

## Supporting Information

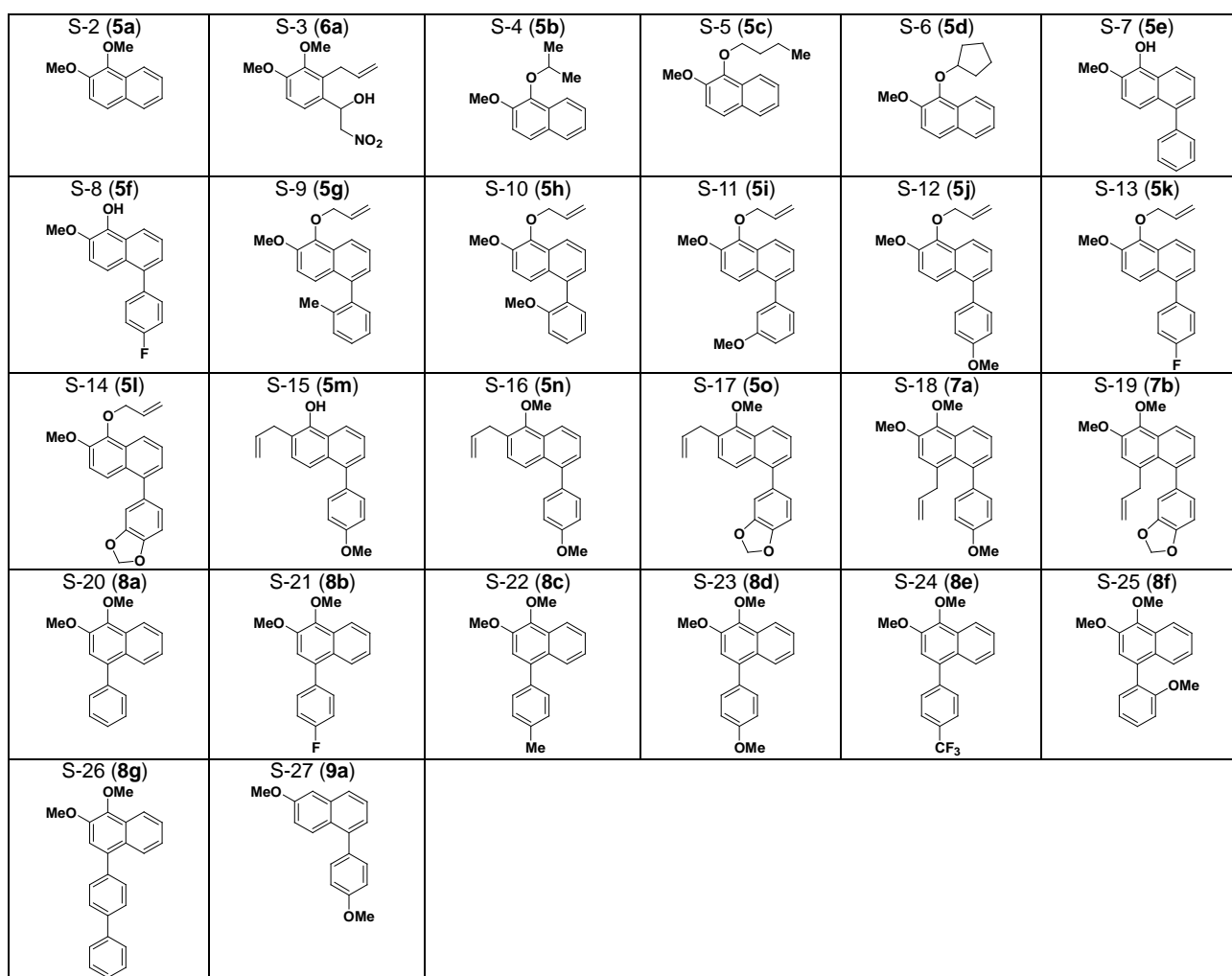
### Metal Triflates Promoted Synthesis of Naphthalenes

Chieh-Kai Chan, Heui-Sin Wang, Yu-Lin Tsai and Meng-Yang Chang\*

Department of Medicinal and Applied Chemistry, Kaohsiung Medical University Hospital, Kaohsiung Medical University, Kaohsiung 807, Taiwan

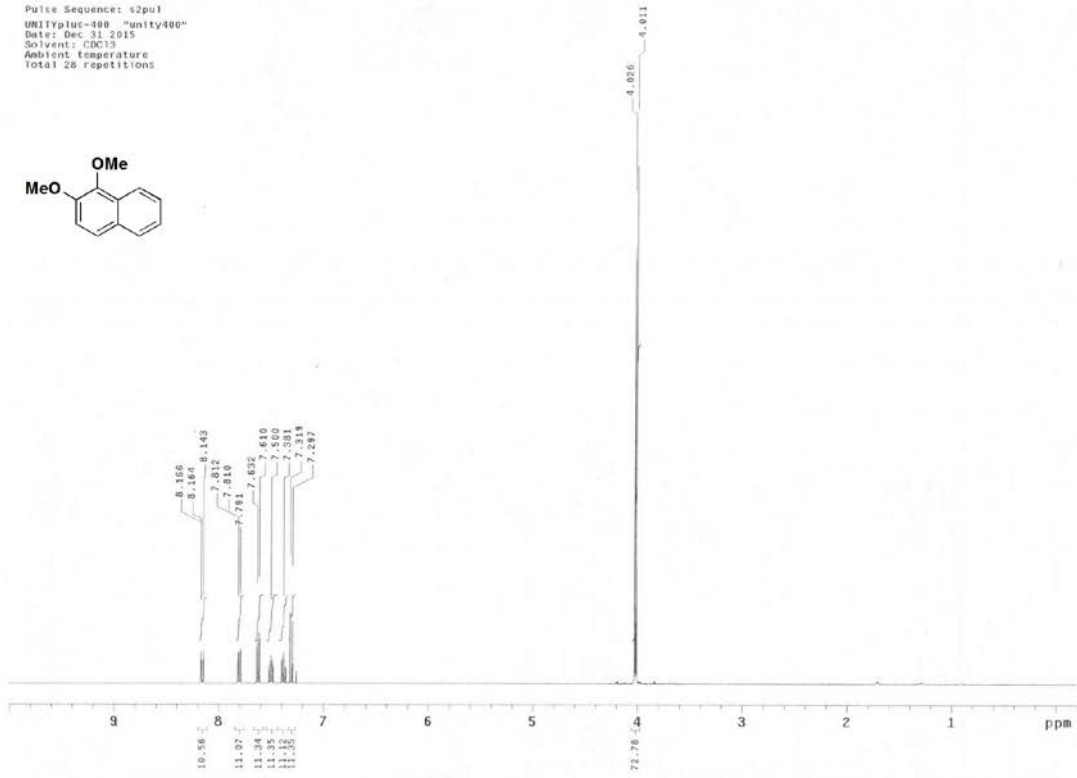
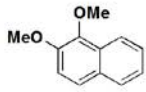
Email: [mychang@kmu.edu.tw](mailto:mychang@kmu.edu.tw)

- (1) Additional scanned photocopies (pages S-2~S-27)
- (2) X-ray crystal data of **5e**, **5f**, **8d**, **8g**, **9a** and **9b** (pages S-28~S-33)

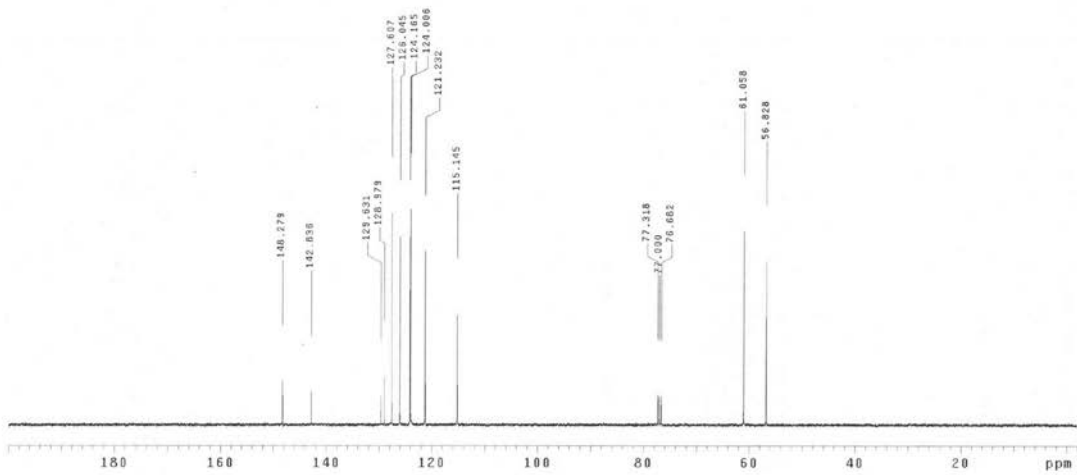
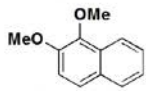


# Compound 5a

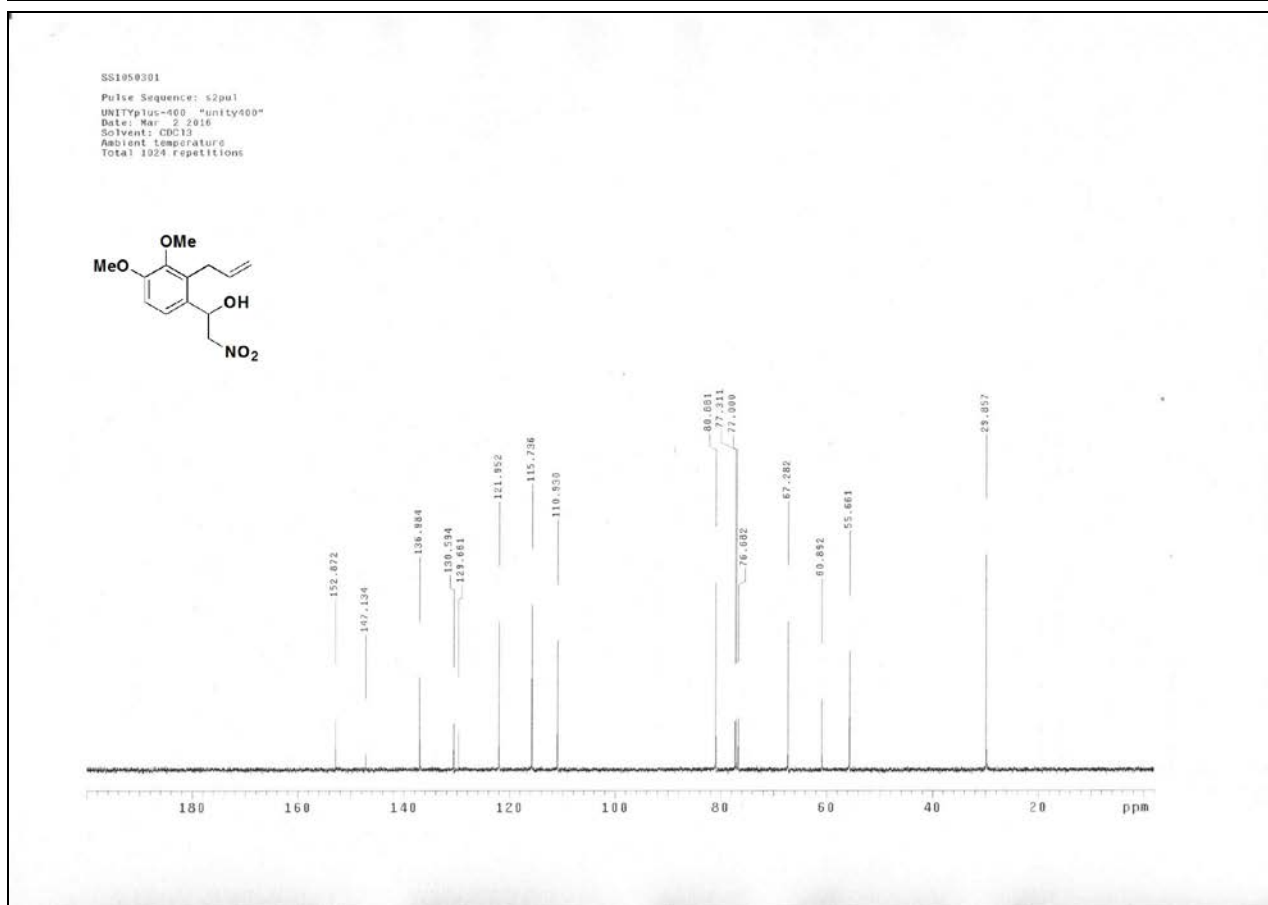
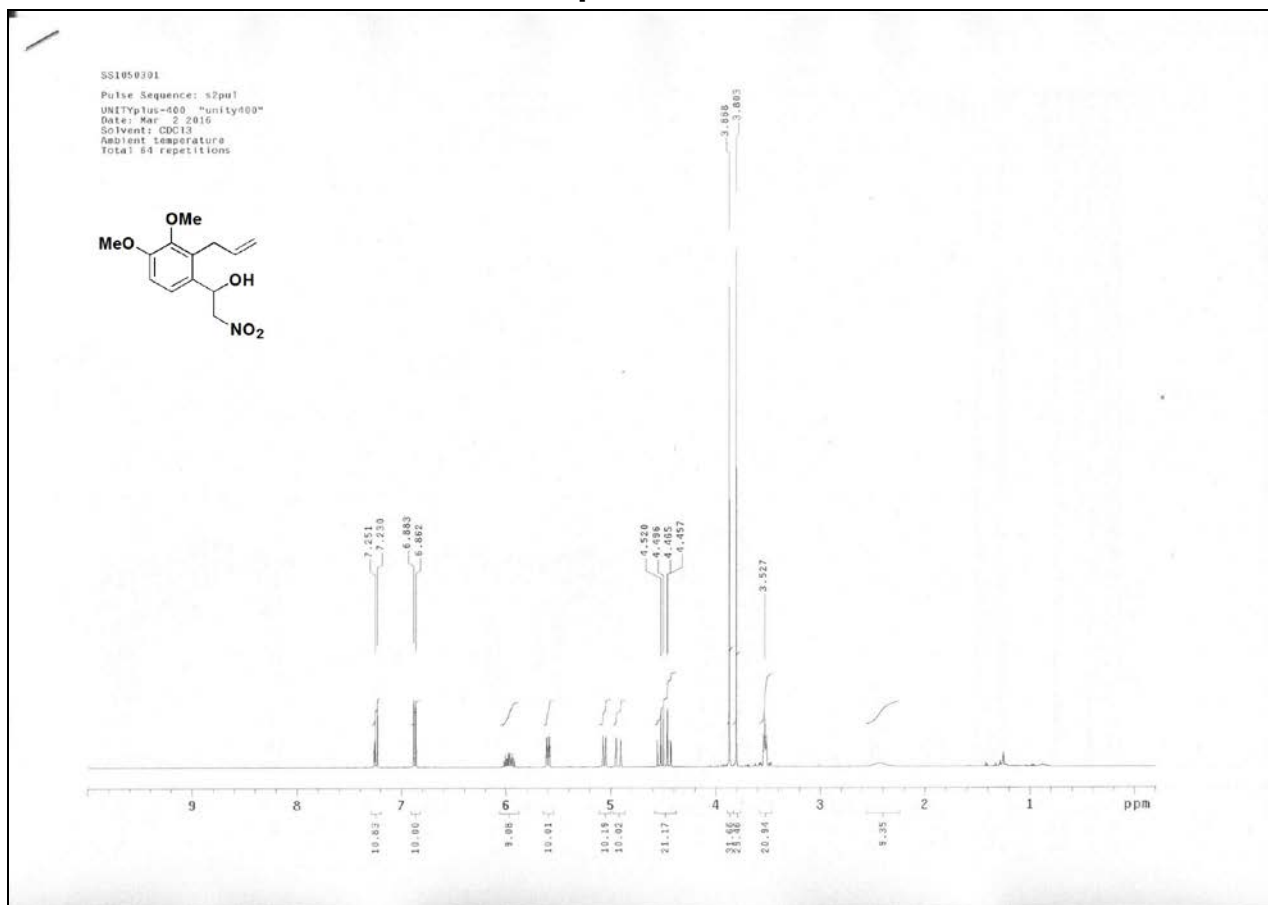
SS1041230  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Dec 31 2015  
Solvent: CDCl3  
Ambient temperature  
Total 26 repetitions



SS1041230  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Dec 31 2015  
Solvent: CDCl3  
Ambient temperature  
Total 1136 repetitions

