

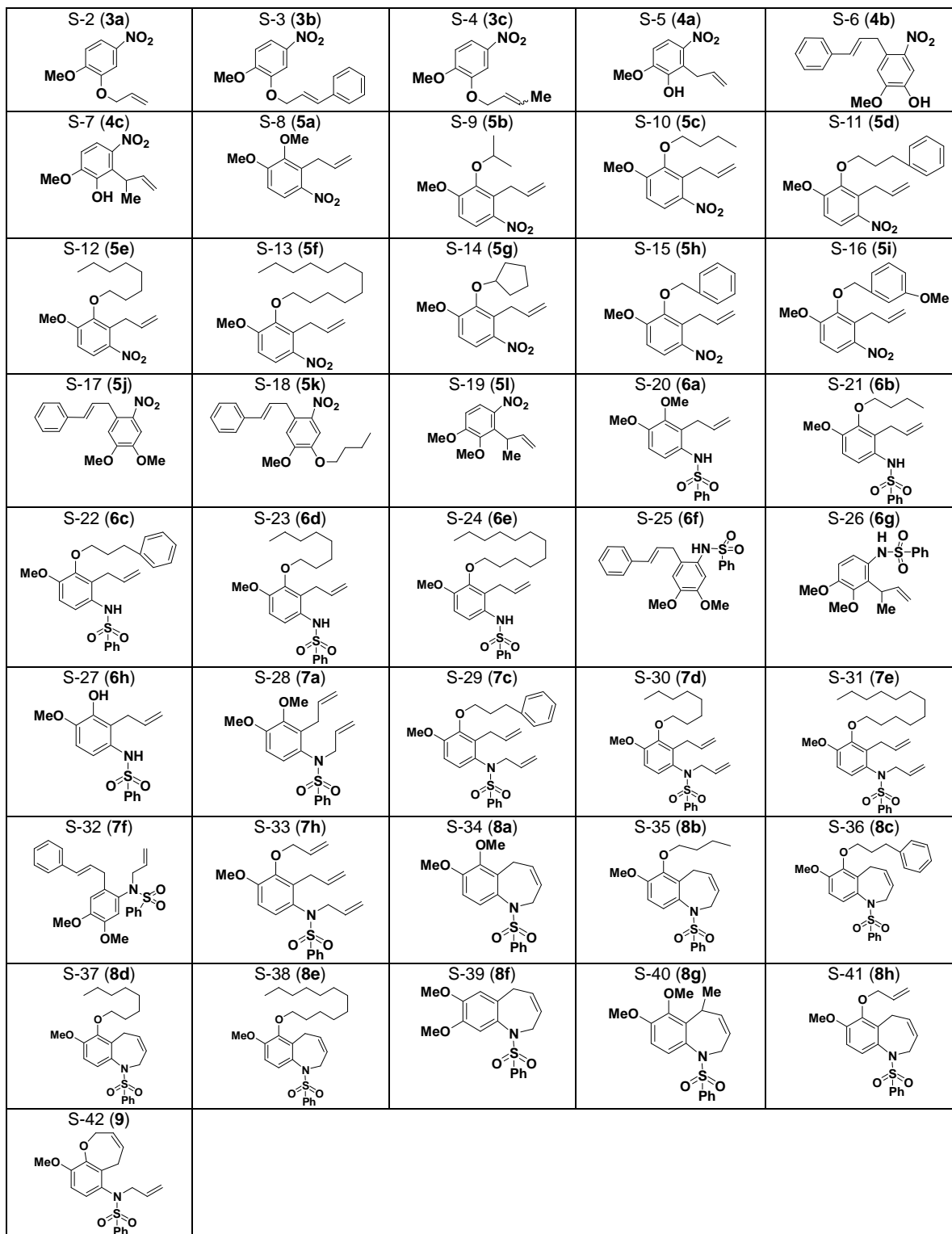
Supporting Information

Synthesis of Dihydro-1-benzazepines

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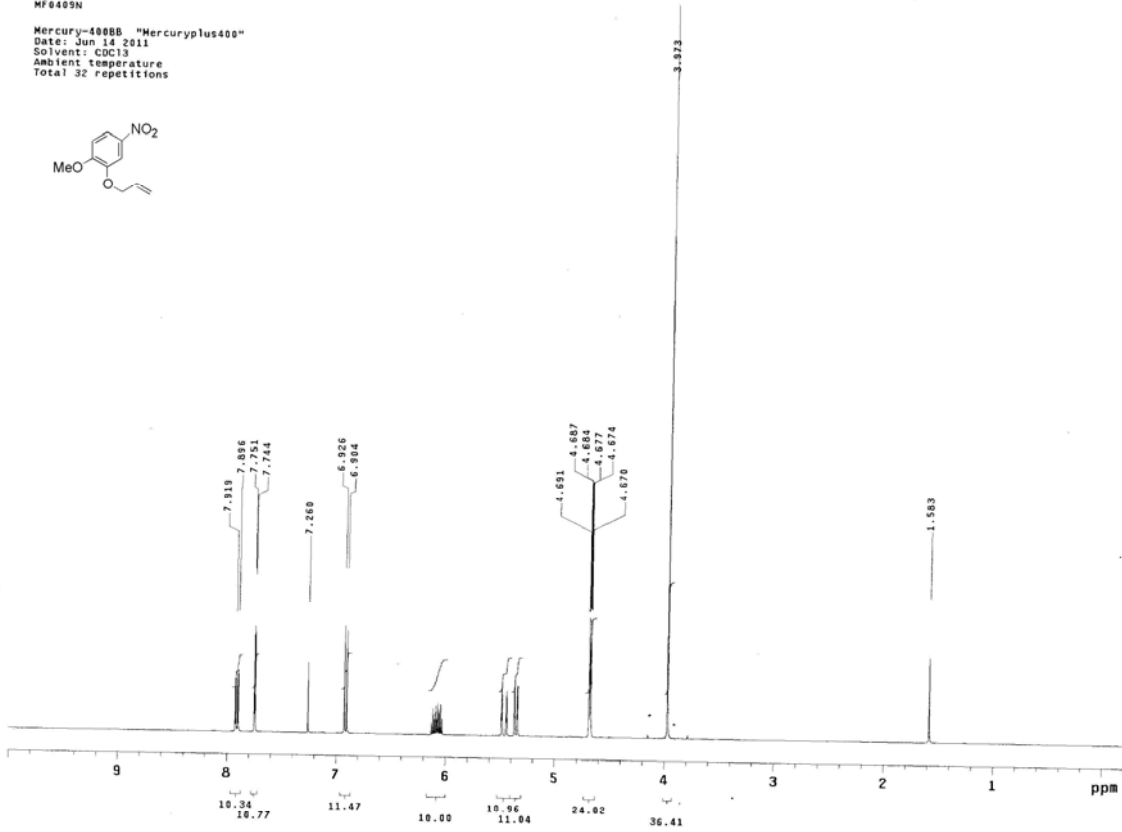
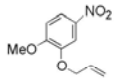
Additional scanned ¹H & ¹³C NMR photocopies (pages S-2~S-42); X-ray crystal data of **6h** (pages S-43~S-49)



Compound 3a

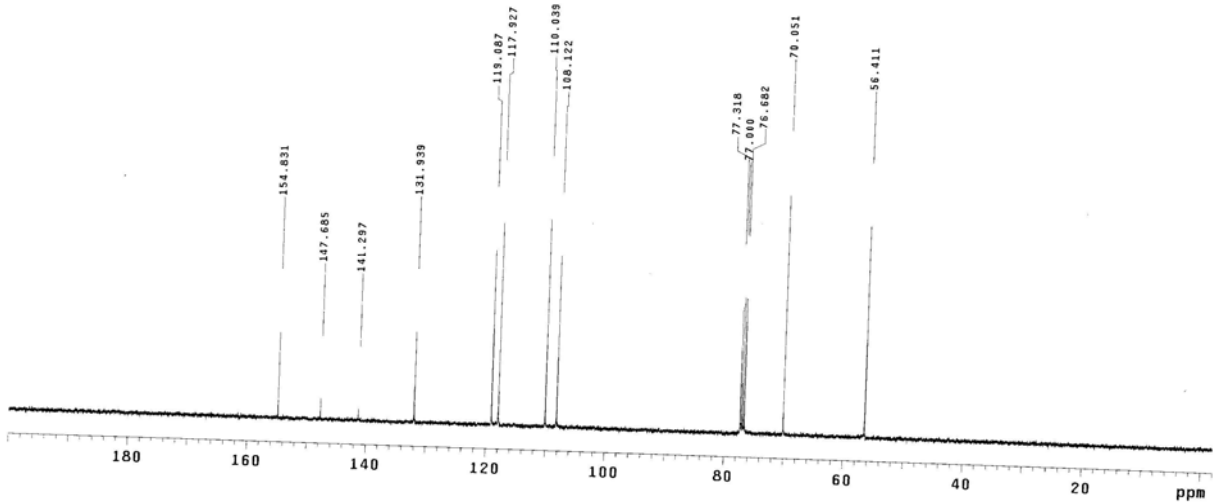
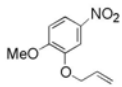
MF0409N

Mercury-40055 "Mercuryplus400"
 Date: Jun 14 2011
 Solvent: CDCl3
 Ambient temperature
 Total 32 repetitions



