27453300	-0.00989800	1.75828000
H	-5.25991700	-1.39147700	1.24107600
H	-3.83997200	-1.63892700	2.26812800
H	-4.53391100	1.32211300	-0.16258000
H	-3.70584900	1.68349400	-1.68368800
H	-5.12094200	0.62782800	-1.67168800
H	-2.30022800	0.72292700	-3.29994900
H	-1.34807300	-0.70398000	-3.72739300
H	-3.09540900	-0.69429400	-3.99584100
H	-0.50457600	-3.63688300	-1.61918300
H	-1.98379400	-4.08597800	-2.50324900

H	-0.91118900	-2.84345700	-3.15430500
C	-0.94958500	3.28926800	-1.37469200
H	-1.79744000	3.03198200	-0.73502000
H	-1.18752900	2.95547300	-2.39156200
C	-0.71461200	4.81268400	-1.35470900
H	-0.44782700	5.10992000	-0.33508700
H	0.14369500	5.04810500	-1.99284200
C	-1.93712700	5.57554500	-1.81814100
C	-2.09853100	5.92920300	-3.16469500
C	-2.95404200	5.91507000	-0.91429600
C	-3.24286300	6.60115800	-3.59845400
H	-1.31527200	5.68162900	-3.87840800
C	-4.10012800	6.58652000	-1.34285600
H	-2.84025800	5.65627300	0.13660000
C	-4.24871400	6.93132500	-2.68811900
H	-3.34568700	6.87173100	-4.64626400
H	-4.87403500	6.84640000	-0.62506400
H	-5.13829100	7.45820900	-3.02287100
F	0.61634600	2.92846100	0.36110900
F	1.33453800	2.79793800	-1.71451700
C	1.54895300	-0.99340700	-1.92147200
C	2.94543700	-0.35032700	-2.08037000
H	1.15231500	-1.27018200	-2.90953400
H	1.60534900	-1.92071700	-1.34113500
C	3.90945600	-1.25264100	-2.86064800
H	2.84744800	0.62195300	-2.57929300
H	3.35265700	-0.14521800	-1.08196300
C	5.30801800	-0.64276000	-3.00350000
H	3.98113200	-2.22686700	-2.35771800
H	3.49313300	-1.45290300	-3.85848000
H	5.97493800	-1.30504500	-3.56718200
H	5.26939500	0.31936700	-3.52885100
H	5.76457100	-0.46570400	-2.02218500
O	0.50893300	-0.49197800	2.38476200
C	0.88704900	-2.43357700	1.18501900
O	0.77113900	-3.22472000	0.22510700
C	1.86247600	-2.72359200	2.31915800
H	2.64401400	-1.95778300	2.36898500
H	1.35601600	-2.72646800	3.28932200
H	2.31333500	-3.69912800	2.12893600

TS-3

Rh	-1.26906000	-0.58413100	0.10784300
N	0.37970900	-1.31226000	1.17358500

C	-3.30535400	-1.57947700	0.60203900
C	-3.49414800	-0.57642500	-0.41988900
C	-2.76908600	-0.98350900	-1.59531000
C	-2.08465100	-2.20365600	-1.29601500
C	-2.42426900	-2.56684900	0.06940800
C	-0.09399200	0.41907000	2.62254900
C	-1.09537400	0.81452500	1.71004700
C	-0.04619300	0.93138500	3.92451900
C	-2.08202000	1.70155500	2.17384200
C	-1.02079300	1.83500300	4.34229900
H	0.73889400	0.59477700	4.59488300
C	-2.05229100	2.20983500	3.47347600
H	-2.86687800	2.02575700	1.49752800
H	-0.98543800	2.23213900	5.35312200
H	-2.82431400	2.89958500	3.80387200
C	0.12769200	0.58995900	-0.84993700
C	-0.24537000	1.52319900	-0.05819600
C	-1.97805500	-3.82353700	0.75366500
C	-1.30739700	-3.05887300	-2.25232300
C	-3.96487400	-1.59083600	1.95028600
C	-4.46553000	0.56644800	-0.34672500
C	-2.79920900	-0.28598500	-2.92430400
C	1.04574100	0.43109400	-2.00778500
H	-1.98719000	-3.71456700	1.84169500
H	-2.65513600	-4.64996800	0.49514200
H	-0.96603100	-4.09200900	0.44485100
H	-3.96310400	-0.59656500	2.40886900
H	-5.00969200	-1.92300400	1.87605900
H	-3.45190200	-2.26871200	2.63771000
H	-4.65573600	0.86933600	0.68610400
H	-4.11499200	1.44228200	-0.90098900
H	-5.43075900	0.27087100	-0.78155200
H	-3.06900400	0.76895900	-2.81811800
H	-1.82903800	-0.33497400	-3.42157000
H	-3.54476000	-0.75134900	-3.58364800
H	-0.40290300	-3.43766200	-1.77171500
H	-1.91755600	-3.90938000	-2.58883600
H	-1.00619800	-2.49042200	-3.13476200
C	2.43867000	-0.09867600	-1.69600300
H	2.93461100	-0.22185600	-2.66591900
H	2.32952600	-1.09280800	-1.25284200
C	3.25296200	0.84355400	-0.79077200
H	3.25654200	1.84146900	-1.24827900
H	2.74632500	0.93826500	0.17616500

C	4.68129100	0.38685500	-0.56540600
C	5.14727000	0.10501400	0.72521400
C	5.57787300	0.25629600	-1.63664400
C	6.46478800	-0.30589700	0.94265100
H	4.47119600	0.21707600	1.56991700
C	6.89399900	-0.15419100	-1.42531400
H	5.24484200	0.48276400	-2.64723600
C	7.34264600	-0.43941400	-0.13317900
H	6.80284700	-0.52000700	1.95331500
H	7.57142700	-0.24883700	-2.27021300
H	8.36788200	-0.75975600	0.03196400
F	0.47296900	-0.39617500	-2.95353500
F	1.16771800	1.66978200	-2.63157700
C	-0.27951300	3.01129400	0.04909000
C	-1.41664800	3.66799500	-0.75793500
H	0.68086300	3.34637800	-0.36885900
H	-0.31557500	3.33483400	1.09290000
C	-1.37876900	5.19980600	-0.68142400
H	-1.33393800	3.34259400	-1.80290600
H	-2.38630700	3.30808600	-0.38932400
C	-2.49683200	5.86508800	-1.49099400
H	-1.44948600	5.51235400	0.36989600
H	-0.40346200	5.55582800	-1.04182900
H	-2.44430100	6.95726200	-1.41938300
H	-2.43085800	5.59680600	-2.55242600
H	-3.48590500	5.55515800	-1.13124400
O	0.85316600	-0.47436000	2.26010300
C	1.23768300	-2.31702200	0.89854700
O	1.07959000	-3.03569400	-0.10545400
C	2.39219200	-2.57244300	1.86024600
H	3.17624100	-1.81866200	1.73002800
H	2.07253000	-2.53792600	2.90528600
H	2.80629500	-3.55382300	1.62148400

TS-3'

Rh	-1.33665200	-0.78782500	0.02352000
N	0.12645300	-1.55943300	1.31581100
C	-3.52777800	-1.53489000	0.36316100
C	-3.48921600	-0.62645100	-0.75635300
C	-2.69526300	-1.22405600	-1.80170500
C	-2.18252900	-2.46290700	-1.31604400
C	-2.69221500	-2.64190900	0.03602800
C	-0.28705600	0.36675800	2.51638400
C	-1.14146200	0.75927200	1.46282800

C	-0.33673000	0.99057800	3.76661400
C	-2.09827800	1.75279100	1.73454000
C	-1.26765800	2.00295700	3.99040500
H	0.33622200	0.65533400	4.54988300
C	-2.16576600	2.37118600	2.98288200
H	-2.78768800	2.05996100	0.95469400
H	-1.30727800	2.48865800	4.96161700
H	-2.90954800	3.14193500	3.16612400
C	-0.03695300	1.09250000	-0.20876100
C	0.32280600	0.06384500	-0.88250900
C	-2.42820400	-3.85013200	0.88389800
C	-1.40139900	-3.48988700	-2.08273900
C	-4.32118700	-1.33858900	1.62225200
C	-4.33059200	0.60804700	-0.91075200
C	-2.52171500	-0.65318200	-3.17945600
C	0.19802500	2.57884700	-0.28406500
H	-2.55099900	-3.63056600	1.94790300
H	-3.13022800	-4.65506100	0.62420600
H	-1.41059600	-4.21419000	0.72644200
H	-4.22960200	-0.31524600	2.00254100
H	-5.38862500	-1.53703500	1.45323100
H	-3.98298900	-2.01270400	2.41381700
H	-4.61733700	1.02544600	0.05792900
H	-3.81817200	1.38906800	-1.48168700
H	-5.25903700	0.37058700	-1.44930900
H	-2.40677300	0.43539400	-3.15519100
H	-1.64627100	-1.07141400	-3.68340100
H	-3.39747100	-0.87482800	-3.80504800
H	-0.55218100	-3.84046100	-1.49161800
H	-2.03795700	-4.34910200	-2.33711400
H	-1.01664400	-3.07986700	-3.02151400
C	-0.84809200	3.37270600	-1.06029500
H	-1.82454600	3.21843000	-0.59326200
H	-0.90012400	2.95015400	-2.06994900
C	-0.52978700	4.88064300	-1.12524600
H	-0.47375400	5.27142100	-0.10387200
H	0.46087800	5.01226200	-1.57338100
C	-1.56869200	5.64200800	-1.92047500
C	-1.43720100	5.80179800	-3.30697400
C	-2.70386400	6.17511500	-1.29415200
C	-2.41152900	6.47255700	-4.04793100
H	-0.55787000	5.40274400	-3.80870700
C	-3.68135600	6.84664100	-2.03045200
H	-2.81741900	6.06941500	-0.21704100

C	-3.53853000	6.99670800	-3.41137000
H	-2.28742600	6.59087200	-5.12133200
H	-4.55110400	7.25801400	-1.52455800
H	-4.29617000	7.52292700	-3.98583200
F	0.36824600	3.13093800	0.95782500
F	1.41525100	2.73764200	-0.92494900
C	1.24175400	-0.59406500	-1.84289300
C	2.52781300	0.18849900	-2.17255100
H	0.68051800	-0.78985300	-2.76863800
H	1.49022500	-1.58552100	-1.44259000
C	3.44806500	-0.59979000	-3.11342100
H	2.26970600	1.15345500	-2.62265200
H	3.05822800	0.41794500	-1.23974000
C	4.73802900	0.15413400	-3.45390900
H	3.69706400	-1.56593700	-2.65286500
H	2.90617500	-0.83543800	-4.04105600
H	5.37611300	-0.43060400	-4.12637600
H	4.52088000	1.11010000	-3.94627300
H	5.31842200	0.37306900	-2.54938700
O	0.59600700	-0.63924300	2.33850000
C	1.01615400	-2.55648700	1.10836100
O	0.85986500	-3.36618000	0.17563600
C	2.19093200	-2.68897700	2.06893600
H	2.86900900	-1.83380500	1.97206800
H	1.85761300	-2.71627900	3.11075900
H	2.72263100	-3.60930700	1.82103600

INT-7

Rh	1.15382300	-1.22349800	0.21611000
N	2.53208600	-0.90619100	-1.22663500
C	2.24165400	-2.57434800	1.76805700
C	1.73821000	-1.29640800	2.27852300
C	0.28473400	-1.34285800	2.27007000
C	-0.08446500	-2.52799900	1.58840100
C	1.14027700	-3.30114300	1.30283700
C	3.04197600	1.30925800	-0.72764300
C	1.95693700	1.95264400	-0.09656800
C	4.36346100	1.59665700	-0.38014400
C	2.26380100	2.89605900	0.89961500
C	4.63888000	2.54069600	0.60906100
H	5.16361000	1.08286700	-0.90413800
C	3.58231400	3.18631500	1.25421600
H	1.45501900	3.40114100	1.41741900
H	5.66821300	2.77033400	0.87119800

H	3.78225600	3.91949600	2.03126400
C	0.11484800	0.39500500	-0.54597700
C	0.56430500	1.66803600	-0.56258600
C	1.19361900	-4.62509100	0.60386000
C	-1.46950300	-3.03907200	1.33334200
C	3.67741800	-3.00229700	1.71264000
C	2.56607400	-0.25381900	2.96214800
C	-0.60915800	-0.32075700	2.90858200
C	-1.18068200	-0.02450900	-1.21487800
H	1.85863700	-4.55485200	-0.26369300
H	1.58348000	-5.40217200	1.27466500
H	0.20473100	-4.94240400	0.26280200
H	4.35265500	-2.15805400	1.87756000
H	3.88527300	-3.74846800	2.49199900
H	3.90899000	-3.43807400	0.73718400
H	3.53406700	-0.12386500	2.47170200
H	2.06531600	0.71655500	2.96676600
H	2.75204300	-0.54821300	4.00547500
H	-0.31042100	0.69742500	2.64291000
H	-1.65157700	-0.44955700	2.60757400
H	-0.56841100	-0.40926900	4.00263800
H	-1.58399600	-3.38237200	0.30178300
H	-1.68804200	-3.88703000	1.99675000
H	-2.22472100	-2.27065300	1.51372700
C	-2.49034000	0.36253500	-0.53276000
H	-2.52577600	1.45248700	-0.44767700
H	-2.47125500	-0.02919900	0.48922000
C	-3.74398200	-0.14739100	-1.27436200
H	-3.73224000	0.25229100	-2.29401300
H	-3.68705500	-1.23741200	-1.35995000
C	-5.02193100	0.25273900	-0.56908200
C	-5.63583000	-0.60722300	0.35193100
C	-5.60446200	1.50824700	-0.79443400
C	-6.79456200	-0.22594700	1.03106200
H	-5.20527800	-1.59076600	0.53070800
C	-6.76242300	1.89500300	-0.11840800
H	-5.14798400	2.18619500	-1.51302400
C	-7.36153900	1.02848500	0.79863000
H	-7.25757900	-0.91117200	1.73668600
H	-7.20037300	2.87086800	-0.31216700
H	-8.26563200	1.32631500	1.32294200
F	-1.18067600	-1.42073000	-1.34718800
F	-1.22455900	0.42467300	-2.52705700
C	-0.17967700	2.86505000	-1.16390700

C	-0.87008400	3.81918800	-0.16476700
H	-0.92755500	2.50403300	-1.87228900
H	0.53820900	3.44876400	-1.75669300
C	-1.72894900	4.87939100	-0.86920500
H	-1.49907400	3.24072200	0.52695500
H	-0.12288100	4.32974400	0.45483900
C	-2.40356200	5.85265600	0.10328800
H	-1.10108900	5.44111600	-1.57511100
H	-2.49493800	4.37820400	-1.47827000
H	-3.00998500	6.59425100	-0.42937900
H	-3.06306200	5.32257100	0.80171800
H	-1.66019000	6.39694600	0.69897700
O	2.80668000	0.41258900	-1.75634600
C	3.30917800	-1.87236600	-1.80170400
O	3.20442700	-3.05525000	-1.44594600
C	4.27065100	-1.46938500	-2.90926100
H	3.75720900	-0.91499900	-3.70013500
H	5.06458400	-0.81965700	-2.52643400
H	4.71180100	-2.38151500	-3.31517600

INT-7'

Rh	-1.18756200	-1.03047700	-0.14796100
N	0.44760500	-1.23775200	1.09885900
C	-3.16033600	-2.22367200	0.33369500
C	-3.31671400	-1.24814300	-0.76245400
C	-2.49417500	-1.65558000	-1.84116300
C	-1.69056600	-2.77187300	-1.35704600
C	-2.20911400	-3.17384100	-0.04513900
C	-0.24236900	0.68174700	2.17323500
C	-0.90898300	1.50702600	1.24309400
C	-0.67048100	0.58017000	3.49969100
C	-2.03496600	2.21648100	1.70606900
C	-1.78224300	1.29950000	3.93045800
H	-0.11583600	-0.06573800	4.17327200
C	-2.46999600	2.11583300	3.02498200
H	-2.56774300	2.86664800	1.01800500
H	-2.11286800	1.22438100	4.96281200
H	-3.33776500	2.68250900	3.35201100
C	-0.36573200	1.66813100	-0.14644200
C	-0.25088600	0.59546400	-0.95982400
C	-1.74769700	-4.37786100	0.72033700
C	-0.70209600	-3.57509900	-2.13942200
C	-3.91272800	-2.13790400	1.62670500
C	-4.32668600	-0.13955100	-0.76842700

C	-2.53351800	-1.12422200	-3.24273800
C	0.05218000	3.08884400	-0.52740600
H	-2.10402600	-4.35687700	1.75400100
H	-2.13471200	-5.29526400	0.25497600
H	-0.65664600	-4.42592400	0.73337100
H	-3.81234700	-1.14442800	2.07918600
H	-4.98453500	-2.31515500	1.46427500
H	-3.55541300	-2.87295600	2.35144400
H	-4.36466800	0.37055400	0.19919700
H	-4.09701400	0.60753700	-1.53294600
H	-5.33274300	-0.53176400	-0.97505200
H	-2.68066300	-0.04066600	-3.26764800
H	-1.61674800	-1.35232200	-3.79103100
H	-3.36514200	-1.58584200	-3.79283800
H	0.15777500	-3.81672500	-1.50743700
H	-1.16368000	-4.51408900	-2.47838400
H	-0.34635500	-3.03670100	-3.02132300
C	-0.92952700	3.86297800	-1.40717400
H	-1.88487300	3.92913000	-0.87438400
H	-1.11642400	3.27946400	-2.31514400
C	-0.43538600	5.27781500	-1.77262800
H	-0.23332000	5.82710000	-0.84686700
H	0.51730100	5.18934200	-2.30528400
C	-1.43926800	6.03118500	-2.61824000
C	-1.41812200	5.93445500	-4.01669700
C	-2.43596400	6.81661800	-2.02224200
C	-2.36469900	6.59967500	-4.79761500
H	-0.64606600	5.33707900	-4.49763300
C	-3.38508800	7.48405100	-2.79817800
H	-2.46215600	6.91148700	-0.93846100
C	-3.35314300	7.37679300	-4.19009500
H	-2.32632400	6.51594900	-5.88080200
H	-4.14563300	8.09287900	-2.31578400
H	-4.08839600	7.89919700	-4.79637400
F	0.25824000	3.82303400	0.62489400
F	1.27895000	3.07011900	-1.17071900
C	0.42276900	0.60580300	-2.31363200
C	1.94566400	0.29899100	-2.27244700
H	0.29382800	1.58818200	-2.78333700
H	-0.05643000	-0.11733800	-2.98099600
C	2.30561600	-1.19016300	-2.31934500
H	2.41087000	0.79822000	-3.13452800
H	2.37755700	0.76536100	-1.38077000
C	3.81809900	-1.43141300	-2.26021100

H	1.82181300	-1.72632100	-1.49676800
H	1.90771500	-1.62432100	-3.24954400
H	4.05257700	-2.50095600	-2.30646700
H	4.33626900	-0.93657700	-3.09197100
H	4.24251000	-1.03905500	-1.32772400
O	0.87326400	-0.03174400	1.78418200
C	1.38738100	-2.21269900	1.14977600
O	1.24351300	-3.26309100	0.49794100
C	2.61078900	-1.99543900	2.02719100
H	3.21772600	-1.16651900	1.64686900
H	2.32899800	-1.73862800	3.05266900
H	3.19877700	-2.91487100	2.01784300

TS-4

Rh	0.42778100	-0.72045400	0.26108100
N	1.72322800	-0.64944100	-1.35296900
C	1.75187500	-2.09893200	1.44912900
C	1.59362900	-0.84281400	2.14309200
C	0.18959100	-0.72230000	2.51247400
C	-0.50478200	-1.84159300	1.97976400
C	0.46418400	-2.70158400	1.31016700
C	2.72612800	1.42320100	-1.08800400
C	2.11819900	2.34717400	-0.21094600
C	4.11691900	1.32506800	-1.17644200
C	2.95981000	3.20690200	0.52008400
C	4.92876200	2.16502600	-0.41643600
H	4.54282500	0.59868300	-1.86147500
C	4.34643300	3.11392500	0.43015800
H	2.51890900	3.94605500	1.18303300
H	6.01010500	2.09270800	-0.49647300
H	4.97241300	3.78103800	1.01634000
C	-0.14210000	1.34188500	-0.11905000
C	0.64259400	2.44003500	-0.14391100
C	0.16211100	-4.00731400	0.64130500
C	-1.97856000	-2.11631000	2.02262900
C	3.04190300	-2.67504800	0.95085300
C	2.70427400	0.04920200	2.61258000
C	-0.39459200	0.38686500	3.33588000
C	-1.46751000	1.12035300	-0.44280700
H	0.64223000	-4.04258200	-0.34060100
H	0.52327600	-4.84885100	1.24893100
H	-0.91400100	-4.13431100	0.49674000
H	3.76791000	-1.88874600	0.72923900
H	3.47846400	-3.33449400	1.71406900

H	2.87766500	-3.24877400	0.03680300
H	3.53883500	0.05255300	1.90679500
H	2.36996300	1.08386000	2.72518300
H	3.08790100	-0.28612600	3.58685700
H	0.11006000	1.33705000	3.14056700
H	-1.45798100	0.52554400	3.12731500
H	-0.28485600	0.16664500	4.40660800
H	-2.37999100	-2.12710800	1.00259300
H	-2.18150200	-3.09026600	2.48406200
H	-2.51661700	-1.35453500	2.59205000
C	-2.10433400	1.37824300	-1.77213900
H	-1.36757700	1.12757200	-2.53800100
H	-2.27100700	2.46546100	-1.84315300
C	-3.42941900	0.62785600	-2.01718100
H	-3.23855400	-0.42956700	-1.82214400
H	-4.18336100	0.97082300	-1.29984100
C	-3.92776100	0.83210400	-3.43140700
C	-4.88502400	1.80988000	-3.73148200
C	-3.41372000	0.05576500	-4.48054600
C	-5.31895800	2.01069800	-5.04363700
H	-5.30052900	2.41524300	-2.92801100
C	-3.84365400	0.25363500	-5.79300900
H	-2.67552000	-0.71246600	-4.26015300
C	-4.79804600	1.23304700	-6.07914800
H	-6.06634400	2.77123900	-5.25535400
H	-3.43733300	-0.36108900	-6.59209800
H	-5.13607900	1.38537900	-7.10076800
F	-2.33189500	0.77875200	0.52062600
F	-1.20366400	-1.00377600	-1.01329300
C	0.02401700	3.83397500	-0.06131700
C	-0.45464800	4.22985100	1.35124900
H	-0.83940400	3.87980700	-0.73820400
H	0.74319300	4.57667300	-0.42620900
C	-1.06387100	5.63675600	1.40580000
H	-1.19456600	3.49231700	1.69100800
H	0.38325200	4.16802900	2.06038000
C	-1.55755400	6.02265400	2.80431800
H	-0.31865900	6.36886000	1.06416500
H	-1.89811100	5.69714500	0.69235700
H	-1.98783400	7.03040900	2.81111500
H	-2.32943100	5.32812900	3.15804700
H	-0.73795700	6.00561700	3.53332300
O	1.93568900	0.67206300	-1.92648500
C	1.77656000	-1.62634800	-2.30613400

O	1.53531300	-2.80483800	-2.01536400
C	2.19501300	-1.24256500	-3.72000000
H	1.47786500	-0.54219600	-4.16108300
H	3.17219100	-0.75006200	-3.73558100
H	2.23318600	-2.15687500	-4.31497400

TS-4'

Rh	0.63956800	-0.92907700	0.26097500
N	2.26005600	-1.07993500	-1.01676300
C	1.77318400	-1.96417200	1.91340400
C	1.40517300	-0.64107000	2.34110800
C	-0.04774600	-0.59887400	2.42559000
C	-0.55391500	-1.85154200	1.99020900
C	0.57494200	-2.70179000	1.64683400
C	3.15991900	1.04236100	-0.94245700
C	2.40282800	2.08527300	-0.36704100
C	4.54246400	0.96903100	-0.75640500
C	3.09681200	3.08784500	0.33915700
C	5.20023200	1.95337100	-0.02172400
H	5.08496400	0.14716000	-1.21277900
C	4.47477000	3.02000300	0.52177000
H	2.54437200	3.91858900	0.76836800
H	6.27752000	1.90142200	0.11127400
H	4.98504500	3.79734800	1.08358000
C	0.15348600	1.03133400	-0.57344000
C	0.94707000	2.13566600	-0.59587600
C	0.49499700	-4.12792400	1.19526600
C	-1.98487600	-2.29018300	1.90384800
C	3.16633800	-2.49468000	1.76683200
C	2.33893200	0.41484900	2.85514900
C	-0.83537800	0.55869400	2.96463400
C	-1.03559100	0.80561200	-1.22627000
H	1.14304200	-4.28157400	0.32808100
H	0.80446400	-4.80856200	2.00083900
H	-0.52549200	-4.39316000	0.90623700
H	3.87949100	-1.69165700	1.56567500
H	3.47405500	-2.99915300	2.69357300
H	3.21853200	-3.20756300	0.94153000
H	3.30478100	0.37942200	2.34477600
H	1.93096400	1.41895600	2.71091200
H	2.52292100	0.28210500	3.93108200
H	-0.44006000	1.51483800	2.60980000
H	-1.89052600	0.50482100	2.68301400
H	-0.78863000	0.57062100	4.06230500

H	-2.21243400	-2.66163600	0.89927900
H	-2.18289800	-3.10385300	2.61350900
H	-2.68187400	-1.47922100	2.13074500
C	-2.39182900	0.43767200	-0.72424000
H	-2.91999000	1.40078700	-0.61278900
H	-2.30176800	0.01276200	0.27446600
C	-3.22327000	-0.47980700	-1.65079200
H	-3.25660800	-0.02950100	-2.64925000
H	-2.68166200	-1.42284200	-1.73324100
C	-4.62959600	-0.68971100	-1.13161700
C	-5.01692100	-1.92066100	-0.58554500
C	-5.57959900	0.34217200	-1.17856300
C	-6.30974600	-2.11545400	-0.09354700
H	-4.29980200	-2.73764000	-0.55847000
C	-6.87174200	0.15408400	-0.68765400
H	-5.30691400	1.30141300	-1.61528000
C	-7.24110400	-1.07731200	-0.14035600
H	-6.58938000	-3.08066200	0.32099200
H	-7.59299900	0.96587400	-0.73870600
H	-8.24827400	-1.22706900	0.23941600
F	-0.53706700	-1.56081900	-1.29533800
F	-1.05197400	1.07348100	-2.54000300
C	0.31296600	3.50511500	-0.82142200
C	-0.38989800	4.09735400	0.41887800
H	-0.42782000	3.40901700	-1.62537200
H	1.07531300	4.20808600	-1.17701800
C	-1.01091300	5.47470300	0.15198900
H	-1.17015500	3.39828900	0.75021200
H	0.32191600	4.17447000	1.25299400
C	-1.72865500	6.05605400	1.37478900
H	-0.22525900	6.16898800	-0.17743600
H	-1.71728900	5.39571400	-0.68651300
H	-2.16093500	7.03819200	1.15304300
H	-2.54350100	5.40050700	1.70596100
H	-1.03890200	6.17883700	2.21895300
O	2.52629800	0.14331800	-1.76213200
C	2.43137800	-2.18584100	-1.81574300
O	2.21635700	-3.31527600	-1.36667700
C	2.95419900	-1.99053000	-3.23078100
H	2.24370400	-1.40191700	-3.82072000
H	3.90629900	-1.45134800	-3.24284000
H	3.08119200	-2.97752800	-3.67911800

TS-4''

Rh	-1.09105700	-0.73543200	0.00476400
N	0.46022600	-0.91528300	1.11605600
C	-2.88611000	-2.31030000	0.25861900
C	-3.27392000	-1.35185800	-0.74197500
C	-2.33786700	-1.41433900	-1.82622400
C	-1.35529500	-2.41642500	-1.49846600
C	-1.71965000	-2.98234000	-0.21546200
C	-1.12176800	0.93235100	2.50257700
C	-1.37823500	1.21020600	1.05160800
C	-2.12689000	1.38170200	3.44537100
C	-2.67879200	1.75580800	0.70647000
C	-3.32627700	1.88678200	3.02452400
H	-1.90339900	1.24609800	4.49886600
C	-3.63084000	2.06192000	1.63826900
H	-2.85474400	1.95935200	-0.34619900
H	-4.07347400	2.16338900	3.76593800
H	-4.59026700	2.47558900	1.34250700
C	0.02926700	0.83447000	-0.73106700
C	-0.24112700	1.76479600	0.17766700
C	-1.05555600	-4.16365200	0.42397400
C	-0.26382600	-2.93069300	-2.39018700
C	-3.65224100	-2.61073900	1.51515700
C	-4.55138600	-0.56752500	-0.71844900
C	-2.47551800	-0.70666100	-3.14324900
C	1.05439900	0.81954200	-1.81859700
H	-1.32255800	-4.25378900	1.48096500
H	-1.37942700	-5.08658400	-0.07712800
H	0.03335900	-4.10317500	0.35224600
H	-4.47531400	-3.31249300	1.31876600
H	-3.01351000	-3.06170300	2.27965600
H	-4.09148300	-1.70438900	1.94359400
H	-4.76767900	-0.16426500	0.27503000
H	-4.53319800	0.26711600	-1.42389400
H	-5.39011700	-1.21862600	-1.00220000
H	-3.02888000	0.23149100	-3.04119300
H	-1.50301100	-0.46961200	-3.57290600
H	-3.02457500	-1.33681900	-3.85694800
H	0.58580600	-3.28310600	-1.79866800
H	-0.62548300	-3.77013300	-3.00155400
H	0.09616700	-2.15060900	-3.06358600
C	2.37819600	0.11520300	-1.53920100
H	2.91876500	0.09871900	-2.49334100
H	2.16540100	-0.91906700	-1.25434200
C	3.24082100	0.79500500	-0.46020400

H	3.33675700	1.85931600	-0.70122900
H	2.71976500	0.72578500	0.50215500
C	4.62617700	0.18559500	-0.35473100
C	5.75558900	0.91695000	-0.74529800
C	4.80972200	-1.12172800	0.12309100
C	7.03639000	0.36603900	-0.66141800
H	5.63012600	1.93177000	-1.11751800
C	6.08848600	-1.67444100	0.20626300
H	3.94766500	-1.71283300	0.42375900
C	7.20713600	-0.93386200	-0.18415000
H	7.89826900	0.95360800	-0.96822300
H	6.21088000	-2.68840500	0.57935600
H	8.20210800	-1.36647200	-0.11633300
F	0.51647200	0.22428100	-2.95966700
F	1.31987400	2.12922600	-2.20005500
C	0.30591600	3.15620900	0.40665900
C	-0.49764700	4.27220000	-0.29022600
H	1.34157900	3.19979200	0.05612900
H	0.32536600	3.34528500	1.48943800
C	0.06192400	5.67282700	-0.00834300
H	-0.48770100	4.08003400	-1.37099100
H	-1.54744000	4.22998500	0.03134900
C	-0.72323100	6.78482200	-0.71218100
H	0.06128000	5.85301200	1.07622300
H	1.11419000	5.71149500	-0.32341700
H	-0.30022900	7.77247900	-0.49511400
H	-0.71179000	6.64895700	-1.80063400
H	-1.77238700	6.79388300	-0.39103600
O	-0.11016800	0.32440500	2.92158100
C	1.19874100	-1.93156800	1.58085500
O	1.75626500	-2.66119900	0.72826300
C	1.44669500	-2.08034000	3.06527100
H	2.12635800	-1.29304900	3.40654000
H	0.52418900	-1.97877300	3.64101600
H	1.90869700	-3.05694700	3.23174300

INT-8

Rh	0.22260900	-0.45252500	-0.11570000
N	1.88245700	-0.31709100	-1.39974200
C	1.33283400	-2.16430600	1.02029200
C	1.31039800	-0.95615000	1.81638900
C	-0.06224700	-0.67202600	2.14082000
C	-0.89005600	-1.63984300	1.47443600
C	-0.01507800	-2.57025500	0.78983800

C	3.01493500	1.63888300	-0.89907800
C	2.39096400	2.52492500	0.00044600
C	4.40116200	1.46700300	-0.89502400
C	3.21237900	3.26893800	0.86658100
C	5.19285800	2.19195000	-0.00598800
H	4.84121800	0.77487500	-1.60623000
C	4.59518600	3.09975200	0.87393700
H	2.75703800	3.97643400	1.55424700
H	6.27161700	2.06151700	-0.00934500
H	5.20661500	3.67720700	1.56180700
C	0.08040200	1.66313800	-0.14100200
C	0.92122600	2.69381400	-0.02256800
C	-0.48891200	-3.68377100	-0.09015000
C	-2.38010700	-1.77669200	1.58228200
C	2.58663000	-2.85679300	0.58992600
C	2.51891000	-0.27747700	2.38802800
C	-0.51146200	0.37317300	3.11648200
C	-1.24566300	1.34304000	-0.30963200
H	0.32588400	-4.35409500	-0.36747100
H	-1.27505500	-4.26711600	0.40307300
H	-0.89189600	-3.24909800	-1.01457300
H	3.28153100	-2.14315900	0.13766500
H	3.07918200	-3.30263300	1.46573500
H	2.38888100	-3.63281600	-0.14773700
H	3.34544500	-0.27309700	1.67286200
H	2.30960300	0.76048500	2.65773600
H	2.86069100	-0.79792900	3.29424400
H	0.02950200	1.31345500	2.97754200
H	-1.57796500	0.58138900	3.03077600
H	-0.31324300	0.02330000	4.13879400
H	-2.79487500	-2.24309600	0.68452600
H	-2.65286900	-2.40566300	2.44121000
H	-2.86263300	-0.80517600	1.70808200
C	-2.01726000	1.38146000	-1.59609500
H	-1.34243100	1.09446200	-2.40128900
H	-2.30952700	2.43144500	-1.76122500
C	-3.27604500	0.48679700	-1.62169200
H	-2.97956200	-0.50360400	-1.27018400
H	-4.02936200	0.88671600	-0.93396900
C	-3.84741200	0.37128800	-3.01878900
C	-5.01651200	1.04342900	-3.39355400
C	-3.18606900	-0.41697600	-3.97440800
C	-5.51999100	0.93397900	-4.69263600
H	-5.54127300	1.65423700	-2.66123800

C	-3.68723100	-0.52738100	-5.27097200
H	-2.27688500	-0.93652800	-3.68086900
C	-4.85610900	0.14792700	-5.63517100
H	-6.43110100	1.46087600	-4.96556600
H	-3.16650000	-1.14484800	-5.99873900
H	-5.24685700	0.05937400	-6.64569700
F	-2.07679600	1.38246500	0.79155400
F	-0.77534700	-1.03533500	-1.76657200
C	0.34714800	4.10939100	0.06586200
C	-0.26865200	4.44695400	1.43886600
H	-0.42773000	4.22700900	-0.70253500
H	1.13470800	4.83312000	-0.17555300
C	-0.82962200	5.87313100	1.50863800
H	-1.06578400	3.72337300	1.65325400
H	0.48647500	4.31401500	2.22749800
C	-1.45510700	6.20518300	2.86767600
H	-0.02711200	6.59123700	1.28813400
H	-1.58094100	6.00427600	0.71704600
H	-1.84904500	7.22760200	2.88640200
H	-2.28327000	5.52422600	3.09932800
H	-0.71841600	6.11733900	3.67590900
O	2.25336500	1.00501400	-1.85553800
C	1.94116900	-1.22470200	-2.44898400
O	1.63613100	-2.39962400	-2.26274400
C	2.46116700	-0.74440700	-3.79547700
H	1.80950200	0.03629000	-4.20166300
H	3.46395400	-0.31414700	-3.71537400
H	2.47917900	-1.60215400	-4.47021400

INT-8'

Rh	0.32663700	-0.70753700	0.42765600
N	1.80679800	-1.12522000	-0.95471600
C	1.48533000	-1.63993300	2.11732200
C	1.24041200	-0.26413200	2.44796500
C	-0.19948000	-0.10142400	2.59324800
C	-0.82353500	-1.33882400	2.29630400
C	0.21857400	-2.30132500	1.97097400
C	2.81339200	0.88876600	-1.30305600
C	2.30081500	2.05082900	-0.67975200
C	4.18922000	0.65437200	-1.38006800
C	3.23940000	2.99694400	-0.19875500
C	5.08428100	1.59168400	-0.87613500
H	4.53302000	-0.25810900	-1.85567800
C	4.60527600	2.76978400	-0.28492500