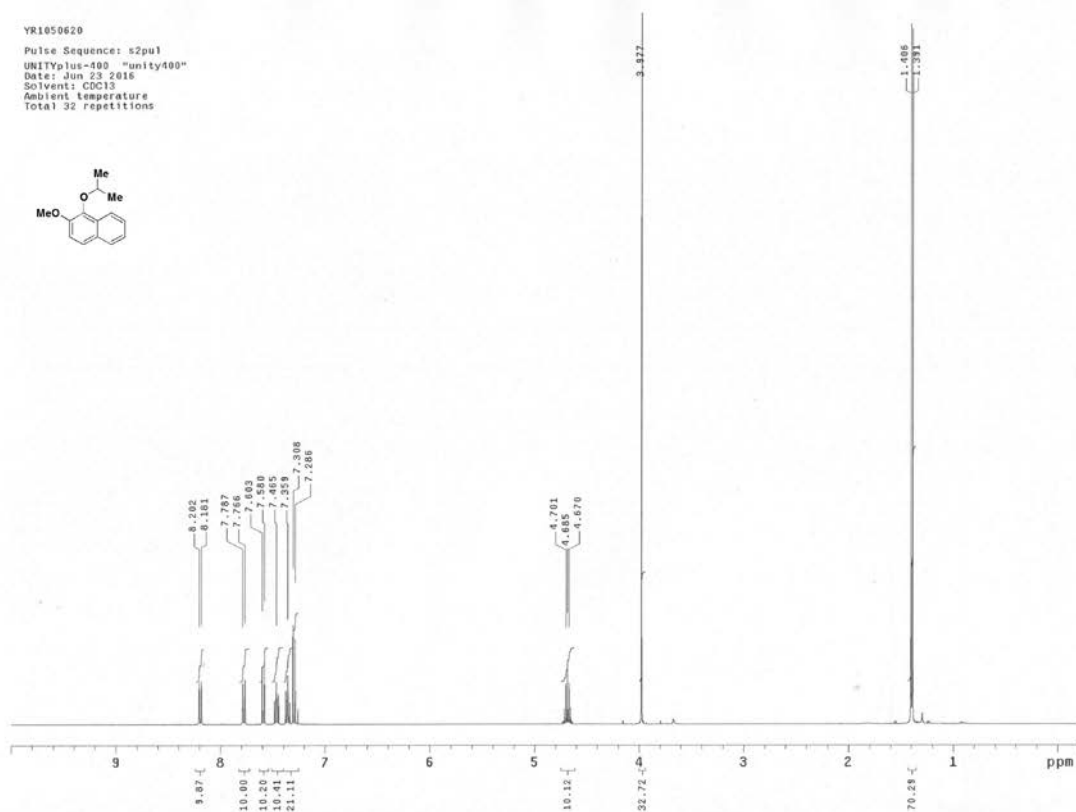


# Compound 6a

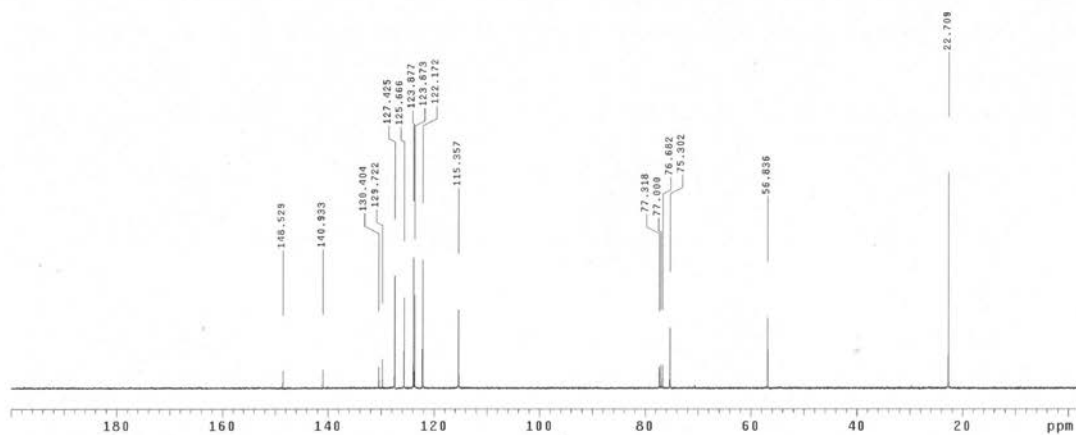
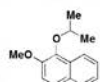


# Compound 5b

YR1050620  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Jun 23 2016  
Solvent: CDCl3  
Ambient temperature  
Total 32 repetitions

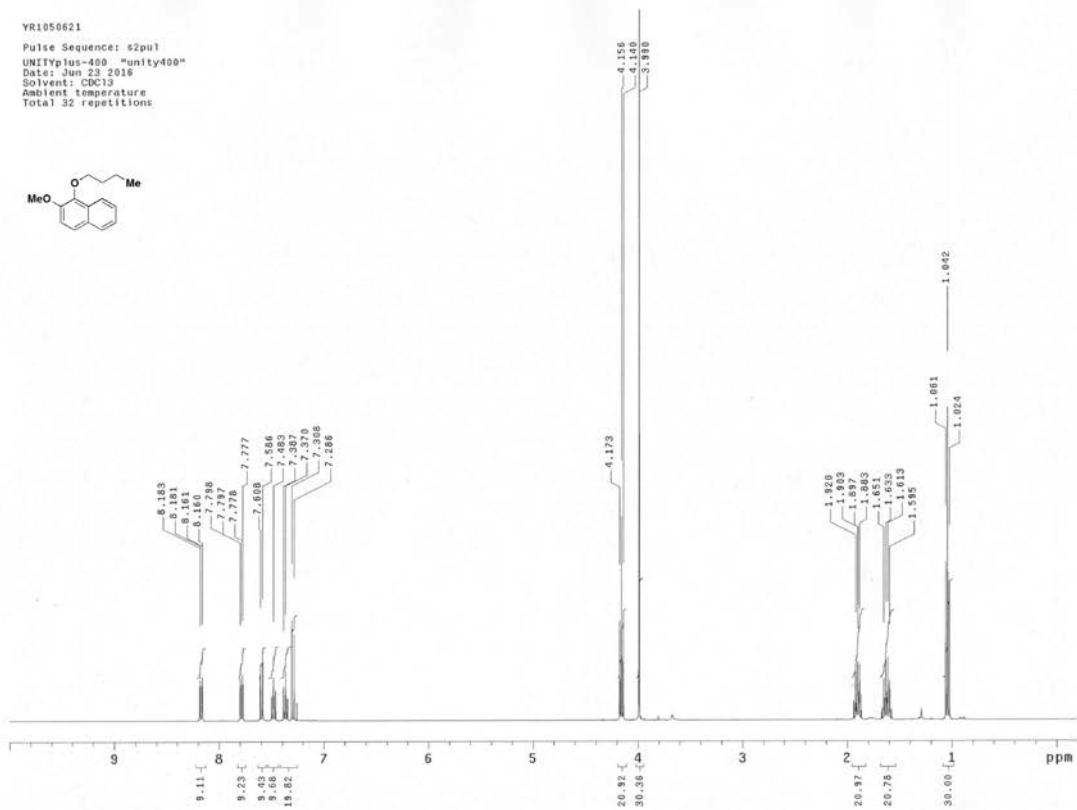
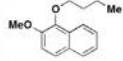


YR1050620  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Jun 23 2016  
Solvent: CDCl3  
Ambient temperature  
Total 688 repetitions

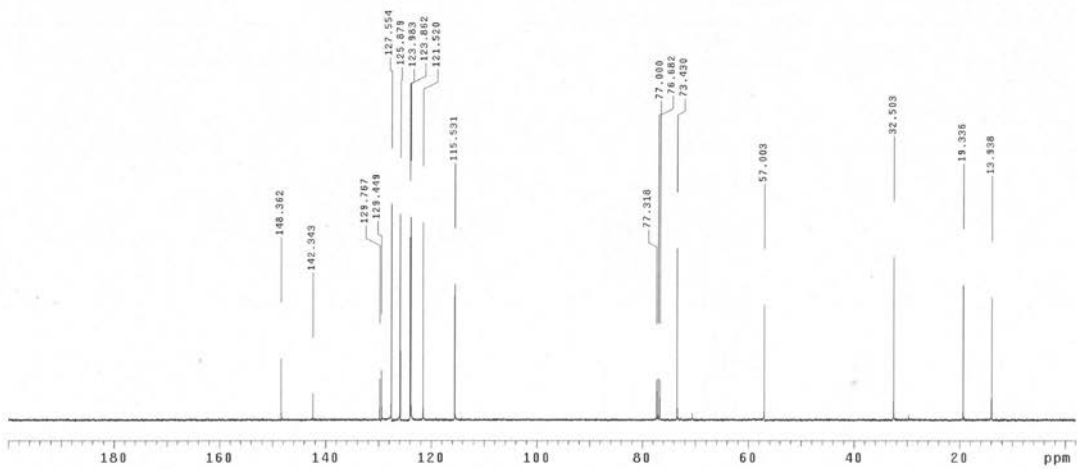
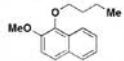


# Compound 5c

YR1050621  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Jun 23 2016  
Solvent: CDCl3  
Ambient temperature  
Total 32 repetitions

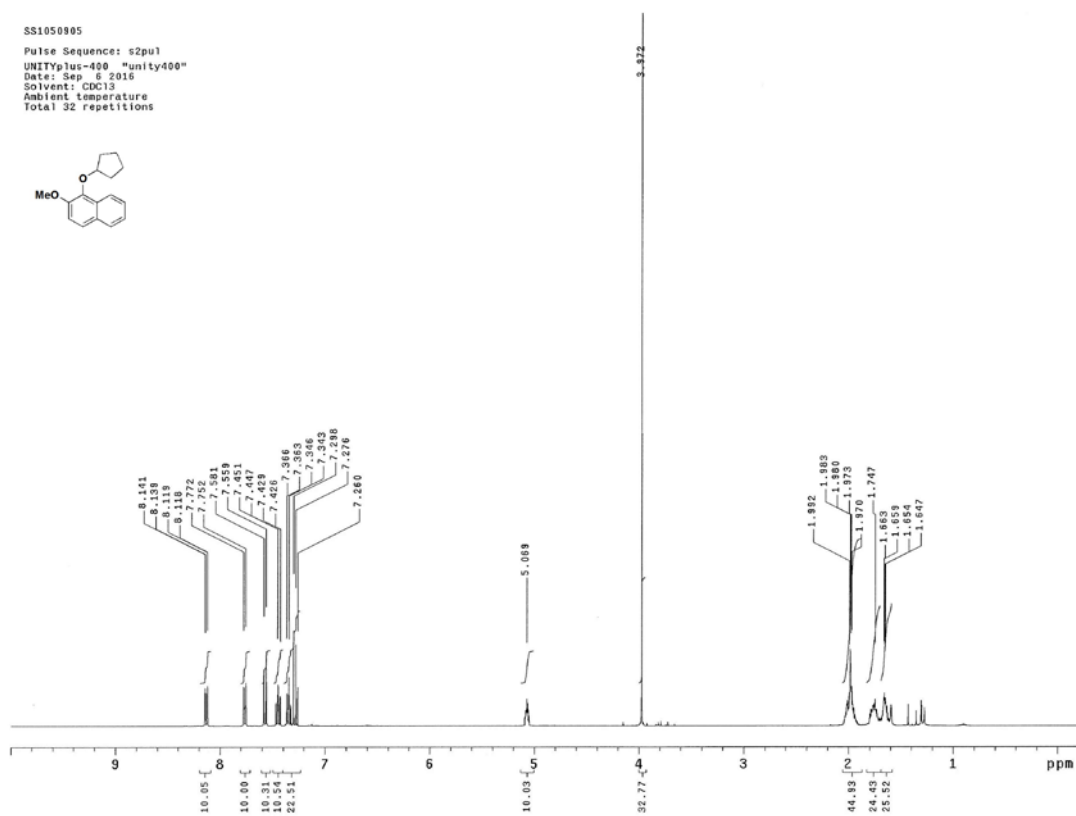


YR1050621  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Jun 23 2016  
Solvent: CDCl3  
Ambient temperature  
Total 1712 repetitions

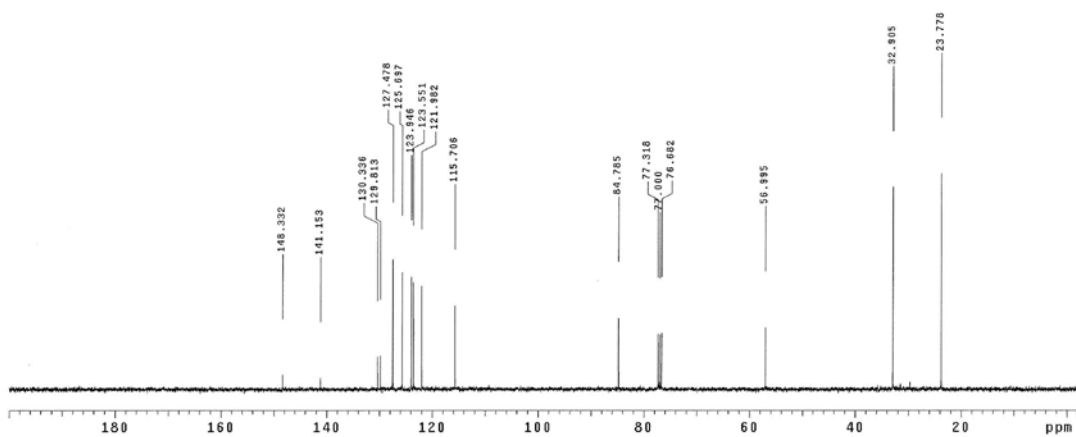


# Compound 5d

SS1050905  
 Pulse Sequence: s2pul  
 UNITYplus-400 "unity400"  
 Date: Sep 6 2016  
 Solvent: CDCl3  
 Ambient temperature  
 Total 32 repetitions



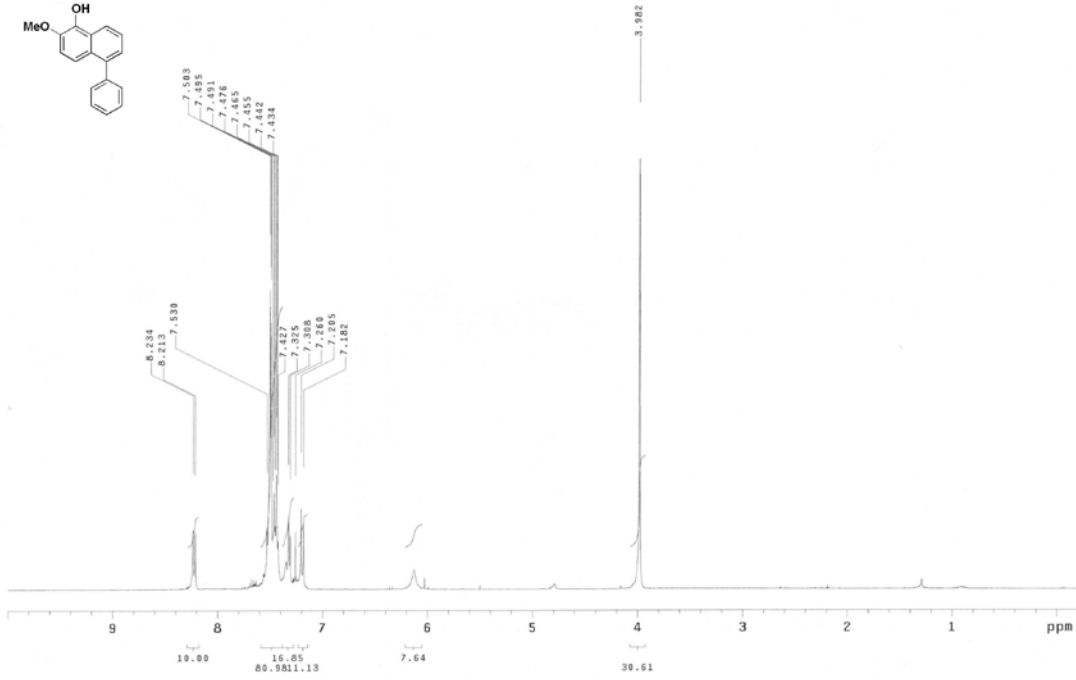
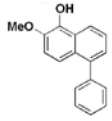
SS1050905  
 Pulse Sequence: s2pul  
 UNITYplus-400 "unity400"  
 Date: Sep 6 2016  
 Solvent: CDCl3  
 Ambient temperature  
 Total 784 repetitions



# Compound 5e

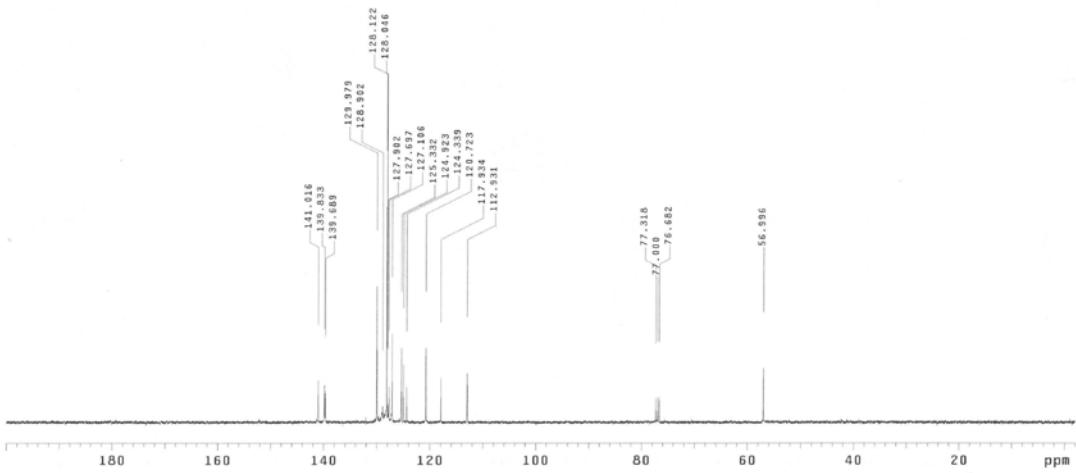
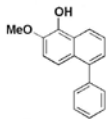
MH101003-1  
STANDARD 1H OBSERVE

Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Oct 15 2012  
Solvent: CDCl3  
Ambient temperature  
Total 32 repetitions



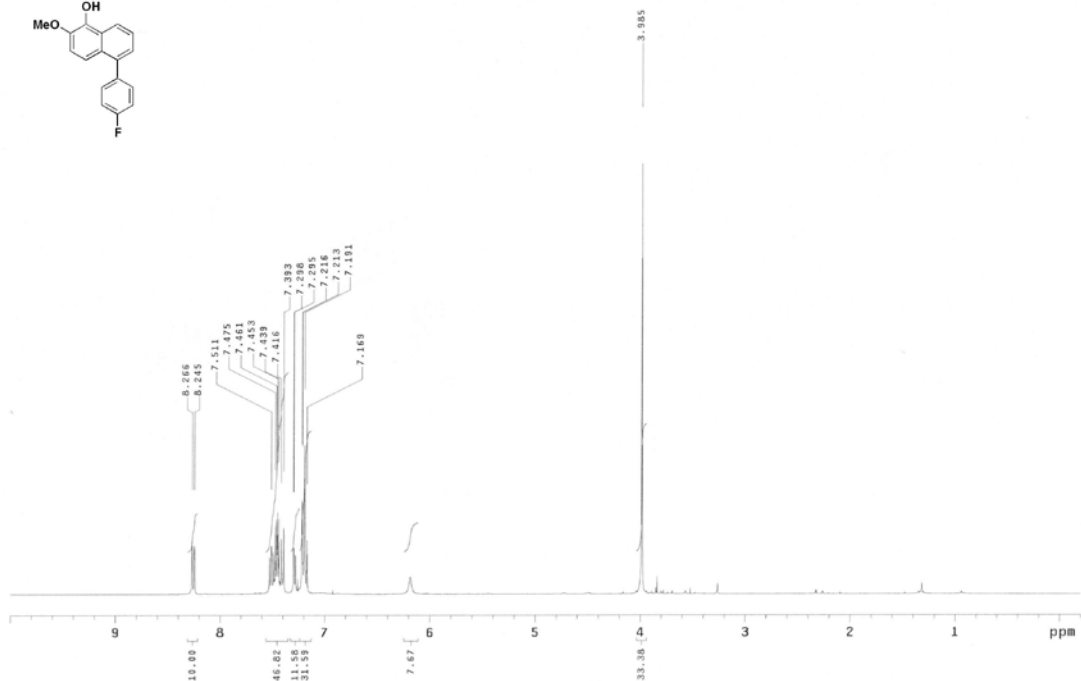
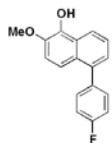
13C OBSERVE