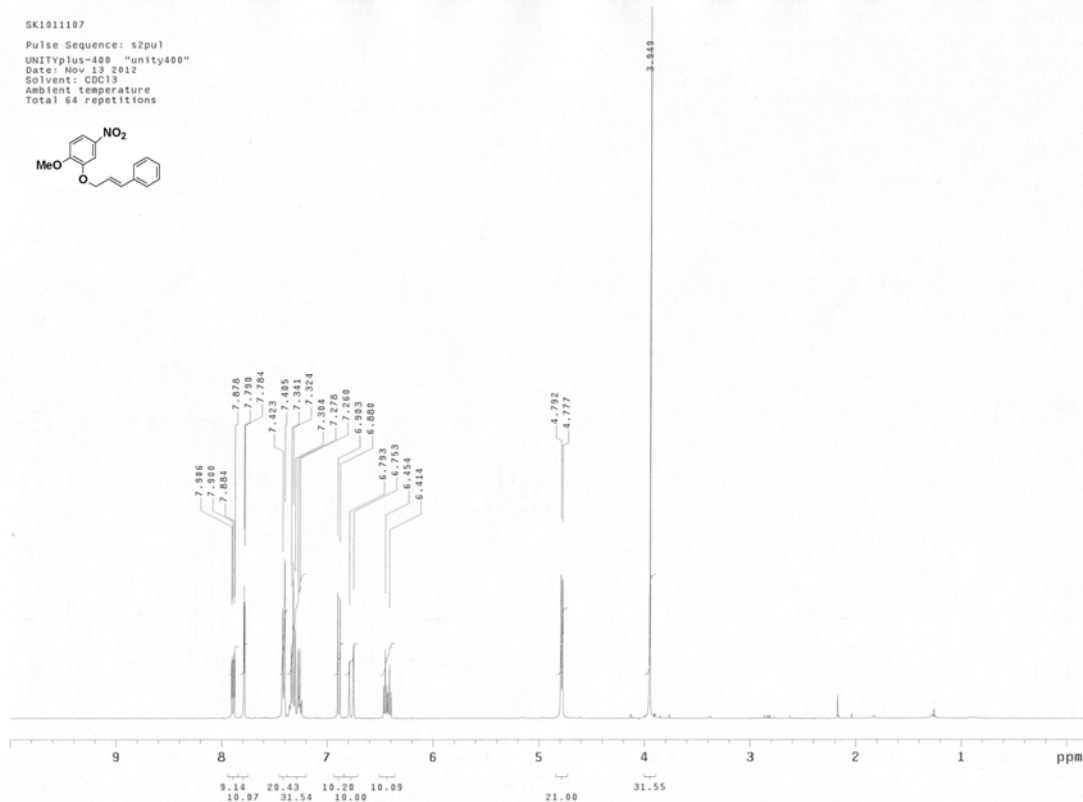
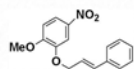
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Mercury-40055 "Mercuryplus400"
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 Ambient temperature
 Total 2313 repetitions

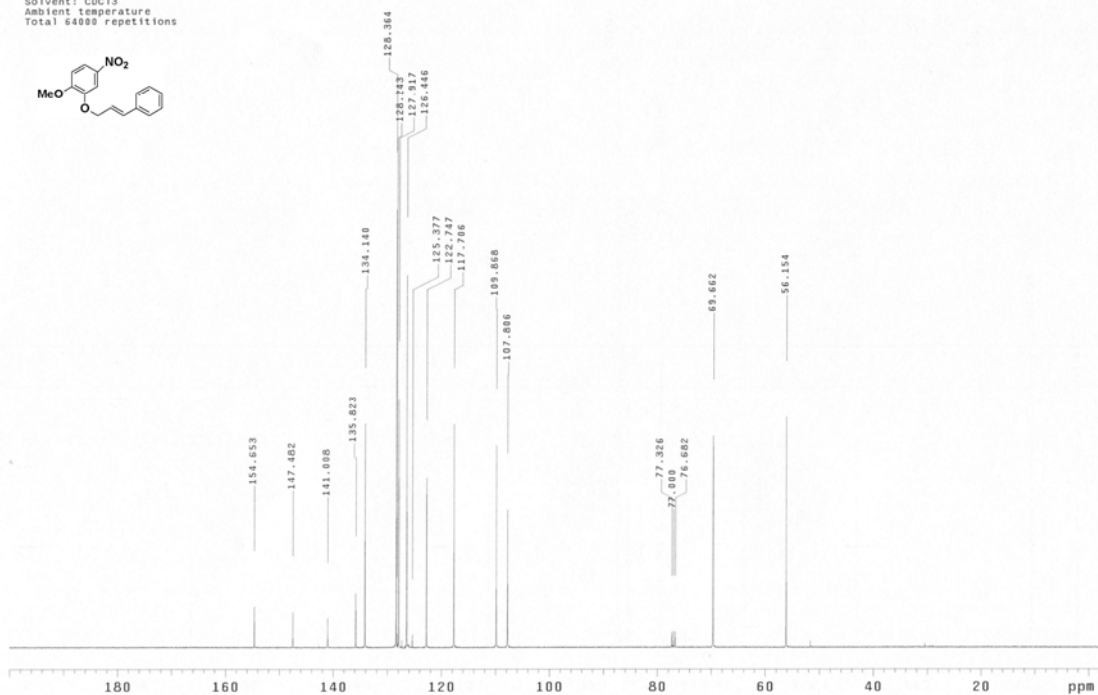
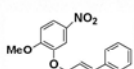


