

Supporting Information

Cycloaddition Reaction of Vinylphenylfurans and Dimethyl Acetylenedicarboxylate to [8+2] Isomers *via* Tandem [4+2]/Diradical Alkene-Alkene Coupling/[1,3]-H Shift Reactions: Experimental Exploration and DFT Understanding of Reaction Mechanism

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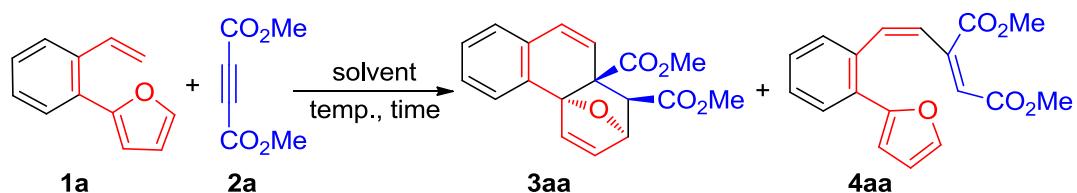
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1. Reaction of Vinylphenylfuran and **DMAD** in Organic Solvent without Catalyst

Table S1. Optimization of reaction conditions^[a]

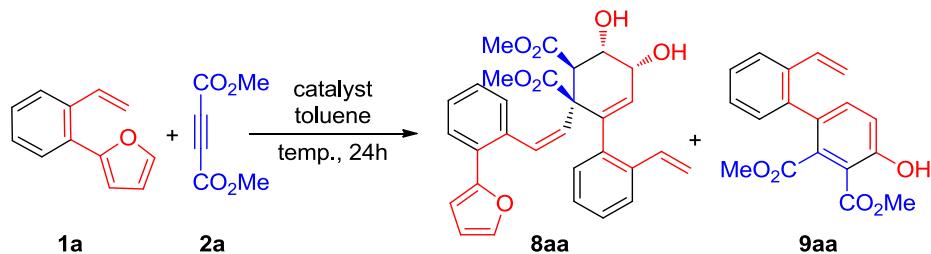


entry	DMAD (eq)	temp. (°C) ^[b]	solv.	Time (h)	yield ^[c] (%) (3aa/4aa) ^[d]
1	1.0	85	Toluene	12	14 ^[e] (1.0:0.3)
2	1.0	100	Toluene	24	60 (1.0:0.5)
3	1.0	110	Toluene	24	65 (1.0:0.7)
4	1.0	120	Toluene	24	77 (1.0:0.8)
5	1.0	120	THF	24	29 (1.0:0.3)
6	1.0	120	DCM	24	67 (1.0:0.4)
7	1.0	120	CH ₃ CN	24	67 (1.0:0.5)
8	1.0	120	Benzene	24	63 (1.0:0.7)
9	1.0	120	n-Hexane	24	53 (1.0:0.6)
10	1.0	120	Chlorobenzene	24	76 (1.0:1.0)
11	1.0	120	Toluene/H ₂ O	24	65 (1.0:0.8)
12	1.2	120	Toluene	24	84 (1.0:1.2)
13	1.5	120	Toluene	24	86 (1.0:0.9)
14	1.5	120	Toluene	48	87 (1.0:1.0)

[a] The reaction was carried out using sealed tubes in the specified solvent under N₂. [b] The oil bath temperature. [c] Isolated yield. [d] The molar ratio of 3aa/4aa was determined by ¹H NMR spectroscopy. [e] Yield determined by ¹H NMR spectroscopy.

2. Reactions of Vinylphenylfuran and **DMAD** in Toluene with Metal Catalyst

Table S2. Optimization of reaction conditions between 2-(2-vinylphenyl)furan and DMAD in toluene with metal catalyst^[a]

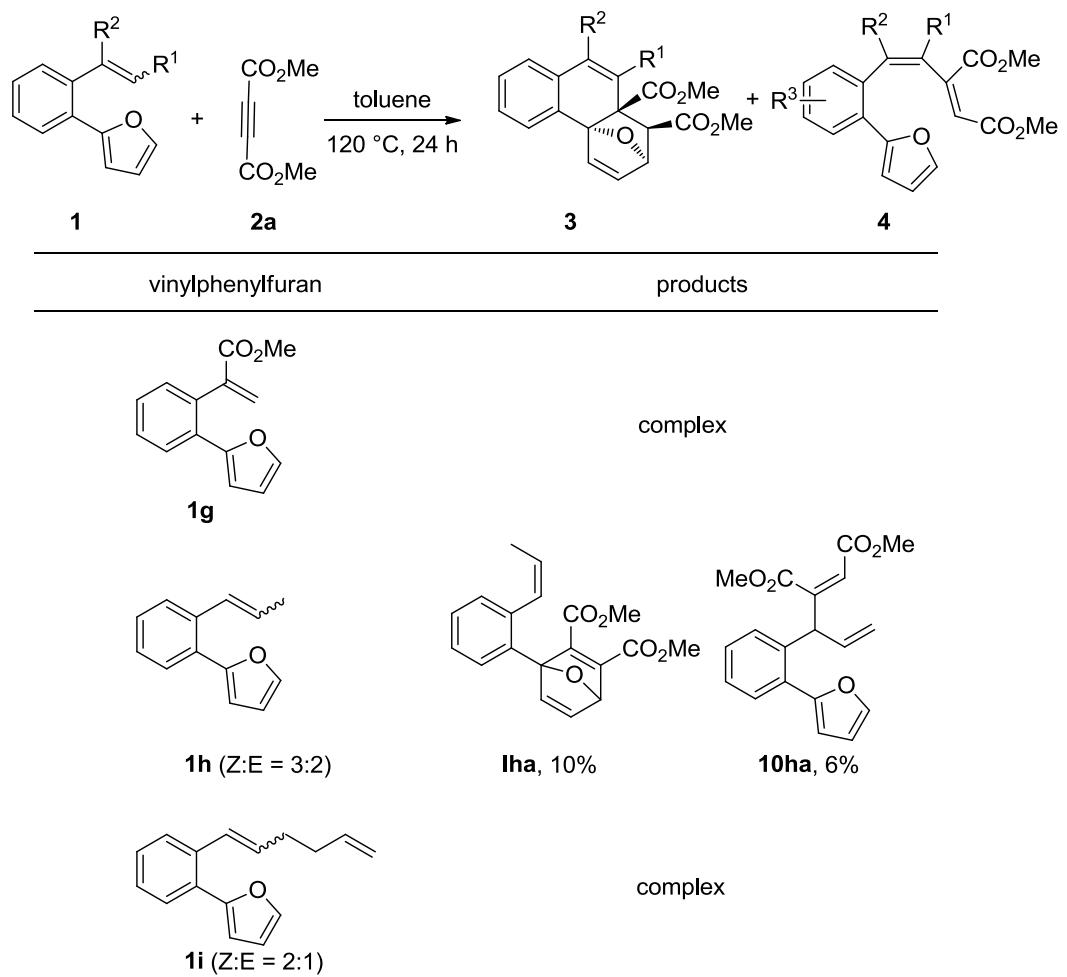


entry	catalyst	DMAD (eq)	temp. (°C) ^[b]	product	yield ^[c] (%)
1	ZnI ₂	1.0	85	8aa:9aa (1:0.9)	30
2	ZnF ₂	1.0	120	3aa:4aa (1:1)	67
3	MnCl ₂	1.0	120	3aa:4aa (1:0.8)	64
4	Ni(acac) ₂	1.0	120	3aa:4aa (1:0.7)	71
5	[Rh(OAc) ₂] ₂	1.0	120	3aa:4aa (1:1)	50
6	SIMes-AuCl	1.0	120	3aa:4aa (1:0.8)	73
7	CuCl ₂ H ₂ O	1.0	120	3aa (trace)	Complex
8	FeCl ₃	1.0	120	9aa	100

[a] The reaction was carried out using sealed tubes in toluene for 24 h using 5 mol% metal catalyst under N₂. The molar ratio of **1a/2a**=1:1. [b] The oil bath temperature. [c] Isolated yield.

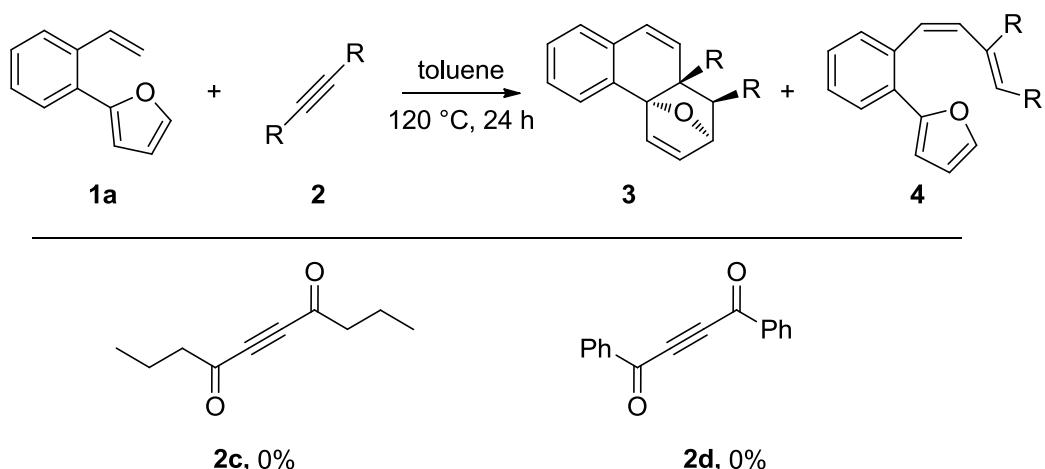
3. Substrate Scope of Vinylphenylfurans and **DMAD** in Toluene

Table S3. Variation of vinylphenylfurans **1**



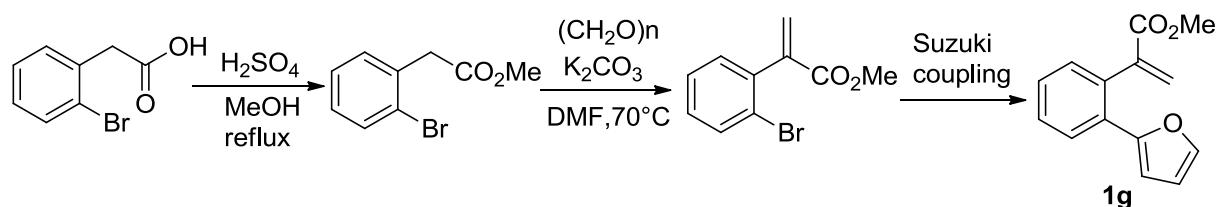
The substrate with an electron-withdrawing group, like ester group, at R^2 (**1g**) was ineffective for this reaction. Internal alkene showed very low reactivity, probably due to the steric hindrance. For **1h**, only the [4+2] product **Iha**, and ene product **10ha** were isolated in yields of 10% and 6%, respectively. Substrate **1i** tethered with a butenyl group, which was designed to trap the possible diradical species intermediate, resulted in a complex system.

Table S4. Variation of alkynes 2



Experimental Section:

Synthesis of 1g



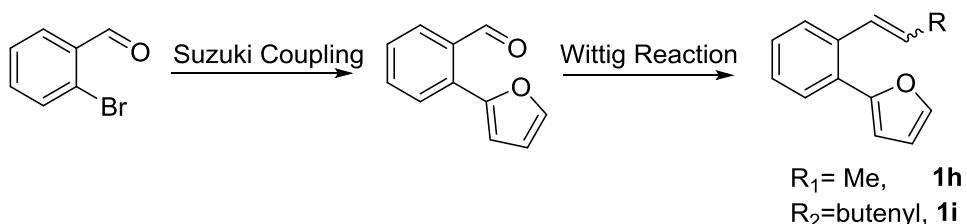
A solution of 2-(2-bromophenyl) acetic acid (1.00 g, 4.65 mmol) in methanol (10 mL) was mixed with 2 mL concentrated sulfuric acid. The reaction was heated for 2 h at 50 °C and complete conversion was detected by TLC. After the reaction completed, the mixture was neutralized with K_2CO_3 (aq.) and extracted with EtOAc (3×10 mL) after methanol was removed by vacuum. The crude product of methyl 2-(2-bromophenyl) acetate was obtained after EtOAc was removed.

A solution of crude 2-(2-bromophenyl) acetate (1.05 g, 4.67 mmol) in DMF (10 mL) was added K_2CO_3 (1.6 g, 9.2 mmol) and paraformaldehyde (276 mg, 9.2 mmol). The reaction was heated for 2 h at 70 °C and complete conversion was detected by GC-MS. After the reaction completed, the reaction was diluted with EtOAc, washed with water and brine. The crude product of methyl 2-(2-bromophenyl) acrylate was obtained after the solvent was removed by vacuum.

The methyl 2-(2-bromophenyl) acrylate (600 mg, 2.63 mmol) and $\text{Pd}(\text{PPh}_3)_4$ (151 mg, 0.131 mmol) was added into a 50 mL schlenk tube, and stirred for 10 min at room temperature. Then 2-furanboronic acid (309.2 mg, 2.763 mmol, dissolved in 2 mL ethanol) and Na_2CO_3 (546 mg, 5.2 mmol, in 2 mL water) were added into the mixture

in sequence. The mixture was heated under reflux for 16 h. After completion of the reaction, the system was filtered, then the solvent was concentrated, and the residue was extracted with 10 mL ether three times, dried over MgSO_4 , and evaporated under reduced pressure to afford methyl 2-(furan-2-yl)phenylacrylate, which was purified by column chromatography over silica gel eluting with petroleum ether and EtOAc (petroleum ether: EtOAc= 10:1).

*Synthesis of **1h** and **1i***



The 2-bromobenzaldehyde (500 mg, 2.5 mmol) and $\text{Pd}(\text{PPh}_3)_4$ (87.1mg, 0.0754 mmol) was added into a 50 mL schlenk tube, and stirred for 10 min at room temperature. Then 2-furanboronic acid (309.2 mg, 2.763 mmol, dissolved in 2 mL ethanol) and Na_2CO_3 (532.6 mg, 5.024 mmol, in 2 mL water) were added into the mixture in sequence. The mixture was heated under reflux for 16 h. After completion of the reaction, the system was filtered, then the solvent was concentrated, and the residue was extracted with 10 mL ether three times, dried over MgSO_4 , and evaporated under reduced pressure to afford 2-(furan-2-yl)benzaldehyde, which was purified by column chromatography over silica gel eluting with petroleum ether and EtOAc (petroleum ether: EtOAc= 10:1).

1h:

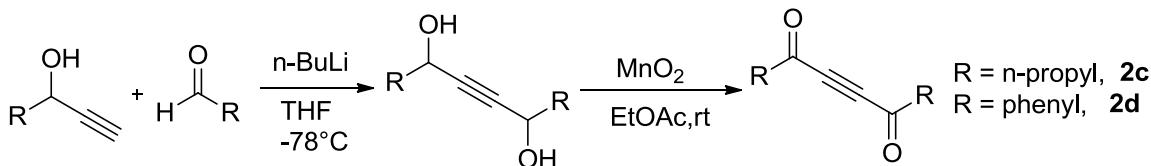
Under a nitrogen atmosphere at 0 °C, *n*-BuLi (1.2 mL, 2.5 M) was dropped into a solution of $\text{CH}_3\text{CH}_2\text{PPh}_3\text{Br}$ (1.16 g, 3.140 mmol) in THF (10 mL) in a 50 mL Schlenk tube, and was stirred for 30 min before being treated with 2-(furan-2-yl)benzaldehyde (464.7 mg, 2.512 mmol) dropwise. The resulting solution was stirred at room temperature for 10 h, and then quenched with water. The product was extracted with petroleum ether, which was dried with MgSO_4 , which was purified by column chromatography over silica gel eluting with petroleum ether.

1i:

Under a nitrogen atmosphere at 0 °C, *n*-BuLi (1.2 mL, 2.5 M) was dropped into a solution of pent-4-en-1-yltriphenylphosphonium bromide (1.21 g, 3.140 mmol) in

THF (10 mL) in a 50 mL Schlenk tube, and was stirred for 30 min before being treated with 2-(furan-2-yl) benzaldehyde (464.7 mg, 2.512 mmol) dropwise. The resulting solution was stirred at room temperature for 10 h, and then quenched with water. The product was extracted with petroleum ether, which was dried with MgSO₄, and purified by column chromatography over silica gel eluting with petroleum ether.

Synthesis of 2c and 2d



Under a nitrogen atmosphere at -78 °C, *n*-BuLi (4.2 mL, 2.5 M) was dropped into a solution of hex-1-yn-3-ol (500 mg, 5.1 mmol) in THF (10 mL) in a 50 mL Schlenk tube, and was stirred for 30 min before being treated with butyraldehyde (550 mg, 7.6 mmol) dropwise. The resulting solution was stirred at room temperature for 10 h, and then quenched with water. The product was extracted with EtOAc, which was dried with MgSO₄. MnO₂ (4.36g, 51 mmol) was added into the extraction and stirred at room temperature until the conversion was completed. After the reaction completed, solid was filtered through Celite pad, and filtrate was evaporated under vacuum and purified by column chromatography over silica gel eluting with petroleum ether and EtOAc .

(E/Z) 2-(2-(hexa-1,5-dien-1-yl)phenyl)furan (1i). Colorless oil, $R_f = 0.9$ (petroleum ether), yield (370 mg, 74%, E/Z=1:2). ¹H NMR (400 MHz, CDCl₃) δ 7.78 (Z, d, *J* = 7.8 Hz, 1H), 7.62 (E, d, *J* = 6.7 Hz, 1H), 7.49 (E, s, 1H), 7.46 (E, s, 1H), 7.46 (Z, s, 1H), 7.32 – 7.19 (E, m, 2H), 7.32 – 7.19 (Z, m, 3H), 6.73 (E, d, *J* = 15.7 Hz, 1H), 6.64 (Z, d, *J* = 3.0 Hz, 1H), 6.56 (Z, d, *J* = 11.5 Hz, 1H), 6.49 (E, m, 2H), 6.44 (Z, d, *J* = 1.5 Hz, 1H), 5.07 (E, d, *J* = 17.1 Hz, 1H), 5.03 – 4.90 (E, m, 1H), 5.03 – 4.90 (Z, m, 2H), 2.31 (Z, ddt, *J* = 21.5, 14.0, 7.1 Hz, 4H), 2.15 (E, q, *J* = 6.9 Hz, 4H). ¹³C NMR (101 MHz, CDCl₃) δ 153.0, 152.7, 142.0, 141.8, 138.2, 138.1, 135.7, 134.2, 132.0, 131.9, 130.3, 129.8, 129.8, 129.6, 128.9, 127.7, 127.4, 127.3, 127.1, 127.0, 126.8, 126.4, 115.0, 114.9, 111.4, 111.4, 109.9, 109.7, 33.9, 33.5, 32.5, 27.7. IR (thin film) ν_{max} (cm⁻¹) 3068, 3009, 2920, 2848, 1722, 1640, 1280, 1211, 1083, 1002, 910, 756. HRMS (EI) mass calcd for C₁₆H₁₆O ([M]⁺): 224.1201; found 224.1199.

dec-5-yne-4,7-dion (2c). colorless oil, $R_f = 0.6$ (petroleum ether: EtOAc = 10:1), yield (210 mg, 65%). ^1H NMR (400 MHz, CDCl_3) δ 2.62 (t, $J = 7.2$ Hz, 1H), 1.72 (dd, $J = 14.6, 7.3$ Hz, 1H), 0.97 (t, $J = 7.4$ Hz, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 186.4, 84.2, 47.1, 17.1, 13.4.

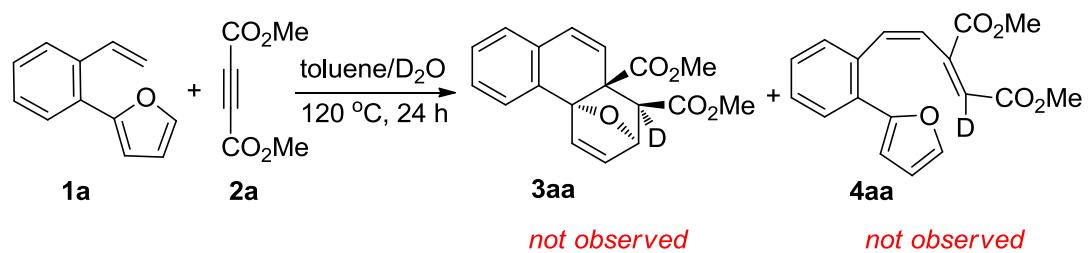
1,4-diphenylbut-2-yne-1,4-dione (2d). Brown powder, $R_f = 0.7$ (petroleum ether: EtOAc = 5:1), yield (420 mg, 70%). ^1H NMR (400 MHz, CDCl_3) δ 8.21 (d, $J = 7.7$ Hz, 2H), 7.71 (t, $J = 7.4$ Hz, 1H), 7.57 (t, $J = 7.5$ Hz, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 176.6, 135.8, 135.2, 129.8, 129.0, 85.9.

(Z)-1-(2-(prop-1-en-1-yl)phenyl)-7-oxabicyclo[2.2.1]hepta-2,5-diene-2,3-dicarboxylate (1ha). Yellow oil, $R_f = 0.3$ (petroleum ether: EtOAc = 10:1), yield (16 mg, 10%). ^1H NMR (400 MHz, CDCl_3) δ 7.66 (d, $J = 5.2$ Hz, 1H), 7.61 (d, $J = 7.5$ Hz, 1H), 7.36 – 7.25 (m, 4H), 6.70 (d, $J = 11.5$ Hz, 1H), 5.87 – 5.72 (m, 2H), 3.80 (s, 3H), 3.59 (s, 3H), 1.74 (d, $J = 7.0$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 164.3, 162.9, 158.0, 149.9, 144.5, 144.4, 137.0, 131.7, 131.0, 129.2, 128.6, 128.4, 128.4, 126.9, 98.3, 84.0, 52.3, 52.0, 14.5. IR (thin film) ν_{max} (cm^{-1}) 3027, 2922, 2854, 2313, 1711, 1434, 1318, 1240, 1104, 983, 756, 705. HRMS (ESI) mass calcd for $\text{C}_{19}\text{H}_{18}\text{O}_5\text{Na}$ ($[\text{M}+\text{Na}]^+$): 349.1055; found 349.1046.

dimethyl 2-(1-(2-(furan-2-yl)phenyl)allyl)maleate (10ha). Yellow oil, $R_f = 0.4$ (petroleum ether: EtOAc = 10:1), yield (14 mg, 6%). ^1H NMR (400 MHz, CDCl_3) δ 7.59 (dd, $J = 5.9, 3.1$ Hz, 1H), 7.52 (d, $J = 1.3$ Hz, 1H), 7.32 (ddd, $J = 7.5, 5.6, 3.3$ Hz, 3H), 7.26 (s, 1H), 6.55 (d, $J = 3.3$ Hz, 1H), 6.49 (dd, $J = 3.3, 1.8$ Hz, 1H), 6.04 (ddd, $J = 17.2, 10.2, 7.0$ Hz, 1H), 5.78 (d, $J = 1.7$ Hz, 1H), 5.26 (d, $J = 10.2$ Hz, 1H), 5.05 (m, 2H), 3.71 (s, 3H), 3.68 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 168.3, 165.6, 152.4, 151.0, 142.4, 136.4, 135.1, 131.0, 129.5, 129.2, 128.1, 127.5, 122.1, 118.9, 111.4, 109.0, 52.3, 51., 49.0. IR (thin film) ν_{max} (cm^{-1}) 2922, 2853, 1728, 1439, 1359, 1262, 1167, 1016, 913, 733. HRMS (MALDI) mass calcd for $\text{C}_{19}\text{H}_{18}\text{O}_5\text{Na}$ ($[\text{M}+\text{Na}]^+$): 349.1055; found 349.1046.

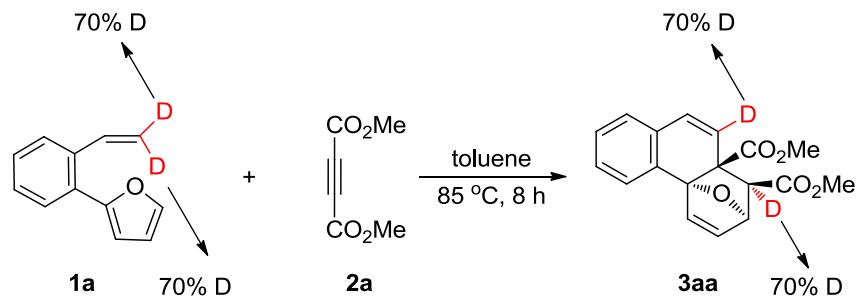
4. H/D Exchange Experiment

Scheme S1. Reaction of vinylphenylfuran and **DMAD** in toluene with equivalents of $\text{D}_2\text{O}^{[\text{a}]}$

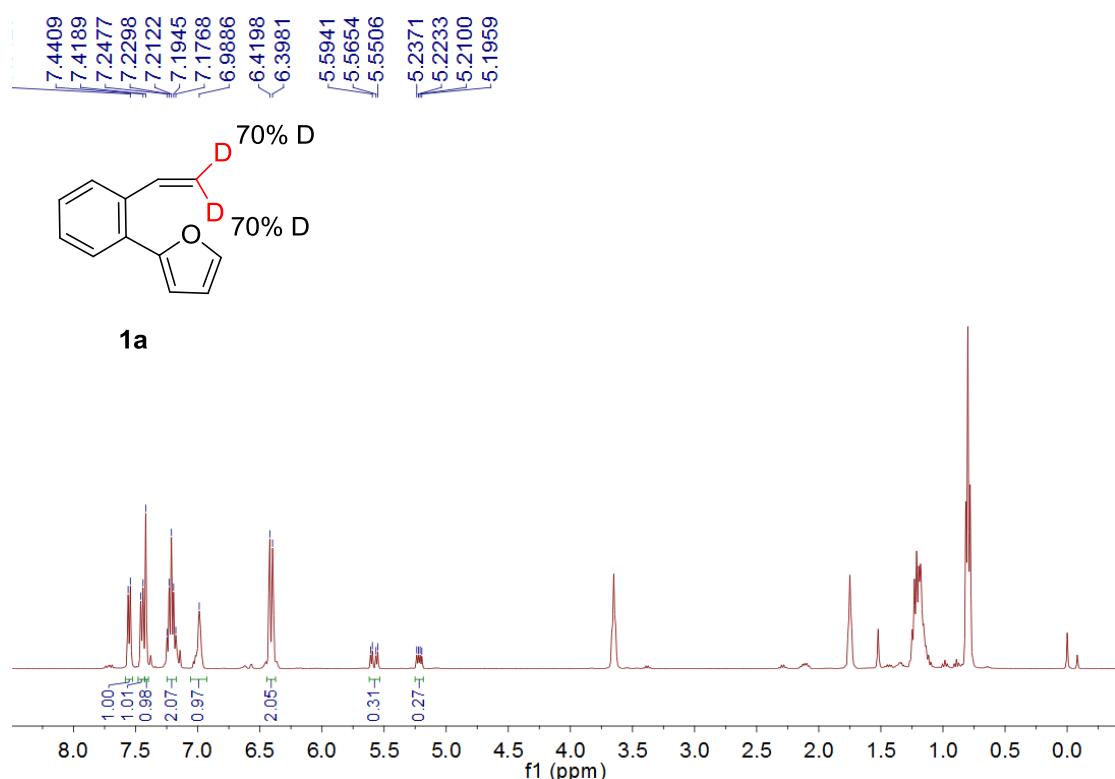


[a] The reaction was conducted at 120 °C in toluene under N_2 for 24 h. The molar ratio of **1a**/**2a**/ D_2O was 1:1.5:10.

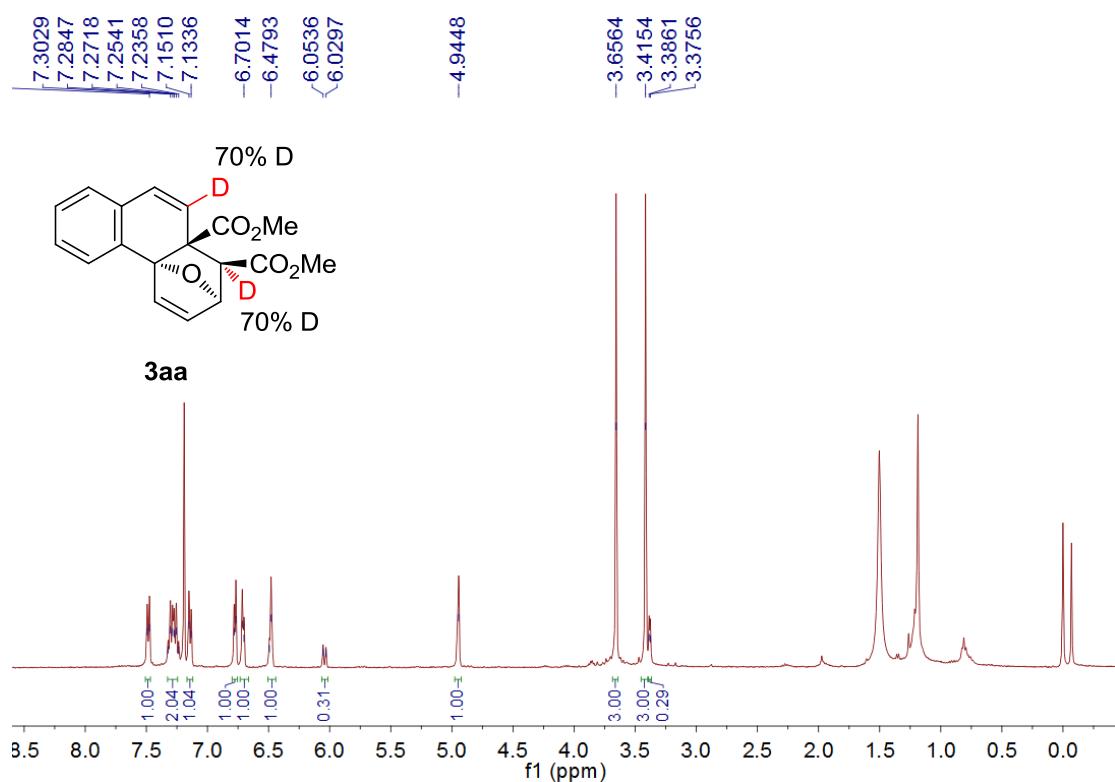
Scheme S2. Deuterium labeling study of the [1,3]-H-shift



Copies of ^1H NMR Spectra for **1a-d₂**

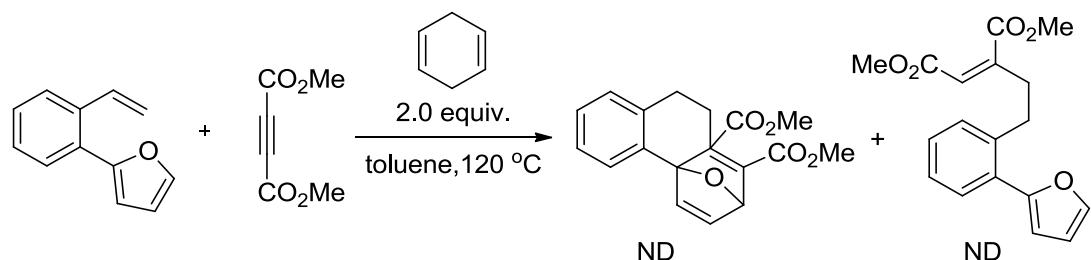


Copies of ^1H NMR Spectra for **3aa-d₂**



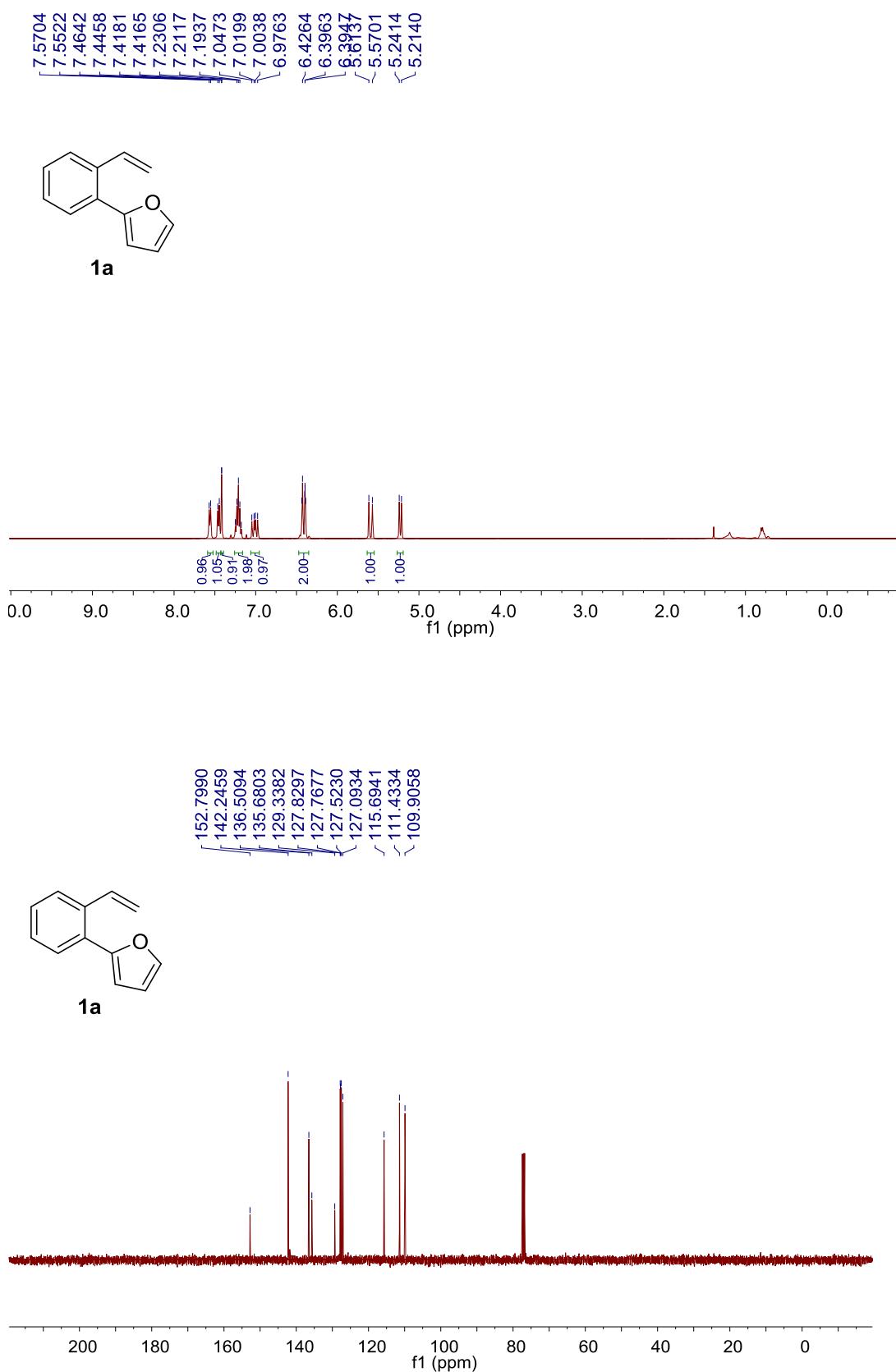
5. Control Experiments

The reaction has been performed in the presence of 1,4-hexadiene. The reduction products, however, were not detected by ^1H NMR and GC-MS.

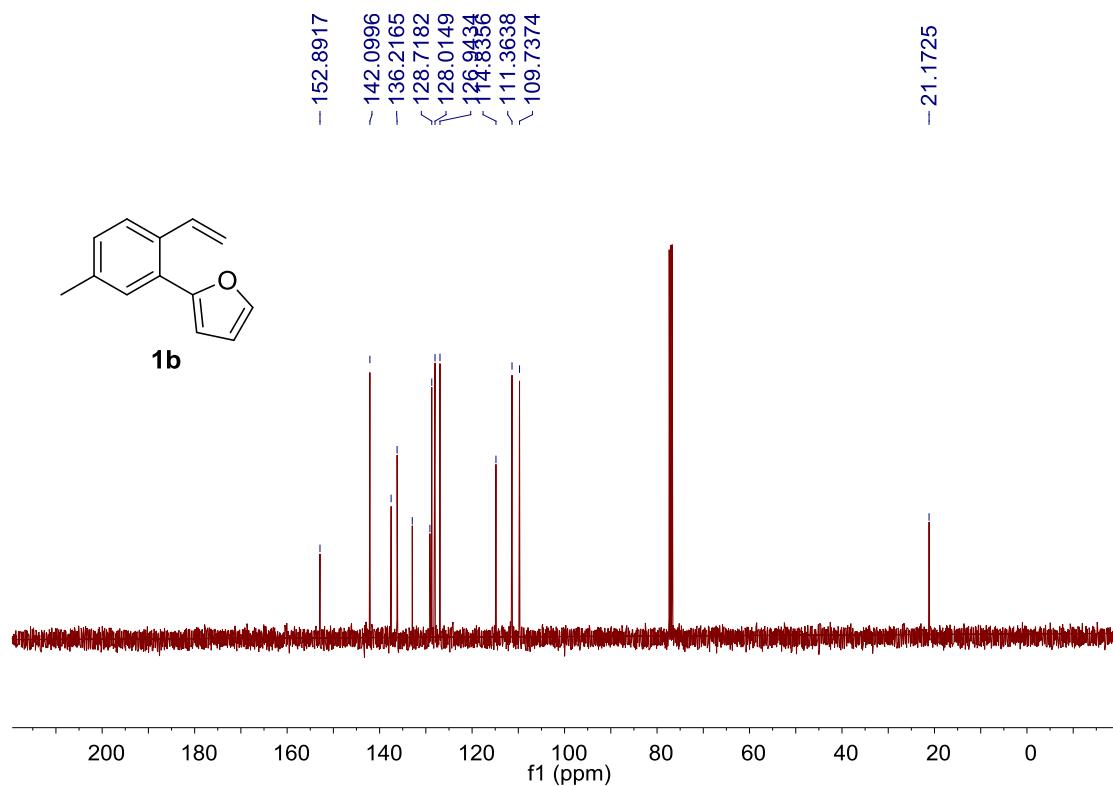
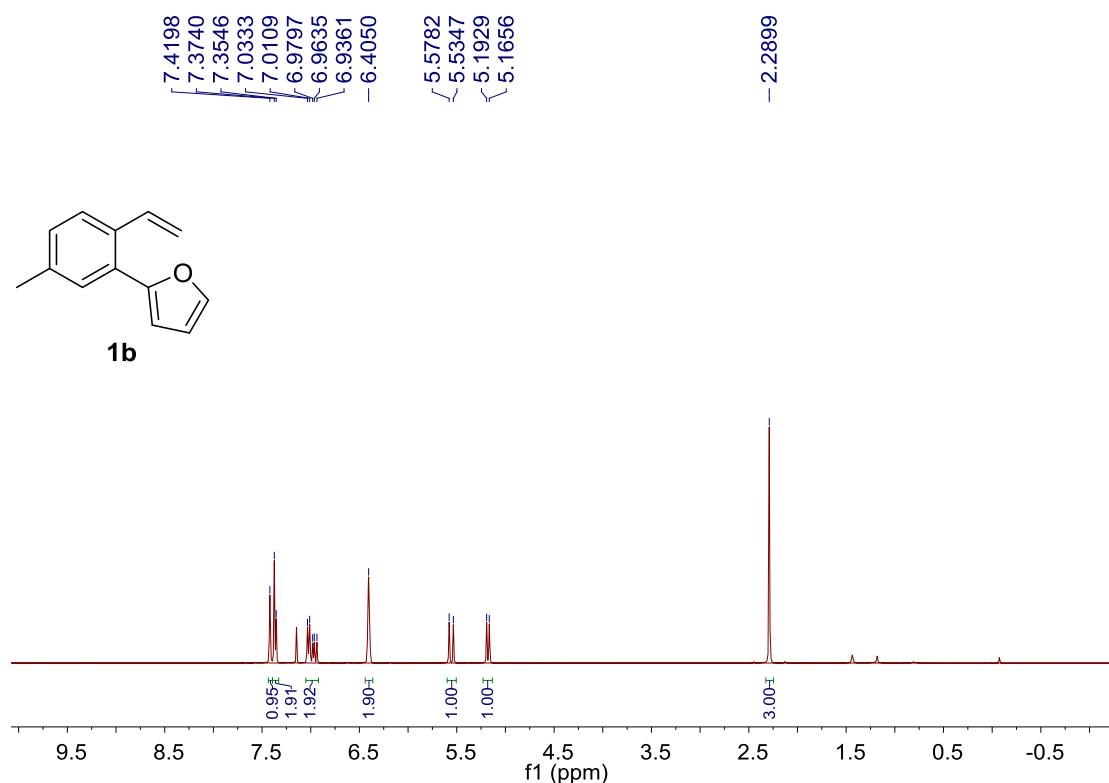


6. ^1H , ^{13}C , and ^{19}F NMR Spectra

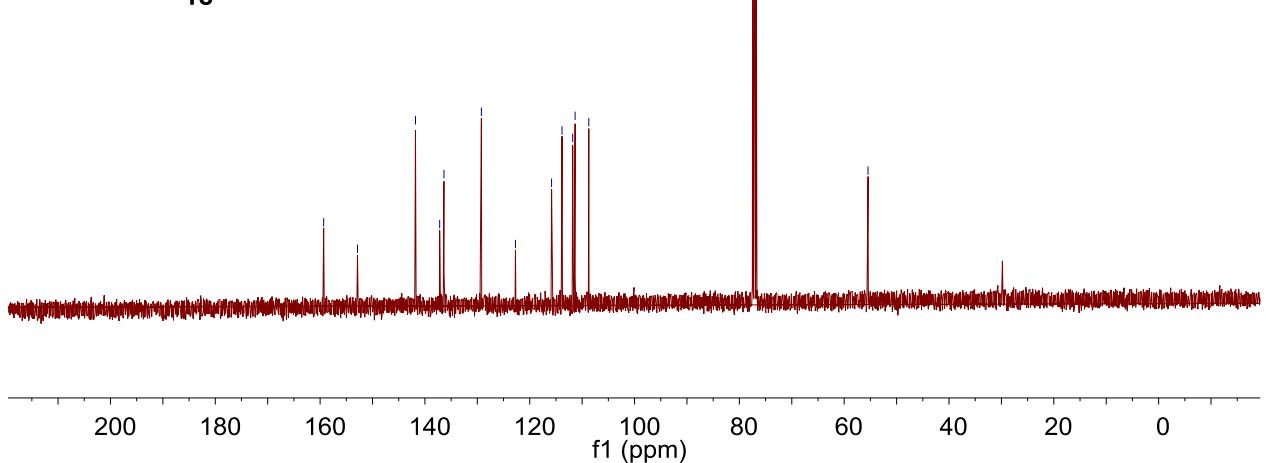
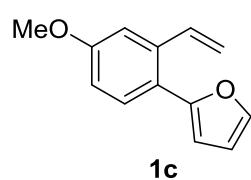
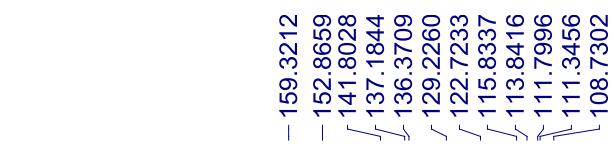
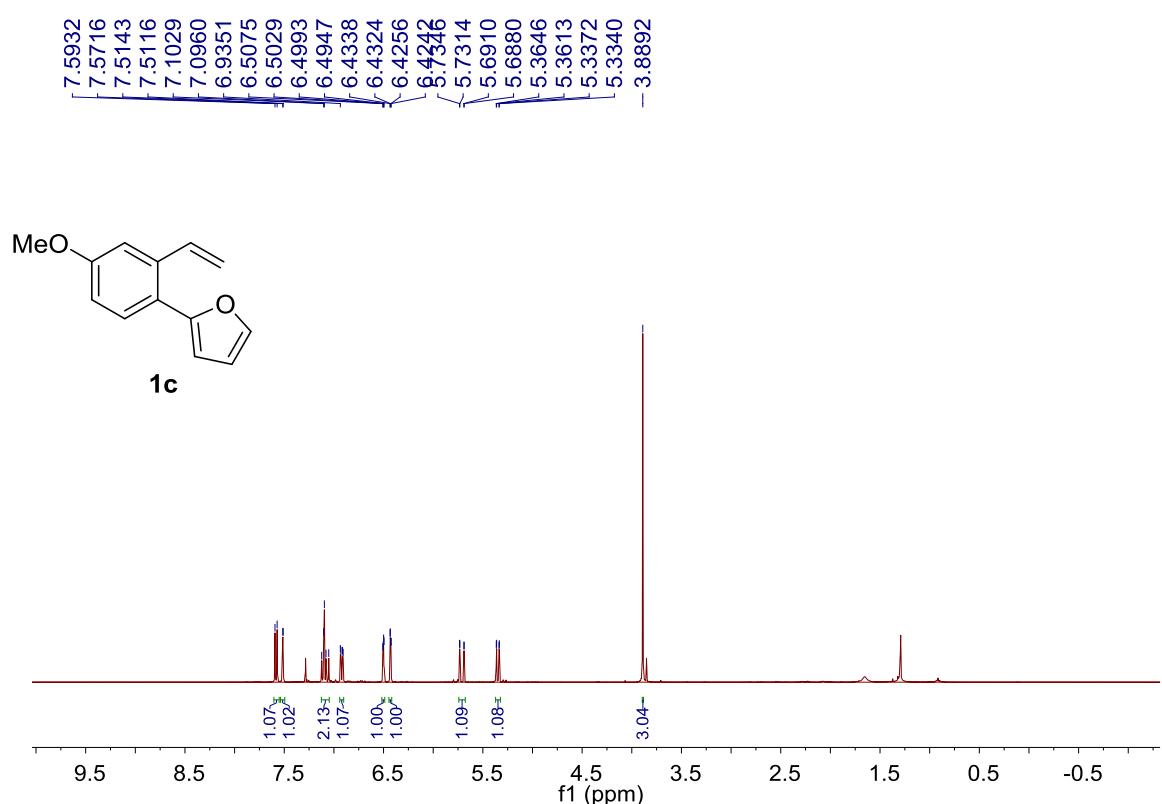
Copies of ^1H and ^{13}C NMR Spectra for **1a**