H	2.88921100	3.90906800	0.27184100
H	6.15383600	1.41681100	-0.95477200
H	5.30161800	3.50678200	0.10452400
C	-0.09948800	1.26993900	-0.55334400
C	0.85816000	2.27531600	-0.58340400
C	0.00600100	-3.74956800	1.65706100
C	-2.28805100	-1.65359900	2.34892500
C	2.82319200	-2.29242700	1.94624400
C	2.28468800	0.75161200	2.80867300
C	-0.89227700	1.13168800	3.09111700
C	-1.32368800	1.33666800	-1.13935700
H	0.62964500	-4.04779300	0.81010400
H	0.25705200	-4.37443300	2.52589700
H	-1.03649300	-3.94336100	1.39223200
H	3.59232800	-1.56344300	1.67908600
H	3.12653600	-2.77779300	2.88450700
H	2.78144300	-3.04474800	1.15583700
H	3.19522600	0.61499900	2.21905000
H	1.93361900	1.77264400	2.63580000
H	2.55948500	0.67230900	3.87022300
H	-0.29232400	2.02752400	2.92285800
H	-1.86372000	1.27937000	2.61004100
H	-1.06884400	1.05337300	4.17290200
H	-2.62058400	-2.14077000	1.42716100
H	-2.50619000	-2.33344000	3.18336300
H	-2.89204700	-0.75302000	2.48983000
C	-2.61193700	0.64128300	-0.87954800
H	-3.35206900	1.40878700	-0.60214400
H	-2.48937200	-0.04311100	-0.04464800
C	-3.13605200	-0.13243200	-2.12331300
H	-3.44189900	0.58764700	-2.88949400
H	-2.30136900	-0.71994500	-2.50911700
C	-4.28177200	-1.05334100	-1.76959000
C	-4.01059800	-2.31107800	-1.20617300
C	-5.61569300	-0.68192300	-1.97713900
C	-5.05297000	-3.17277700	-0.86356800
H	-2.97117500	-2.58750100	-1.04606500
C	-6.66046400	-1.54334800	-1.63184800
H	-5.83953100	0.28621400	-2.42153200
C	-6.38168300	-2.79198200	-1.07402300
H	-4.82840300	-4.14815900	-0.43829100
H	-7.69042600	-1.24085300	-1.80499000
H	-7.19280500	-3.46611400	-0.81054000
F	-0.91533400	-1.57431400	-0.91151900

F	-1.43072000	2.11170200	-2.25989500
C	0.39136900	3.72205400	-0.44503700
C	0.12447200	4.20623100	0.99603500
H	-0.53695100	3.82430800	-1.01340300
H	1.12469400	4.38514900	-0.91727500
C	-0.26582300	5.68954800	1.05091600
H	-0.68222200	3.60006800	1.42486500
H	1.00967700	4.03863400	1.62575600
C	-0.57263400	6.17474500	2.47166500
H	0.54509800	6.29533900	0.62258000
H	-1.14145300	5.85513300	0.40790500
H	-0.84623200	7.23567500	2.47863200
H	-1.40579200	5.61325500	2.91179100
H	0.29571500	6.05070000	3.13055200
O	1.93605400	0.01343100	-1.87352200
C	1.76796100	-2.31293000	-1.66233800
O	1.67112700	-3.37871600	-1.05275700
C	1.91166300	-2.27673800	-3.17397500
H	1.07048000	-1.73096100	-3.61398000
H	2.82780900	-1.76767800	-3.48794200
H	1.91673900	-3.30652000	-3.53548800

INT-8"

Rh	-1.21502100	-0.81175600	-0.04107900
N	0.19732100	-1.07625500	1.46683200
C	-3.05370300	-2.26640900	0.05025600
C	-3.22411600	-1.19999900	-0.95161800
C	-2.24908700	-1.36006600	-1.96683700
C	-1.33938600	-2.39767100	-1.50679300
C	-1.93017300	-3.01731900	-0.30562500
C	-1.00269000	0.62626600	2.46313300
C	-1.36744200	1.50924600	1.41847400
C	-1.84308700	0.40981500	3.56130000
C	-2.62576500	2.14064200	1.52231000
C	-3.07136300	1.05982900	3.64061900
H	-1.50693700	-0.26885700	4.33902300
C	-3.46654600	1.92262300	2.61026700
H	-2.93258000	2.82213400	0.73476500
H	-3.71942400	0.89486900	4.49707800
H	-4.42404800	2.43378900	2.66436700
C	-0.10480700	0.84591900	-0.52779800
C	-0.39482300	1.85113600	0.31629600
C	-1.37112100	-4.22276600	0.38707600
C	-0.17282200	-2.95960800	-2.25608300

C	-3.95702800	-2.45408400	1.23224500
C	-4.36814500	-0.23183600	-0.96491800
C	-2.25804700	-0.67429700	-3.30202700
C	0.92404100	0.86427900	-1.62271800
H	-1.81664300	-4.36133600	1.37593700
H	-1.58152700	-5.12561600	-0.20313900
H	-0.28896300	-4.13093500	0.50577000
H	-4.09377400	-1.51718700	1.78468200
H	-4.95195700	-2.79353300	0.91335500
H	-3.55828100	-3.19530100	1.92901600
H	-4.56847400	0.16703000	0.03433000
H	-4.17215600	0.60964600	-1.63452600
H	-5.28466500	-0.73032900	-1.31164000
H	-2.38943700	0.40723900	-3.20869700
H	-1.33373400	-0.84545800	-3.85124900
H	-3.09028100	-1.06358000	-3.90452700
H	0.60542300	-3.27144700	-1.55468000
H	-0.48408800	-3.83158600	-2.84983900
H	0.25237100	-2.21548700	-2.93240700
C	2.24412300	0.15235700	-1.34175000
H	2.79291000	0.14734600	-2.29136900
H	2.02022800	-0.88461500	-1.07706700
C	3.10239100	0.81314300	-0.25037200
H	3.21017800	1.87906000	-0.47934600
H	2.57063500	0.74980600	0.70794300
C	4.48496600	0.19694500	-0.12956900
C	5.62766700	0.99798900	-0.25643700
C	4.65762500	-1.17643200	0.10925600
C	6.90866600	0.45312700	-0.14395500
H	5.51180000	2.06322900	-0.44566100
C	5.93729700	-1.72281200	0.22071200
H	3.79014800	-1.82465300	0.20844900
C	7.06804200	-0.91213700	0.09555000
H	7.77963200	1.09592100	-0.24599300
H	6.04966100	-2.78822000	0.40636100
H	8.06303800	-1.34114300	0.18263400
F	0.39134200	0.26940500	-2.76436000
F	1.21176900	2.16500500	-2.02563200
C	0.13509100	3.28347700	0.32150900
C	-0.61213800	4.25780100	-0.61202100
H	1.19134700	3.28387000	0.03949800
H	0.08126000	3.66298100	1.35099300
C	-0.02532200	5.67525400	-0.57931300
H	-0.56682300	3.86339200	-1.63350700

H	-1.67532500	4.30498900	-0.33694800
C	-0.75871000	6.64986100	-1.50715500
H	-0.05244600	6.05858600	0.45090100
H	1.03614800	5.63058200	-0.86063400
H	-0.31444900	7.65119000	-1.46814700
H	-0.72042700	6.30820500	-2.54881300
H	-1.81598400	6.74394100	-1.22873900
O	0.22200000	-0.00639100	2.45385100
C	1.26314700	-1.89412500	1.56487800
O	1.49139800	-2.74591200	0.67938400
C	2.16248200	-1.77260500	2.78667300
H	2.80711900	-0.89025100	2.70566100
H	1.58427500	-1.66922700	3.70861700
H	2.79117700	-2.66393200	2.82968800

INT-9

Rh	0.43690100	-0.88928700	-0.24199600
N	2.56374000	-0.78999100	-0.46625900
C	0.70396800	-2.97999800	0.59717400
C	0.11672700	-2.15391000	1.62118300
C	-1.19347500	-1.76136600	1.15679600
C	-1.37428800	-2.26314600	-0.17122500
C	-0.18505900	-3.01108700	-0.52852900
C	3.03840700	0.36055000	1.58484500
C	1.98369400	1.27246600	1.40527300
C	3.80086600	0.38388200	2.76454600
C	1.68639000	2.16434700	2.45322200
C	3.51267500	1.30253100	3.76574100
H	4.60773100	-0.33478100	2.87186900
C	2.44161400	2.19339100	3.62058800
H	0.86002200	2.85555900	2.31086400
H	4.11838900	1.31665000	4.66779900
H	2.20580400	2.90583800	4.40538200
C	-0.16563900	1.16983100	0.15065100
C	1.19727300	1.36931000	0.15316400
C	0.01461300	-3.76188000	-1.80963500
C	-2.57062100	-2.13430700	-1.06681600
C	1.99557200	-3.72739800	0.70898500
C	0.65226000	-1.92942700	3.00484700
C	-2.19745000	-1.04664600	2.00877300
C	-1.26655700	1.89364400	0.04282200
H	-0.23114300	-4.82492500	-1.67685300
H	-0.62716900	-3.35812500	-2.59628200
H	1.04564700	-3.66506100	-2.15622300

H	2.73434400	-3.16830800	1.28892000
H	1.81951200	-4.68503800	1.21842700
H	2.41445900	-3.94020500	-0.27666500
H	1.74437400	-1.96358800	3.02076400
H	0.35015000	-0.95397200	3.39718300
H	0.28323500	-2.69818800	3.69859700
H	-1.78190700	-0.13055900	2.43861900
H	-3.09665900	-0.78445800	1.44900500
H	-2.49927700	-1.69646500	2.84104700
H	-2.30282400	-1.59046900	-1.98020200
H	-2.93466900	-3.12596500	-1.36197400
H	-3.39837800	-1.61066600	-0.58233400
C	-2.66358800	1.57559000	-0.37060700
H	-2.76029600	0.49820200	-0.50423300
H	-2.82941400	2.02160400	-1.36201500
C	-3.74595700	2.11754400	0.59578800
H	-3.57707200	1.70945200	1.59937200
H	-3.62252500	3.20312100	0.67540100
C	-5.14804800	1.78136900	0.13397100
C	-5.73075100	2.46815900	-0.94172200
C	-5.88794500	0.76171900	0.74760700
C	-7.00924100	2.14161800	-1.39390300
H	-5.17805800	3.27066900	-1.42586400
C	-7.16910400	0.43109800	0.29954000
H	-5.46208100	0.22976800	1.59620600
C	-7.73329400	1.11938200	-0.77509200
H	-7.44285200	2.68866700	-2.22702700
H	-7.72671100	-0.36020600	0.79405300
H	-8.73040900	0.86612700	-1.12494600
F	-1.12961000	3.23967900	0.32705700
F	0.18283200	-0.29990500	-2.13269700
C	1.80014400	1.98052000	-1.11277000
C	3.28504800	2.35353500	-1.08296100
H	1.20546500	2.89072200	-1.29005900
H	1.56628700	1.30280100	-1.94039200
C	3.72624000	3.01241000	-2.39786400
H	3.48813800	3.03853700	-0.24786900
H	3.89274700	1.45870300	-0.90942700
C	5.20761400	3.40383500	-2.40396200
H	3.52294700	2.32456800	-3.22998900
H	3.11114100	3.90490500	-2.58257000
H	5.49404200	3.86996200	-3.35381400
H	5.43383800	4.11639000	-1.60078800
H	5.84951700	2.52621900	-2.25738100

O	3.34494800	-0.65578300	0.73440800
C	3.26144000	-1.54931200	-1.37348800
O	2.69912100	-2.11012300	-2.31393000
C	4.77637200	-1.64117400	-1.20336300
H	5.23326400	-0.66633300	-1.01079000
H	5.03006900	-2.29059000	-0.35760000
H	5.18227300	-2.07215200	-2.12045000

INT-9'

Rh	-0.59086600	-0.92911500	-0.00688500
N	-1.74421700	0.33384400	1.26965700
C	-2.50473700	-1.77878600	-0.86255000
C	-1.82084200	-1.06653900	-1.91612400
C	-0.57862600	-1.75547200	-2.16406500
C	-0.45503900	-2.82766900	-1.21839800
C	-1.65567000	-2.83945300	-0.40556900
C	-1.57459300	2.32709800	-0.06230700
C	-0.20231200	2.14859100	-0.32511400
C	-2.28120900	3.37740000	-0.67392400
C	0.40859500	3.01418600	-1.25243300
C	-1.64033600	4.24051800	-1.55189500
H	-3.33773500	3.48389600	-0.44738300
C	-0.28678400	4.05434300	-1.85882900
H	1.46238900	2.86631200	-1.47263000
H	-2.19991600	5.05268500	-2.00793700
H	0.21923900	4.71701600	-2.55445100
C	1.27416700	0.14418300	-0.36018900
C	0.62878000	1.12153600	0.35675600
C	-1.96690100	-3.82270400	0.68082100
C	0.64341600	-3.84126100	-1.09928700
C	-3.88973000	-1.49846900	-0.36995300
C	-2.38789900	0.05061900	-2.74224400
C	0.35019700	-1.43986400	-3.29700100
C	2.44560000	-0.27528700	-0.79760000
H	-2.40128100	-3.30952800	1.54236700
H	-2.66691700	-4.58923700	0.32027100
H	-1.05741600	-4.32283900	1.02110200
H	-4.13109500	-0.43408000	-0.43324400
H	-4.61510900	-2.04528000	-0.98855300
H	-4.01144400	-1.82137600	0.66588400
H	-3.09289800	0.65344700	-2.16442800
H	-1.60360700	0.72218700	-3.10296000
H	-2.92244700	-0.34076600	-3.61921900
H	0.41185000	-0.36248600	-3.47386000

H	1.35708300	-1.81274000	-3.11369600
H	-0.02973000	-1.90402300	-4.21764700
H	1.06504200	-3.82251300	-0.08869700
H	0.25169500	-4.84912400	-1.28666900
H	1.45248900	-3.65111800	-1.80488200
C	3.70744500	0.52407700	-0.94487400
H	3.52300800	1.55175200	-0.61581000
H	3.98715600	0.57229600	-2.00715400
C	4.88951800	-0.08221600	-0.14549000
H	4.61152100	-0.12510100	0.91433300
H	5.03973900	-1.11538000	-0.47623300
C	6.16360500	0.71476500	-0.32224200
C	7.04275900	0.43786400	-1.37860400
C	6.47576600	1.77193000	0.54370700
C	8.19955500	1.19574700	-1.56696100
H	6.82137100	-0.38513900	-2.05529200
C	7.63165600	2.53253500	0.36019000
H	5.80974300	1.99524400	1.37475700
C	8.49740400	2.24715200	-0.69756500
H	8.87110700	0.96119400	-2.38890600
H	7.85851000	3.34423600	1.04660100
H	9.39977300	2.83571000	-0.83989600
F	2.62464100	-1.56799300	-1.21045900
F	0.41859200	-1.59108300	1.58327400
C	1.00959000	1.27175100	1.83290700
C	0.40408700	2.44890000	2.60292100
H	2.10753200	1.37026300	1.83930600
H	0.79450000	0.31318500	2.31687300
C	0.92664900	2.50644200	4.04563600
H	0.63393300	3.39634700	2.09527900
H	-0.68749200	2.36046400	2.62154100
C	0.34099100	3.67262300	4.84857700
H	0.69476000	1.55817000	4.54929200
H	2.02357200	2.58509100	4.03396600
H	0.73047300	3.68807600	5.87305400
H	0.58375400	4.63680500	4.38437900
H	-0.75205600	3.60139700	4.90942700
O	-2.35198700	1.50045800	0.68448600
C	-2.55704900	-0.14300100	2.26652400
O	-2.46478900	-1.30115500	2.67709300
C	-3.56555100	0.82284600	2.88441600
H	-3.12198100	1.79490500	3.11825000
H	-4.39724600	1.00417500	2.19381800
H	-3.95007500	0.35643400	3.79333800

TS-5

Rh	0.35430400	-1.11324100	-0.28676500
N	2.43595400	-0.69940400	0.04522100
C	0.57641500	-3.28122300	0.26443800
C	-0.09426100	-2.59601600	1.35455300
C	-1.36334000	-2.13478900	0.86131400
C	-1.43996300	-2.43024900	-0.53948200
C	-0.23216900	-3.16041800	-0.90188400
C	2.70190600	0.61801700	1.95902000
C	1.96612400	1.61629500	1.31194000
C	3.26834200	0.84645800	3.21756000
C	1.79309600	2.85289100	1.95421600
C	3.10423900	2.08523500	3.83057800
H	3.83274700	0.04888100	3.69061500
C	2.36655500	3.09292700	3.20129700
H	1.18884400	3.61338300	1.46917900
H	3.55287000	2.26322000	4.80396000
H	2.23090600	4.05745000	3.68110100
C	-0.03260400	0.99524900	-0.02312000
C	1.31139200	1.39973500	-0.00584100
C	0.08928000	-3.61317700	-2.29311900
C	-2.57714100	-2.19621800	-1.48914800
C	1.88530700	-4.00423200	0.36216000
C	0.36640500	-2.55460200	2.78213600
C	-2.42894100	-1.52226000	1.72084200
C	-1.10696900	1.76371700	-0.12426600
H	-0.72104800	-4.23079900	-2.70010500
H	0.21831900	-2.72913500	-2.92988500
H	1.01535900	-4.19092600	-2.32552900
H	2.49982800	-3.60330000	1.17272000
H	1.71259800	-5.06891800	0.57125600
H	2.45318400	-3.92359300	-0.56738200
H	1.44453000	-2.38316800	2.84286900
H	-0.12606000	-1.74872800	3.33404600
H	0.14249700	-3.49850800	3.29869300
H	-2.03828300	-0.69796100	2.32537800
H	-3.26771600	-1.14593900	1.13254900
H	-2.82434000	-2.27881600	2.41182700
H	-2.22456300	-1.67189500	-2.38390800
H	-3.01310100	-3.15155100	-1.81062600
H	-3.37929600	-1.60511200	-1.04040500
C	-2.55343100	1.47066700	-0.33081600
H	-2.68957800	0.39077400	-0.38377500

H	-2.84777500	1.87201800	-1.31126100
C	-3.47349000	2.09116600	0.75025100
H	-3.18806400	1.69929100	1.73395900
H	-3.28815900	3.17096200	0.77705100
C	-4.94039800	1.81900900	0.49279700
C	-5.61712900	2.47335200	-0.54801200
C	-5.65439400	0.89545200	1.26803100
C	-6.96114000	2.20782900	-0.80977600
H	-5.08567500	3.20316200	-1.15534100
C	-7.00100900	0.62628300	1.01092000
H	-5.15331700	0.39123200	2.09176100
C	-7.65863500	1.28050000	-0.03125000
H	-7.46630800	2.72872800	-1.61910100
H	-7.53568900	-0.09073900	1.62876200
H	-8.70648300	1.07489400	-0.23276600
F	-0.90369400	3.14025800	-0.05633800
F	0.45782900	-0.51102500	-2.21277200
C	1.91669800	1.88934400	-1.29228400
C	3.39352400	2.28564900	-1.29699100
H	1.28888100	2.75682500	-1.56304500
H	1.67564100	1.12325300	-2.04294900
C	3.84630800	2.77020100	-2.68159500
H	3.57908800	3.07304800	-0.55362300
H	4.00660900	1.42748300	-0.99859000
C	5.32277100	3.17730600	-2.71851500
H	3.66405600	1.97414500	-3.41578200
H	3.22350100	3.62187400	-2.99130700
H	5.61754700	3.51771700	-3.71774000
H	5.52867900	3.99284500	-2.01381500
H	5.97179800	2.33495900	-2.44922700
O	2.84958200	-0.62699300	1.41935300
C	3.43236600	-1.26683100	-0.72821600
O	3.19046100	-1.69899200	-1.85013000
C	4.84011600	-1.33193200	-0.13933200
H	5.14941000	-0.38597400	0.31455000
H	4.89315800	-2.09796000	0.64251900
H	5.52192500	-1.59997500	-0.94868600

TS-5'

Rh	-0.71134500	-1.09573700	-0.16651600
N	-1.65468300	0.66044900	0.63224700
C	-2.55326700	-2.27950000	-0.60865900
C	-2.14772300	-1.60509100	-1.83248600
C	-0.86140600	-2.10947400	-2.20441100

C	-0.42972100	-3.04706600	-1.19223400
C	-1.50666900	-3.17411400	-0.23209600
C	-1.25328000	2.59088700	-0.61985700
C	0.07826500	2.51599600	-0.19116400
C	-1.72320900	3.70685500	-1.31889300
C	0.92227200	3.60962800	-0.43858000
C	-0.86214400	4.77043600	-1.57624100
H	-2.76181600	3.72772800	-1.63371100
C	0.46074400	4.73056700	-1.12739300
H	1.95389200	3.57410200	-0.09981000
H	-1.23081600	5.63925000	-2.11429700
H	1.13121500	5.56421500	-1.31249000
C	1.01490700	0.21937300	-0.37193100
C	0.62321800	1.28757300	0.45197700
C	-1.44947100	-4.00950600	1.00986500
C	0.79803900	-3.90846600	-1.20931200
C	-3.86345300	-2.10852700	0.10144000
C	-2.99946100	-0.65932900	-2.62658500
C	-0.12913500	-1.78067300	-3.47077400
C	2.17075100	-0.06226000	-0.95105200
H	-2.43055700	-4.08952100	1.48463000
H	-1.08806000	-5.01968300	0.78680500
H	-0.75988400	-3.53241600	1.71914300
H	-4.35687300	-1.17947300	-0.19696500
H	-4.54340700	-2.93610500	-0.14367300
H	-3.72664400	-2.07916000	1.18499900
H	-3.54580700	0.02755100	-1.97581500
H	-2.39505600	-0.05176800	-3.30523000
H	-3.73151200	-1.21107000	-3.23233400
H	-0.40665600	-0.79379000	-3.85095400
H	0.95000600	-1.79365100	-3.32252200
H	-0.38065600	-2.51759200	-4.24628800
H	1.15672600	-4.08779900	-0.19138800
H	0.58131100	-4.88462800	-1.66635300
H	1.60954700	-3.44114200	-1.76722500
C	3.45077400	0.72291300	-0.97947600
H	3.31578200	1.66589300	-0.44098600
H	3.69316100	0.98495200	-2.01929400
C	4.64627300	-0.05705900	-0.37386300
H	4.40529400	-0.32126700	0.66296900
H	4.75836600	-0.99831000	-0.92243000
C	5.93331200	0.73664500	-0.42565700
C	6.74058200	0.72125600	-1.57214000
C	6.33046300	1.53534600	0.65558300

C	7.90826000	1.48261300	-1.63851900
H	6.45322400	0.10025200	-2.41831100
C	7.49798600	2.29830700	0.59498100
H	5.72220100	1.55189400	1.55782800
C	8.29073800	2.27523700	-0.55407400
H	8.52255700	1.45234900	-2.53483400
H	7.79087300	2.90602400	1.44735000
H	9.20195300	2.86544900	-0.60219700
F	2.33158600	-1.23550800	-1.65553700
F	0.16522300	-1.49090900	1.60725000
C	1.01465100	1.26205300	1.90291300
C	0.46068900	2.35052900	2.82416500
H	2.12004900	1.28534800	1.90414500
H	0.75919600	0.24740700	2.24654800
C	0.93661900	2.16542000	4.27183800
H	0.75259200	3.34721200	2.46646300
H	-0.63490300	2.32149700	2.80123500
C	0.39175800	3.23785900	5.22053400
H	0.63046700	1.17133900	4.62321100
H	2.03618600	2.17654300	4.29945600
H	0.74738600	3.08135500	6.24534200
H	0.70448700	4.24237700	4.90839100
H	-0.70471700	3.22391700	5.24315900
O	-2.13666200	1.58326100	-0.36498800
C	-2.51276500	0.63870500	1.72192000
O	-2.42094500	-0.24168500	2.56944000
C	-3.55467900	1.74892900	1.83711000
H	-3.11045400	2.74400200	1.73469000
H	-4.31384300	1.65308700	1.05317200
H	-4.03023600	1.65309400	2.81493900

INT-10

Rh	0.24308300	-1.32856500	-0.27982700
N	2.23159000	-0.26342500	-0.46110100
C	0.56657700	-3.42389400	0.73836500
C	0.15331100	-2.41775800	1.72058000
C	-1.14922200	-1.96344900	1.36589600
C	-1.49391100	-2.57204300	0.10007900
C	-0.43787200	-3.53119500	-0.23580900
C	2.91116800	0.37552300	1.60937500
C	1.97593100	1.32855800	1.23722900
C	3.53076000	0.37149900	2.85377900
C	1.60338600	2.32091400	2.13742300
C	3.15840000	1.37956500	3.75052000

H	4.26776300	-0.38166200	3.11278800
C	2.20069600	2.33930900	3.40367500
H	0.85822700	3.05765300	1.85273400
H	3.62038700	1.40898800	4.73335300
H	1.92074700	3.10580400	4.12019100
C	0.08336800	0.71361100	-0.31447200
C	1.54444600	1.11536400	-0.19965900
C	-0.41658300	-4.31307000	-1.51391100
C	-2.80153200	-2.50021600	-0.63276100
C	1.86287000	-4.17585900	0.80726200
C	0.87213800	-2.13035400	3.00544700
C	-2.01800100	-1.07074100	2.19963100
C	-0.93050900	1.56575100	-0.43091700
H	-1.34428100	-4.88209400	-1.64777000
H	-0.31530100	-3.60925100	-2.35188500
H	0.41901600	-5.01776200	-1.54796000
H	2.70203500	-3.50218500	1.01329800
H	1.83943300	-4.91943100	1.61555900
H	2.07353800	-4.70657500	-0.12508700
H	1.95689100	-2.16852400	2.87571800
H	0.62142500	-1.14148400	3.39816300
H	0.60562100	-2.87278800	3.77169400
H	-1.44050000	-0.26804300	2.66687700
H	-2.81026200	-0.61143200	1.60560000
H	-2.49777000	-1.65005400	3.00068000
H	-2.63869600	-2.33845400	-1.70308300
H	-3.35716900	-3.44116500	-0.51577200
H	-3.44175800	-1.69629900	-0.26158800
C	-2.38048600	1.33177700	-0.70450700
H	-2.57006500	0.25750200	-0.69546100
H	-2.60036000	1.67297700	-1.72700800
C	-3.33260200	2.07290700	0.26728800
H	-3.11657500	1.76181400	1.29656200
H	-3.11104100	3.14451400	0.21244600
C	-4.79204800	1.82562900	-0.04928500
C	-5.39833000	2.44193800	-1.15464100
C	-5.56847900	0.95811700	0.73097300
C	-6.73352200	2.19442800	-1.47332500
H	-4.81703200	3.12658500	-1.76879500
C	-6.90644400	0.70696400	0.41723600
H	-5.12374000	0.48339500	1.60343800
C	-7.49343400	1.32350700	-0.68830100
H	-7.18295700	2.68523200	-2.33286200
H	-7.48982300	0.03340600	1.04005500

H	-8.53449300	1.13184400	-0.93421000
F	-0.68555400	2.93826900	-0.34650500
F	0.16883000	-1.33149000	-2.27444800
C	2.03310600	2.26615200	-1.11371100
C	3.53382000	2.58578100	-1.05735200
H	1.46994100	3.14647100	-0.79380500
H	1.72828700	2.04532800	-2.13757200
C	3.91737000	3.70166800	-2.04024300
H	3.81541500	2.88824900	-0.03982600
H	4.13141500	1.69505600	-1.29165900
C	5.40523400	4.06367500	-1.98649700
H	3.65076500	3.38952000	-3.05895900
H	3.31429000	4.59534800	-1.82563300
H	5.64835700	4.86073900	-2.69857000
H	5.69435800	4.41030800	-0.98639400
H	6.03272400	3.19734000	-2.23050900
O	3.16459000	-0.55862100	0.63233200
C	2.88142600	-0.59094100	-1.72197100
O	2.57473400	-0.02366300	-2.73826600
C	3.88469800	-1.71975300	-1.64819900
H	4.78549500	-1.39892500	-1.11561200
H	3.47464600	-2.58066200	-1.11383800
H	4.14032800	-1.99956700	-2.67125600

INT-10'

Rh	-0.73807500	-1.21453700	-0.23978400
N	-0.88769000	0.47946500	1.19248500
C	-2.79723200	-1.91380800	-1.15343700
C	-2.05048600	-1.05422800	-2.07674800
C	-0.82965900	-1.71745100	-2.41101500
C	-0.74250600	-2.90263300	-1.59365300
C	-2.01217900	-3.04236000	-0.87197700
C	-1.72157700	2.24537100	0.07505800
C	-0.39437200	2.15242500	-0.32823900
C	-2.62296700	3.14048400	-0.48816700
C	0.06808200	2.96683600	-1.35471400
C	-2.14386400	3.96112900	-1.51611200
H	-3.64999500	3.19500900	-0.14212000
C	-0.81832700	3.87186100	-1.95397400
H	1.10066800	2.90091400	-1.68674200
H	-2.81931500	4.67234200	-1.98314400
H	-0.47161800	4.51177600	-2.75993400
C	0.91594600	-0.02359100	-0.16522200
C	0.35161100	1.17621200	0.57329600

C	-2.27735900	-4.13161400	0.12333000
C	0.32541600	-3.95451000	-1.63854100
C	-4.15459400	-1.57640800	-0.60877500
C	-2.61097900	0.16552400	-2.74751900
C	0.15239800	-1.29080000	-3.46170900
C	2.15333300	-0.27300400	-0.58150700
H	-3.30427300	-4.10001100	0.49832000
H	-2.10895200	-5.12139500	-0.31696900
H	-1.59399200	-4.01126100	0.97486500
H	-4.17501400	-0.56417700	-0.18840800
H	-4.91526900	-1.61449300	-1.40015700
H	-4.45911800	-2.27194900	0.17783800
H	-3.27319600	0.72350300	-2.08036500
H	-1.82234000	0.84899500	-3.07261800
H	-3.19679600	-0.11679700	-3.63430600
H	0.10604500	-0.21238700	-3.63690000
H	1.17415100	-1.54108400	-3.17343100
H	-0.07161200	-1.79352700	-4.41289500
H	0.44988700	-4.42099500	-0.65682500
H	0.06617100	-4.74407400	-2.35873000
H	1.28790500	-3.52782500	-1.92399600
C	3.45142400	0.48025200	-0.55014700
H	3.29870900	1.51338200	-0.23310100
H	3.85140800	0.52004100	-1.57338100
C	4.50828100	-0.19206300	0.36568800
H	4.11384200	-0.22577700	1.38813600
H	4.63448400	-1.23009700	0.03995500
C	5.83631600	0.53183600	0.33989500
C	6.80268100	0.22711200	-0.62946300
C	6.11837900	1.55097000	1.26042100
C	8.01331500	0.91977200	-0.68014500
H	6.60508900	-0.56686700	-1.34693500
C	7.32777100	2.24662200	1.21479800
H	5.38404100	1.79559600	2.02528800
C	8.27993200	1.93357900	0.24261700
H	8.75098000	0.66365500	-1.43654200
H	7.52844300	3.02918600	1.94224300
H	9.22383600	2.47117000	0.20769400
F	2.38444800	-1.49797700	-1.19256600
F	-0.19699300	-2.11092700	1.48945400
C	1.27718100	1.95435800	1.54353500
C	0.61636700	3.02140700	2.43011300
H	2.00678100	2.46429200	0.90230800
H	1.82192400	1.23785600	2.16029500

C	1.63441000	3.70277700	3.35623400
H	0.13373300	3.78310900	1.80353400
H	-0.17084400	2.57122600	3.04412700
C	1.00767600	4.78779900	4.23817800
H	2.10689600	2.94136900	3.99164200
H	2.44050200	4.14316100	2.75143100
H	1.75551800	5.25419600	4.88978200
H	0.55349300	5.58055000	3.63067200
H	0.22153900	4.37032000	4.87923100
O	-2.04365900	1.37887100	1.09113400
C	-0.87792500	-0.05194300	2.57737400
O	0.09812000	0.03316000	3.27279600
C	-2.20627200	-0.61112200	3.02125600
H	-2.74947800	0.16235100	3.57713800
H	-2.82050500	-0.93788700	2.18259100
H	-2.00443000	-1.44984500	3.68935900

INT-11

Rh	0.16445700	1.48908200	-0.65635300
N	-2.75352500	-0.06971500	-0.41719500
C	0.13236200	3.72904100	-0.05042600
C	-0.34947400	2.81493000	0.99602100
C	0.76263900	2.01077100	1.42799400
C	1.85966100	2.30006900	0.55260600
C	1.46423800	3.40335700	-0.33020900
C	-3.03035900	-0.27820800	1.78750200
C	-2.01541800	-1.16987400	1.45749700
C	-3.52002300	-0.12935700	3.08183100
C	-1.45882100	-1.96807500	2.45249500
C	-2.95072900	-0.93661900	4.07293500
H	-4.31624000	0.57456200	3.30106400
C	-1.93354900	-1.84674500	3.76499800
H	-0.66250600	-2.66234500	2.20944100
H	-3.31130700	-0.85396600	5.09465500
H	-1.50751300	-2.46566600	4.54932700
C	-0.27218700	-0.55045300	-0.29340900
C	-1.72138000	-1.07655000	-0.03652400
C	2.36483900	4.00083000	-1.36920300
C	3.27401700	1.83016500	0.70427100
C	-0.74807600	4.71096300	-0.75821000
C	-1.67374200	2.97317100	1.67802900
C	0.79987000	1.10235900	2.61873600
C	0.76287600	-1.39748600	-0.20427100
H	1.84234100	4.74202200	-1.97897100

H	3.22733400	4.49380200	-0.90214300
H	2.75196400	3.22580800	-2.04047200
H	-1.47477900	4.16251100	-1.37085900
H	-1.29794400	5.33329800	-0.04270000
H	-0.17488800	5.37234300	-1.41343100
H	-2.49279400	3.00834400	0.95521800
H	-1.87461700	2.15458600	2.37072800
H	-1.68646000	3.91143700	2.25106300
H	-0.19564500	0.74733700	2.89074300
H	1.42041300	0.22225000	2.43340600
H	1.21889900	1.63758100	3.48223200
H	3.75823700	1.65949400	-0.26185800
H	3.86313100	2.59237800	1.23437200
H	3.33601500	0.90668800	1.28115900
C	2.22068600	-1.28649700	-0.55443100
H	2.48390600	-0.24947100	-0.75113300
H	2.37090700	-1.81680300	-1.50626100
C	3.17021500	-1.91900700	0.49379700
H	3.06747300	-1.39615200	1.45340200
H	2.84422700	-2.94895300	0.67247900
C	4.62347500	-1.91220800	0.06368400
C	5.04367200	-2.66331500	-1.04569600
C	5.58794700	-1.16905200	0.75704900
C	6.37749600	-2.66228000	-1.45307700
H	4.31815600	-3.26257300	-1.59153300
C	6.92603200	-1.16517500	0.35502500
H	5.29070500	-0.59438400	1.63166600
C	7.32561700	-1.91009000	-0.75463400
H	6.67887800	-3.25453000	-2.31343900
H	7.65508800	-0.58254600	0.91265900
H	8.36569400	-1.91055900	-1.06967400
F	0.54950600	-2.72323100	0.20502600
F	-1.47743300	1.95863000	-1.91121200
C	-2.03323800	-2.42688800	-0.76957500
C	-3.47184100	-2.93965500	-0.62189200
H	-1.35551600	-3.17850500	-0.37078900
H	-1.79784000	-2.29133800	-1.82662000
C	-3.66278400	-4.29871700	-1.31191500
H	-3.73060400	-3.03898200	0.44167500
H	-4.18291300	-2.22647500	-1.05445000
C	-5.09070900	-4.84025000	-1.18462100
H	-3.40127400	-4.20200500	-2.37470300
H	-2.95619600	-5.02636100	-0.88747300
H	-5.19846700	-5.80923100	-1.68627100

H	-5.37133600	-4.97644300	-0.13254400
H	-5.81633500	-4.15050500	-1.63327700
O	-3.47971600	0.44481000	0.71995800
C	-3.32380500	0.15926300	-1.64207200
O	-2.87823200	-0.37335500	-2.65257400
C	-4.50378400	1.11150600	-1.65874200
H	-5.30720400	0.77416700	-0.99670000
H	-4.18613400	2.10461400	-1.32800300
H	-4.86461900	1.16774700	-2.68691100
C	0.70791400	0.83380800	-3.66446800
O	1.19229600	0.85472200	-2.51067200
O	-0.48394500	1.22257900	-3.97844800
H	-1.01110700	1.52753800	-3.11117400
C	1.53285900	0.30751500	-4.81324300
H	1.41716100	0.95339300	-5.68797000
H	2.58293900	0.22901400	-4.52837600
H	1.15836300	-0.68592000	-5.08592300

INT-11'