Compound 3b

SK1011107
 Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Nov 13 2012
 Solvent: CDCl3
 Ambient temperature
 Total 64 repetitions

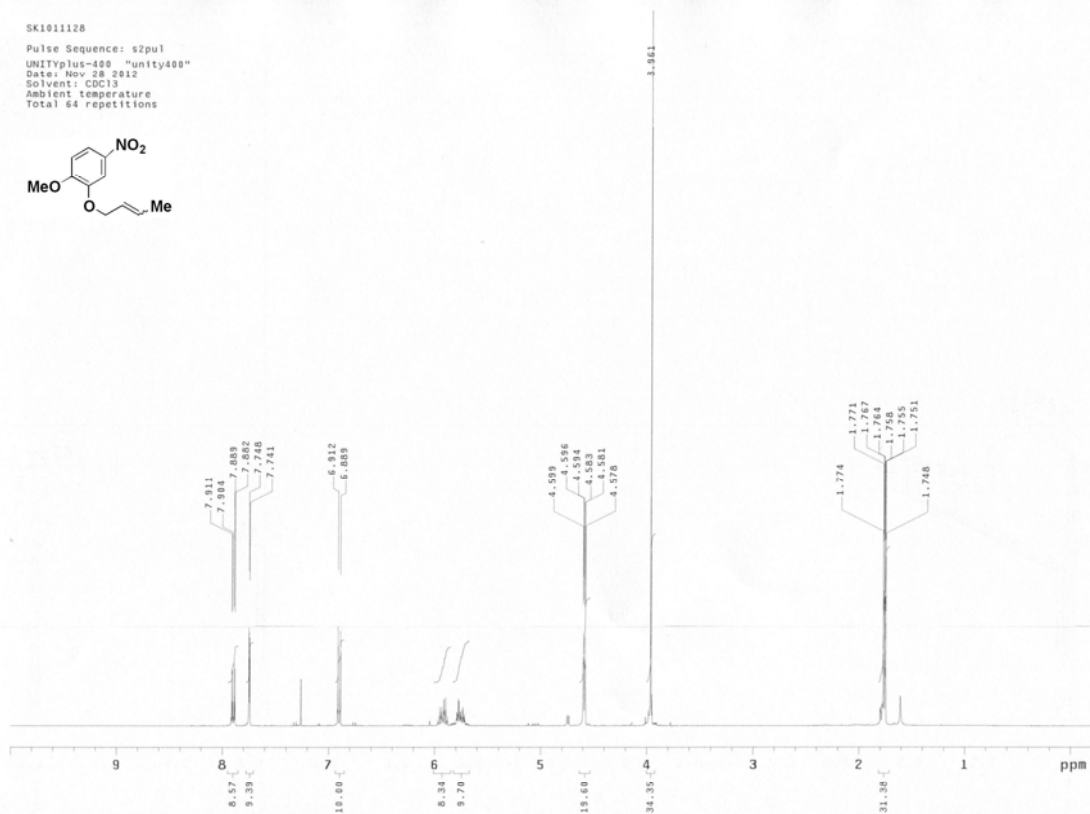
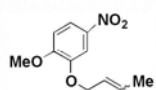


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 Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Nov 13 2012
 Solvent: CDCl3
 Ambient temperature
 Total 64000 repetitions

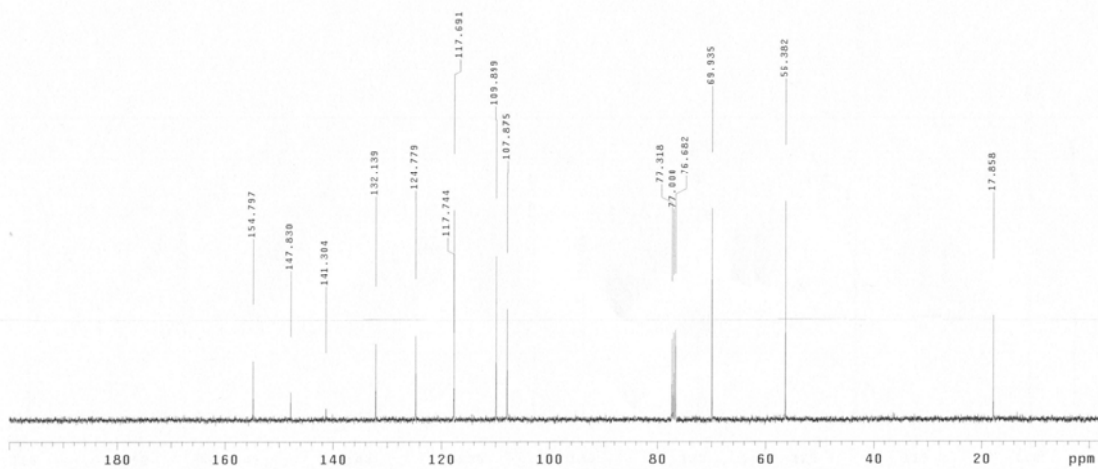
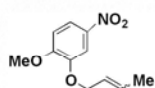