MH101003-1  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Oct 15 2012  
Solvent: CDCl3  
Ambient temperature  
Total 1384 repetitions

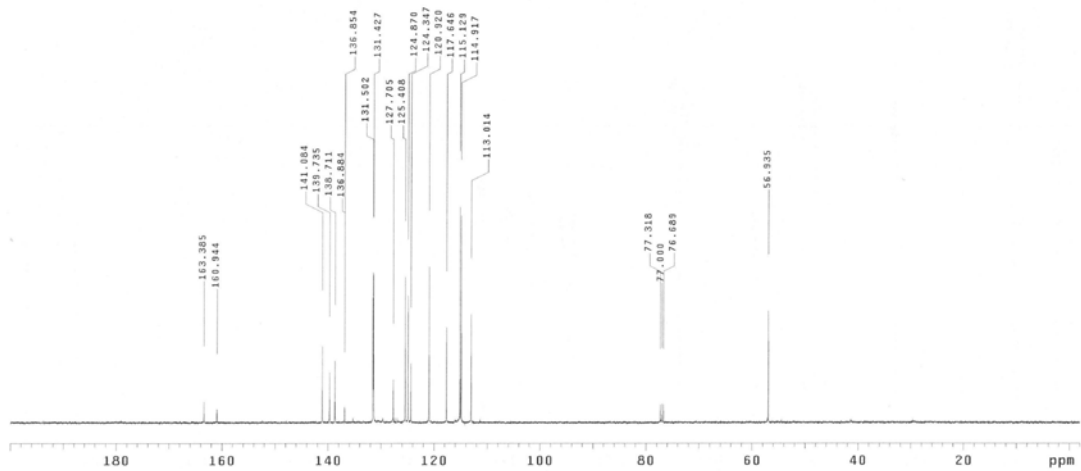
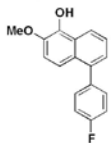


# Compound 5f

MH1011002-H  
 Pulse Sequence: s2pul  
 UNITYplus-400 "unity400"  
 Date: Oct 15 2012  
 Solvent: CDCl3  
 Ambient temperature  
 Total 32 repetitions



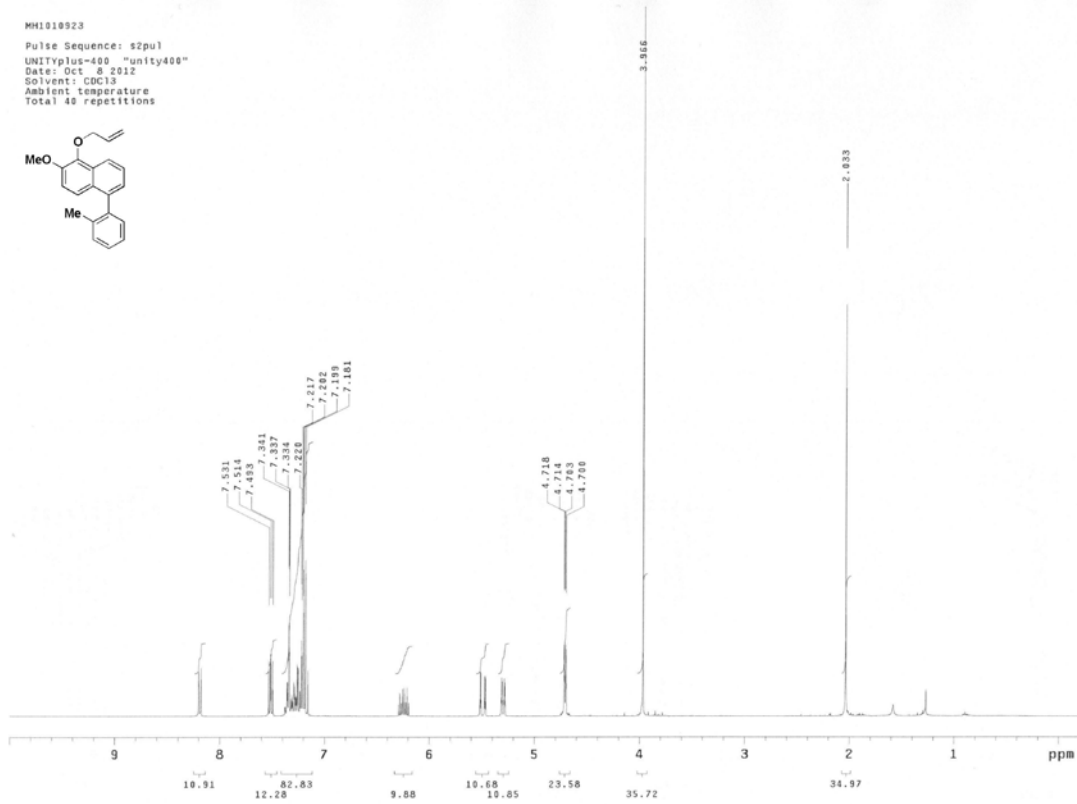
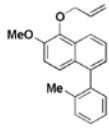
MH1011002-H  
 Pulse Sequence: s2pul  
 UNITYplus-400 "unity400"  
 Date: Oct 15 2012  
 Solvent: CDCl3  
 Ambient temperature  
 Total 896 repetitions



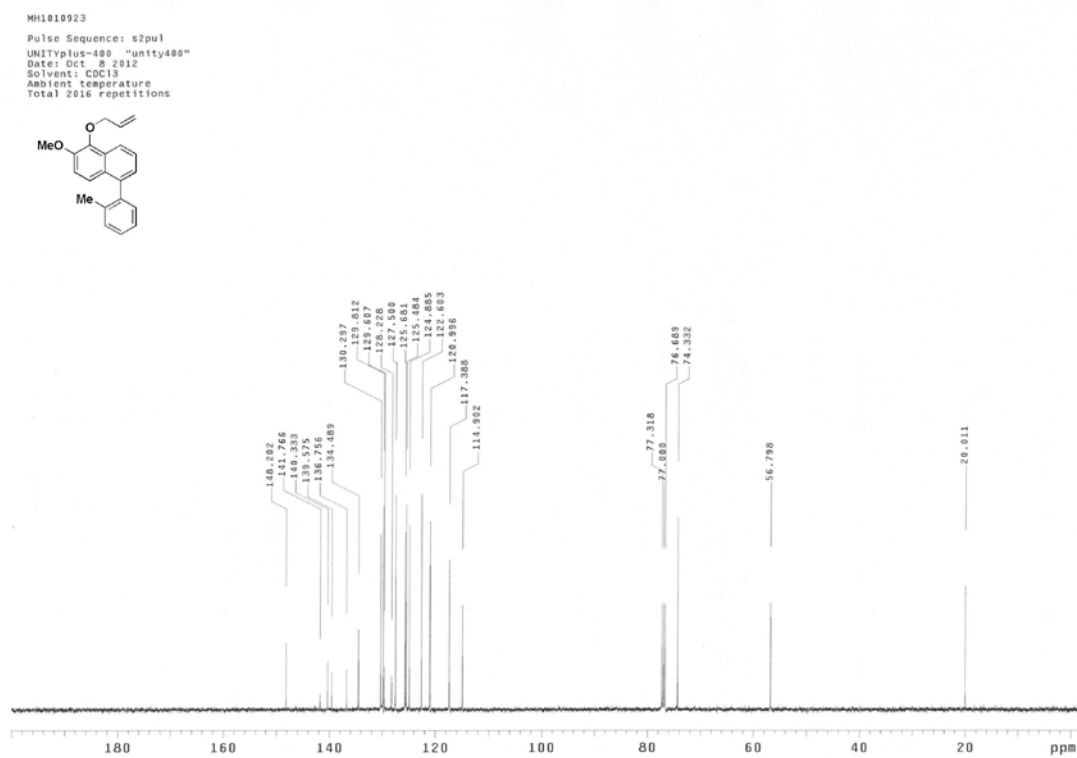
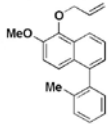


# Compound 5g

MH1010923  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Oct 8 2012  
Solvent: CDCl3  
Ambient temperature  
Total 40 repetitions

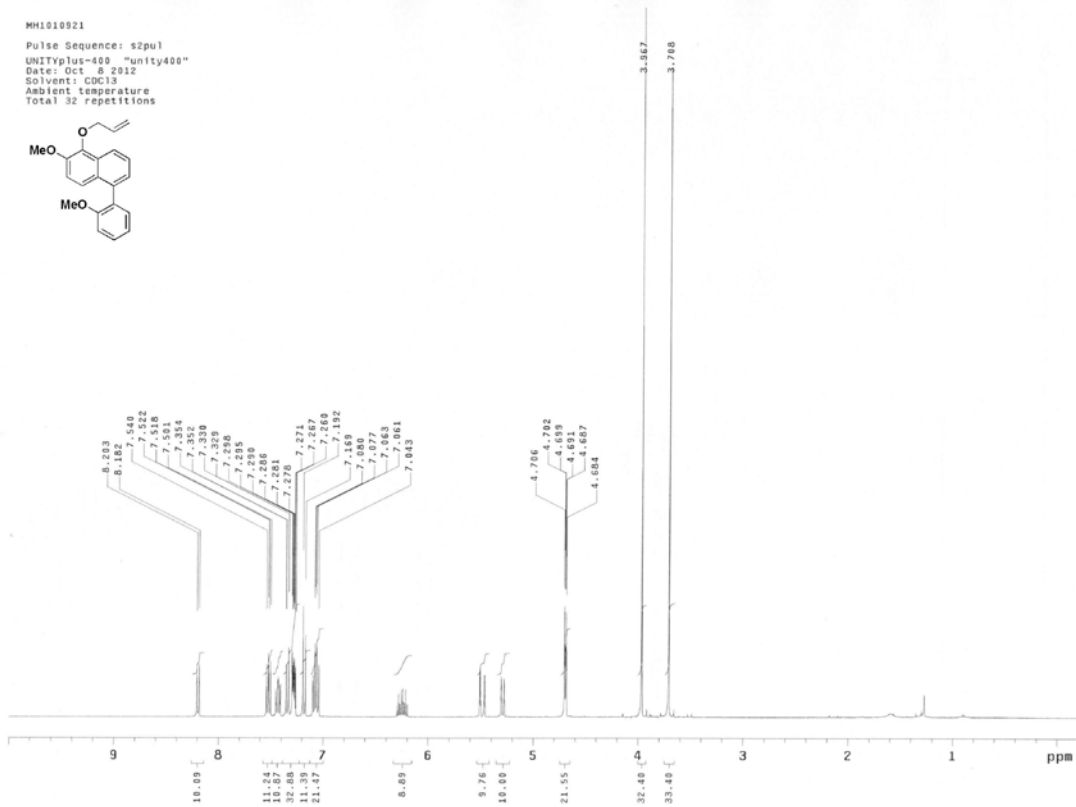
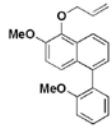


MH1010923  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Oct 8 2012  
Solvent: CDCl3  
Ambient temperature  
Total 2016 repetitions

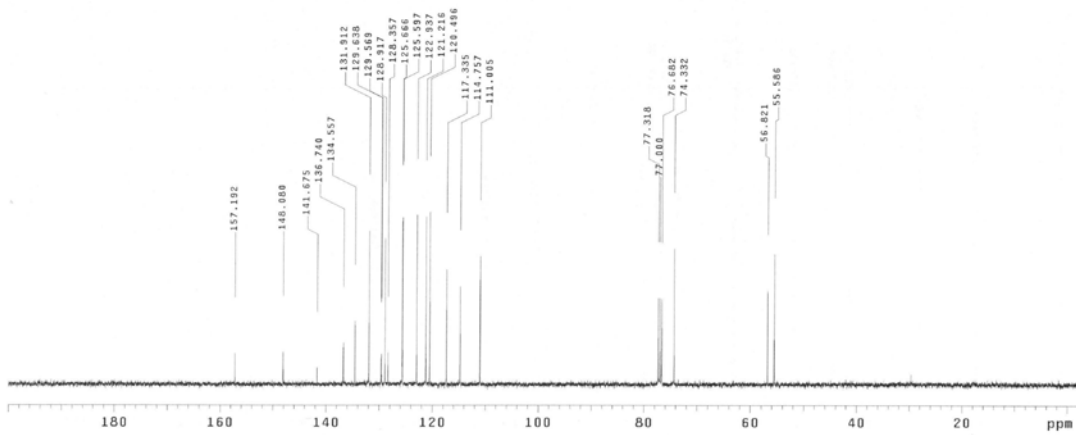
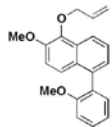


# Compound 5h

MH1010921  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Oct 8 2012  
Solvent: CDCl3  
Ambient temperature  
Total 32 repetitions

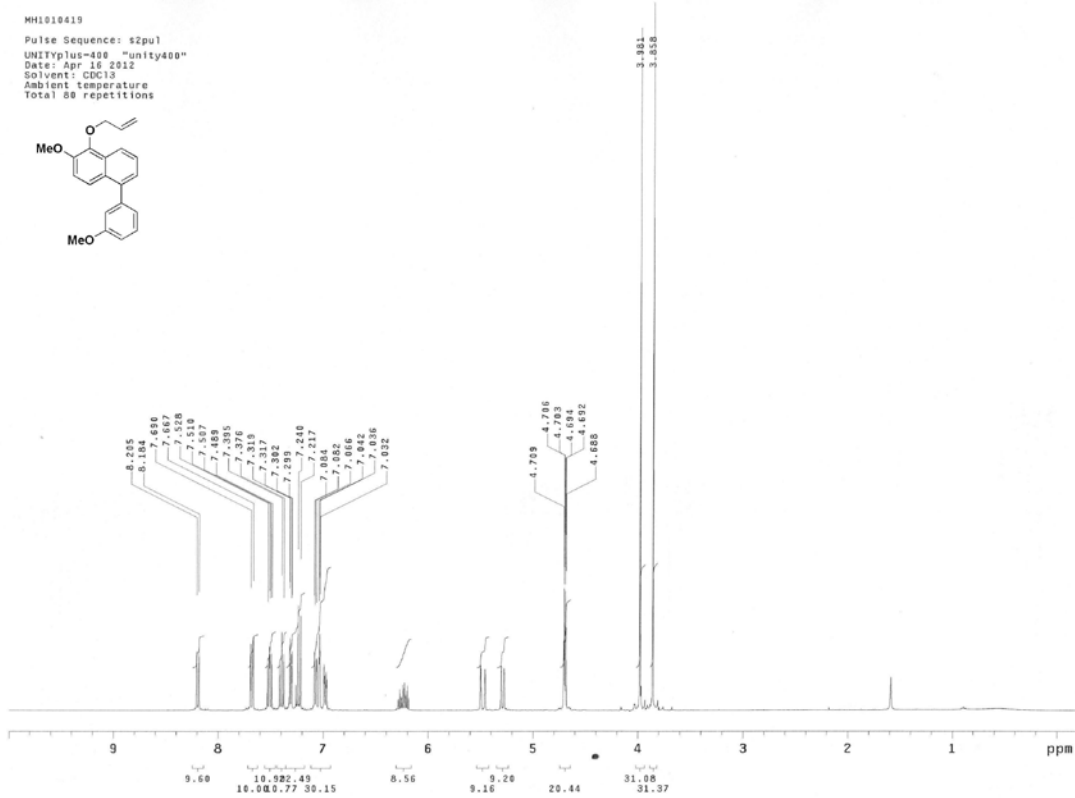
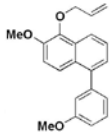


MH1010921  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Oct 8 2012  
Solvent: CDCl3  
Ambient temperature  
Total 138 repetitions

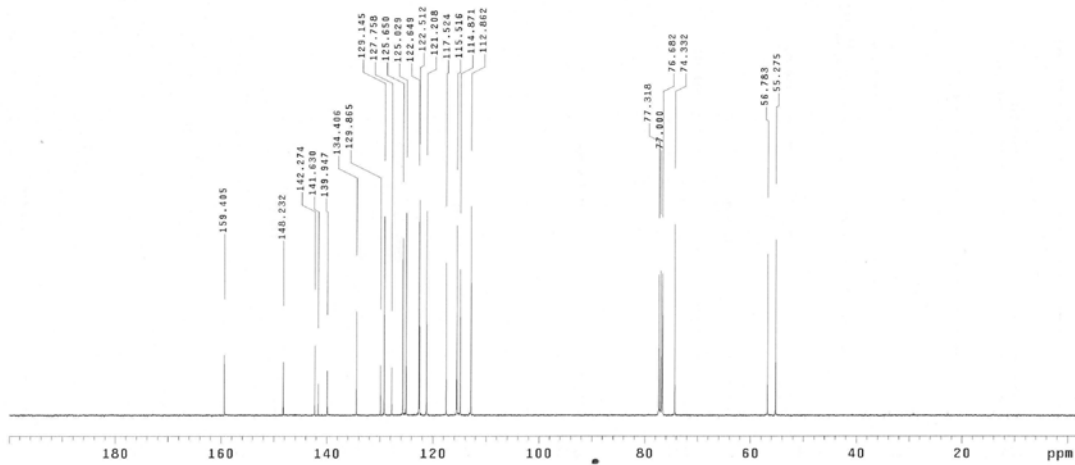
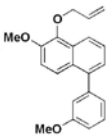


# Compound 5i

MH1010419  
 Pulse Sequence: s2pul  
 UNITYplus-400 "unity400"  
 Date: Apr 16 2012  
 Solvent: CDCl3  
 Ambient temperature  
 Total 80 repetitions