Rh	-0.64482300	-1.42314700	-0.70380800
N	-0.09287500	0.86791100	2.00031900
C	-2.43906500	-2.26494400	-1.87453800
C	-1.86951500	-1.04666300	-2.46416100
C	-0.54104000	-1.36046700	-2.93149000
C	-0.24160100	-2.68896300	-2.49569200
C	-1.44866800	-3.25529300	-1.88089200
C	-1.82858600	1.99545100	1.17717700
C	-0.89060000	1.97669600	0.15229200
C	-3.06034000	2.62744300	1.06142600
C	-1.15705200	2.64828300	-1.03231700
C	-3.32491800	3.28860900	-0.14368300
H	-3.77237400	2.61847300	1.87976500
C	-2.38419500	3.31060900	-1.17839900
H	-0.41876000	2.66790300	-1.83009200
H	-4.27482700	3.80156900	-0.26759300
H	-2.60582100	3.84147800	-2.09981500
C	0.77484900	0.07764500	-0.22359600
C	0.38226400	1.29811700	0.63771200
C	-1.52523400	-4.64750100	-1.32934800
C	0.98157500	-3.50134700	-2.79634200
C	-3.79963000	-2.32372200	-1.25003200
C	-2.68878000	0.15720500	-2.81444400
C	0.33521200	-0.47984900	-3.77028100
C	2.02340000	-0.20283800	-0.62174600

H	-2.46454400	-4.82155500	-0.79833700
H	-1.44920300	-5.39087700	-2.13386700
H	-0.70276100	-4.83479500	-0.63023100
H	-3.81115800	-1.70481100	-0.34391200
H	-4.56495700	-1.94344000	-1.93667600
H	-4.07291700	-3.34460300	-0.96993300
H	-3.30038900	0.48733800	-1.97067500
H	-2.06466000	0.99889700	-3.11713400
H	-3.36401600	-0.07937200	-3.64988900
H	0.11812600	0.57732000	-3.59810900
H	1.38932500	-0.64741600	-3.54431600
H	0.17190800	-0.68656800	-4.83700500
H	1.36953900	-3.97846300	-1.89091800
H	0.73361300	-4.29521200	-3.51450600
H	1.78086700	-2.89343100	-3.22014500
C	3.42110800	0.32778900	-0.43328000
H	3.44225300	1.35633600	-0.08888200
H	3.91526400	0.31277700	-1.41438900
C	4.23053100	-0.55947800	0.55290600
H	3.67748000	-0.60228900	1.49554600
H	4.27321100	-1.57670800	0.14761500
C	5.62658600	-0.02680200	0.78563100
C	6.66803800	-0.30091500	-0.11282500
C	5.90372200	0.78491000	1.89506600
C	7.94669500	0.22157300	0.08714200
H	6.47435700	-0.93676600	-0.97473800
C	7.18109800	1.30995600	2.09985600
H	5.10823100	0.99563500	2.60678000
C	8.20758200	1.03096800	1.19524800
H	8.74099300	-0.00722200	-0.61927800
H	7.37589700	1.93278100	2.96952500
H	9.20350700	1.43618400	1.35464300
F	2.19089200	-1.36182900	-1.37883900
F	-1.94703500	-0.87284700	0.85661300
C	1.47756800	2.39609600	0.83852500
C	1.03976500	3.64898100	1.61355800
H	1.83381000	2.69830100	-0.15356000
H	2.31172300	1.94170400	1.37464800
C	2.21687500	4.60382800	1.86390300
H	0.25352600	4.18393300	1.06735800
H	0.60457900	3.36013800	2.57978400
C	1.80888200	5.86647300	2.63048300
H	3.00381700	4.07535900	2.41990500
H	2.66478500	4.88965000	0.90131700

H	2.66640800	6.52932100	2.79412400
H	1.04727800	6.43469800	2.08221100
H	1.38954400	5.61518100	3.61261100
O	-1.38970700	1.39544500	2.32155800
C	0.63972300	0.42302200	3.05892700
O	1.80247600	0.03825300	2.90518000
C	-0.06560800	0.39369300	4.40124100
H	-0.44204900	1.38421300	4.67518900
H	-0.91823300	-0.29057200	4.36975800
H	0.65569800	0.05020200	5.14458600
C	0.16993000	-2.74604300	1.99954400
O	0.45658900	-2.65029200	0.79041800
O	-0.89234300	-2.22888200	2.54701900
H	-1.41582600	-1.62972900	1.84067700
C	1.09927700	-3.45898300	2.94572900
H	1.75343200	-2.69745900	3.38745600
H	0.54059500	-3.94537300	3.74901800
H	1.71488800	-4.18046000	2.40594700

INT-11"

Rh	-0.21028100	-1.13419800	-0.61575100
N	-0.71572300	1.64551100	2.15573200
C	-1.40821600	-2.52269500	-1.73390200
C	-1.74156200	-1.19560500	-2.23642200
C	-0.56398800	-0.64065200	-2.80837900
C	0.50443900	-1.63096400	-2.70550100
C	-0.03866300	-2.80582300	-2.10079600
C	-2.44742900	2.16950800	0.85450700
C	-1.32216500	2.48816900	0.10151600
C	-3.73893900	2.46473400	0.42688300
C	-1.46233400	3.14097800	-1.11601900
C	-3.87094400	3.11135500	-0.80548200
H	-4.59889400	2.20999800	1.03681500
C	-2.75014300	3.45450000	-1.57188500
H	-0.58859000	3.41265300	-1.70227200
H	-4.86489100	3.36325900	-1.16528300
H	-2.87802500	3.97626400	-2.51583300
C	0.65304300	0.89446900	0.22565600
C	-0.08532000	2.03732800	0.85660900
C	0.70885700	-4.04450800	-1.71430400
C	1.87303000	-1.48282800	-3.30277100
C	-2.36820300	-3.43883800	-1.03779300
C	-3.08293200	-0.55631800	-2.05904900
C	-0.42582900	0.67875200	-3.50475200

C	1.63897200	0.17220100	0.04752200
H	0.94495300	-3.97872500	-0.64228000
H	0.10404600	-4.94034800	-1.88792600
H	1.64126000	-4.14699400	-2.27579500
H	-2.86168100	-2.90200100	-0.22107700
H	-3.13721100	-3.80793500	-1.72936100
H	-1.85160400	-4.29940500	-0.60595600
H	-3.31688100	-0.51129500	-0.98918000
H	-3.10873800	0.46189900	-2.45290400
H	-3.86122000	-1.14347000	-2.56242500
H	-1.25475700	1.34759800	-3.26748400
H	0.50452300	1.18250900	-3.22315700
H	-0.40466900	0.53209200	-4.59324800
H	2.59941200	-2.13782400	-2.81500800
H	1.85774100	-1.73802100	-4.37145800
H	2.23777500	-0.45475300	-3.21852400
C	2.91941700	-0.54220700	0.12127200
H	3.40561700	-0.58487700	-0.86163900
H	2.67633400	-1.56582200	0.42716600
C	3.87674300	0.10685700	1.15810500
H	4.11187000	1.13086800	0.84380300
H	3.34259600	0.17356300	2.11089700
C	5.15025300	-0.69655000	1.30548400
C	5.17622400	-1.84407700	2.11214200
C	6.31835700	-0.33679900	0.62033300
C	6.33708000	-2.60899600	2.22997600
H	4.27904100	-2.13263800	2.65536200
C	7.48293200	-1.09878800	0.73628900
H	6.31739900	0.55470000	-0.00399500
C	7.49524900	-2.23877500	1.54171700
H	6.33907700	-3.49180600	2.86423500
H	8.38068600	-0.79895100	0.20139100
H	8.40109200	-2.83187500	1.63651800
F	0.66035000	-2.29903400	0.75224600
F	-1.61899900	-0.74648000	0.75546600
C	0.95386400	3.17635800	1.08887200
C	0.40042700	4.42837400	1.77693300
H	1.37255600	3.43823200	0.10764100
H	1.76510600	2.74922400	1.68552700
C	1.48632900	5.48955400	2.00681300
H	-0.40969300	4.86183300	1.17557300
H	-0.04246500	4.14395700	2.73932500
C	0.95239600	6.74725600	2.70070300
H	2.29670800	5.05510900	2.60856000

H	1.93724700	5.76735900	1.04301500
H	1.74676200	7.48686400	2.85362900
H	0.16264200	7.22326800	2.10631100
H	0.52711400	6.50624000	3.68254400
O	-2.15431300	1.60330200	2.04995600
C	-0.16294700	0.72075800	3.03546900
O	1.05485400	0.67259800	3.14211800
C	-1.12751100	-0.13968800	3.80853100
H	-1.90297800	0.45146900	4.30444000
H	-1.61006900	-0.80402300	3.08339500
H	-0.55983700	-0.71478400	4.54135500

TS-6

Rh	0.24142400	1.68864900	-0.53417700
N	-2.81171900	-0.14412600	-0.64798600
C	0.07346400	3.76387400	0.23326200
C	-0.33118700	2.83170600	1.26758900
C	0.82766300	2.04323100	1.62716000
C	1.91130600	2.43126800	0.78252000
C	1.43884600	3.50408400	-0.08344400
C	-3.15694900	-0.07177700	1.53717000
C	-2.18472700	-1.05227100	1.35156700
C	-3.76777500	0.18092500	2.76120400
C	-1.81069800	-1.83647600	2.44171700
C	-3.36927300	-0.60487400	3.84668000
H	-4.52914200	0.94833600	2.85494900
C	-2.40341300	-1.60401700	3.69010500
H	-1.07025900	-2.61802200	2.33105700
H	-3.82766300	-0.44147500	4.81823400
H	-2.11505300	-2.21498400	4.54058300
C	-0.32968700	-0.57430400	-0.43237500
C	-1.77982600	-1.07405800	-0.12587000
C	2.28054900	4.18651200	-1.11714300
C	3.33740500	1.97573200	0.84930000
C	-0.85185000	4.72298800	-0.44808000
C	-1.63672800	2.90535000	1.99684100
C	0.87898300	1.05147600	2.74940900
C	0.72140300	-1.32847100	-0.03404500
H	1.72172500	4.96832100	-1.63687900
H	3.16217500	4.64627900	-0.65285500
H	2.62210200	3.46504000	-1.86732500
H	-1.50105200	5.22327200	0.27849500
H	-0.30552400	5.48892800	-1.00485100
H	-1.47651700	4.15732600	-1.15298100

H	-2.47879900	2.92539400	1.30020900
H	-1.77624900	2.05543100	2.66596500
H	-1.67396800	3.82077200	2.60458200
H	-0.05042700	0.48280700	2.82919300
H	1.69717000	0.33776100	2.62448600
H	1.03634100	1.57540800	3.70219000
H	3.75302500	1.80456400	-0.14878100
H	3.96002500	2.73731500	1.33906400
H	3.43965300	1.05151900	1.42159300
C	2.14298700	-1.32284600	-0.53509700
H	2.41427400	-0.31861700	-0.86454500
H	2.15116800	-1.94777200	-1.44148400
C	3.19345100	-1.88856800	0.44727900
H	3.23664300	-1.26605500	1.34921700
H	2.86792600	-2.88129200	0.77469300
C	4.57191900	-1.98388400	-0.17668800
C	4.83354300	-2.93273800	-1.17713400
C	5.61400800	-1.13586400	0.21874500
C	6.09295000	-3.02442800	-1.76902400
H	4.04324400	-3.61152700	-1.49127400
C	6.87825800	-1.22446100	-0.36924300
H	5.43870800	-0.40374300	1.00371500
C	7.12134000	-2.16792600	-1.36764800
H	6.27347100	-3.76869300	-2.54029800
H	7.67256400	-0.55772800	-0.04340600
H	8.10383400	-2.23989600	-1.82626300
F	0.53708600	-2.41542400	0.79097800
F	-1.28215200	2.03551800	-1.77936500
C	-1.98123600	-2.48592500	-0.77081200
C	-3.40183900	-3.05620200	-0.69035600
H	-1.28918200	-3.16887900	-0.27024200
H	-1.68142300	-2.41237600	-1.81837700
C	-3.48531000	-4.46959600	-1.28500300
H	-3.74314000	-3.08292800	0.35370300
H	-4.09235000	-2.40071700	-1.23319000
C	-4.89942600	-5.05792100	-1.23292200
H	-3.13831300	-4.44276600	-2.32713600
H	-2.79278500	-5.13456200	-0.74845900
H	-4.93082700	-6.06544700	-1.66420000
H	-5.26354600	-5.12564100	-0.19996100
H	-5.60703600	-4.43369300	-1.79227700
O	-3.44414900	0.61793500	0.39604900
C	-3.18382000	0.14672900	-1.93501700
O	-2.73996600	-0.50951500	-2.86881600

C	-4.19089200	1.26624000	-2.09587900
H	-5.09106300	1.09467900	-1.49732200
H	-3.72948700	2.20268600	-1.77396000
H	-4.45057500	1.32490700	-3.15401800
C	0.99735900	0.56989300	-3.22848500
O	1.35610800	1.42641700	-2.36140200
O	0.23452000	-0.41288000	-2.99296200
H	-0.09969000	-0.38362500	-1.75652600
C	1.50804100	0.73897200	-4.64298900
H	0.76326700	1.31569300	-5.20407500
H	2.45231300	1.28775900	-4.65325000
H	1.61914200	-0.23353800	-5.12759300

TS-6'

Rh	-0.71502500	-1.87337800	-0.20900700
N	-0.92516100	1.04469700	1.93934800
C	-2.40183200	-2.11408300	-1.63203600
C	-1.49331500	-1.13269300	-2.16491400
C	-0.22721200	-1.80083500	-2.43298000
C	-0.33587700	-3.14951600	-2.00547300
C	-1.68529200	-3.34854200	-1.48171200
C	-1.53618100	2.27120200	0.20992800
C	-0.15114200	2.14476500	0.09923000
C	-2.29775000	3.10950400	-0.59758700
C	0.50821200	2.91093100	-0.85942500
C	-1.61869800	3.85554400	-1.56449000
H	-3.37182900	3.18358000	-0.46204900
C	-0.22976500	3.76107700	-1.69512200
H	1.58657700	2.87875900	-0.96453900
H	-2.17868000	4.52645600	-2.21016600
H	0.28715500	4.36145900	-2.43793700
C	0.80197600	-0.22658000	0.60599500
C	0.34076300	1.15542200	1.16439500
C	-2.21312200	-4.64460800	-0.94699800
C	0.71140600	-4.21829100	-2.07241500
C	-3.79636300	-1.85141200	-1.15120400
C	-1.85872500	0.24323800	-2.62893800
C	0.93675000	-1.18049200	-3.14384700
C	1.96792900	-0.38634900	-0.05584600
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H	-4.25240600	-1.01475000	-1.68763200

H	-4.43431500	-2.73064500	-1.28272100
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H	-1.02721200	0.94403200	-2.52726000
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H	4.66374900	-0.90820900	0.01580000
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C	1.04260500	3.02964700	2.86238900
H	2.31105700	1.99021000	1.47415700
H	1.73245100	0.98420000	2.80353100
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C	0.69944300	-3.20899400	2.11147000
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TS-6''

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C	-1.85472500	-1.30717100	-1.69712800
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C	-0.42965300	2.61645300	-0.90750200
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H	2.22355100	5.07006100	2.01305700
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H	-0.18166600	6.02580200	3.68807400
O	-2.33694100	2.43328400	0.36433100

C	-1.51538300	1.30278700	2.29522200
O	-0.61619100	0.81458600	2.96115900
C	-2.90680300	1.57678600	2.83354100
H	-3.10040000	2.65468500	2.86210500
H	-3.68313500	1.12763900	2.20710600
H	-2.95765000	1.16740900	3.84343500

Cp*RhF₂

Rh	-0.24261900	-1.41212500	-0.39640200
C	-1.58415600	-2.57153900	-1.58786000
C	-1.64673500	-1.20830900	-2.08765500
C	-0.33372500	-0.85779600	-2.50595500
C	0.53477100	-2.03328800	-2.34158400
C	-0.24871100	-3.09855500	-1.82067000
C	0.21459600	-4.48742000	-1.49998800
C	1.98447300	-2.08351900	-2.71411000
C	-2.73804200	-3.34789700	-1.03490000
C	-2.85833200	-0.32595100	-2.08728400
C	0.10662700	0.45794000	-3.06955400
H	-0.29023300	-4.87962900	-0.61282200
H	0.00888700	-5.16970900	-2.33529800
H	1.28849900	-4.51134900	-1.29910700
H	-3.26926200	-3.85966400	-1.84965600
H	-2.40472900	-4.10679100	-0.32260300
H	-3.45198800	-2.69566100	-0.52582200
H	-3.51408600	-0.55182600	-1.24200900
H	-2.58134100	0.72838600	-2.00959500
H	-3.43830600	-0.45917200	-3.01001000
H	-0.55156500	1.26993000	-2.75168000
H	1.12306700	0.70789000	-2.75240400
H	0.09834600	0.42354800	-4.16759800
H	2.51034300	-2.87215400	-2.17084800
H	2.09488500	-2.27941600	-3.78943700
H	2.48571100	-1.13628800	-2.49559700
F	0.81213400	-2.07557200	1.06925200
F	-0.77010600	0.01761400	0.77813600

Cp*RhF(OAc)

Rh	1.07767200	2.17635900	-1.35688100
C	0.38954000	3.74085000	0.01906000
C	0.23288600	2.44319700	0.61776800
C	1.56308000	1.85925700	0.78704800
C	2.51133800	2.76191800	0.23436500
C	1.78344900	3.91858000	-0.28607200

C	2.40595300	5.12321600	-0.92464700
C	3.99930700	2.59371100	0.17123200
C	-0.72417500	4.65003600	-0.40912000
C	-1.05167500	1.83212500	1.08982200
C	1.83632900	0.53496200	1.43356400
H	1.69460500	5.63781400	-1.57547100
H	2.74800500	5.83555200	-0.16098700
H	3.27131800	4.84567200	-1.53354900
H	-1.03609400	4.36733000	-1.42440000
H	-1.58514900	4.56533000	0.26015300
H	-0.40173000	5.69525400	-0.41780500
H	-1.90375100	2.21428900	0.52211300
H	-1.03796200	0.74436800	0.97487600
H	-1.22112600	2.05486500	2.15248400
H	1.11345100	-0.21946200	1.10877500
H	2.83474200	0.16478400	1.18802200
H	1.76652100	0.61808200	2.52639400
H	4.38864000	2.89131600	-0.80709000
H	4.48970000	3.21645700	0.93130000
H	4.29579400	1.55634200	0.34462400
F	-0.21261600	2.70020700	-2.74008700
C	1.71168300	0.44110000	-3.08857300
O	2.34303000	1.54455300	-3.02439600
O	0.86972700	0.15897100	-2.17676800
C	1.92587900	-0.49628300	-4.24845800
H	1.73532500	-1.52917000	-3.94693100
H	1.21838700	-0.23405600	-5.04379700
H	2.93954400	-0.39279200	-4.64318700

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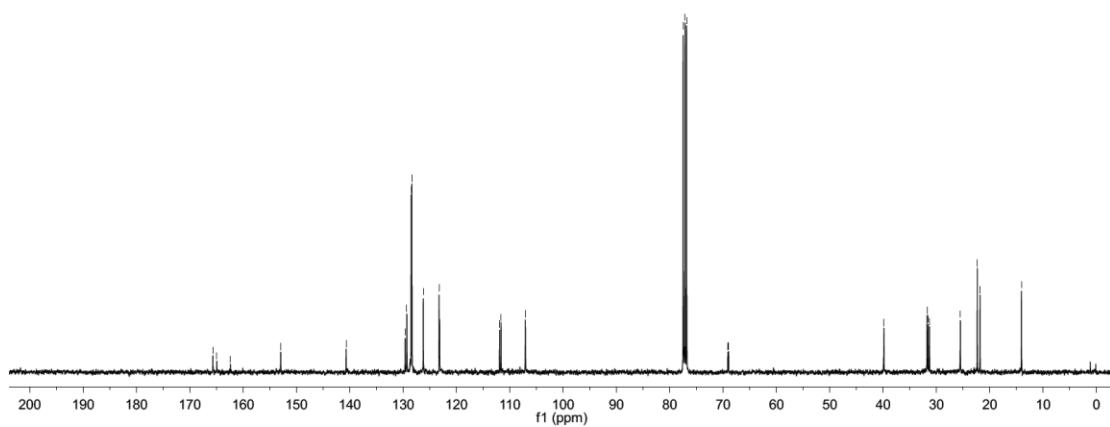
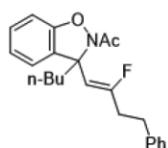
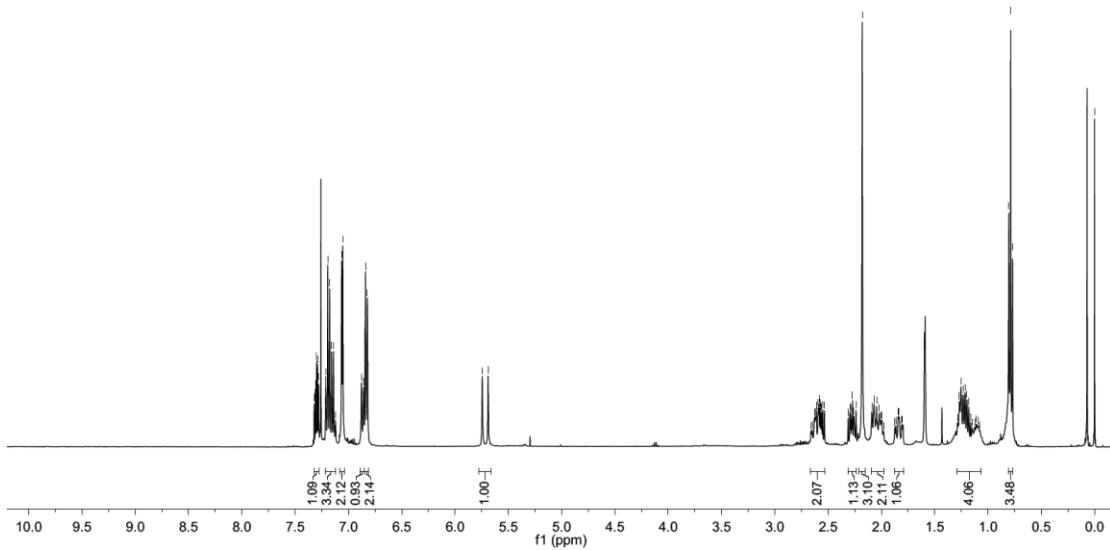
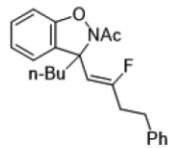
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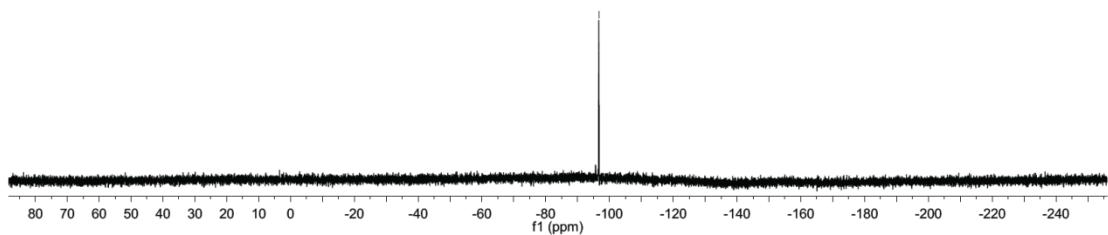
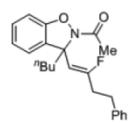
VI. Copies of ^1H and ^{13}C NMR Spectra

3a

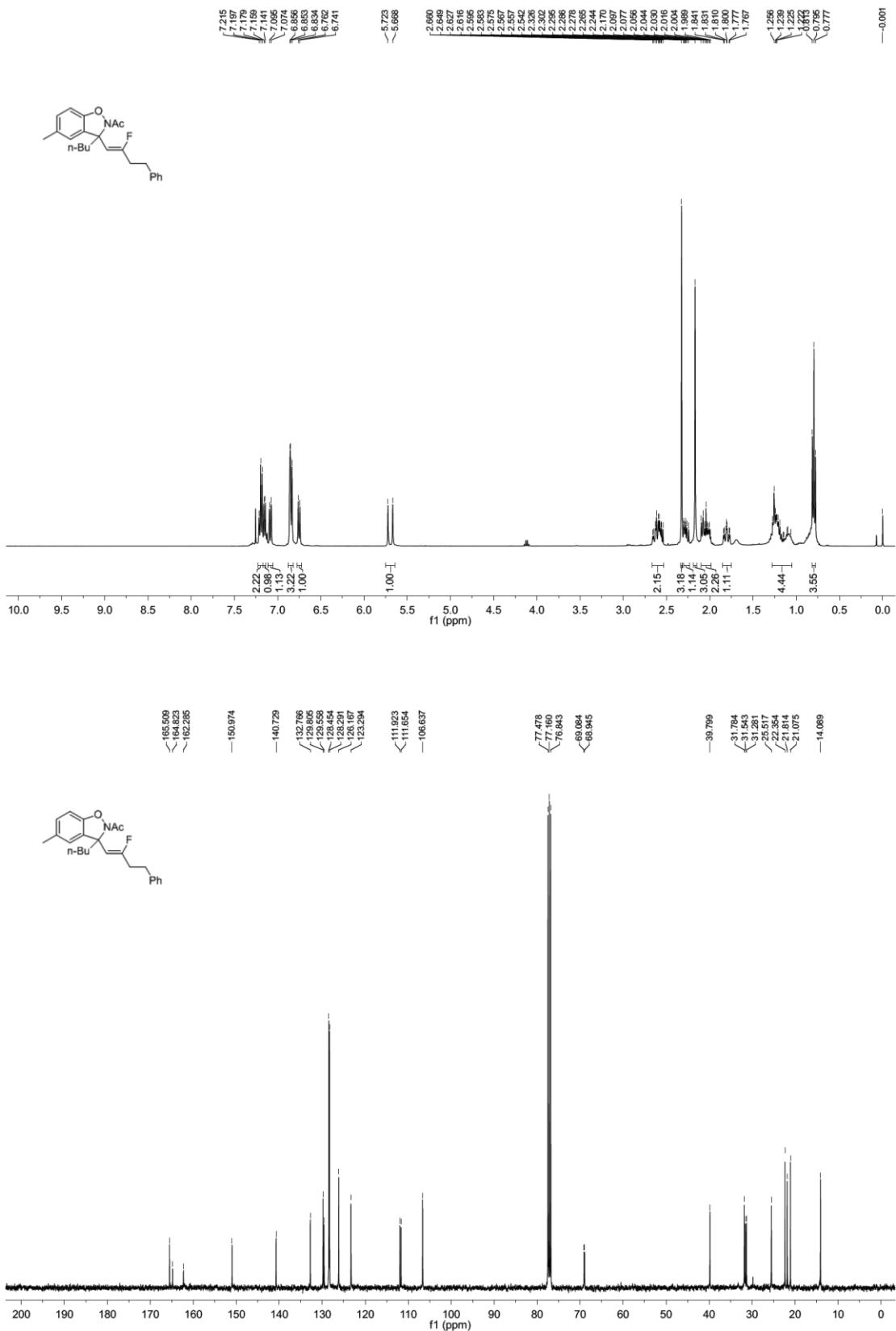


¹⁹F NMR spectrum of 3a

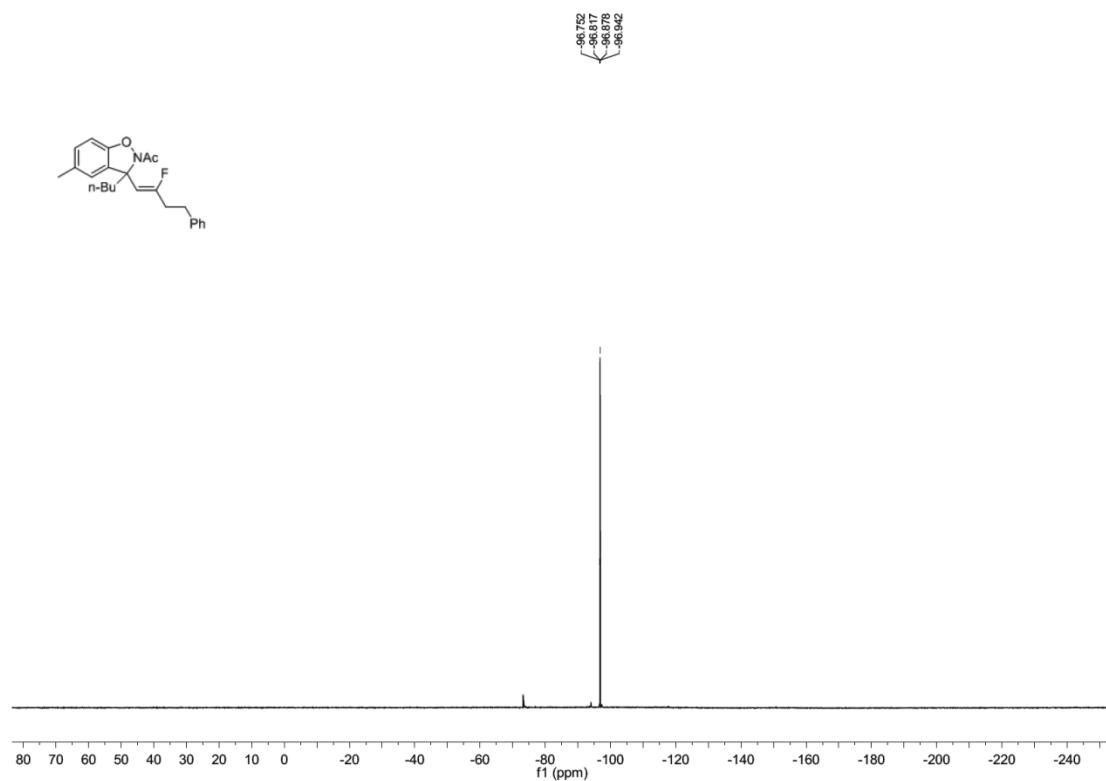
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98.775