Compound 3c

SK1011128
 Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Nov 28 2012
 Solvent: CDCl3
 Ambient temperature
 Total 64 repetitions

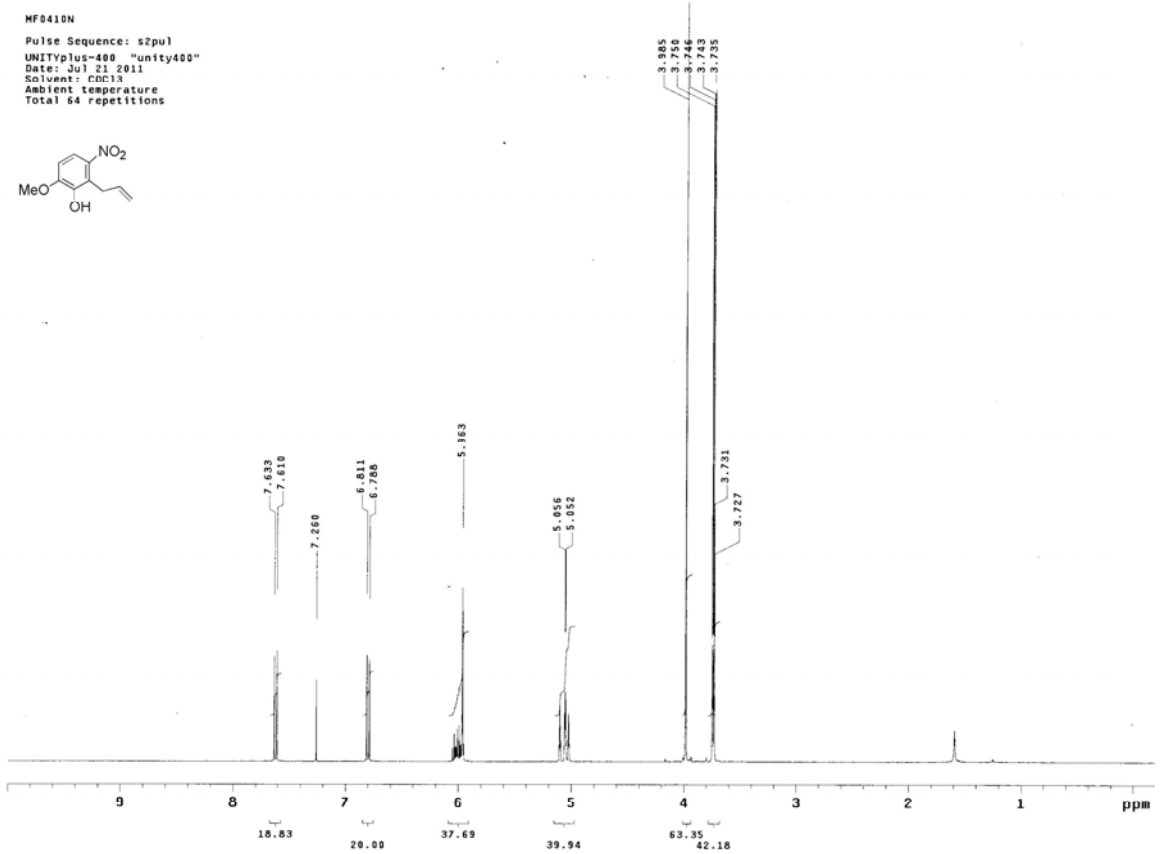
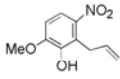


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 UNITYplus-400 "unity400"
 Date: Nov 28 2012
 Solvent: CDCl3
 Ambient temperature
 Total 2016 repetitions