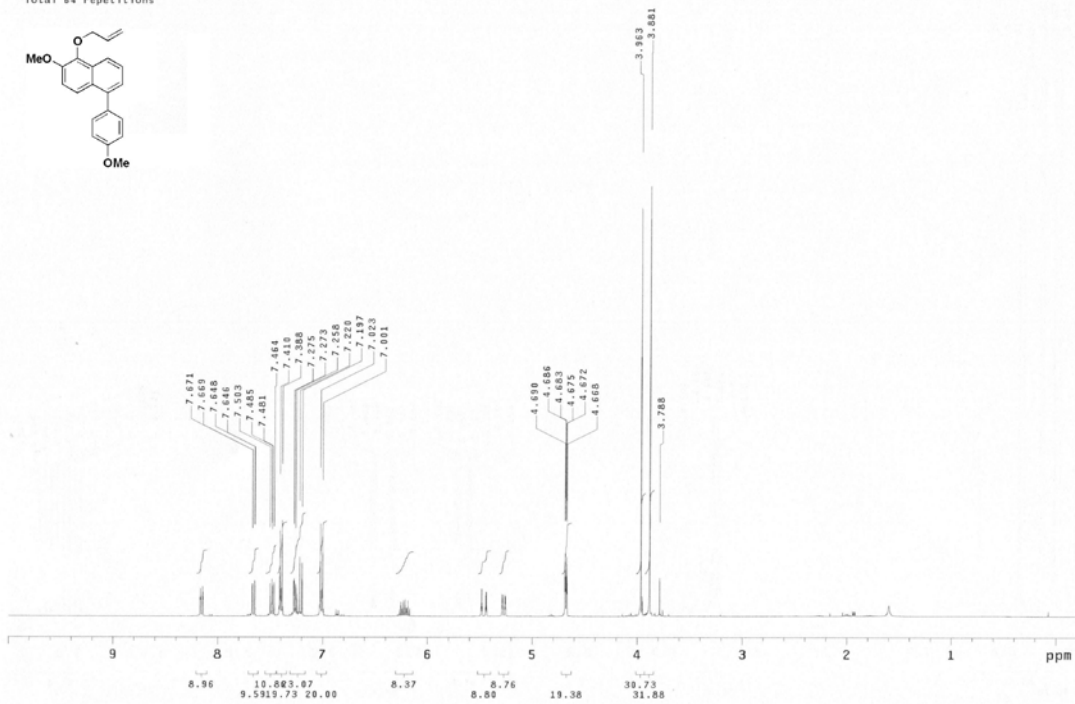
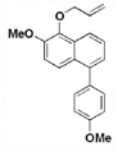


MH1010419  
 Pulse Sequence: s2pul  
 UNITYplus-400 "unity400"  
 Date: Apr 16 2012  
 Solvent: CDCl3  
 Ambient temperature  
 Total 14080 repetitions

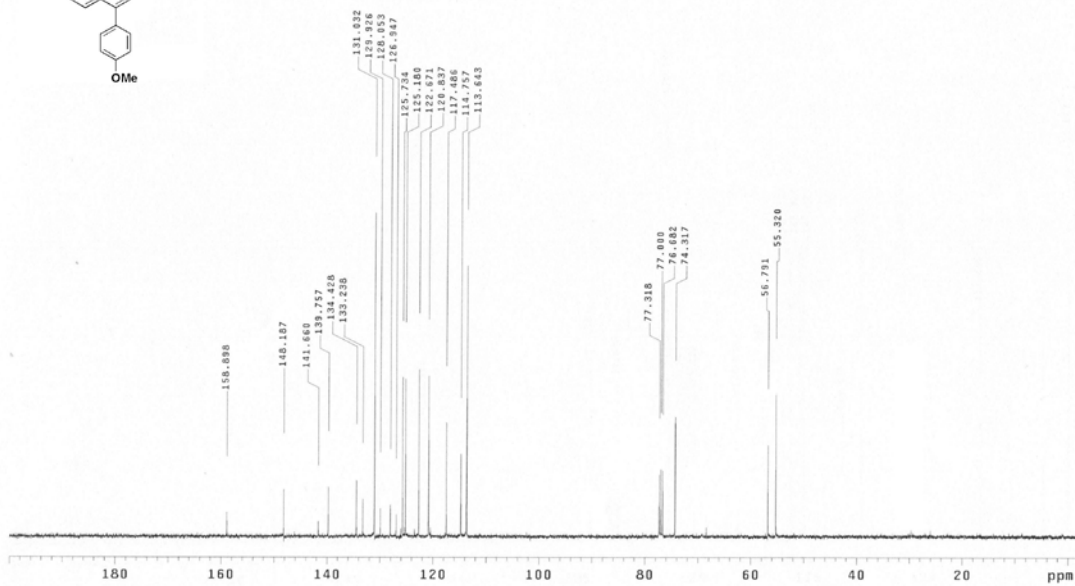
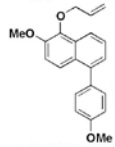


# Compound 5j

MH4NHM  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Jul 26 2012  
Solvent: CDCl3  
Ambient temperature  
Total 64 repetitions

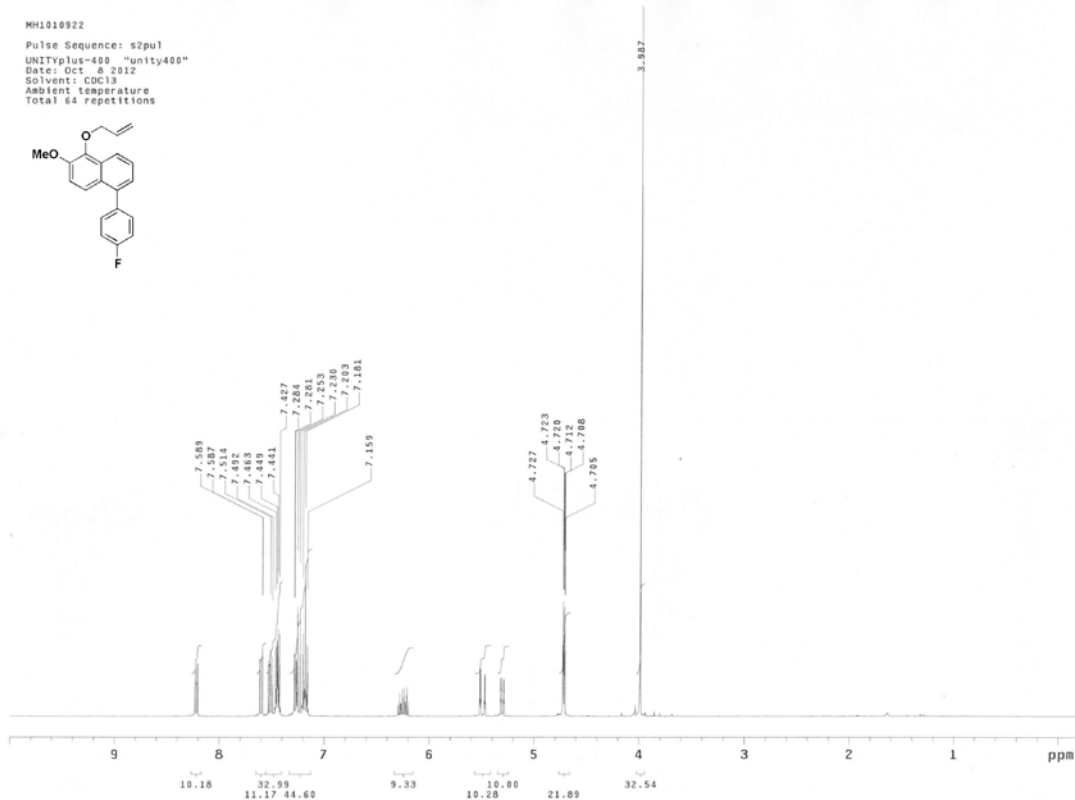
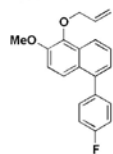


MH4NHM  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Jul 26 2012  
Solvent: CDCl3  
Ambient temperature  
Total 1984 repetitions

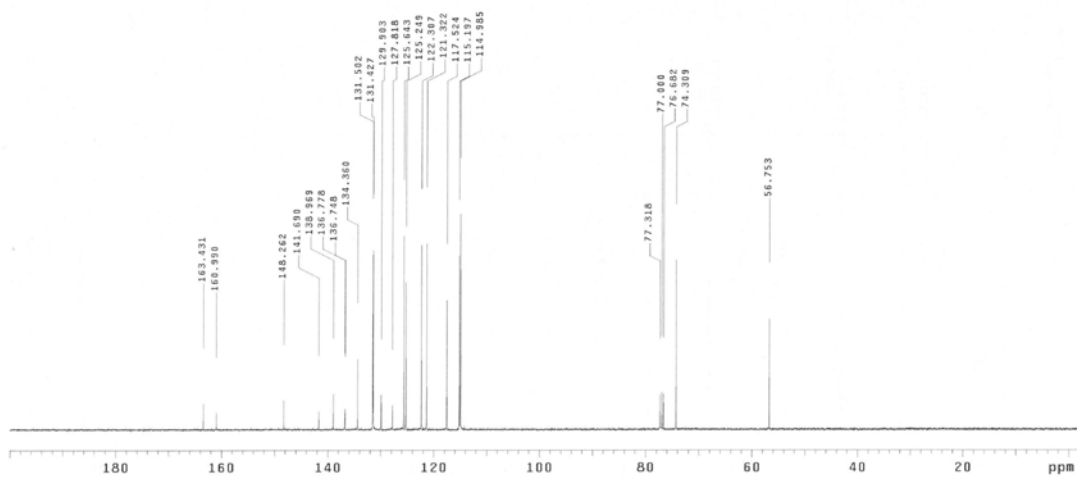
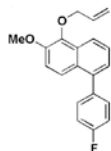


# Compound 5k

MH1010922  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Oct 8 2012  
Solvent: CDCl3  
Ambient temperature  
Total 64 repetitions



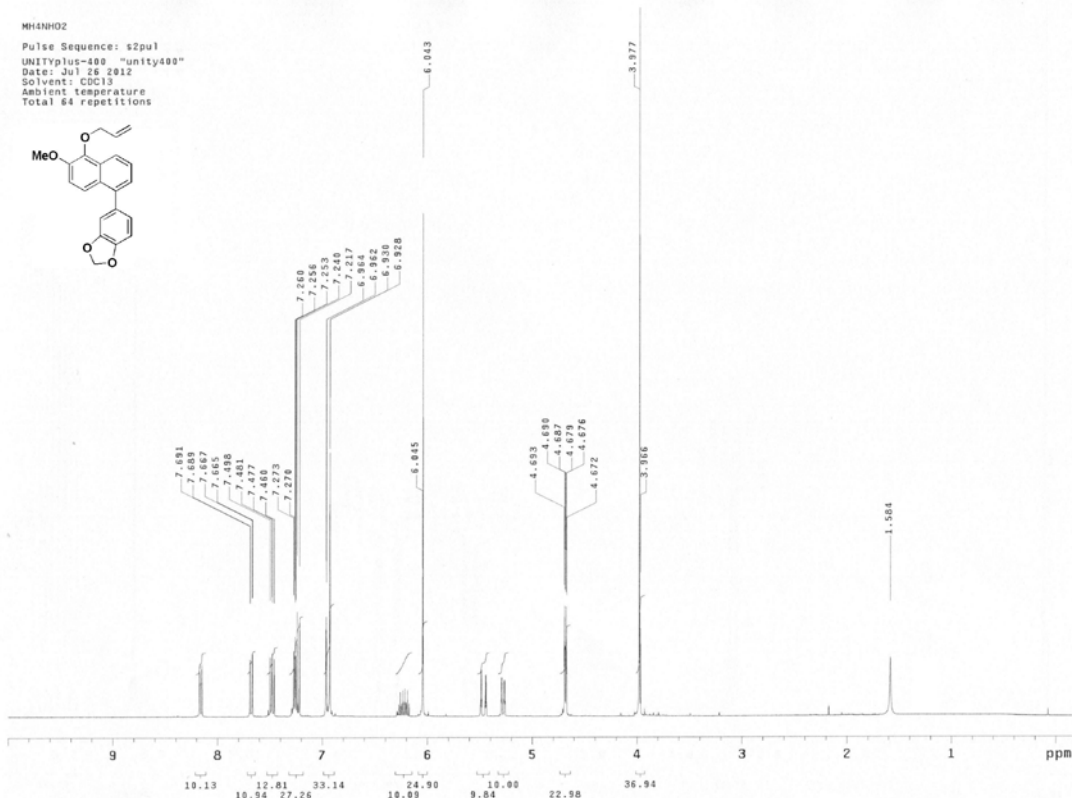
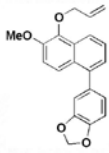
MH1010922  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Oct 8 2012  
Solvent: CDCl3  
Ambient temperature  
Total 1152 repetitions



# Compound 5l

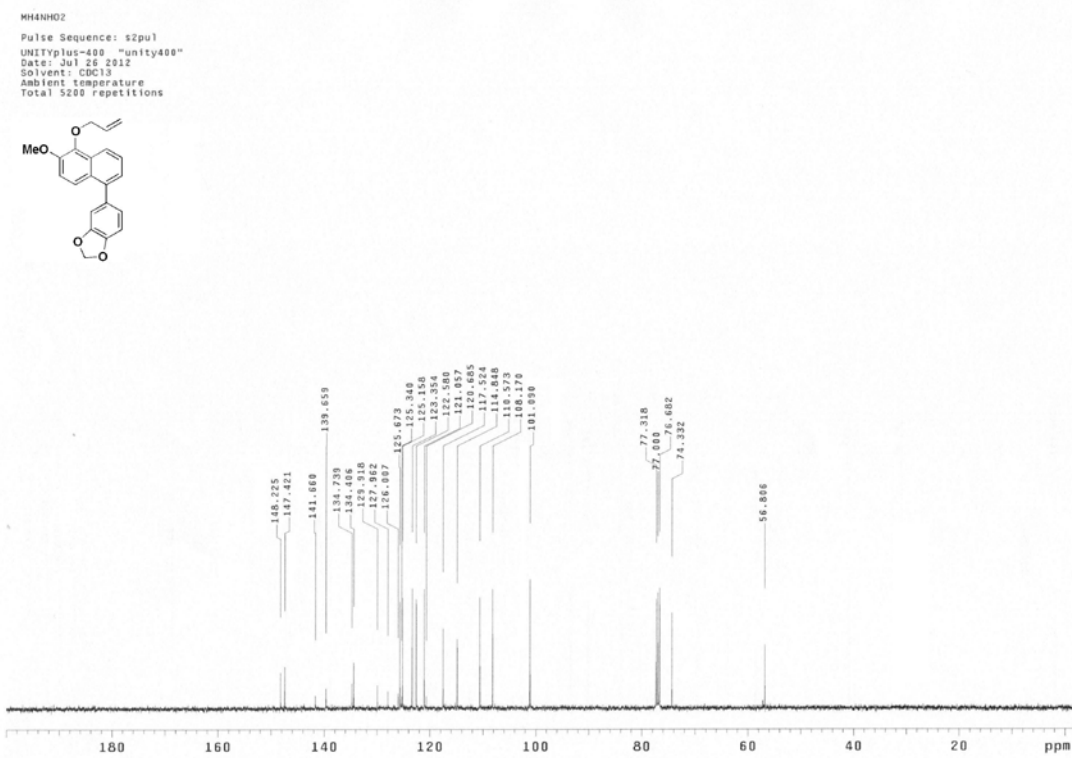
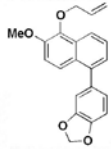
MH4NH02

Pulse Sequence: s2pul  
 UNITYplus-400 "unity400"  
 Date: Jul 26 2012  
 Solvent: CDCl3  
 Ambient temperature  
 Total 64 repetitions



MH4NH02

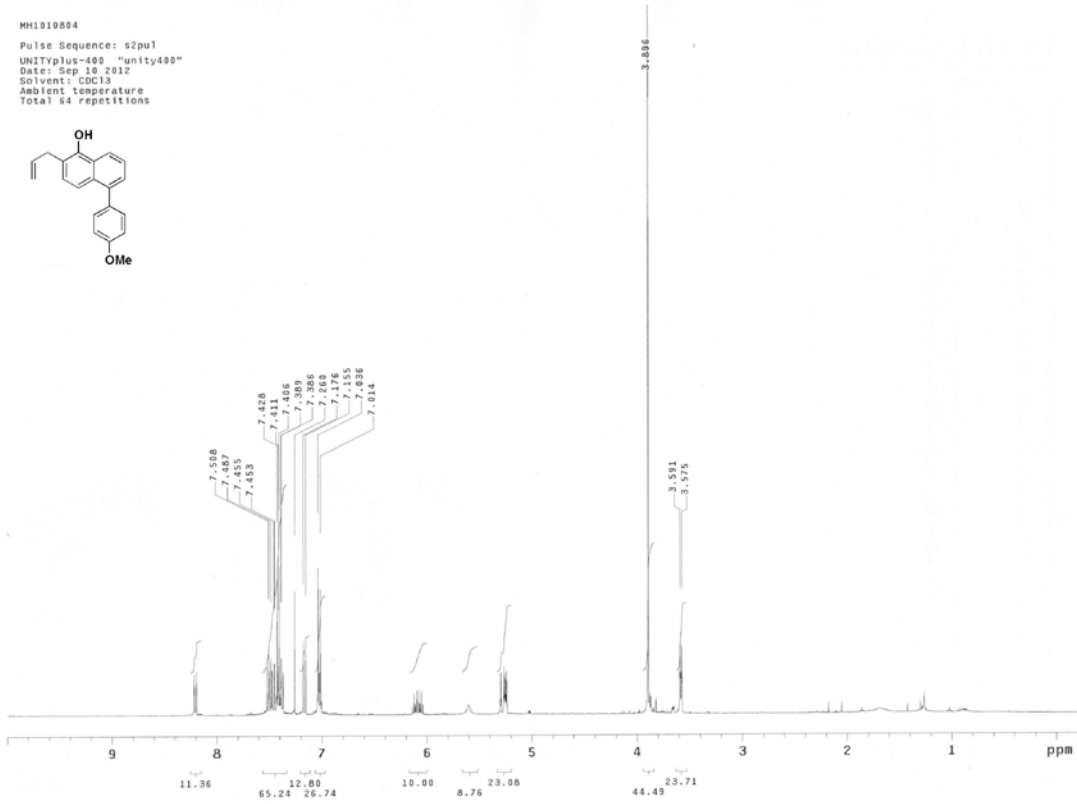
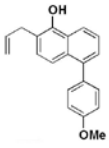
Pulse Sequence: s2pul  
 UNITYplus-400 "unity400"  
 Date: Jul 26 2012  
 Solvent: CDCl3  
 Ambient temperature  
 Total 5200 repetitions