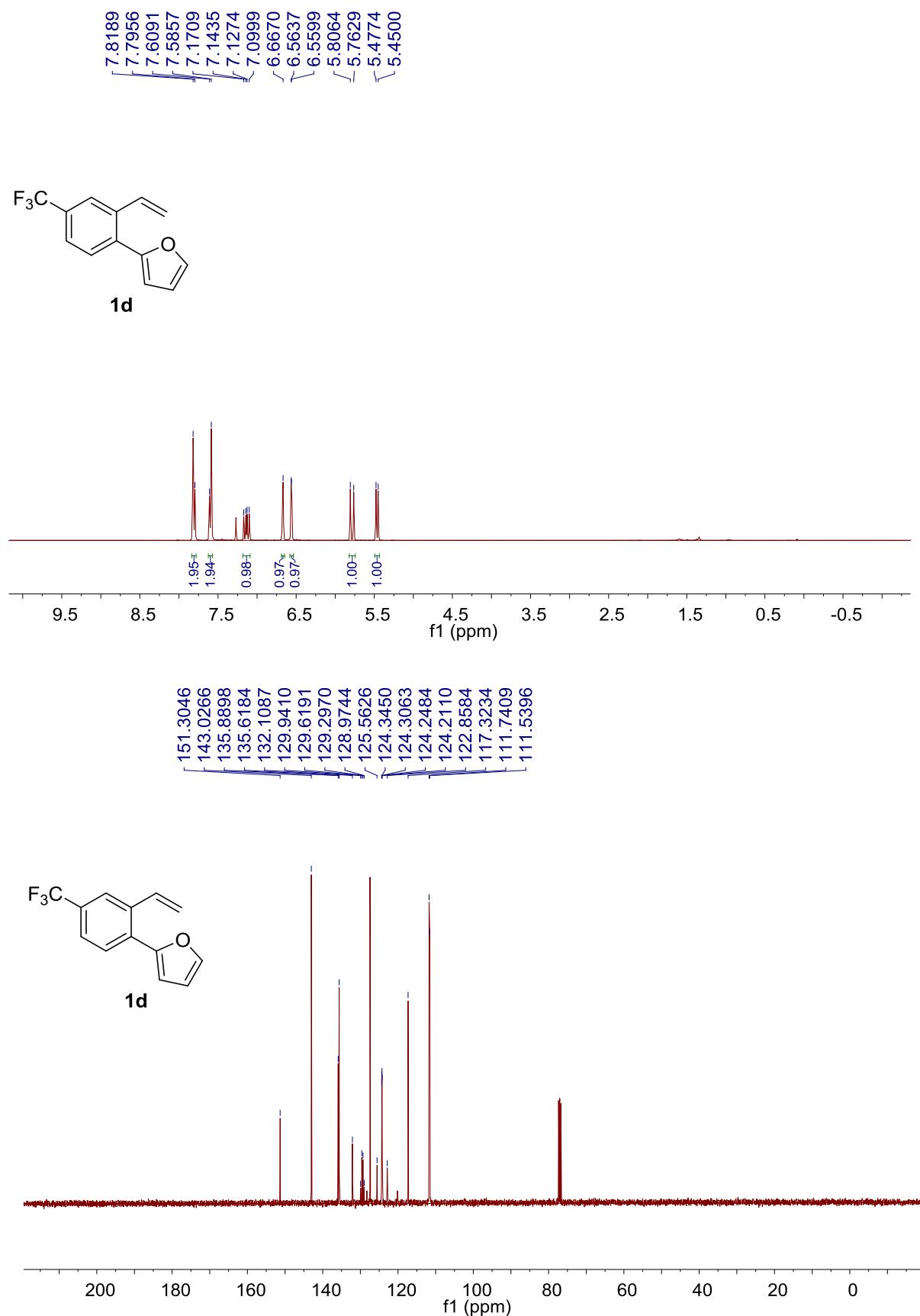
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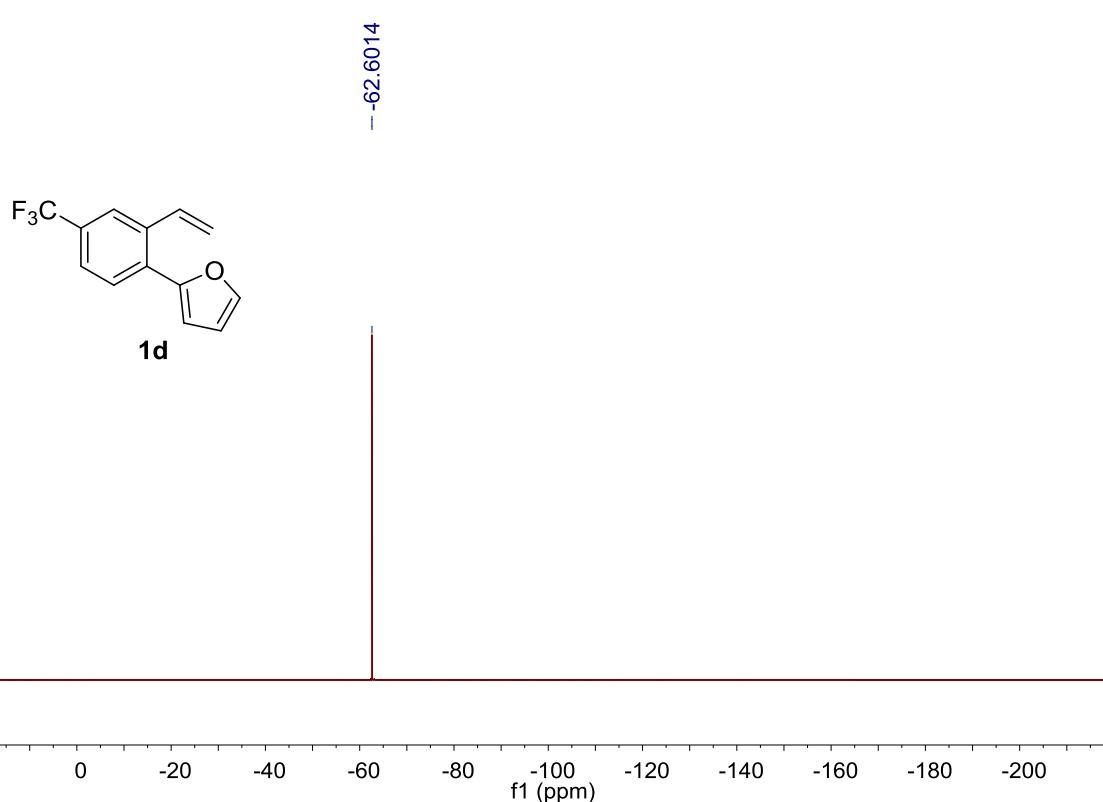


Copies of ^1H and ^{13}C NMR Spectra for **1c**

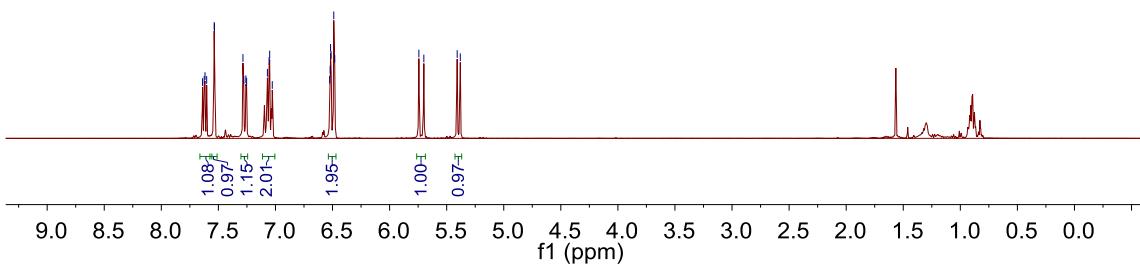
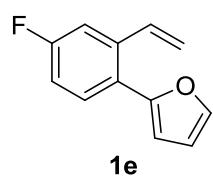
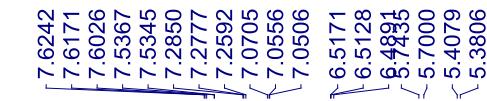


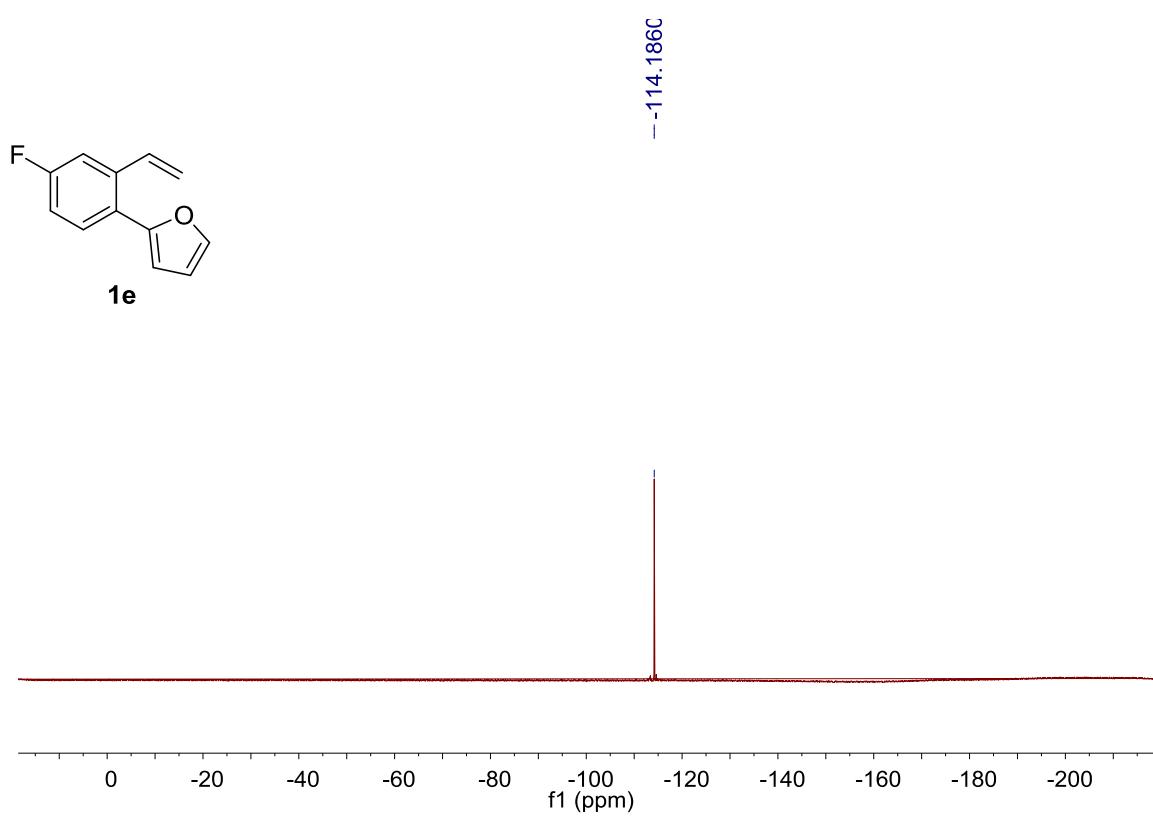
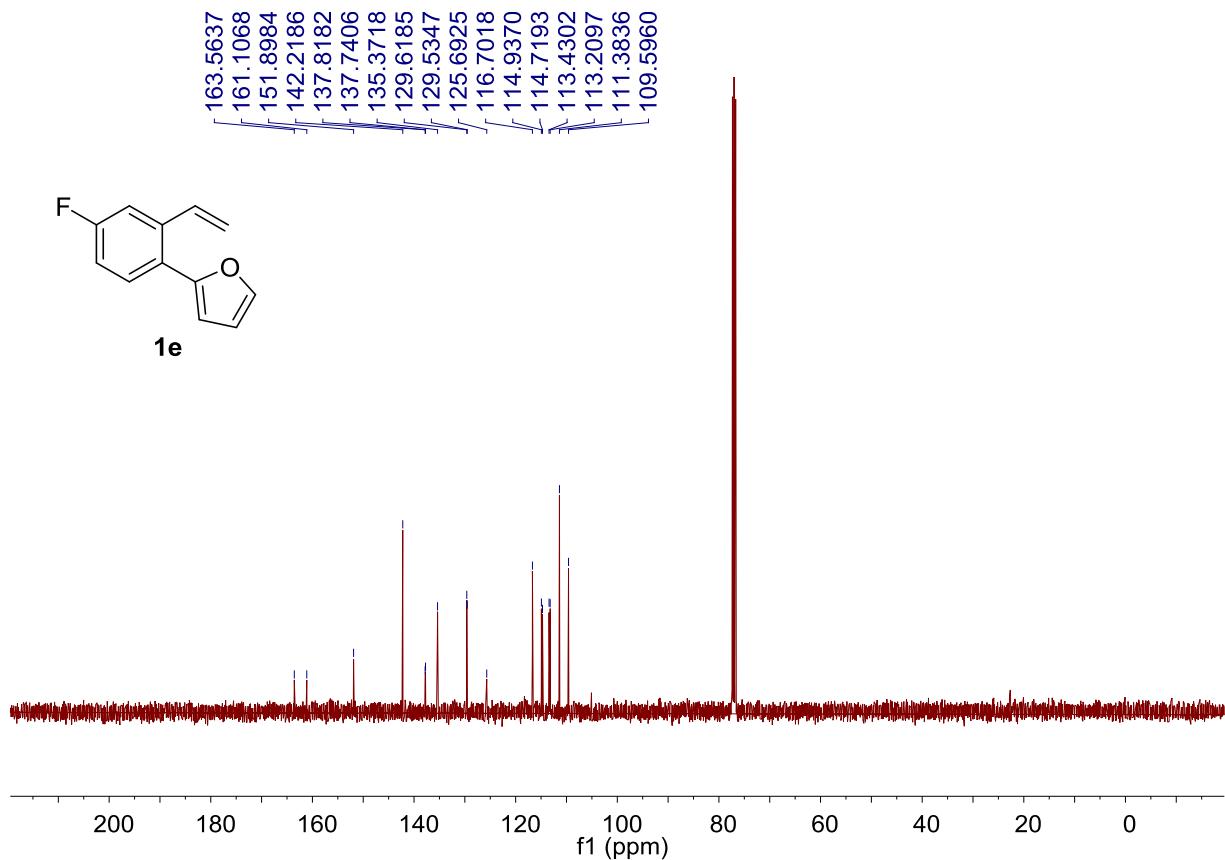
Copies of ^1H , ^{13}C NMR and ^{19}F NMR Spectra for **1d**



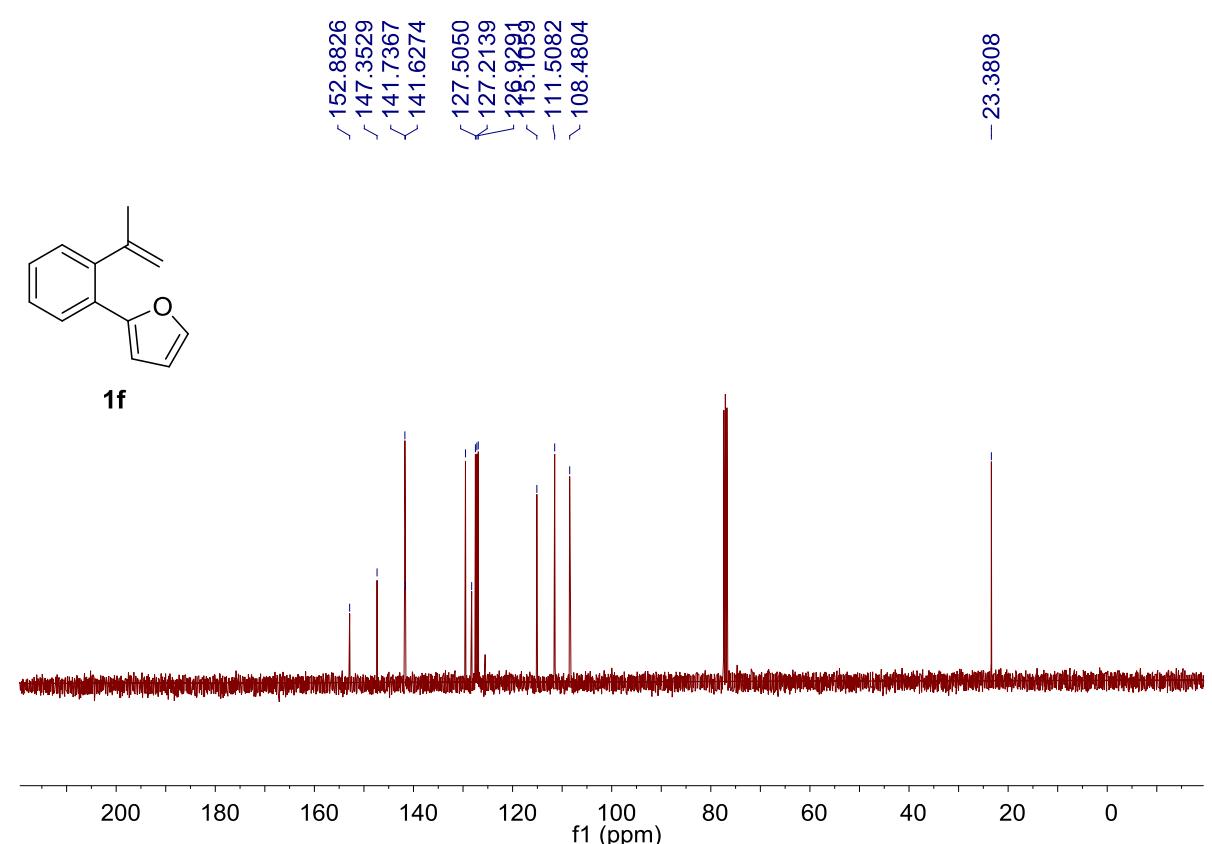
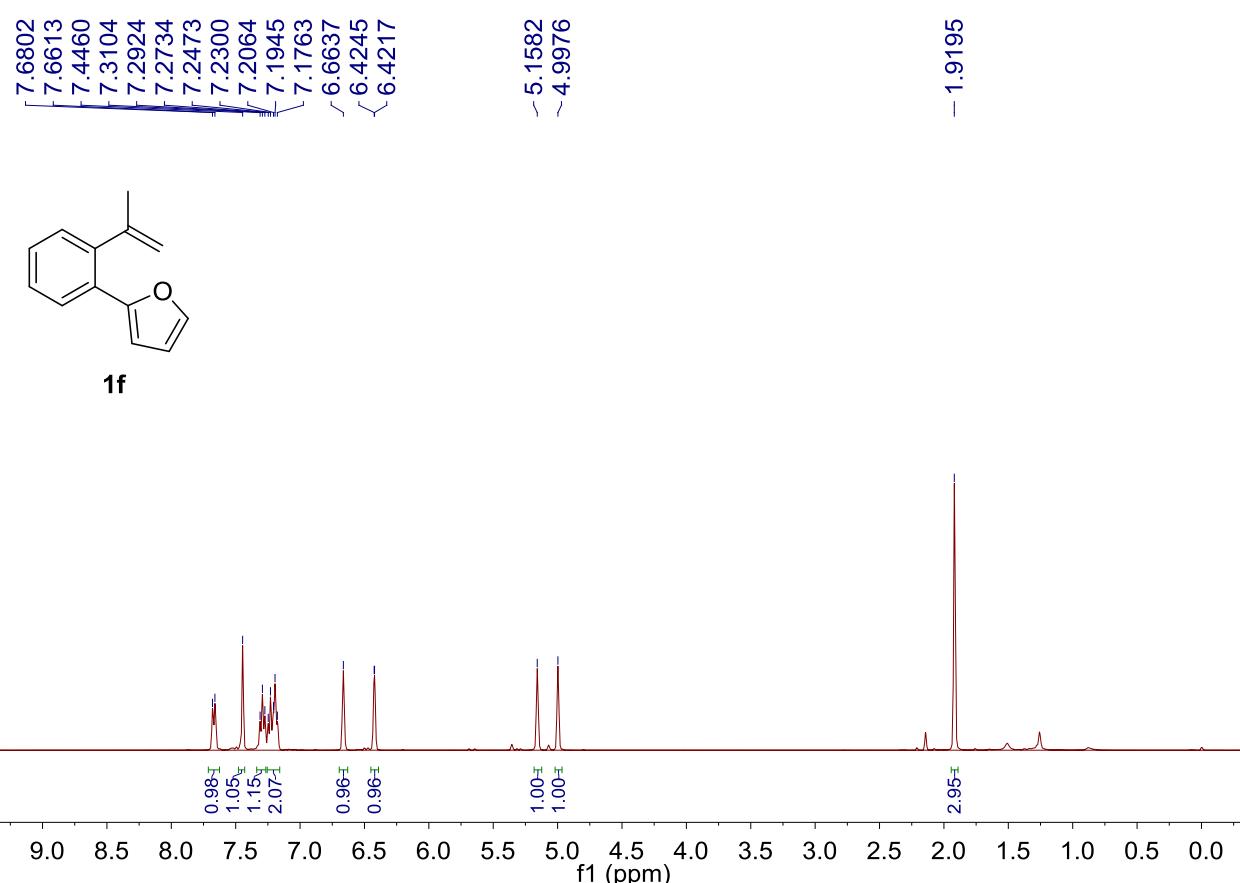


Copies of ^1H , ^{13}C and ^{19}F NMR NMR Spectra for **1e**

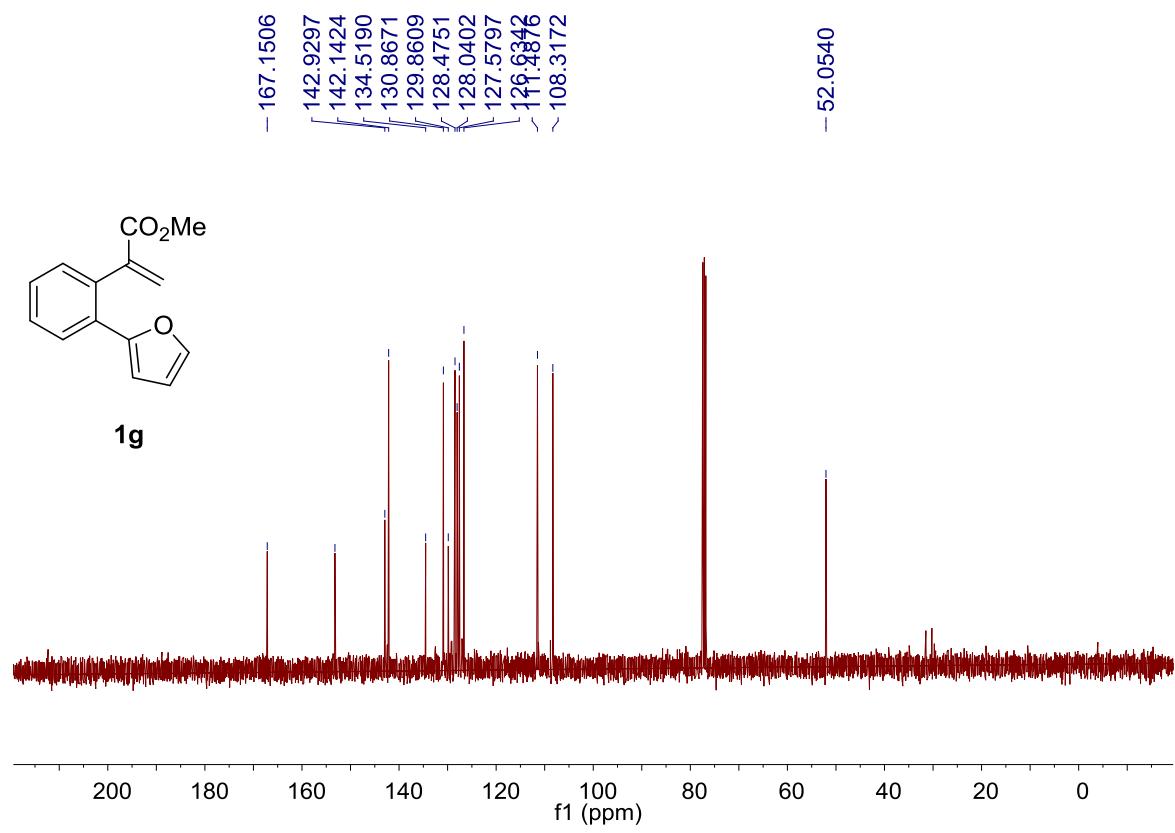
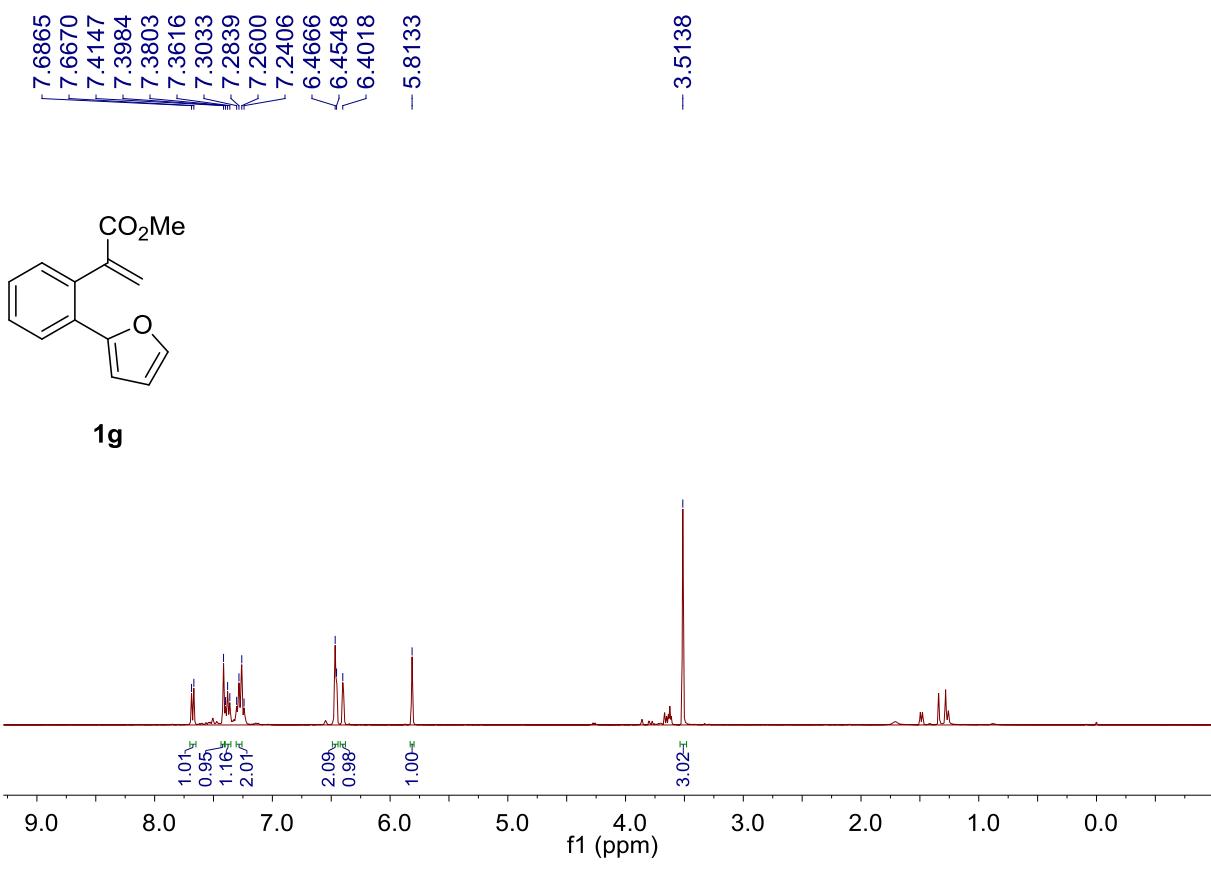




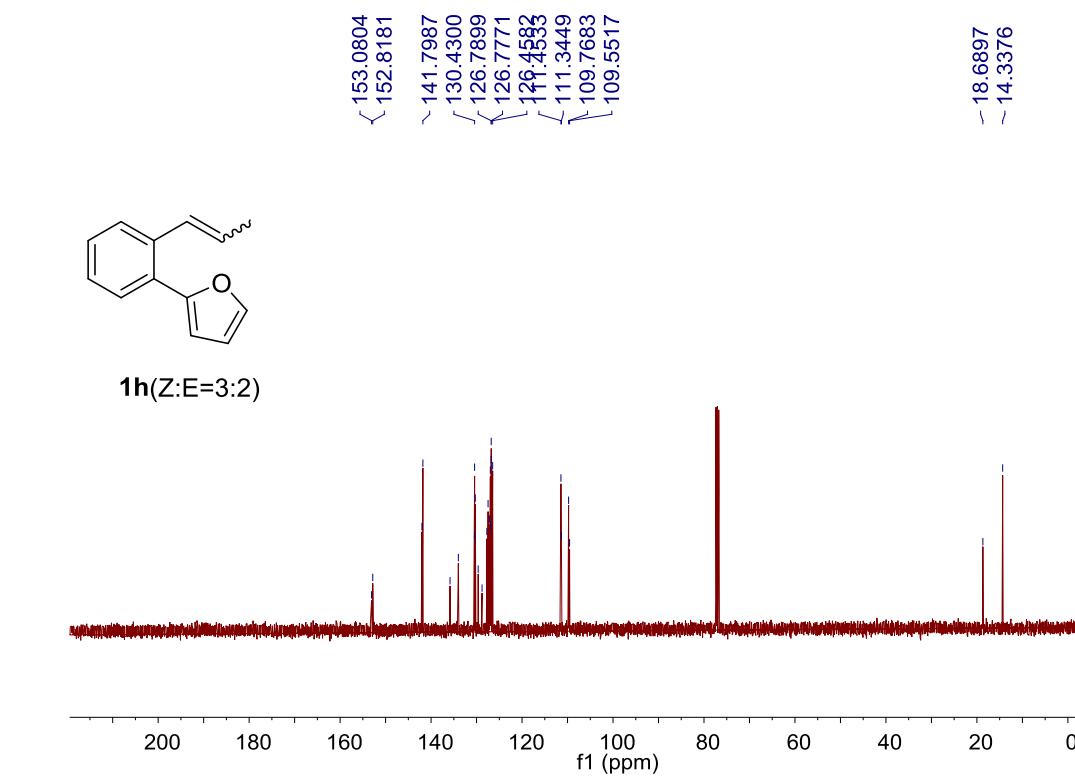
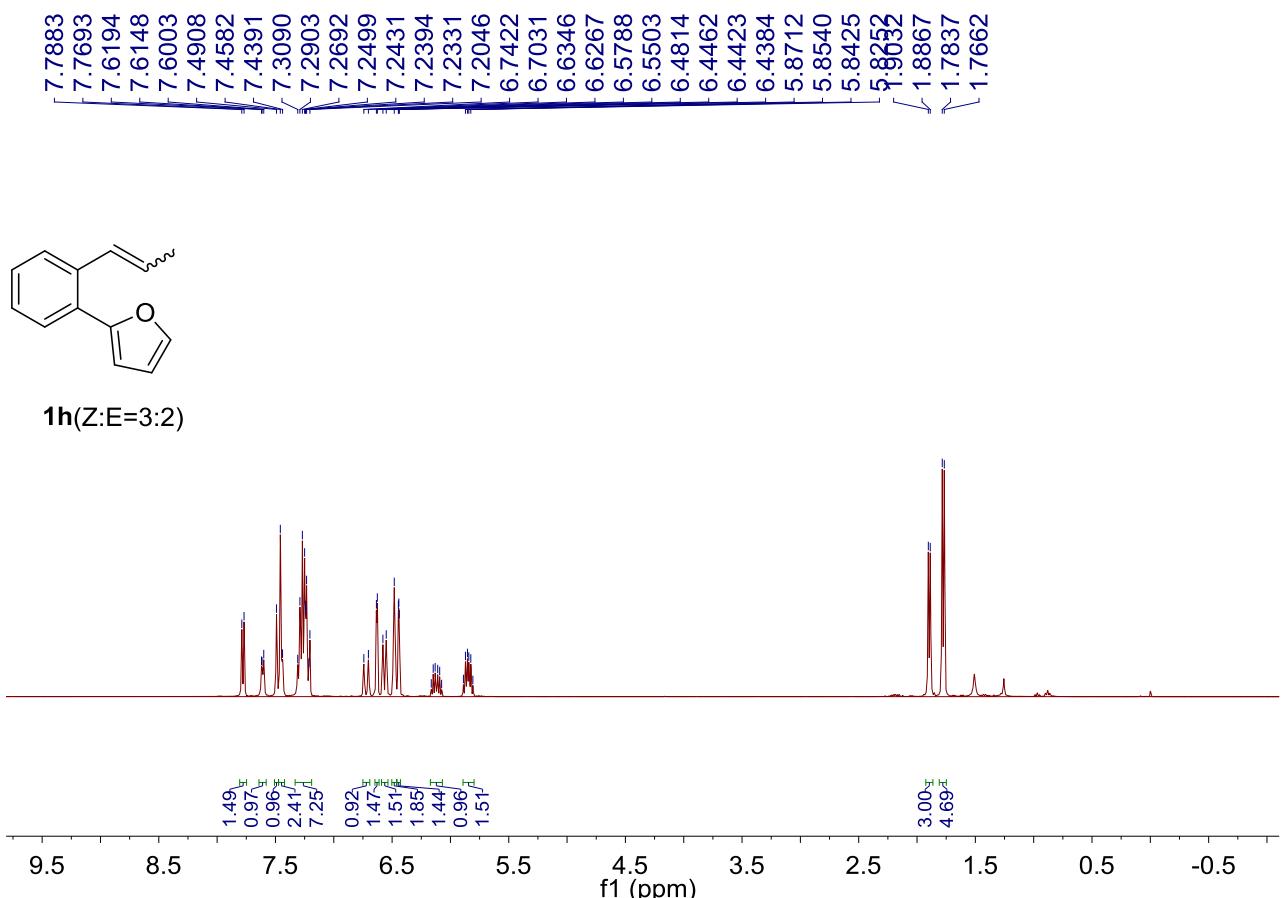
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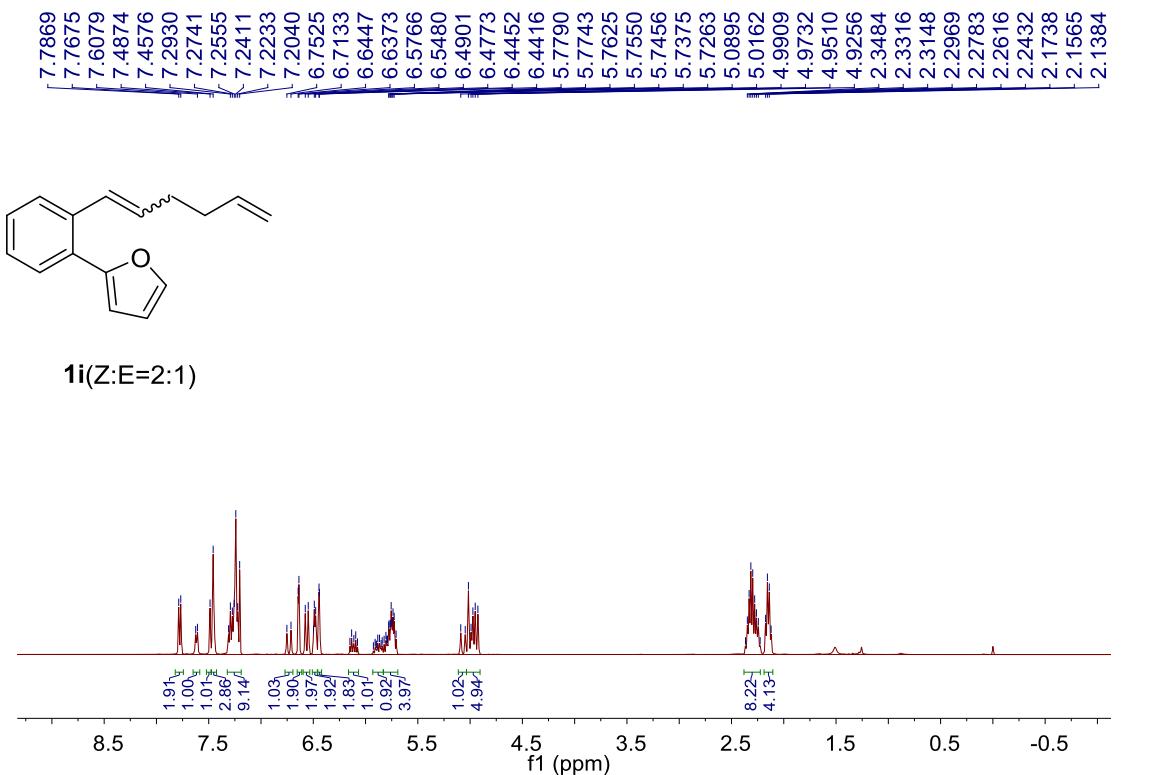
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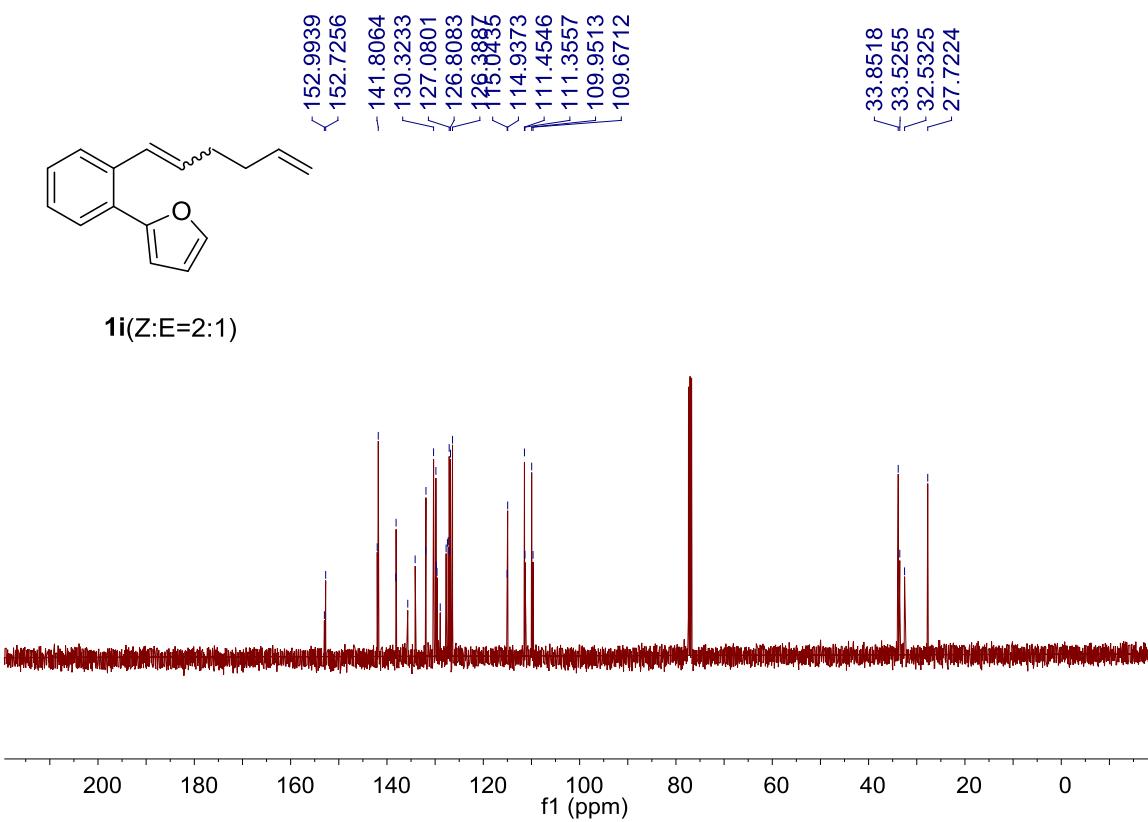
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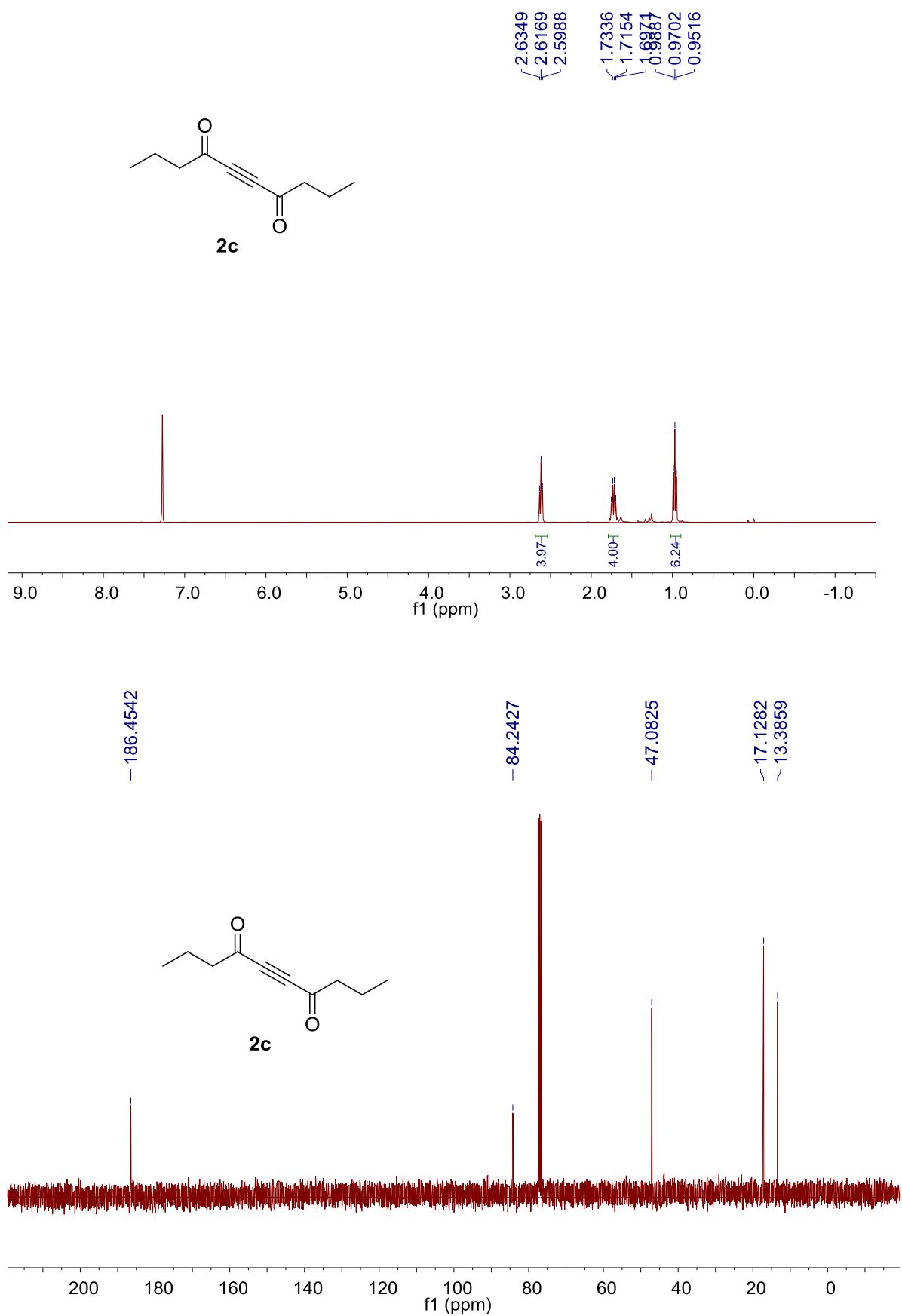
Copies of ^1H and ^{13}C NMR Spectra for **1i**



1i(Z:E=2:1)

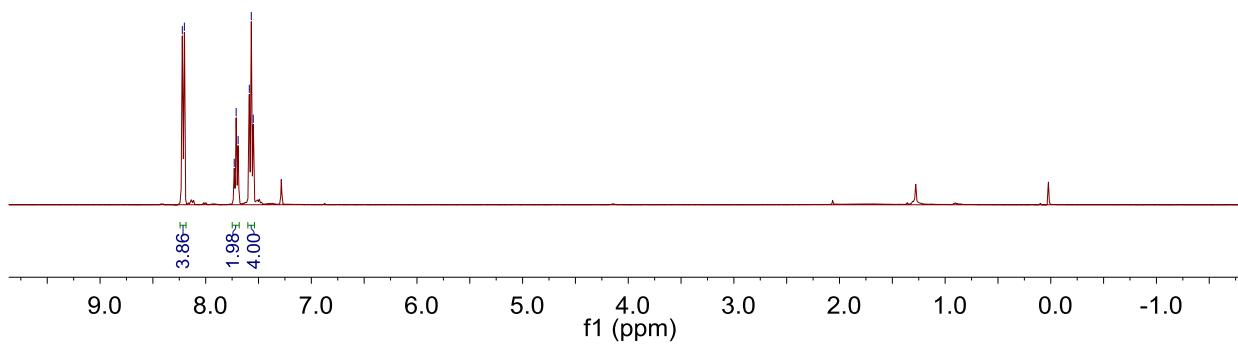
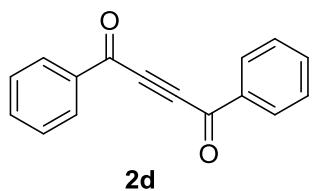


Copies of ^1H and ^{13}C NMR Spectra for **2c**



Copies of ^1H and ^{13}C NMR Spectra for **2d**

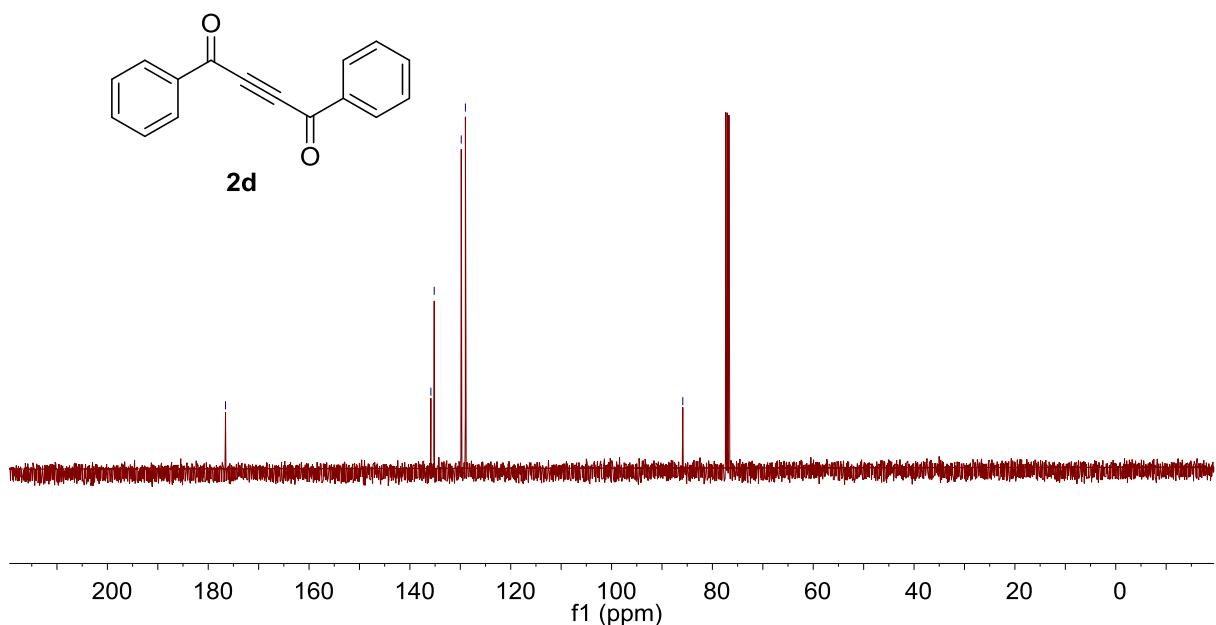
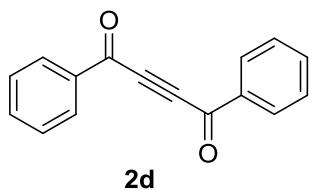
8.2213
8.2020
7.7300
7.7118
7.6932
7.5873
7.5684
7.5498