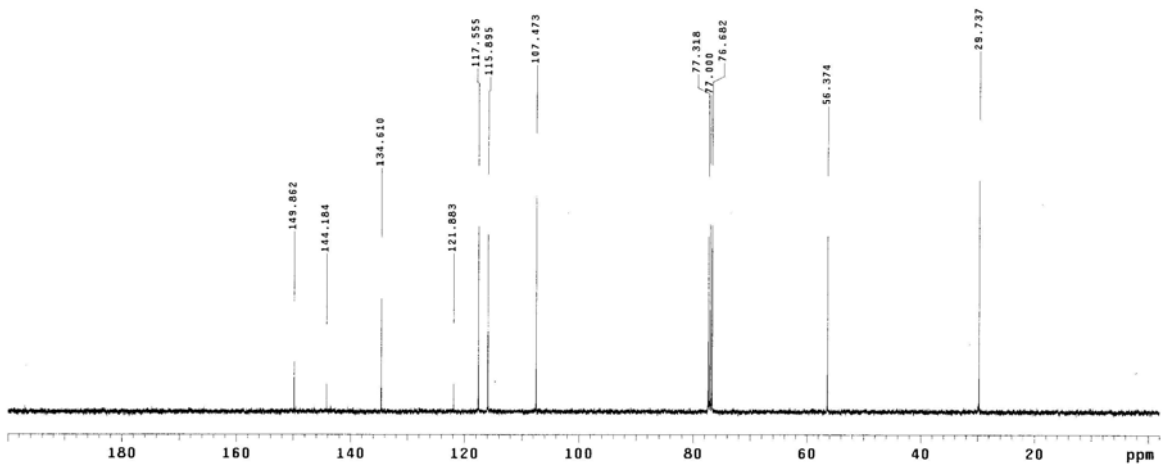
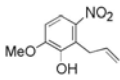


Compound 4a

MF0410N
 Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jul 21 2011
 Solvent: CDCl3
 Ambient temperature
 Total 64 repetitions



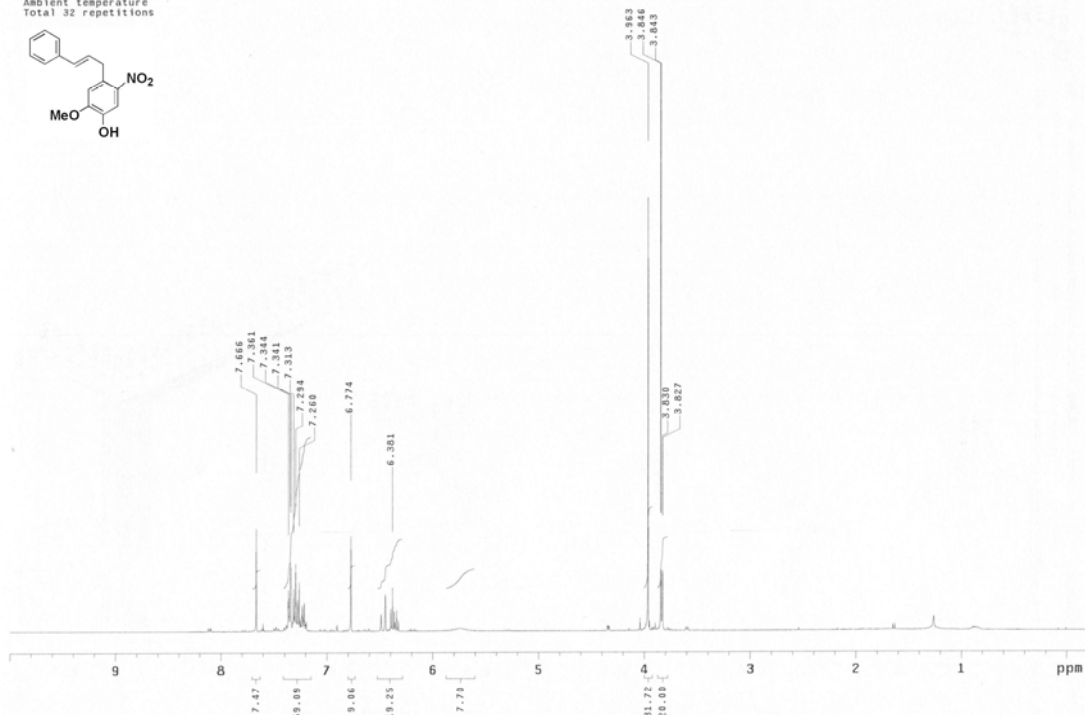
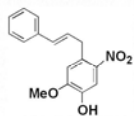
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 UNITYplus-400 "unity400"
 Date: Jul 21 2011
 Solvent: CDCl3
 Ambient temperature
 Total 3200 repetitions