# Compound 5m

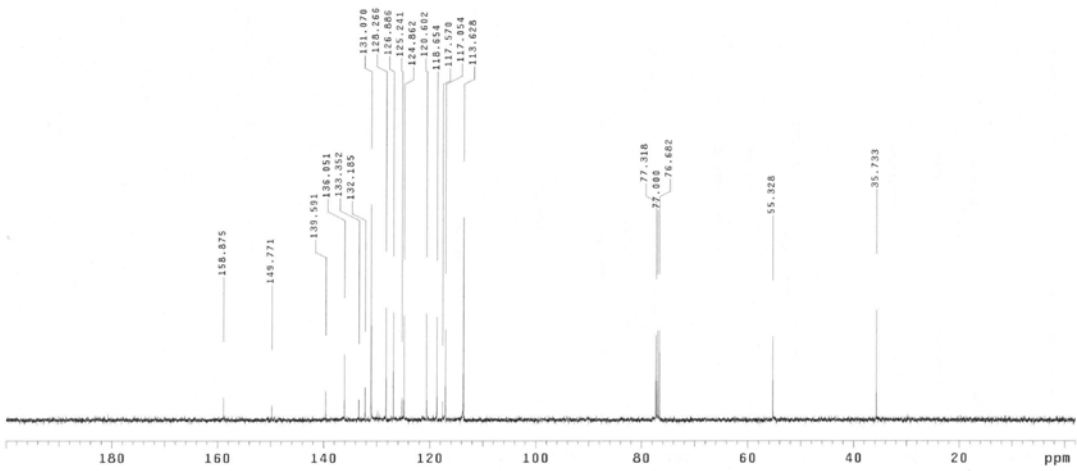
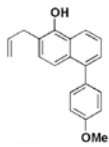
MH1010884

Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Sep 10 2012  
Solvent: CDCl3  
Ambient temperature  
Total 64 repetitions



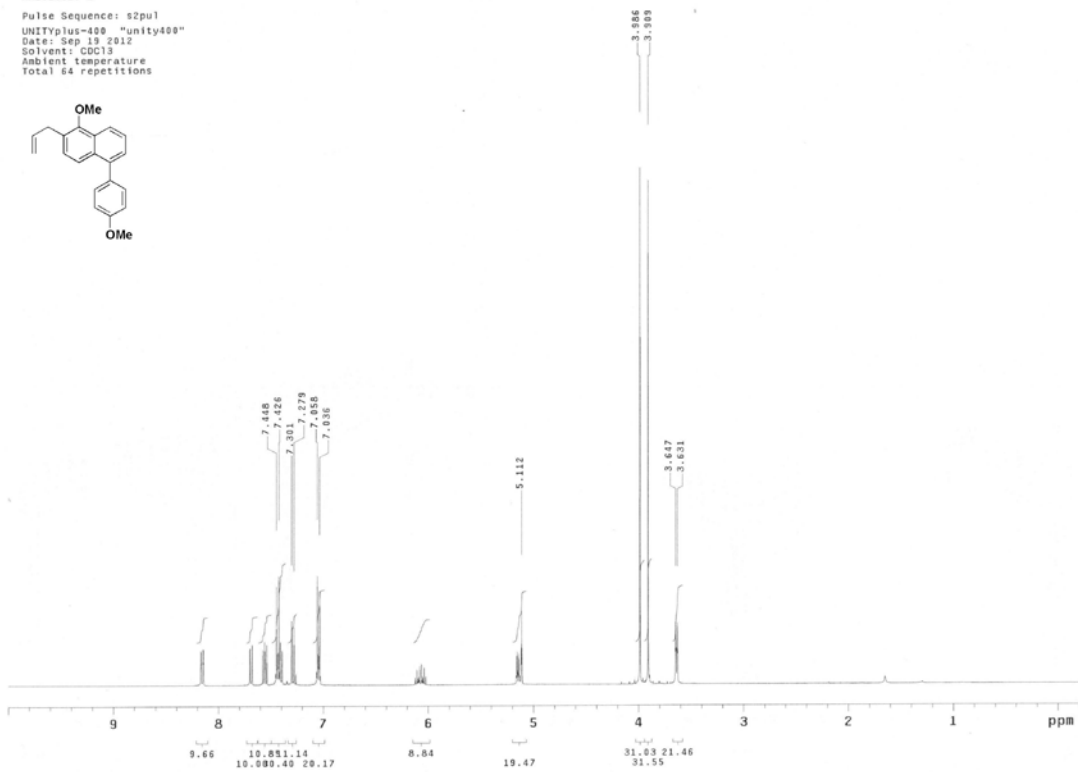
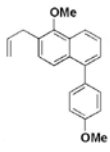
MH1010884

Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Sep 10 2012  
Solvent: CDCl3  
Ambient temperature  
Total 2008 repetitions

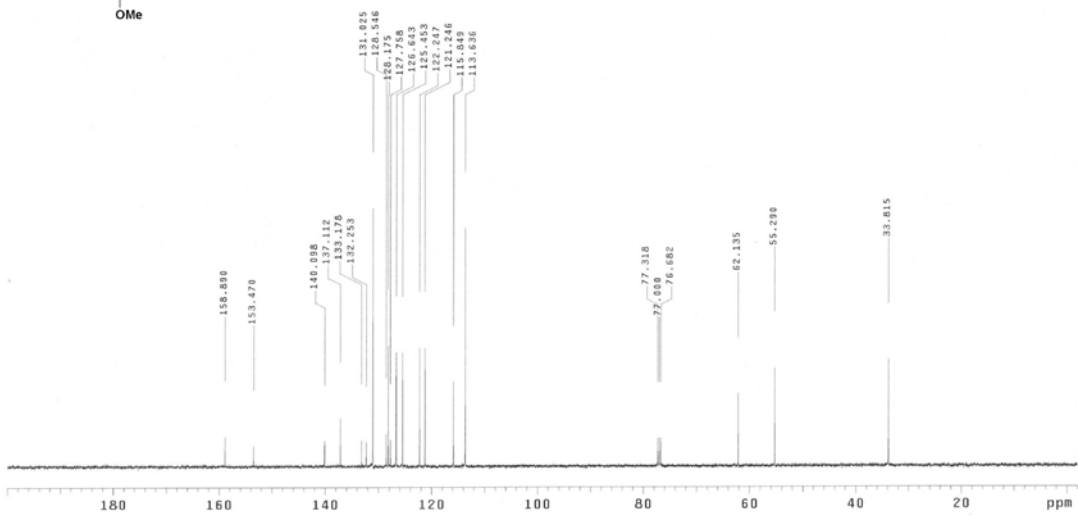
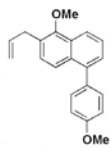


# Compound 5n

MH1010815-1  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Sep 19 2012  
Solvent: CDCl3  
Ambient temperature  
Total 64 repetitions



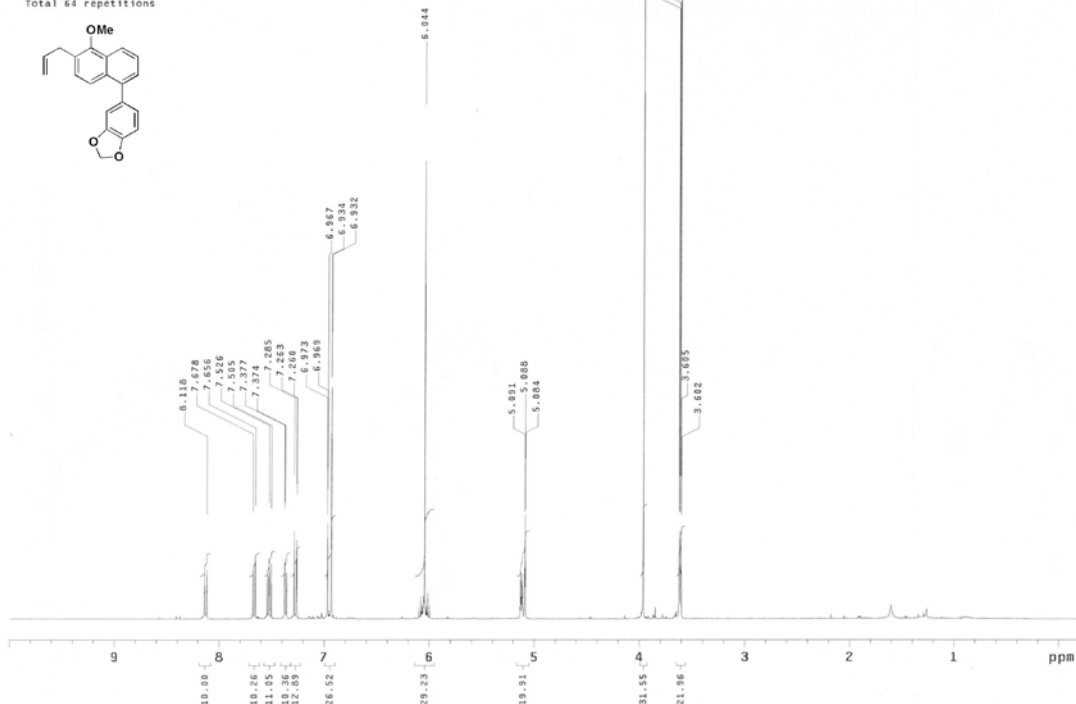
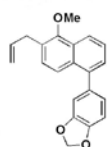
MH1010815-1  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Sep 19 2012  
Solvent: CDCl3  
Ambient temperature  
Total 256 repetitions



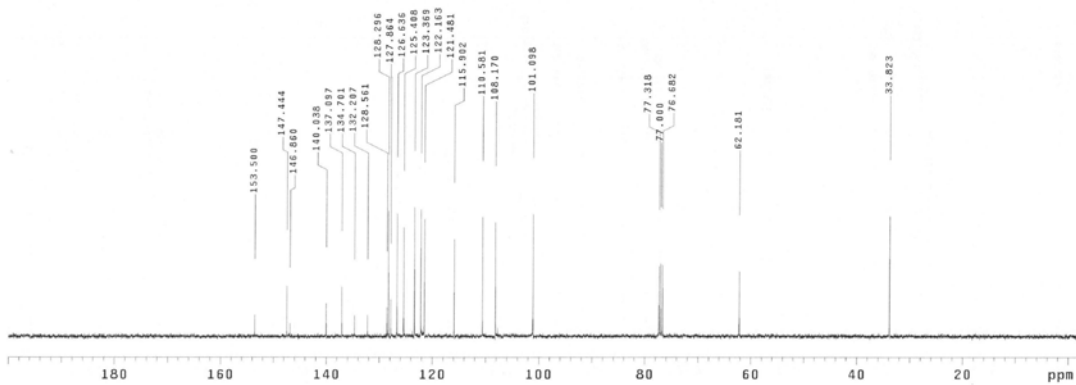
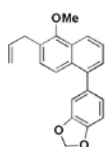


# Compound 5o

MH1010915-1  
 Pulse Sequence: s2pul  
 UNITYplus-400 "unity400"  
 Date: Oct 2 2012  
 Solvent: CDCl3  
 Ambient temperature  
 Total 64 repetitions

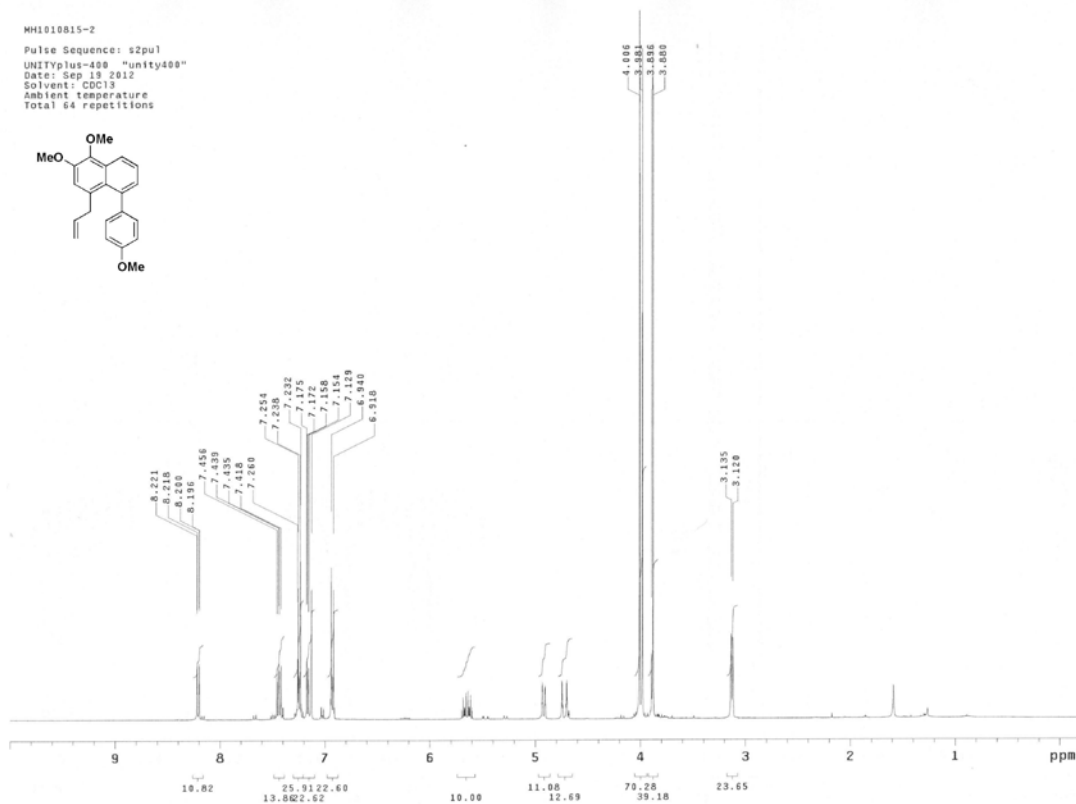
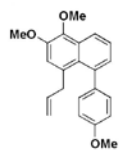


MH1010915-1  
 Pulse Sequence: s2pul  
 UNITYplus-400 "unity400"  
 Date: Oct 2 2012  
 Solvent: CDCl3  
 Ambient temperature  
 Total 2480 repetitions

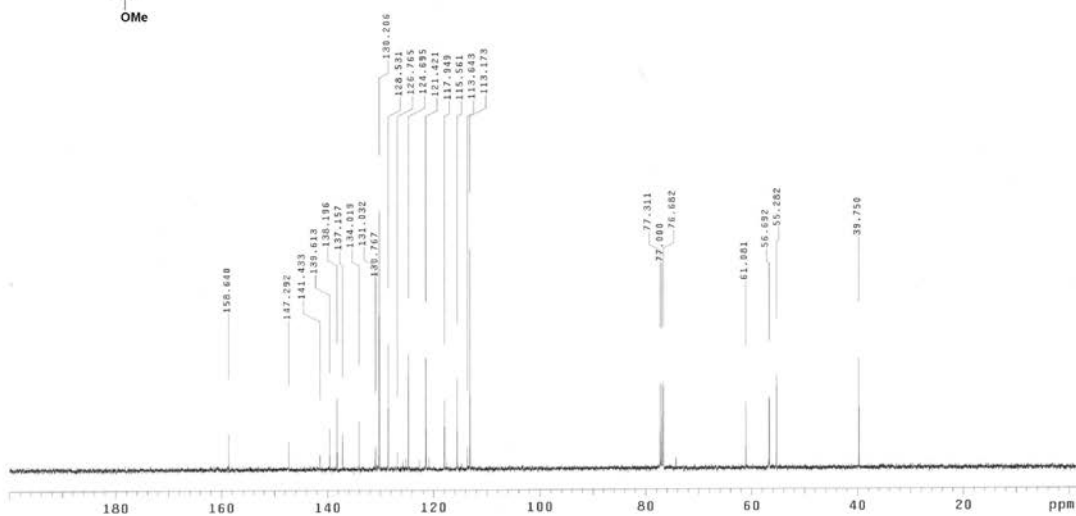
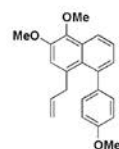


# Compound 7a

MH1010815-2  
 Pulse Sequence: s2pul  
 UNITYplus-400 "unity400"  
 Date: Sep 19 2012  
 Solvent: CDCl3  
 Ambient Temperature  
 Total 64 repetitions

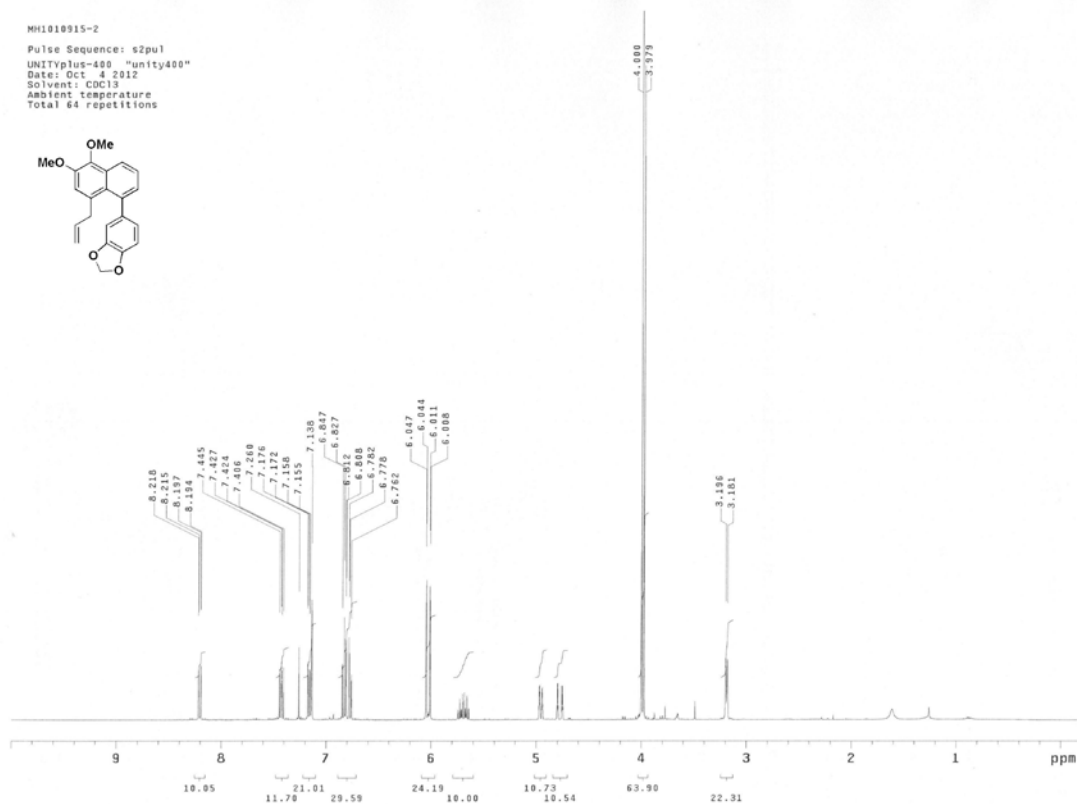
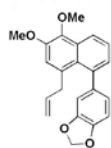


MH1010815-2  
 Pulse Sequence: s2pul  
 UNITYplus-400 "unity400"  
 Date: Sep 19 2012  
 Solvent: CDCl3  
 Ambient Temperature  
 Total 1568 repetitions