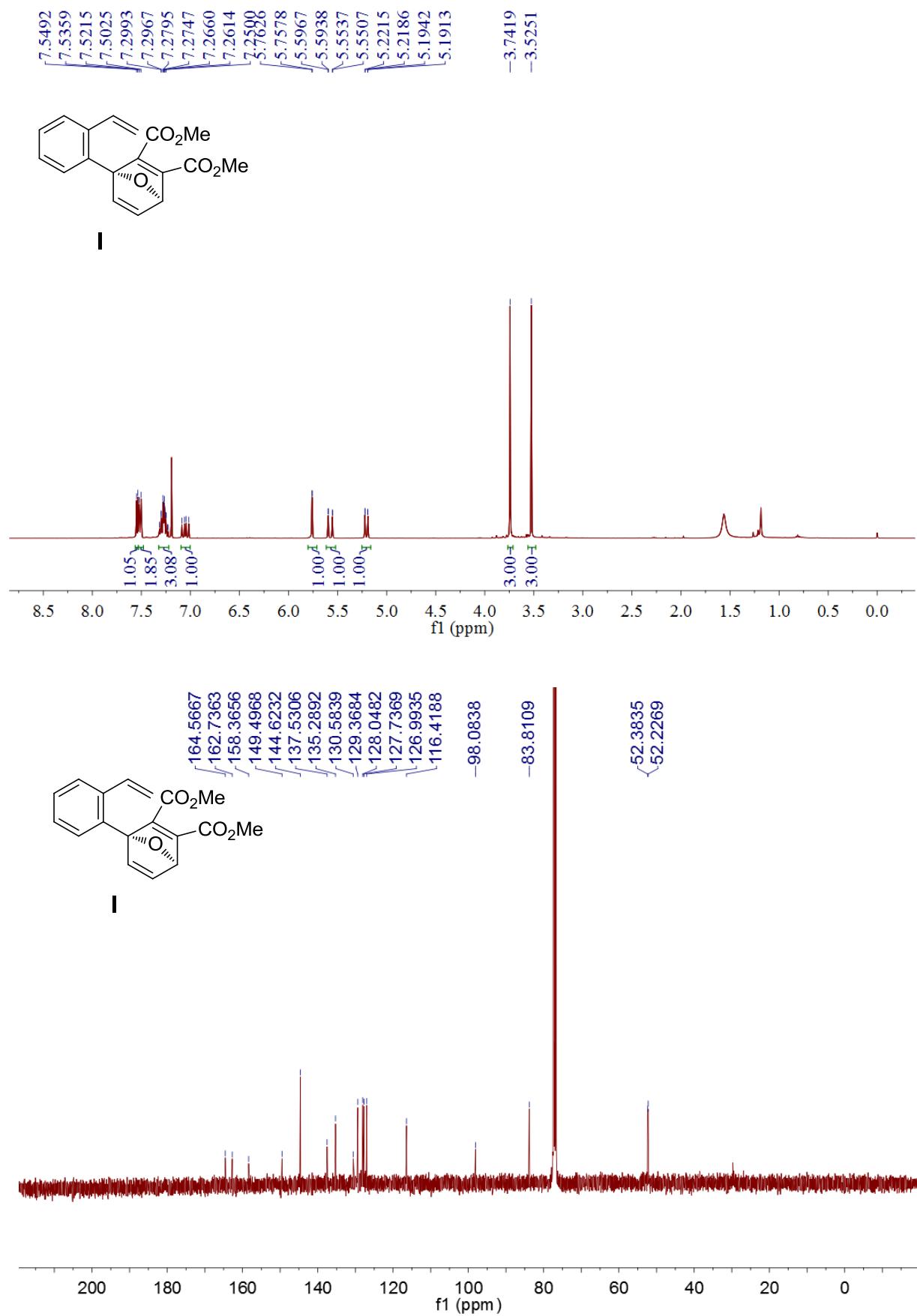
-176.5687

135.8370
135.1766
129.8144
128.9906

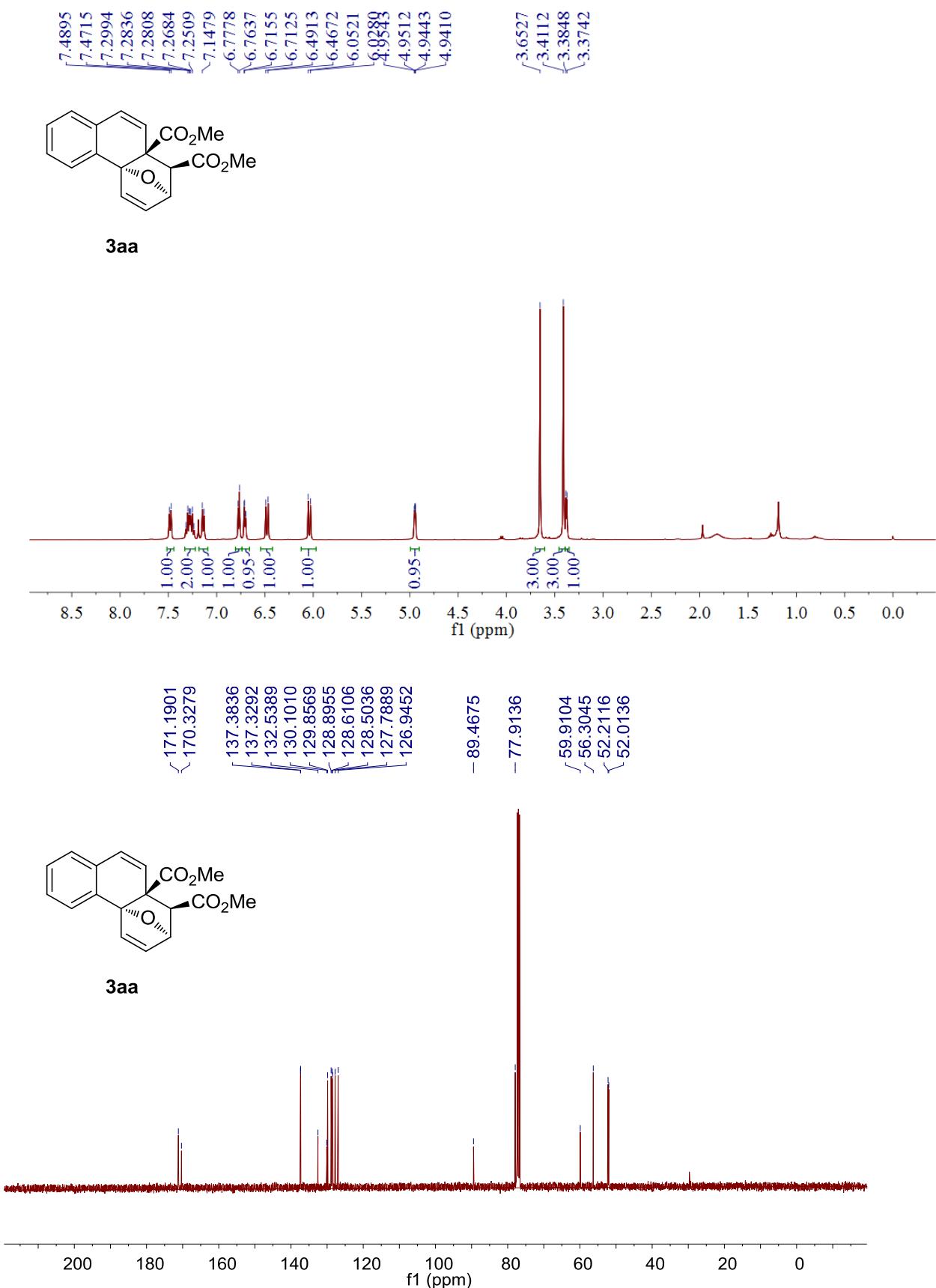
-85.8720



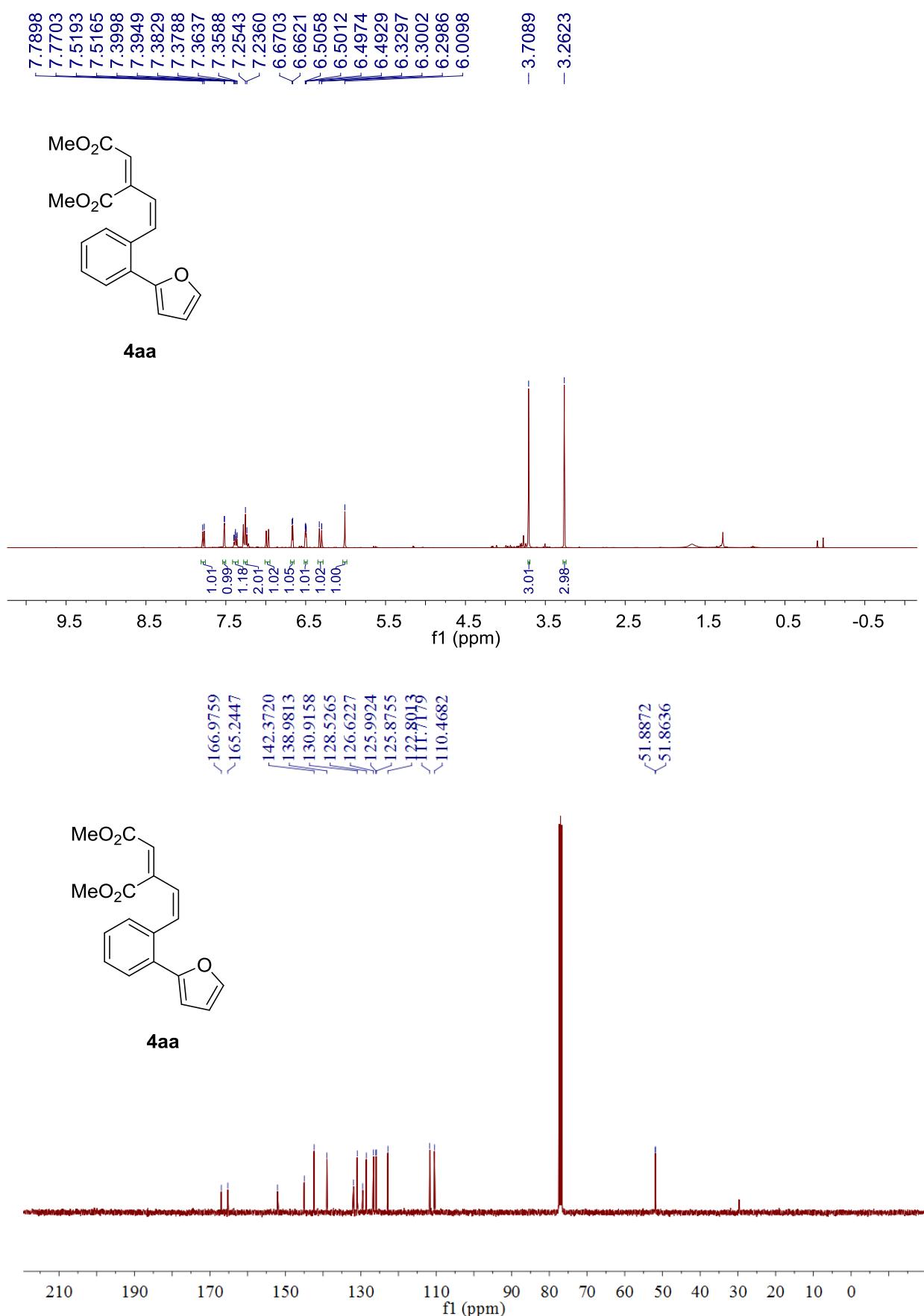
Copies of ^1H and ^{13}C NMR Spectra for **I**



Copies of ^1H and ^{13}C NMR Spectra for **3aa**



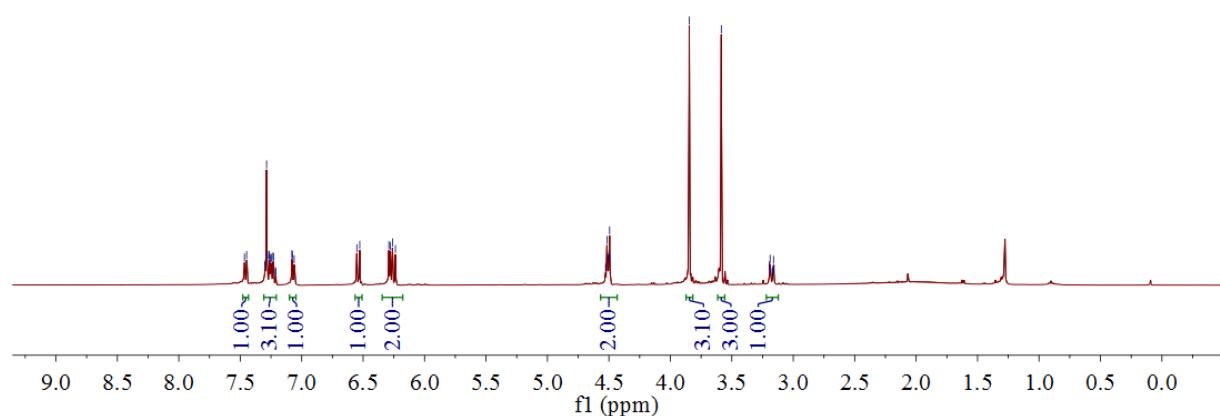
Copies of ^1H and ^{13}C NMR Spectra for **4aa**



Copies of ^1H and ^{13}C NMR Spectra for **5aa**



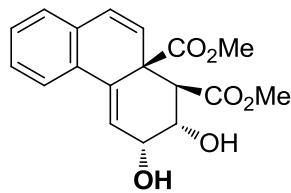
5aa



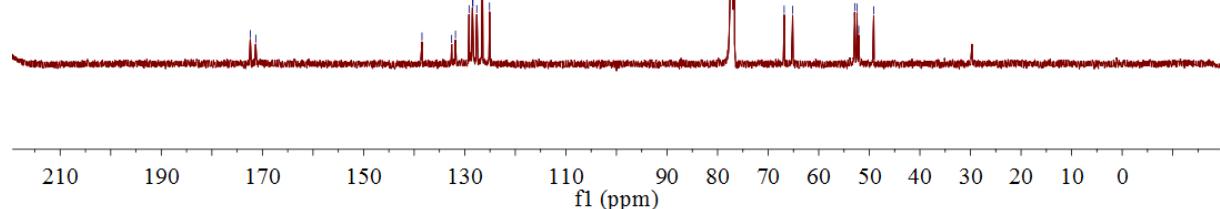
$^{172}_{171}3927$
 $^{171}_{172}3166$

$^{138}_{132}4492$
 $^{132}_{131}5858$
 $^{131}_{129}8284$
 $^{129}_{128}1396$
 $^{128}_{128}4638$
 $^{128}_{128}3738$
 $^{127}_{127}6156$
 $^{126}_{126}5230$
 $^{125}_{125}0956$

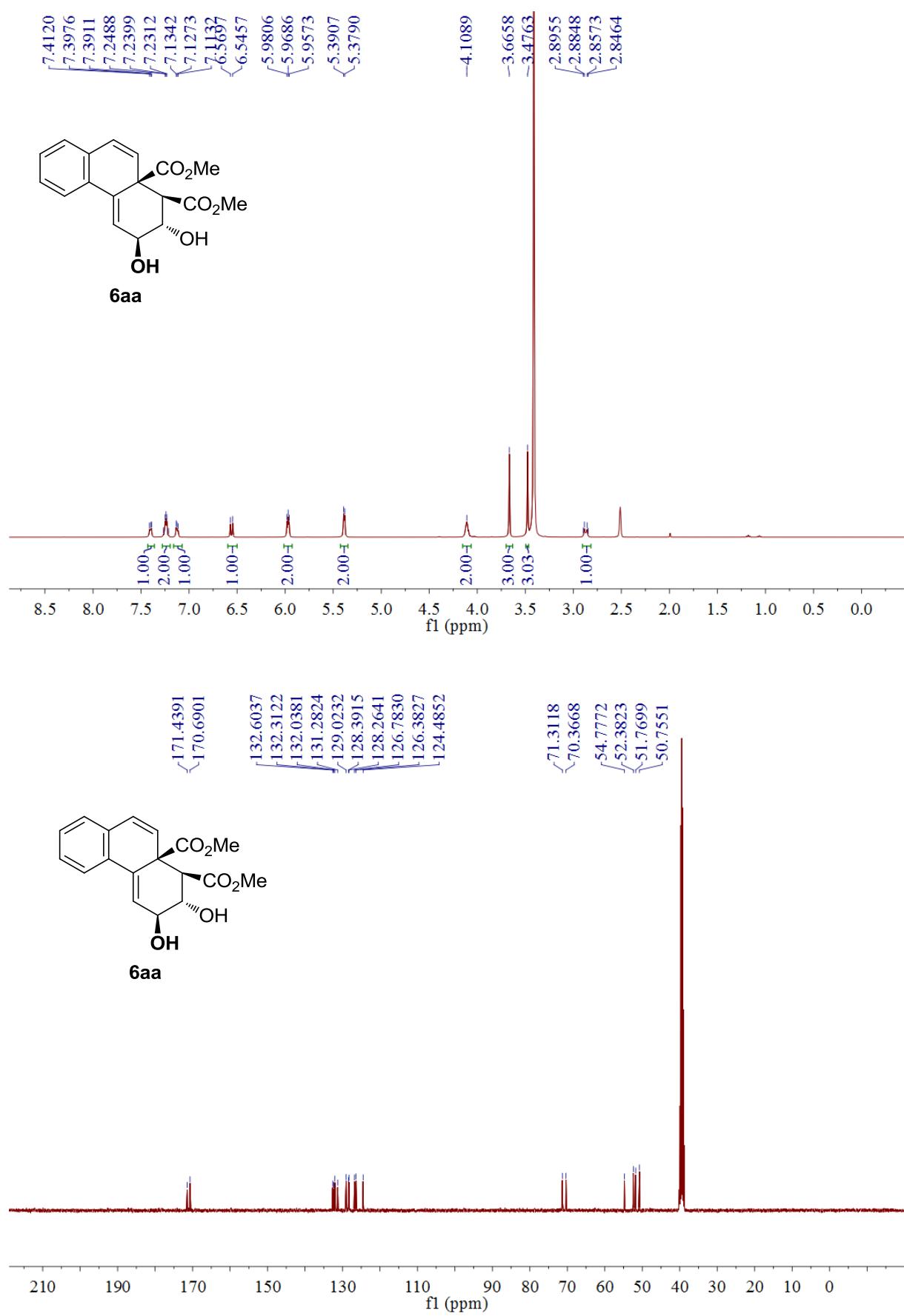
$^{66}_{65}8360$
 $^{65}_{65}1610$
 $^{52}_{52}8886$
 $^{52}_{52}4286$
 $^{52}_{52}0936$
 $^{49}_{49}1220$



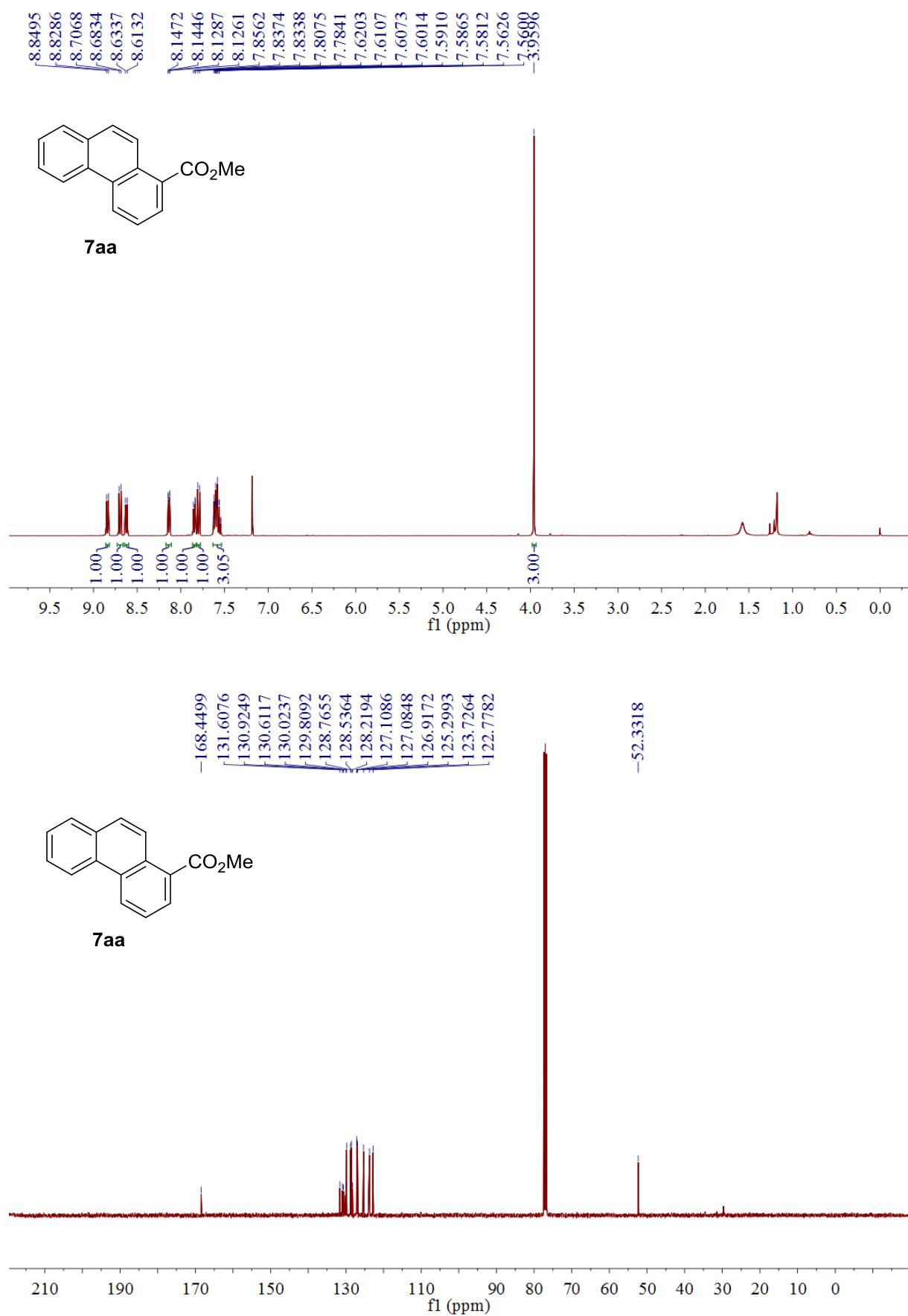
5aa



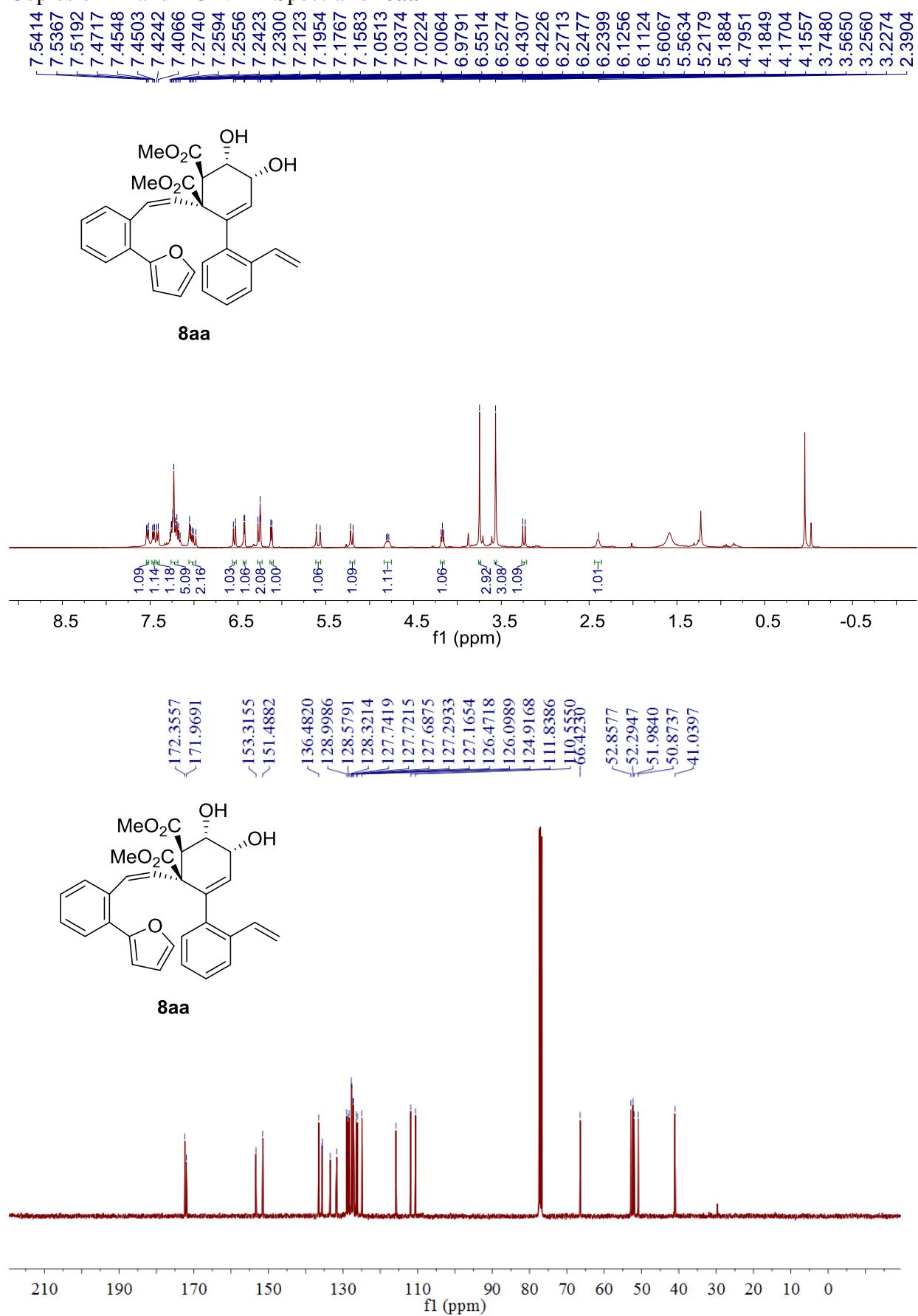
Copies of ^1H and ^{13}C NMR Spectra for **6aa**



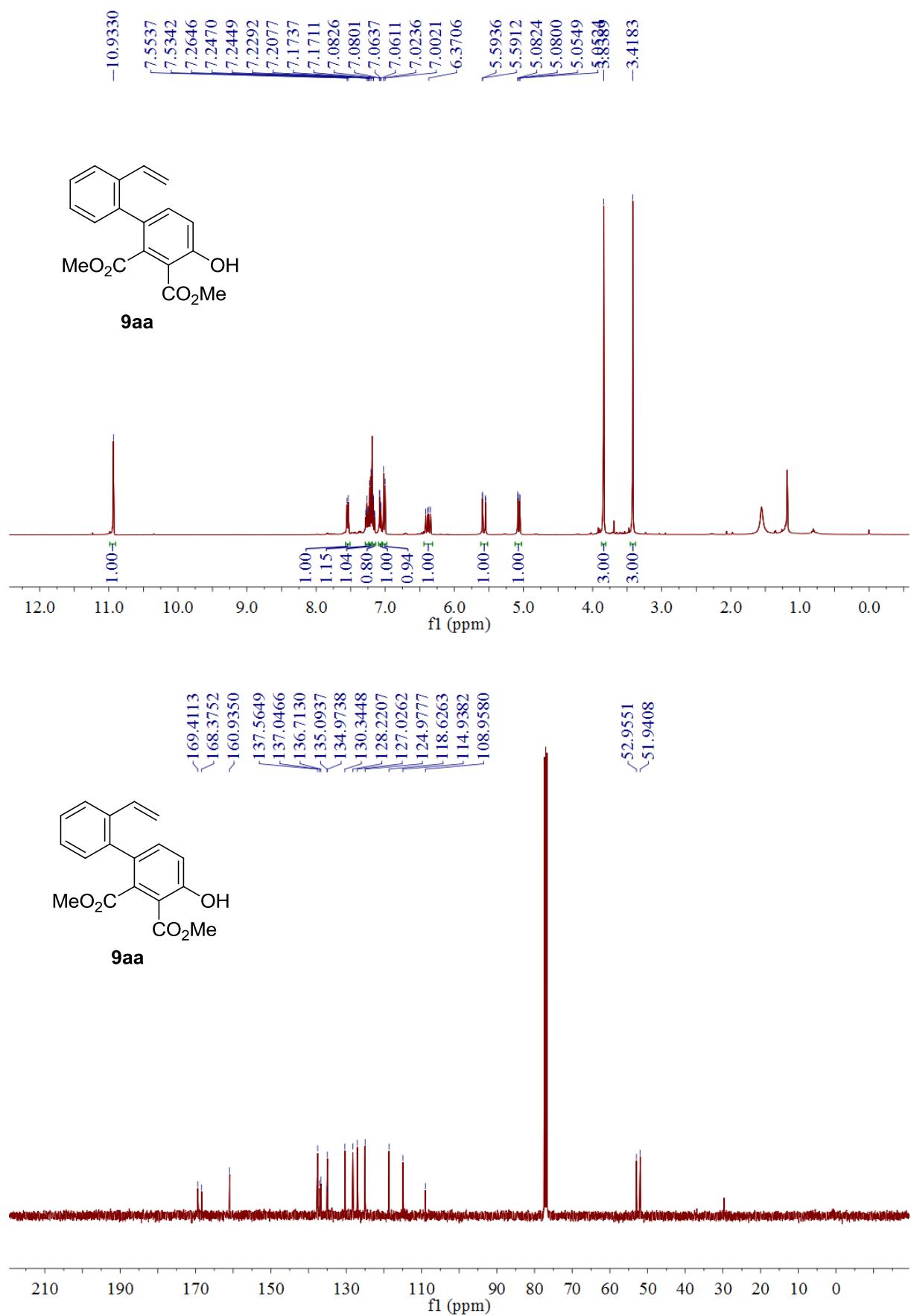
Copies of ^1H and ^{13}C NMR Spectra for **7aa**



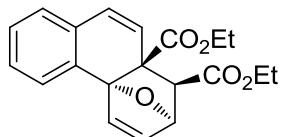
Copies of ^1H and ^{13}C NMR Spectra for **8aa**



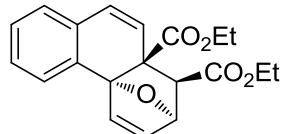
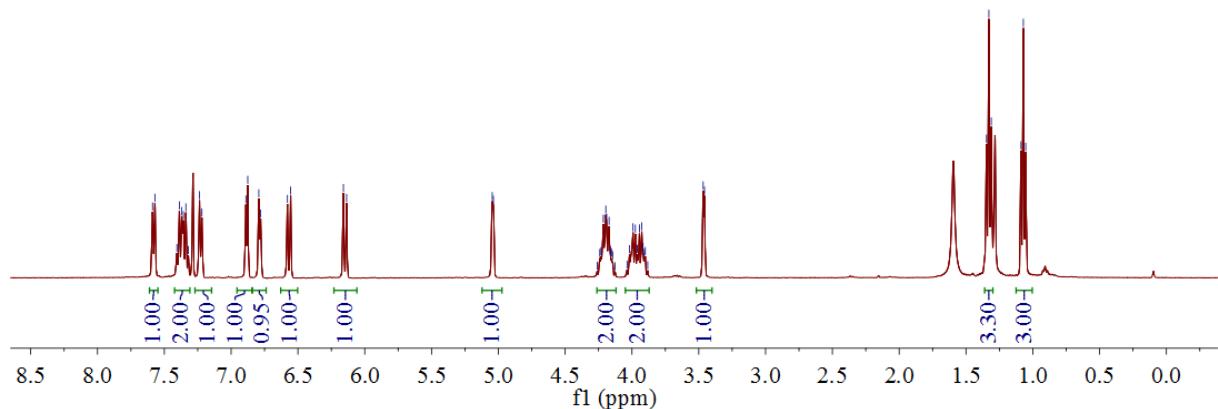
Copies of ^1H and ^{13}C NMR Spectra for **9aa**



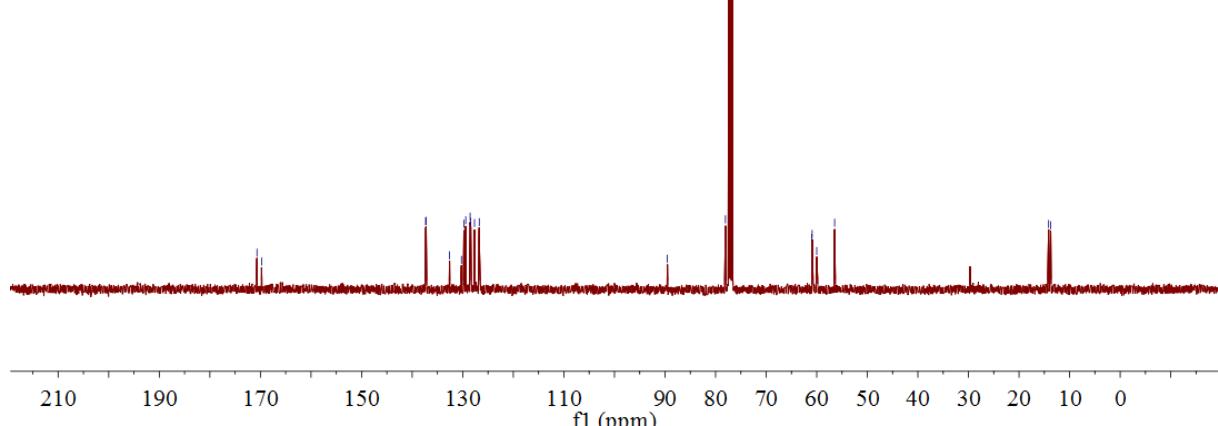
Copies of ^1H and ^{13}C NMR Spectra for **3ab**



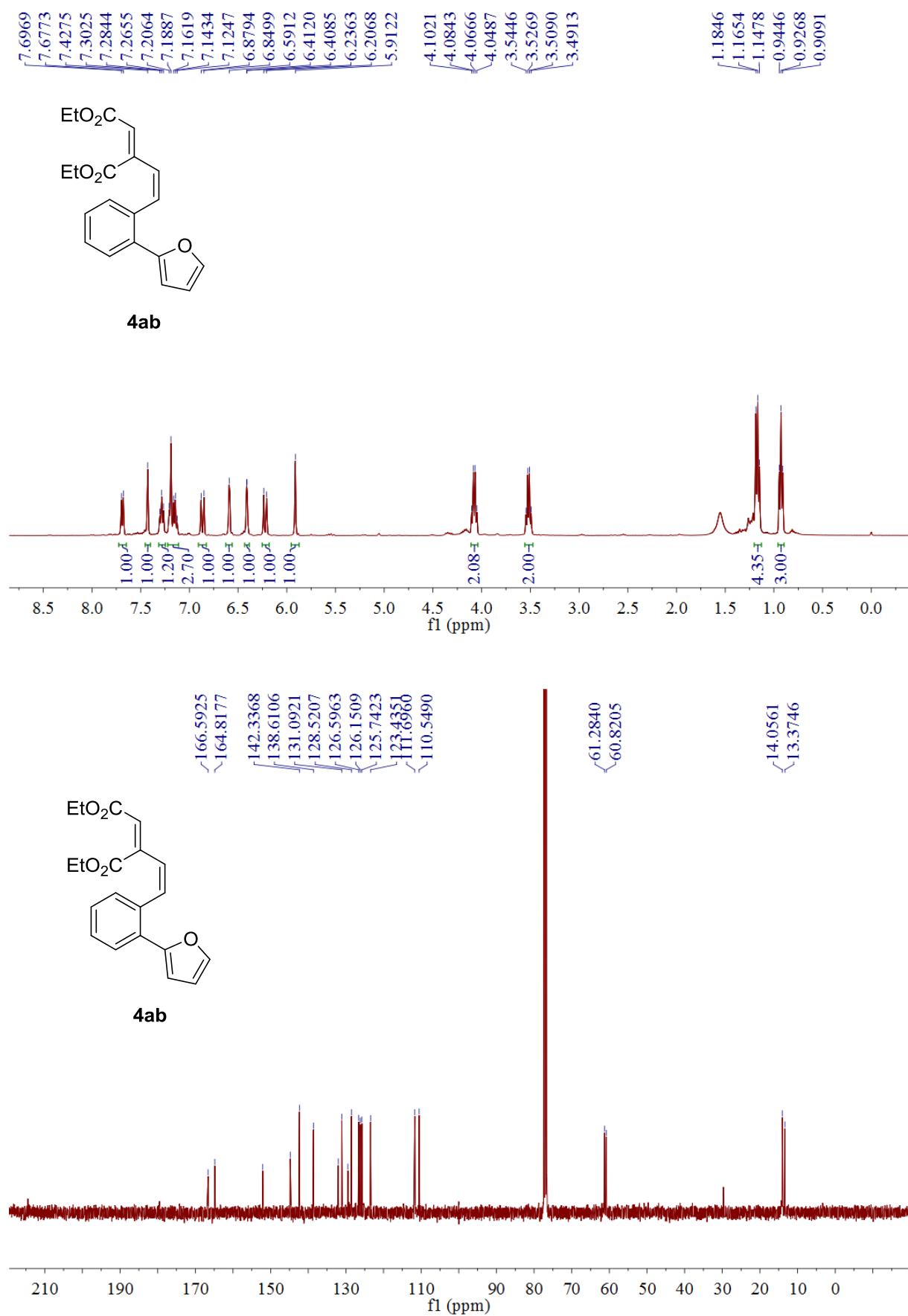
3ab



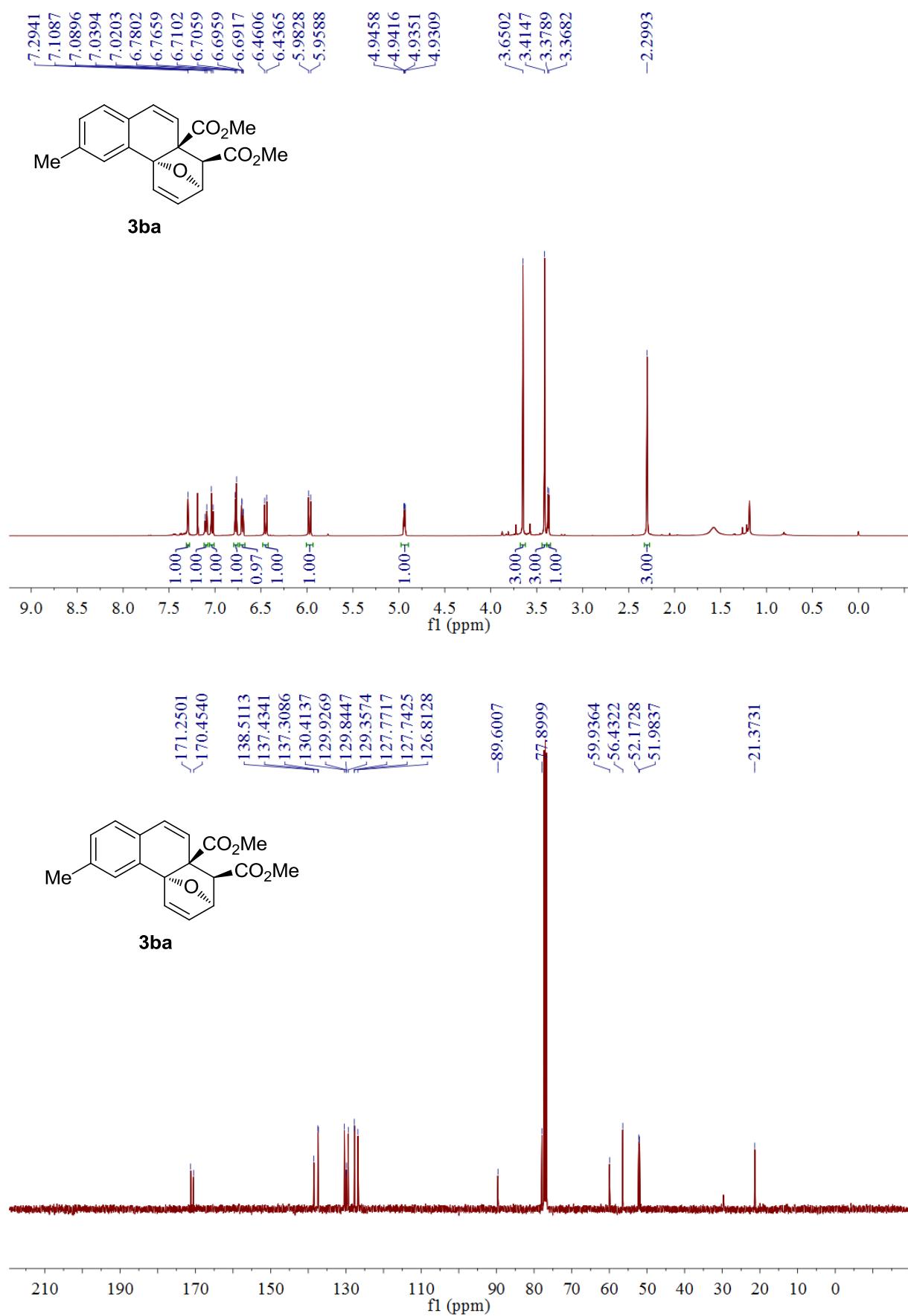
3ab



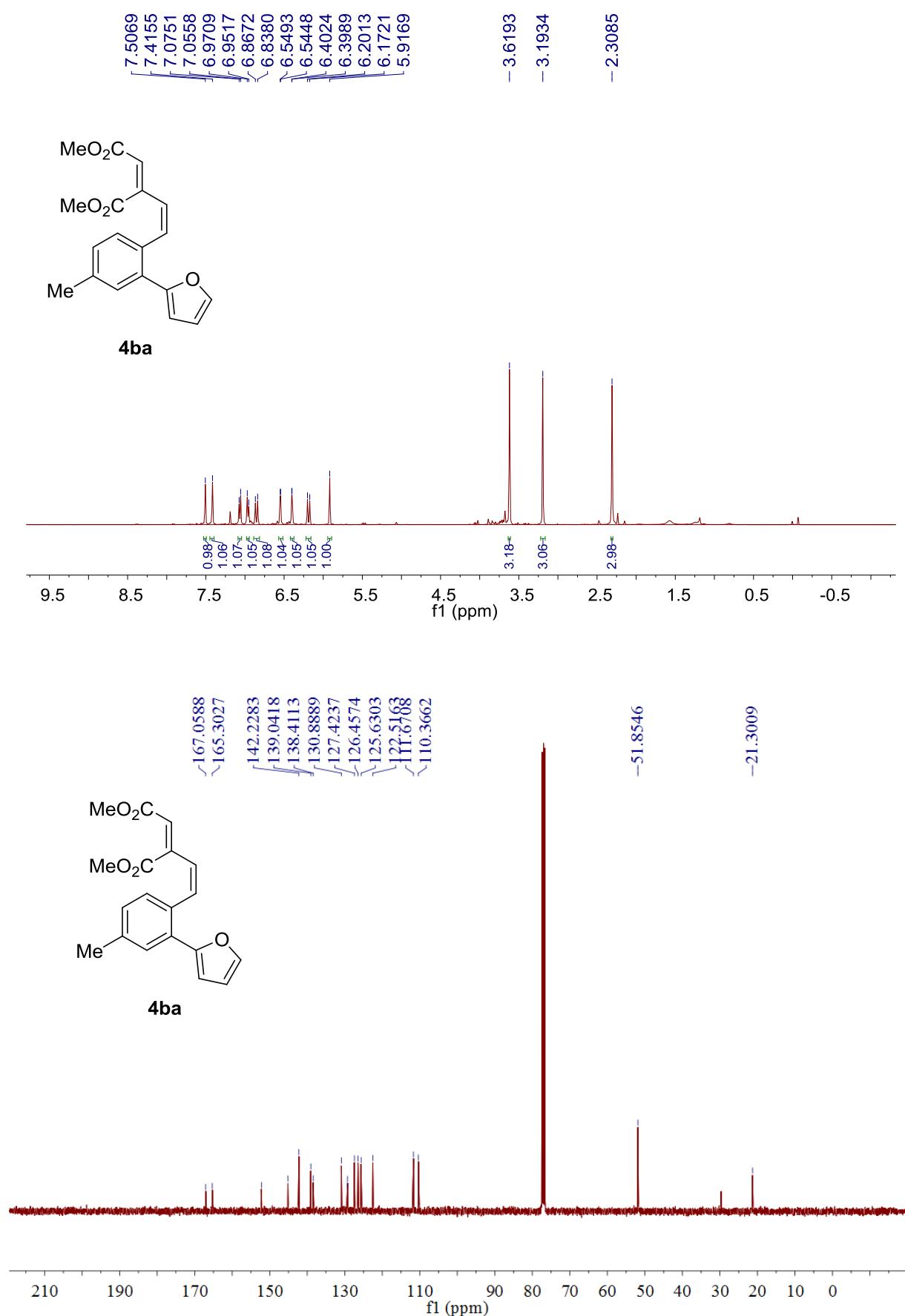
Copies of ^1H and ^{13}C NMR Spectra for **4ab**



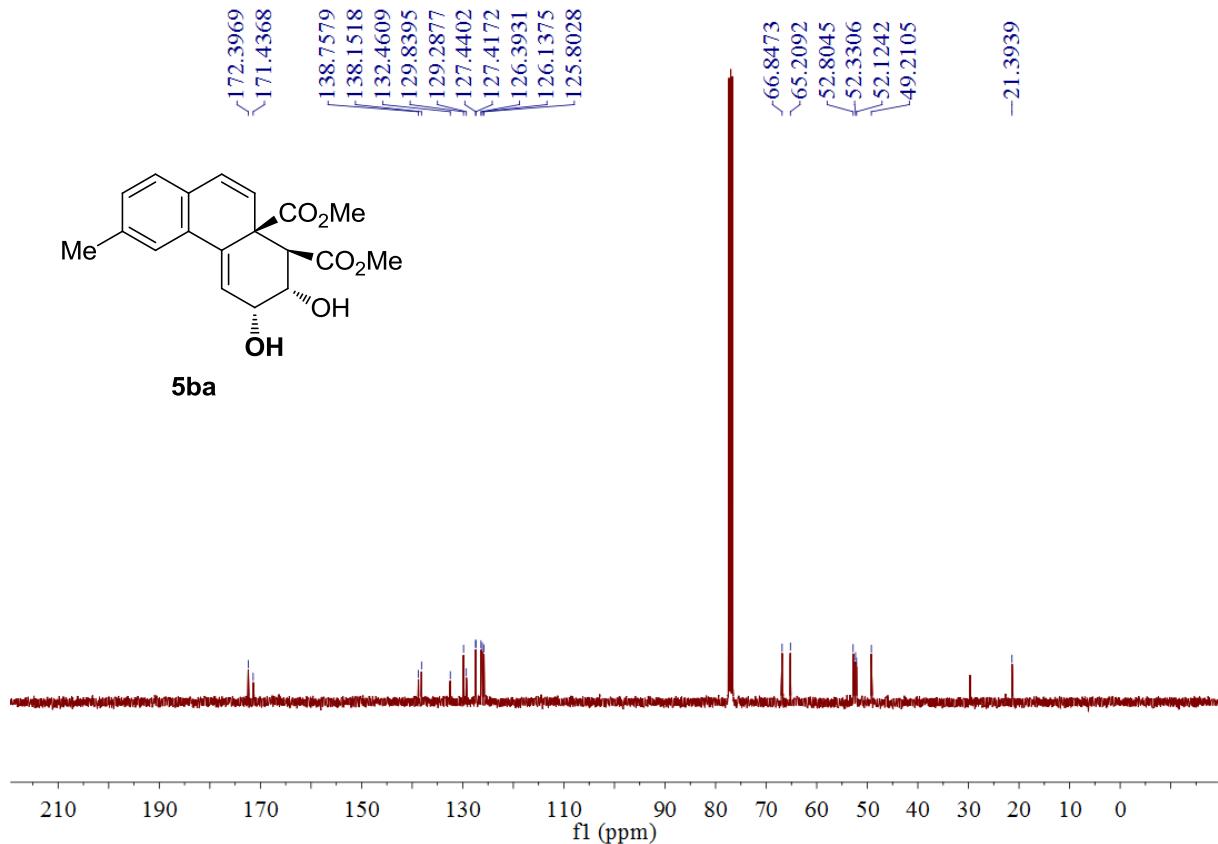
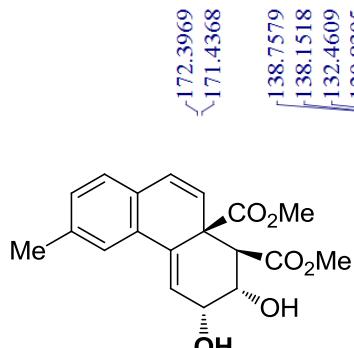
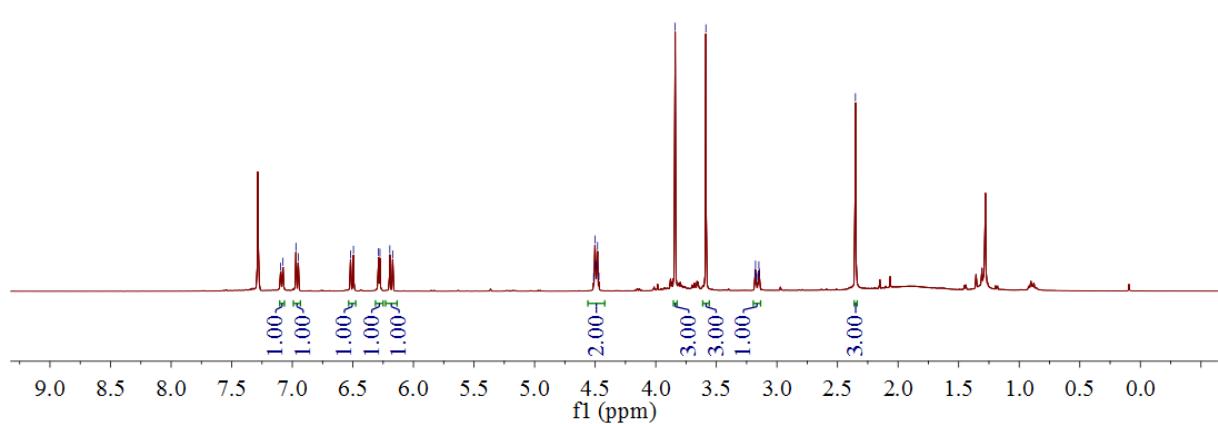
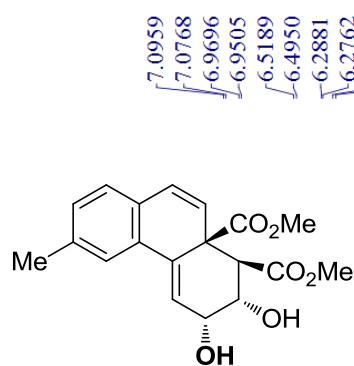
Copies of ^1H and ^{13}C NMR Spectra for **3ba**