Compound 4b

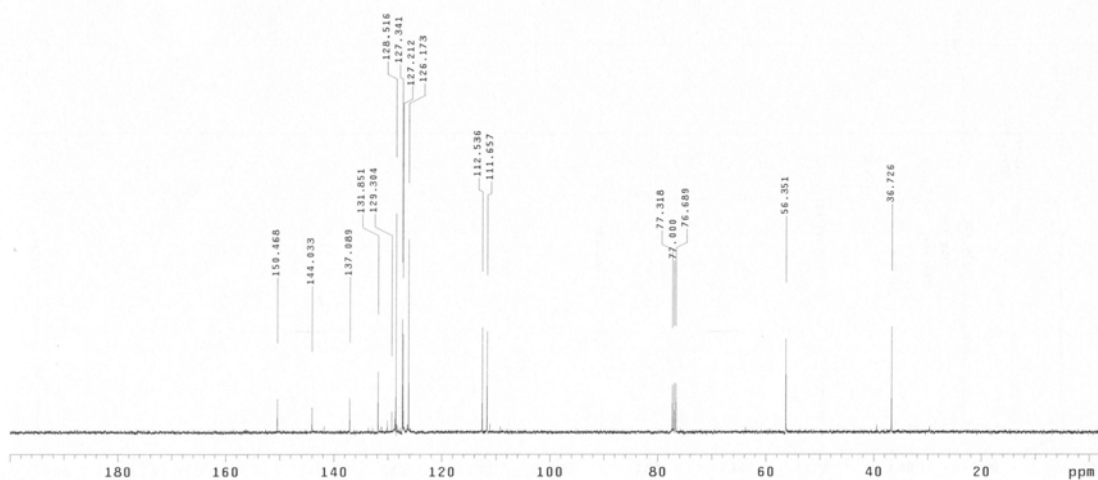
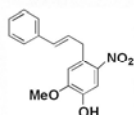
SK1011108

Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Nov 14 2012
 Solvent: CDCl3
 Ambient temperature
 Total 32 repetitions



SK1011108

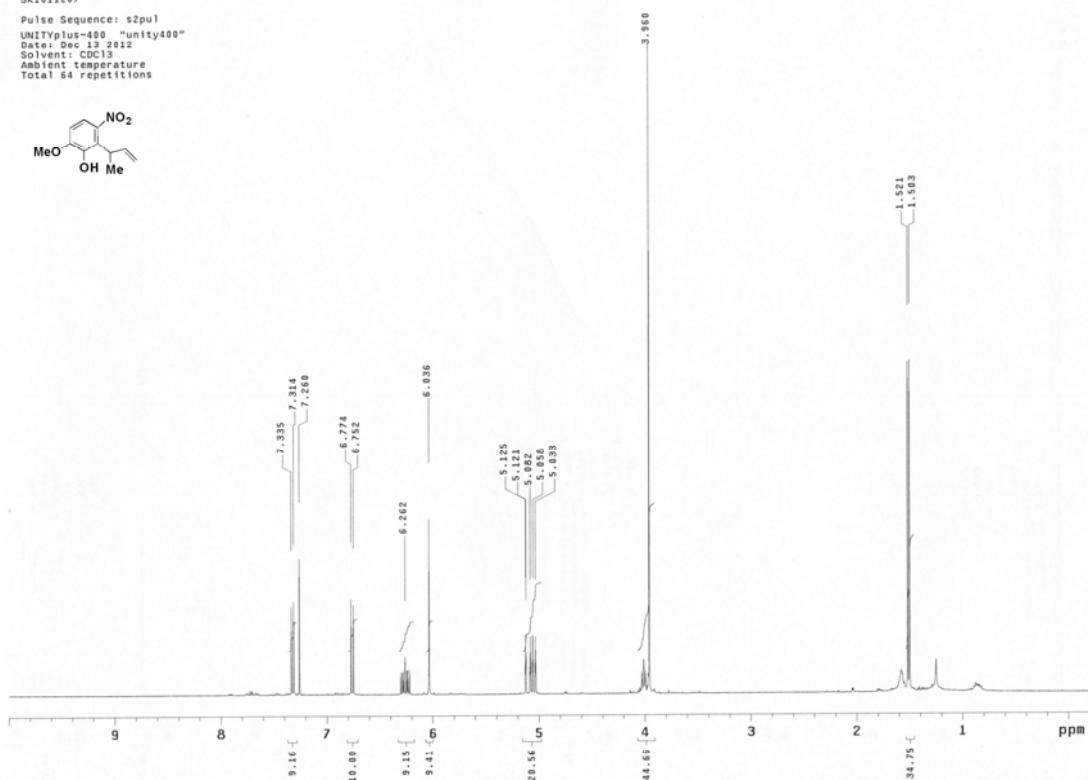
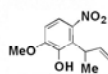
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 Date: Nov 14 2012
 Solvent: CDCl3
 Ambient temperature
 Total 1688 repetitions