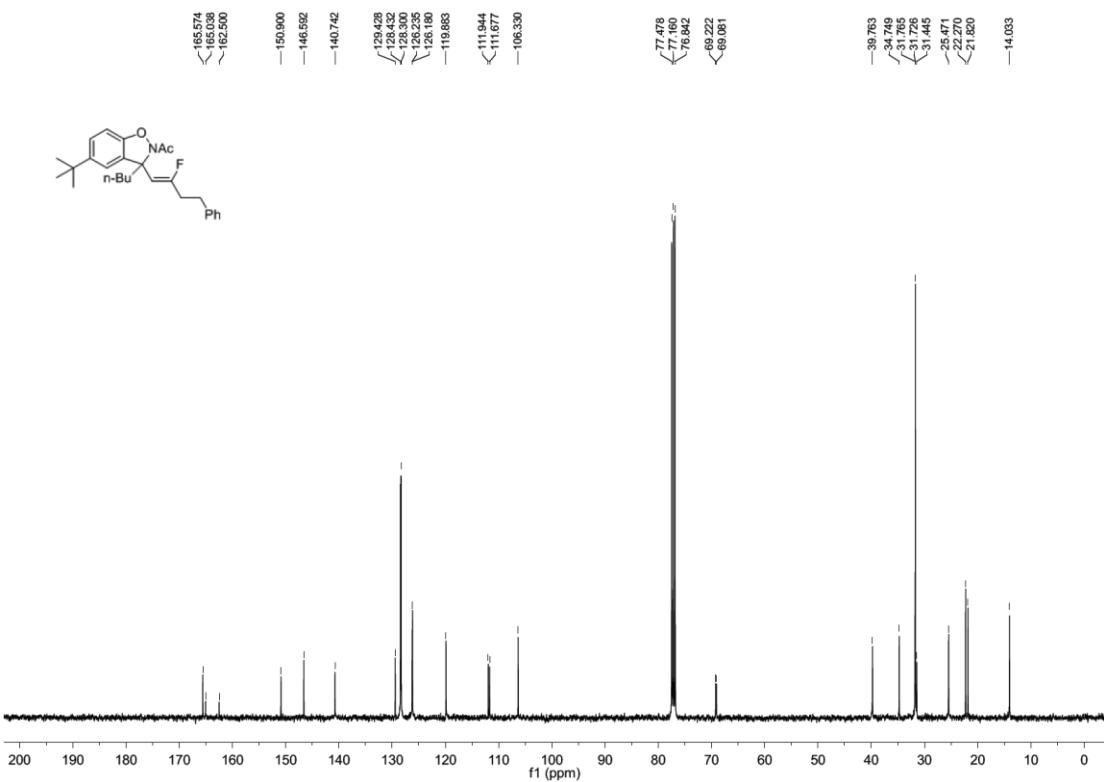
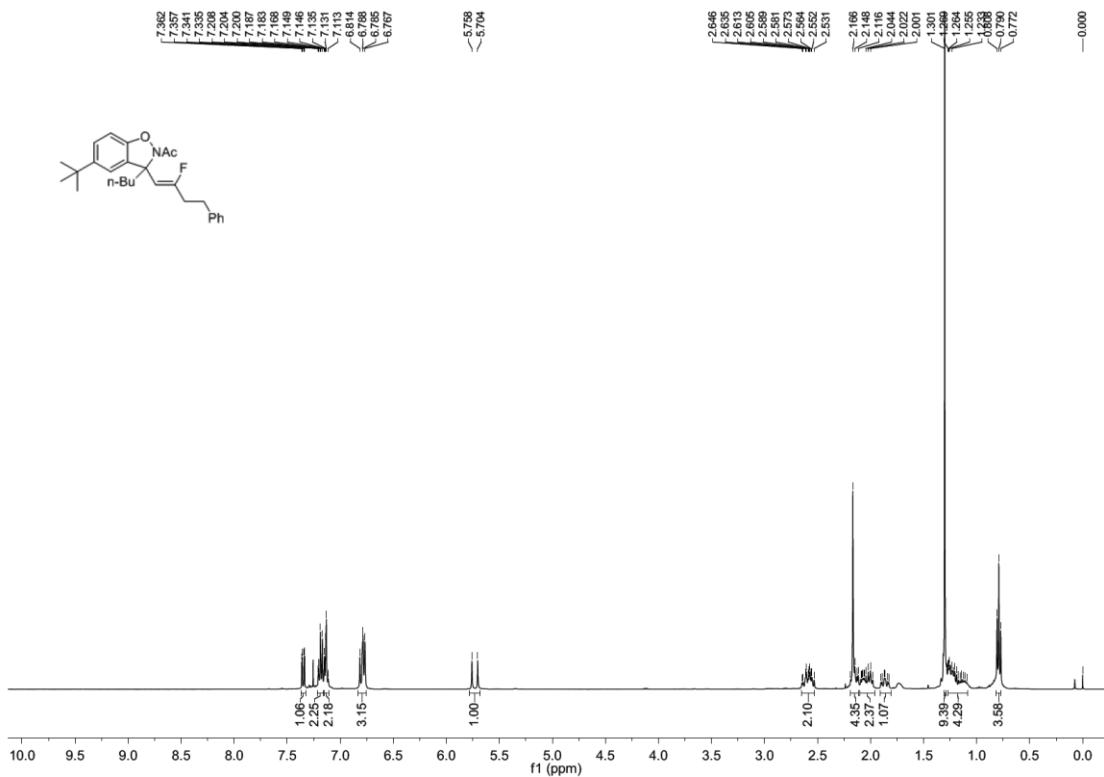
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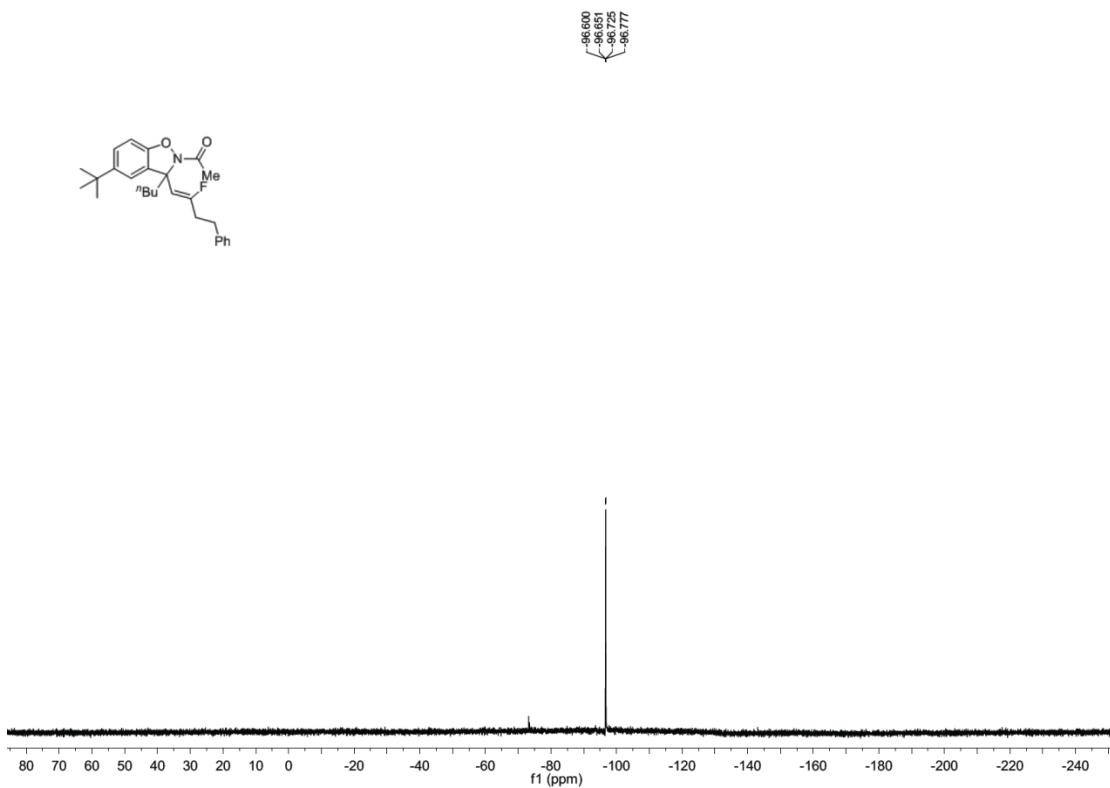
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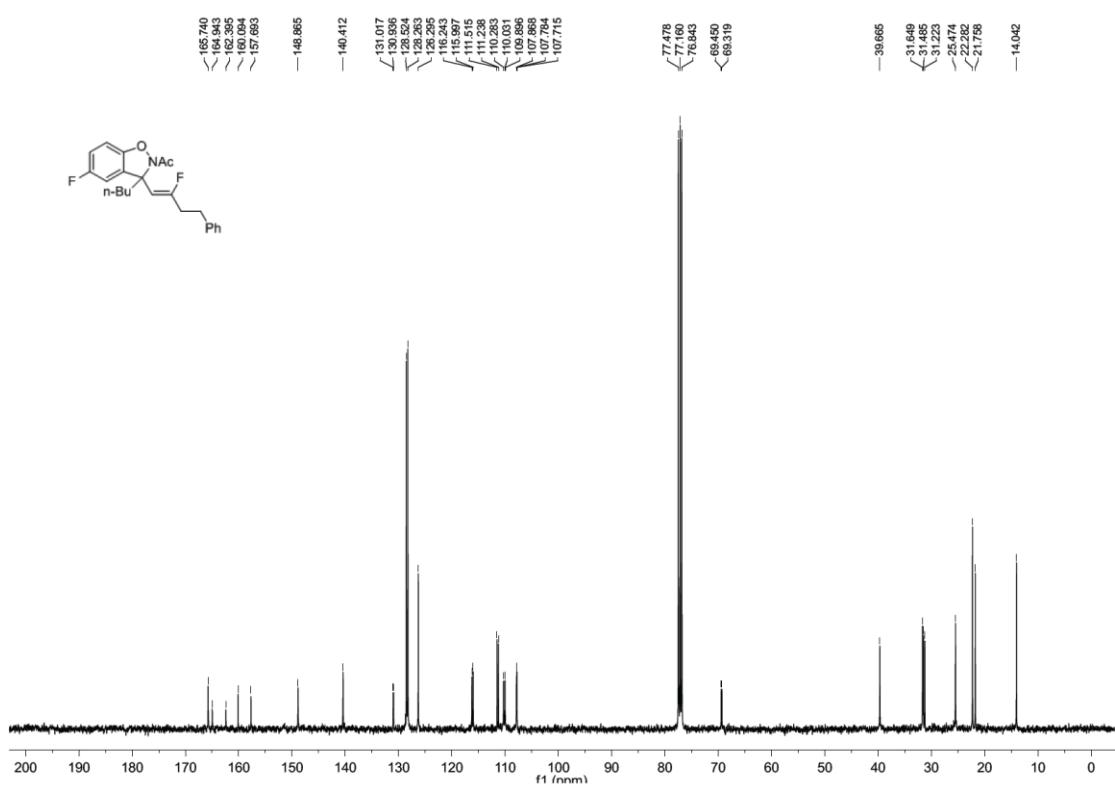
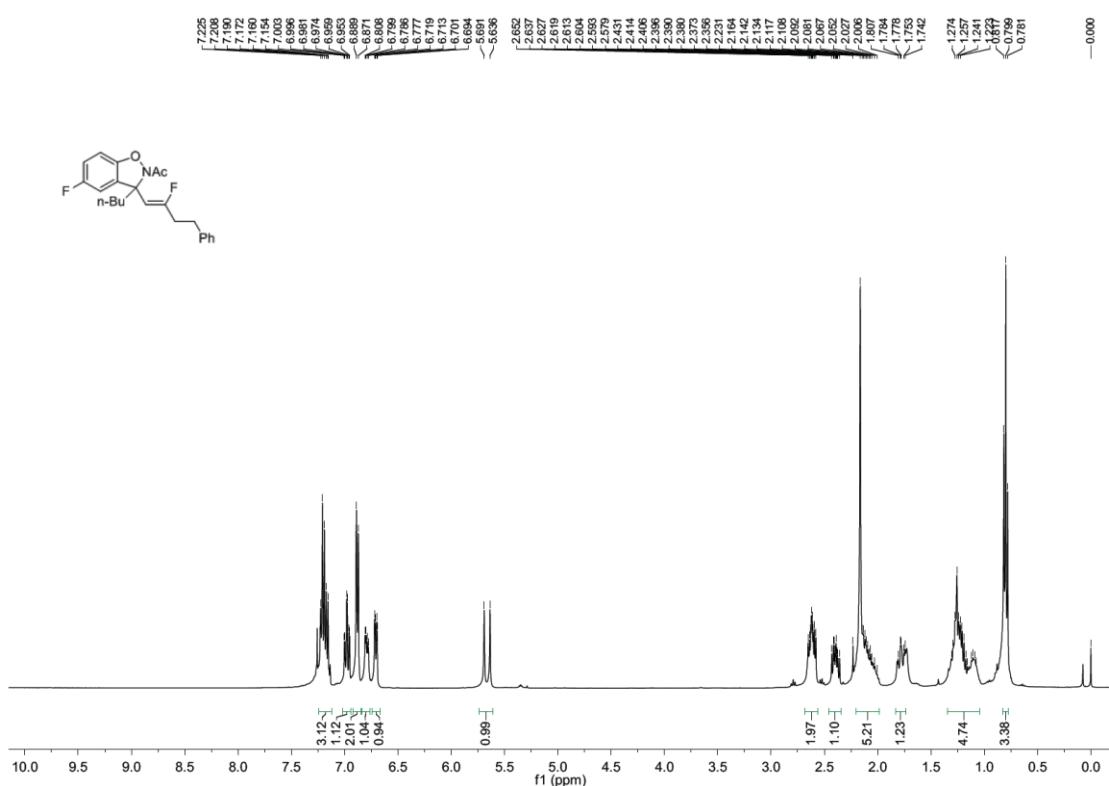
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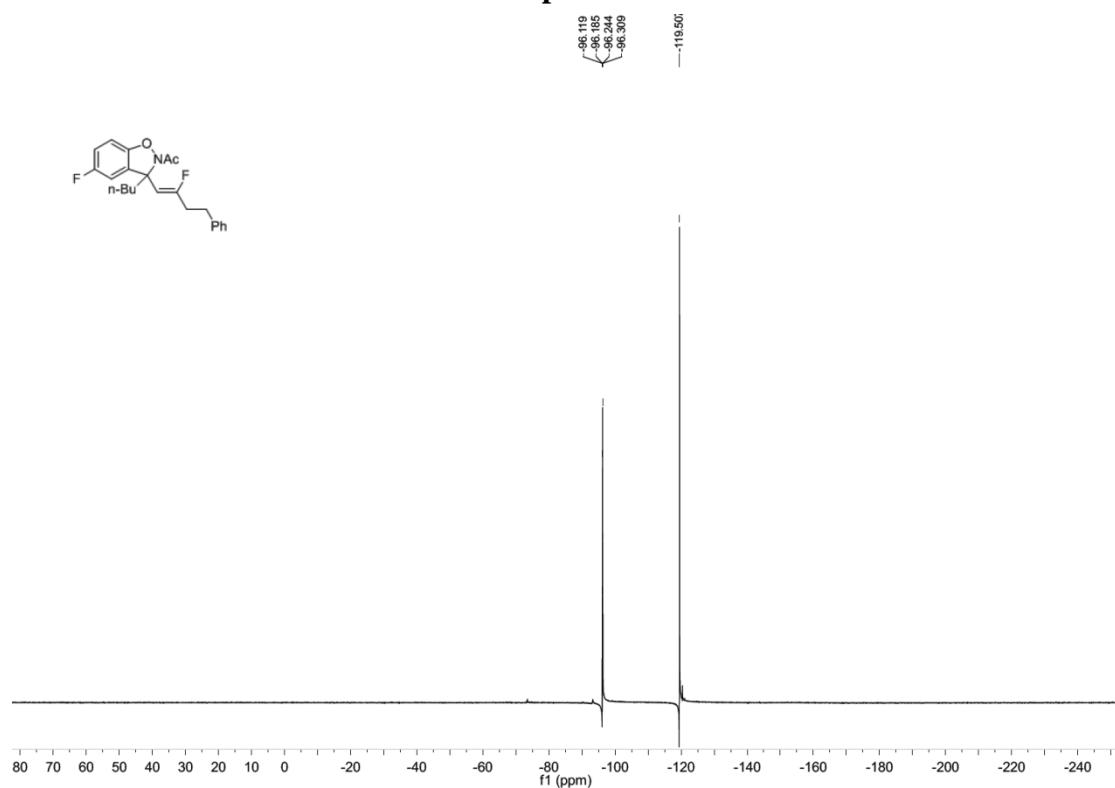
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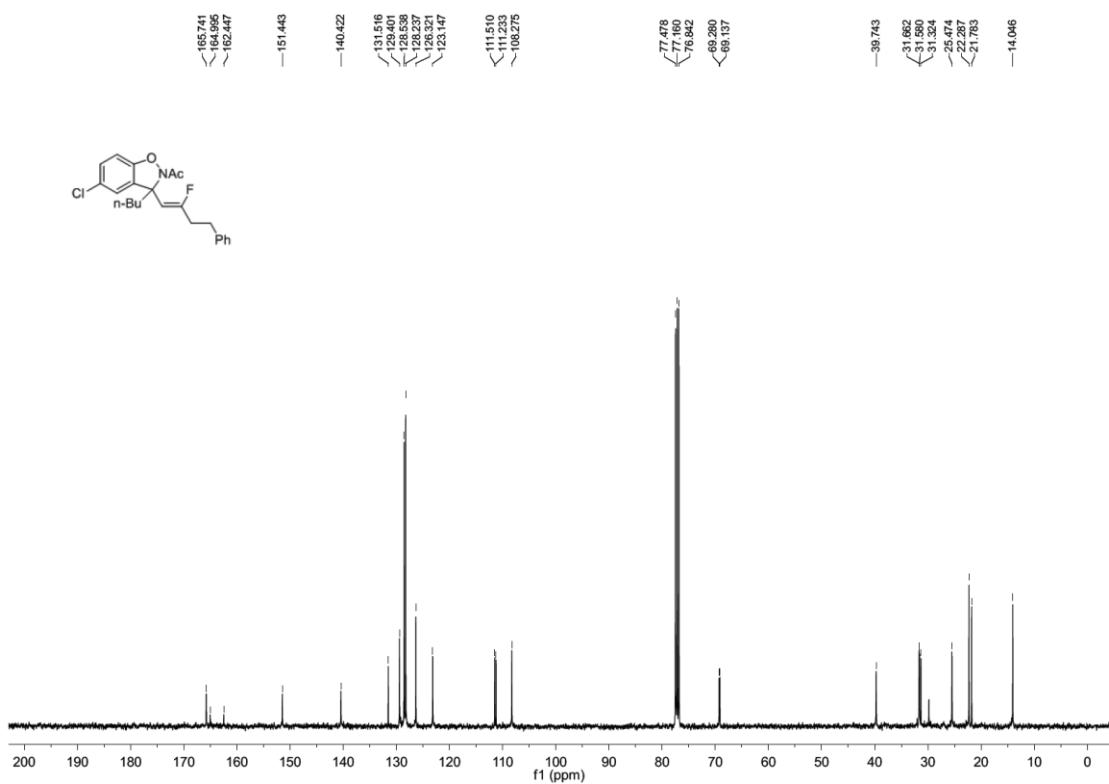
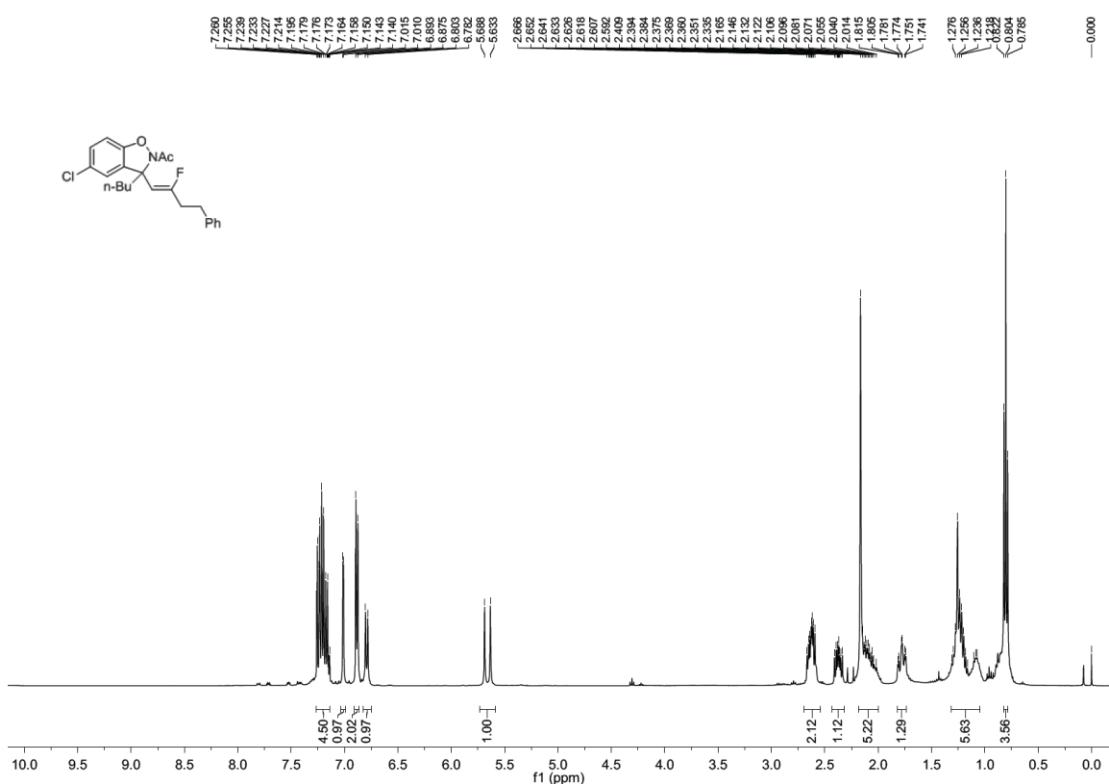
3d



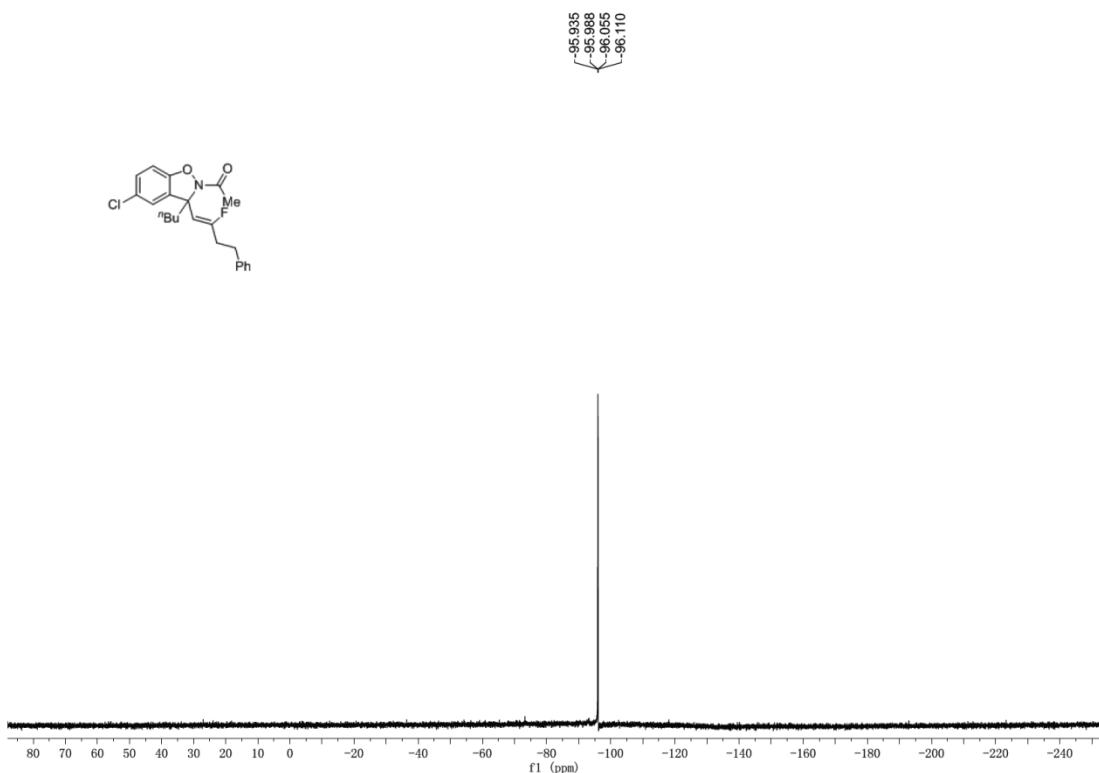
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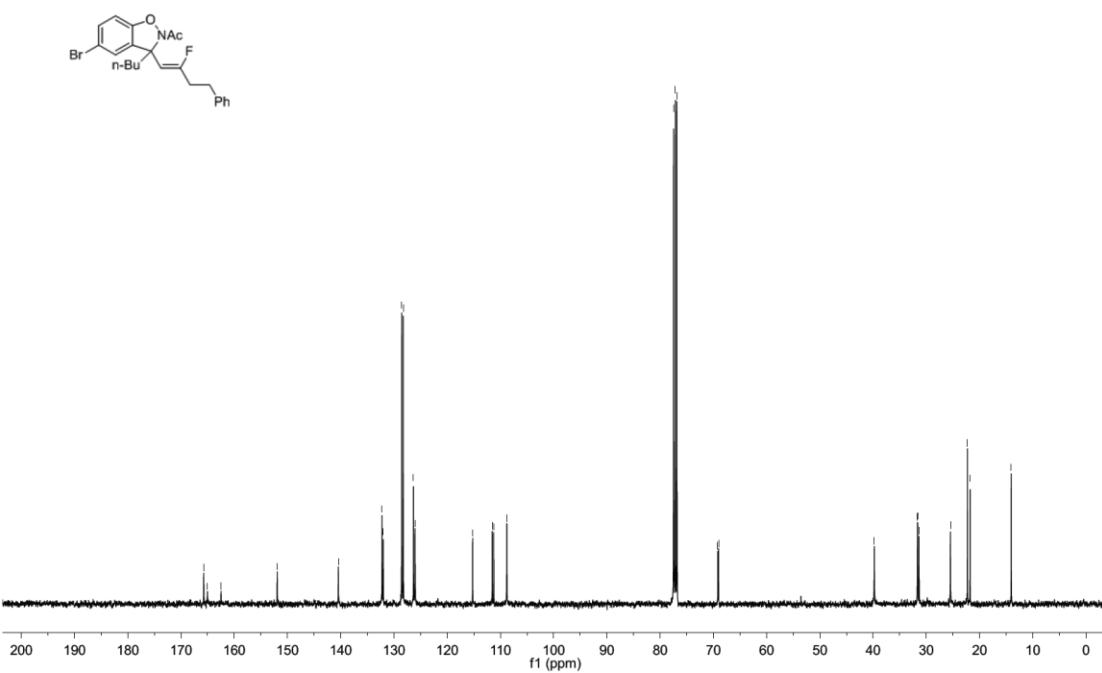
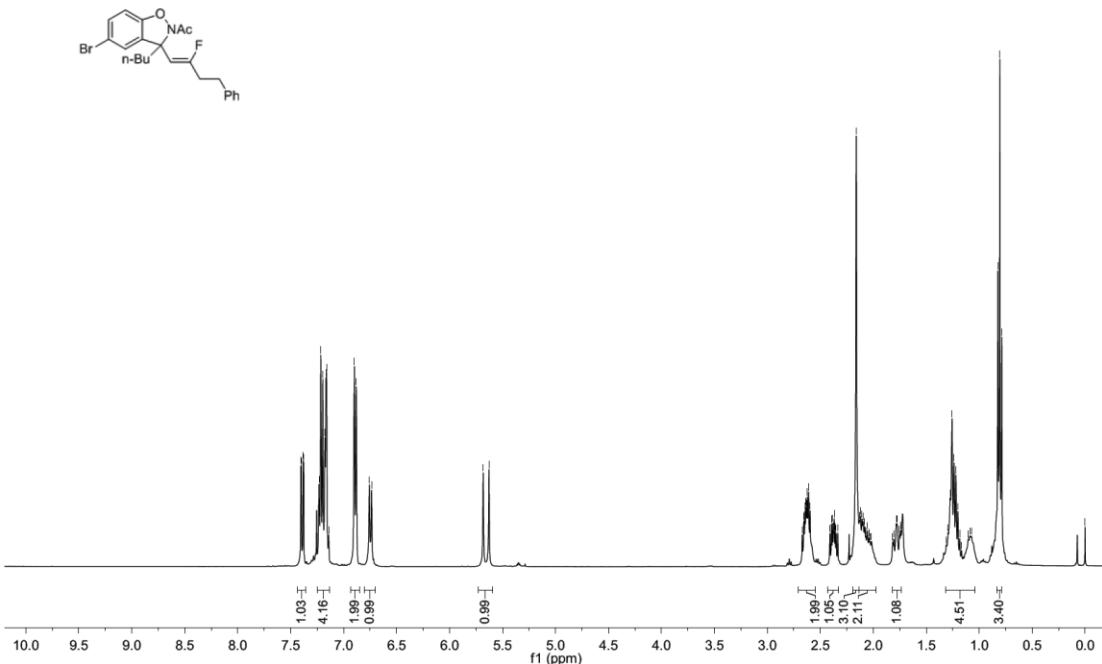
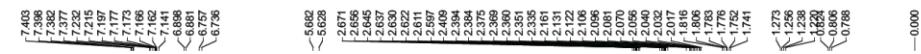
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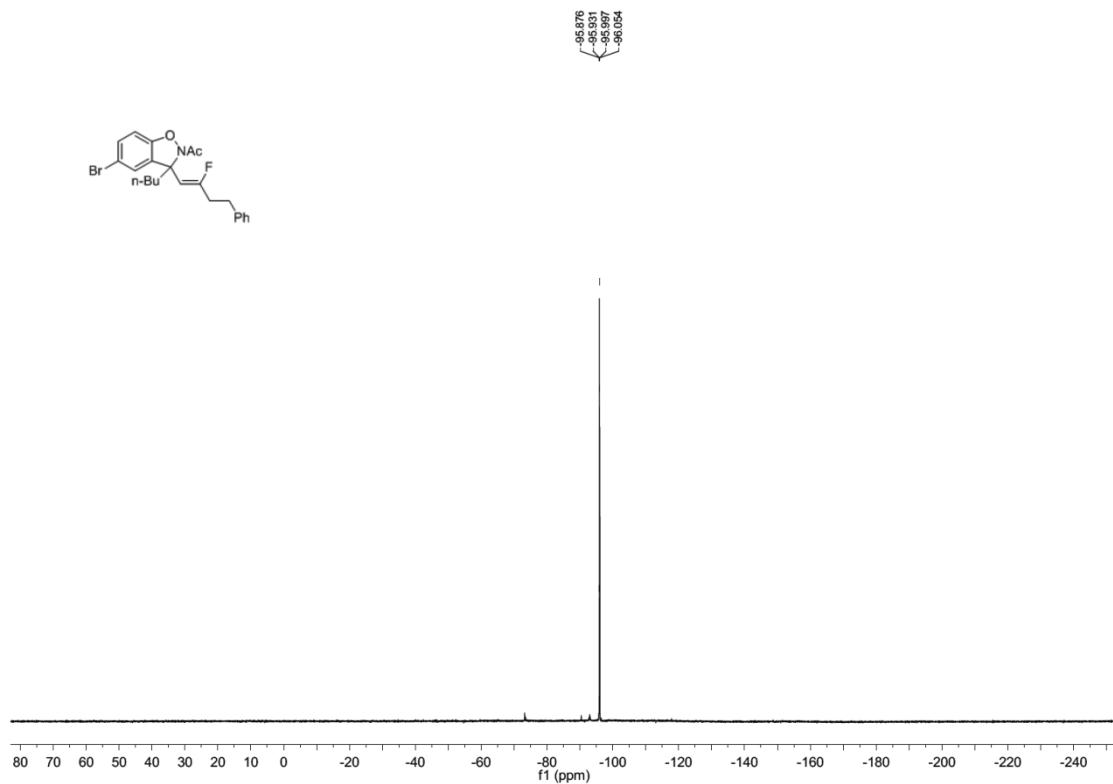
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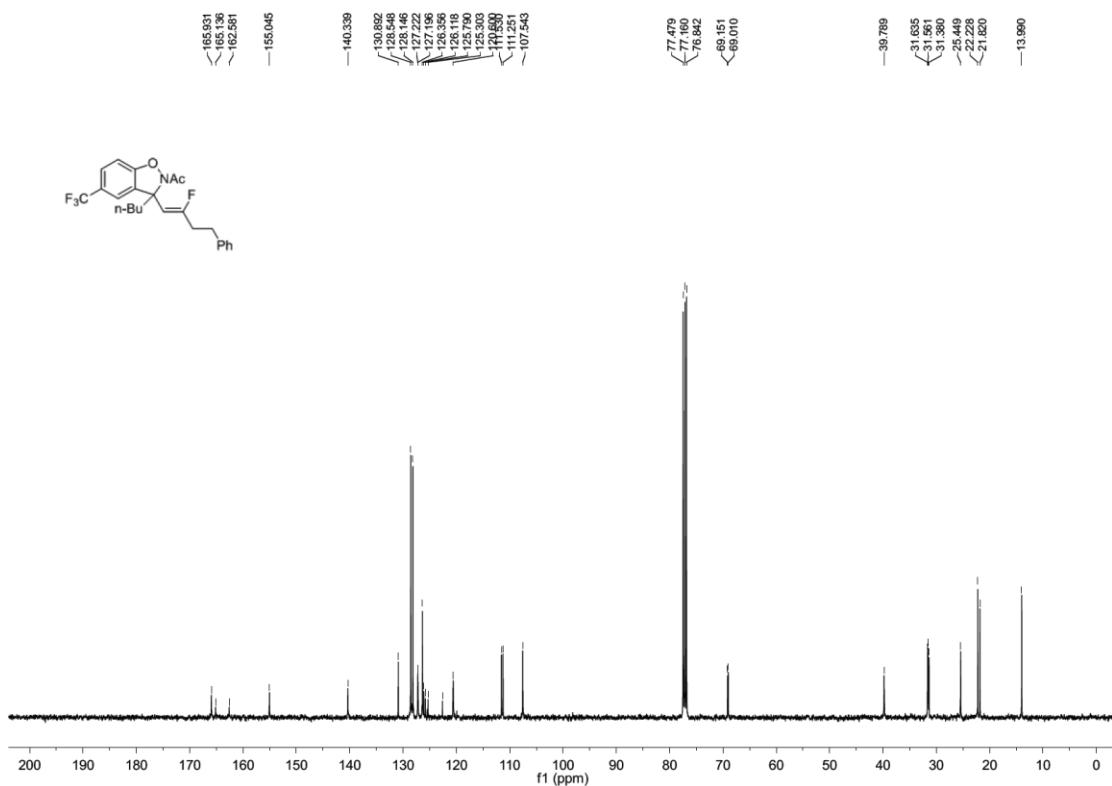
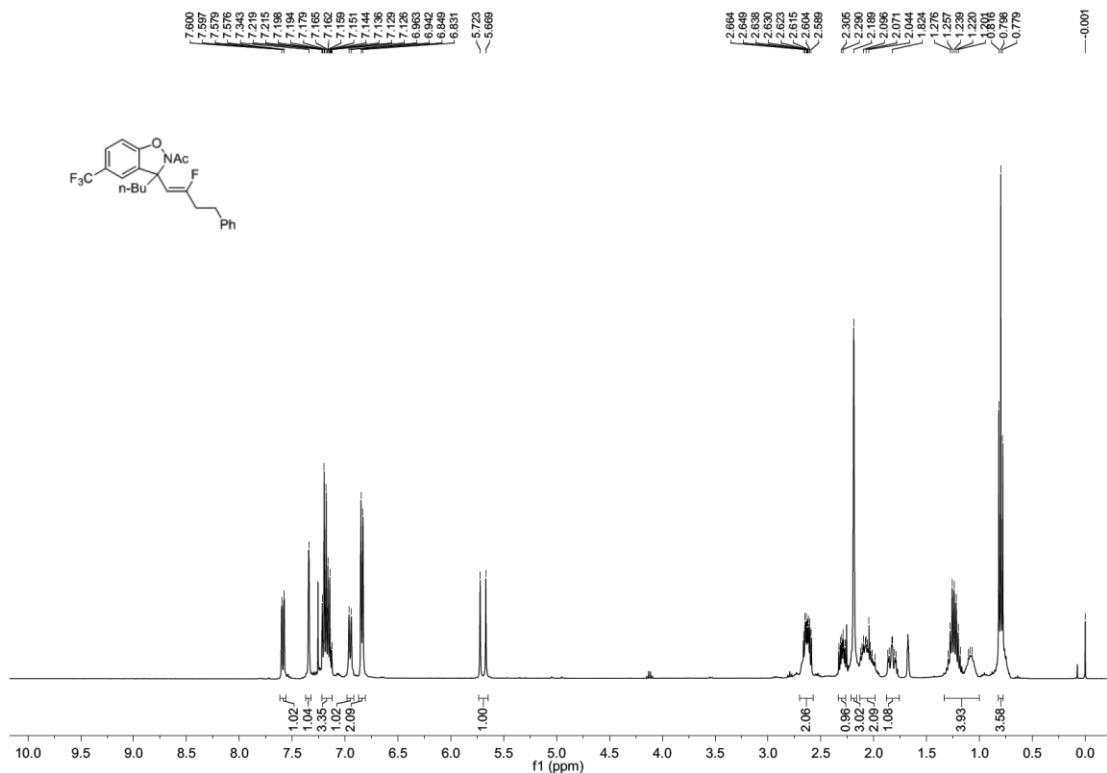
3f



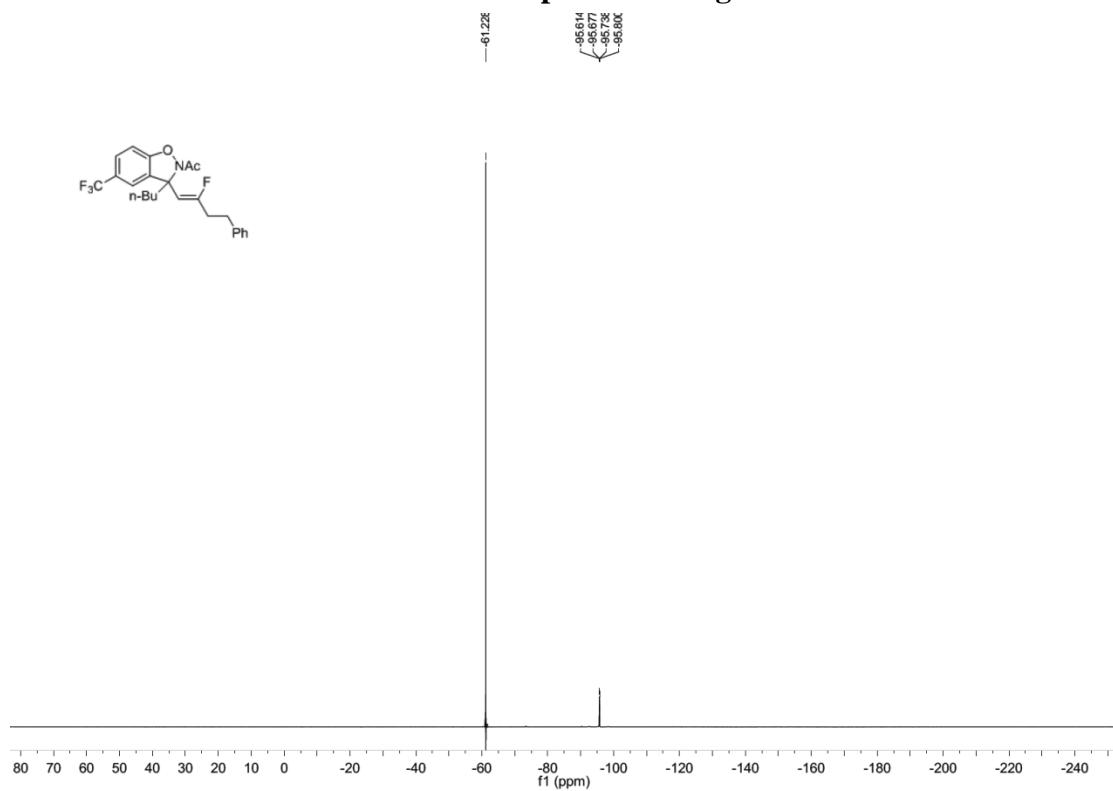
¹⁹F NMR spectrum of 3f



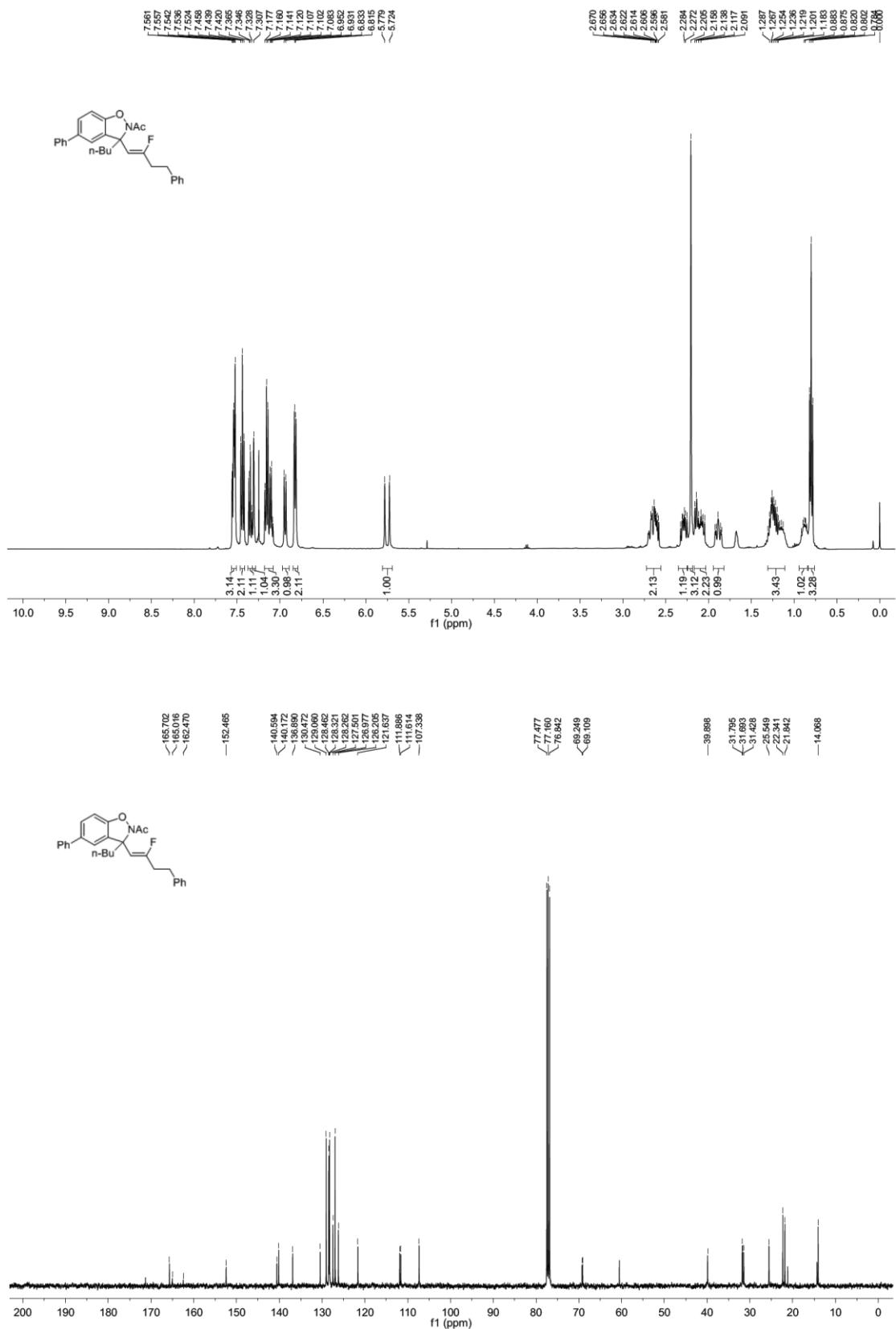
3g



¹⁹F NMR spectrum of 3g

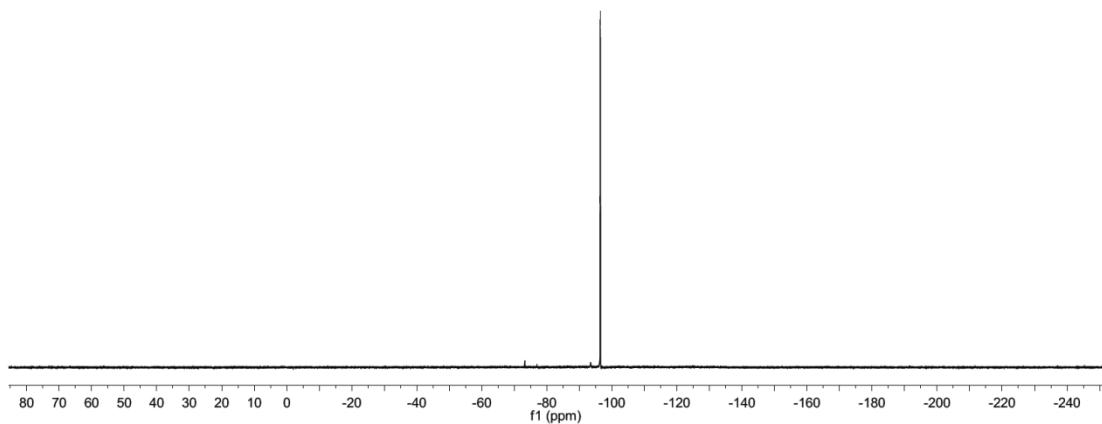
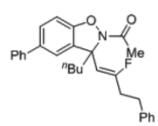