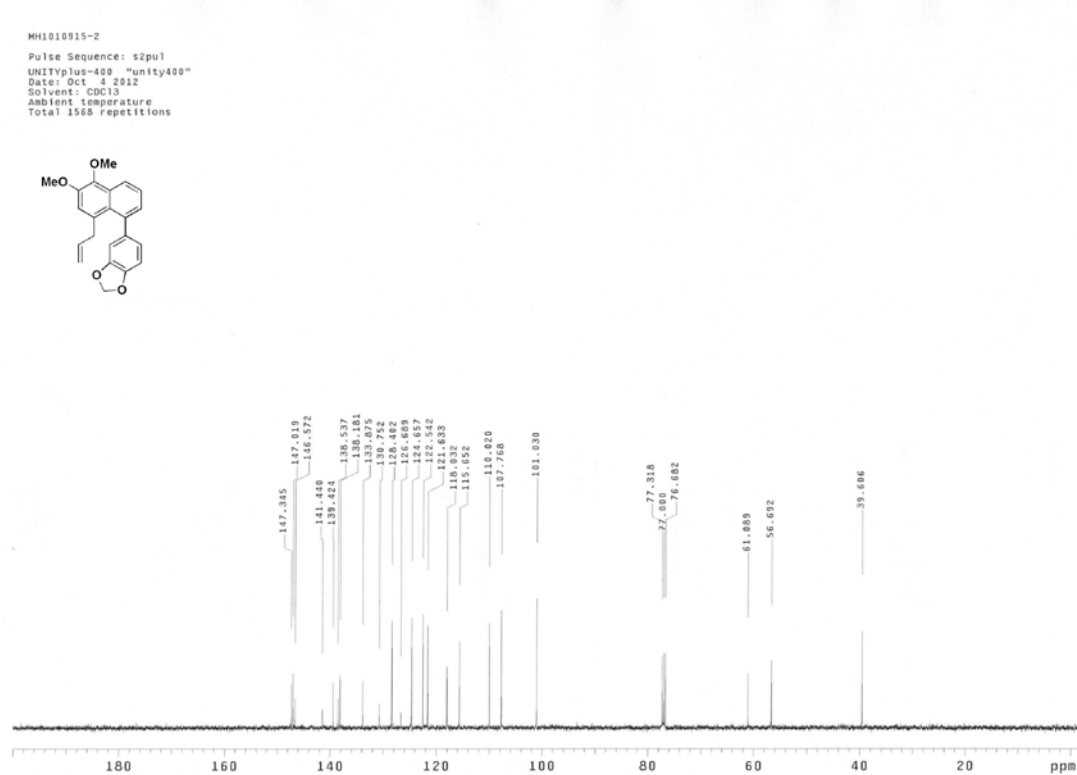
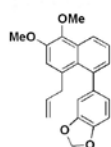


# Compound 7b

MH1010915-2  
 Pulse Sequence: s2pul  
 UNITYplus-400 "unity400"  
 Date: Oct 4 2012  
 Solvent: CDCl3  
 Ambient temperature  
 Total 64 repetitions

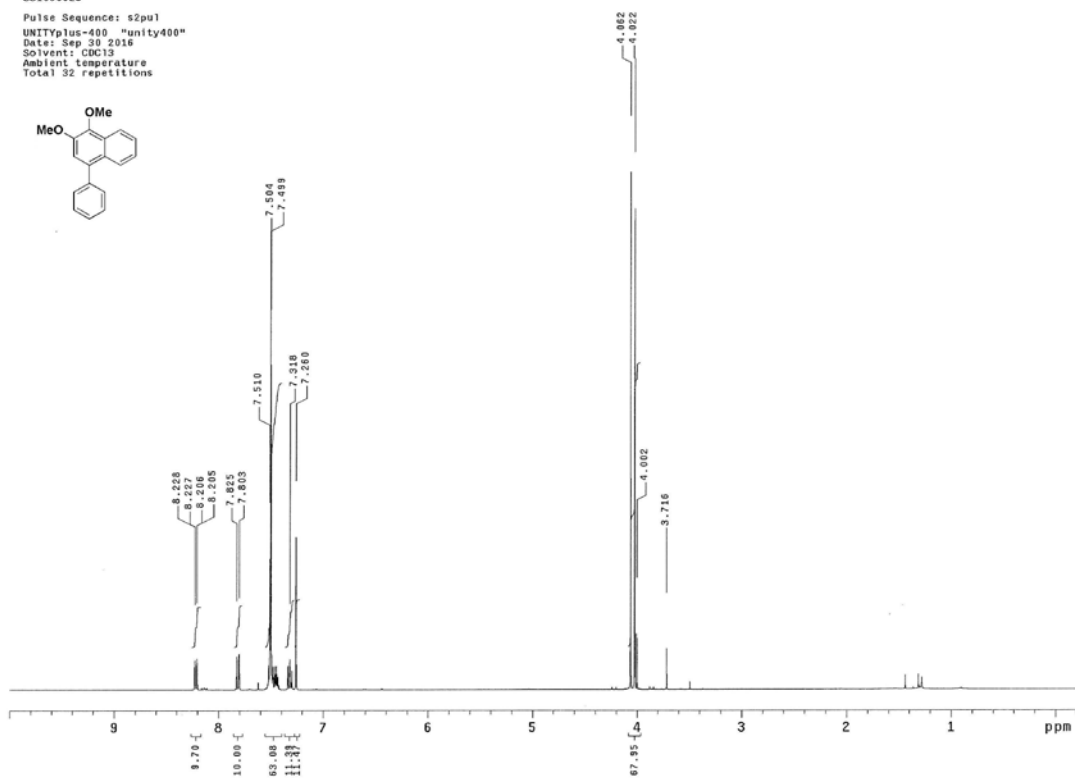
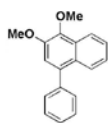


MH1010915-2  
 Pulse Sequence: s2pul  
 UNITYplus-400 "unity400"  
 Date: Oct 4 2012  
 Solvent: CDCl3  
 Ambient temperature  
 Total 1568 repetitions

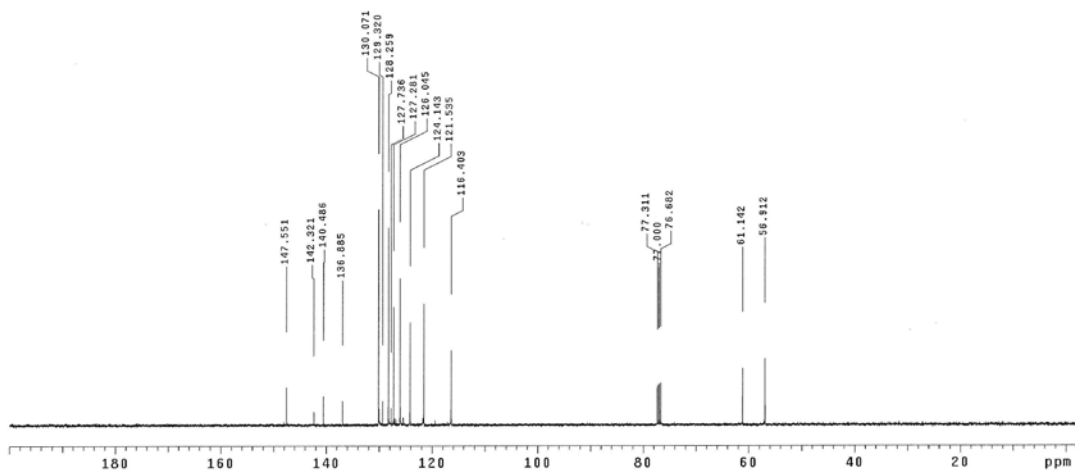
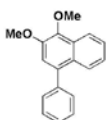


# Compound 8a

SS1050928  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Sep 30 2016  
Solvent: CDCl3  
Ambient temperature  
Total 32 repetitions

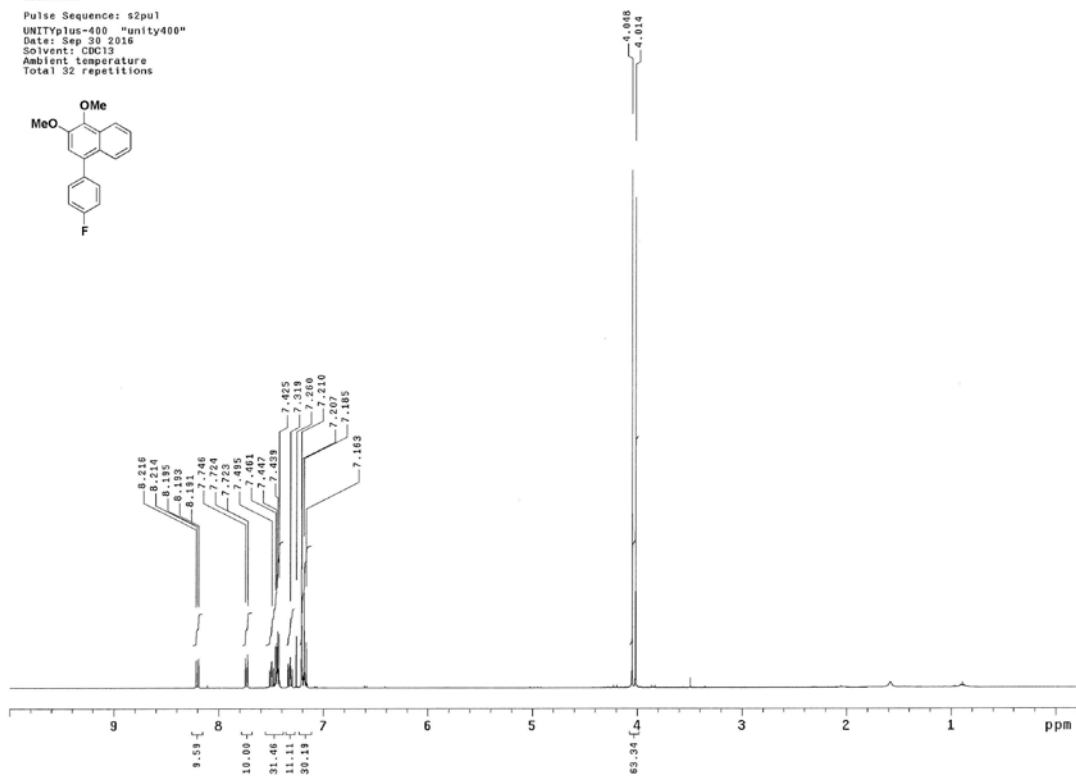
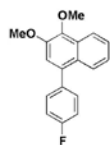


SS1050928  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Sep 30 2016  
Solvent: CDCl3  
Ambient temperature  
Total 1200 repetitions

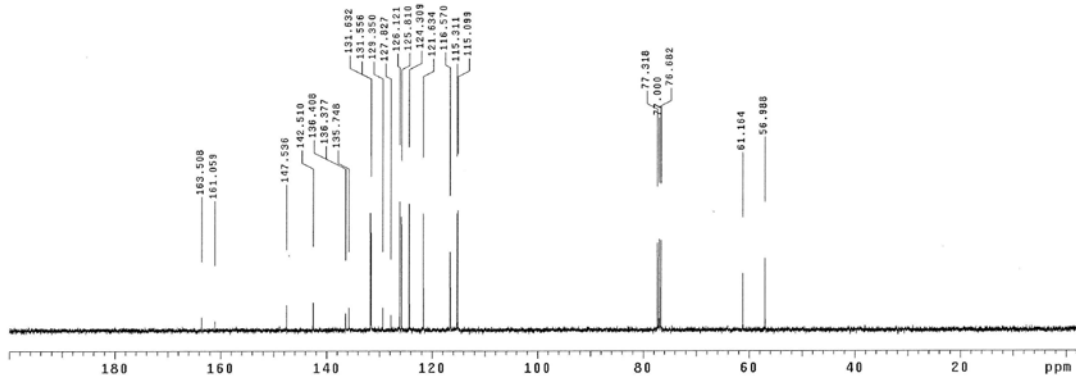
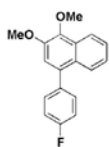


# Compound 8b

SS1050929  
 Pulse Sequence: s2pul  
 UNITYplus-400 "unity400"  
 Date: Sep 30 2016  
 Solvent: CDCl3  
 Ambient temperature  
 Total 32 repetitions

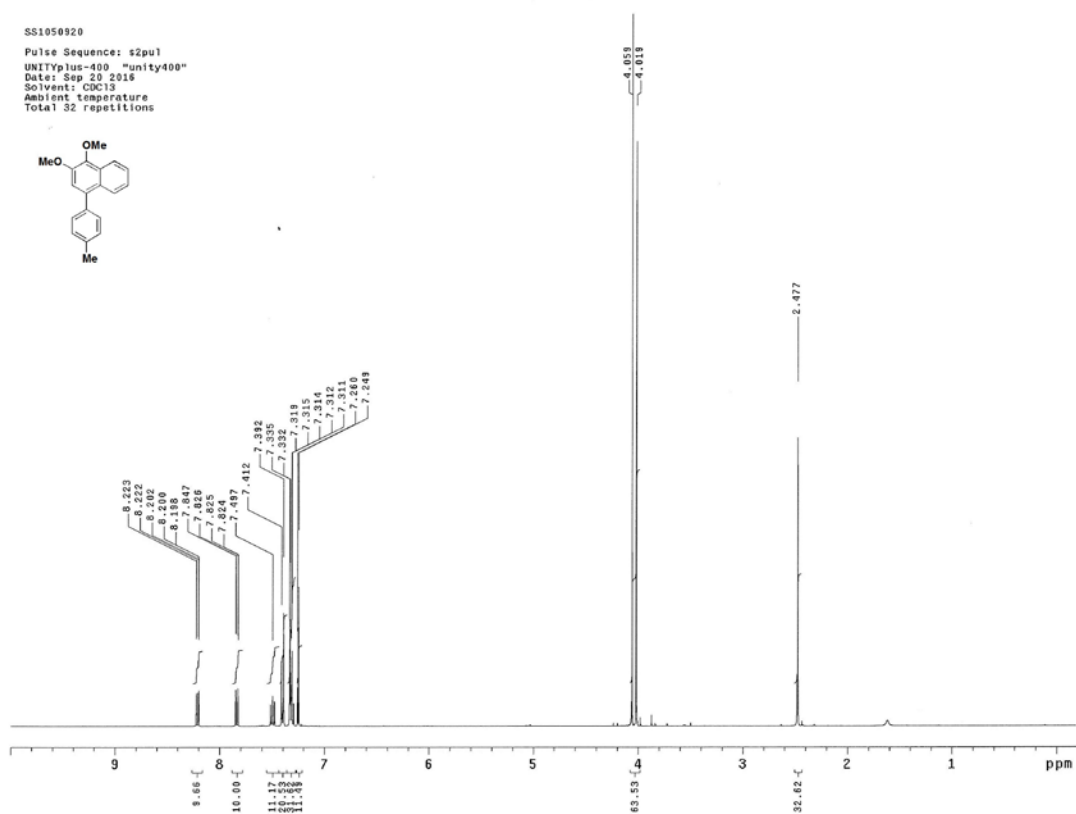
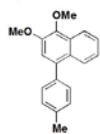


SS1050929  
 Pulse Sequence: s2pul  
 UNITYplus-400 "unity400"  
 Date: Sep 30 2016  
 Solvent: CDCl3  
 Ambient temperature  
 Total 1455 repetitions

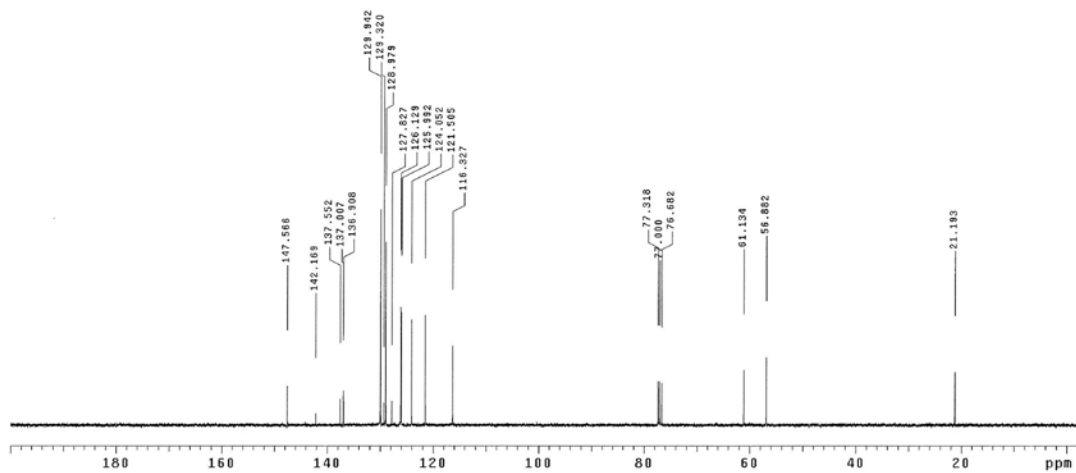
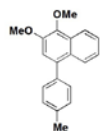


# Compound 8c

SS1050920  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Sep 20 2016  
Solvent: CDCl3  
Ambient temperature  
Total 32 repetitions

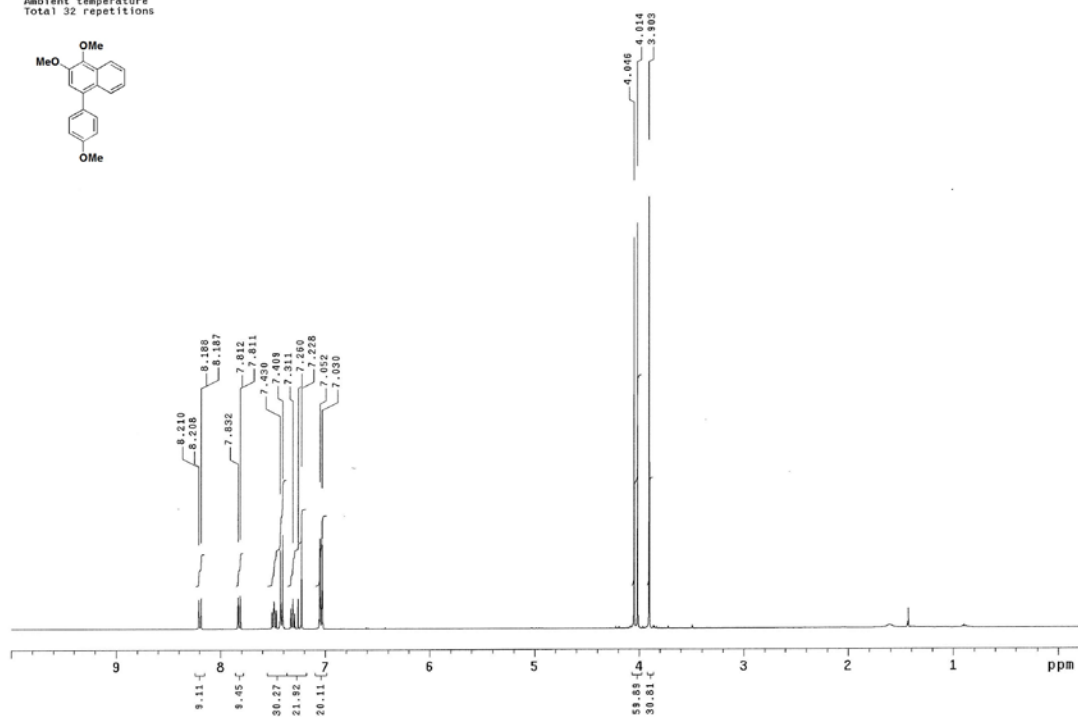
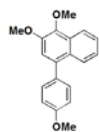