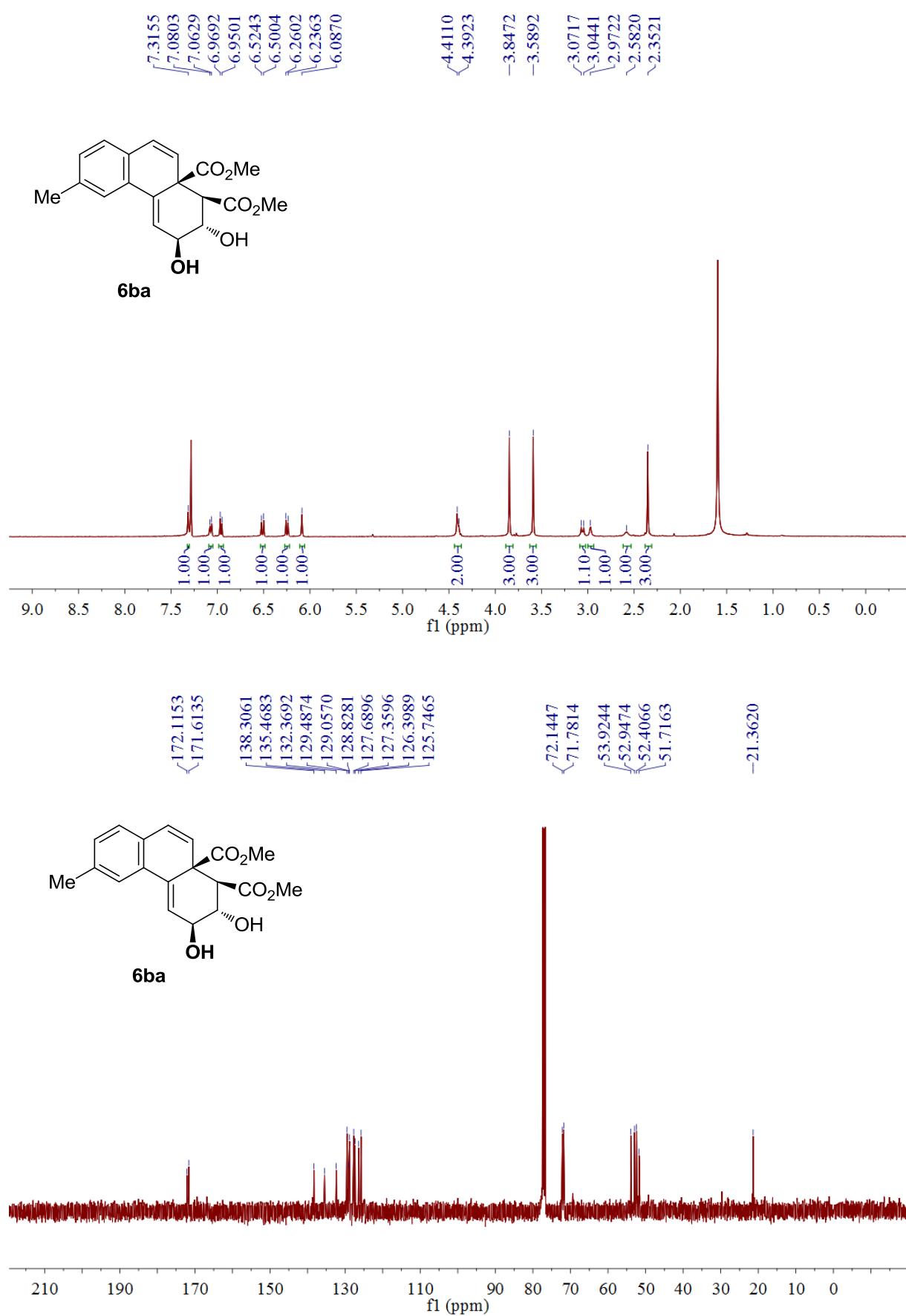
Copies of ^1H and ^{13}C NMR Spectra for **4ba**



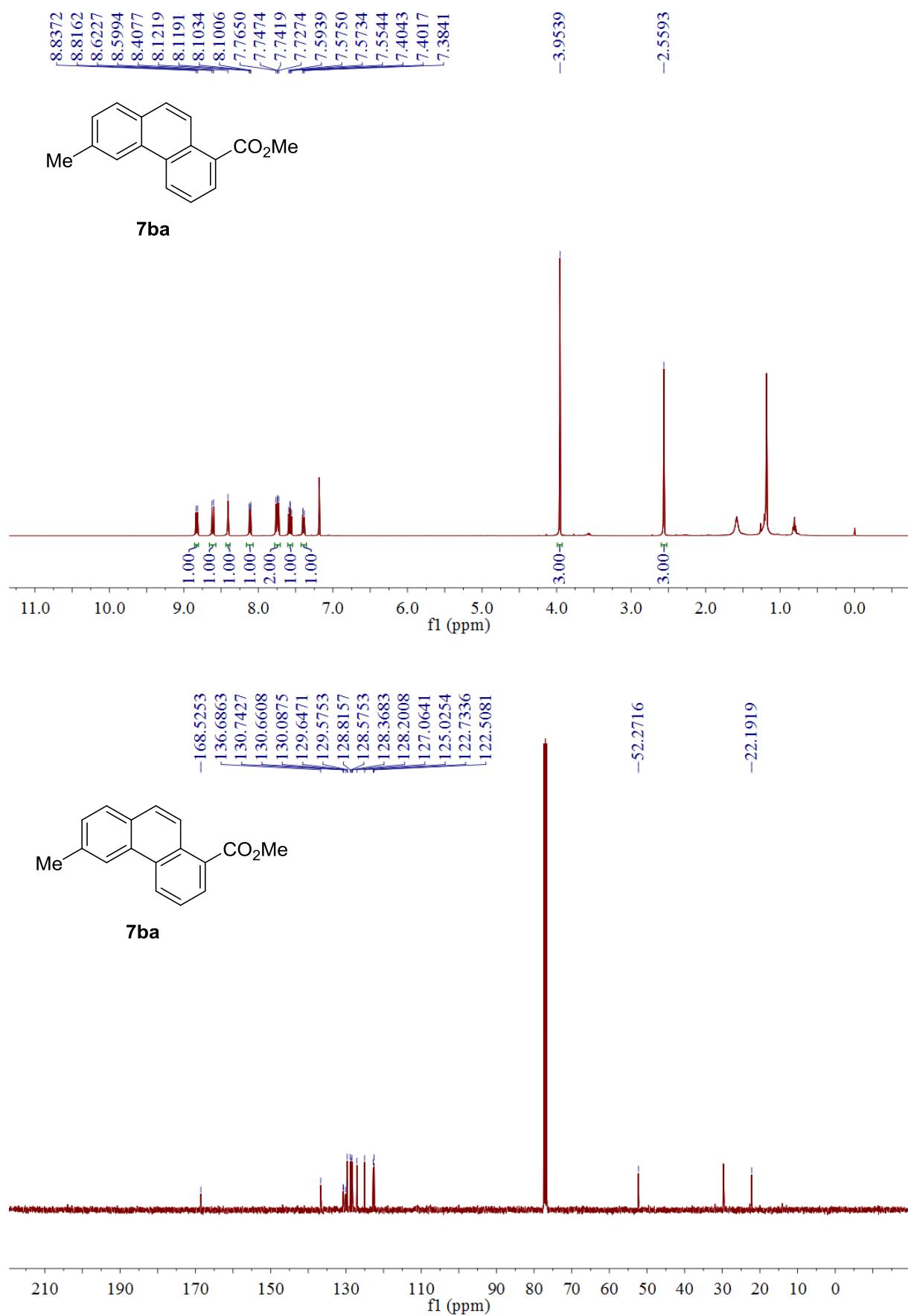
Copies of ^1H and ^{13}C NMR Spectra for **5ba**



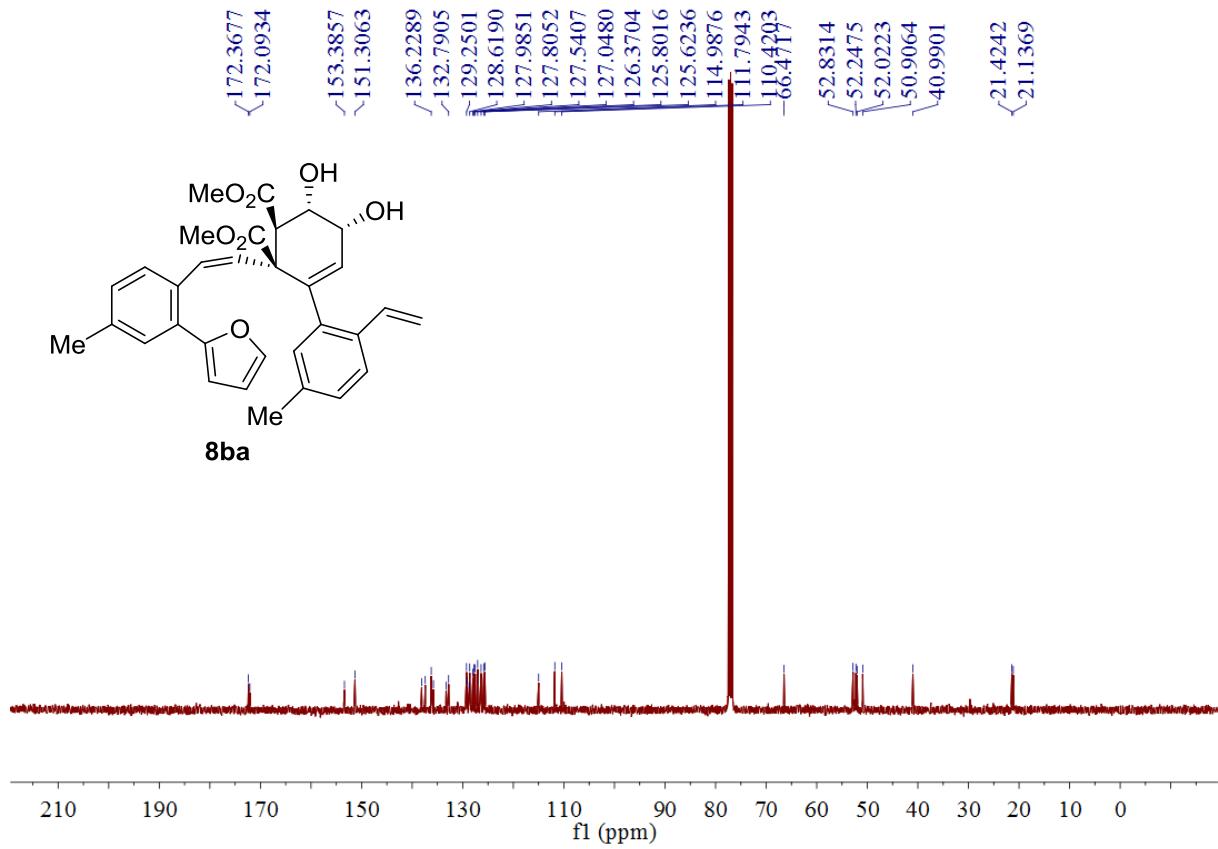
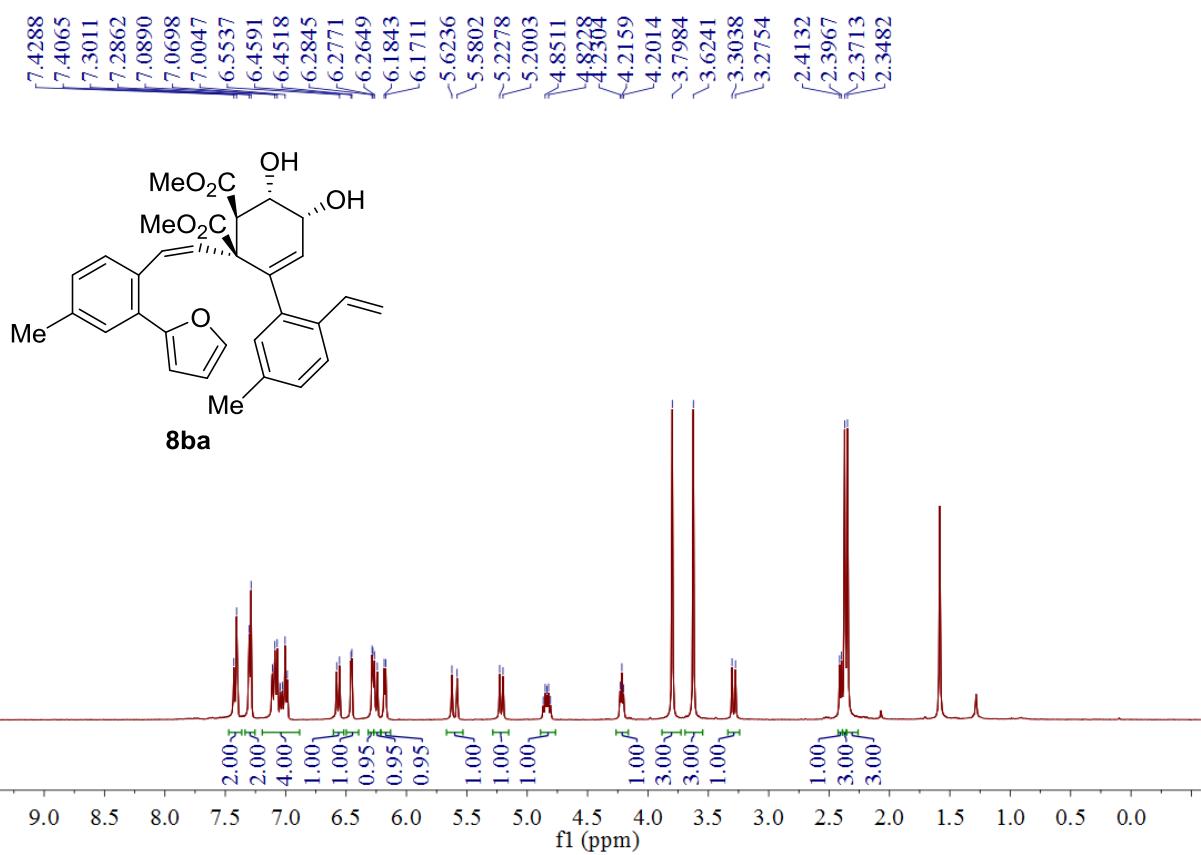
Copies of ^1H and ^{13}C NMR Spectra for **6ba**



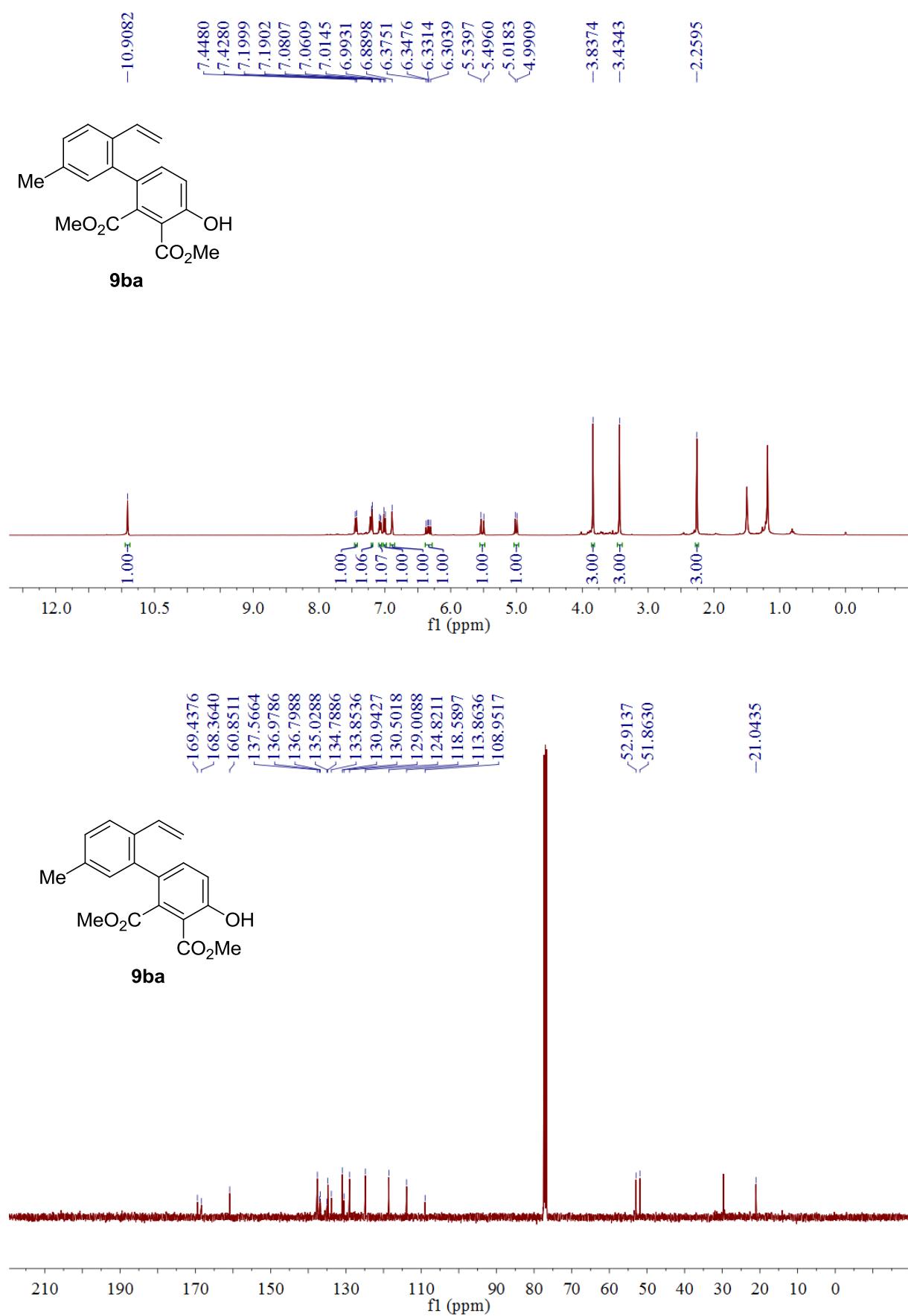
Copies of ^1H and ^{13}C NMR Spectra for **7ba**



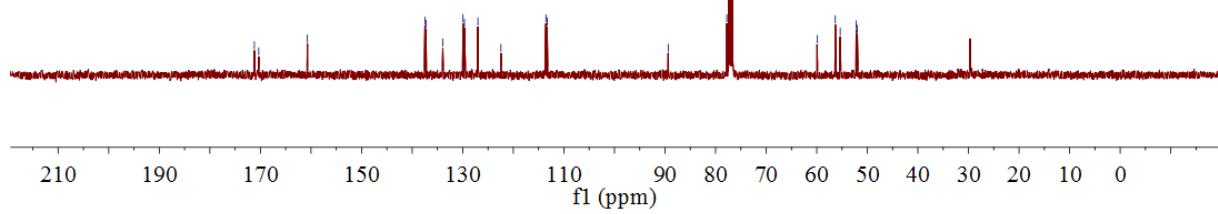
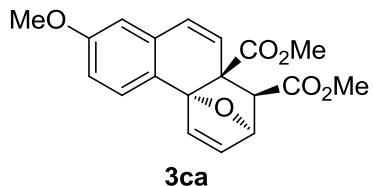
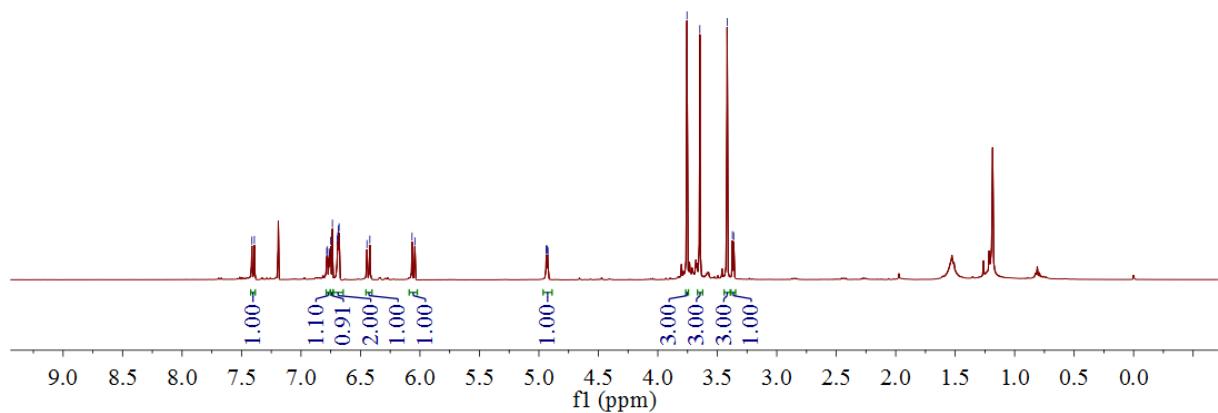
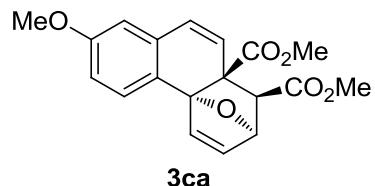
Copies of ^1H and ^{13}C NMR Spectra for **8ba**



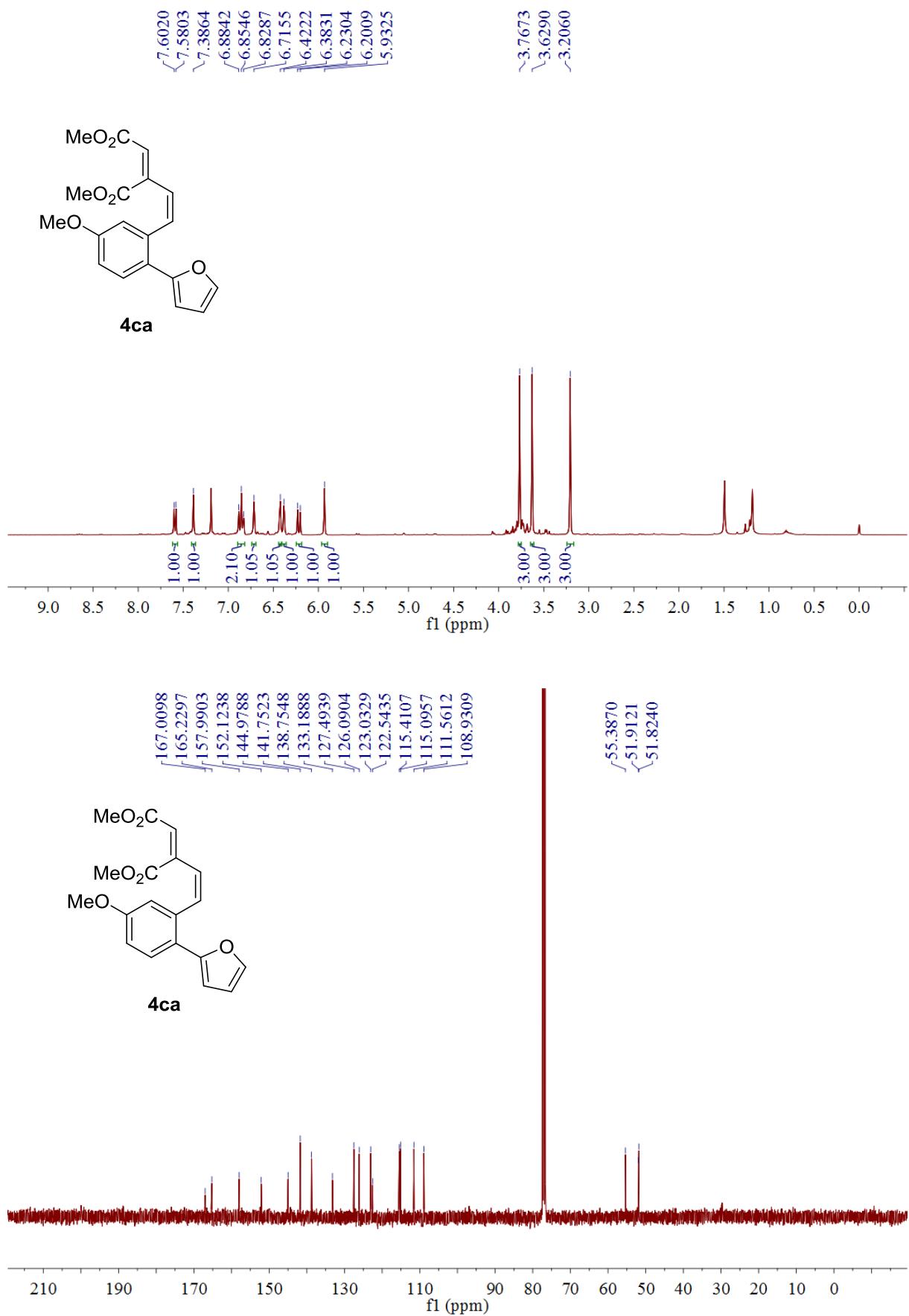
Copies of ^1H and ^{13}C NMR Spectra for **9ba**



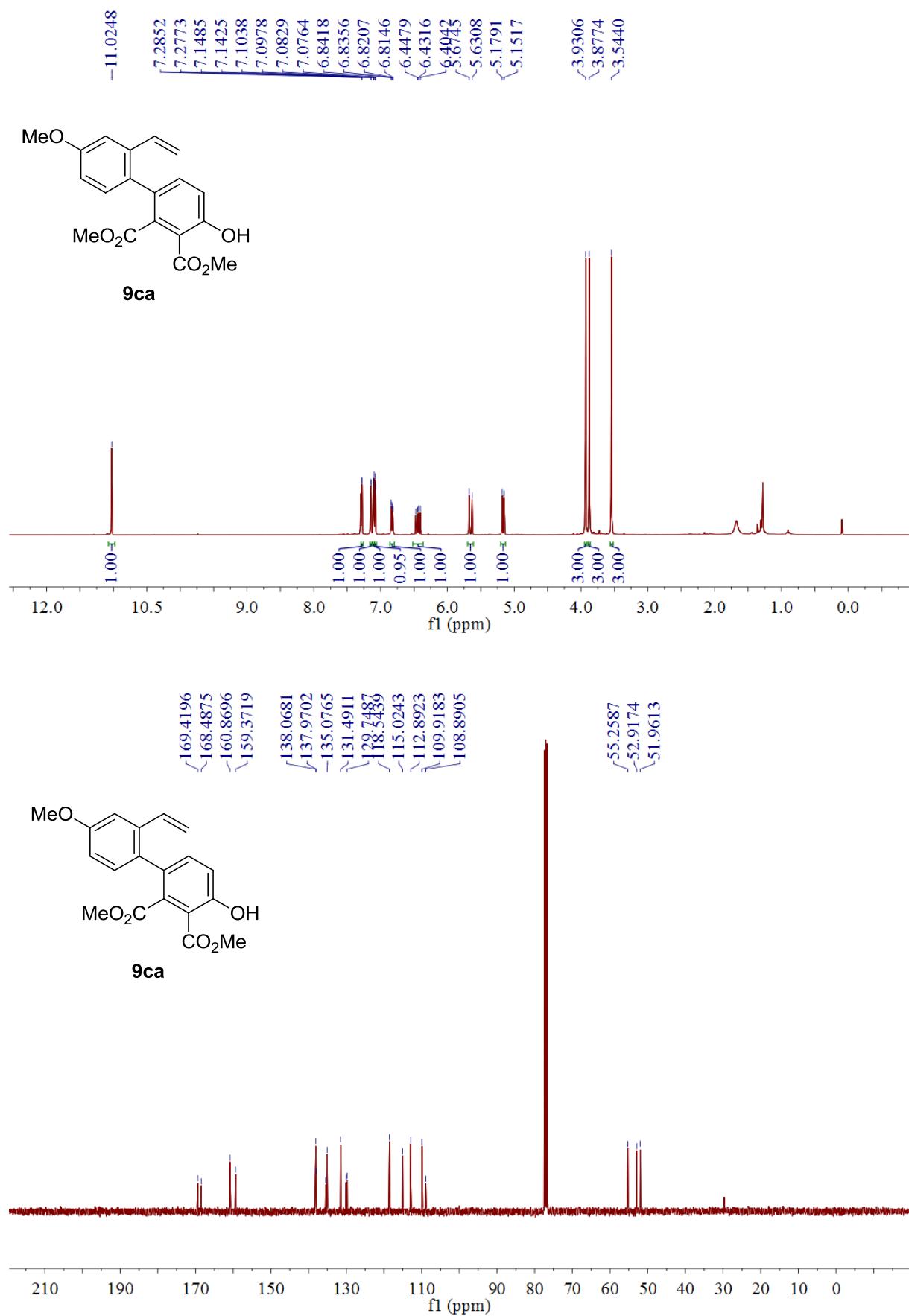
Copies of ^1H and ^{13}C NMR Spectra for **3ca**



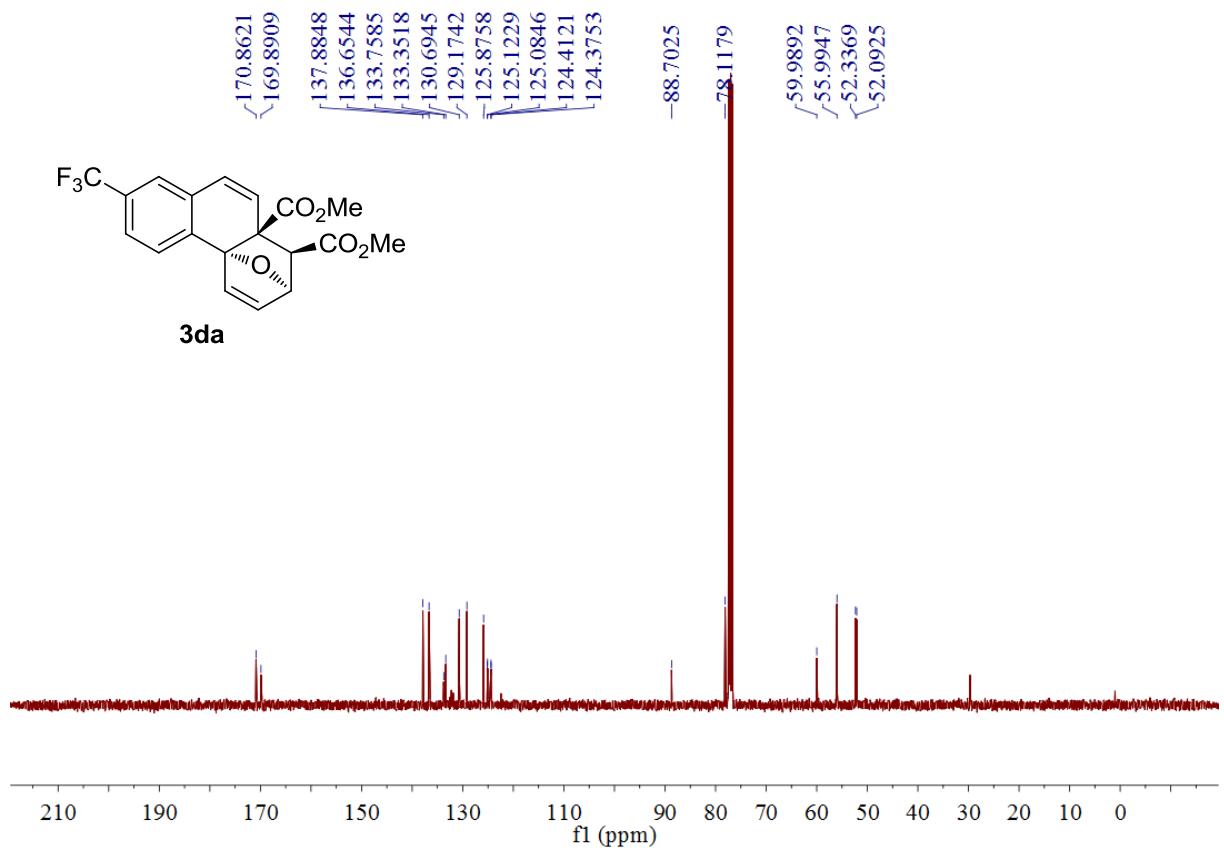
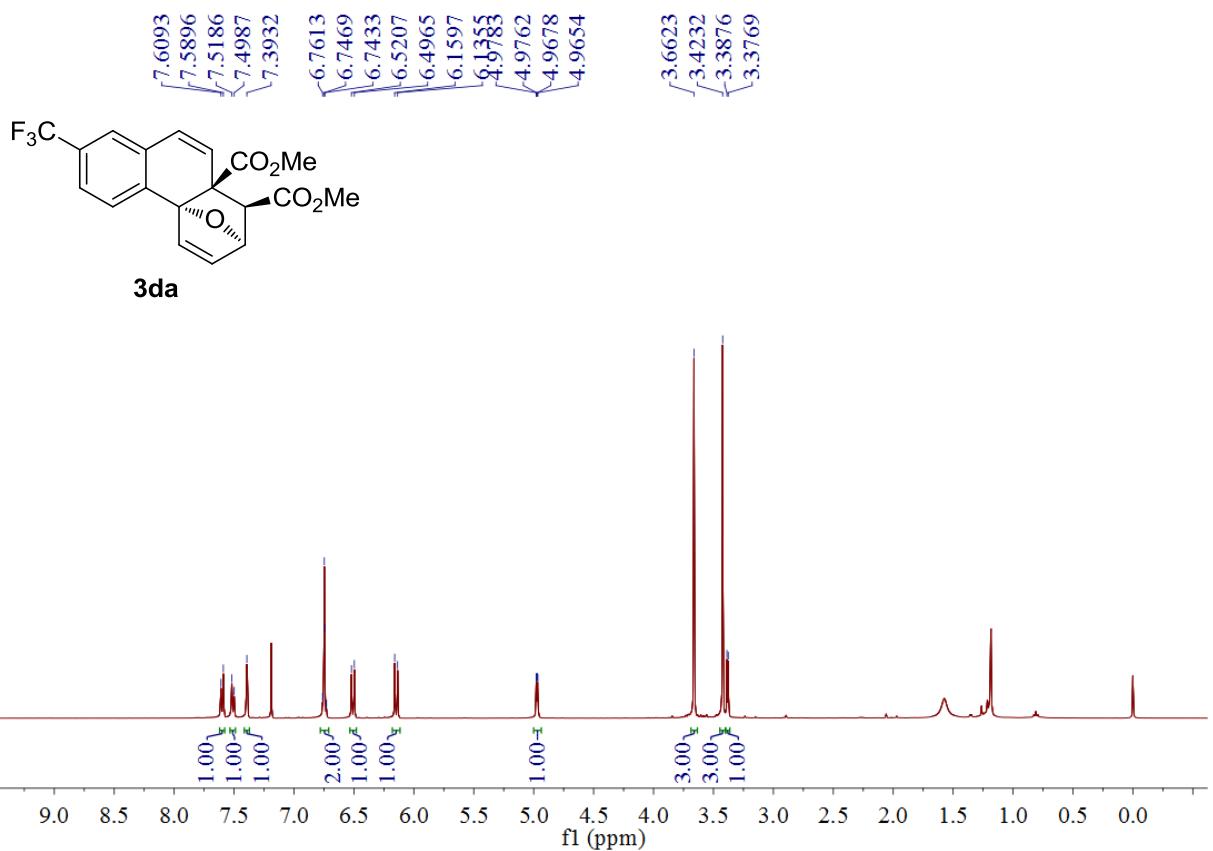
Copies of ^1H and ^{13}C NMR Spectra for **4ca**

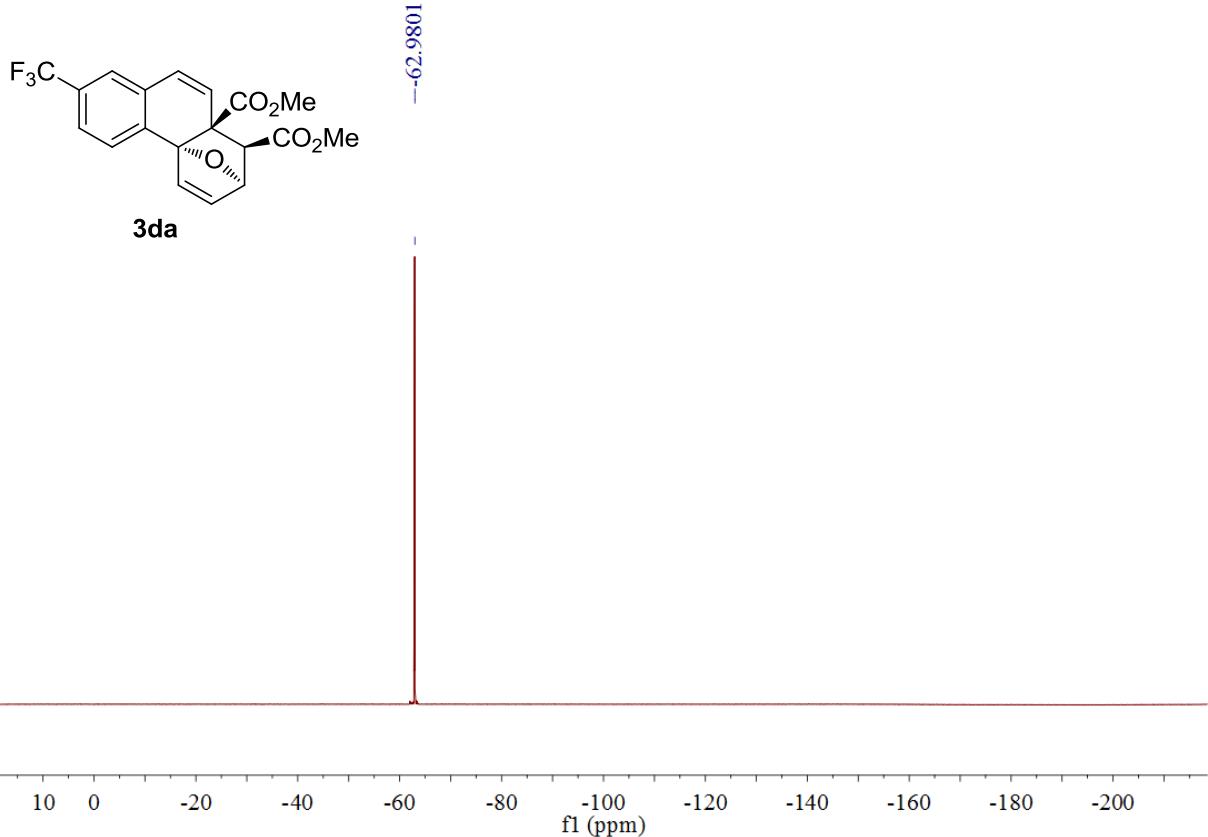


Copies of ^1H and ^{13}C NMR Spectra for **9ca**

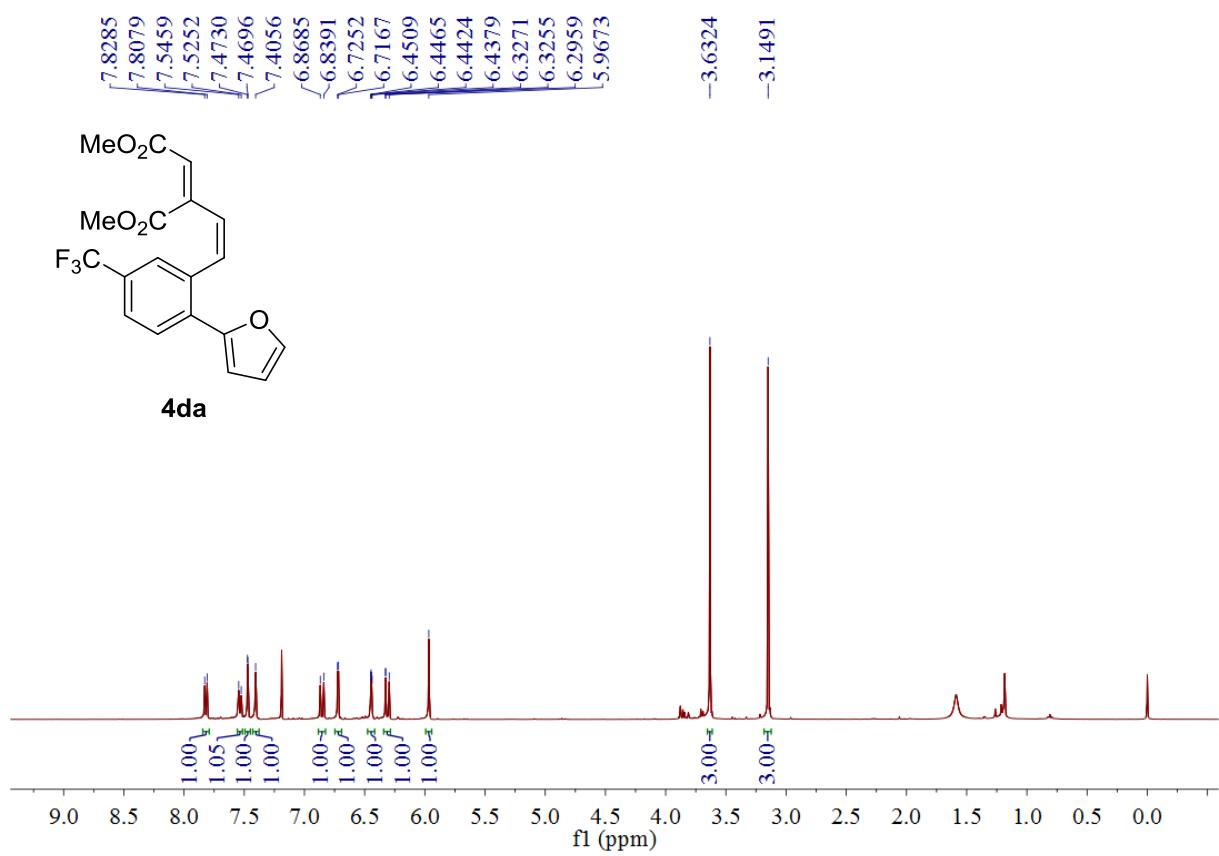


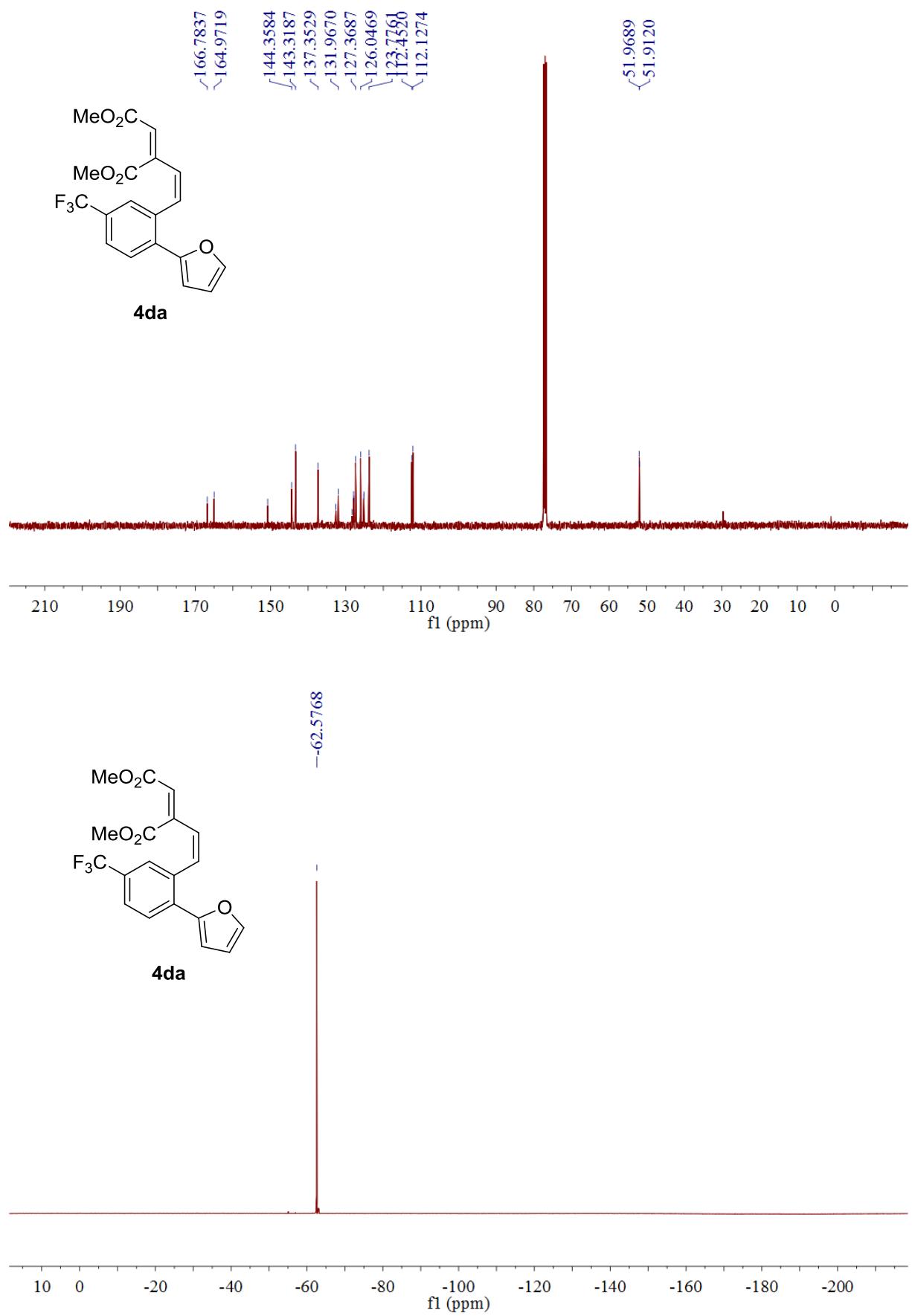
Copies of ^1H , ^{13}C and ^{19}F NMR Spectra for **3da**



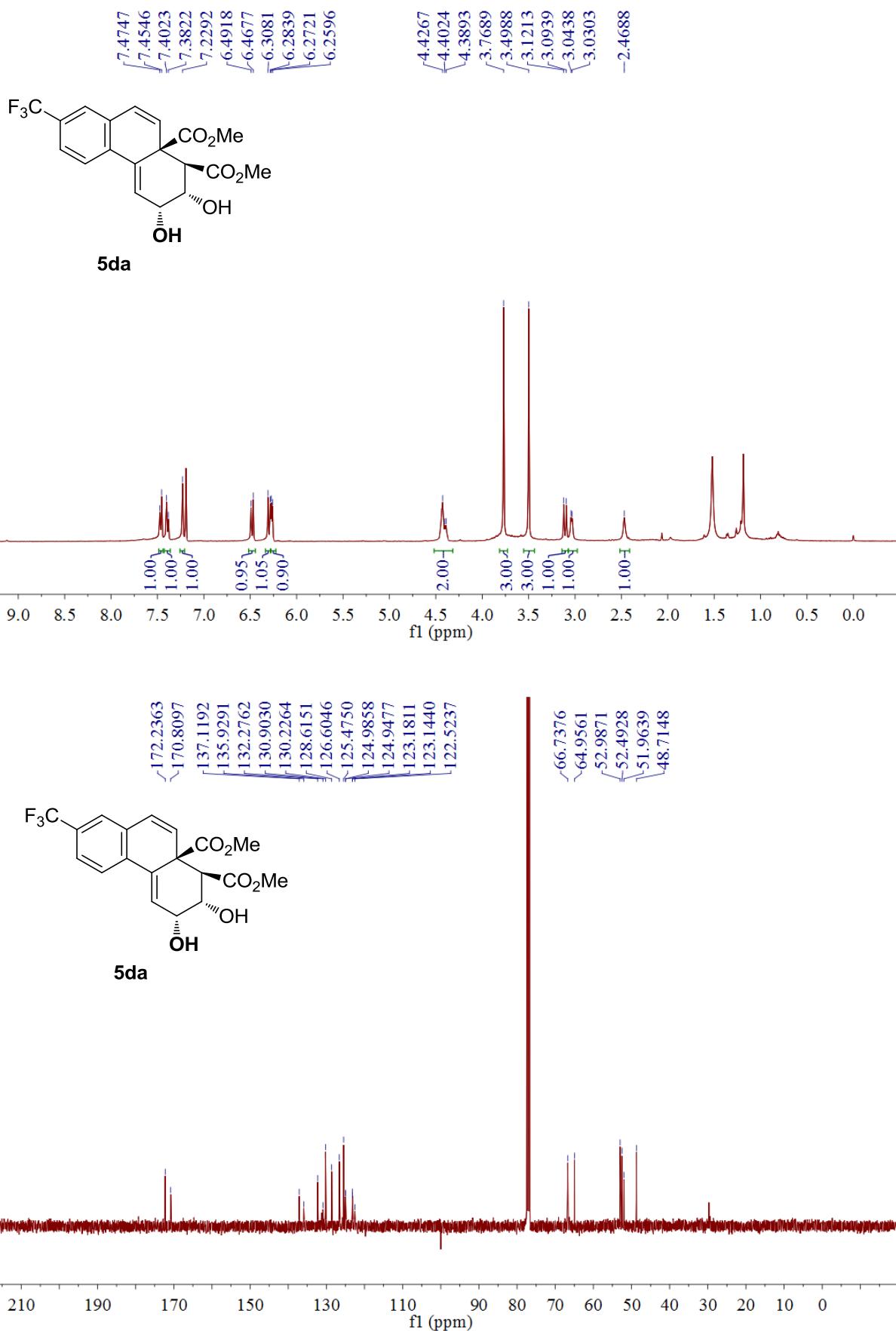


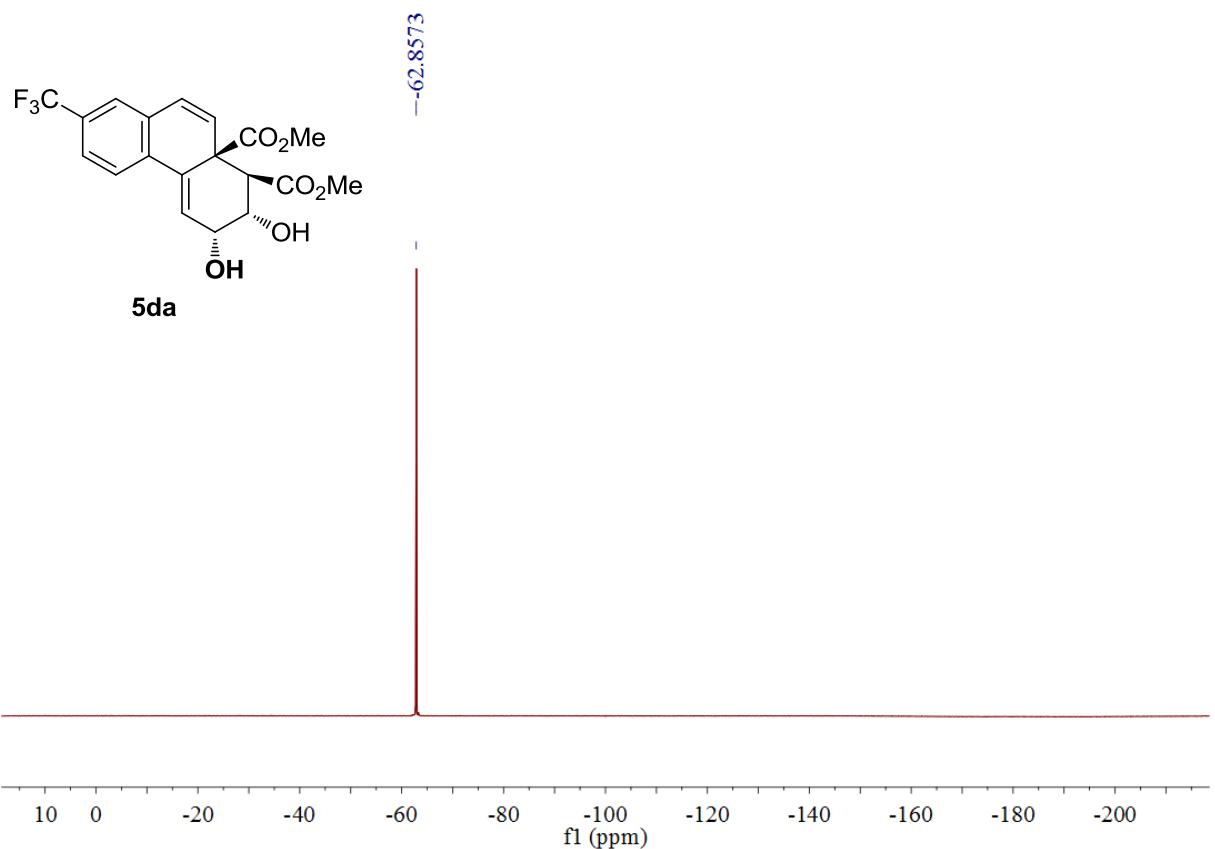
Copies of ^1H , ^{13}C and ^{19}F NMR Spectra for **4da**