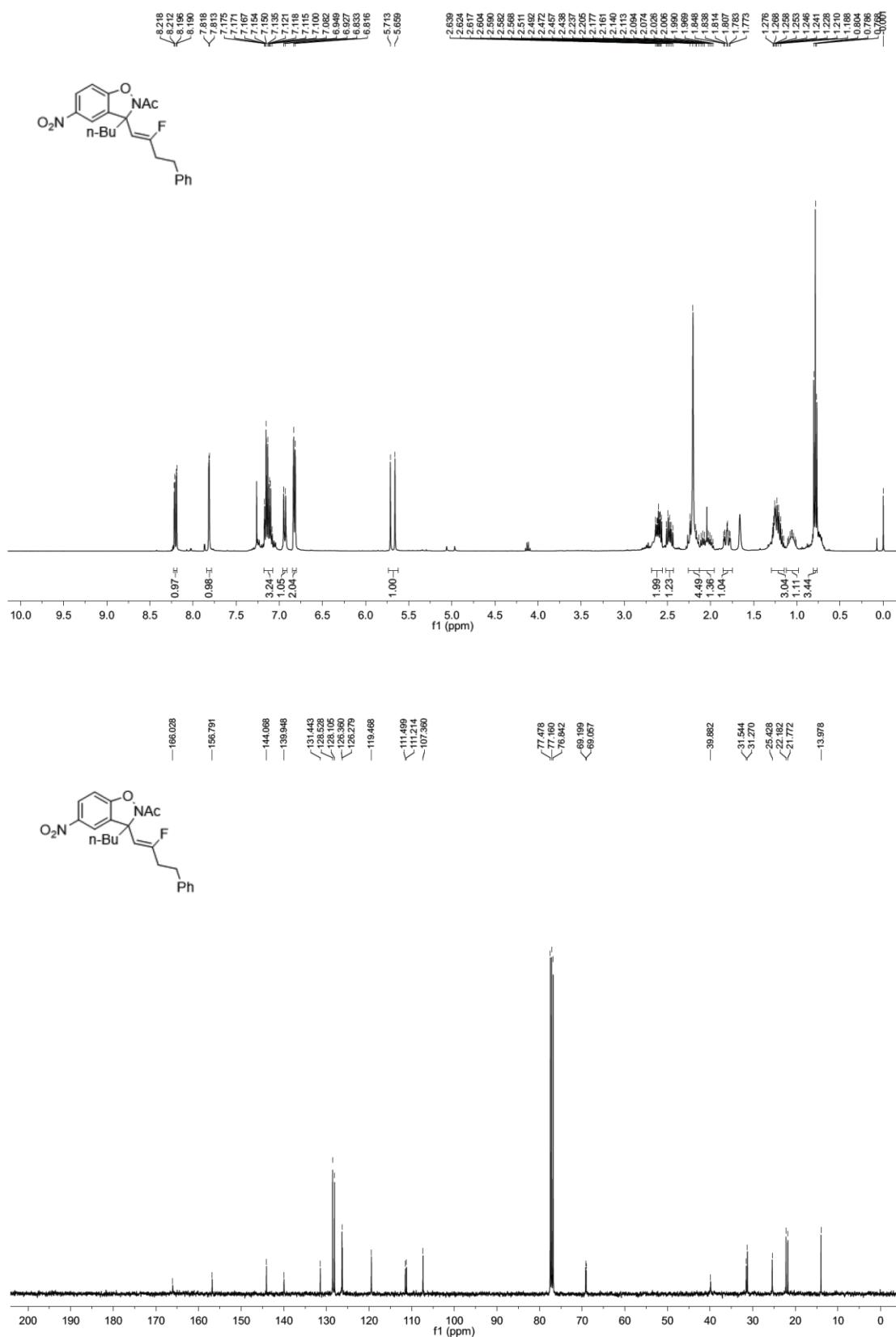
3h



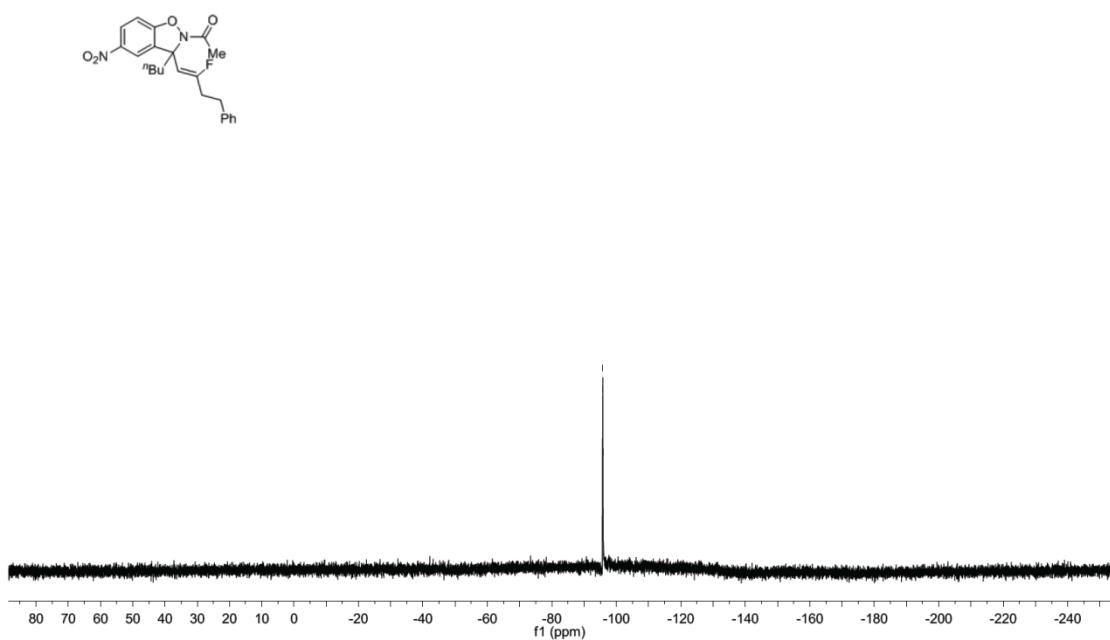
¹⁹F NMR spectrum of 3h

-96.138
-96.399
-96.464
-96.526

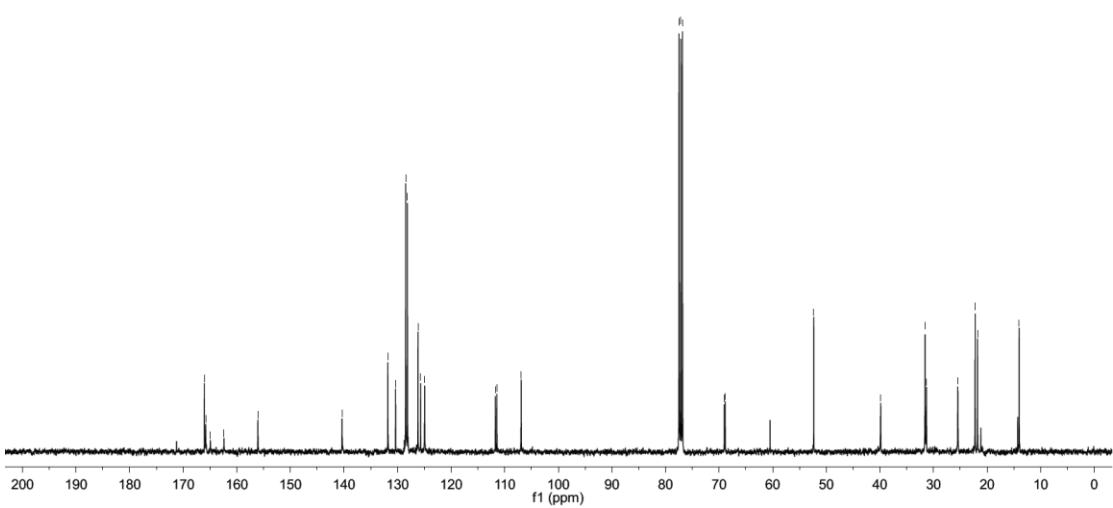
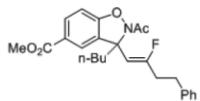
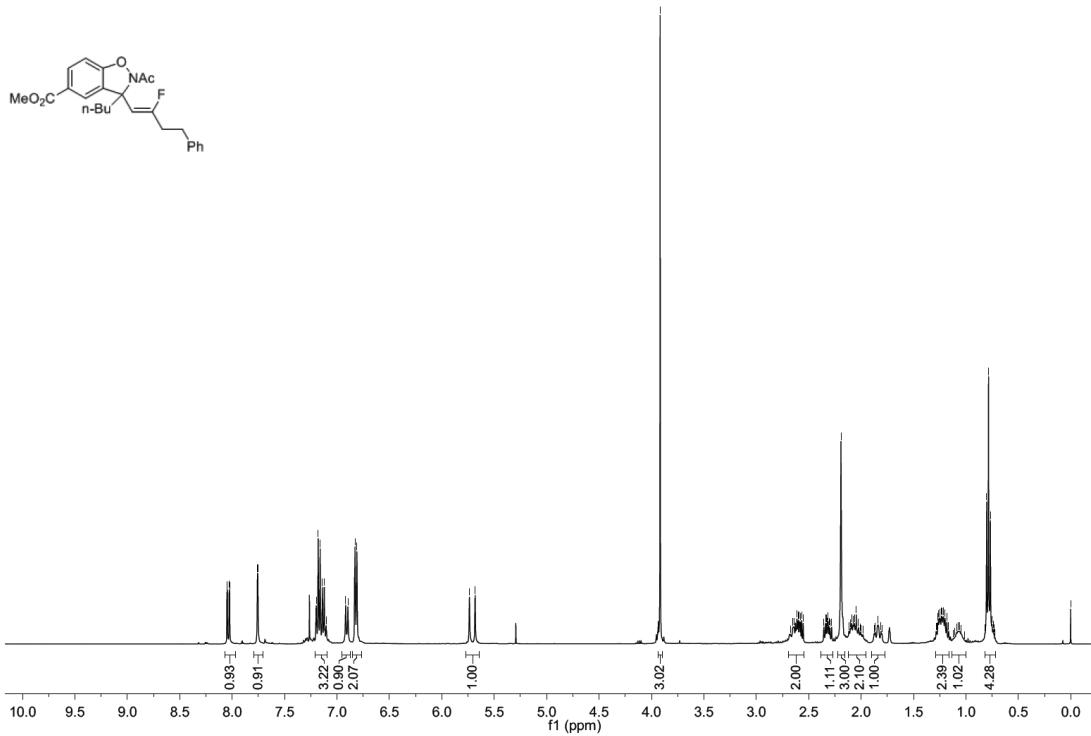
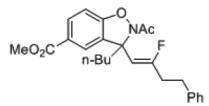


3i

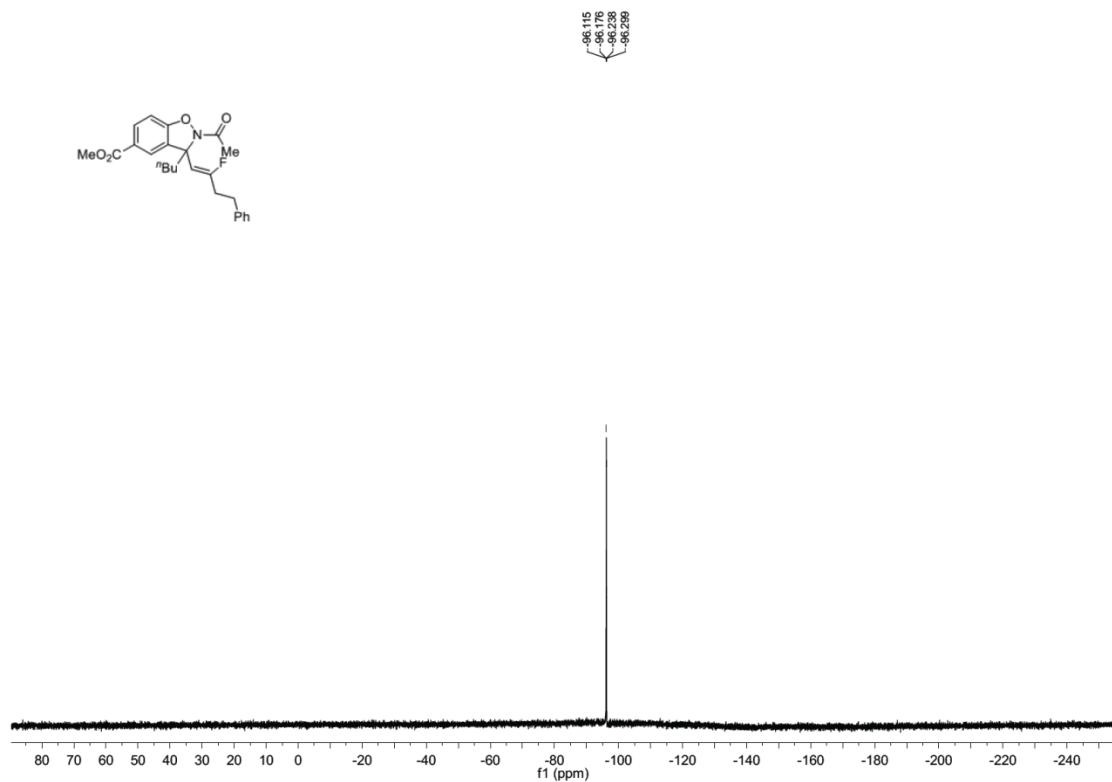
¹⁹F NMR spectrum of 3i



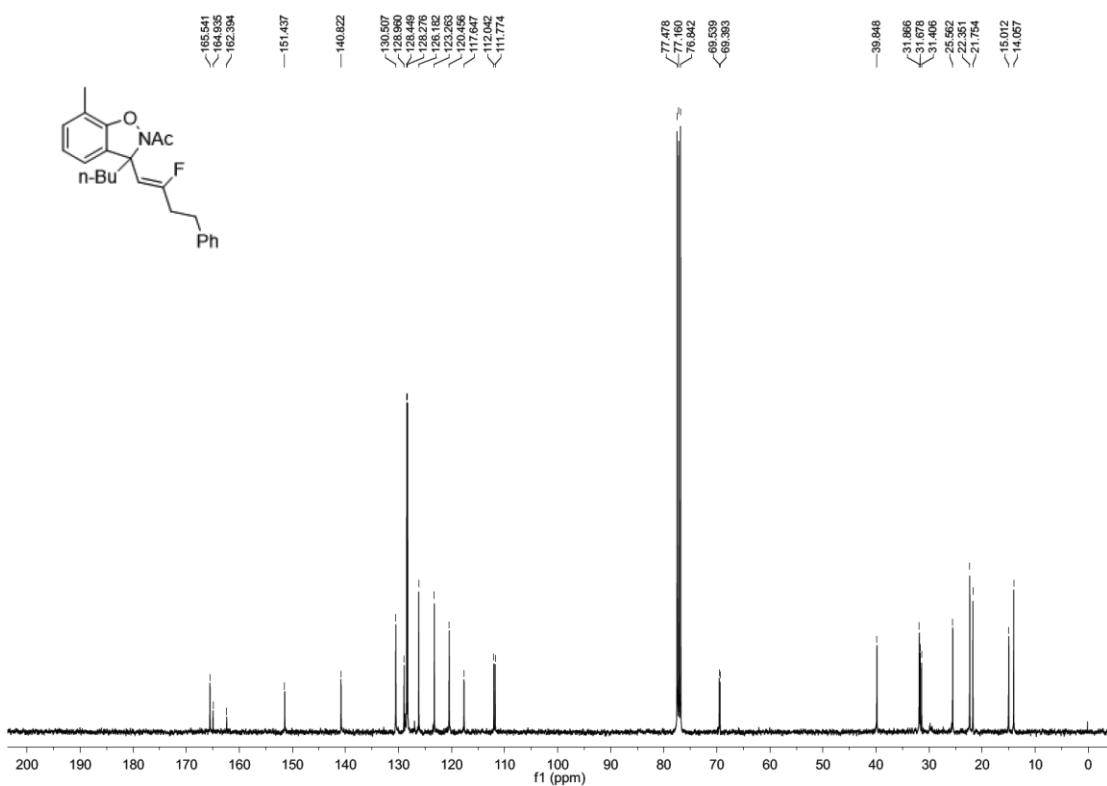
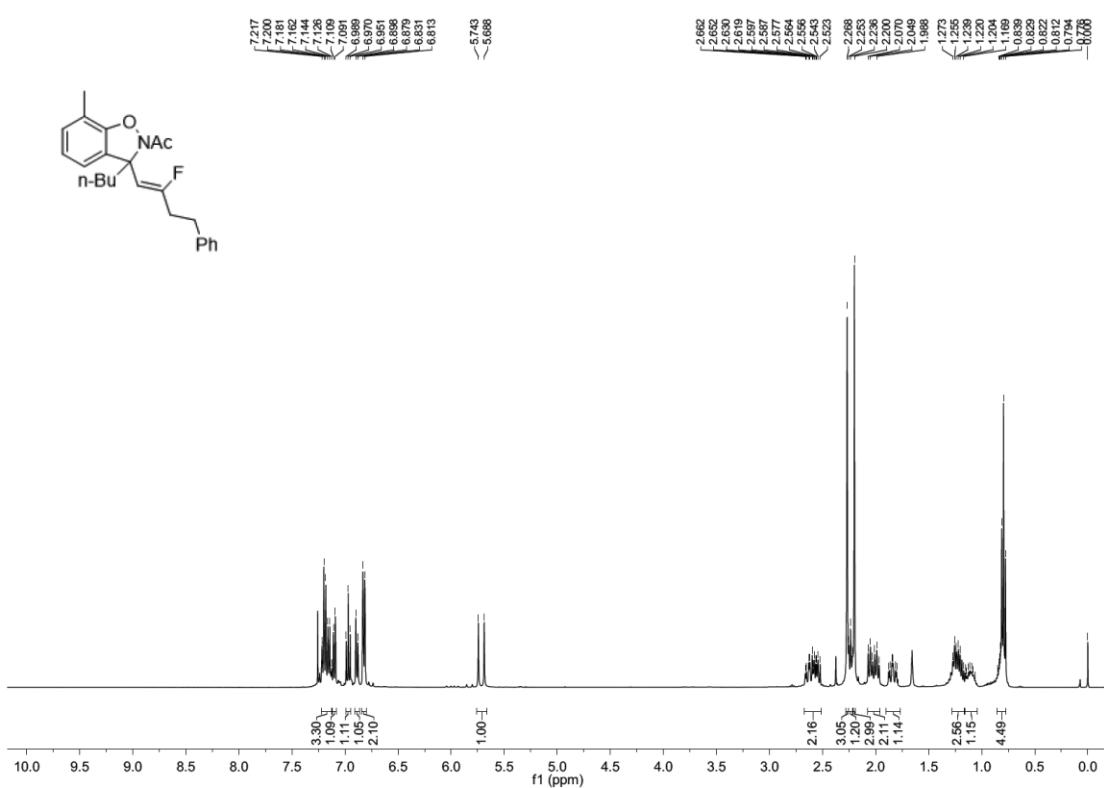
3j



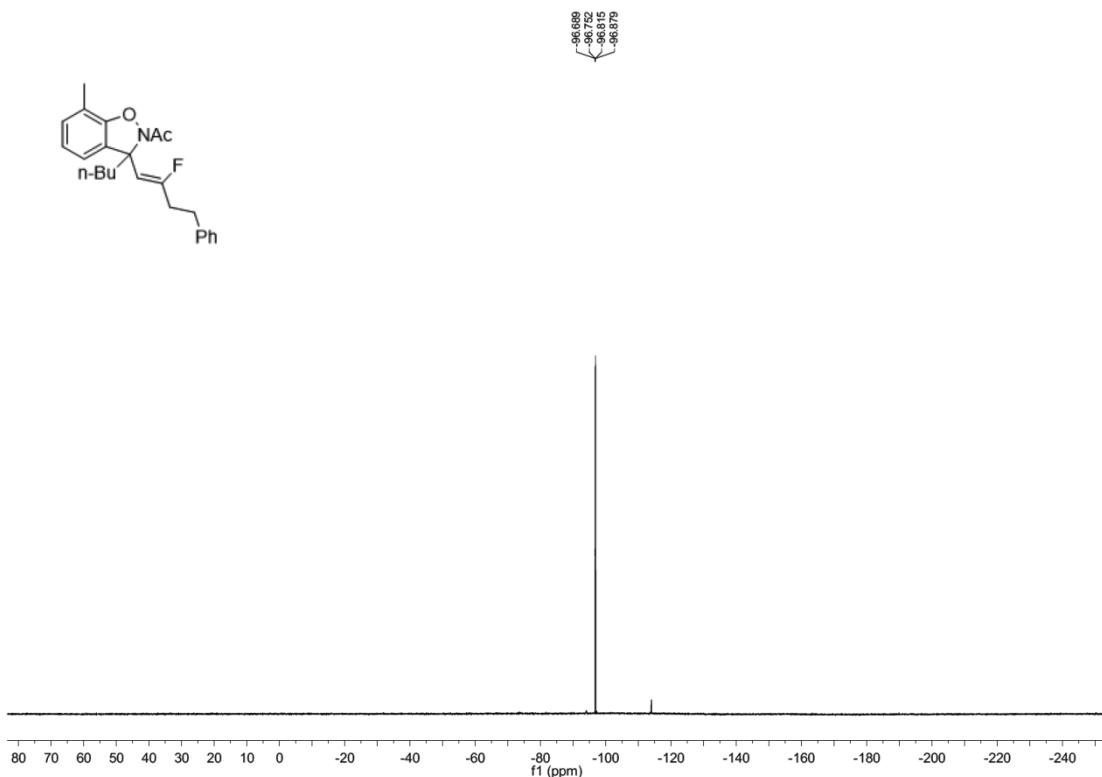
¹⁹F NMR spectrum of 3j



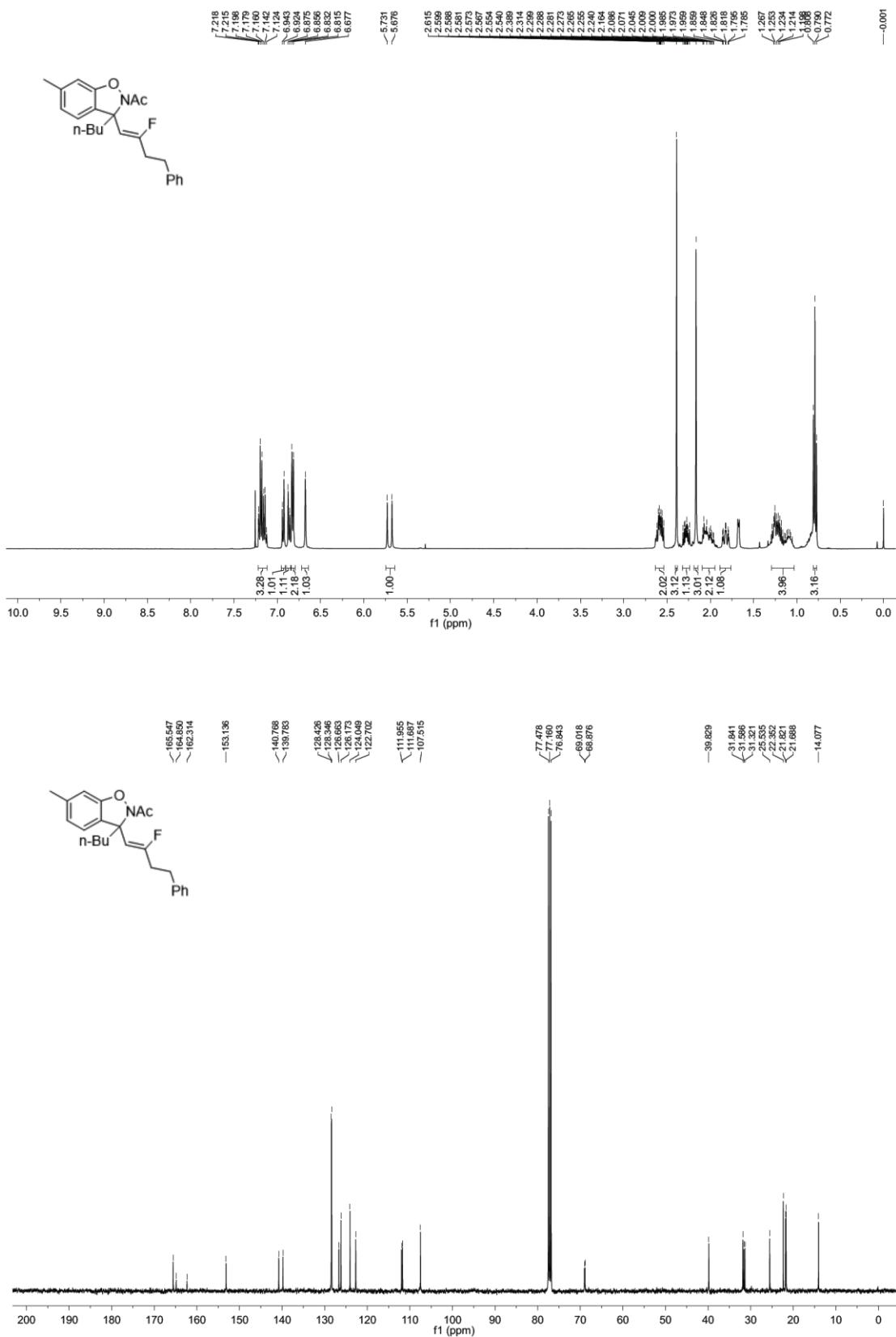
3k



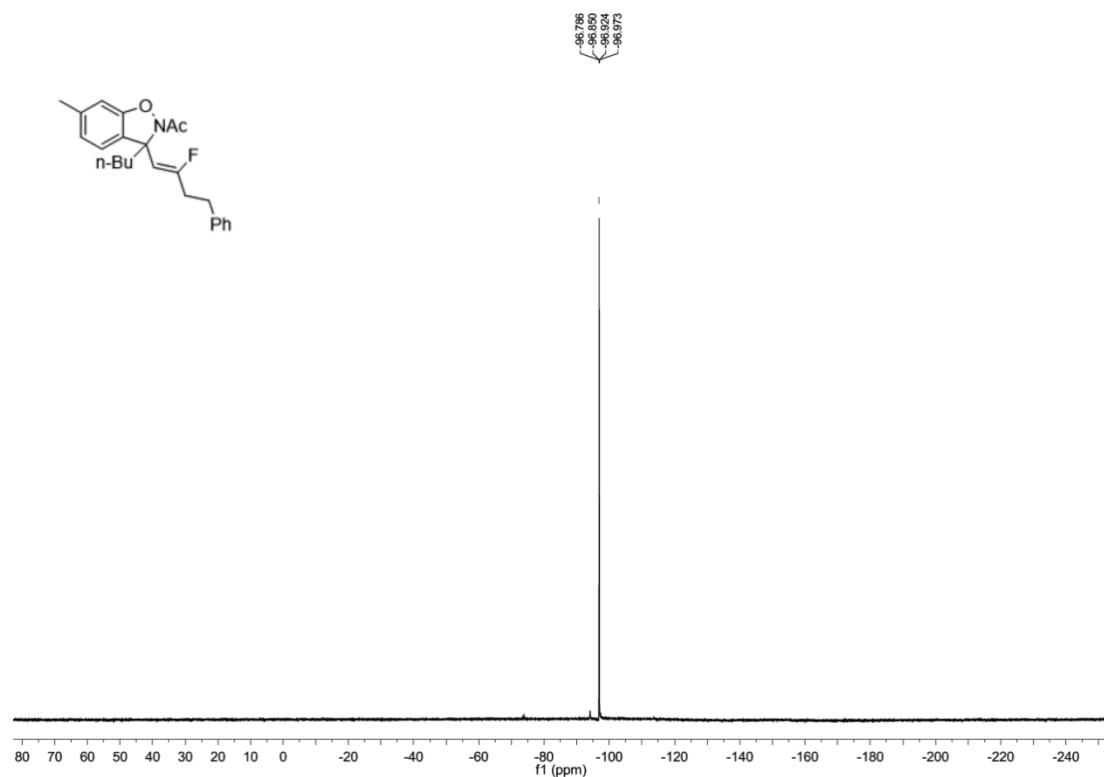
¹⁹F NMR spectrum of 3k

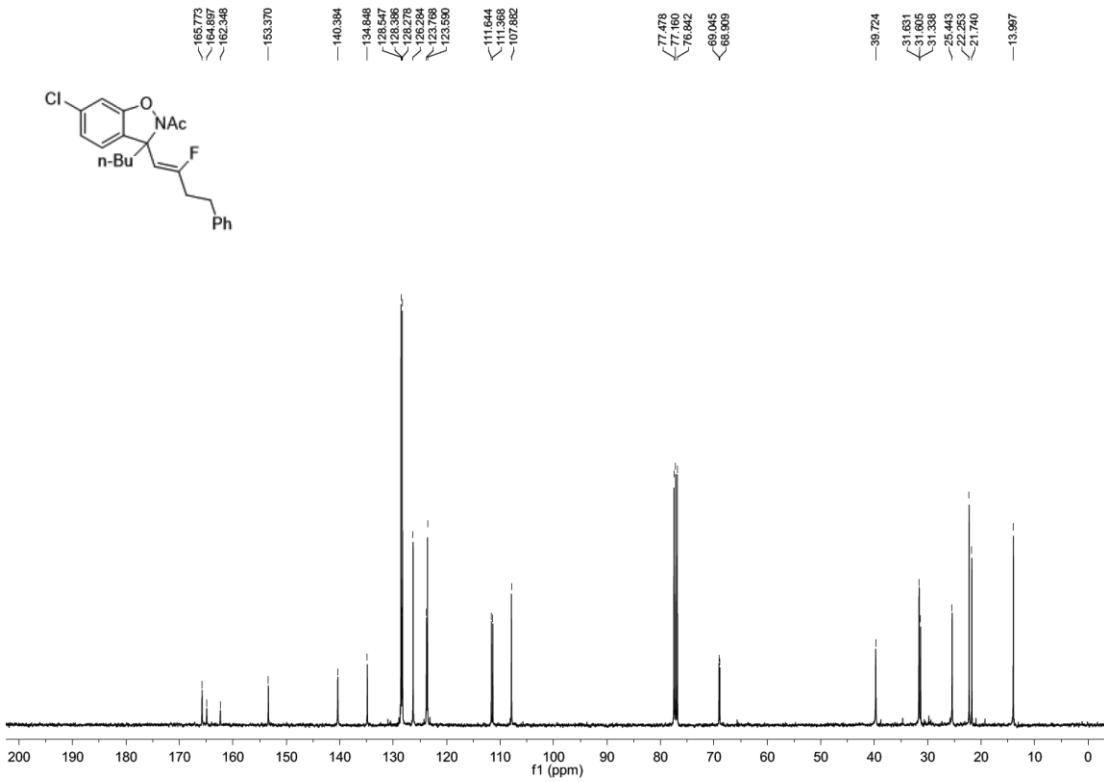
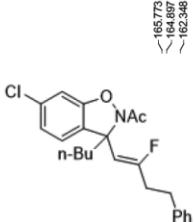
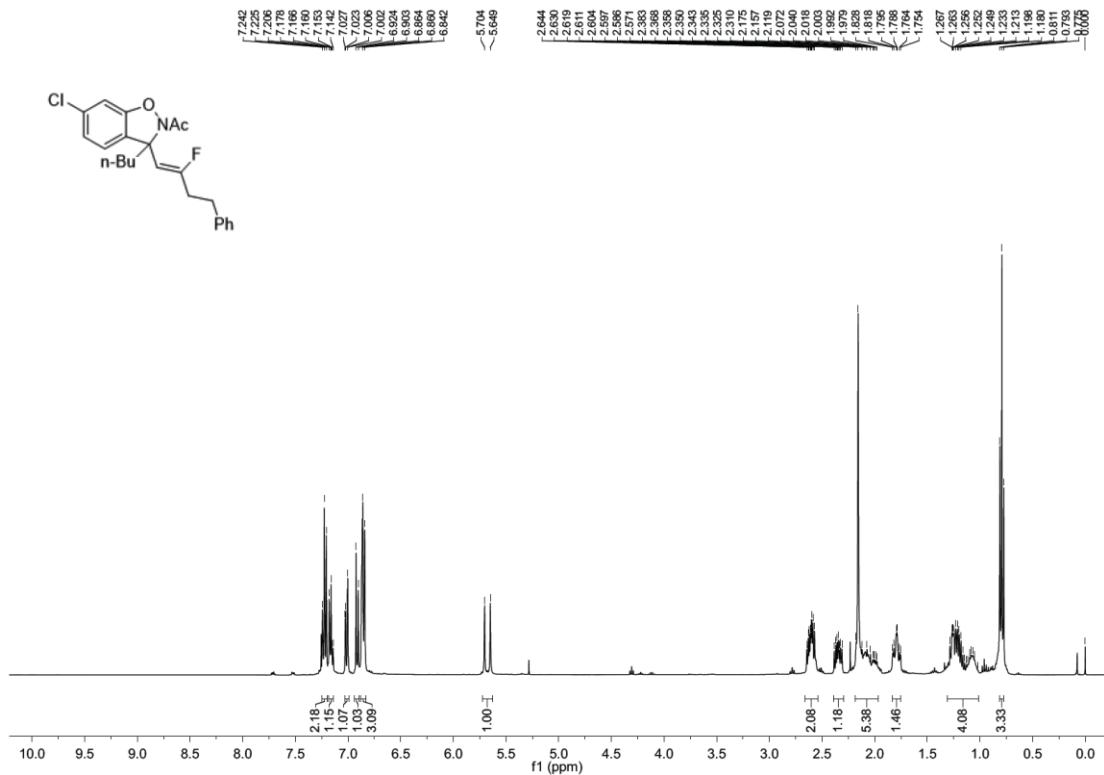
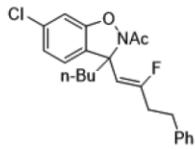