SS1050920  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Sep 20 2016  
Solvent: CDCl3  
Ambient temperature  
Total 640 repetitions

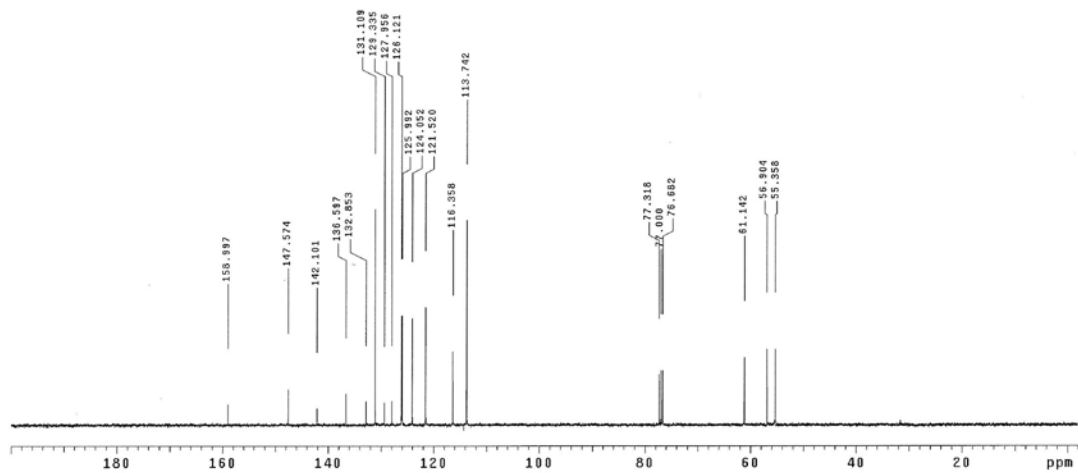
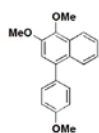


# Compound 8d

SS1051006  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Oct 6 2016  
Solvent: CDCl3  
Ambient temperature  
Total 32 repetitions

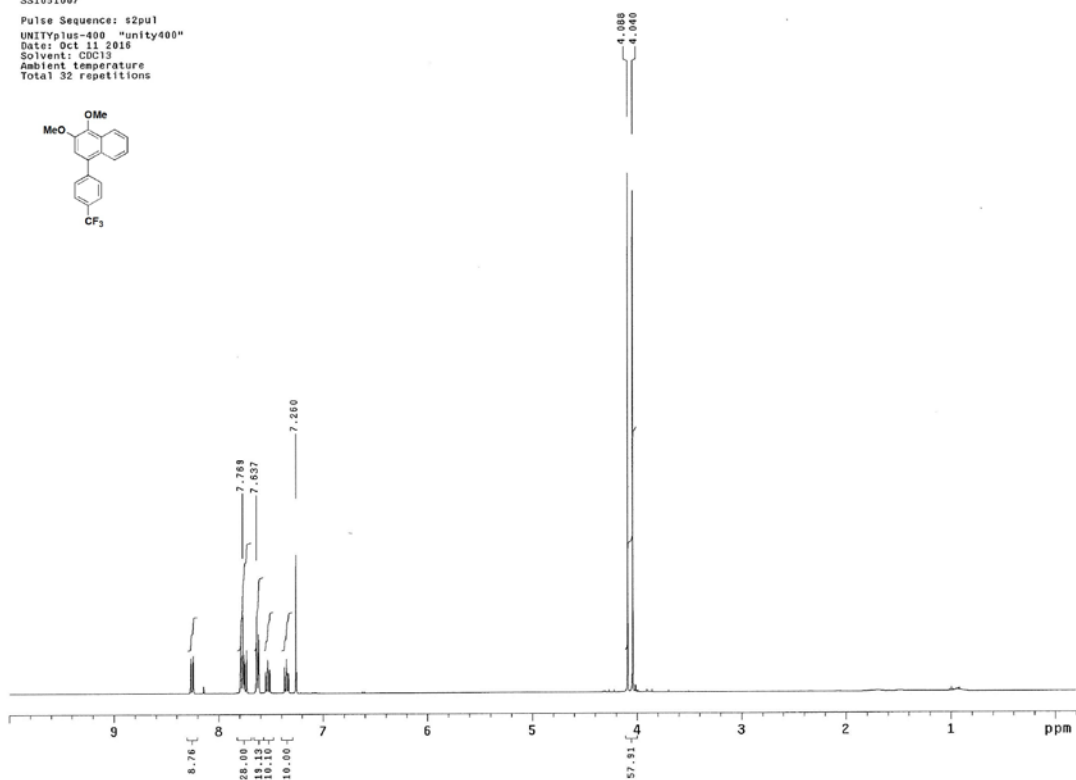
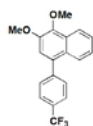


SS1051006  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Oct 6 2016  
Solvent: CDCl3  
Ambient temperature  
Total 1312 repetitions

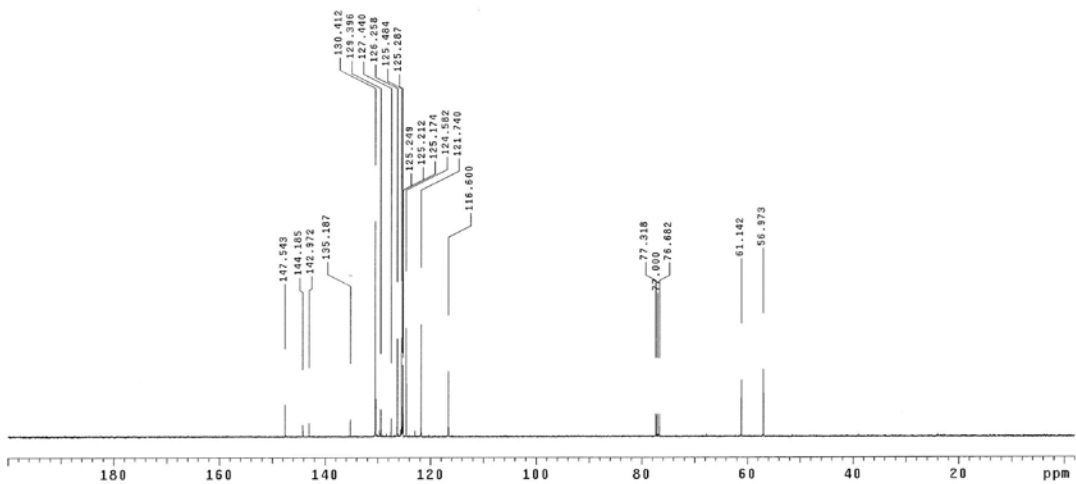
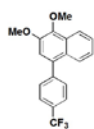


# Compound 8e

SS1051007  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Oct 11 2016  
Solvent: CDCl3  
Ambient temperature  
Total 32 repetitions



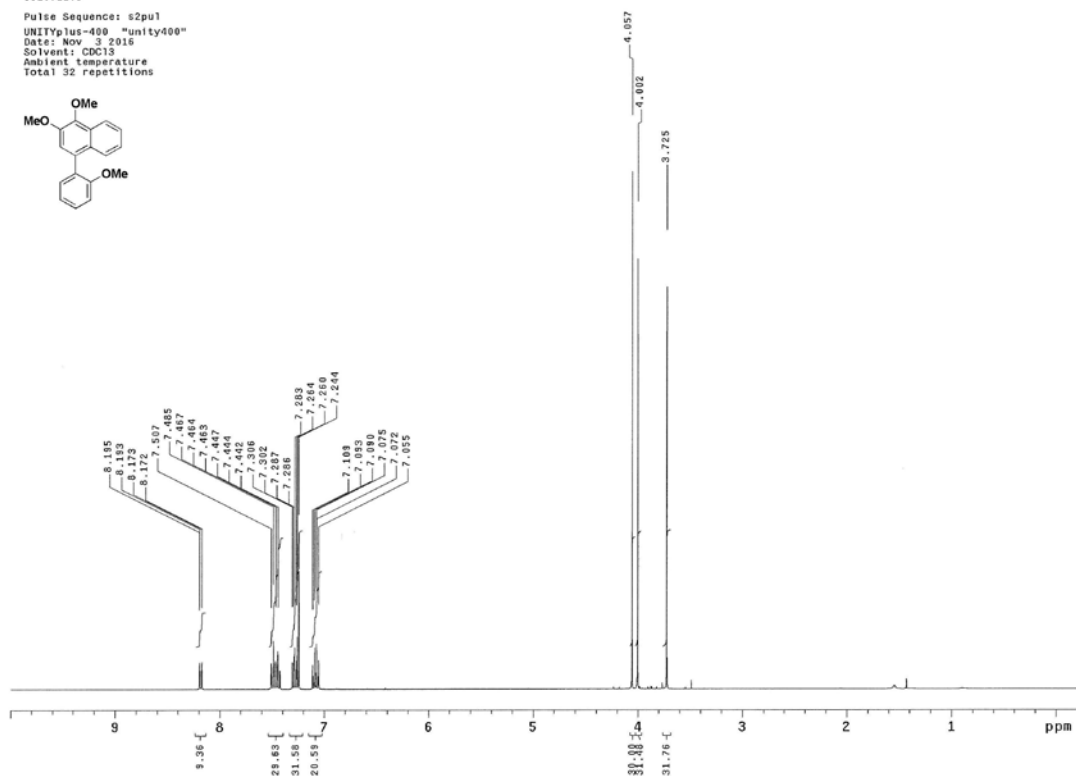
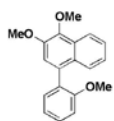
SS1051007  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Oct 11 2016  
Solvent: CDCl3  
Ambient temperature  
Total 480 repetitions



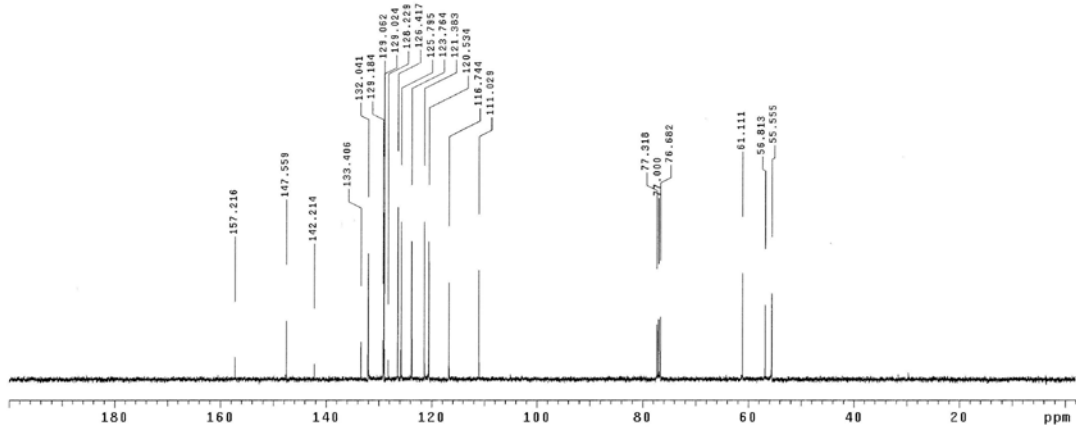
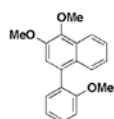


# Compound 8f

SS1051103  
 Pulse Sequence: s2pul  
 UNITYplus-400 "unity400"  
 Date: Nov 3 2016  
 Solvent: CDCl3  
 Ambient temperature  
 Total 32 repetitions

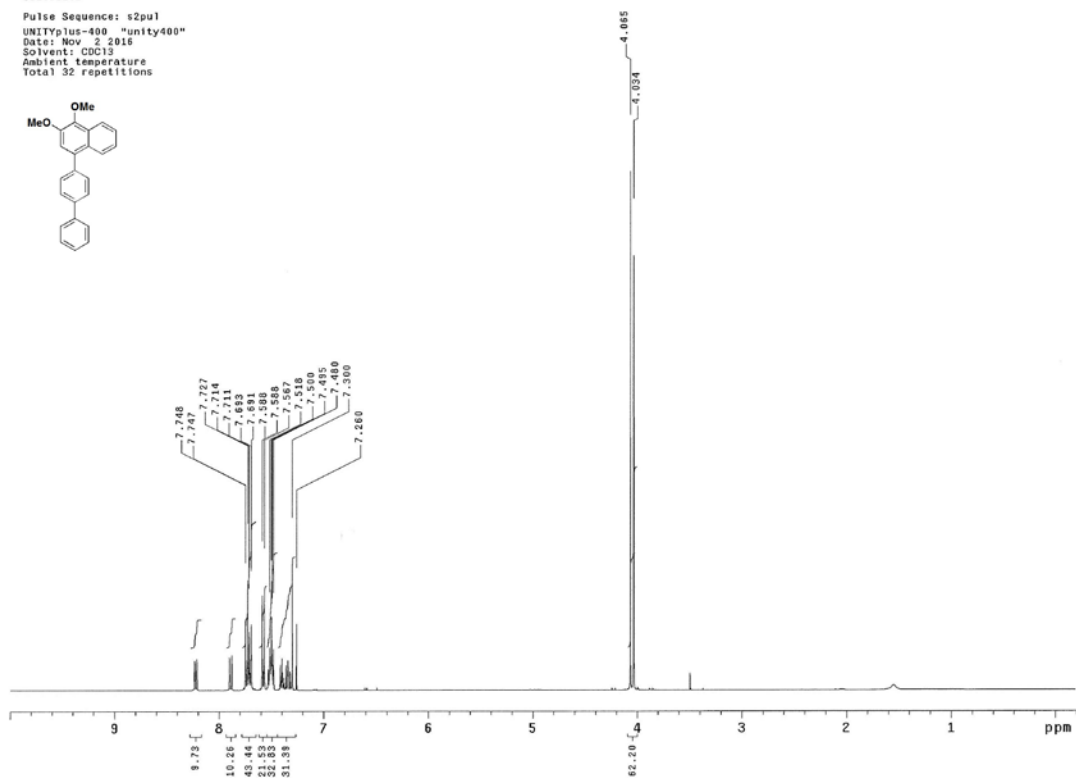
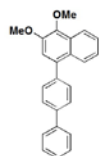


SS1051103  
 Pulse Sequence: s2pul  
 UNITYplus-400 "unity400"  
 Date: Nov 3 2016  
 Solvent: CDCl3  
 Ambient temperature  
 Total 1568 repetitions

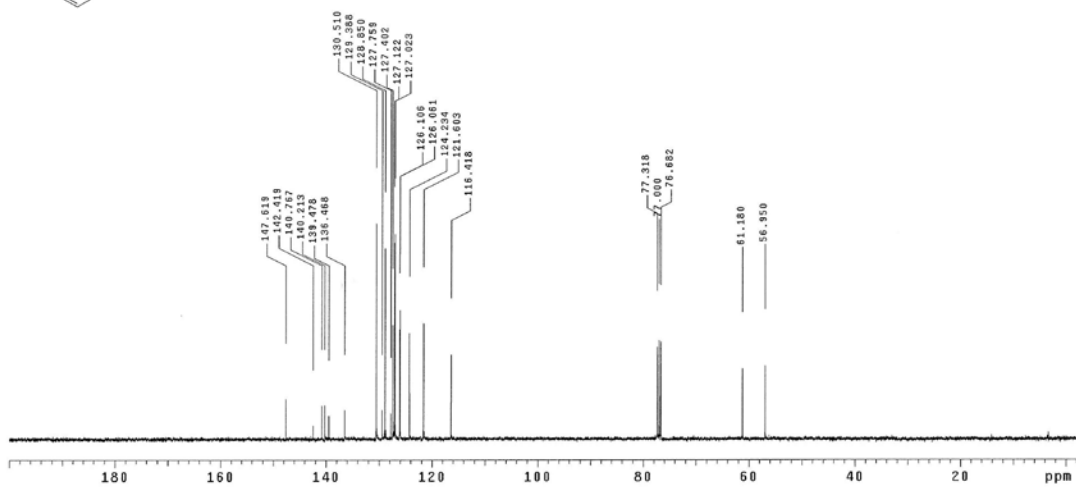
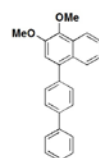


# Compound 8g

SS1051102  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Nov 2 2016  
Solvent: CDCl3  
Ambient temperature  
Total 32 repetitions