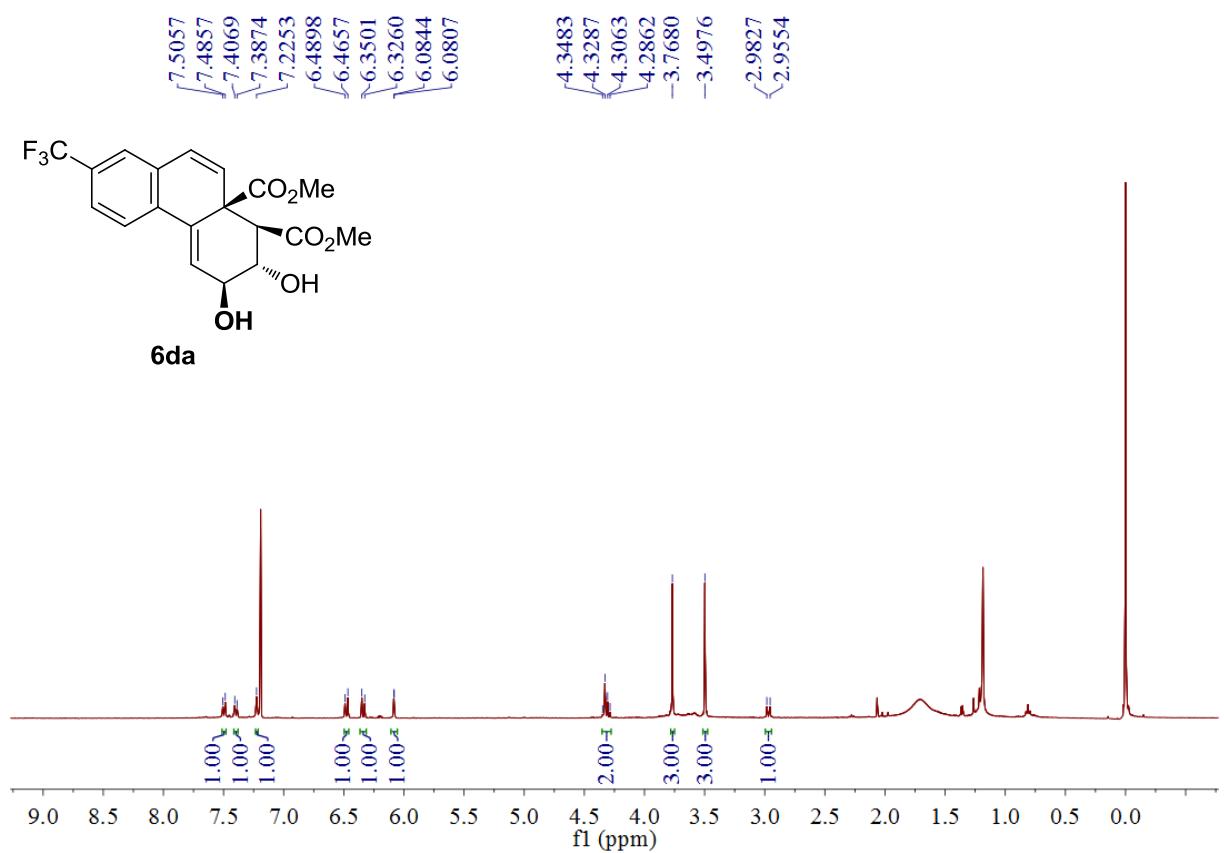


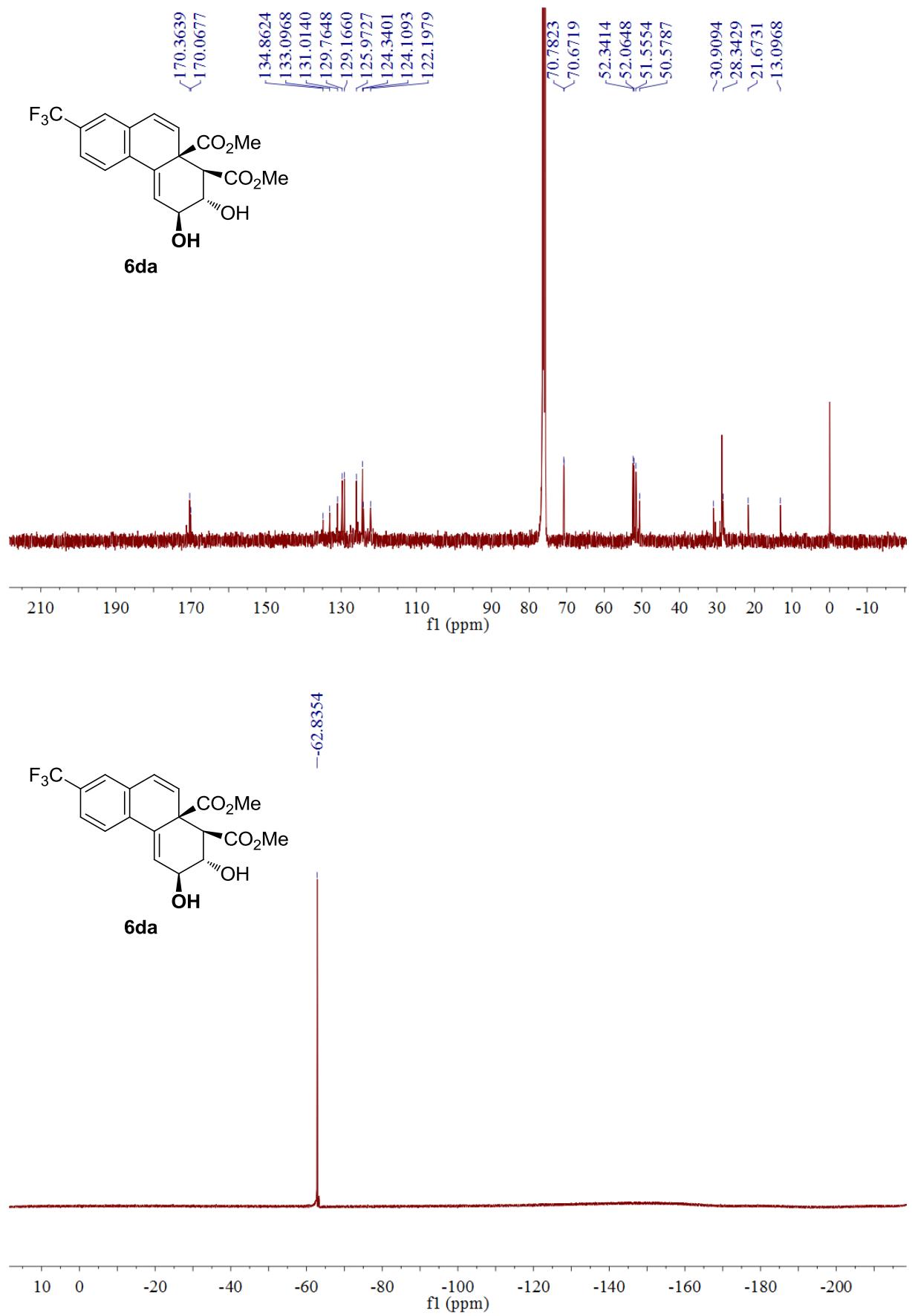
Copies of ^1H , ^{13}C and ^{19}F NMR Spectra for **5da**



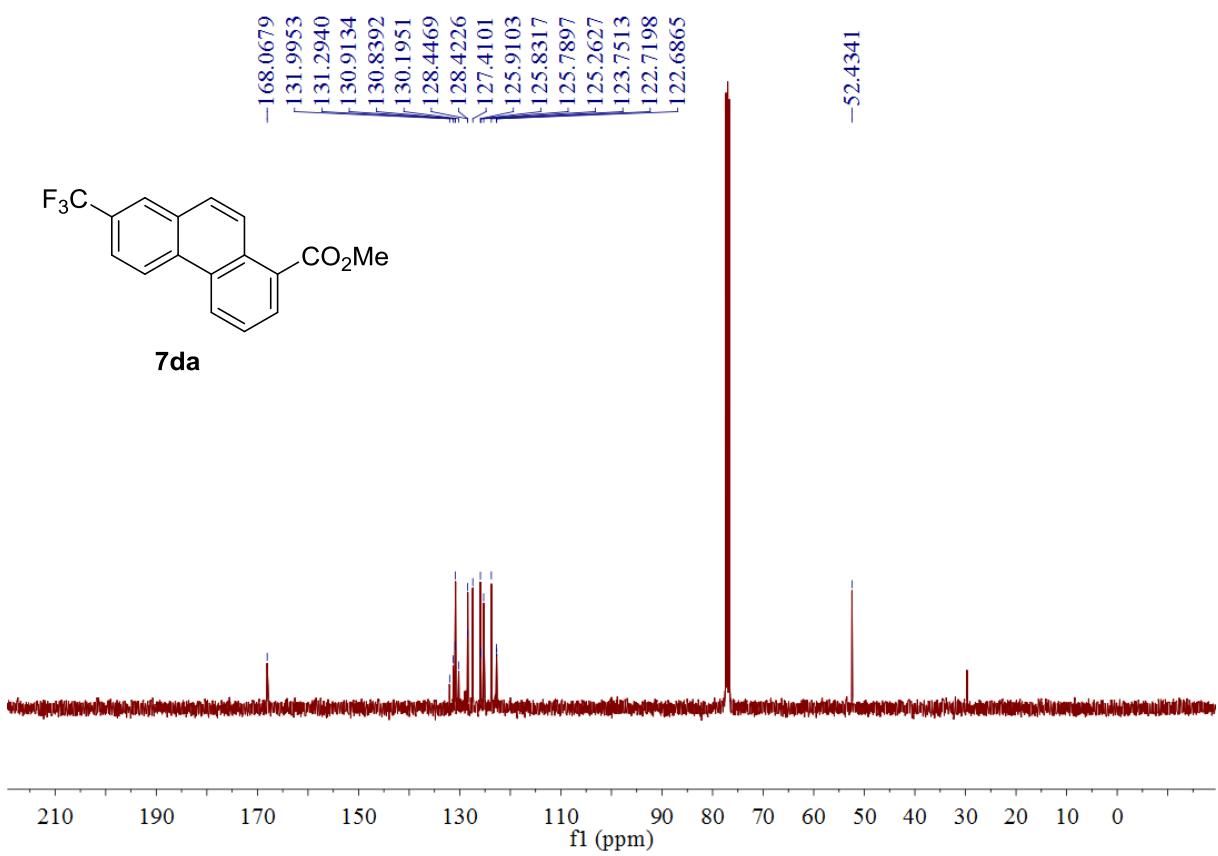
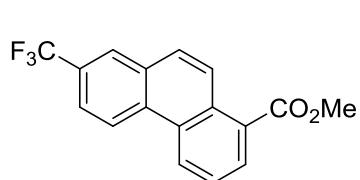
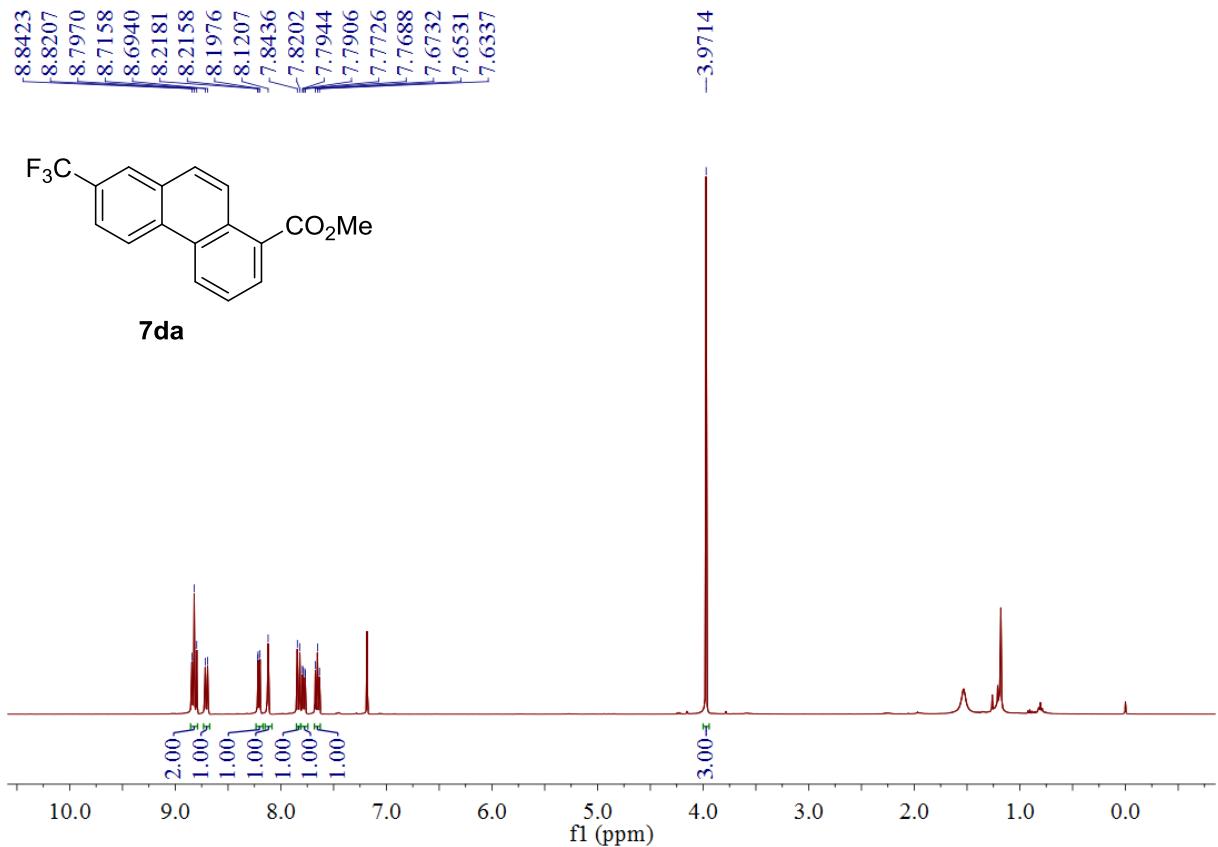
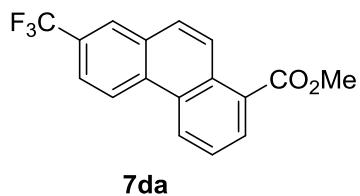


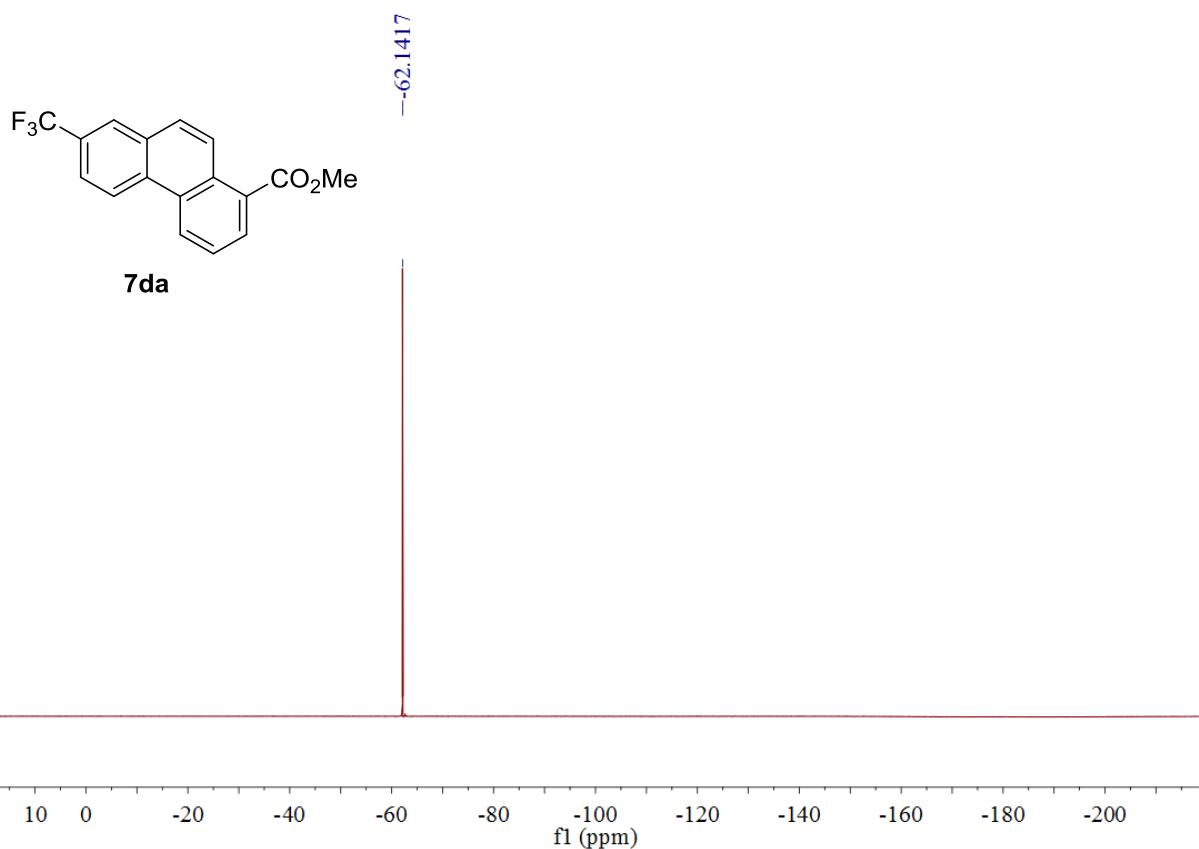
Copies of ^1H , ^{13}C and ^{19}F NMR Spectra for **6da**



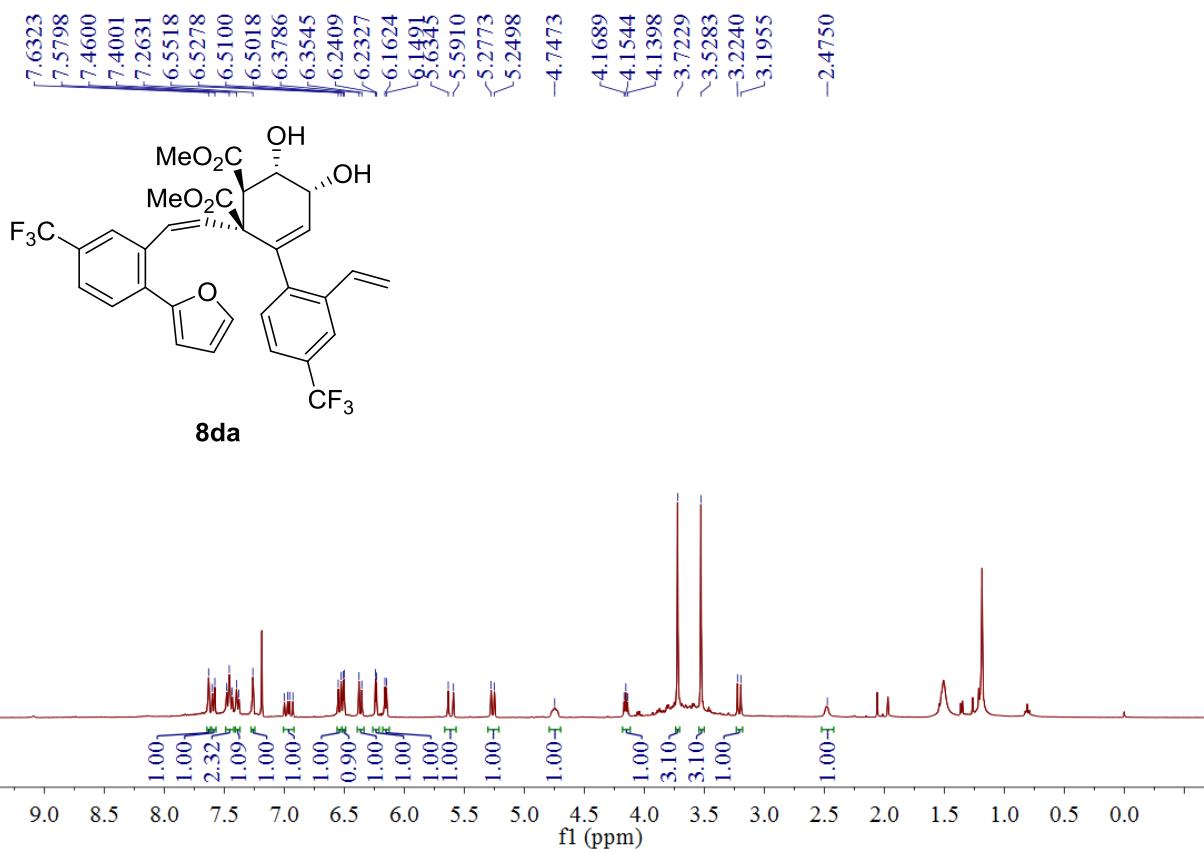


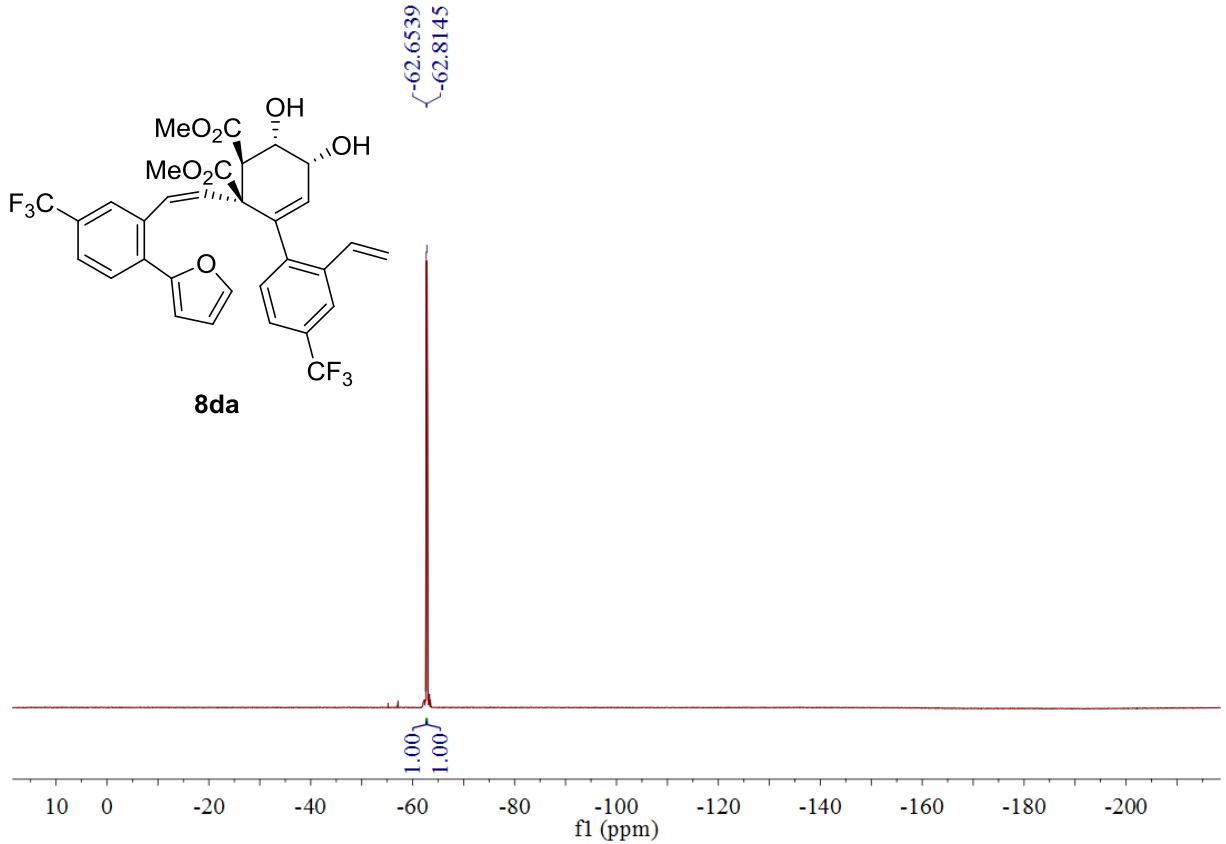
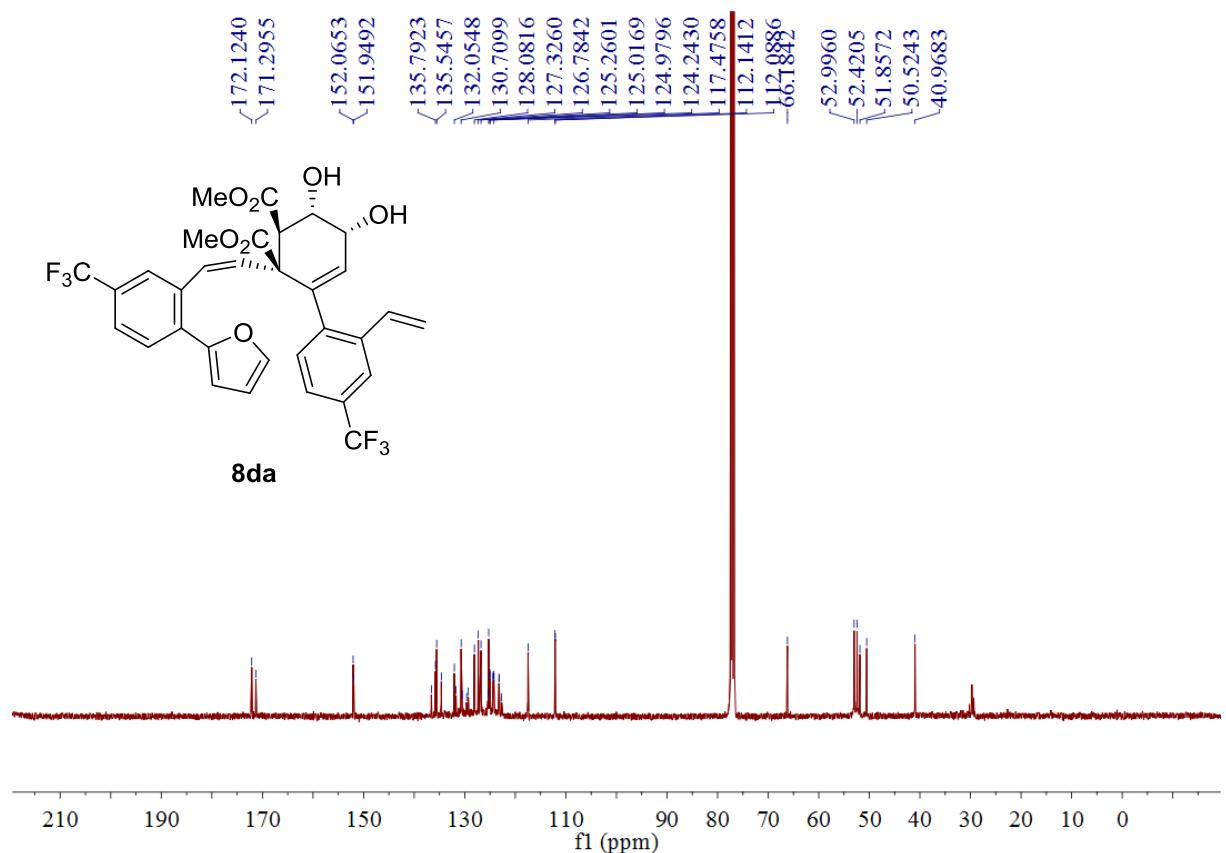
Copies of ^1H , ^{13}C and ^{19}F NMR Spectra for **7da**



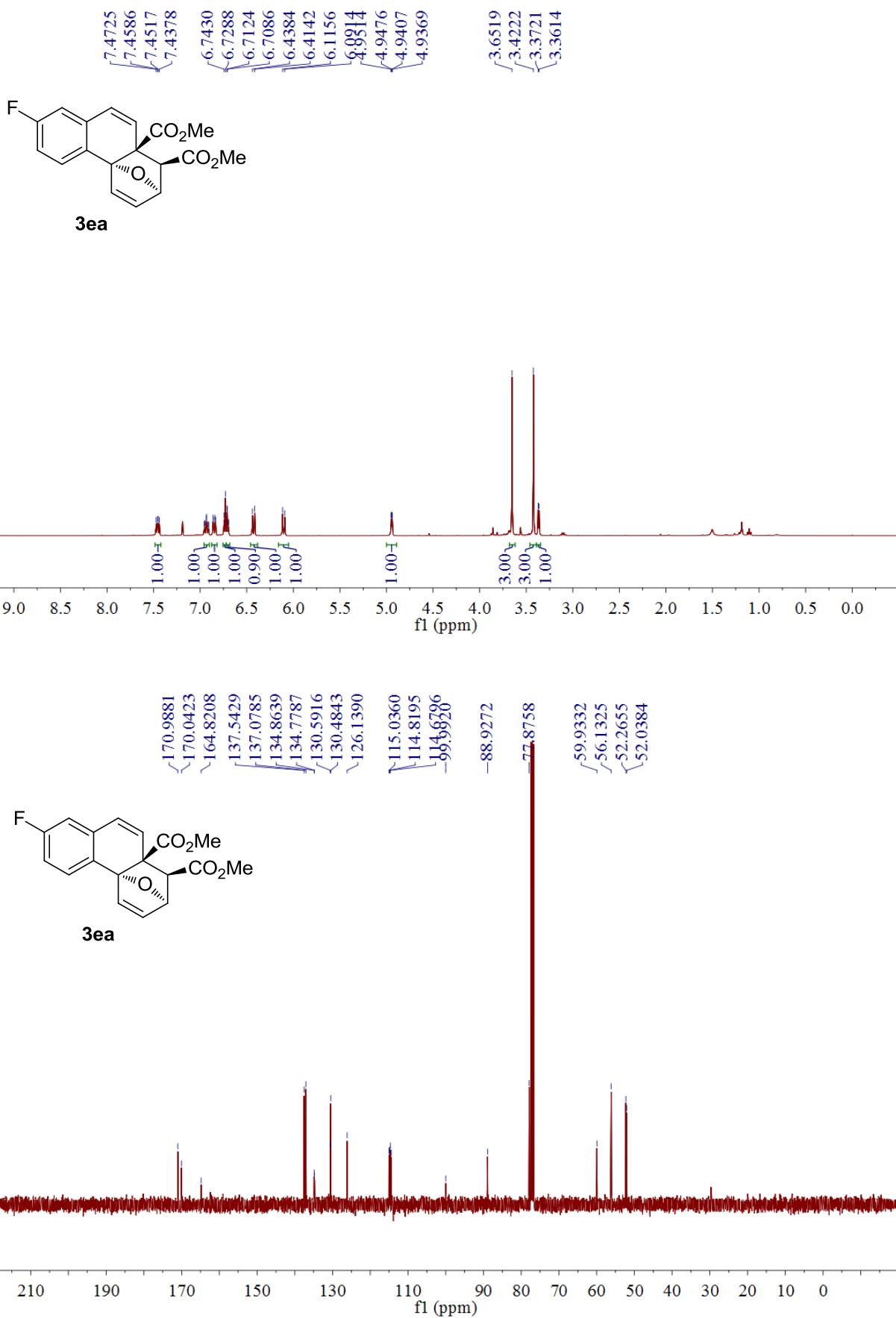


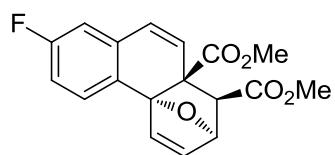
Copies of ^1H , ^{13}C and ^{19}F NMR Spectra for **8da**



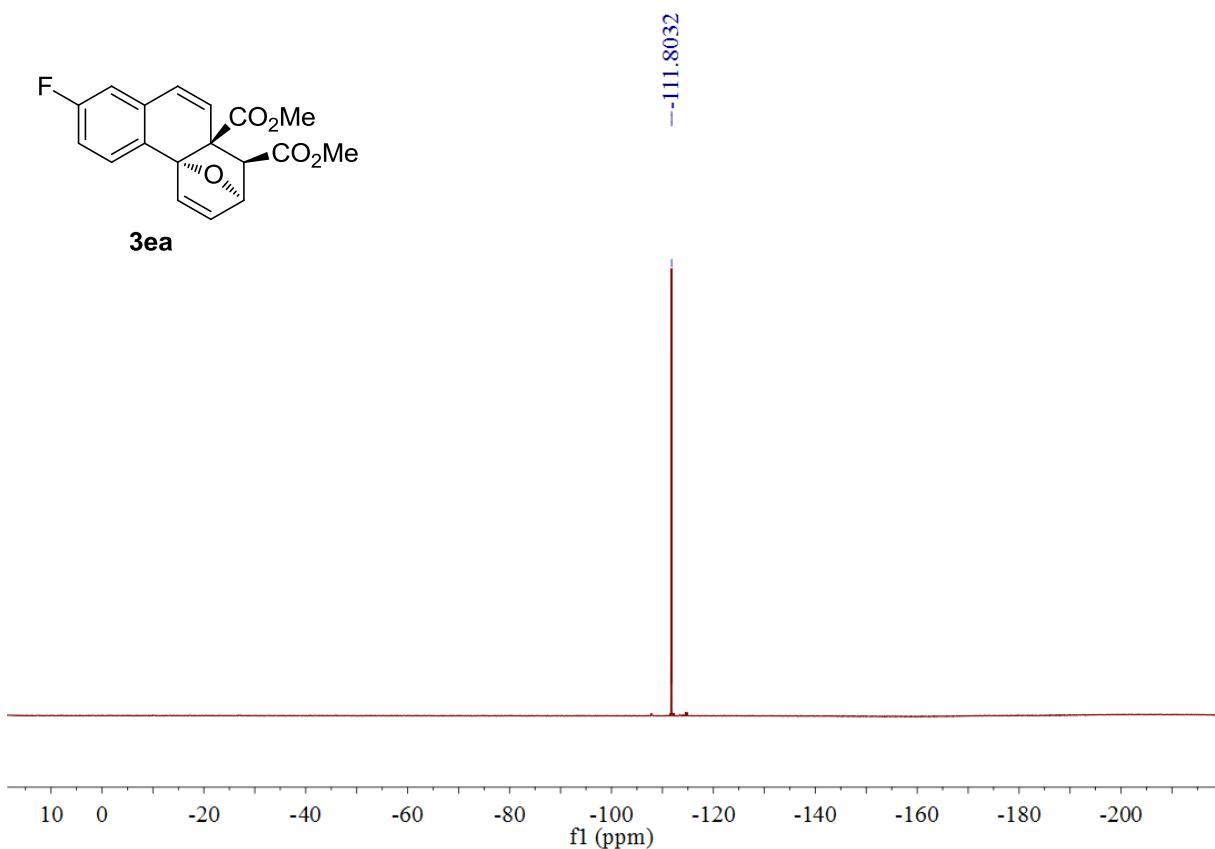


Copies of ^1H , ^{13}C and ^{19}F NMR Spectra for **3ea**

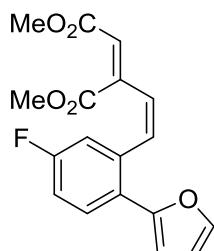




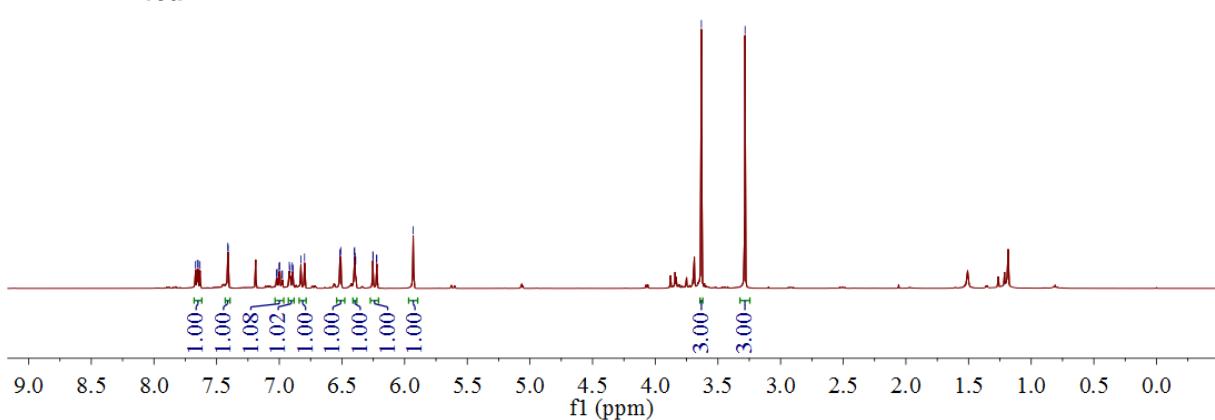
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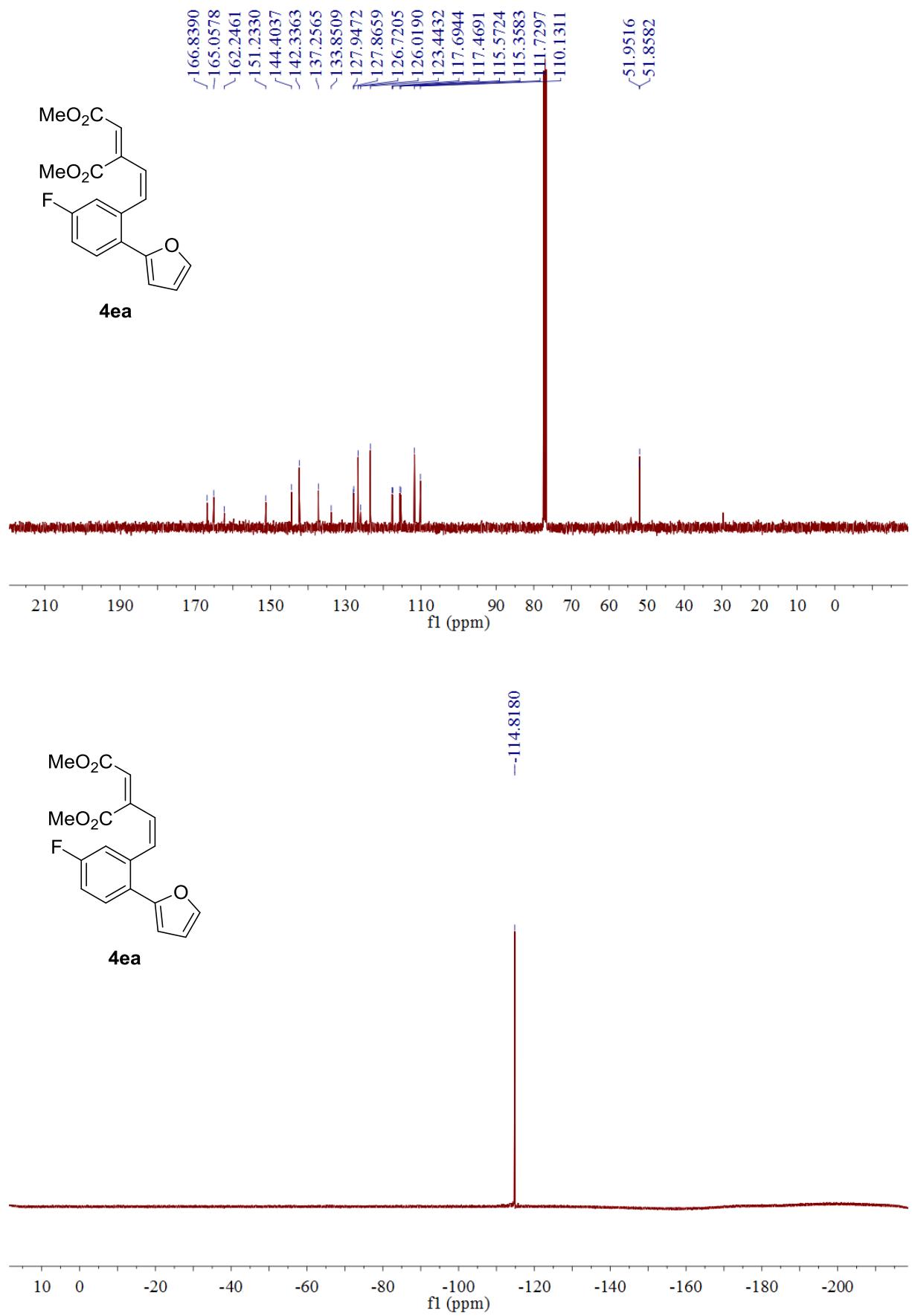