3l

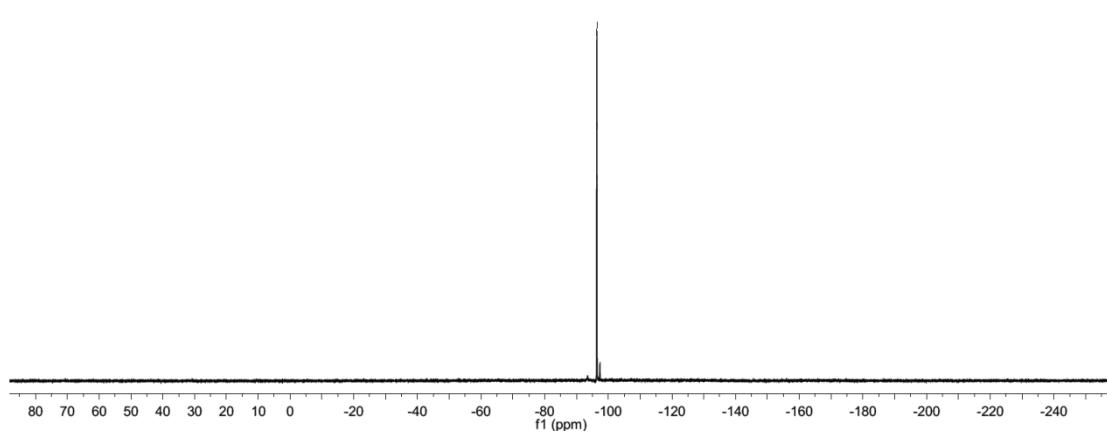


¹⁹F NMR spectrum of 3l

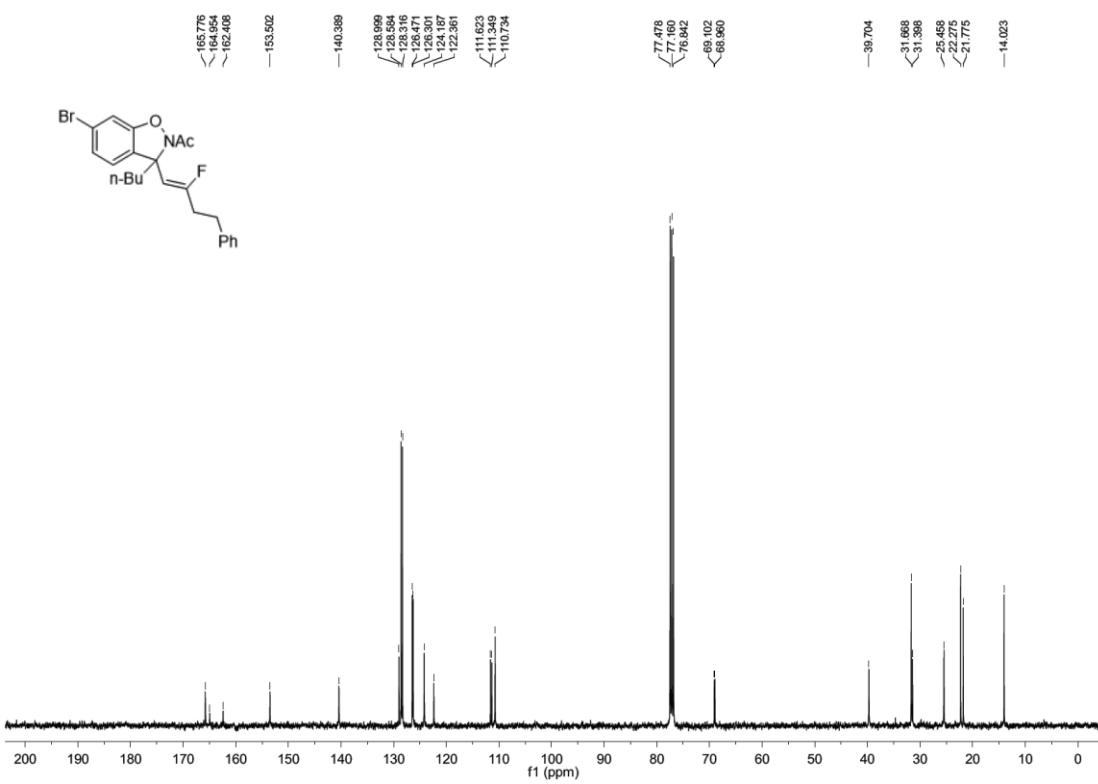
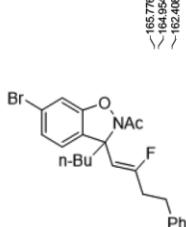
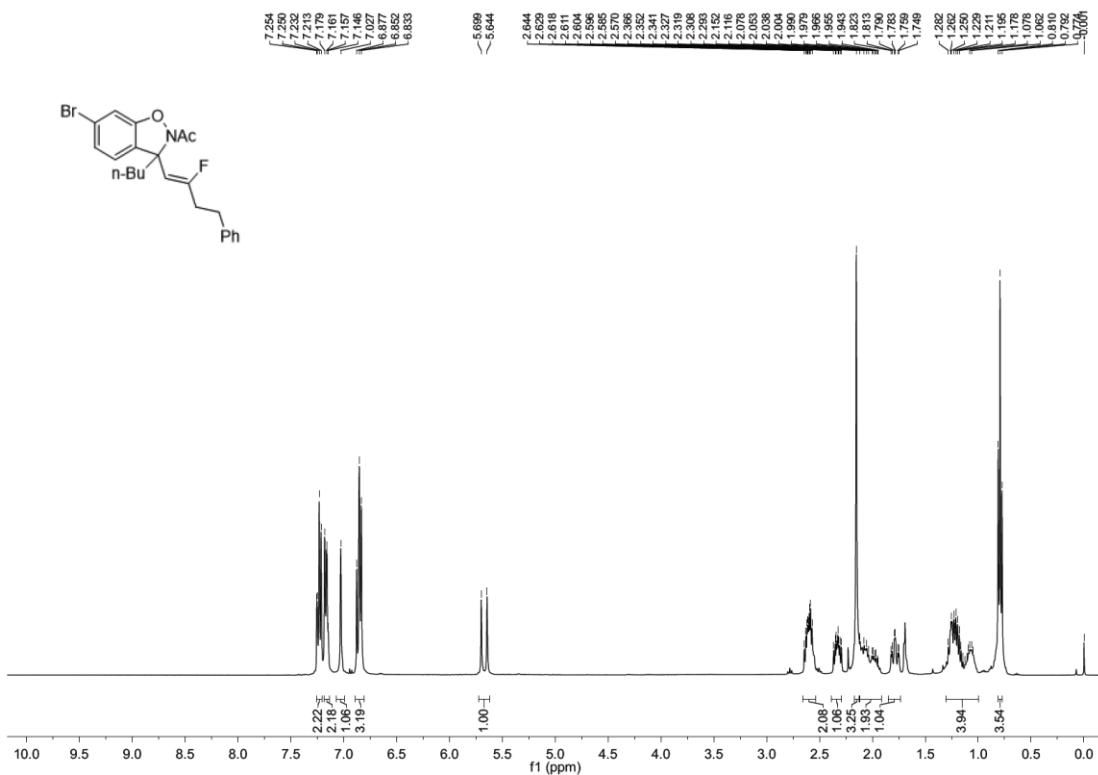
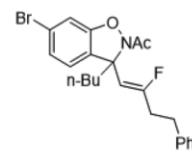




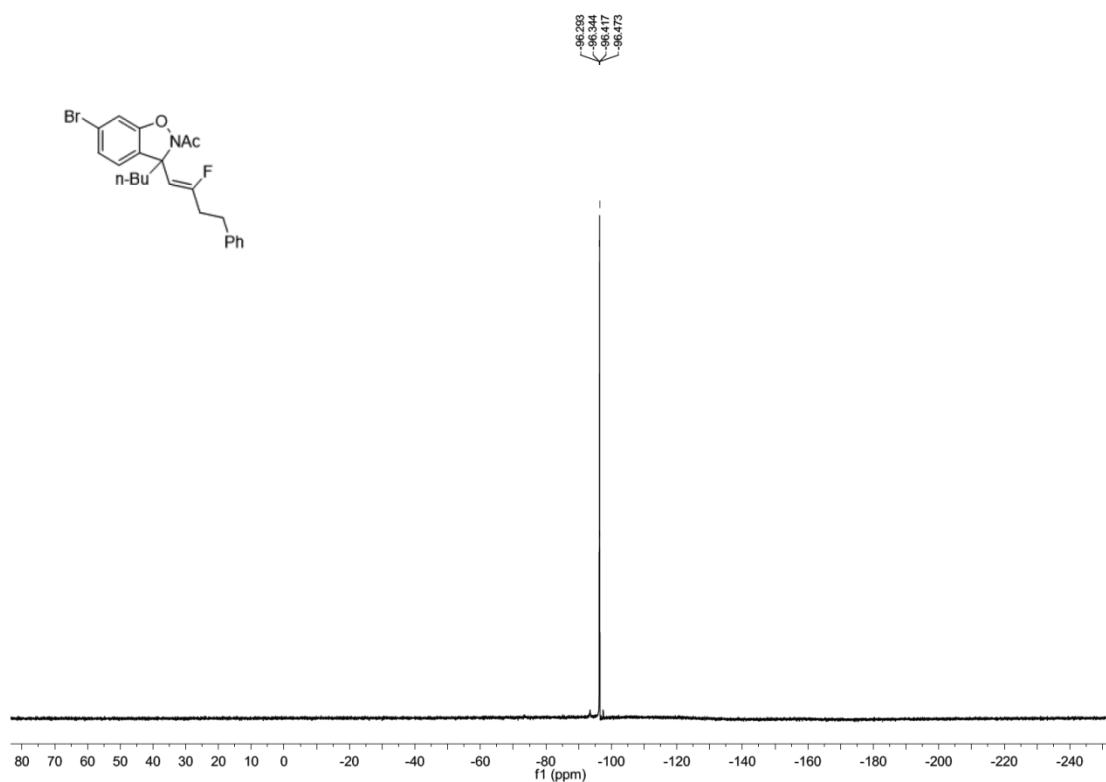
¹⁹F NMR spectrum of 3m



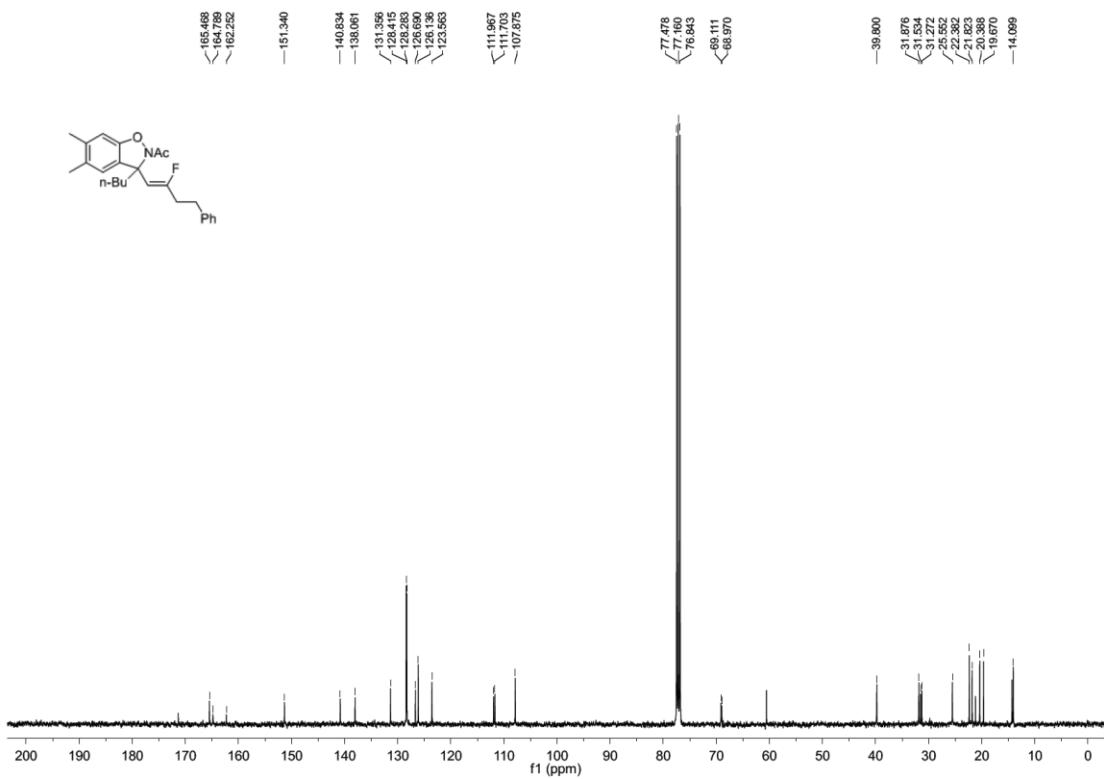
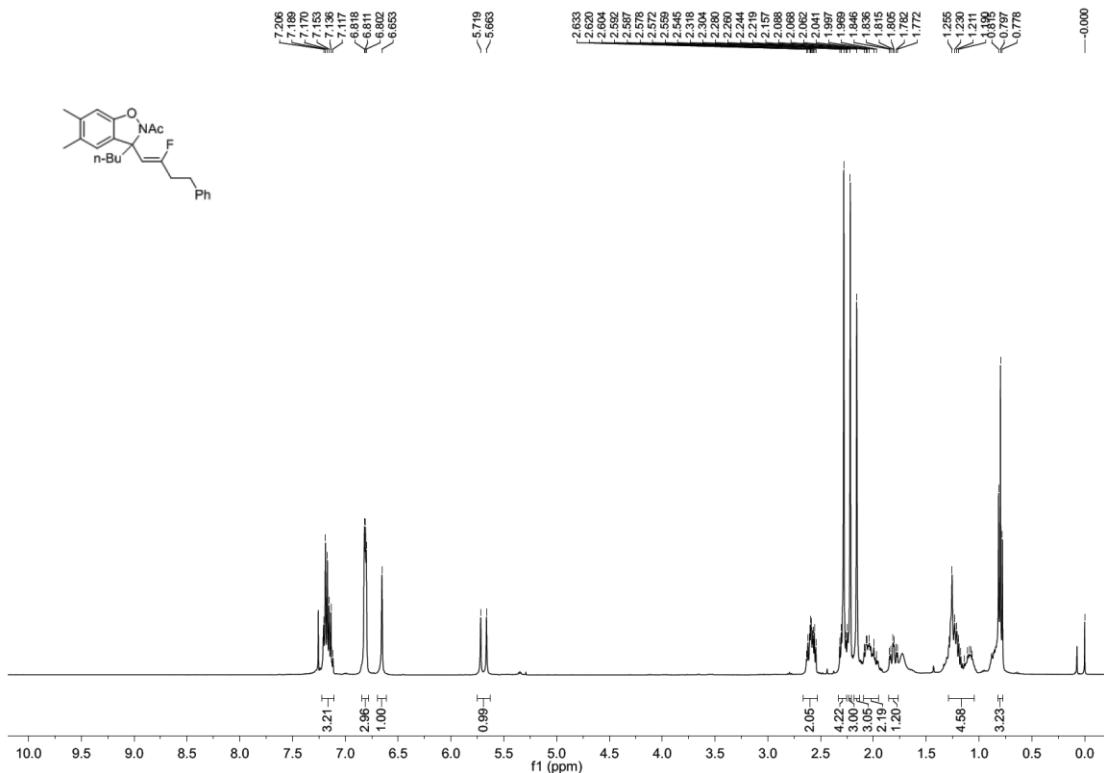
3n



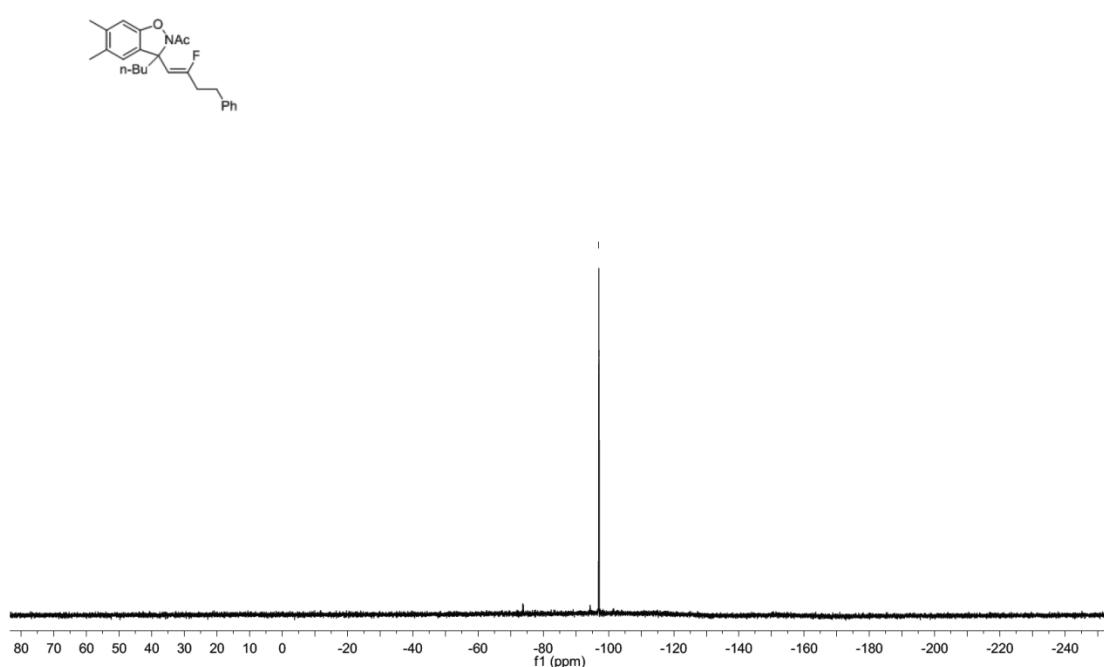
¹⁹F NMR spectrum of 3n



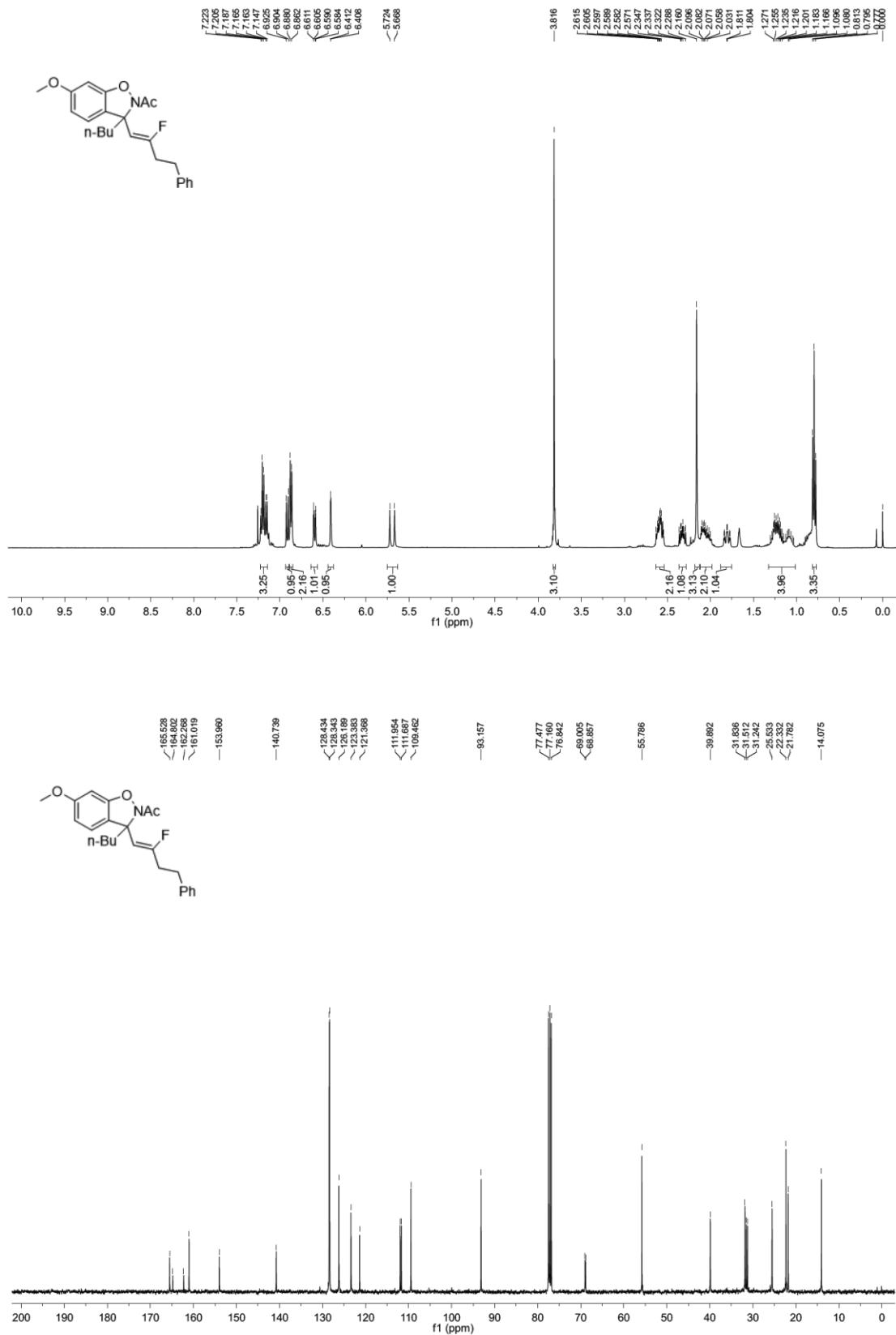
3o



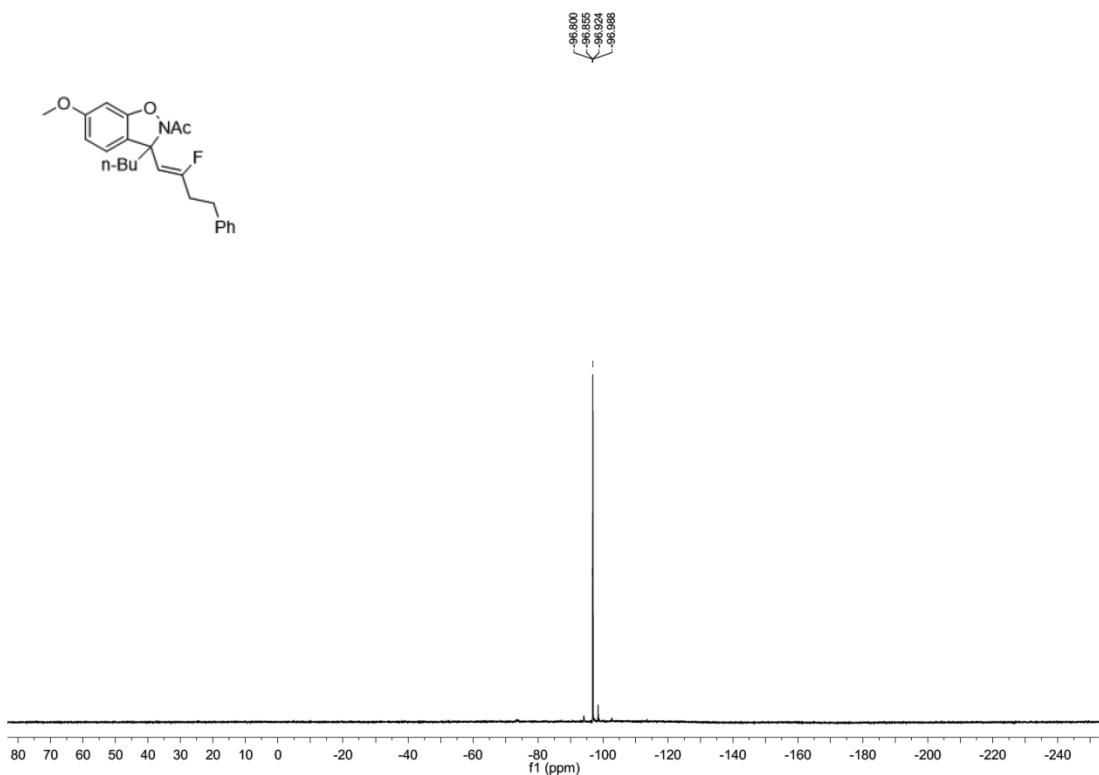
¹⁹F NMR spectrum of 3o



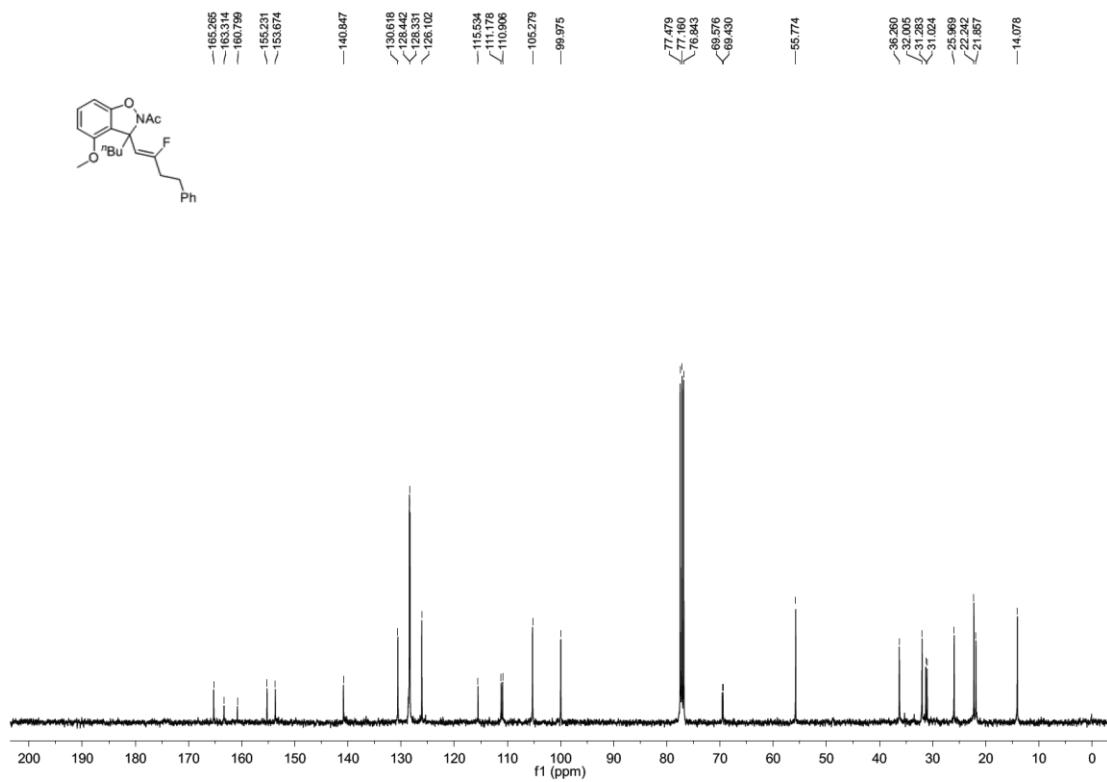
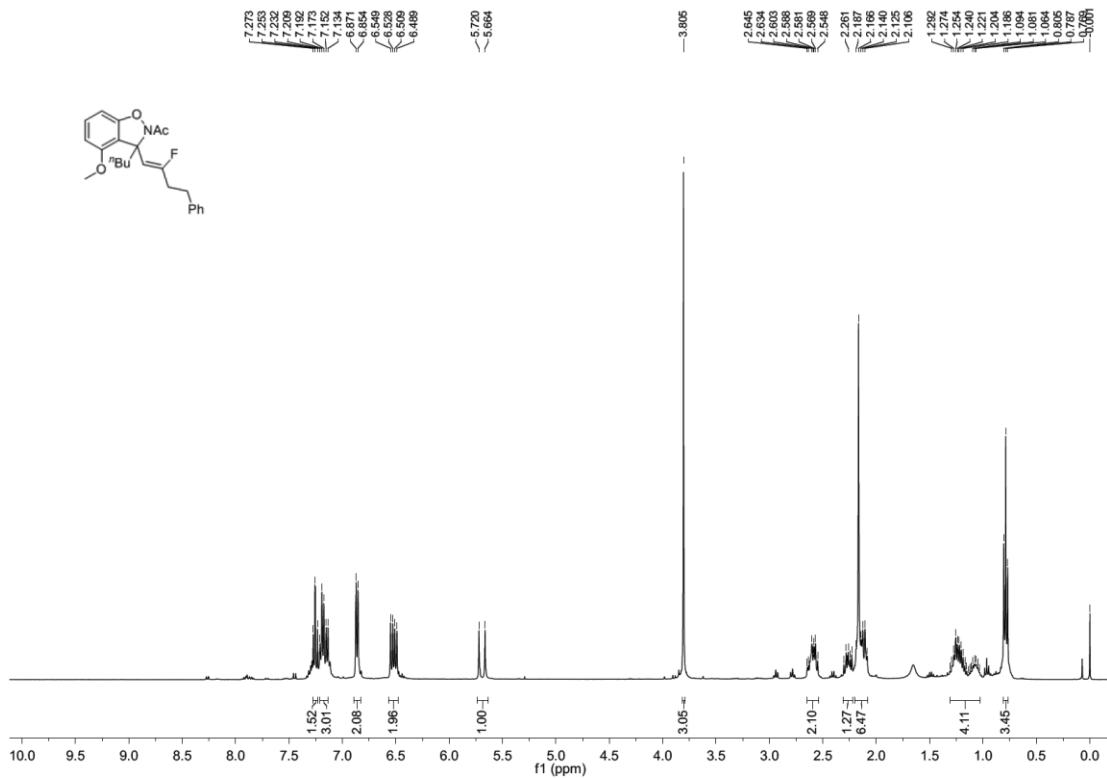
3p



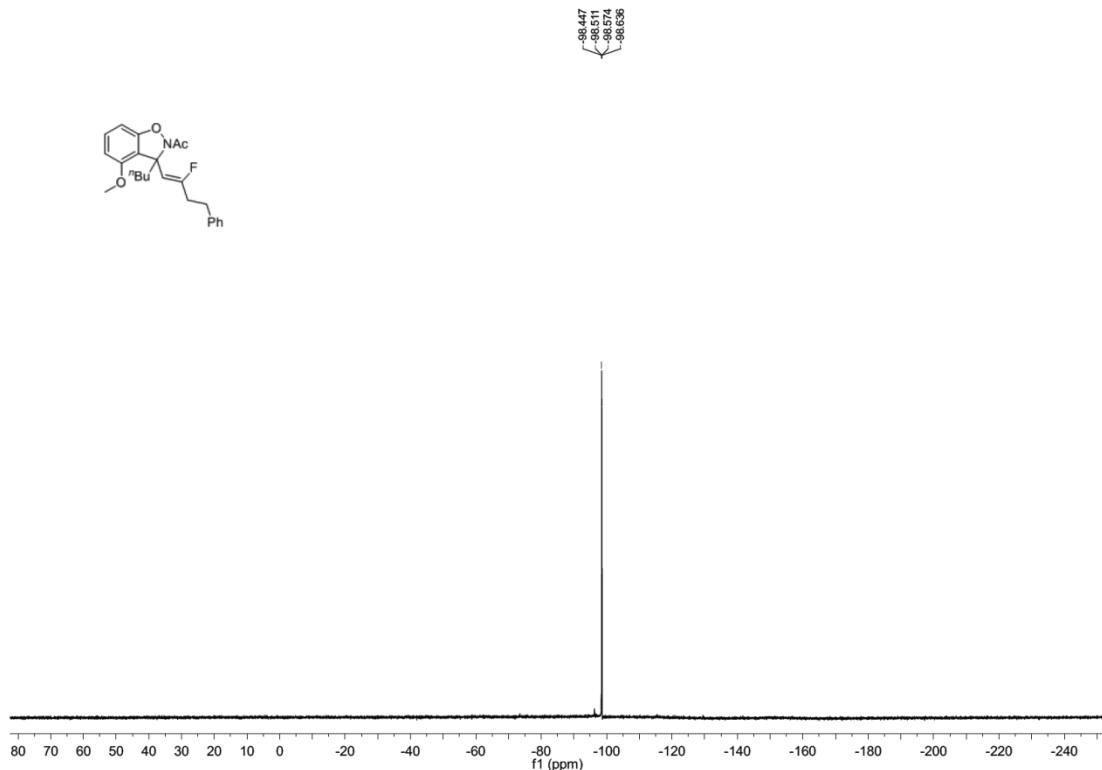
¹⁹F NMR spectrum of 3p



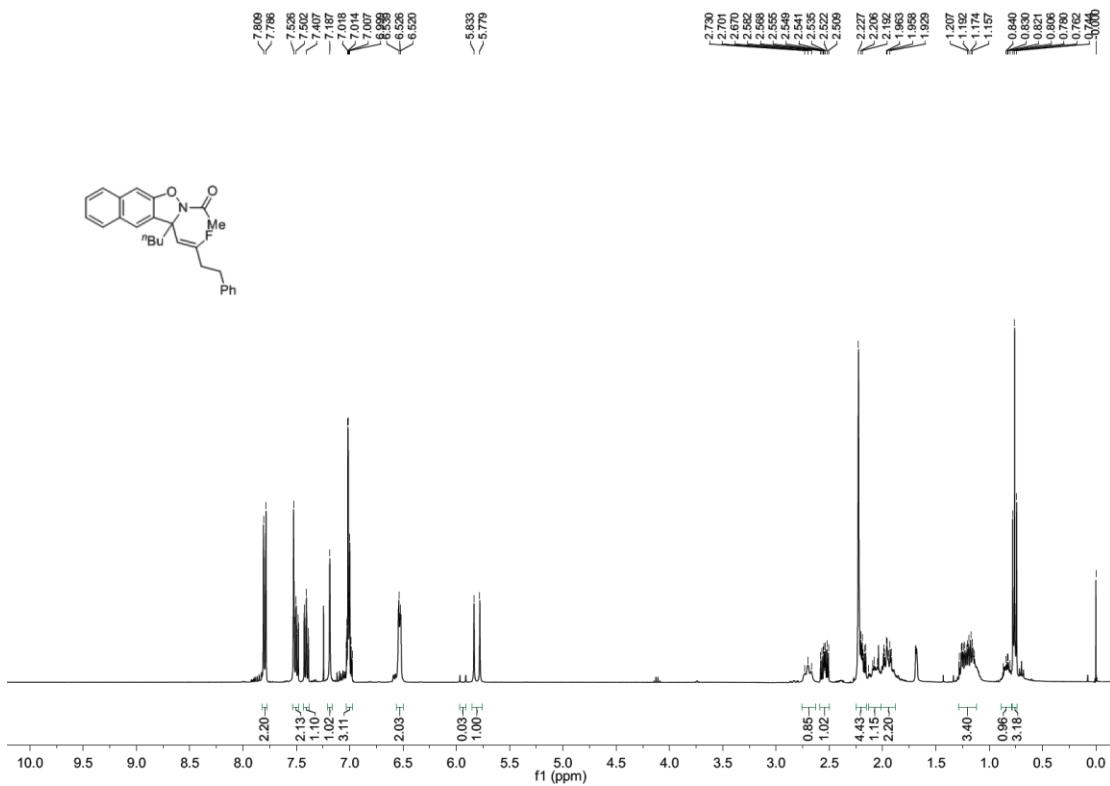
3p'



¹⁹F NMR spectrum of 3p'

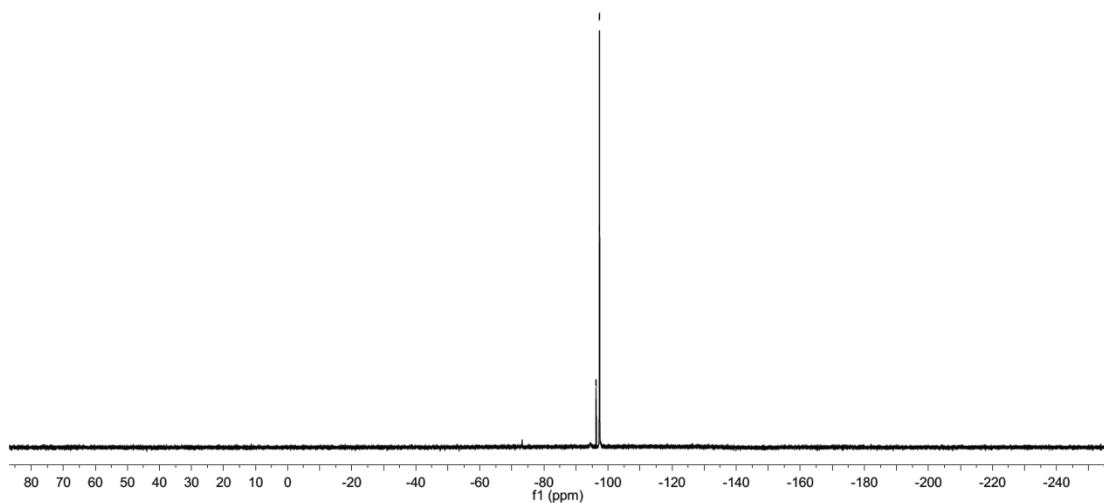
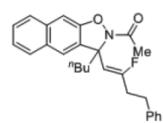