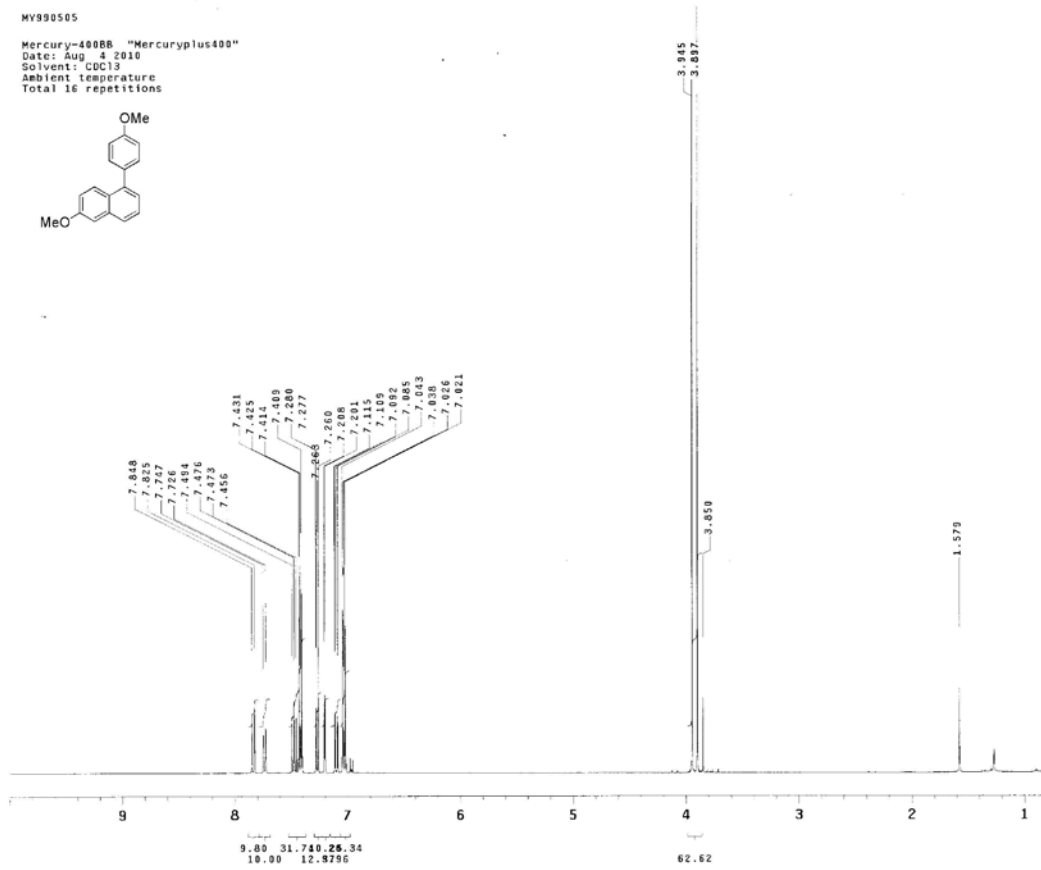
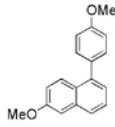
SS1051102  
Pulse Sequence: s2pul  
UNITYplus-400 "unity400"  
Date: Nov 2 2016  
Solvent: CDCl3  
Ambient temperature  
Total 3120 repetitions



# Compound 9a

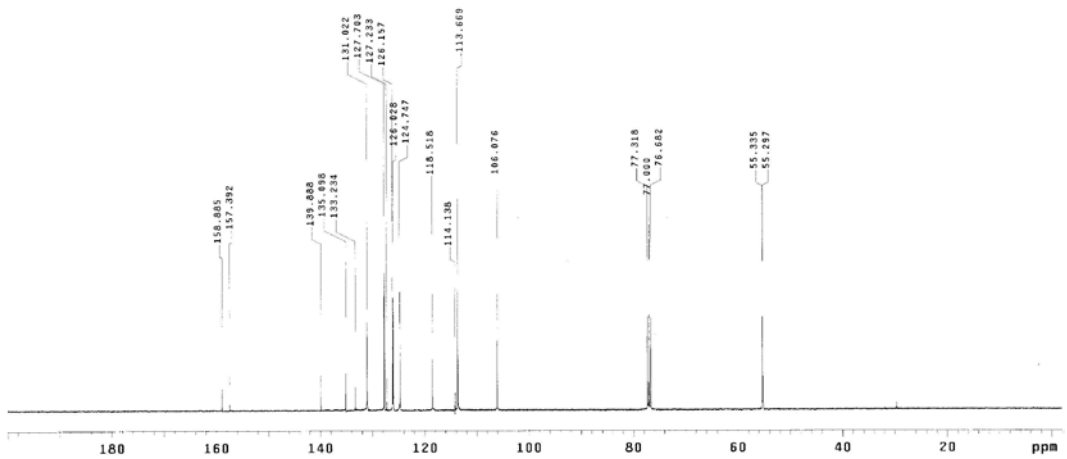
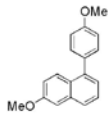
MY990505

Mercury-40088 "Mercuryplus400"  
Date: Aug 4 2010  
Solvent: CDCl3  
Ambient temperature  
Total 16 repetitions

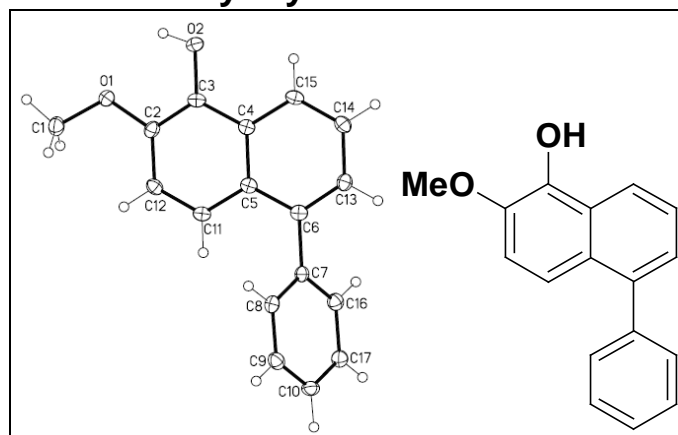


MY990505

Mercury-40088 "Mercuryplus400"  
Date: Aug 4 2010  
Solvent: CDCl3  
Ambient temperature  
Total 32000 repetitions

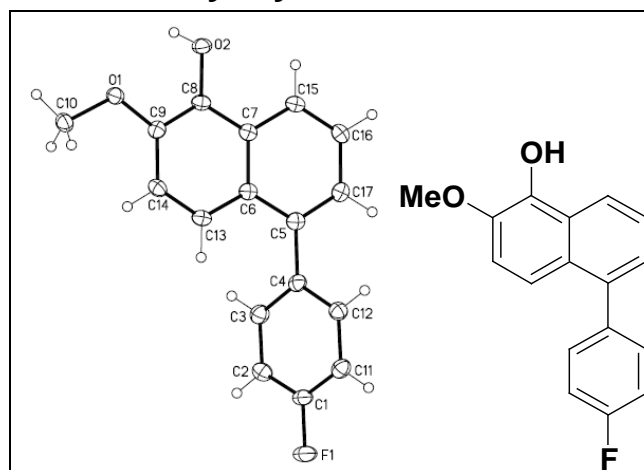


## X-ray crystal data of 5e



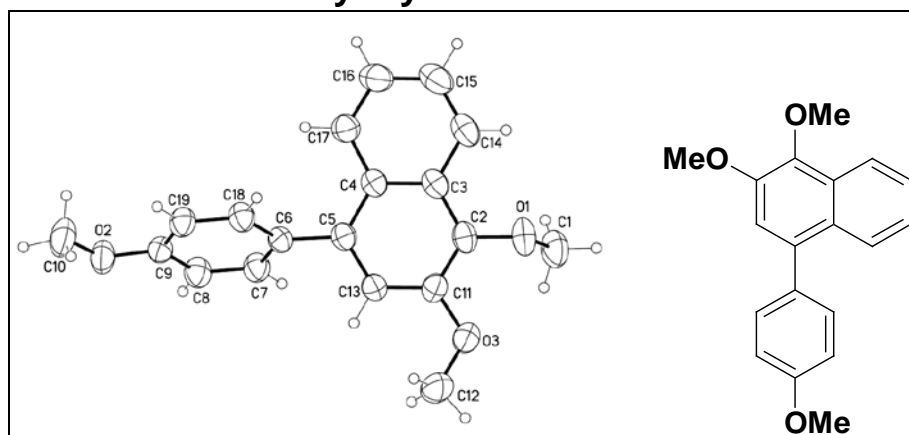
Empirical formula	C <sub>17</sub> H <sub>14</sub> O <sub>2</sub>	
Formula weight	250.28	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	F d d 2	
Unit cell dimensions	a = 13.3885(3) Å	α = 90°.
	b = 66.3135(18) Å	β = 90°.
	c = 5.5816(2) Å	γ = 90°.
Volume	4955.6(2) Å <sup>3</sup>	
Z	16	
Density (calculated)	1.342 Mg/m <sup>3</sup>	
Absorption coefficient	0.087 mm <sup>-1</sup>	
F(000)	2112	
Crystal size	0.25 x 0.25 x 0.12 mm <sup>3</sup>	
Theta range for data collection	1.23 to 26.39°.	
Index ranges	-10 ≤ h ≤ 16, -82 ≤ k ≤ 82, -6 ≤ l ≤ 6	
Reflections collected	11029	
Independent reflections	2518 [R(int) = 0.0603]	
Completeness to theta = 26.39°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9486 and 0.8690	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	2518 / 1 / 174	
Goodness-of-fit on F <sup>2</sup>	1.168	
Final R indices [I > 2σ(I)]	R <sub>1</sub> = 0.0325, wR <sub>2</sub> = 0.0807	
R indices (all data)	R <sub>1</sub> = 0.0428, wR <sub>2</sub> = 0.1154	
Absolute structure parameter	0.2(13)	
Largest diff. peak and hole	0.404 and -0.542 e.Å <sup>-3</sup>	

## X-ray crystal data of 5f



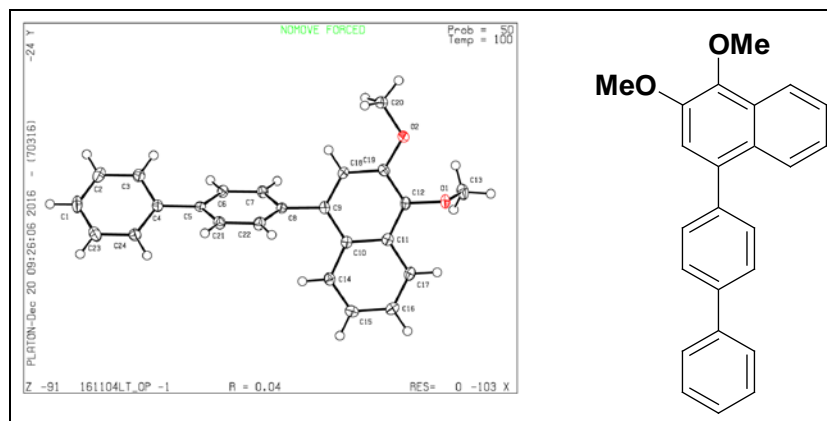
Empirical formula	C <sub>17</sub> H <sub>13</sub> F O <sub>2</sub>	
Formula weight	268.27	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 6.7021(11) Å	α = 85.327(6)°.
	b = 7.9371(12) Å	β = 80.530(6)°.
	c = 12.170(2) Å	γ = 82.517(6)°.
Volume	631.92(18) Å <sup>3</sup>	
Z	2	
Density (calculated)	1.410 Mg/m <sup>3</sup>	
Absorption coefficient	0.101 mm <sup>-1</sup>	
F(000)	280	
Crystal size	0.18 x 0.10 x 0.10 mm <sup>3</sup>	
Theta range for data collection	1.70 to 26.38°.	
Index ranges	-8 ≤ h ≤ 7, -9 ≤ k ≤ 7, -15 ≤ l ≤ 15	
Reflections collected	9259	
Independent reflections	2547 [R(int) = 0.0243]	
Completeness to theta = 26.38°	98.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9486 and 0.9019	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	2547 / 0 / 183	
Goodness-of-fit on F <sup>2</sup>	1.089	
Final R indices [I > 2σ(I)]	R1 = 0.0343, wR2 = 0.0907	
R indices (all data)	R1 = 0.0431, wR2 = 0.1097	
Largest diff. peak and hole	0.231 and -0.223 e.Å <sup>-3</sup>	

## X-ray crystal data of 8d



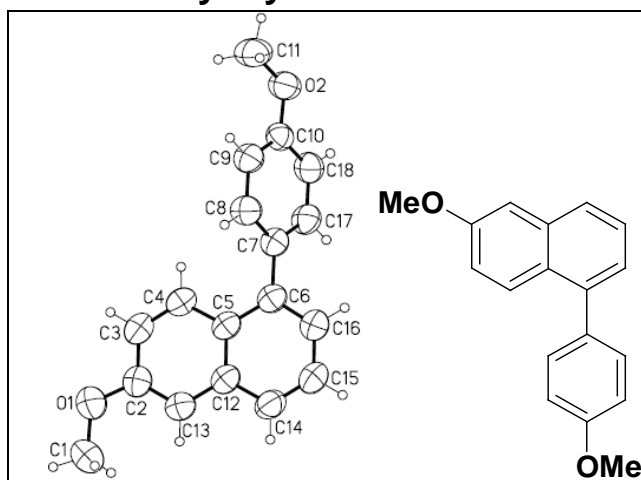
Empirical formula	C <sub>19</sub> H <sub>18</sub> O <sub>3</sub>	
Formula weight	294.33	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2 <sub>1</sub> /c	
Unit cell dimensions	a = 13.3450(12) Å	α = 90°.
	b = 15.2538(14) Å	β = 99.819(2)°.
	c = 7.5723(7) Å	γ = 90°.
Volume	1518.9(2) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.287 Mg/m <sup>3</sup>	
Absorption coefficient	0.086 mm <sup>-1</sup>	
F(000)	624	
Crystal size	0.15 x 0.10 x 0.10 mm <sup>3</sup>	
Theta range for data collection	2.045 to 26.421°.	
Index ranges	-16 ≤ h ≤ 16, -18 ≤ k ≤ 19, -9 ≤ l ≤ 4	
Reflections collected	12198	
Independent reflections	3116 [R(int) = 0.0580]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.8689	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	3116 / 0 / 202	
Goodness-of-fit on F <sup>2</sup>	0.996	
Final R indices [I > 2σ(I)]	R <sub>1</sub> = 0.0504, wR <sub>2</sub> = 0.1026	
R indices (all data)	R <sub>1</sub> = 0.1172, wR <sub>2</sub> = 0.1285	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.146 and -0.186 e.Å <sup>-3</sup>	

## X-ray crystal data of 8g



Empirical formula	C <sub>24</sub> H <sub>20</sub> O <sub>2</sub>	
Formula weight	340.40	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 6.6111(3) Å	$\alpha = 106.574(2)^\circ$ .
	b = 9.8830(5) Å	$\beta = 94.682(2)^\circ$ .
	c = 14.4700(8) Å	$\gamma = 104.105(2)^\circ$ .
Volume	867.14(8) Å <sup>3</sup>	
Z	2	
Density (calculated)	1.304 Mg/m <sup>3</sup>	
Absorption coefficient	0.082 mm <sup>-1</sup>	
F(000)	360	
Crystal size	0.12 x 0.10 x 0.10 mm <sup>3</sup>	
Theta range for data collection	1.488 to 26.356°.	
Index ranges	-7<=h<=8, -12<=k<=10, -17<=l<=18	
Reflections collected	11883	
Independent reflections	3534 [R(int) = 0.0262]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.8919	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	3534 / 0 / 237	
Goodness-of-fit on F <sup>2</sup>	1.072	
Final R indices [I>2sigma(I)]	R1 = 0.0386, wR2 = 0.1084	
R indices (all data)	R1 = 0.0460, wR2 = 0.1231	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.231 and -0.211 e.Å <sup>-3</sup>	

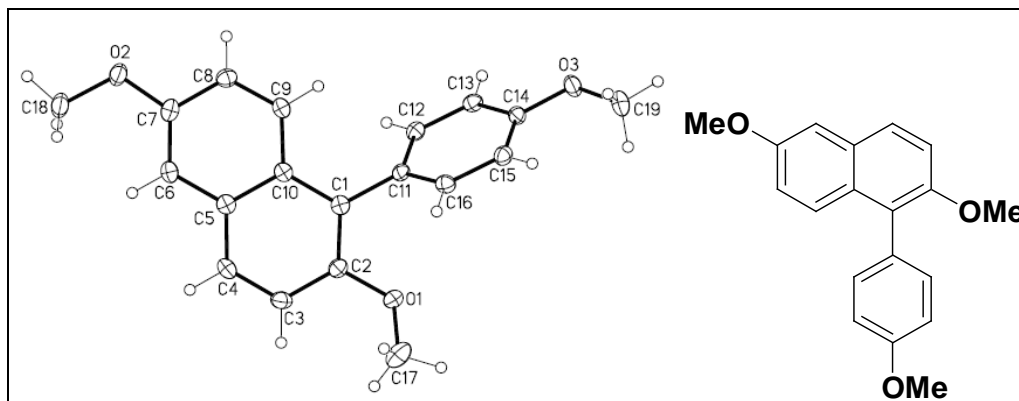
## X-ray crystal data of 9a



Empirical formula	C <sub>18</sub> H <sub>16</sub> O <sub>2</sub>	
Formula weight	264.31	
Temperature	295(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 2 <sub>1</sub> /c 1	
Unit cell dimensions	a = 7.654(4) Å	α = 90°.
	b = 13.820(8) Å	β = 98.379(9)°.
	c = 13.657(8) Å	γ = 90°.
Volume	1429.0(14) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.229 Mg/m <sup>3</sup>	
Absorption coefficient	0.079 mm <sup>-1</sup>	
F(000)	560	
Crystal size	0.30 x 0.20 x 0.18 mm <sup>3</sup>	
Theta range for data collection	2.11 to 26.46°.	
Index ranges	-9 ≤ h ≤ 9, -17 ≤ k ≤ 15, -12 ≤ l ≤ 17	
Reflections collected	8979	
Independent reflections	2937 [R(int) = 0.0271]	
Completeness to theta = 26.46°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9486 and 0.8266	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	2937 / 0 / 183	
Goodness-of-fit on F <sup>2</sup>	1.049	
Final R indices [I > 2σ(I)]	R <sub>1</sub> = 0.0475, wR <sub>2</sub> = 0.1271	
R indices (all data)	R <sub>1</sub> = 0.0711, wR <sub>2</sub> = 0.1581	
Largest diff. peak and hole	0.160 and -0.175 e.Å <sup>-3</sup>	



## X-ray crystal data of 9b



Empirical formula	C <sub>19</sub> H <sub>18</sub> O <sub>3</sub>	
Formula weight	294.33	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 1 c 1	
Unit cell dimensions	a = 8.6905(3) Å	α = 90°.
	b = 21.9250(7) Å	β = 108.3260(10)°.
	c = 8.2652(3) Å	γ = 90°.
Volume	1494.97(9) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.308 Mg/m <sup>3</sup>	
Absorption coefficient	0.088 mm <sup>-1</sup>	
F(000)	624	
Crystal size	0.30 x 0.25 x 0.25 mm <sup>3</sup>	
Theta range for data collection	1.86 to 26.52°.	
Index ranges	-8 ≤ h ≤ 10, -27 ≤ k ≤ 27, -10 ≤ l ≤ 10	
Reflections collected	5988	
Independent reflections	2742 [R(int) = 0.0146]	
Completeness to theta = 26.52°	99.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9486 and 0.8716	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	2742 / 2 / 202	
Goodness-of-fit on F <sup>2</sup>	1.052	
Final R indices [I > 2σ(I)]	R1 = 0.0277, wR2 = 0.0732	
R indices (all data)	R1 = 0.0291, wR2 = 0.0743	
Absolute structure parameter	0.9(7)	
Largest diff. peak and hole	0.194 and -0.156 e.Å <sup>-3</sup>	