Copies of ^1H , ^{13}C and ^{19}F NMR Spectra for **4ea**

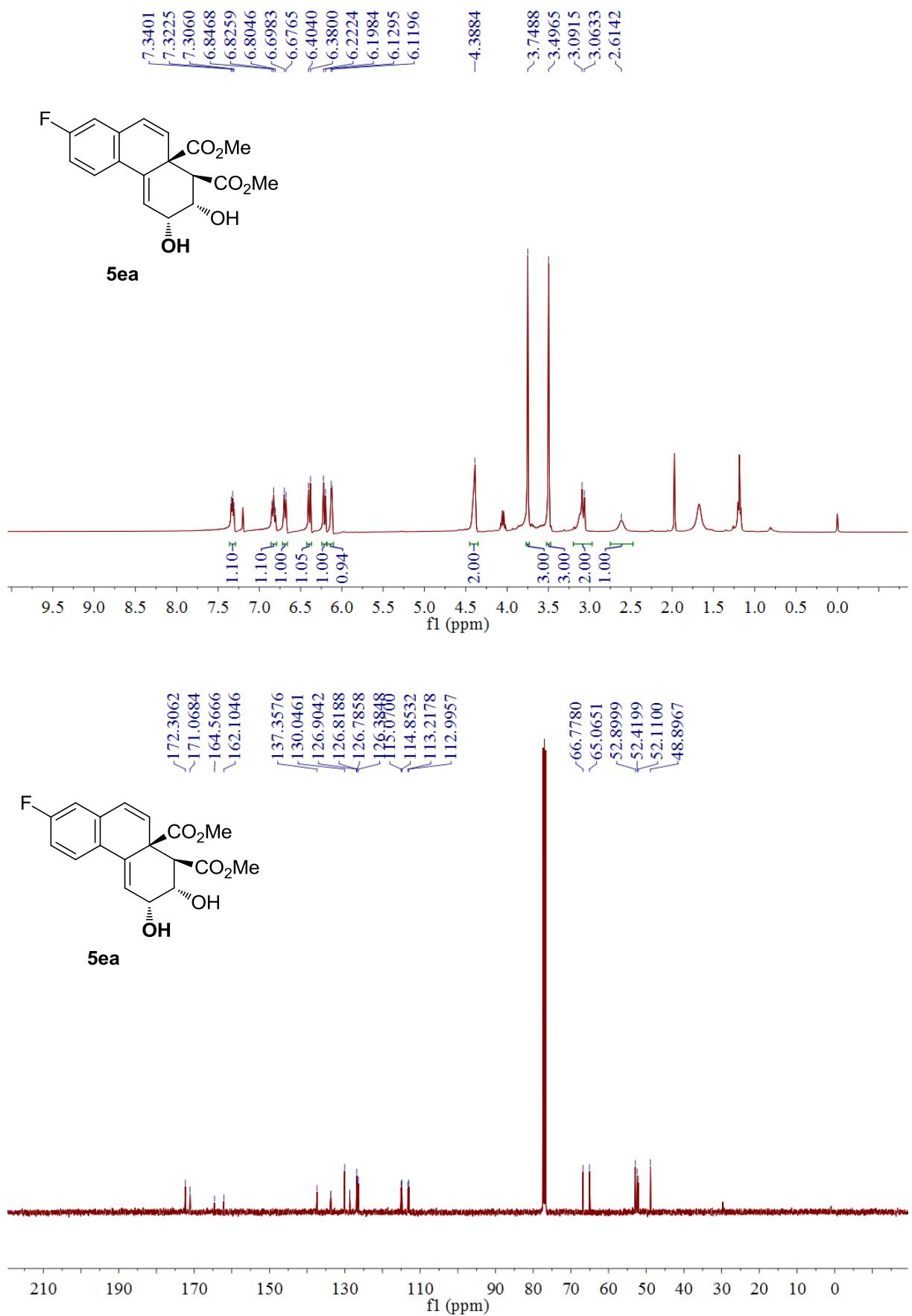


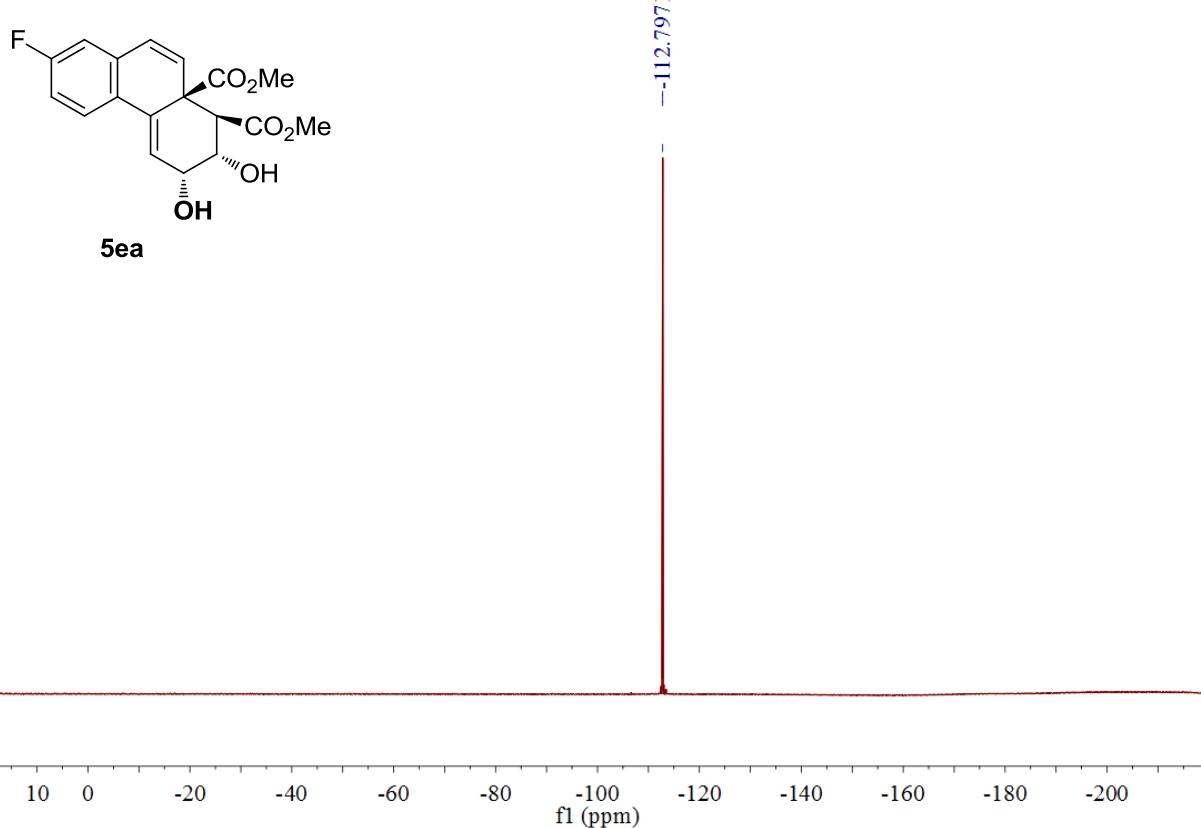
4ea



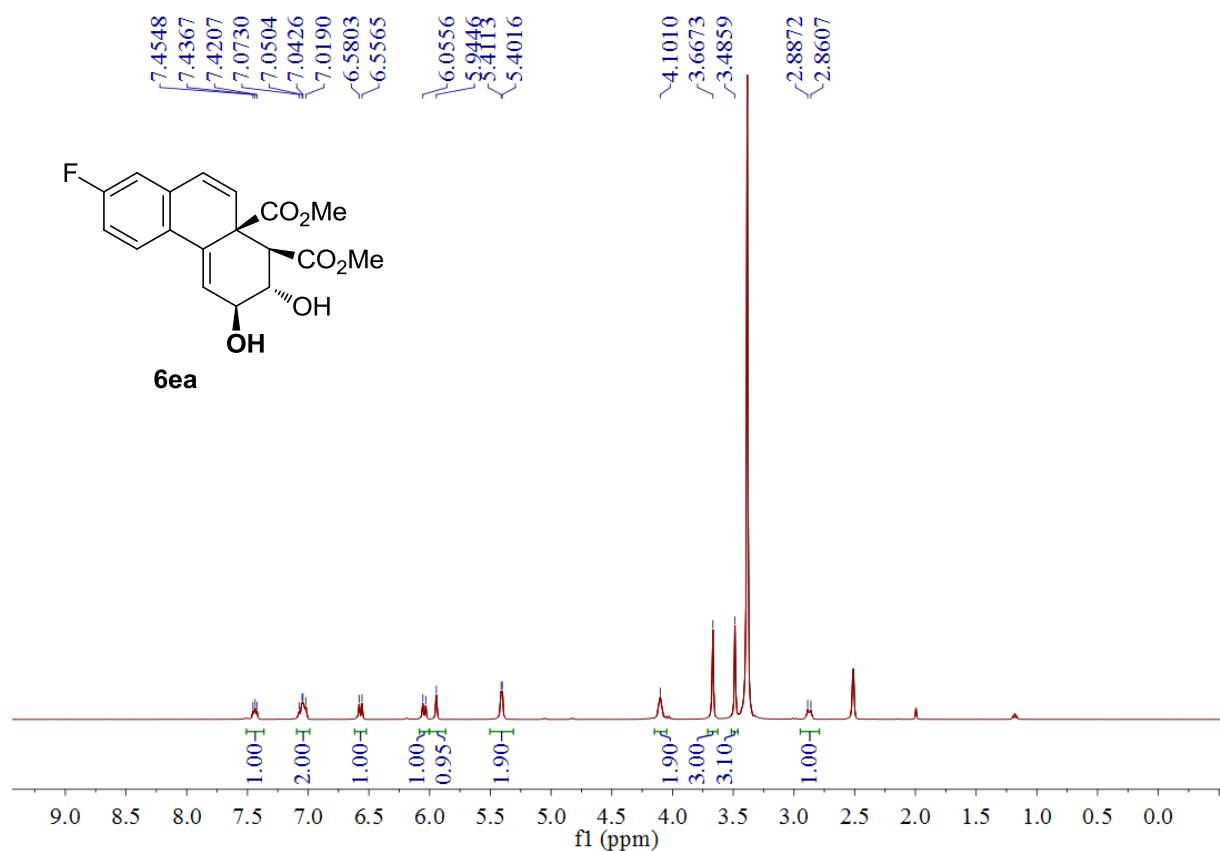


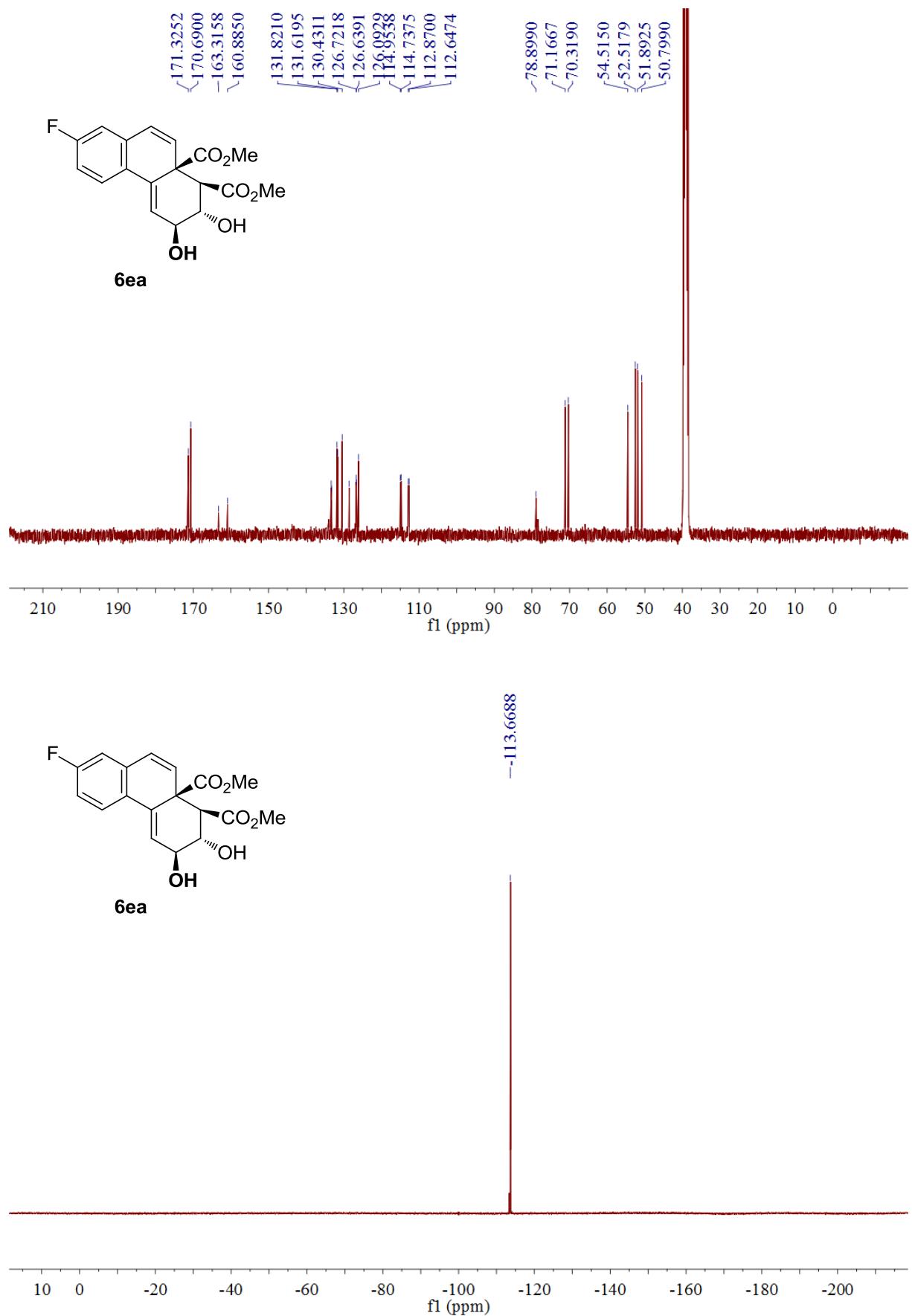
Copies of ^1H , ^{13}C and ^{19}F NMR Spectra for **5ea**



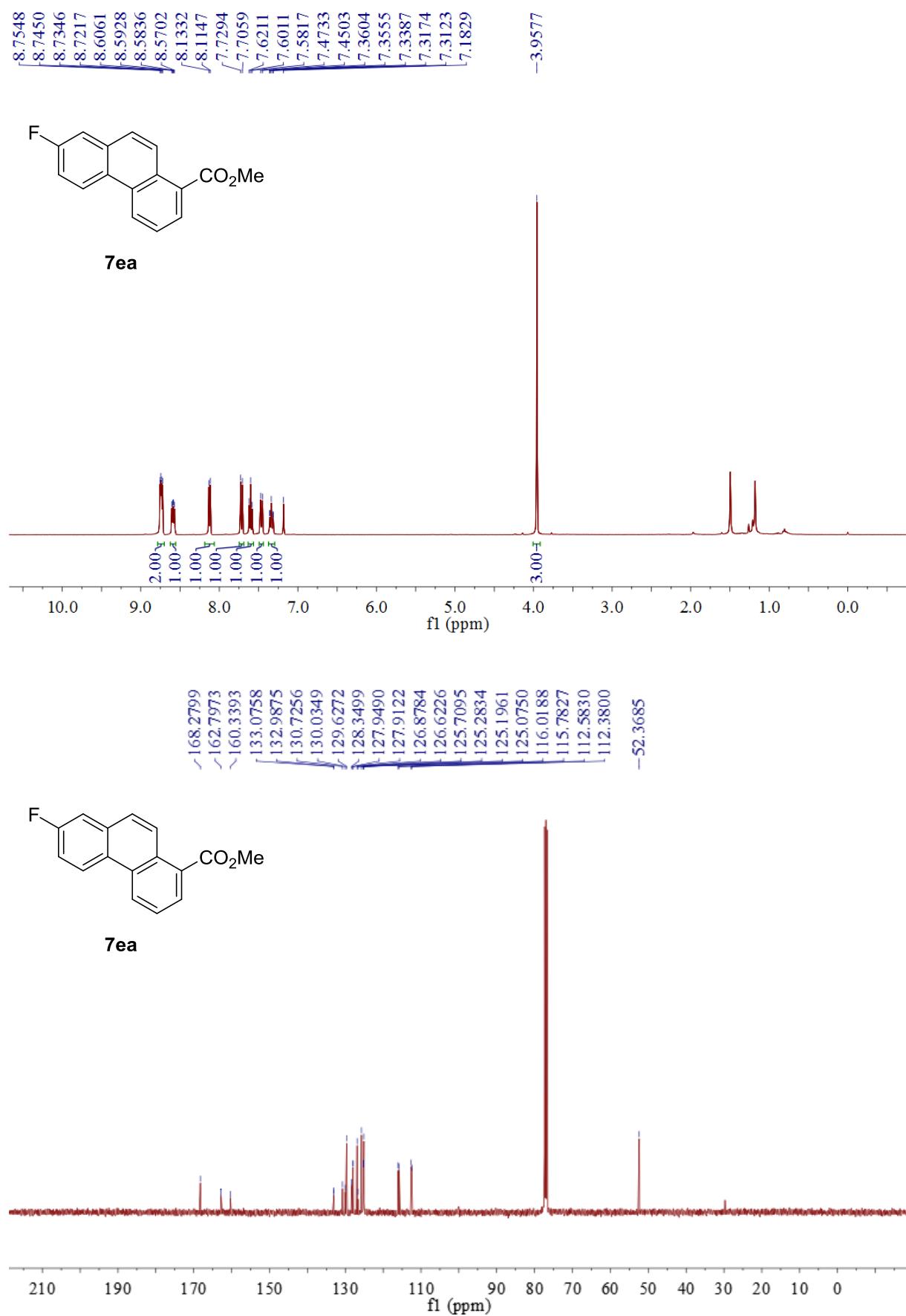


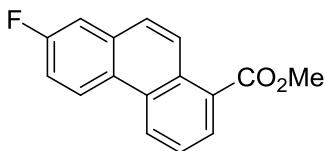
Copies of ¹H, ¹³C and ¹⁹F NMR Spectra for 6ea



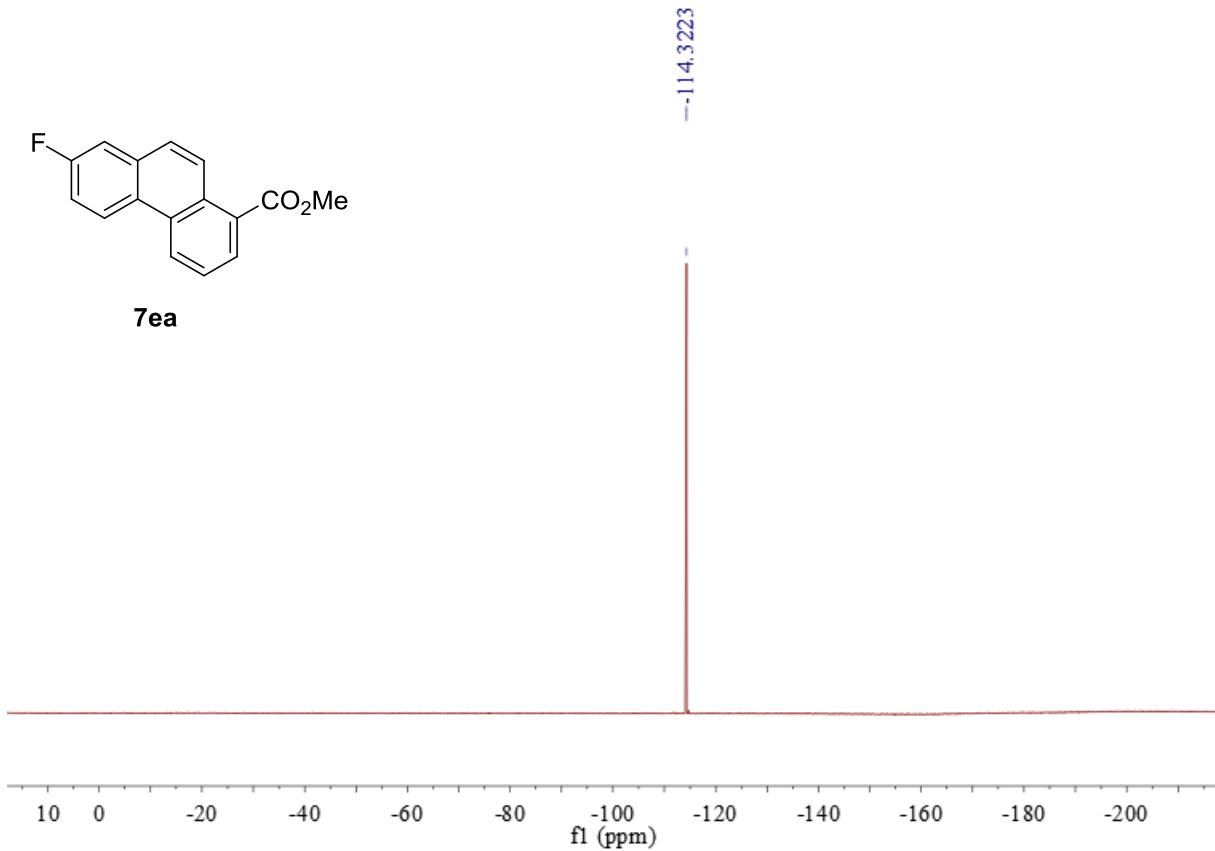


Copies of ^1H , ^{13}C and ^{19}F NMR Spectra for **7ea**

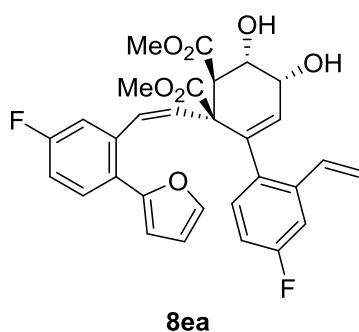




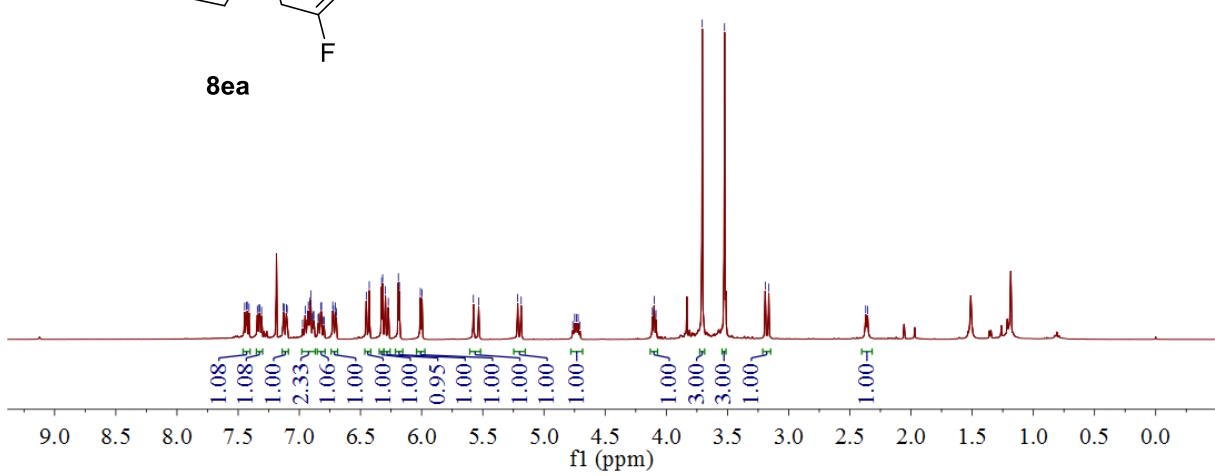
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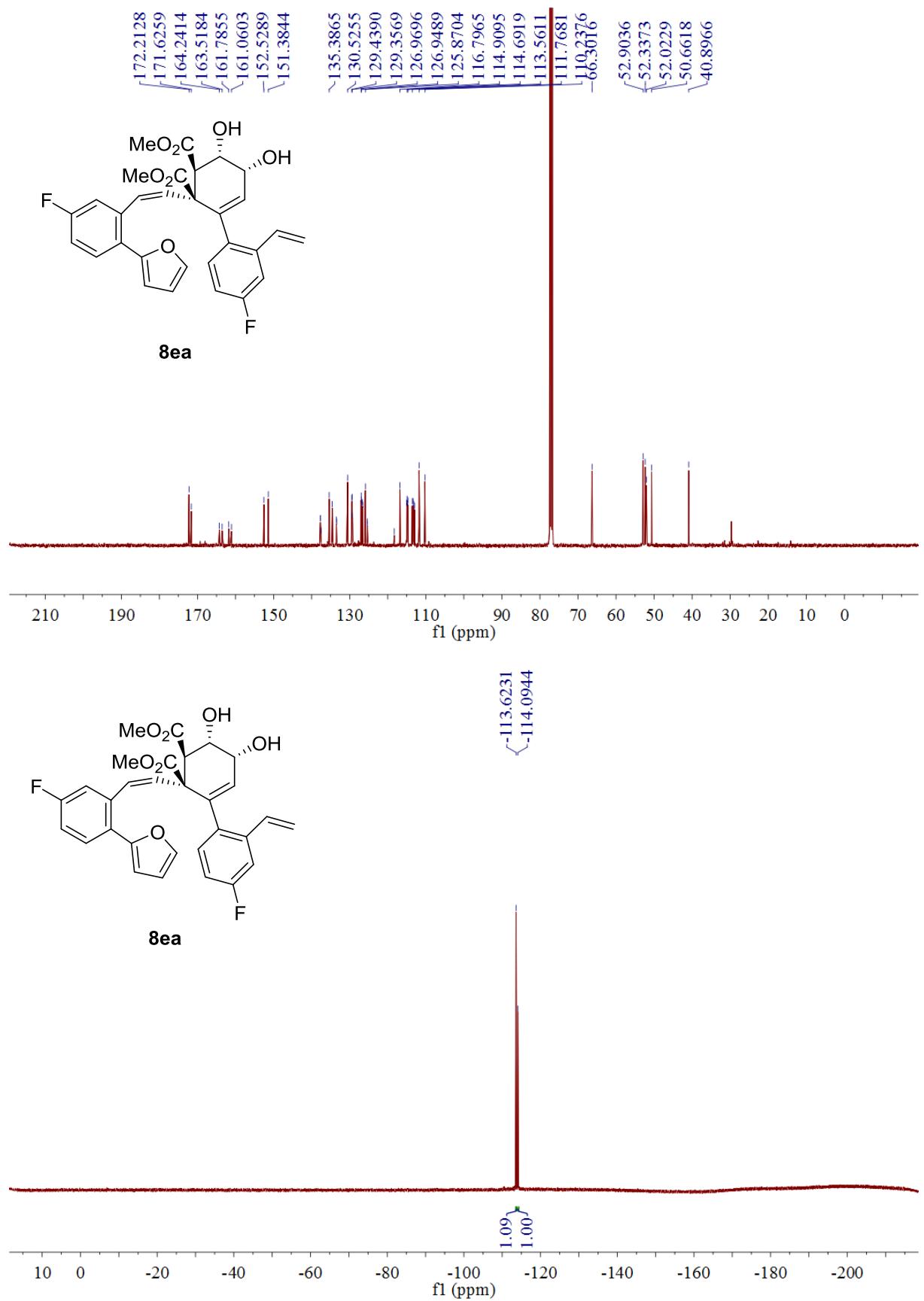


Copies of ^1H , ^{13}C and ^{19}F NMR Spectra for **8ea**

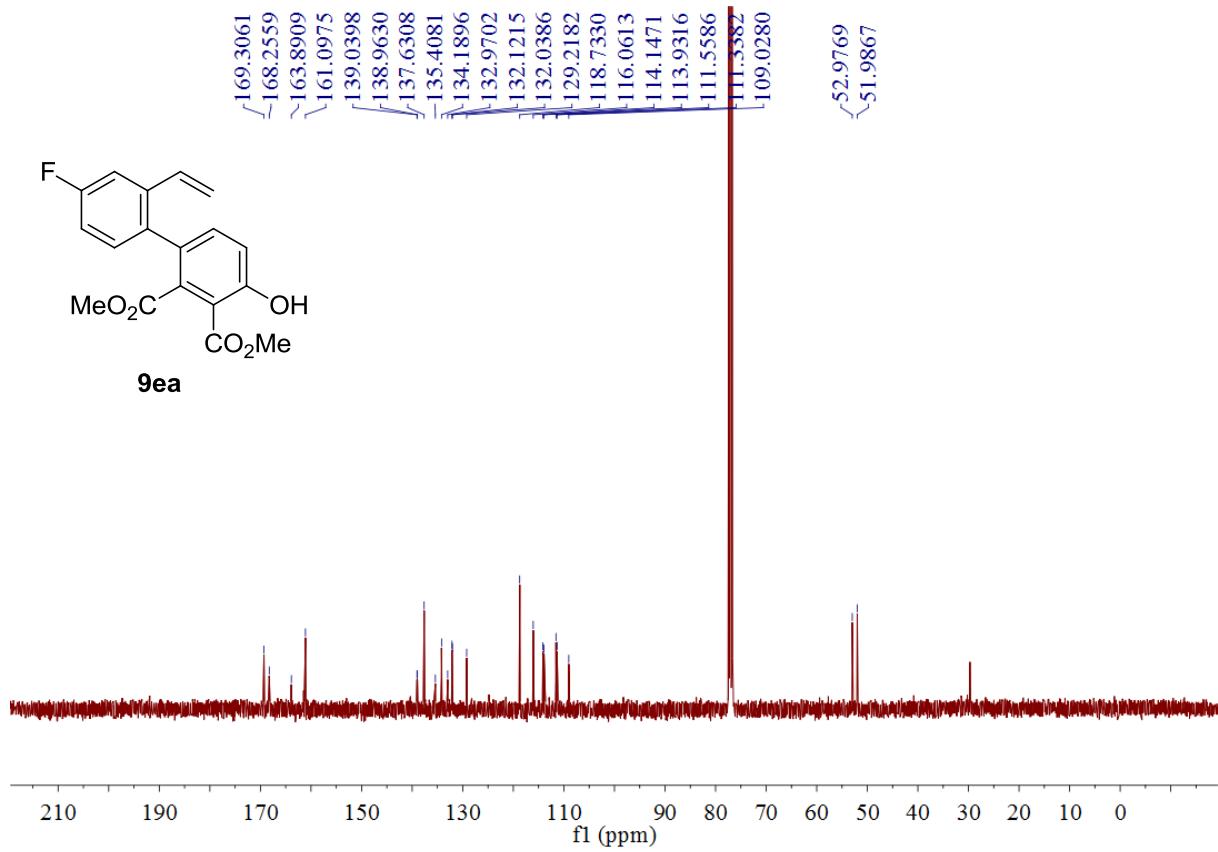
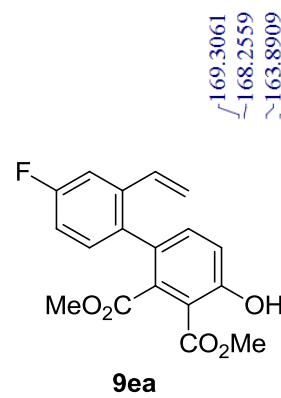
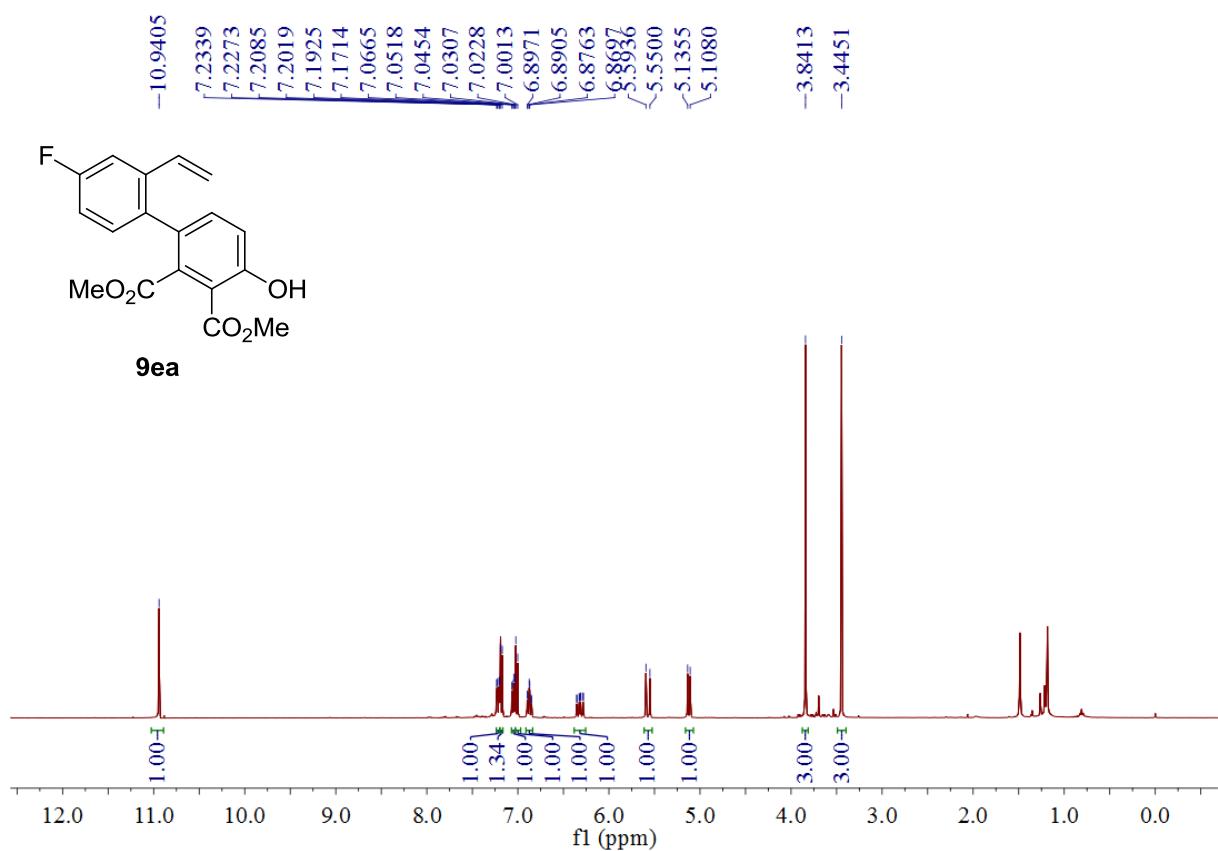
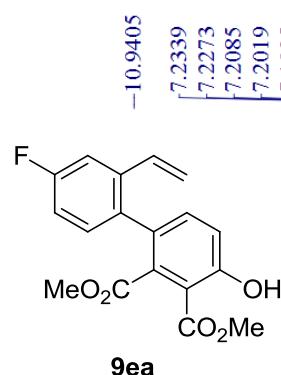


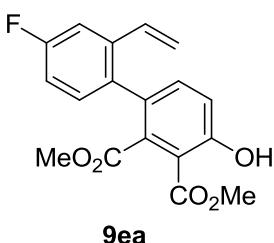
8ea





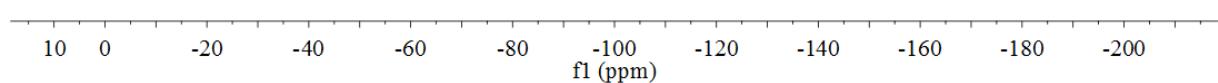
Copies of ^1H , ^{13}C and ^{19}F NMR Spectra for **9ea**



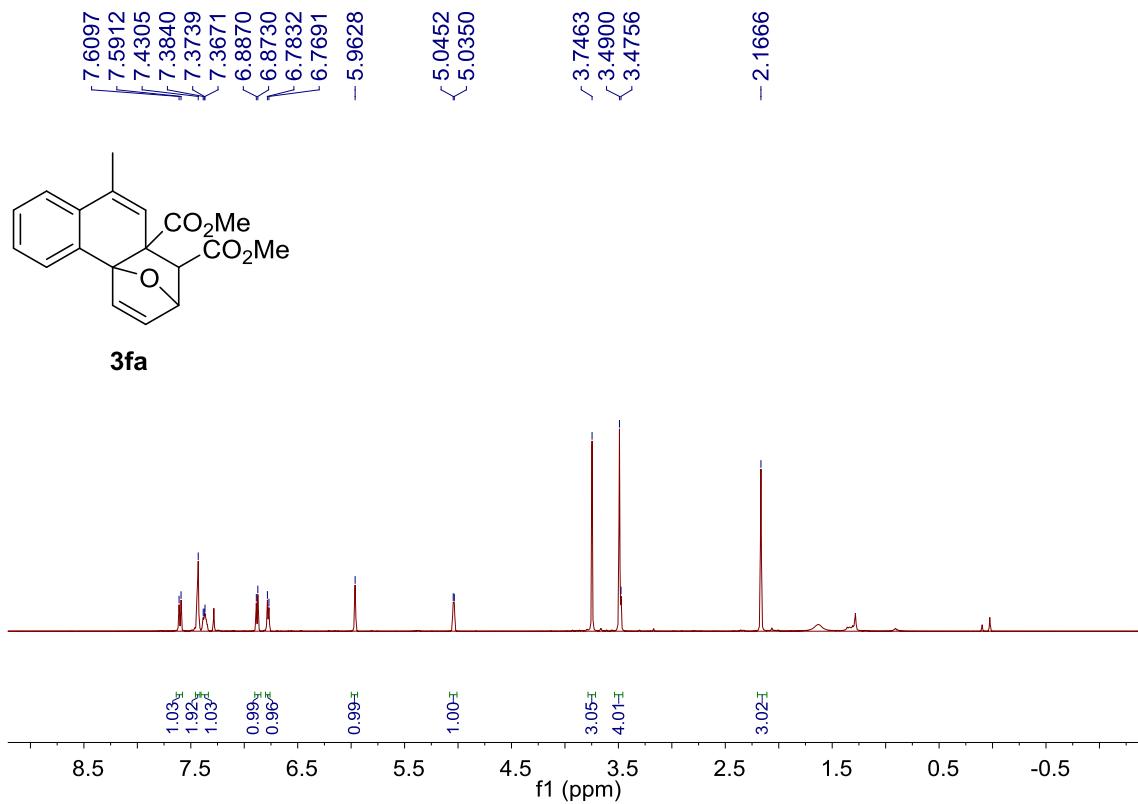


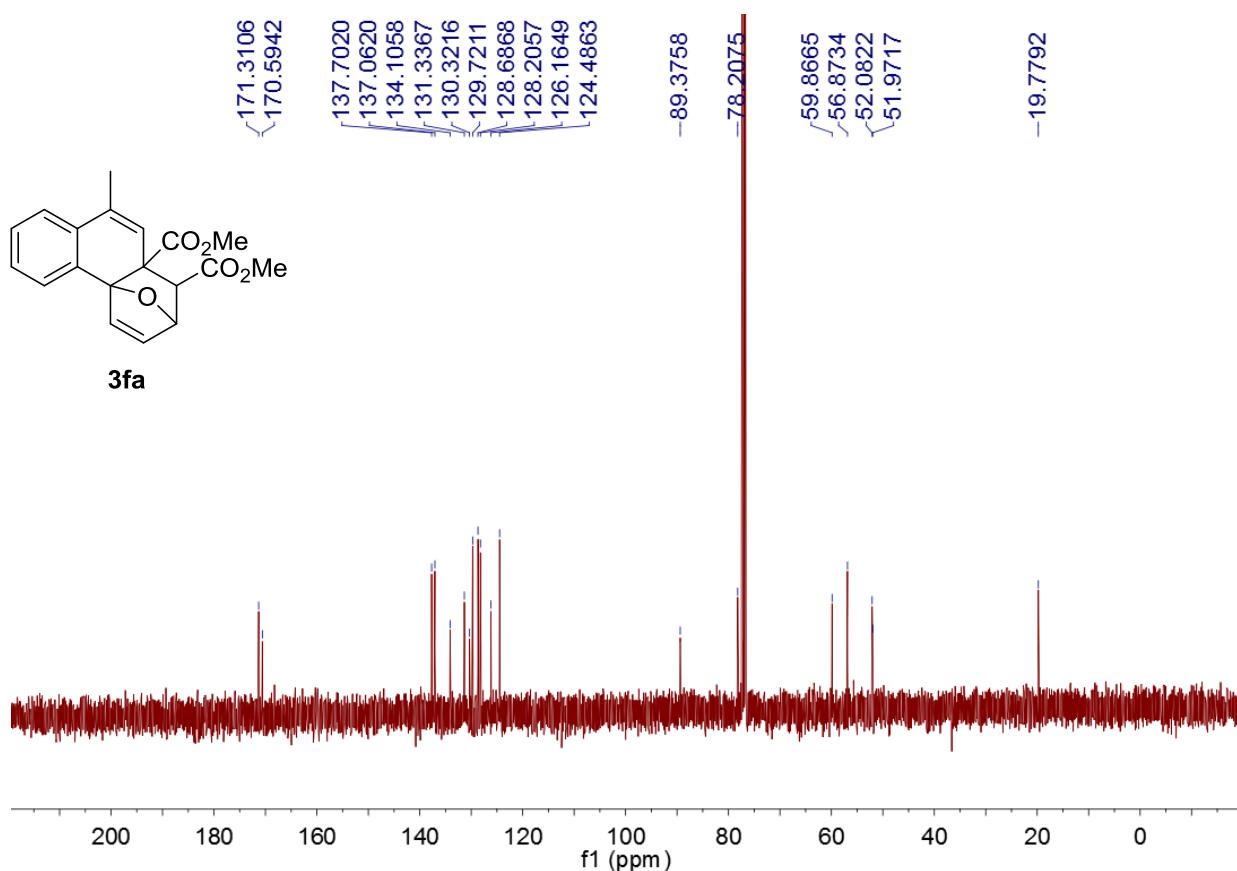
9ea

-113.9582

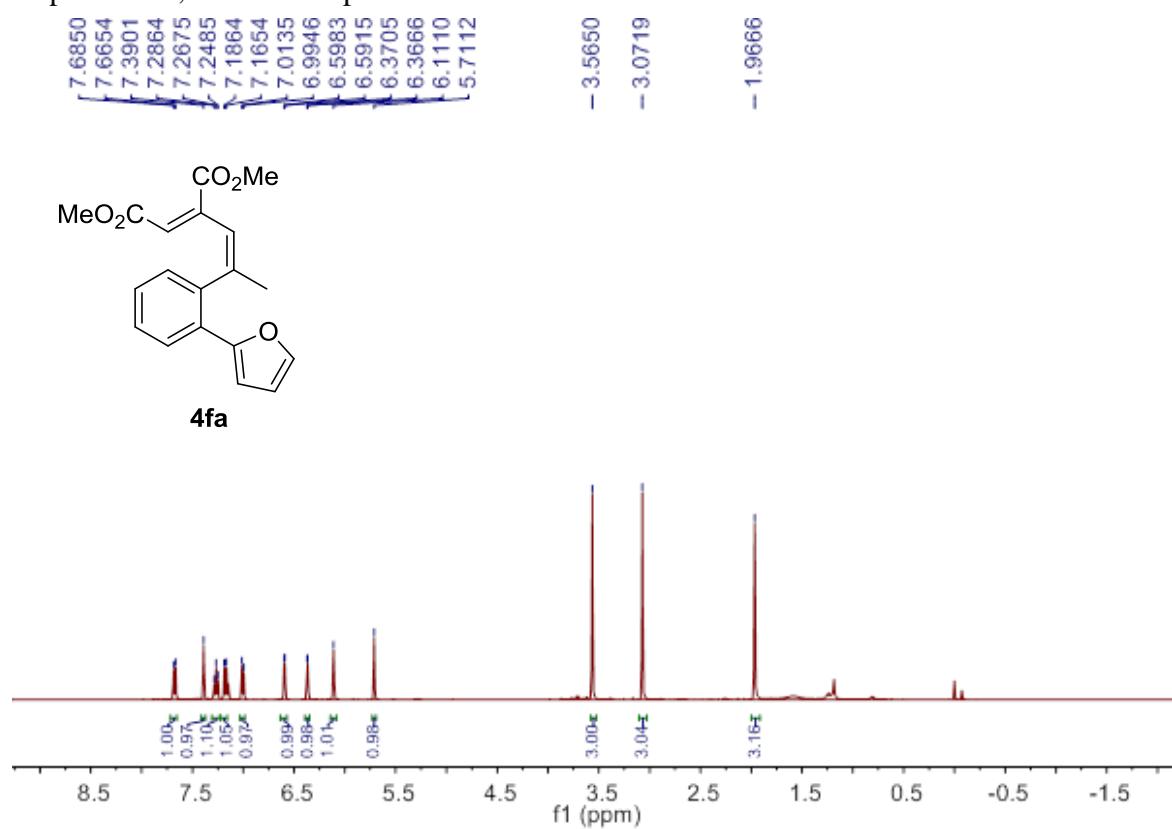


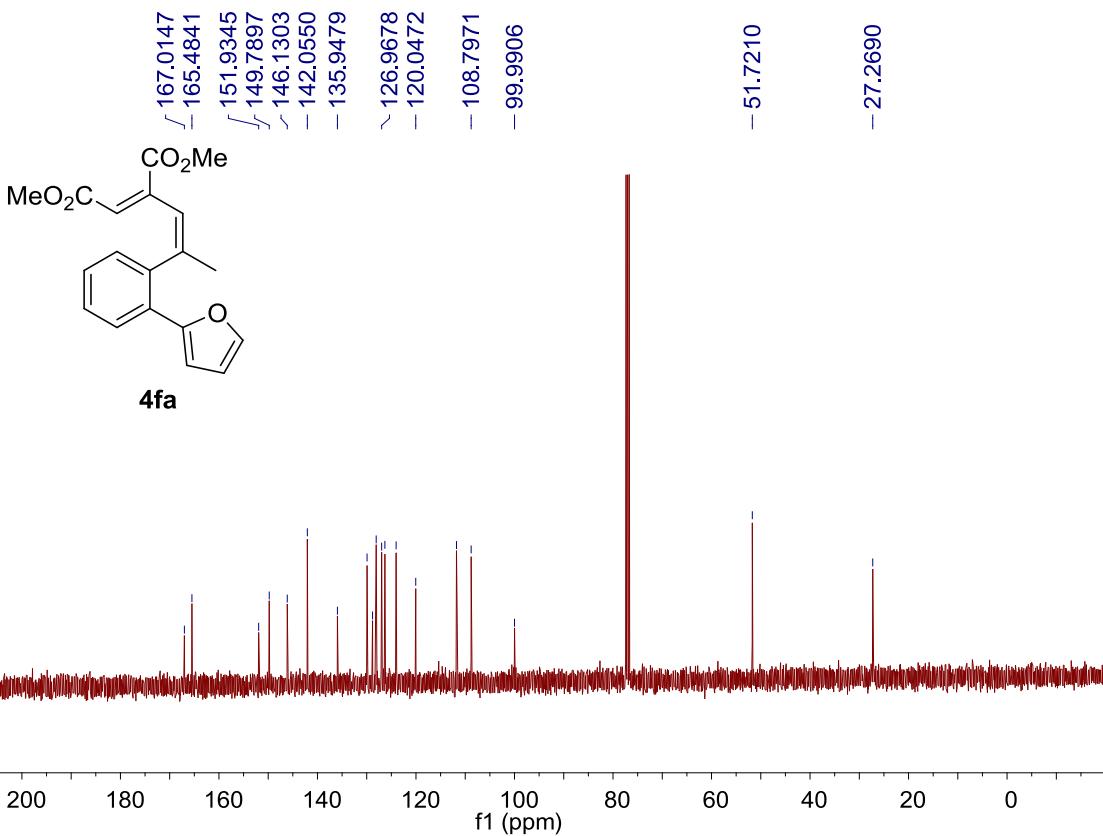
Copies of ^1H , ^{13}C NMR Spectra for **3fa**



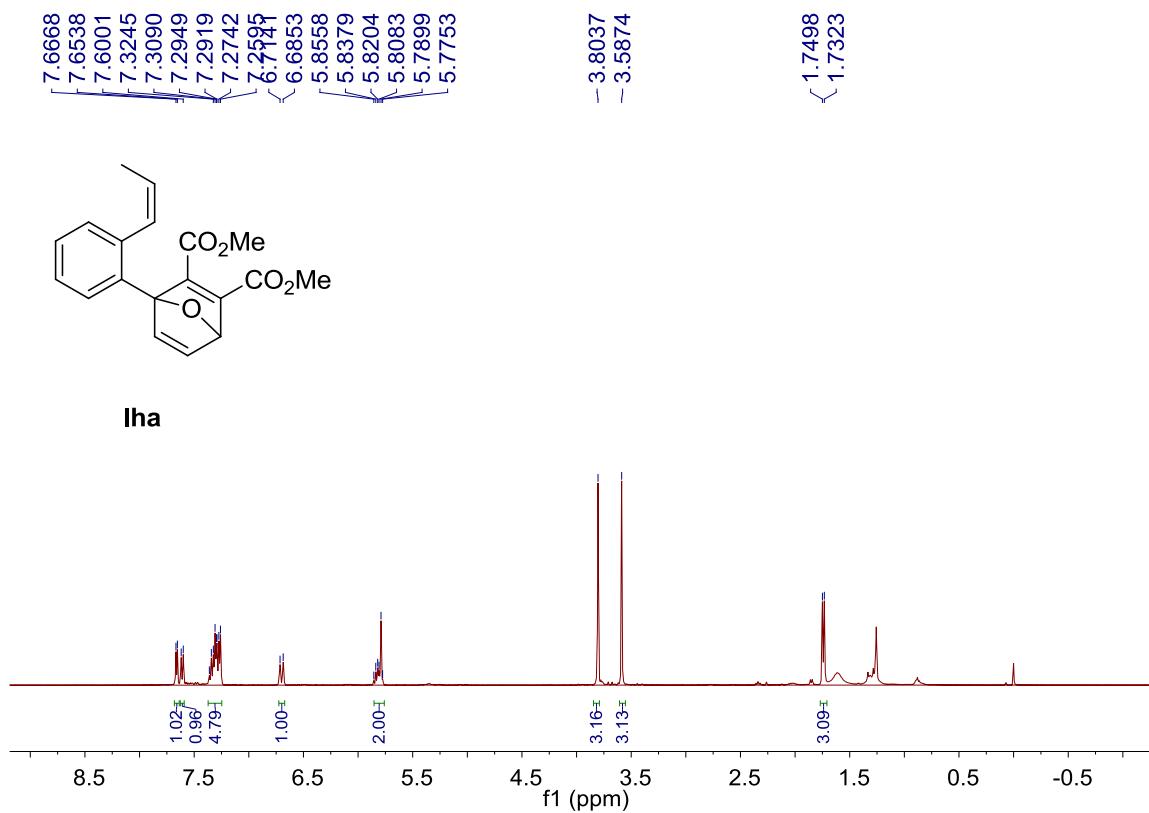


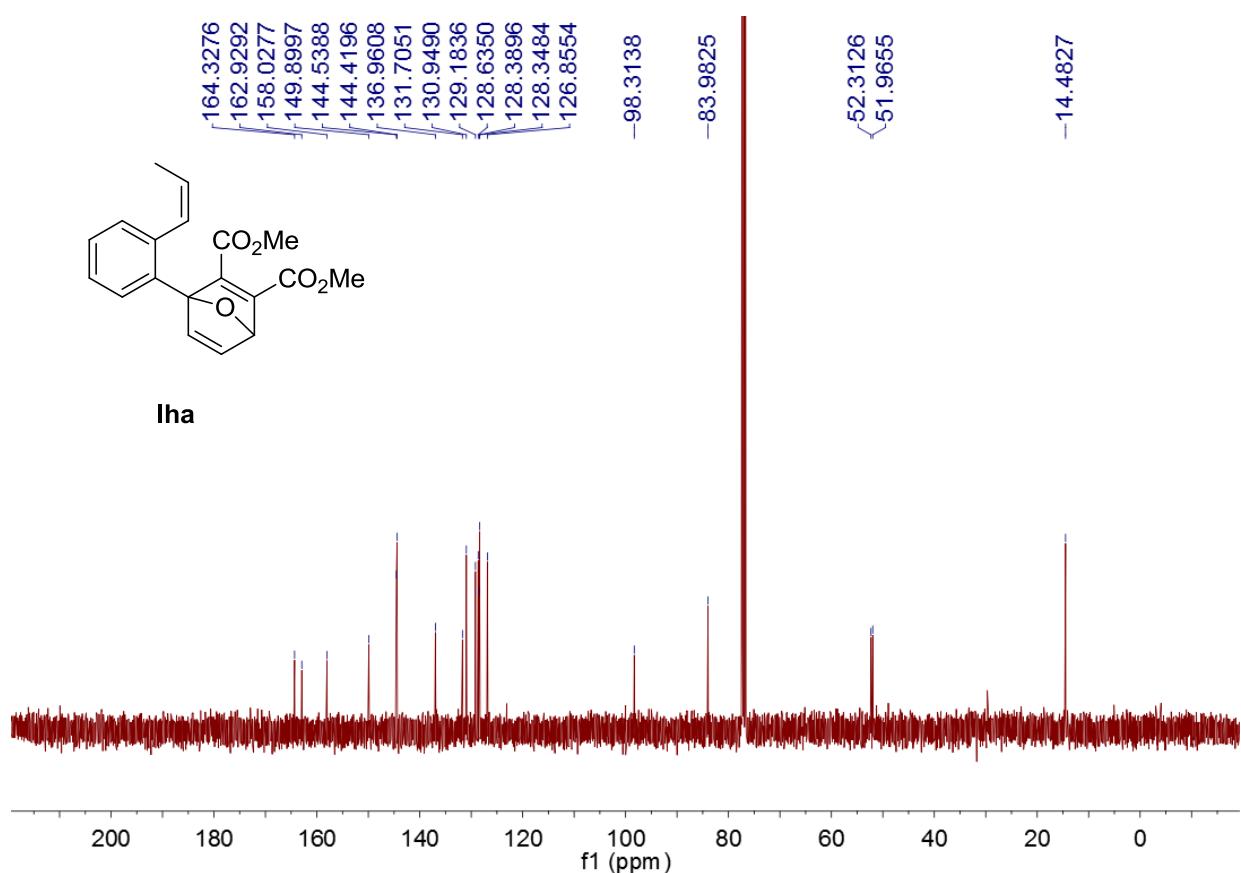
Copies of ^1H , ^{13}C NMR Spectra for **4fa**