3q

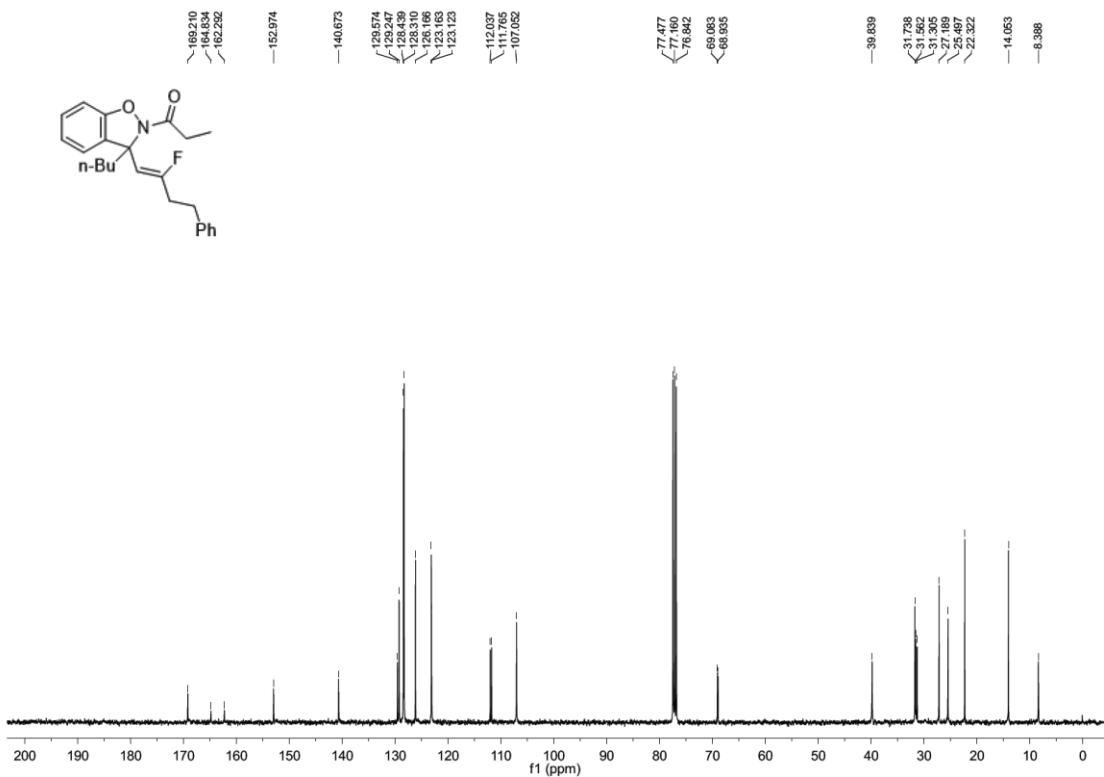
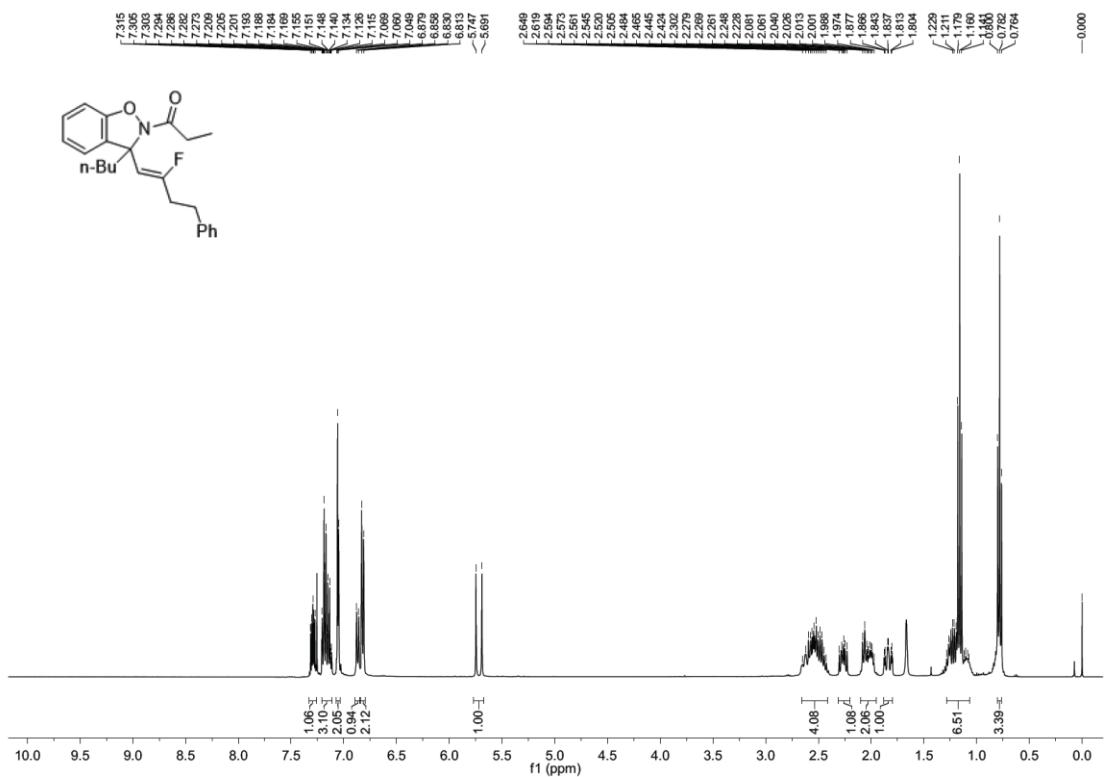


¹⁹F NMR spectrum of 3q

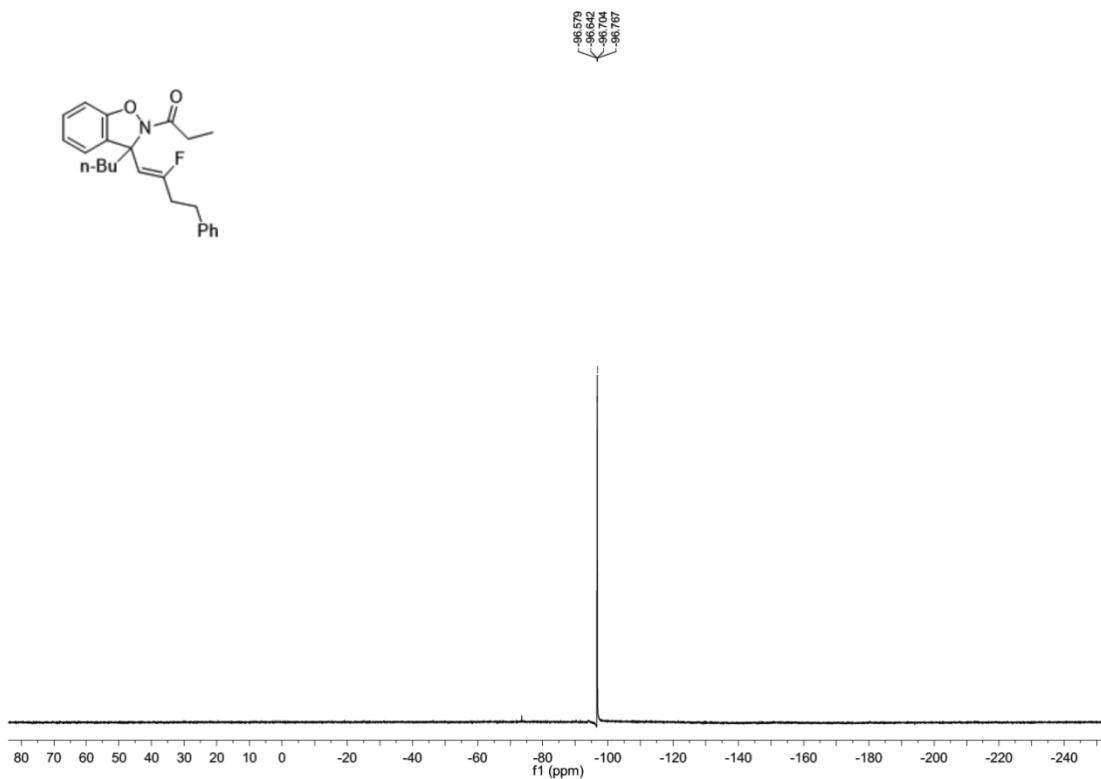
-96.196
-96.241
-96.263
-96.297
-96.318
-96.373
-97.258
-97.313
-97.387
-97.441



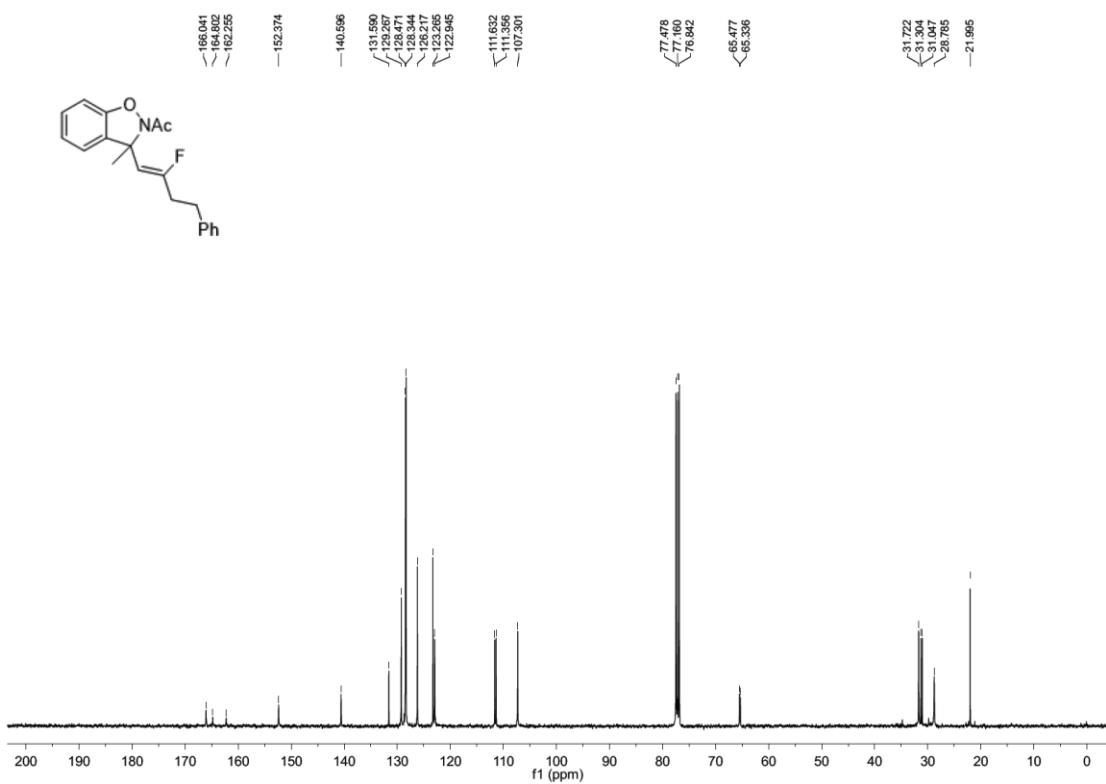
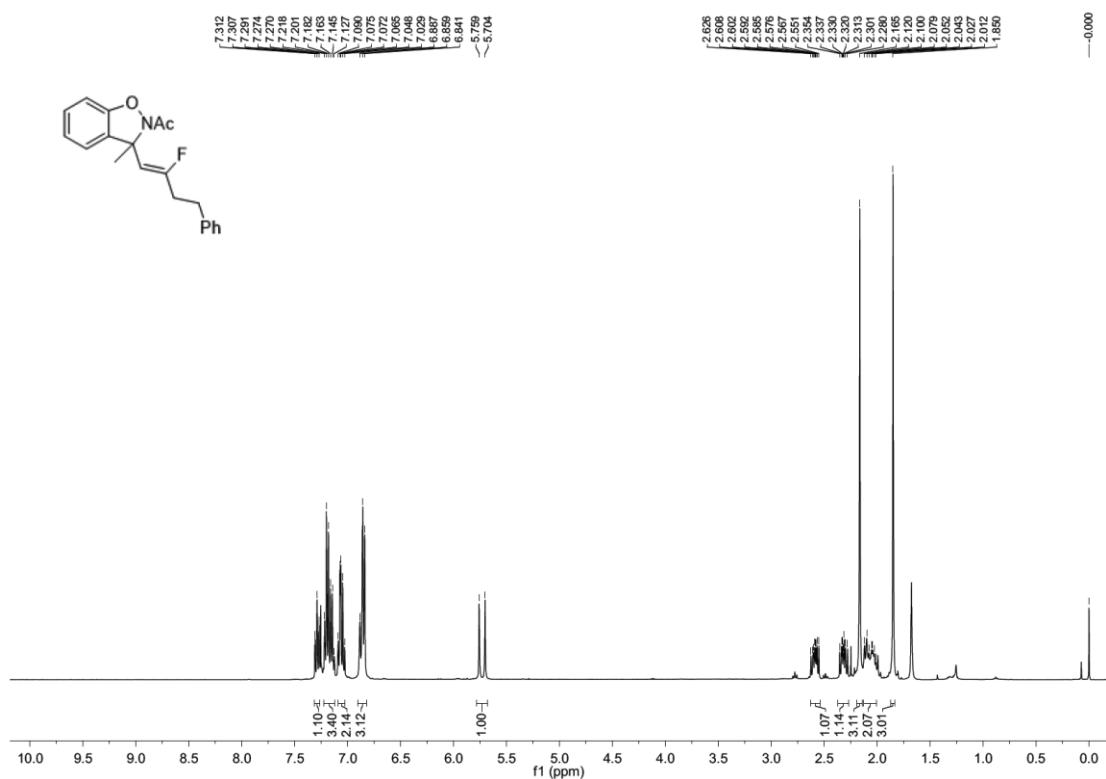
3r



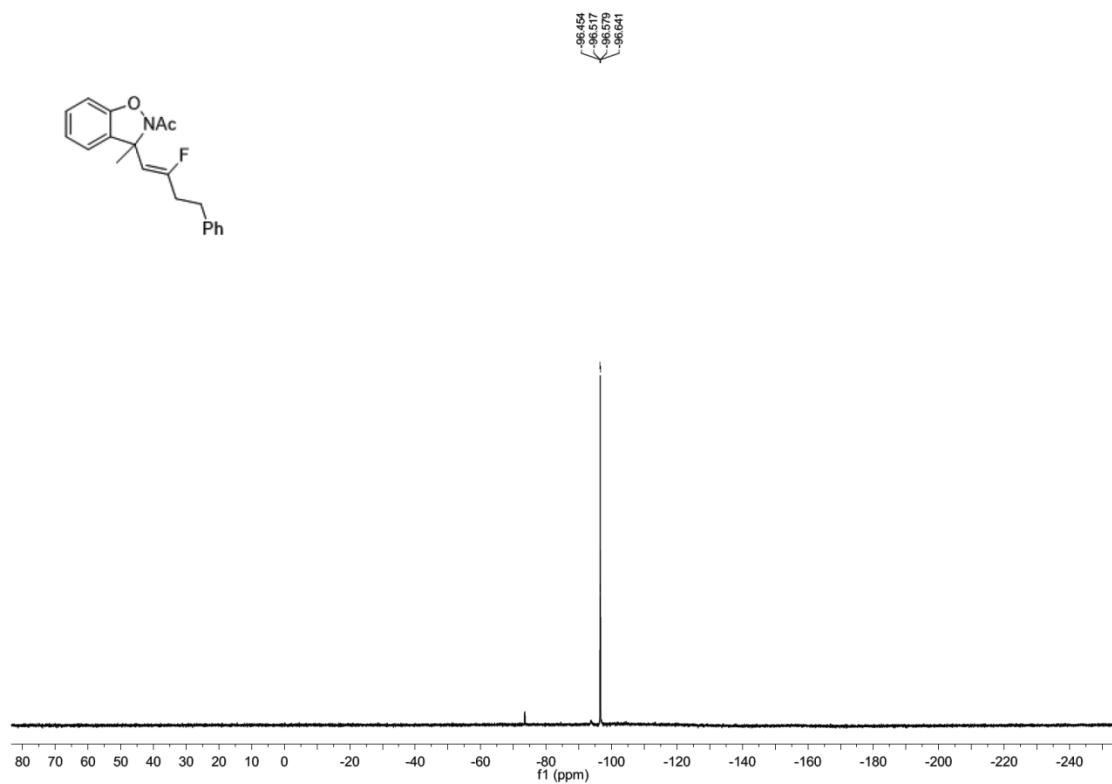
¹⁹F NMR spectrum of 3r



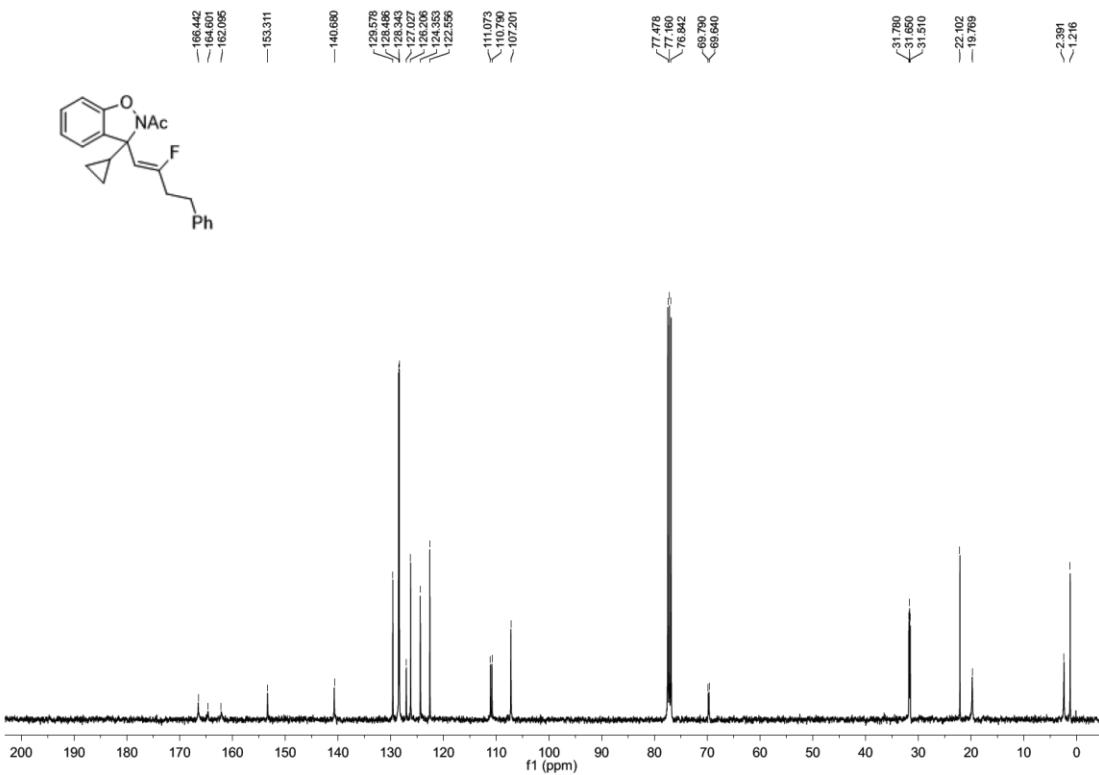
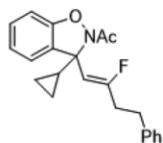
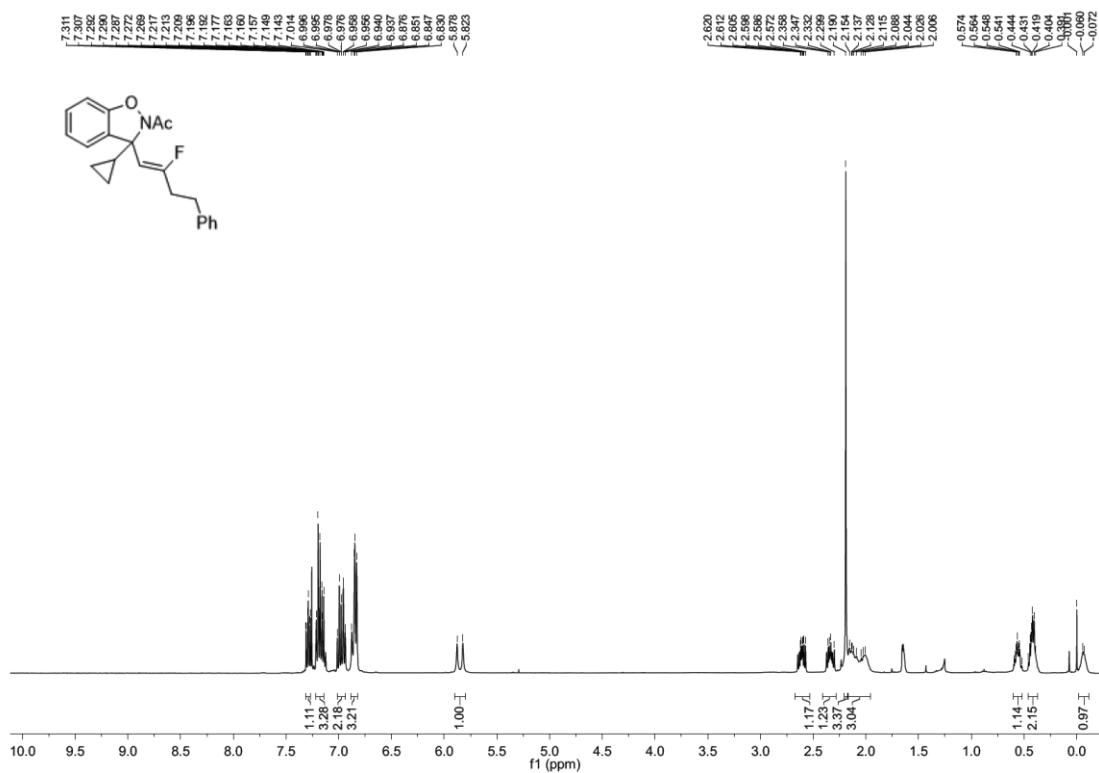
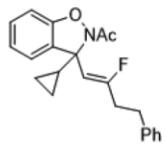
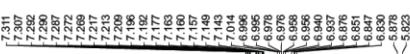
3s



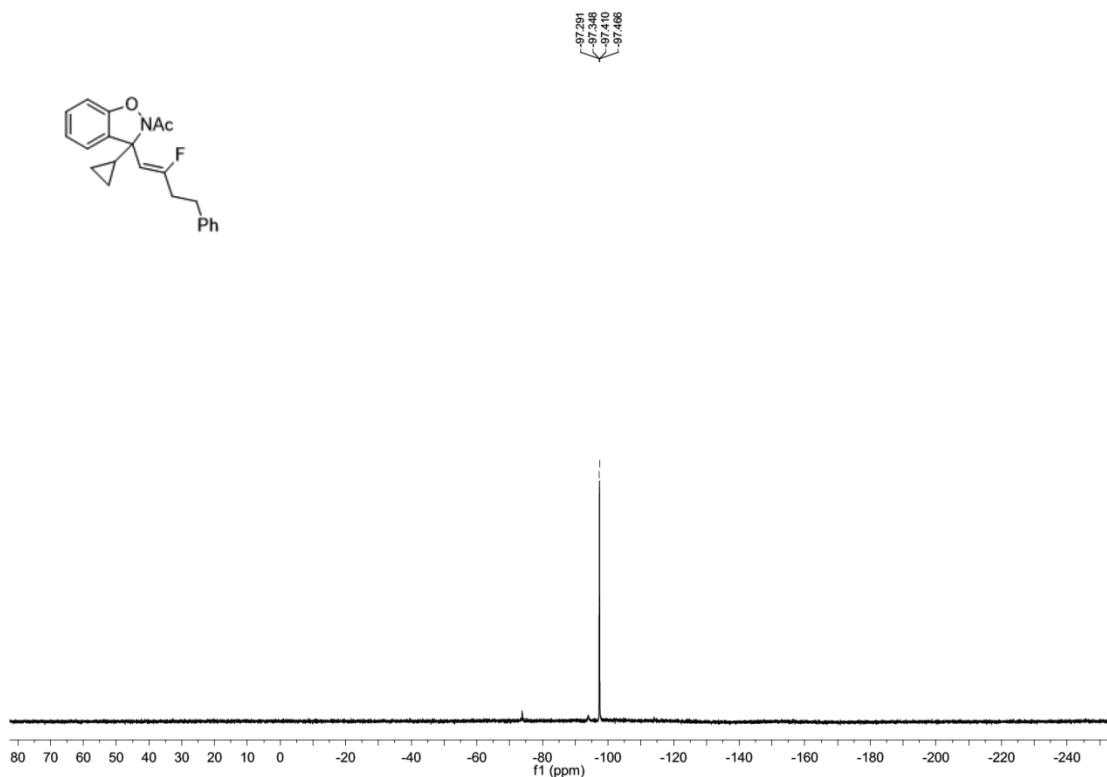
¹⁹F NMR spectrum of 3s



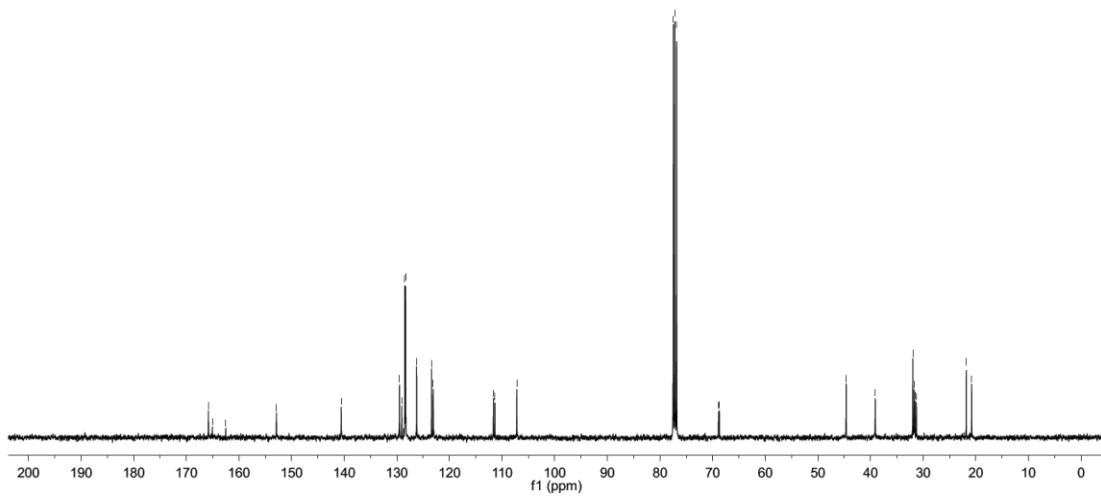
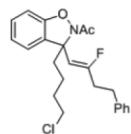
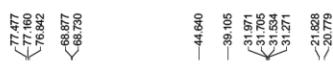
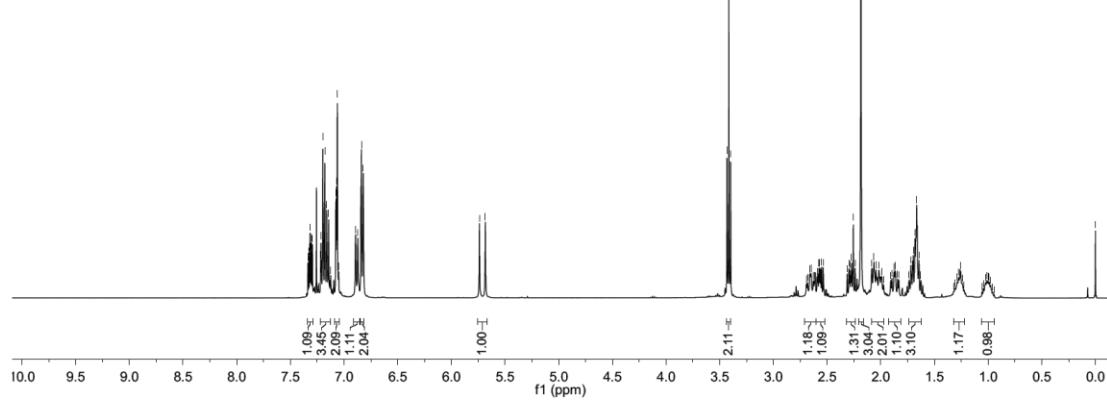
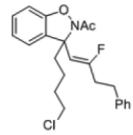
3t



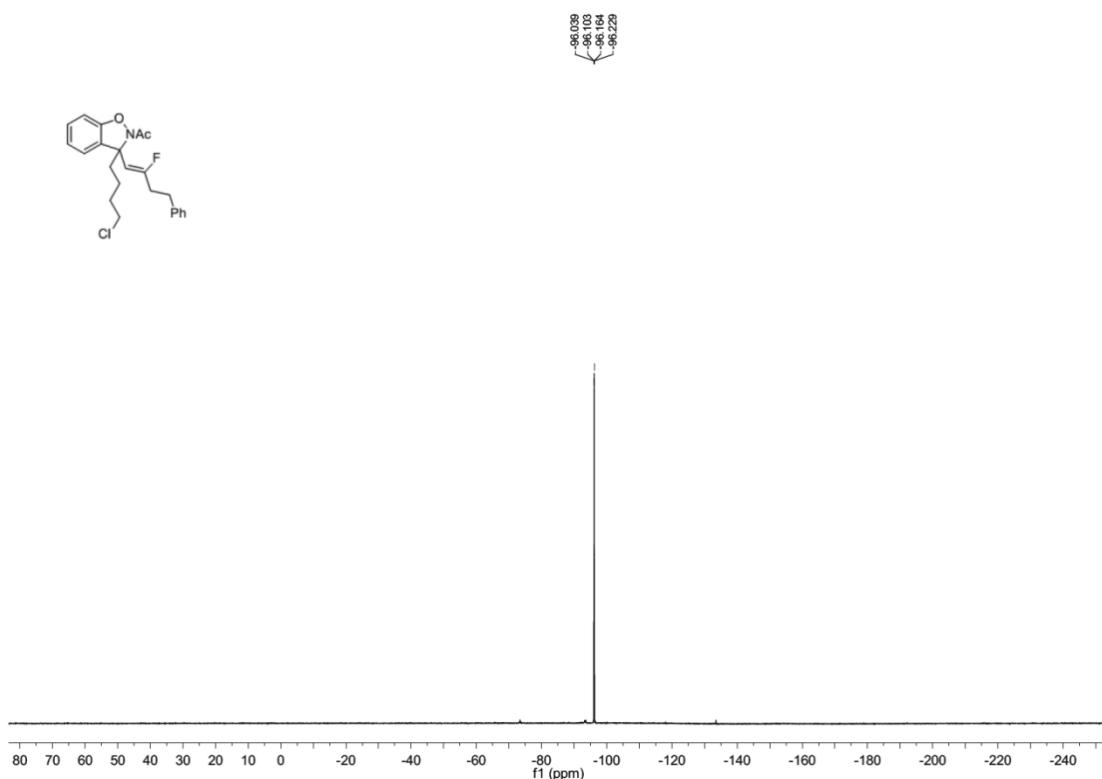
¹⁹F NMR spectrum of 3t



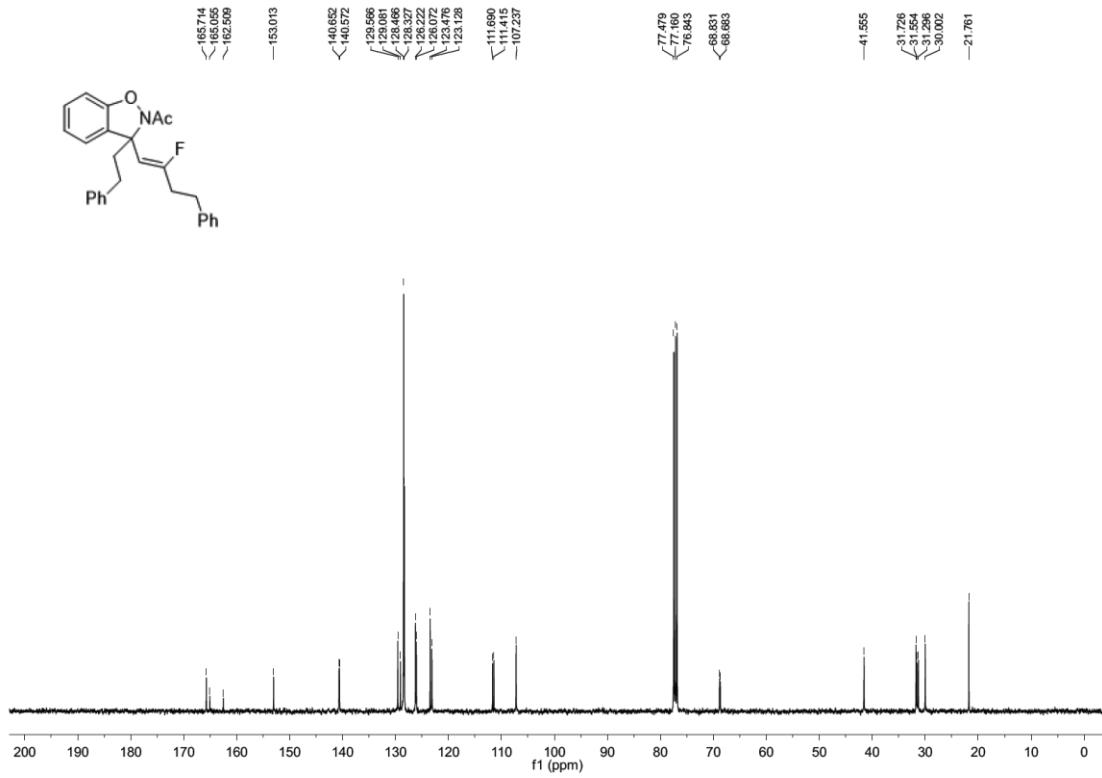
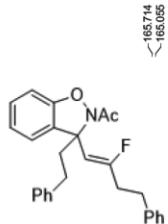
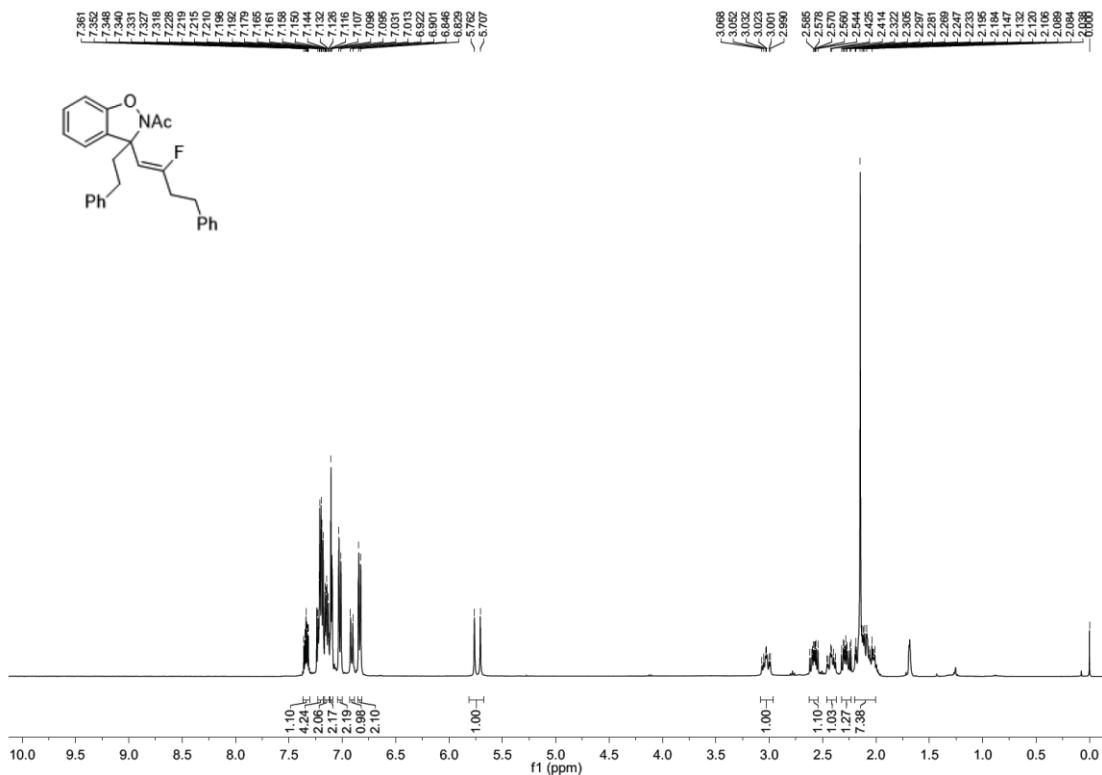
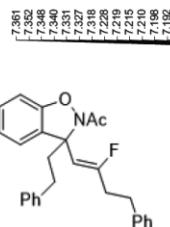
3u



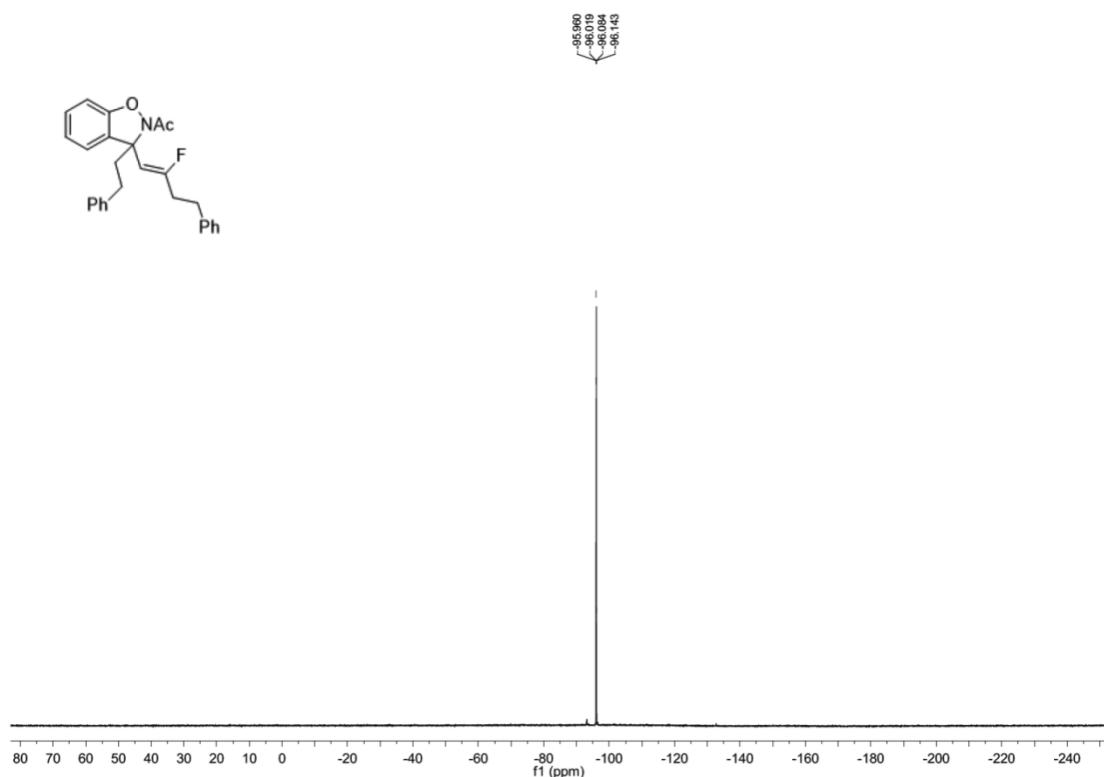
¹⁹F NMR spectrum of 3u



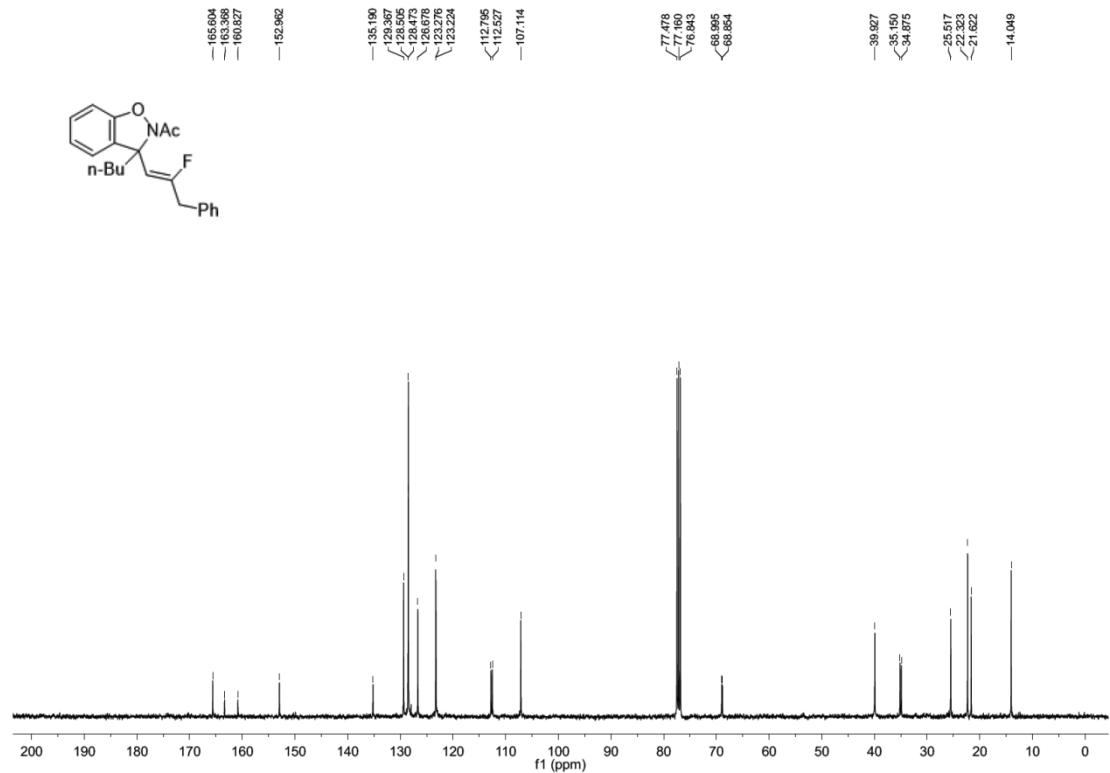
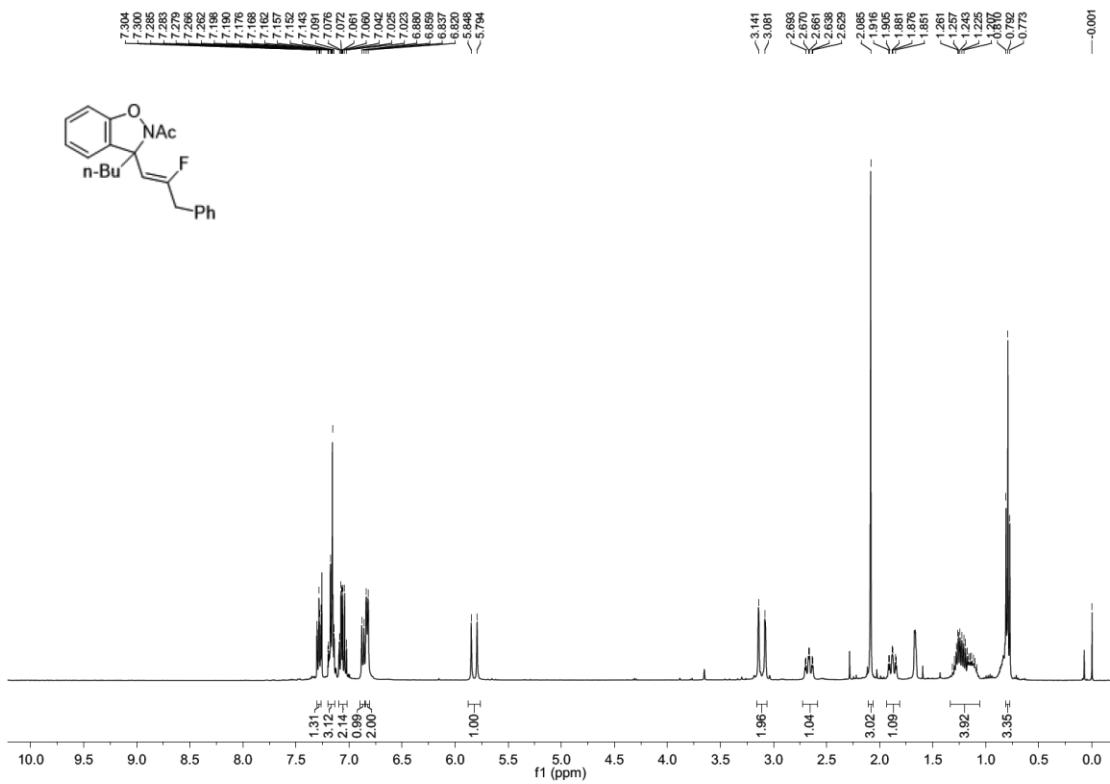
3v



¹⁹F NMR spectrum of 3v

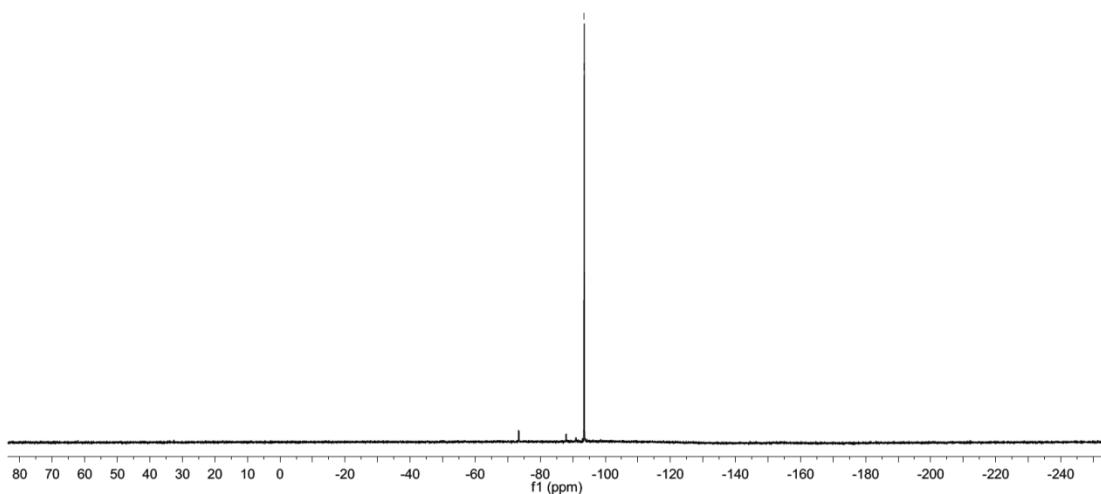
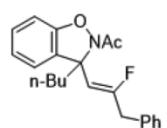


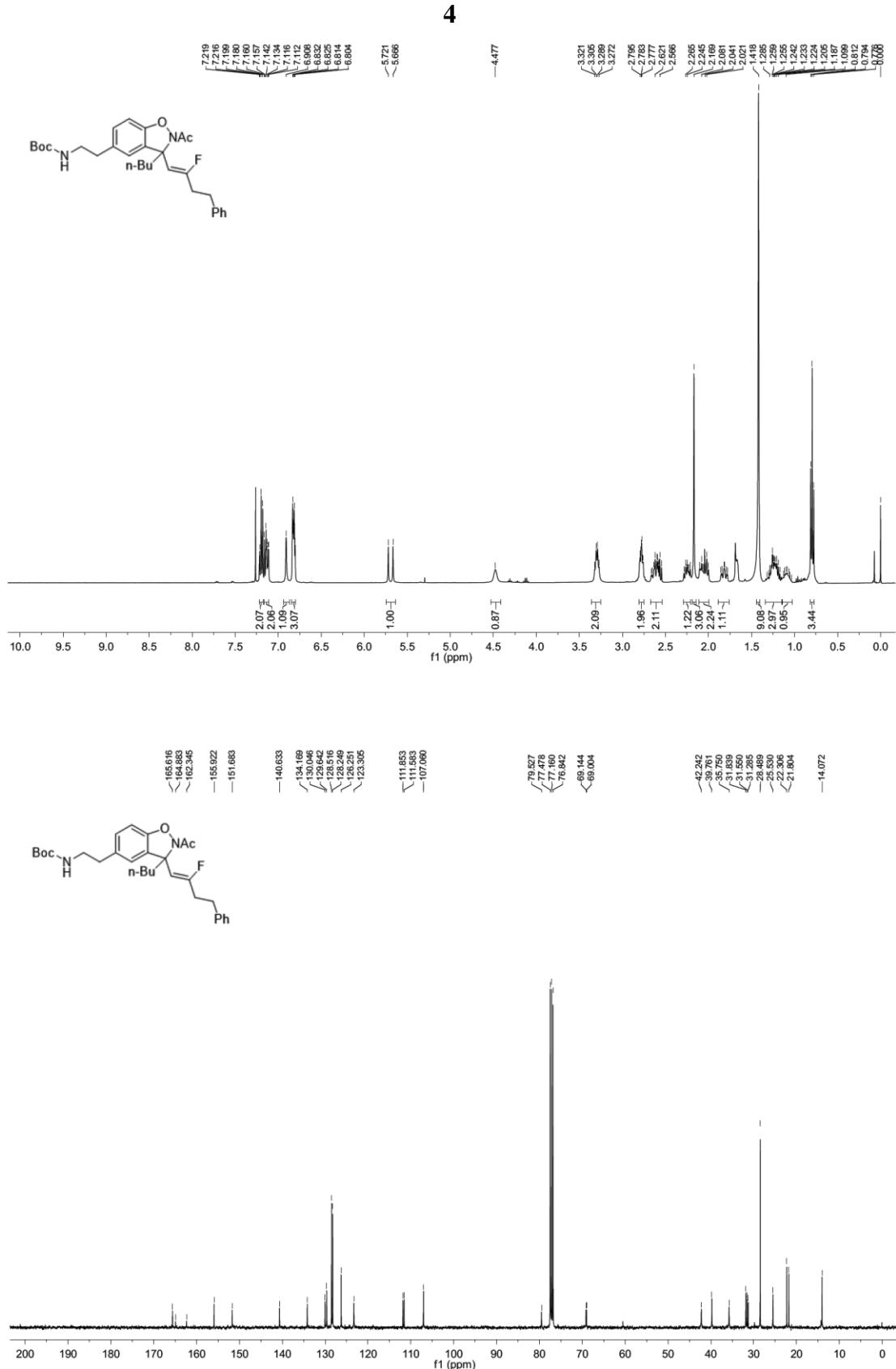
3w



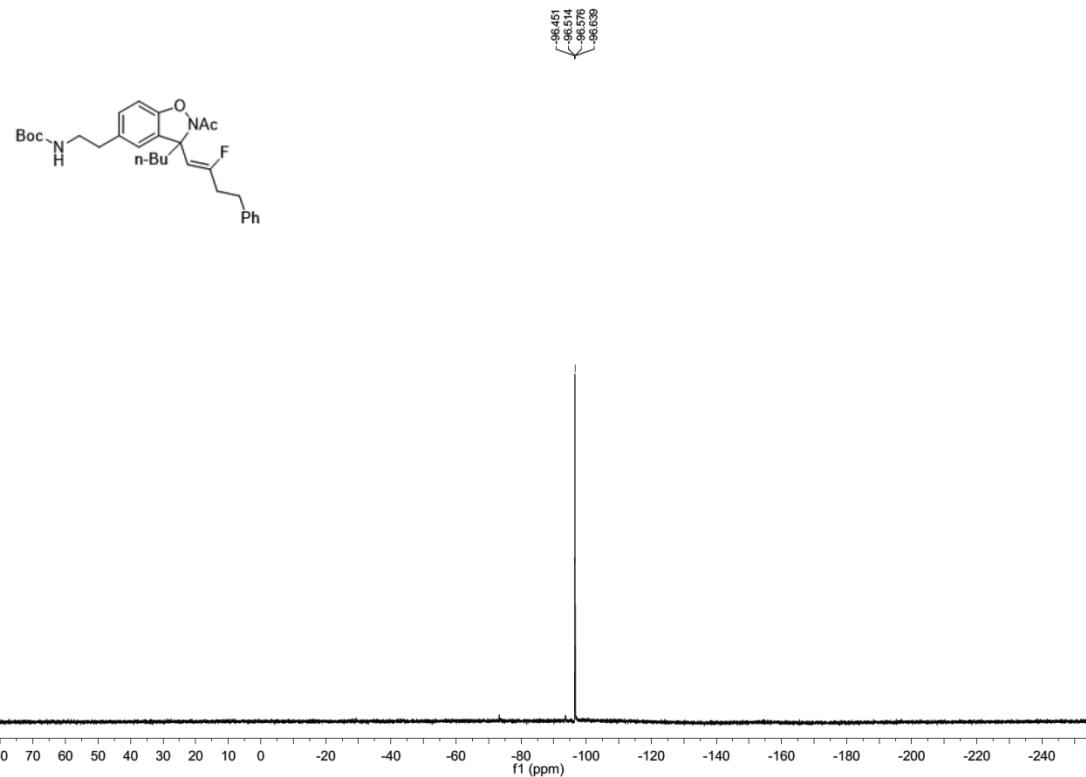
¹⁹F NMR spectrum of 3w

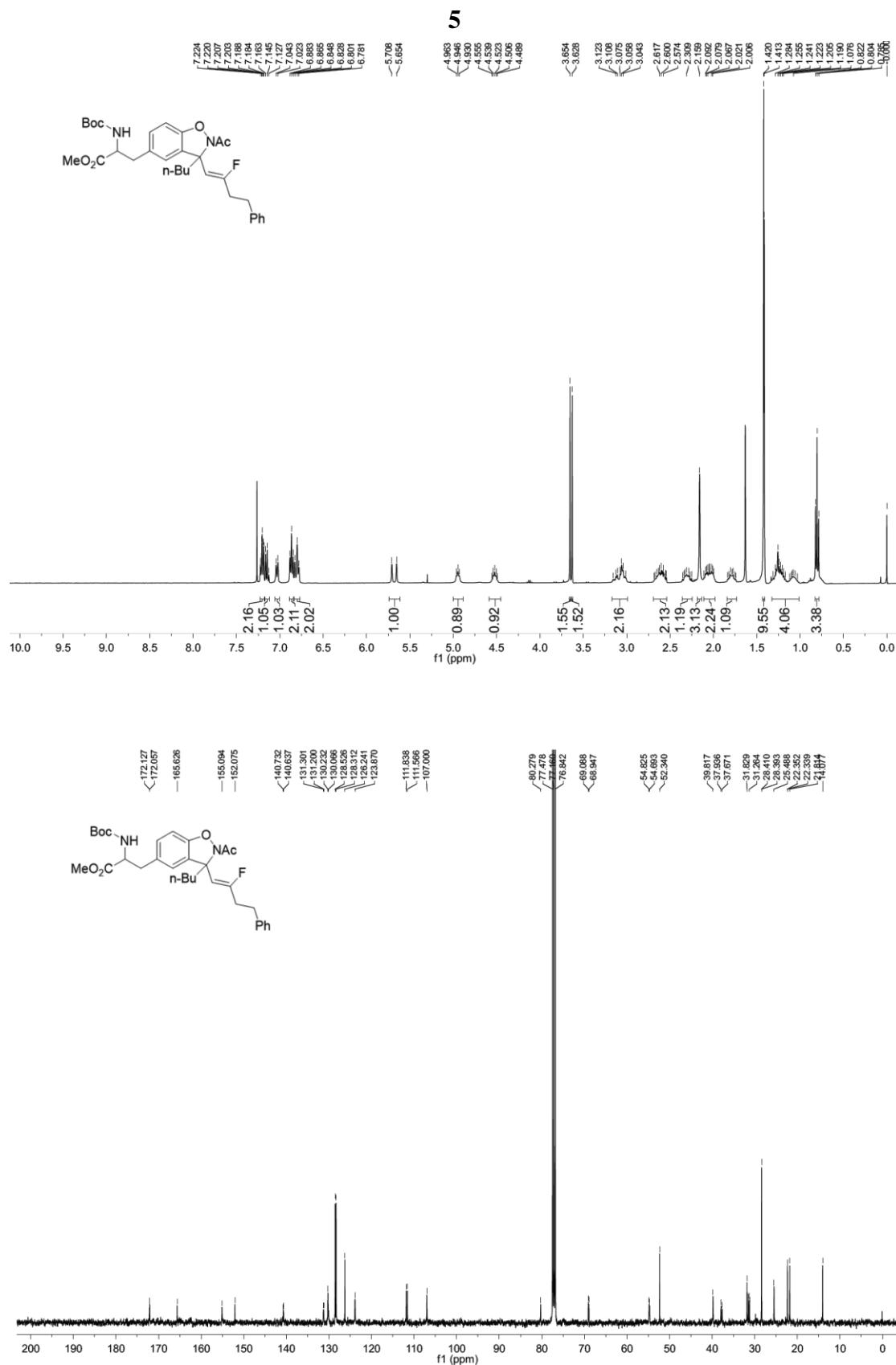
-93.394
-93.458
-93.521
-93.583



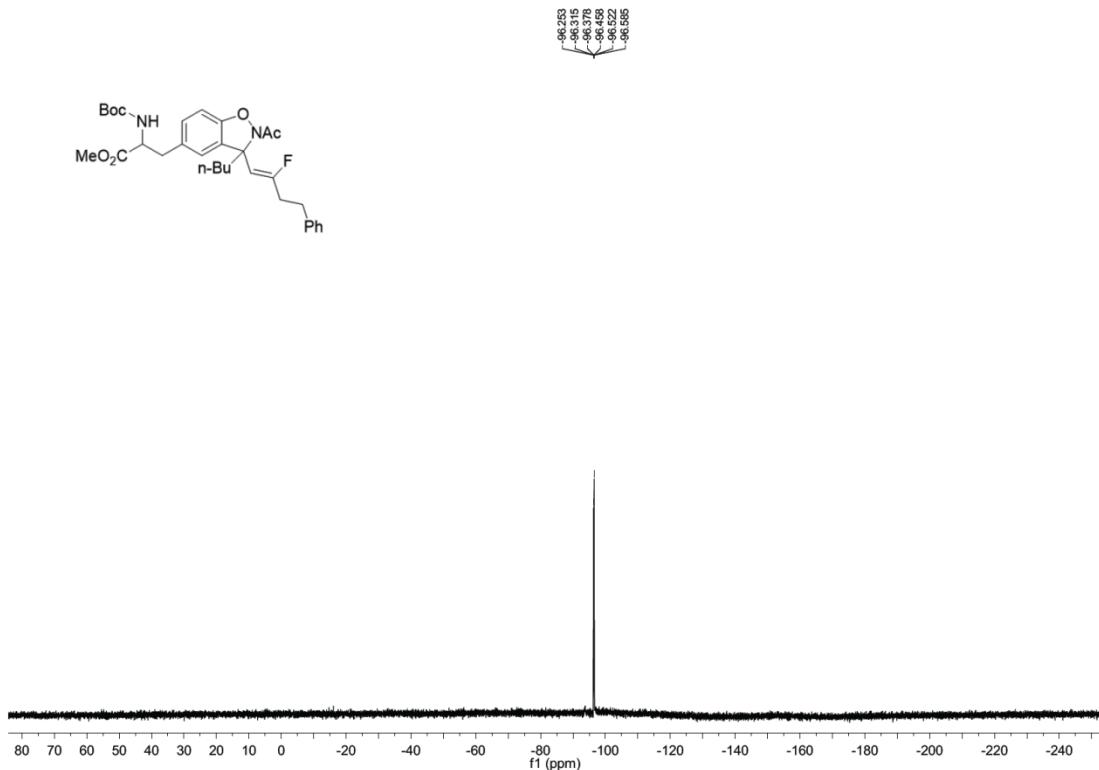


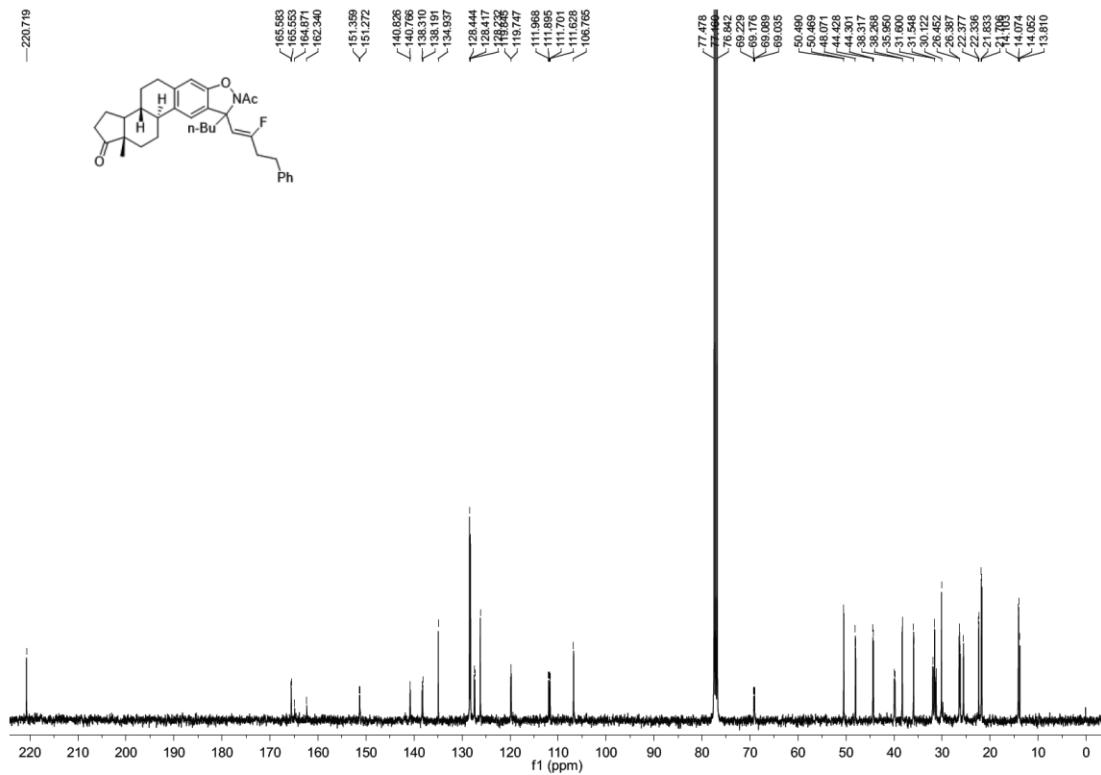
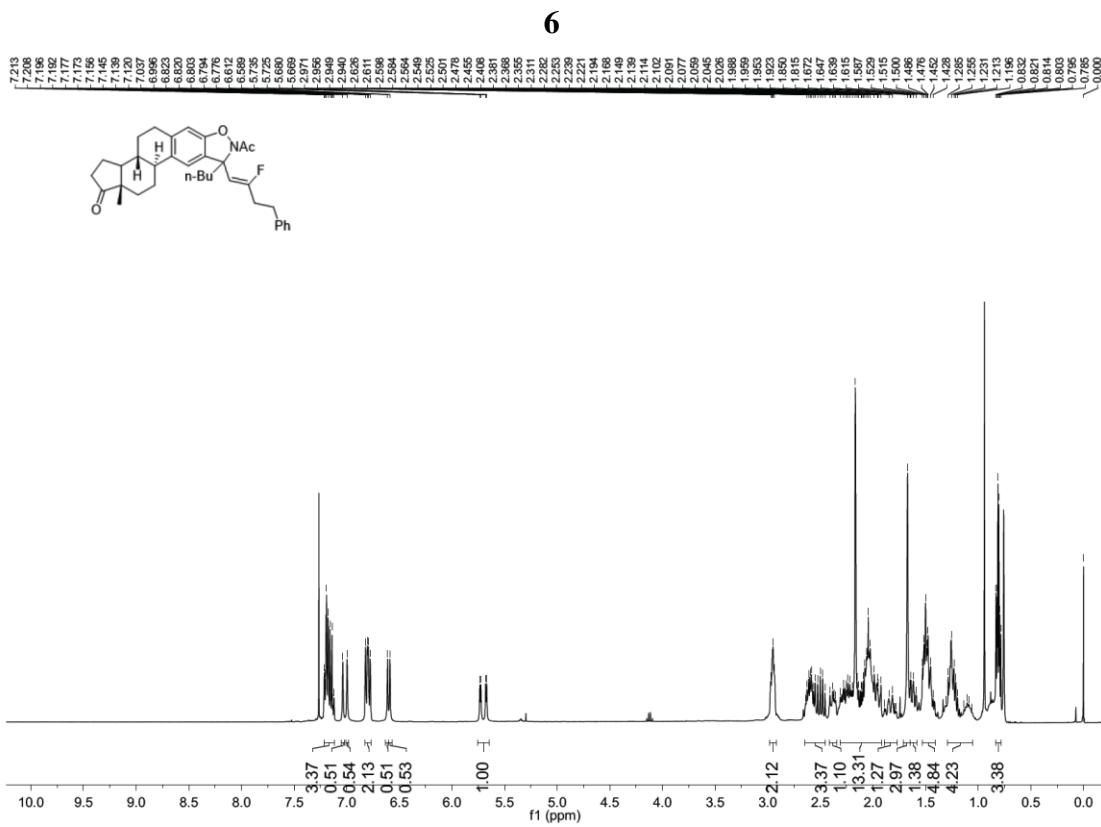
¹⁹F NMR spectrum of 4



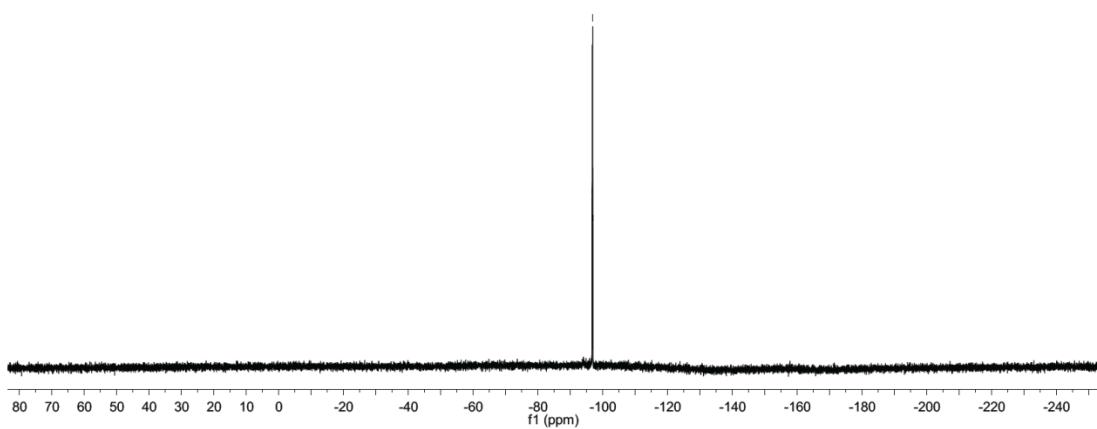
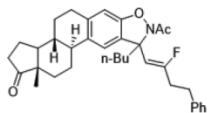


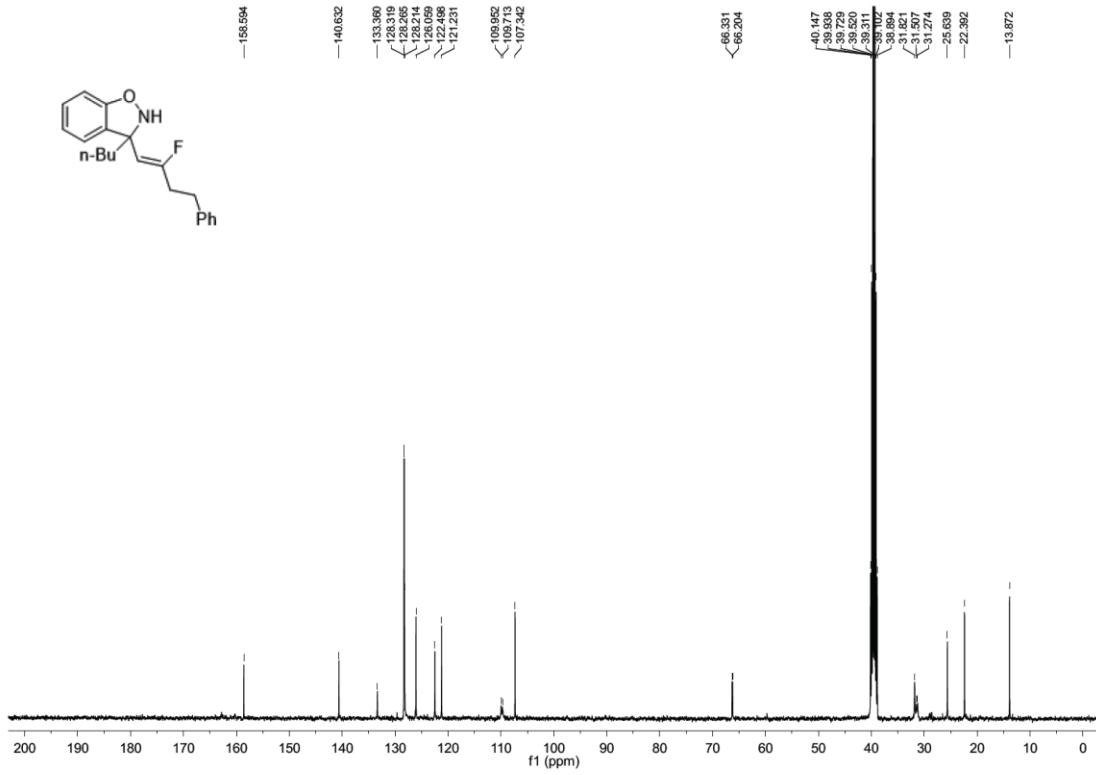
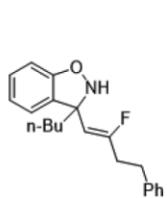
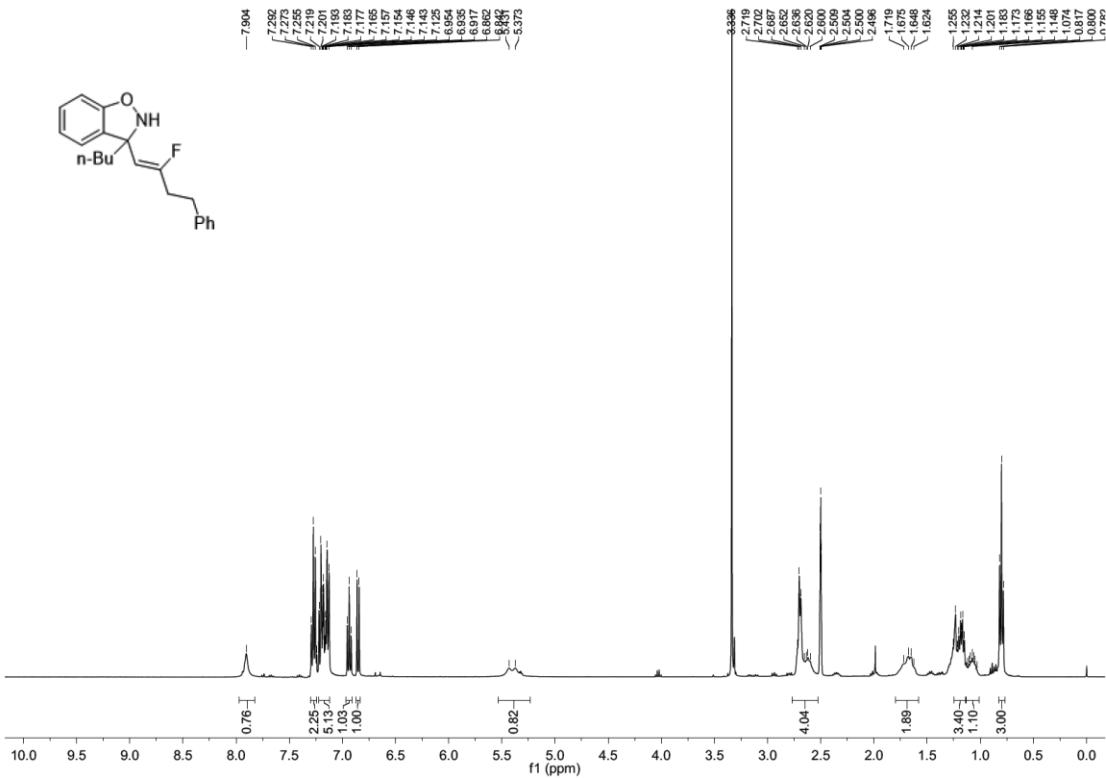
¹⁹F NMR spectrum of 5





¹⁹F NMR spectrum of 6





¹⁹F NMR spectrum of 7