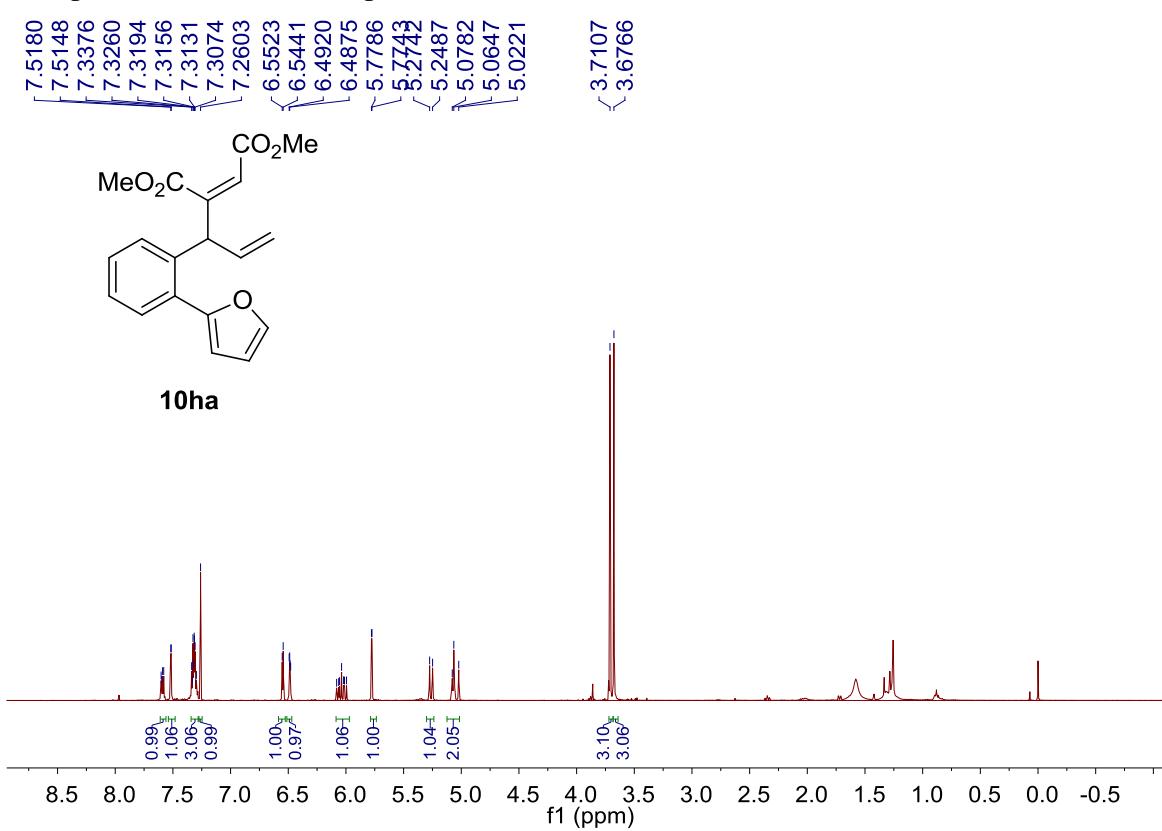


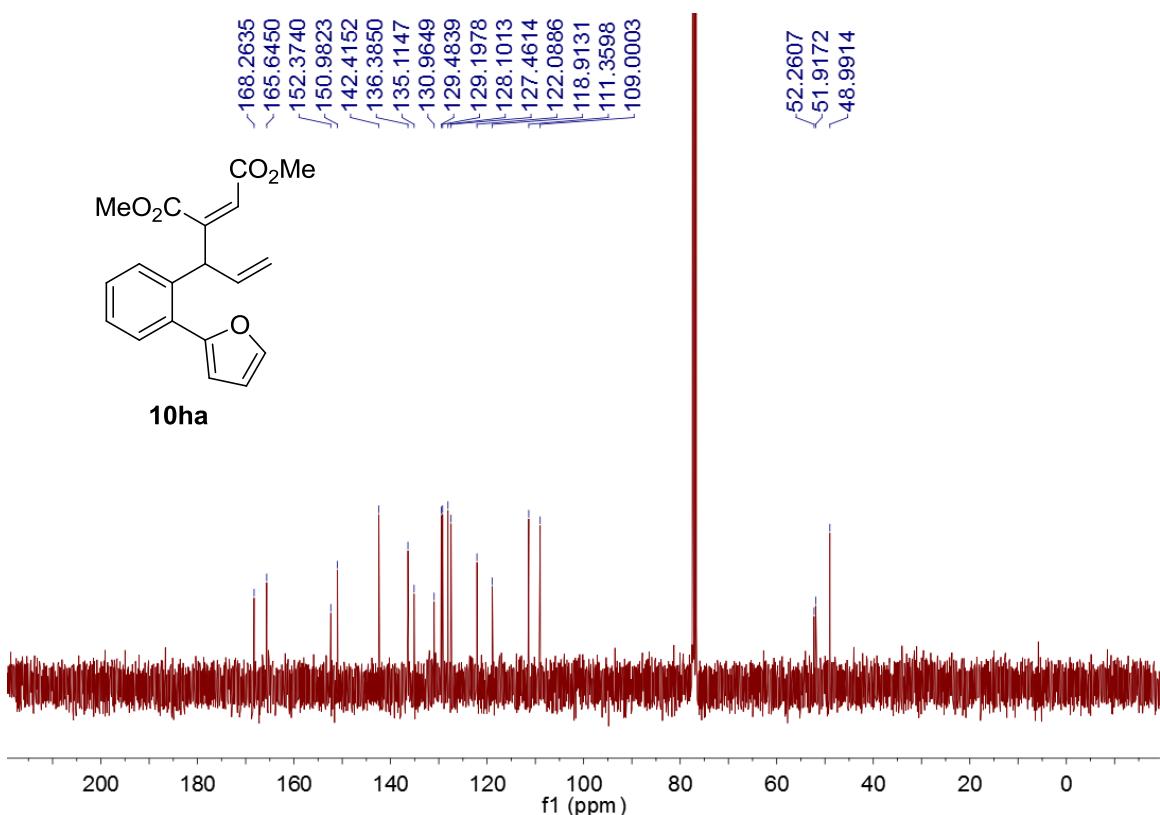
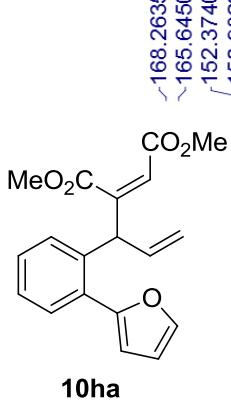
Copies of ^1H , ^{13}C NMR Spectra for **Iha**





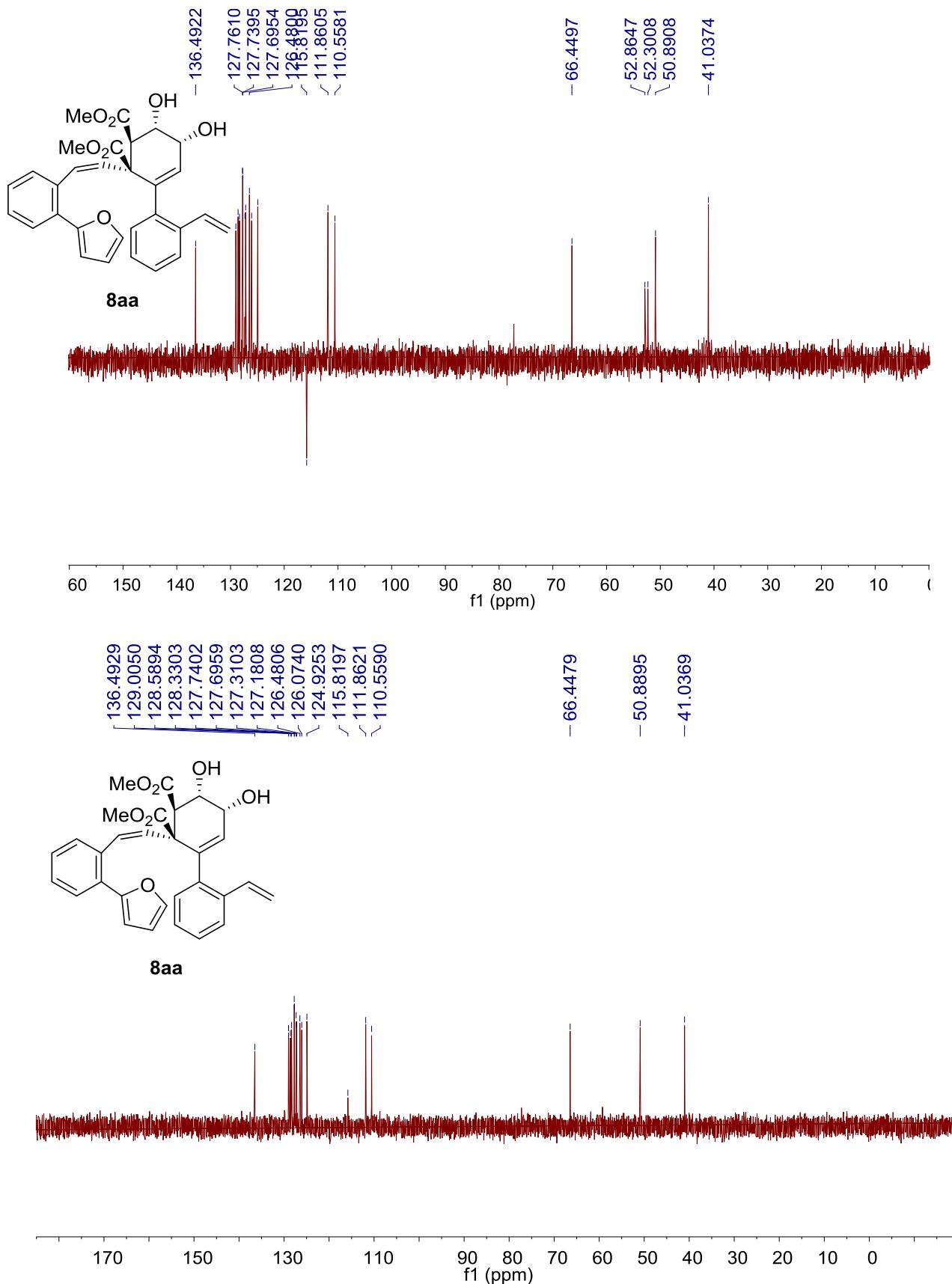
Copies of ^1H , ^{13}C NMR Spectra for **10ha**



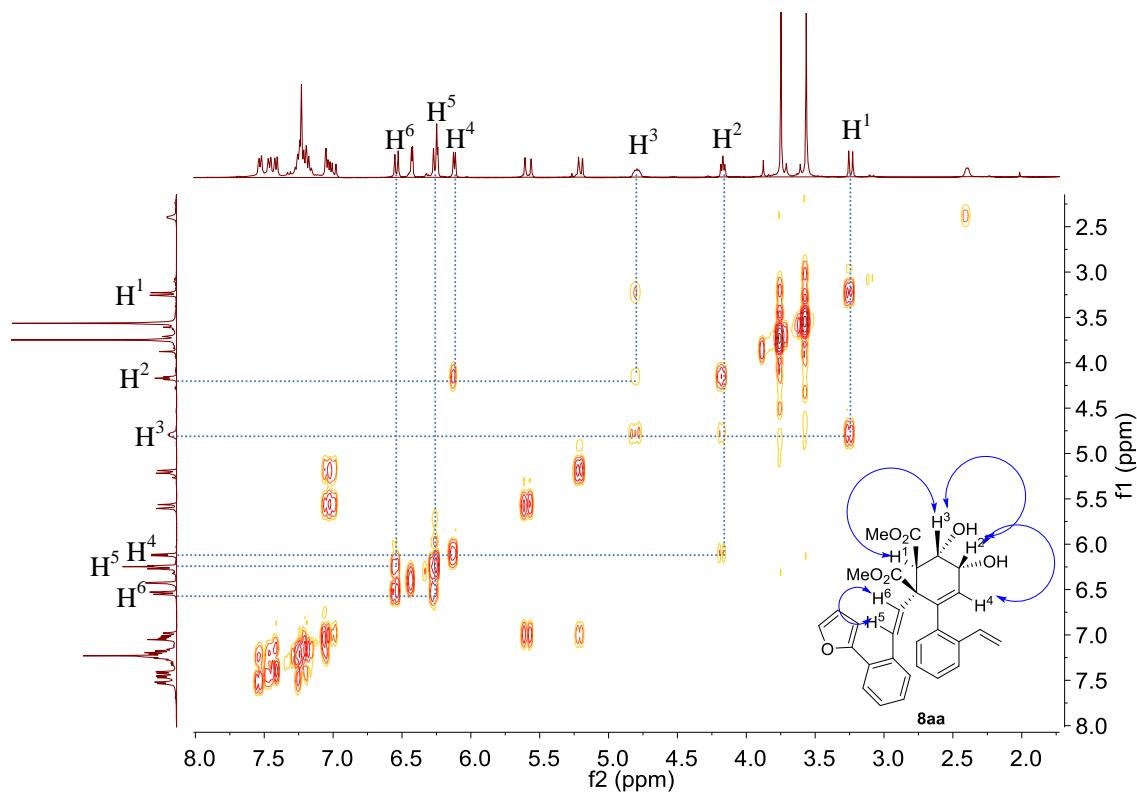


7. ^{13}C DEPT NMR,COSY,HSQC,HMBC and NOE spectra for compound **8aa**

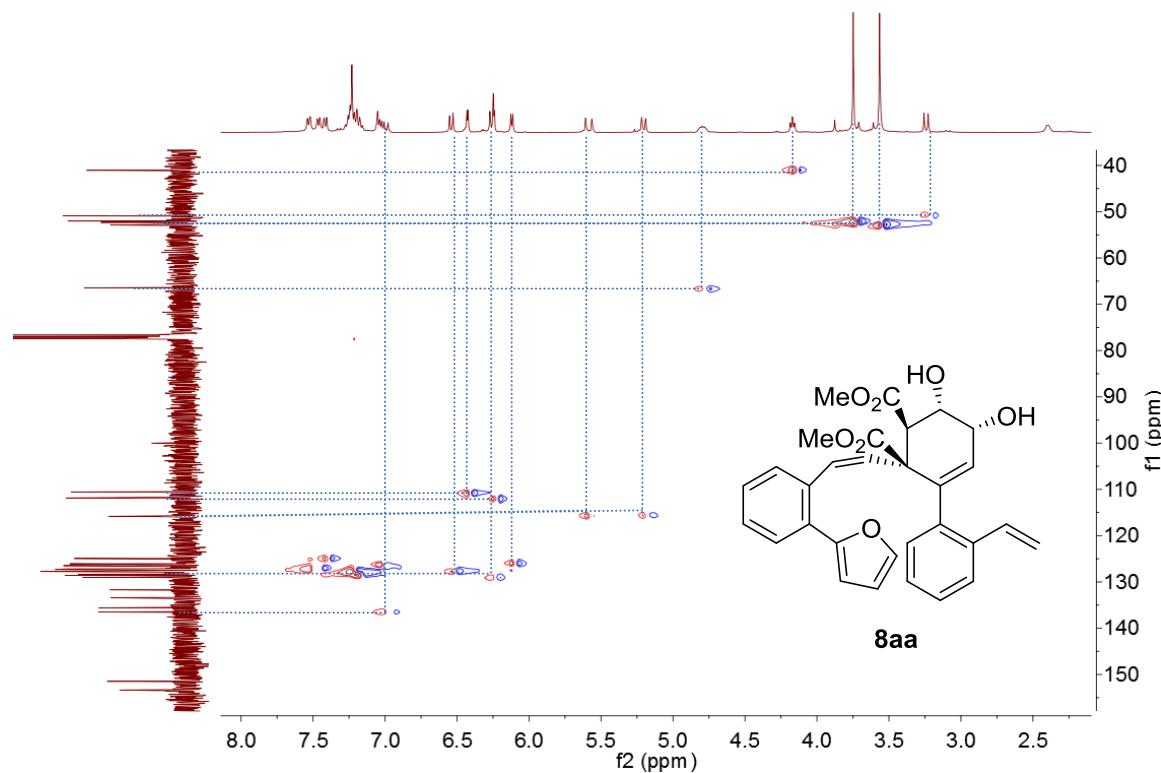
Copies of ^{13}C DEPT-135 and DEPT- 90 NMR Spectra for **8aa**



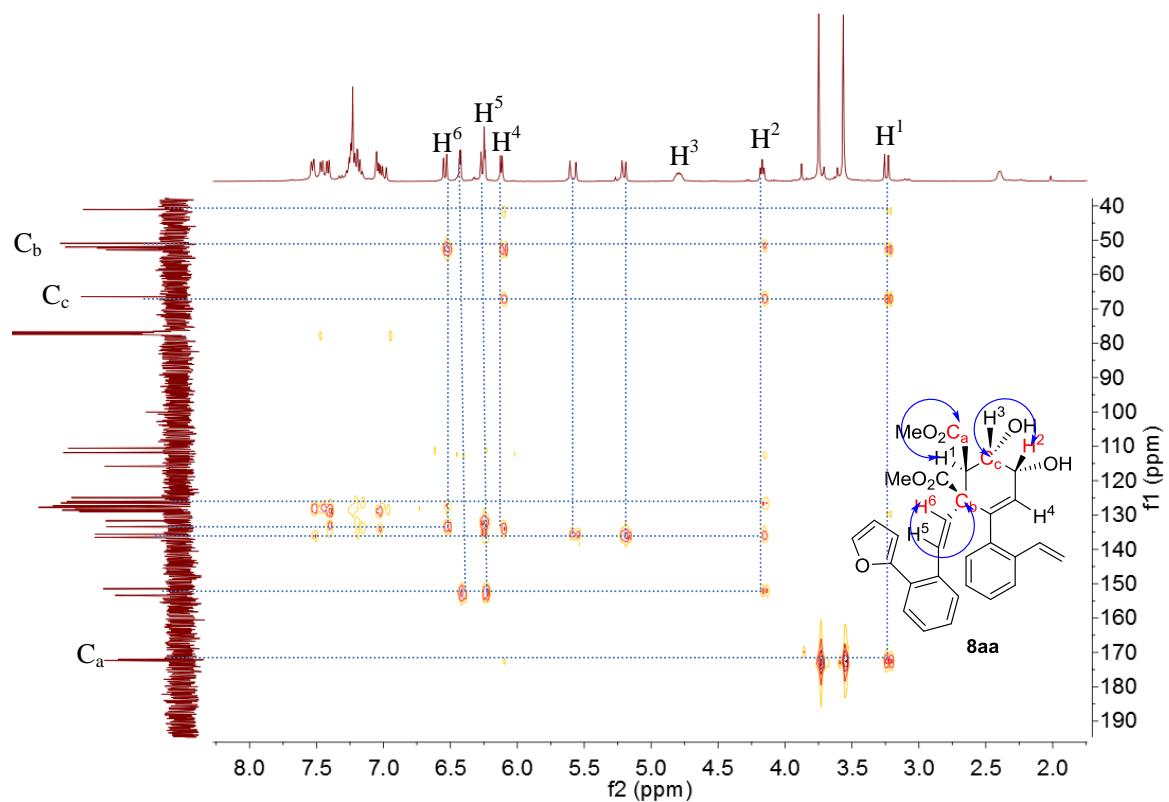
Copy of HSQC NMR Spectra for **8aa**



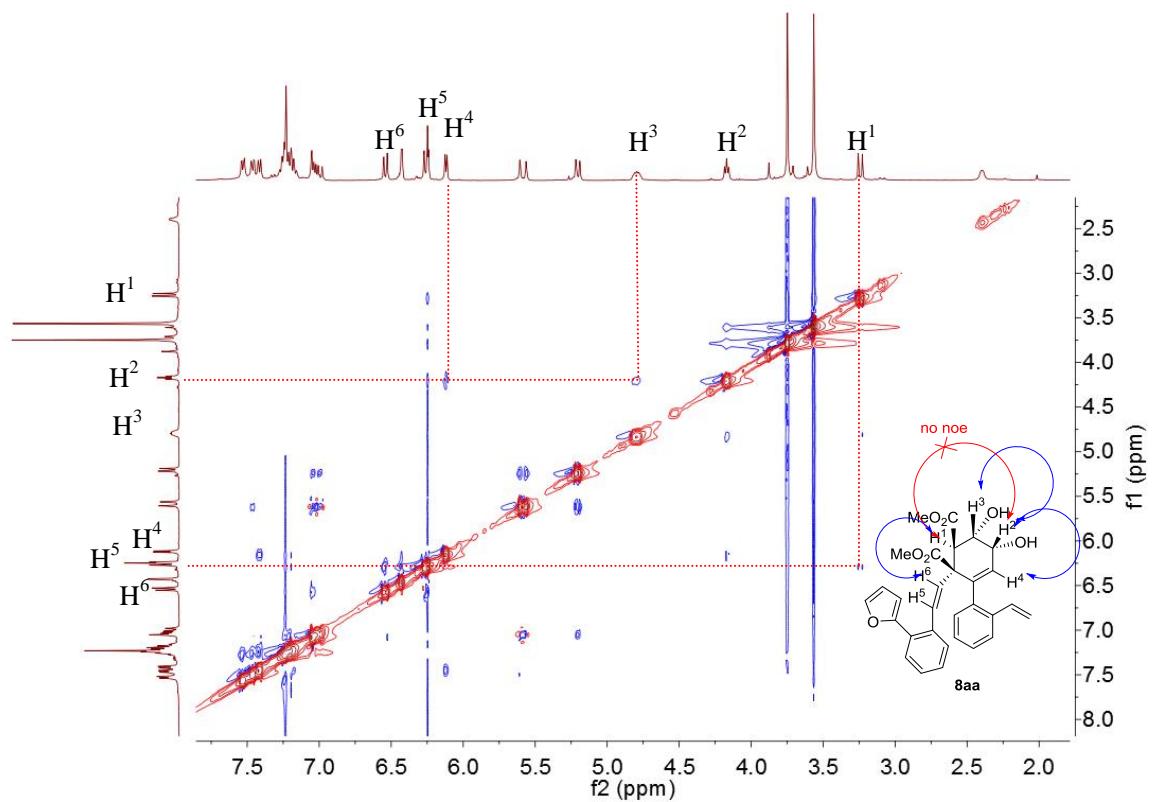
Copy of ^1H - ^{13}C COSY NMR Spectra for **8aa**



Copy of HMBC NMR Spectra for **8aa**

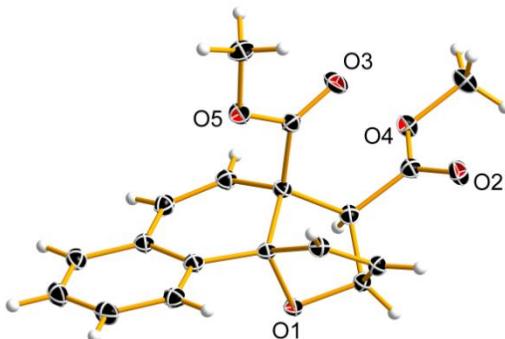


Copy of NOE Spectra for **8aa**



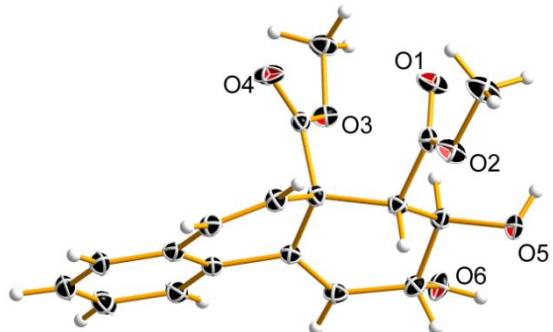
8. Crystal Data for **3aa** and **6aa**

Crystal data and structure refinement for **3aa** (thermal ellipsoid plot at the 30% probability level).



Identification code	zsfhjld
Empirical formula	C ₁₈ H ₁₆ O ₅
Formula weight	312.31
Temperature	293(2) K
Wavelength	1.54178 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 8.1905(3) Å alpha = 90 deg. b = 22.6990(8) Å beta = 108.004(5) deg. c = 8.3591(4) Å gamma = 90 deg.
Volume	1478.00(10) Å ³
Z, Calculated density	4, 1.404 Mg/m ³
Absorption coefficient	0.852 mm ⁻¹
F(000)	656
Crystal size	0.20 x 0.10 x 0.10 mm
Theta range for data collection	3.89 to 62.32 deg.
Limiting indices	-6 ≤ h ≤ 9, -25 ≤ k ≤ 21, -9 ≤ l ≤ 9
Reflections collected / unique	4035 / 2275 [R(int) = 0.0290]
Completeness to theta = 25.25	96.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9196 and 0.8481
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2275 / 0 / 210
Goodness-of-fit on F ²	1.065
Final R indices [I>2sigma(I)]	R1 = 0.0424, wR2 = 0.1335
R indices (all data)	R1 = 0.0477, wR2 = 0.1411
Extinction coefficient	0.0264(13)
Largest diff. peak and hole	0.177 and -0.249 e.Å ⁻³

Crystal data and structure refinement for **6aa** (thermal ellipsoid plot at the 30% probability level).



Identification code	exp17810	
Empirical formula	C ₁₈ H ₁₈ O ₆	
Formula weight	330.32	
Temperature	293(2) K	
Wavelength	1.54178 Å	
Crystal system, space group	Triclinic, P -1	
Unit cell dimensions	a = 7.7687(4) Å	alpha = 78.673(5) deg.
	b = 8.5018(5) Å	beta = 80.463(5) deg.
	c = 13.4014(8) Å	gamma = 63.227(5) deg.
Volume	771.83(8) Å ³	
Z, Calculated density	2, 1.421 Mg/m ³	
Absorption coefficient	0.895 mm ⁻¹	
F(000)	348	
Crystal size	0.20 x 0.10 x 0.10 mm	
Theta range for data collection	3.38 to 61.07 deg.	
Limiting indices	-8<=h<=8, -9<=k<=9, -15<=l<=15	
Reflections collected / unique	11078 / 2365 [R(int) = 0.0375]	
Completeness to theta = 25.25	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9196 and 0.8481	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	2365 / 0 / 221	
Goodness-of-fit on F ²	1.015	
Final R indices [I>2sigma(I)]	R1 = 0.0415, wR2 = 0.1595	
R indices (all data)	R1 = 0.0455, wR2 = 0.1695	
Extinction coefficient	0.0264(13)	
Largest diff. peak and hole	0.224 and -0.233 e.Å ⁻³	

9. PES of Pathway I and II without Corrections of Spin Contamination.

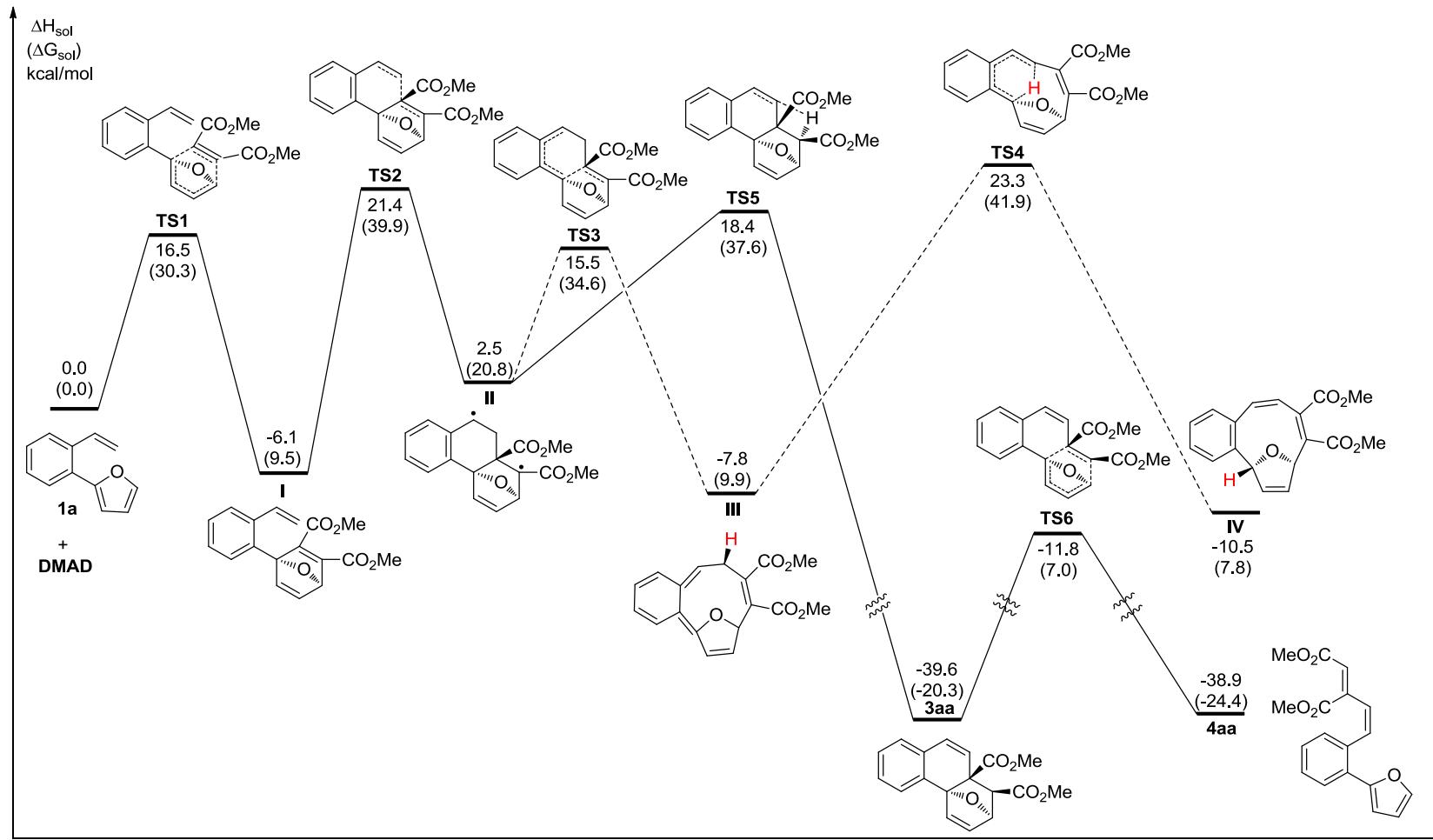


Figure S1. Full Potential Energy Surfaces of Pathways I and II without Corrections of Spin Contamination at the (U)B3LYP level.

10. PES of the Water-assisted [1,3]-H shift in pathway I.

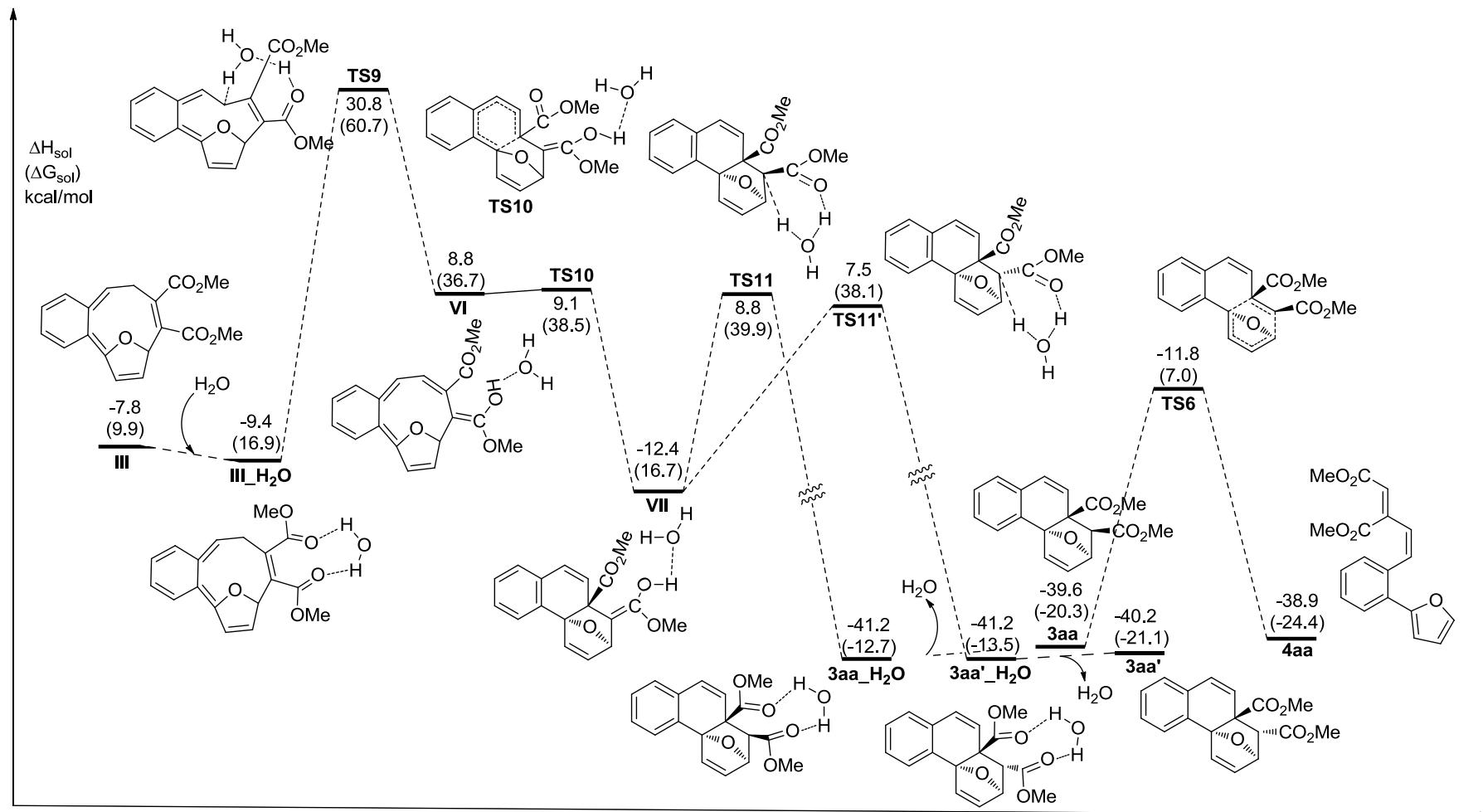
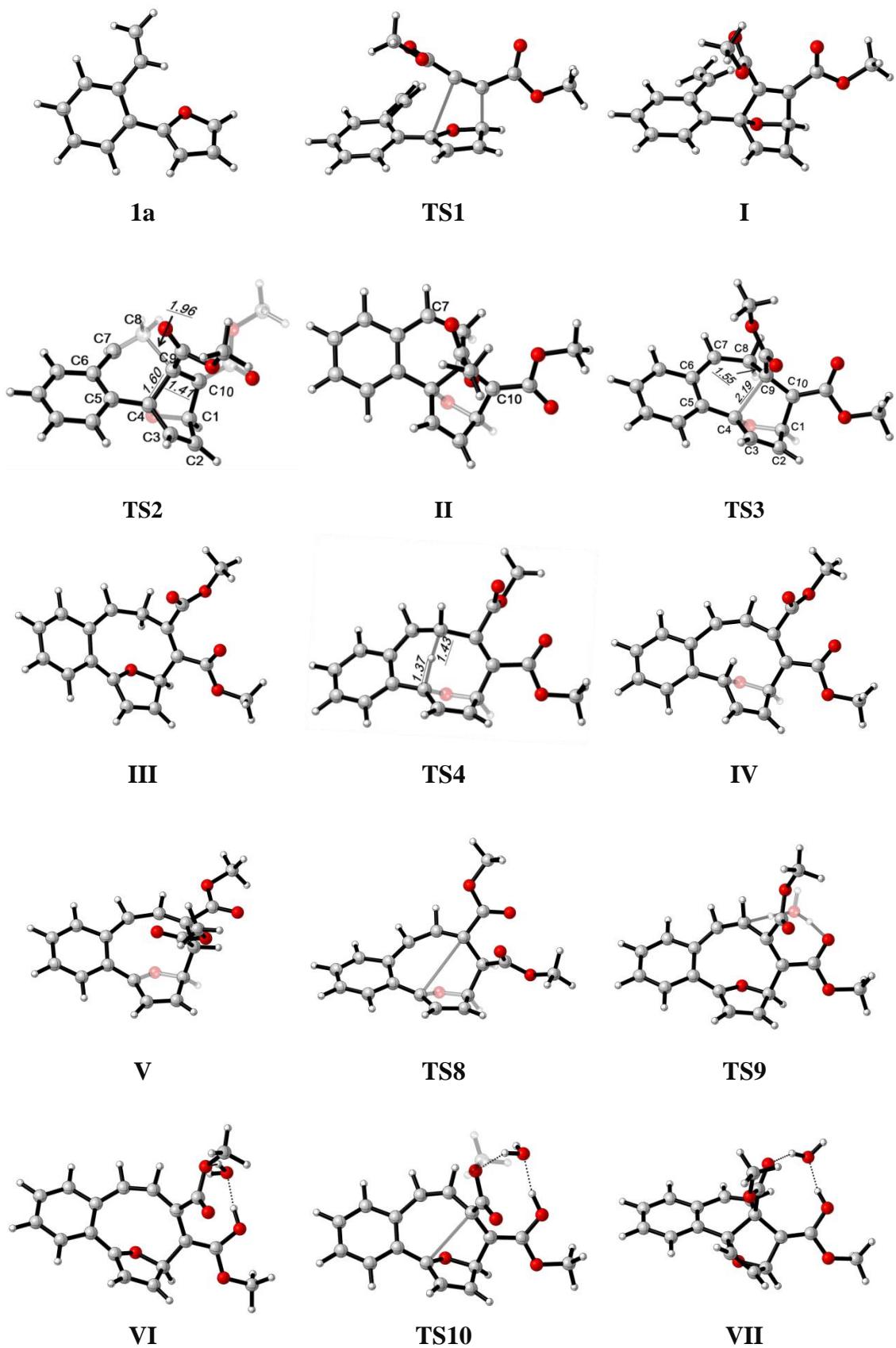


Figure S2. Computed energy profile of water-assisted [1,3]-H shift in pathway I at the B3LYP/6-31+G(d) level in toluene.

11. The Computed Geometries of Stationary Points





TS11



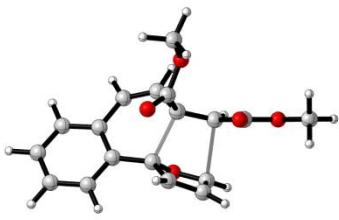
TS11'



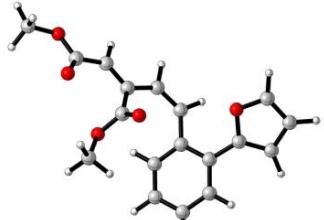
TS5



3aa



TS6

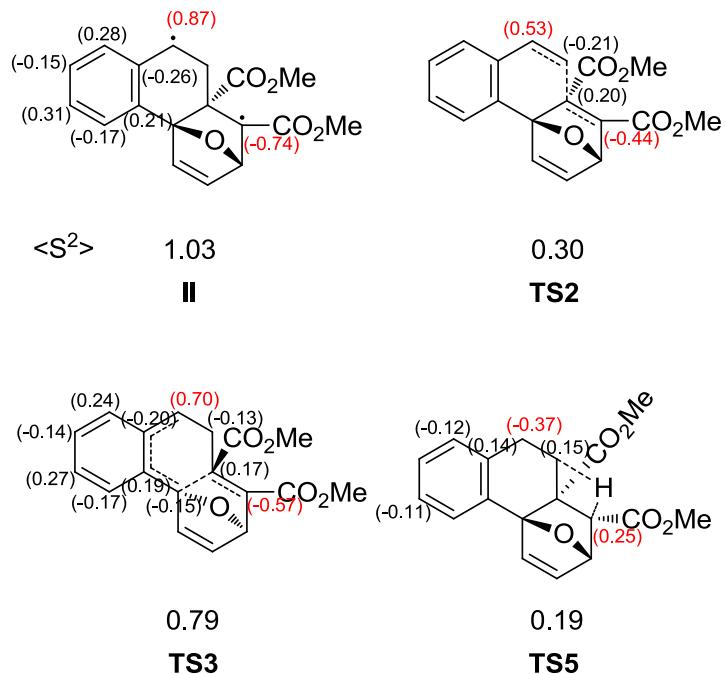


4aa

12. Energies and Other Thermodynamic Parameters

Unit: Hartree	E _{ele}	E _{ele(sol)}	E	H	G
1a	-538.498107	-538.506524	-538.303568	-538.302624	-538.351172
2a	-533.10005	-533.109854	-532.973932	-532.972988	-533.023576
TS1	-1071.564358	-1071.590419	-1071.242483	-1071.241539	-1071.318671
I	-1071.603719	-1071.62894	-1071.279285	-1071.278341	-1071.352588
TS2	-1071.557491	-1071.58236	-1071.235841	-1071.234896	-1071.304503
II	-1071.587973	-1071.614231	-1071.264582	-1071.263638	-1071.3336
TS3	-1071.563034	-1071.591995	-1071.241061	-1071.240116	-1071.308878
III	-1071.606279	-1071.633018	-1071.280545	-1071.2796	-1071.350406
TS4	-1071.551843	-1071.577896	-1071.231634	-1071.230689	-1071.300189
IV	-1071.607583	-1071.637916	-1071.281223	-1071.280279	-1071.35023
V	-1071.610137	-1071.641108	-1071.283772	-1071.282828	-1071.354104
TS8	-1071.604352	-1071.635595	-1071.279271	-1071.278327	-1071.345663
TS5	-1071.556573	-1071.584801	-1071.237267	-1071.236323	-1071.304789
3aa	-1071.657606	-1071.684338	-1071.331189	-1071.330245	-1071.398557
TS6	-1071.617621	-1071.637069	-1071.294143	-1071.293199	-1071.362422
4aa	-1071.663633	-1071.682111	-1071.338218	-1071.337274	-1071.413324
H₂O	-76.422572	-76.433282	-76.398639	-76.397694	-76.419134
III_H₂O	-1148.04061	-1148.071545	-1147.687186	-1147.686242	-1147.764971
TS9	-1147.971495	-1147.999857	-1147.62568	-1147.624735	-1147.697686
VI	-1148.013988	-1148.041889	-1147.661298	-1147.660354	-1147.736404
TS10	-1148.011193	-1148.039948	-1147.659944	-1147.659	-1147.732662
VII	-1148.049187	-1148.076371	-1147.695748	-1147.694804	-1147.769081
TS11	-1148.008489	-1148.034772	-1147.662821	-1147.661877	-1147.732916
3aa_H₂O	-1148.092201	-1148.123007	-1147.737976	-1147.737032	-1147.812227
TS11'	-1148.011141	-1148.036913	-1147.665481	-1147.664537	-1147.736274
3aa'_H₂O	-1148.090246	-1148.122856	-1147.736191	-1147.735247	-1147.811761
3aa'	-1071.657187	-1071.685175	-1071.330869	-1071.329925	-1071.398546

13. The Computed Spin Distributions of the Diradical Species



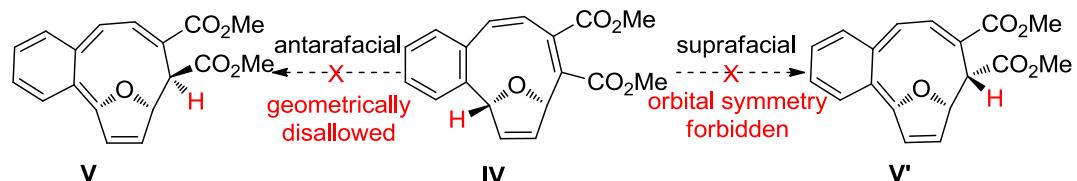
Singlet and triplet diradical energies and the spin correction energies using Yamaguchi-Houk method

	II	TS2	TS3	TS5
$E_{ele}(\text{Singlet})$	-1071.587973	-1071.557491	-1071.563034	-1071.556573
$E_{ele}(\text{Triplet})$	-1071.588046	-1071.532047	-1071.555007	-1071.527237
Spin-correction energy(kcal/mol)	0.05	-2.82	-3.29	-1.90

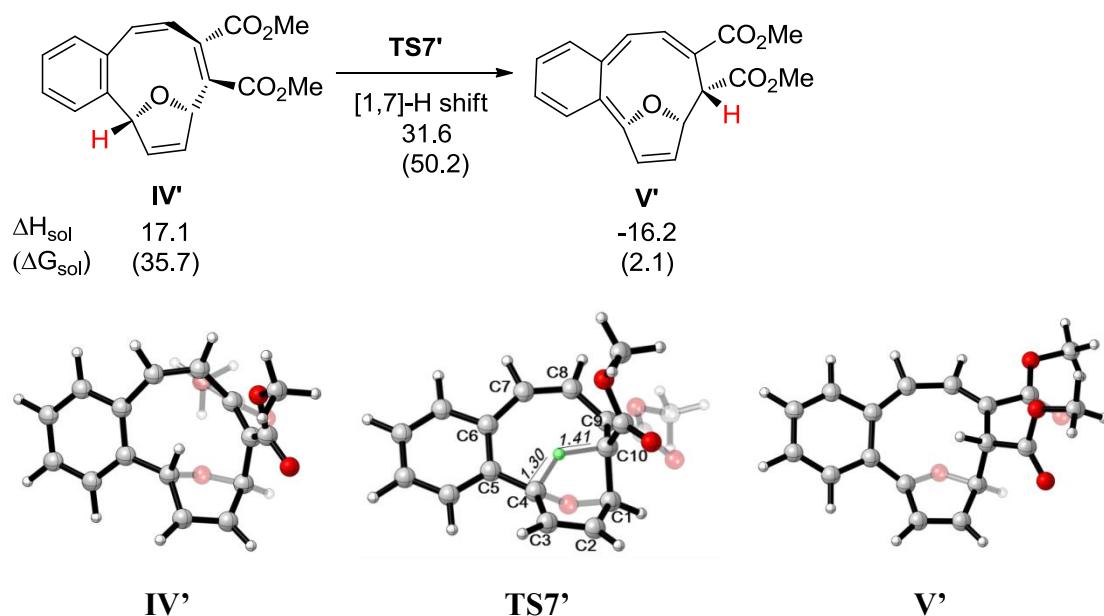
14. Studies About [1,7]-H Shifts.

An antarafacial [1,7]-H shift is not allowed geometrically from **IV** to **V**, while a suprafacial one is forbidden according to the theory of conservation of orbital symmetry. However, **IV'**, the stereoisomer of **IV**, which has the two ester groups in a trans configuration can have a antarafacial [1,7]-H shift (see Scheme S4). But **IV'** cannot be reached from the reaction of **1a** and **2a** (see pathway I).

Scheme S3. Conversion from **IV** to **V** (or **V'**)



Scheme S4. [1,7]-H Shift from **IV'** to **V'** (ΔH_{sol} or ΔG_{sol} are given relative to the initial state: **1a** and **2a**)



15. Cartesian Coordinates of All Computed Structures

1a

C	1.200579	-0.394415	0.046760
C	3.131115	0.554095	-0.459902
C	-0.259239	-0.537551	0.009009
C	-1.155157	0.558023	0.133769
C	-2.536660	0.294296	0.082795
C	-3.035080	-0.995031	-0.085220
C	-2.149183	-2.070901	-0.198779
C	-0.777590	-1.836059	-0.156376
H	-0.084348	-2.663715	-0.278186
H	-2.523218	-3.083026	-0.328570
H	-4.108889	-1.161470	-0.112811
H	-3.230129	1.119359	0.217279
O	1.780110	0.672972	-0.597908
C	2.188523	-1.179491	0.586588
C	-0.670961	1.931492	0.377228
C	-1.312627	3.061983	0.045949
H	0.295148	2.014581	0.868912
H	-0.891891	4.033087	0.291072
H	-2.257035	3.064811	-0.493291
C	3.438554	-0.562968	0.258786
H	3.719042	1.331840	-0.923679
H	4.429404	-0.903165	0.527913
H	2.037387	-2.076917	1.170992

2a

C	-0.602633	0.187904	-0.061332
C	0.602635	0.188138	0.061262
H	-4.401493	-0.908589	-0.626886
C	2.034511	0.248281	0.278934
O	2.557443	0.983634	1.091035
O	2.686359	-0.606456	-0.526940
C	4.124435	-0.621355	-0.388814
H	4.534216	0.365550	-0.617457
H	4.401590	-0.906984	0.628907
H	4.469209	-1.362531	-1.109183
O	-2.557183	0.980725	-1.093659
O	-2.686517	-0.605018	0.528543
H	-4.534364	0.367285	0.616033
C	-2.034461	0.247551	-0.279455
C	-4.124562	-0.620242	0.390129
H	-4.469524	-1.359474	1.112402

3aa

C	-0.199861	0.737416	0.607842
C	1.094953	0.784065	-0.337801
O	1.189979	0.646603	2.541370
H	-1.369057	2.591539	0.541062
C	-1.133337	1.771665	-0.143158
H	-0.722595	2.586843	-2.195718
C	1.952897	-0.449150	-0.367132
C	1.378214	-1.693460	-0.035095
C	-0.006398	-1.755843	0.432807
H	-0.439777	-2.745370	0.567663
C	-0.744481	-0.671874	0.718740
H	-1.754545	-0.778855	1.102870
O	0.461048	0.971404	-1.622111
C	-2.461376	1.235817	-0.657634
O	-3.312765	0.982848	0.363107
O	-2.766760	1.101959	-1.823805
C	-4.622130	0.512198	-0.010610
H	-5.125937	1.251220	-0.639153
H	-5.157815	0.375640	0.929222
C	0.078490	1.222329	2.041150
O	-0.613256	1.995704	2.670962
H	-4.546126	-0.432540	-0.555958
C	1.735227	2.157742	-0.116534
C	1.518020	0.977250	3.904617
H	0.712430	0.663738	4.573893
H	1.676088	2.054130	4.008010
H	2.434797	0.428118	4.120191
C	3.274033	-0.392164	-0.811072
H	3.703830	0.566372	-1.090077
C	2.154782	-2.856678	-0.150469
C	4.042337	-1.556351	-0.915954
H	5.071011	-1.497943	-1.261813
C	3.479506	-2.791315	-0.584294
H	4.068860	-3.700951	-0.667031
H	1.712851	-3.817519	0.104843
H	0.977416	4.118298	-0.709856
H	2.604373	2.347659	0.501892
C	0.926086	3.035013	-0.719491
C	-0.203976	2.207020	-1.317799

3aa'

C	-0.199861	0.737416	0.607842
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C	1.094953	0.784065	-0.337801
O	1.189979	0.646603	2.541370
H	-1.369057	2.591539	0.541062
C	-1.133337	1.771665	-0.143158
H	-0.722595	2.586843	-2.195718
C	1.952897	-0.449150	-0.367132
C	1.378214	-1.693460	-0.035095
C	-0.006398	-1.755843	0.432807
H	-0.439777	-2.745370	0.567663
C	-0.744481	-0.671874	0.718740
H	-1.754545	-0.778855	1.102870
O	0.461048	0.971404	-1.622111
C	-2.461376	1.235817	-0.657634
O	-3.312765	0.982848	0.363107
O	-2.766760	1.101959	-1.823805
C	-4.622130	0.512198	-0.010610
H	-5.125937	1.251220	-0.639153
H	-5.157815	0.375640	0.929222
C	0.078490	1.222329	2.041150
O	-0.613256	1.995704	2.670962
H	-4.546126	-0.432540	-0.555958
C	1.735227	2.157742	-0.116534
C	1.518020	0.977250	3.904617
H	0.712430	0.663738	4.573893
H	1.676088	2.054130	4.008010
H	2.434797	0.428118	4.120191
C	3.274033	-0.392164	-0.811072
H	3.703830	0.566372	-1.090077
C	2.154782	-2.856678	-0.150469
C	4.042337	-1.556351	-0.915954
H	5.071011	-1.497943	-1.261813
C	3.479506	-2.791315	-0.584294
H	4.068860	-3.700951	-0.667031
H	1.712851	-3.817519	0.104843
H	0.977416	4.118298	-0.709856
H	2.604373	2.347659	0.501892
C	0.926086	3.035013	-0.719491
C	-0.203976	2.207020	-1.317799

3aa_H2O

C	0.055755	-0.051467	-0.568472
C	-1.017736	-0.718909	0.408478
C	-0.550250	0.219624	-1.933181
O	-0.875925	-2.109265	-0.000129

C	0.502057	-2.256341	0.351895
C	0.537723	-1.705300	1.766917
C	-0.406570	-0.760543	1.805612
H	0.837543	-3.280916	0.187209
C	-2.441434	-0.272785	0.225943
C	-2.852511	0.205090	-1.036346
C	-1.873717	0.346697	-2.116050
H	-2.256790	0.580226	-3.107822
H	0.141597	0.369135	-2.758012
C	1.137314	-1.206970	-0.643624
C	2.574060	-0.858981	-0.322331
O	3.396786	-1.219799	-1.324765
O	2.977393	-0.369009	0.718254
C	4.803152	-0.974019	-1.115146
H	4.980639	0.093821	-0.965867
H	5.293112	-1.325888	-2.022940
C	0.574980	1.298384	-0.058584
O	0.150682	1.887771	0.916603
H	5.158335	-1.527141	-0.242033
O	1.523245	1.794209	-0.872566
C	2.065949	3.088214	-0.516935
H	1.263689	3.829030	-0.474709
H	2.770274	3.327471	-1.313890
H	2.572121	3.028206	0.449604
C	-3.375888	-0.407291	1.252913
H	-3.059365	-0.794642	2.217415
C	-4.199990	0.542385	-1.234300
C	-4.715021	-0.059502	1.048661
H	-5.431575	-0.164995	1.858811
C	-5.126825	0.415643	-0.198741
H	-6.166619	0.684801	-0.365507
H	-4.518346	0.909925	-2.207539
H	1.111506	-1.641465	-1.644345
H	-0.634738	-0.066767	2.603264
H	1.258366	-1.968137	2.531259
O	2.590481	1.757457	2.781241
H	2.762066	0.968245	2.238052
H	1.670590	1.984615	2.567691

3aa' _H2O

C	-0.188714	0.654089	0.629932
C	1.100887	0.757160	-0.318027
O	1.248188	0.570845	2.526867
H	-1.405712	2.492761	0.609495

C	-1.149025	1.690569	-0.087141
H	-0.761728	2.571013	-2.118982
C	1.983873	-0.456649	-0.385521
C	1.435734	-1.721983	-0.090176
C	0.054119	-1.827932	0.378882
H	-0.358551	-2.829813	0.483380
C	-0.706993	-0.769419	0.698105
H	-1.713713	-0.910087	1.081655
O	0.457757	0.966409	-1.592940
C	-2.454703	1.119388	-0.620329
O	-3.346085	0.900580	0.385041
O	-2.719140	0.915026	-1.783314
C	-4.628212	0.366685	-0.016274
H	-5.129854	1.061888	-0.693562
H	-5.193600	0.250502	0.908600
C	0.088822	1.079410	2.079961
O	-0.649663	1.752847	2.774832
H	-4.494246	-0.596026	-0.515533
C	1.710370	2.138388	-0.058598
C	1.578485	0.839459	3.905504
H	0.812203	0.422993	4.564126
H	1.657179	1.916638	4.073125
H	2.538013	0.349153	4.069108
C	3.302033	-0.358802	-0.830756
H	3.711536	0.616269	-1.081373
C	2.234843	-2.865298	-0.243575
C	4.093132	-1.503601	-0.973081
H	5.119253	-1.413775	-1.319588
C	3.556617	-2.759409	-0.678414
H	4.163970	-3.653737	-0.791190
H	1.813283	-3.842380	-0.017440
H	0.905853	4.097532	-0.595408
H	2.578627	2.330239	0.560173
C	0.879548	3.014100	-0.633961
C	-0.232167	2.177687	-1.253550
O	-3.374993	2.945484	2.633229
H	-2.483392	2.715296	2.945759
H	-3.537408	2.284125	1.940744

4aa

C	3.500487	-0.717034	-0.115633
C	-1.545660	-0.579206	0.543928
C	3.657695	-2.834239	-0.722583
C	-2.784098	-1.080738	0.782380

C	-0.408876	-1.122128	1.285485
C	4.937797	-2.367050	-0.655885
C	4.838570	-0.996040	-0.262336
H	3.220522	-3.787847	-0.977582
C	2.786017	0.510975	0.232951
C	1.518180	0.519050	0.876590
C	0.882863	-0.722958	1.350532
H	1.554705	-1.405791	1.868747
H	-0.650989	-2.033249	1.830793
O	2.776240	-1.849779	-0.395805
C	-4.001847	-0.734291	0.028304
O	-5.093815	-1.277781	0.626793
O	-4.065278	-0.079274	-0.997449
C	-6.350578	-1.031580	-0.025946
H	-6.337165	-1.433312	-1.042978
H	-6.555691	0.041877	-0.066184
C	-1.325405	0.402476	-0.586665
O	-0.752913	0.106059	-1.612261
H	-7.097140	-1.543813	0.581878
O	-1.825998	1.616046	-0.307530
C	-1.777027	2.570785	-1.385436
H	-0.741946	2.750310	-1.687507
H	-2.227896	3.479180	-0.984801
H	-2.353654	2.194127	-2.233821
C	3.394320	1.738195	-0.087544
H	4.343231	1.731855	-0.616103
C	0.930856	1.757692	1.190849
C	2.793854	2.953156	0.233123
H	3.289797	3.885423	-0.024186
C	1.553601	2.964368	0.876532
H	1.078228	3.904680	1.142894
H	-0.013873	1.765304	1.724438
H	-2.914354	-1.820742	1.567397
H	5.656012	-0.310136	-0.087032
H	5.839826	-2.928625	-0.857815

I

C	0.619899	0.291108	0.057536
C	-0.446778	-0.531018	0.887118
C	1.752717	-0.419580	0.135237
C	1.390246	-1.650493	1.008112
C	-1.906428	-0.326130	0.550078
C	-2.460538	-0.769514	-0.680477
C	-3.828073	-0.532464	-0.914863

C	-4.638957	0.108235	0.018644
C	-4.088101	0.545496	1.223148
C	-2.733840	0.325007	1.475911
H	-2.322790	0.670525	2.417690
H	-4.700688	1.056643	1.961006
H	-5.689651	0.278918	-0.201895
H	-4.248986	-0.833401	-1.869523
H	-0.954784	3.917370	-0.702903
C	3.086797	-0.035628	-0.349865
O	3.354359	0.995728	-0.937459
O	4.006623	-0.985239	-0.044763
C	5.354829	-0.708049	-0.468203
H	5.395377	-0.600438	-1.555268
H	5.718233	0.210850	-0.000369
H	5.941763	-1.567034	-0.142091
O	0.031872	-1.861875	0.585049
C	0.028035	-0.419084	2.368718
C	-1.659990	-1.441609	-1.727738
C	-2.128200	-2.369712	-2.573910
H	-0.618451	-1.148352	-1.810622
H	-1.486904	-2.799041	-3.338500
H	-3.145524	-2.750873	-2.522071
C	1.155132	-1.127036	2.439815
O	0.134612	1.732333	-1.785578
O	0.307813	2.591522	0.306032
H	1.994699	-2.544772	0.876357
H	0.794373	4.193621	-0.940328
C	0.347789	1.596605	-0.600669
C	0.025237	3.906878	-0.219152
H	0.038702	4.568993	0.646640
H	1.825708	-1.265754	3.279009
H	-0.441972	0.174929	3.139971

II

C	2.213431	0.385866	-0.017731
C	3.266107	0.961719	0.691232
C	4.581911	0.511994	0.530796
C	4.849405	-0.546875	-0.353269
C	3.819550	-1.130765	-1.072606
C	2.474084	-0.675519	-0.943862
H	3.060573	1.781156	1.375339
H	5.388062	0.978078	1.090366
H	5.867569	-0.908016	-0.475632
H	4.027276	-1.947569	-1.760022

C	1.437051	-1.249050	-1.703732
H	1.670493	-2.072126	-2.374318
C	0.028768	-0.750380	-1.661741
C	0.812108	0.883071	0.171818
C	0.420708	1.485679	1.524048
C	-0.598732	2.319977	1.289718
H	0.840307	1.185737	2.476521
C	-0.850334	2.228257	-0.213442
H	-1.226459	2.848745	1.997243
H	-1.333522	3.062822	-0.717151
O	0.475710	1.981953	-0.721322
C	-0.357251	-0.145046	-0.280584
C	-1.478868	0.858378	-0.400600
C	-0.605537	-1.286304	0.711310
C	-2.884074	0.643531	-0.635430
O	-1.305582	-0.889346	1.794225
O	-3.192703	-0.667991	-0.837232
O	-0.212668	-2.424360	0.558912
O	-3.722236	1.541547	-0.658865
C	-1.574962	-1.908894	2.775402
H	-0.639670	-2.312458	3.172561
H	-2.156884	-2.719165	2.328491
H	-2.145186	-1.409545	3.559243
C	-4.580767	-0.952604	-1.079418
H	-5.188640	-0.648158	-0.222612
H	-4.633071	-2.032143	-1.224955
H	-4.929296	-0.425415	-1.972015
H	-0.673177	-1.551292	-1.911437
H	-0.104137	0.036711	-2.418826

III

C	-0.839815	0.772012	0.518935
C	1.591282	-1.501466	0.335092
C	0.252224	1.313093	1.460634
O	0.777925	-1.214499	1.402372
C	-0.539701	-1.684586	1.081417
C	-0.253393	-2.788815	0.079848
C	1.017299	-2.645671	-0.348502
H	-1.016310	-2.023959	2.006929
C	2.600292	-0.639884	-0.021675
C	2.663683	0.768850	0.444359
C	1.674428	1.549003	0.995244
H	1.984820	2.578203	1.167057
H	0.266351	0.676986	2.349365

H	-0.123616	2.290141	1.789760
C	-1.293626	-0.497264	0.444908
C	-2.558205	-0.789954	-0.286111
O	-3.078127	-1.983456	0.099884
O	-3.102614	-0.068662	-1.099157
C	-4.328031	-2.350657	-0.515238
H	-4.588582	-3.317466	-0.083598
H	-4.209457	-2.427475	-1.599266
C	-1.473871	1.878898	-0.284964
O	-0.994578	2.300344	-1.314964
H	-5.094835	-1.605837	-0.287351
O	-2.531158	2.420707	0.348956
C	-3.201464	3.485798	-0.355020
H	-2.511065	4.311526	-0.546432
H	-4.010161	3.801705	0.304514
H	-3.596747	3.109434	-1.301908
C	3.628972	-1.115149	-0.926164
H	3.531387	-2.119085	-1.330077
C	3.923538	1.459230	0.154764
C	4.731274	-0.376520	-1.217422
H	5.501958	-0.774396	-1.871907
C	4.895980	0.930371	-0.629172
H	5.801770	1.496597	-0.830765
H	4.046894	2.457066	0.569059
H	-0.998159	-3.484992	-0.279420
H	1.498985	-3.207654	-1.138275

III_H2O

C	-0.650586	-0.511713	-0.842237
C	1.918055	1.502454	-0.164967
C	0.477009	-1.019813	-1.761150
O	1.184712	1.423915	-1.322721
C	-0.115934	1.962006	-1.048447
C	0.160414	2.903083	0.110031
C	1.372575	2.597138	0.616195
H	-0.482722	2.452004	-1.956171
C	2.823269	0.518842	0.151558
C	2.820805	-0.820044	-0.491556
C	1.828985	-1.435760	-1.218473
H	2.073718	-2.458670	-1.499067
H	0.617615	-0.278232	-2.551446
H	0.059747	-1.910300	-2.247876
C	-1.010146	0.772699	-0.632813
C	-2.301034	1.087868	0.036994

O	-2.715111	2.338064	-0.266307
O	-2.948272	0.338462	0.748042
C	-3.976779	2.745425	0.303894
H	-4.140410	3.760140	-0.059095
H	-3.922148	2.725692	1.395272
C	-1.433869	-1.656314	-0.252116
O	-1.082164	-2.236007	0.756649
H	-4.774842	2.079395	-0.032795
O	-2.455169	-2.027663	-1.035884
C	-3.239153	-3.156613	-0.576866
H	-2.603841	-4.042225	-0.492015
H	-4.001218	-3.299656	-1.342887
H	-3.690704	-2.927247	0.391106
C	3.801592	0.785802	1.187931
H	3.745592	1.735664	1.712332
C	3.993190	-1.648920	-0.197961
C	4.814413	-0.076616	1.462834
H	5.552927	0.167704	2.221369
C	4.930118	-1.308898	0.721901
H	5.768890	-1.972311	0.916466
H	4.076197	-2.593392	-0.730339
H	-0.557530	3.613042	0.496447
H	1.822273	3.012063	1.509010
O	-3.357480	-1.862448	2.751852
H	-3.335891	-1.036530	2.239472
H	-2.497324	-2.265478	2.548668

IV

C	-0.889301	0.833143	0.097458
C	1.420416	-1.108243	-0.462534
C	0.320761	1.598114	0.526879
O	0.862126	-1.089633	0.863555
C	-0.441184	-1.611213	0.698334
C	-0.216539	-2.700799	-0.362598
C	0.933680	-2.440472	-0.995680
H	-0.791748	-2.006519	1.657079
C	2.804083	-0.580694	-0.319120
C	2.848933	0.740384	0.196565
C	1.688769	1.585154	0.559113
H	2.057156	2.532747	0.952846
H	0.899334	-0.358871	-1.084730
H	-0.041448	2.572016	0.862431
C	-1.323923	-0.456026	0.218543
C	-2.742312	-0.776096	-0.101907

O	-3.044782	-2.050726	0.257001
O	-3.568293	-0.025951	-0.589752
C	-4.404922	-2.459971	0.024465
H	-4.457182	-3.493947	0.367036
H	-4.646244	-2.390360	-1.039478
C	-1.829571	1.850303	-0.542852
O	-1.794204	2.120161	-1.723466
H	-5.093560	-1.829204	0.592853
O	-2.568227	2.500649	0.373676
C	-3.494554	3.473259	-0.149943
H	-2.961303	4.248319	-0.706906
H	-3.992115	3.895932	0.723352
H	-4.214337	2.976866	-0.805665
C	3.969385	-1.272462	-0.628160
H	3.903745	-2.288179	-1.009792
C	4.120839	1.316404	0.384446
C	5.220231	-0.671483	-0.442054
H	6.127916	-1.216738	-0.686835
C	5.291755	0.625587	0.067888
H	6.256787	1.101489	0.220553
H	4.190826	2.326781	0.781205
H	-0.912108	-3.507465	-0.557039
H	1.356400	-2.979234	-1.836759

V

C	-0.982457	1.193615	1.256557
C	1.197973	0.728116	-1.584376
O	-2.470840	0.554697	3.030690
H	-1.462778	3.096901	0.419738
C	-0.671471	2.355758	0.297914
H	-1.732979	1.743606	-1.487101
C	2.143601	-0.132614	-1.067326
C	1.844093	-0.917587	0.138446
C	0.801855	-0.812223	1.080454
H	0.906978	-1.610161	1.814886
C	-0.326787	-0.006588	1.480951
H	-0.809186	-0.520574	2.308098
O	-0.073029	0.581722	-1.171677
C	0.641087	3.042515	0.694749
O	0.455264	4.367748	0.887984
O	1.714737	2.494541	0.831893
C	1.616680	5.112498	1.303763
H	1.999898	4.718696	2.248714
H	1.271681	6.139686	1.424442

C	-2.142699	1.516224	2.125398
O	-2.787920	2.558247	2.053637
H	2.400384	5.052273	0.543581
C	1.286758	1.945069	-2.380360
C	-3.597392	0.847272	3.870079
H	-4.497291	1.001052	3.267888
H	-3.410045	1.743317	4.468457
H	-3.710276	-0.027111	4.512962
C	3.422594	-0.253204	-1.717143
H	3.629485	0.389046	-2.569268
C	2.832107	-1.935733	0.439356
C	4.335827	-1.185942	-1.325076
H	5.287902	-1.282740	-1.838762
C	4.011069	-2.062234	-0.238715
H	4.721656	-2.829508	0.058724
H	2.629596	-2.598205	1.277001
H	-0.064552	3.656630	-2.492098
H	2.151045	2.257206	-2.952374
C	0.168760	2.659323	-2.137964
C	-0.694807	1.881283	-1.167062

VI

C	-0.320824	1.404662	-0.425238
H	2.139079	1.853939	-2.571438
O	2.871565	2.011170	-1.954794
H	2.473381	2.497520	-1.202824
O	1.918880	2.638742	0.626238
H	3.215934	0.559061	-1.093882
C	1.156984	-0.774129	-0.153372
H	0.570578	-2.720862	-0.915075
C	-2.983174	-0.483854	0.148950
C	-2.828081	0.658061	-0.741839
C	-1.636393	1.370126	-0.986088
H	-1.849111	2.316008	-1.486562
C	0.723392	0.605711	0.065633
H	-0.065859	2.456115	-0.282456
O	-1.042987	-1.457708	-0.713473
C	2.476000	-1.085803	-0.334594
O	2.846203	-2.386157	-0.264121
O	3.494092	-0.251326	-0.585625
C	4.107229	-2.772605	-0.837812
H	4.138215	-3.858727	-0.738879
H	4.937070	-2.318284	-0.291801
C	1.627750	1.343562	1.014736

O	2.081605	0.888440	2.044027
H	4.161700	-2.487692	-1.893252
C	-1.434668	-2.133643	1.428244
C	2.692648	3.409241	1.568534
H	3.662421	2.936096	1.741135
H	2.155295	3.492456	2.516433
H	2.815287	4.390768	1.108398
C	-4.241339	-0.722901	0.789671
H	-4.309769	-1.527144	1.518683
C	-4.060414	1.272455	-1.177567
C	-5.362949	-0.032745	0.413540
H	-6.324815	-0.253154	0.867773
C	-5.270493	0.945332	-0.626725
H	-6.171365	1.452892	-0.963121
H	-4.001534	2.062319	-1.923533
H	0.532841	-3.050486	1.761038
H	-1.961690	-2.259421	2.365760
C	-1.910039	-1.351590	0.322003
C	-0.172109	-2.528411	1.126536
C	0.191062	-1.971253	-0.217011

VII

H	2.978602	3.732443	-1.066141
O	2.322256	3.044651	-1.253830
H	2.898005	1.467254	-0.750581
O	3.396580	0.700937	-0.368112
C	0.813957	-2.132175	-0.277572
C	0.450343	-2.457026	1.166438
C	-0.618967	-1.702645	1.439865
H	1.358561	-2.875952	-0.855251
C	-2.339840	-0.488353	-0.122994
C	-2.556040	0.484027	-1.123954
C	-1.408720	1.092834	-1.799435
H	-1.608443	1.675183	-2.697166
H	0.662102	1.451962	-1.893593
C	1.412748	-0.721017	-0.266787
C	2.733996	-0.475288	-0.343509
O	3.581603	-1.544403	-0.313779
O	-0.486416	-1.879202	-0.845191
C	4.791591	-1.446233	-1.079996
H	5.265606	-2.425663	-0.992052
H	5.451175	-0.671818	-0.680822
C	0.387539	1.231370	1.043519
O	0.735294	2.393107	0.862536

H	4.569180	-1.234574	-2.132927
O	0.147009	0.763772	2.271735
C	0.362778	1.680130	3.365309
H	1.408656	1.995732	3.389892
H	0.108193	1.115503	4.262396
H	-0.282899	2.555191	3.259432
C	-3.431790	-1.077432	0.516346
H	-3.263555	-1.846218	1.265195
C	-3.871573	0.843456	-1.453986
C	-4.739316	-0.704013	0.187467
H	-5.580035	-1.170995	0.693774
C	-4.957739	0.258523	-0.801020
H	-5.970975	0.549458	-1.066700
H	-4.039403	1.589148	-2.228236
H	1.039961	-3.068024	1.840570
H	-1.112177	-1.553101	2.390767
C	0.199346	0.205964	-0.086790
C	-0.929714	-0.931769	0.155558
C	-0.148962	0.971705	-1.356440
H	1.649009	3.091241	-0.537544

IV'

C	0.883771	1.120268	0.360223
C	-0.371972	-1.207674	-0.803230
O	-1.042706	2.518895	0.186563
H	0.262833	-1.150819	0.087672
C	1.763188	0.362150	-0.370441
H	1.488849	0.696466	-2.586598
C	-1.734319	-1.213460	-0.189669
C	-1.843340	-0.577982	1.085329
C	-0.746255	0.021460	1.926268
H	-0.972831	-0.100472	2.986273
C	0.385315	0.743327	1.713423
H	0.930254	1.077674	2.592703
O	-0.191851	0.006190	-1.570906
C	2.914090	-0.379527	0.193349
O	3.011335	-0.315789	1.541048
O	3.752309	-0.929111	-0.503904
C	4.168608	-0.951974	2.114696
H	4.181930	-2.016442	1.865968
H	4.070635	-0.808570	3.191244
C	0.141280	2.214845	-0.372762
O	0.618998	2.830449	-1.307901
H	5.083482	-0.482548	1.743334

C	0.411697	-2.195198	-1.664406
C	-1.781825	3.571493	-0.458302
H	-2.012951	3.290873	-1.489336
H	-1.204370	4.499965	-0.455355
H	-2.695545	3.680097	0.126640
C	-2.857610	-1.764767	-0.807218
H	-2.740473	-2.236951	-1.779699
C	-3.119021	-0.559733	1.681956
C	-4.112252	-1.716765	-0.195731
H	-4.977914	-2.153375	-0.686822
C	-4.238383	-1.108339	1.054375
H	-5.205639	-1.067804	1.548890
H	-3.234293	-0.100094	2.661114
H	2.295123	-1.867515	-2.709921
H	0.260411	-3.267756	-1.716377
C	1.441569	-1.492054	-2.160382
C	1.243094	-0.012374	-1.797298

V'

C	1.055754	0.815319	-0.024161
C	-1.900164	-0.965679	-0.919859
O	2.645846	2.570797	-0.366233
H	0.095254	-0.872598	0.848687
C	0.866825	-0.702866	0.083355
H	1.011085	-1.114153	-2.068904
C	-2.831098	-0.219444	-0.224363
C	-2.539654	1.143173	0.270151
C	-1.340836	1.865926	0.370687
H	-1.548479	2.871104	0.737105
C	0.080618	1.770948	0.122810
H	0.502029	2.773304	0.075223
O	-0.829406	-0.353151	-1.460736
C	2.072245	-1.504807	0.556389
O	2.586510	-1.002469	1.692545
O	2.449921	-2.536365	0.035768
C	3.749653	-1.677154	2.207509
H	3.513953	-2.718195	2.444318
H	4.024843	-1.129019	3.109017
C	2.416730	1.233761	-0.410390
O	3.284457	0.442741	-0.766548
H	4.555846	-1.642036	1.470230
C	-1.679749	-2.410825	-0.977631
C	3.952306	2.994488	-0.786258
H	4.137101	2.699589	-1.822991

H	4.722996	2.556819	-0.145690
H	3.945687	4.081190	-0.690903
C	-4.118056	-0.819604	0.046084
H	-4.281169	-1.843746	-0.278278
C	-3.702973	1.840087	0.798638
C	-5.134273	-0.121499	0.622146
H	-6.102325	-0.584544	0.789370
C	-4.920095	1.252568	0.976485
H	-5.737475	1.828591	1.403168
H	-3.567457	2.876157	1.098084
H	0.194165	-3.527661	-1.147269
H	-2.424056	-3.169287	-0.772016
C	-0.357492	-2.596806	-1.155594
C	0.306821	-1.240576	-1.243918

TS1

C	1.116786	0.923952	-0.176480
C	-0.647426	-0.971083	0.926737
C	2.012897	0.030985	-0.125110
C	1.432350	-1.597959	0.559663
C	-2.045286	-0.713436	0.597826
C	-2.571941	-0.775535	-0.724775
C	-3.950046	-0.548445	-0.894580
C	-4.794507	-0.273024	0.177462
C	-4.271681	-0.204704	1.472833
C	-2.914413	-0.422898	1.671834
H	-2.520131	-0.390374	2.682344
H	-4.916134	0.014444	2.319651
H	-5.852510	-0.096529	0.001884
H	-4.349238	-0.554757	-1.904154
H	-0.304212	4.756423	1.234791
C	3.461853	0.011883	-0.421121
O	4.039566	0.829727	-1.105555
O	4.094491	-1.029927	0.182062
C	5.517002	-1.099614	-0.032020
H	5.849615	-1.978761	0.520892
H	5.735590	-1.206019	-1.097764
H	6.002019	-0.196435	0.347352
O	0.132534	-1.653893	0.062321
C	0.044886	-0.826021	2.153678
C	-1.740952	-1.017857	-1.922938
C	-2.123264	-1.767323	-2.966137
H	-0.773800	-0.525326	-1.949698
H	-1.485469	-1.873359	-3.839229

H	-3.064626	-2.312713	-2.978648
C	1.321073	-1.312202	1.959214
O	-0.417361	2.160055	-1.436185
O	0.339238	2.965690	0.559644
H	2.080593	-2.344700	0.120510
H	-1.528132	3.862138	0.270023
C	0.287912	2.040258	-0.439959
C	-0.472242	4.134852	0.354143
H	-0.163603	4.662752	-0.552543
H	2.148232	-1.299662	2.656221
H	-0.343935	-0.361318	3.048444

TS2

C	-2.209234	-0.045259	0.250755
C	-3.209231	0.534239	1.033708
C	-4.523990	0.616268	0.563974
C	-4.854353	0.078496	-0.682716
C	-3.867187	-0.517213	-1.468215
C	-2.533128	-0.555809	-1.031961
H	-2.976980	0.901594	2.028709
H	-5.290475	1.076000	1.182087
H	-5.879247	0.122170	-1.042036
H	-4.118977	-0.929210	-2.442402
C	-1.451403	-1.134115	-1.825381
H	-1.553214	-2.162333	-2.168736
C	-0.239237	-0.452711	-1.952816
C	-0.827118	-0.327857	0.782041
C	-0.425252	0.082439	2.211162
C	0.520942	-0.783947	2.587237
H	-0.778904	0.962368	2.734167
C	0.713347	-1.722059	1.387102
H	1.126353	-0.781776	3.485899
H	1.104736	-2.721207	1.566399
O	-0.630713	-1.758338	0.857597
C	0.418624	0.024096	-0.165403
C	1.392952	-0.886726	0.299383
C	0.749945	1.500839	-0.329256
C	2.785508	-1.007933	-0.044477
O	1.617144	1.901623	0.618114
O	3.133489	-0.247262	-1.126149
O	0.263213	2.264533	-1.140528
O	3.589965	-1.719982	0.550481
C	1.968074	3.299792	0.597629
H	1.079506	3.918495	0.748644

H	2.431244	3.557648	-0.358231
H	2.674124	3.427625	1.418398
C	4.516766	-0.304970	-1.506745
H	5.155828	0.045199	-0.690823
H	4.606397	0.351107	-2.373851
H	4.801513	-1.328216	-1.768462
H	-0.305313	0.611497	-2.178853
H	0.582480	-0.960963	-2.453154

TS3

C	2.057497	-0.849535	-0.123322
C	2.924561	-1.328093	-1.125942
C	4.277320	-1.011611	-1.131295
C	4.810813	-0.174947	-0.124984
C	3.980949	0.354933	0.837809
C	2.574194	0.071991	0.863718
H	2.534987	-2.004283	-1.880832
H	4.926816	-1.427580	-1.896470
H	5.872222	0.058714	-0.119470
H	4.380549	1.026279	1.594235
C	1.753555	0.788218	1.738170
H	2.238514	1.528198	2.371806
C	0.270185	0.689766	1.836866
C	0.664753	-1.253106	-0.138344
C	-0.063679	-1.767593	-1.299309
C	-1.257631	-2.210671	-0.851175
H	0.255877	-1.664378	-2.327951
C	-1.288610	-1.869259	0.621245
H	-2.115578	-2.536099	-1.423312
H	-1.857748	-2.499898	1.301910
O	0.101146	-1.872578	0.977067
C	-0.511600	0.469927	0.514182
C	-1.662397	-0.362227	0.561198
C	-0.493432	1.561486	-0.495200
C	-3.026799	0.065023	0.284578
O	0.163444	2.668123	-0.061734
O	-3.864225	-0.999394	0.083664
O	-0.950778	1.465692	-1.621133
O	-3.425935	1.219983	0.306234
C	0.266788	3.740384	-1.013138
H	-0.728781	4.084123	-1.306533
H	0.811016	3.410926	-1.902713
H	0.812580	4.532572	-0.498738
C	-5.247893	-0.668605	-0.116618

H	-5.644876	-0.138300	0.753815
H	-5.758391	-1.623366	-0.250929
H	-5.365544	-0.039626	-1.003396
H	-0.119697	1.601437	2.307088
H	0.011252	-0.138880	2.504612

TS4

C	-0.937783	0.658393	-0.400310
C	1.559939	-1.180604	-0.456800
C	0.451080	1.135537	-0.805288
O	0.723610	-1.187754	0.680595
C	-0.519818	-1.742070	0.263528
C	-0.115584	-2.658436	-0.890528
C	1.139955	-2.353759	-1.258538
H	-0.941656	-2.296833	1.106034
C	2.824337	-0.578823	-0.145231
C	2.744462	0.799121	0.275348
C	1.625552	1.586579	-0.108981
H	1.869249	2.637011	-0.266887
H	1.028694	-0.124253	-1.144557
H	0.238519	1.856350	-1.604943
C	-1.427978	-0.566705	-0.074272
C	-2.899372	-0.779345	0.015976
O	-3.186836	-2.077906	0.288719
O	-3.765308	0.058756	-0.155793
C	-4.586476	-2.406454	0.367942
H	-4.619369	-3.476136	0.576812
H	-5.083637	-2.179323	-0.578689
C	-1.905779	1.814733	-0.610403
O	-2.213820	2.239996	-1.704524
H	-5.063673	-1.840146	1.171984
O	-2.250077	2.377711	0.557348
C	-3.195395	3.462285	0.472660
H	-2.798491	4.267183	-0.151649
H	-3.336153	3.800999	1.499342
H	-4.135216	3.096725	0.050968
C	4.081807	-1.202779	-0.279812
H	4.127914	-2.225902	-0.644519
C	3.950256	1.417898	0.728274
C	5.231439	-0.559583	0.143572
H	6.189501	-1.070433	0.098424
C	5.154770	0.750993	0.677008
H	6.059797	1.241249	1.026888
H	3.908350	2.443287	1.088240

H	-0.780899	-3.387219	-1.337742
H	1.699380	-2.767322	-2.090189

TS5

C	-2.237345	-0.094902	0.268979
C	-3.305366	0.252524	1.090457
C	-4.602666	0.342085	0.571920
C	-4.836174	0.054917	-0.778733
C	-3.779105	-0.305007	-1.608058
C	-2.456710	-0.364021	-1.112249
H	-3.132307	0.434027	2.147735
H	-5.428545	0.615466	1.222940
H	-5.844707	0.109564	-1.180070
H	-3.959347	-0.522421	-2.658349
C	-1.354998	-0.639265	-1.988622
H	-1.573877	-1.015356	-2.985861
C	-0.010633	-0.455033	-1.613374
C	-0.860616	-0.350458	0.795405
C	-0.377211	0.071255	2.179865
C	0.597647	-0.792949	2.495987
H	-0.666156	0.975680	2.702271
C	0.701160	-1.765752	1.323062
H	1.280864	-0.759427	3.336649
H	1.076820	-2.768383	1.514567
O	-0.671350	-1.782082	0.860741
C	0.321993	0.067847	-0.220949
C	1.334966	-1.020618	0.158219
C	0.681595	1.540453	-0.192721
C	2.749425	-1.054439	-0.146653
O	1.600405	1.850649	0.741750
O	3.089551	-0.188010	-1.149251
O	0.184507	2.360614	-0.940740
O	3.563442	-1.799123	0.388642
C	1.989238	3.235495	0.805130
H	1.125300	3.865218	1.034967
H	2.421313	3.550838	-0.148261
H	2.730969	3.289743	1.602458
C	4.467032	-0.219026	-1.555945
H	5.120873	0.029032	-0.715212
H	4.553325	0.530216	-2.344252
H	4.733967	-1.209490	-1.936071
H	0.695220	-0.147898	-2.387534
H	0.600447	-1.531822	-1.245431

TS6

C	-0.419806	0.383829	0.588188
C	0.819896	-1.011903	-0.228562
C	-1.577290	-0.370452	0.941347
C	-0.753777	-2.407081	0.336002
O	0.465611	-1.969738	0.733466
C	-0.883180	-2.236149	-1.062475
C	0.117646	-1.367492	-1.428723
H	-1.245079	-3.109074	0.996393
C	2.235791	-0.555849	-0.156612
C	2.668604	0.309446	0.872032
C	1.734599	0.862832	1.856319
H	2.186385	1.311205	2.739947
H	-0.177455	1.340865	2.558242
C	0.396154	0.880665	1.755409
C	-2.819696	-0.299826	0.173474
O	-3.861344	-0.848883	0.863003
O	-2.950485	0.163686	-0.950500
C	-5.132581	-0.824371	0.196200
H	-5.434055	0.204587	-0.020087
H	-5.832991	-1.290438	0.890784
C	-0.543361	1.482220	-0.471227
O	0.009745	1.518247	-1.549237
H	-5.089161	-1.387130	-0.741045
O	-1.287898	2.498573	0.014113
C	-1.486303	3.609494	-0.879663
H	-0.526387	4.054117	-1.156208
H	-2.095952	4.321595	-0.322242
H	-2.008203	3.273404	-1.779410
C	3.159357	-1.032397	-1.092114
H	2.820338	-1.706189	-1.873977
C	4.028208	0.652612	0.939340
C	4.506594	-0.664655	-1.026319
H	5.208177	-1.041966	-1.765416
C	4.942393	0.176524	-0.001460
H	5.988957	0.462062	0.066644
H	4.365483	1.313851	1.734582
H	-1.688020	-0.674104	1.977416
H	0.262641	-0.891914	-2.387363
H	-1.699195	-2.600642	-1.671959

TS8

C	-0.345091	0.676380	1.683097
C	1.349748	0.722961	-1.283131

O	-0.072472	0.342689	4.054612
H	-2.066047	1.473842	0.752685
C	-0.997490	1.709970	0.753018
H	-1.511927	1.831483	-1.362162
C	2.195930	-0.359657	-1.160079
C	1.737566	-1.527612	-0.413139
C	0.832520	-1.538960	0.652404
H	0.776083	-2.530447	1.102469
C	0.219434	-0.582014	1.543494
H	0.215474	-1.061117	2.520681
O	0.025498	0.512020	-1.078730
C	-0.872614	3.137944	1.302179
O	-1.984892	3.849831	1.013740
O	0.121326	3.615660	1.805554
C	-1.994577	5.213195	1.476601
H	-1.910973	5.235879	2.566158
H	-2.953485	5.620735	1.154992
C	-0.743834	1.012771	3.088226
O	-1.617612	1.826087	3.365209
H	-1.166467	5.776253	1.036969
C	1.574435	2.130867	-1.506165
C	-0.482039	0.617948	5.404581
H	-1.535855	0.362531	5.547067
H	-0.332392	1.675313	5.638141
H	0.155208	-0.008698	6.029938
C	3.478267	-0.383650	-1.811217
H	3.847135	0.527312	-2.275970
C	2.462419	-2.752940	-0.679216
C	4.175642	-1.551015	-1.931607
H	5.123924	-1.575561	-2.460830
C	3.625184	-2.764450	-1.395589
H	4.159075	-3.699950	-1.543330
H	2.089888	-3.672330	-0.233131
H	0.267930	3.844152	-1.167460
H	2.524324	2.572896	-1.777553
C	0.433619	2.774568	-1.185593
C	-0.594814	1.754986	-0.770359

TS9

C	-0.277084	1.422913	-0.409312
H	0.773881	1.462264	-1.487025
O	1.771502	1.448445	-2.196482
H	2.097755	2.365280	-2.224107
O	2.020682	2.593466	0.565233

H	2.476815	0.905011	-1.642797
C	1.178940	-0.745229	-0.055505
H	0.679817	-2.587842	-1.119486
C	-2.913637	-0.529344	0.194552
C	-2.806457	0.659058	-0.651161
C	-1.643672	1.386518	-0.908777
H	-1.859665	2.324150	-1.423902
C	0.727698	0.569548	0.191023
H	-0.103980	2.460214	-0.104844
O	-0.977194	-1.408830	-0.790654
C	2.567844	-0.921133	-0.306788
O	3.021932	-2.193538	-0.223010
O	3.332579	-0.002228	-0.726865
C	4.361683	-2.438361	-0.684418
H	4.507602	-3.514378	-0.579964
H	5.081996	-1.892908	-0.069428
C	1.695840	1.363938	1.055407
O	2.115218	0.963020	2.120714
H	4.473642	-2.134438	-1.728970
C	-1.361007	-2.300639	1.275118
C	2.901949	3.371835	1.397493
H	3.851729	2.848057	1.533119
H	2.444103	3.551710	2.373570
H	3.050184	4.311498	0.863260
C	-4.145033	-0.788472	0.885841
H	-4.182126	-1.614393	1.592419
C	-4.065171	1.271730	-1.029603
C	-5.280495	-0.089761	0.582140
H	-6.219728	-0.326844	1.074279
C	-5.244456	0.921631	-0.436110
H	-6.164578	1.428289	-0.716794
H	-4.042080	2.078476	-1.759464
H	0.614627	-3.233788	1.509358
H	-1.880438	-2.527127	2.197933
C	-1.847452	-1.411596	0.261309
C	-0.094451	-2.652488	0.933848
C	0.265409	-1.941133	-0.341495

TS10

C	0.605134	0.539853	-0.143228
C	-1.601486	-1.364628	0.374469
O	3.026928	2.469566	-1.426156
H	2.305369	2.818604	-0.861122
O	1.104146	2.755119	0.637723

H	3.223019	0.825890	-0.830091
C	1.222146	-0.762922	-0.289378
H	0.807232	-2.835202	-0.969757
C	-2.785539	-0.603843	0.156079
C	-2.803012	0.373830	-0.889520
C	-1.650407	1.064246	-1.432676
H	-1.953957	1.830248	-2.146077
C	-0.343839	1.215304	-1.022681
H	0.035155	2.186371	-1.352824
O	-0.913863	-1.718593	-0.735991
C	2.576882	-0.960335	-0.324377
O	3.048775	-2.222163	-0.186579
O	3.543838	-0.063233	-0.526486
C	4.408863	-2.495032	-0.563169
H	4.585470	-2.230396	-1.610334
H	4.527928	-3.570182	-0.420577
C	1.225782	1.388317	0.887568
O	1.798941	1.002917	1.894849
H	5.105671	-1.947907	0.076149
C	-0.990232	-1.915520	1.529243
C	1.543531	3.616192	1.704081
H	2.609355	3.476733	1.904451
H	0.977206	3.406508	2.615152
H	1.344960	4.631670	1.356461
C	-3.954428	-0.870130	0.910540
H	-3.901791	-1.591902	1.721886
C	-4.077324	0.899024	-1.240535
C	-5.163547	-0.292482	0.570766
H	-6.062225	-0.529822	1.133262
C	-5.226396	0.573267	-0.542074
H	-6.178914	1.004686	-0.839421
H	-4.133324	1.615378	-2.057200
H	0.997527	-2.853982	1.745761
H	-1.365932	-1.810981	2.538852
H	2.697496	2.506773	-2.337150
C	0.211043	-2.440295	1.129183
C	0.387769	-2.085077	-0.302010

TS11

C	1.447181	-0.808603	0.104978
H	1.588395	-1.882428	-0.894789
O	2.073422	-2.351648	-1.893703
H	2.789086	-1.188556	-1.848305
O	3.311493	-0.364426	-1.299683

C	-0.807138	-0.297816	0.806241
C	0.233832	0.043191	-0.383513
H	1.520178	-2.143208	1.897547
C	-2.264983	-0.316281	0.442136
C	-2.648648	-0.493533	-0.903515
C	-1.634384	-0.547136	-1.957003
H	-1.981525	-0.762652	-2.966294
C	-0.331200	-0.308707	-1.743341
H	0.364294	-0.293848	-2.580086
O	-0.375811	-1.623465	1.179716
C	2.785787	-0.369118	-0.114510
O	3.586754	-0.166407	0.921352
O	-0.555629	2.296318	-0.523957
C	5.001242	0.004409	0.669564
H	5.166554	0.919527	0.097415
H	5.396716	-0.854543	0.122727
C	0.563574	1.553093	-0.415320
O	1.677941	2.034894	-0.382326
H	5.454082	0.079363	1.658130
C	-0.331316	0.516793	2.012830
C	-0.366848	3.721619	-0.608614
H	0.225891	3.972847	-1.492324
H	0.141724	4.092216	0.285581
H	-1.370596	4.140333	-0.685038
C	-3.241300	-0.250610	1.437321
H	-2.936481	-0.137068	2.474399
C	-4.013720	-0.592126	-1.216393
C	-4.598673	-0.344074	1.114748
H	-5.348051	-0.289436	1.900062
C	-4.984538	-0.515254	-0.217267
H	-6.037450	-0.591289	-0.476701
H	-4.311542	-0.726978	-2.254166
H	1.486318	0.241466	3.192331
H	-0.764579	1.454529	2.340089
H	1.372876	-2.416573	-2.560491
C	0.786390	-0.087186	2.432747
C	0.987869	-1.277964	1.502030

TS7*

C	-1.328161	-0.555924	0.308268
C	1.186428	0.482086	-1.151295
O	-2.599364	-2.537878	0.240559
H	0.414654	0.794164	-0.153976
C	-0.994818	0.751289	-0.198125

H	-1.729133	0.504331	-2.309798
C	2.273301	-0.196801	-0.463635
C	2.047674	-0.994010	0.716999
C	0.825167	-1.300371	1.452655
H	1.073888	-1.908497	2.321433
C	-0.553262	-1.194963	1.316562
H	-1.093886	-1.852918	1.994992
O	0.188879	-0.245682	-1.825072
C	-1.306709	1.978181	0.601905
O	-0.971736	1.876495	1.902709
O	-1.844251	2.957467	0.114262
C	-1.340907	2.992436	2.735759
H	-0.849784	3.906000	2.390253
H	-1.000545	2.726385	3.736754
C	-2.440672	-1.305352	-0.314674
O	-3.186298	-0.894583	-1.193911
H	-2.424742	3.135337	2.720649
C	1.197136	1.824112	-1.837824
C	-3.717572	-3.298052	-0.244578
H	-3.610022	-3.493844	-1.314881
H	-4.654368	-2.760917	-0.070590
H	-3.697336	-4.230875	0.320653
C	3.594602	0.059822	-0.896991
H	3.734486	0.679719	-1.778142
C	3.216868	-1.558900	1.314079
C	4.693915	-0.503738	-0.274369
H	5.694044	-0.322798	-0.658653
C	4.495620	-1.333519	0.843519
H	5.344421	-1.791515	1.344357
H	3.086780	-2.189016	2.190063
H	-0.526571	2.926885	-2.616323
H	2.037793	2.505124	-1.891643
C	-0.078393	2.040339	-2.187779
C	-0.853139	0.801011	-1.742731

TS11'

C	1.397745	-0.743904	0.037848
H	2.463604	-0.818536	1.072129
O	3.373479	-1.433082	1.549052
H	3.489108	-1.861167	0.353070
O	3.266161	-1.899629	-0.802757
C	-0.931240	-0.393860	0.605545
C	0.354846	0.404911	0.057772
H	0.931680	-2.937929	0.280213

C	-2.282766	0.139669	0.223987
C	-2.407772	0.947215	-0.924623
C	-1.213426	1.339296	-1.671272
H	-1.368326	1.877466	-2.605154
C	0.040021	1.095617	-1.257012
H	0.883493	1.446869	-1.839359
O	-0.714137	-1.679859	-0.027430
C	2.336739	-1.012791	-0.988757
O	2.397908	-0.291947	-2.106731
O	-0.190599	2.223025	1.520902
C	3.554513	-0.451462	-2.956718
H	3.604906	-1.471721	-3.342449
H	4.469032	-0.219399	-2.405392
C	0.837420	1.524761	0.997915
O	2.002997	1.798270	1.210722
H	3.403270	0.259861	-3.769068
C	-0.647570	-0.737101	2.071208
C	0.159263	3.348669	2.347704
H	0.732051	4.079198	1.769965
H	0.751658	3.021142	3.206393
H	-0.791001	3.773629	2.672096
C	-3.422921	-0.226887	0.940617
H	-3.322108	-0.869156	1.811623
C	-3.684176	1.375582	-1.322463
C	-4.689713	0.209212	0.539956
H	-5.569141	-0.083414	1.107715
C	-4.818809	1.013368	-0.595617
H	-5.800120	1.354762	-0.915586
H	-3.781962	1.999945	-2.208257
H	0.811964	-2.153292	2.873936
H	-1.047620	-0.197912	2.921296
H	4.077904	-0.799703	1.765638
C	0.270364	-1.707560	2.048028
C	0.563819	-1.954634	0.570933