Compound 4c

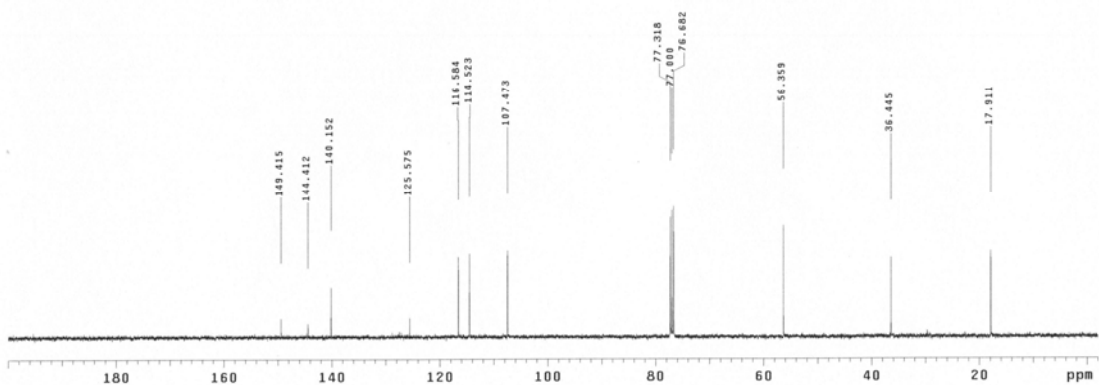
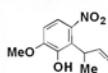
SK1011207

Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Dec 13 2012
 Solvent: CDCl3
 Ambient temperature
 Total 64 repetitions

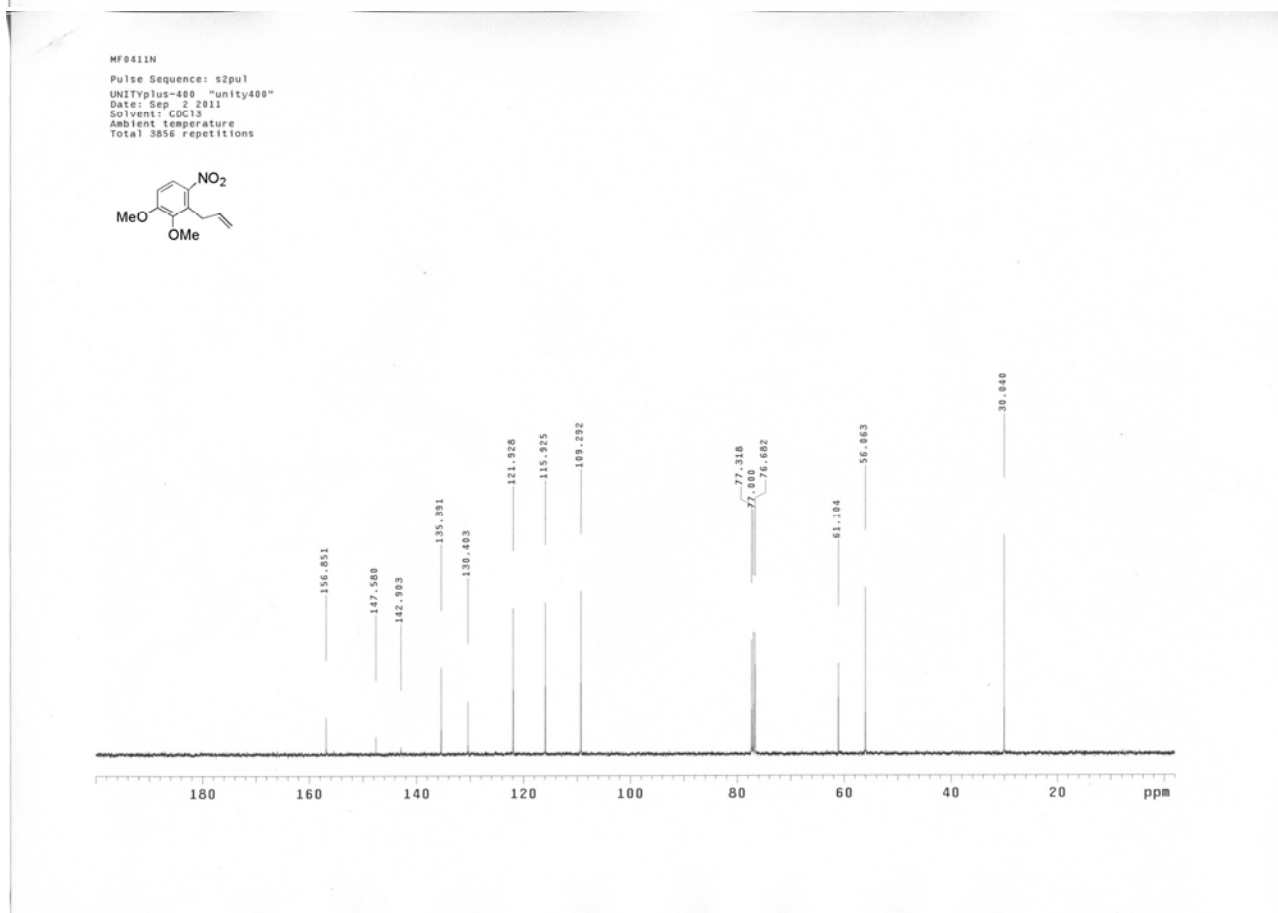
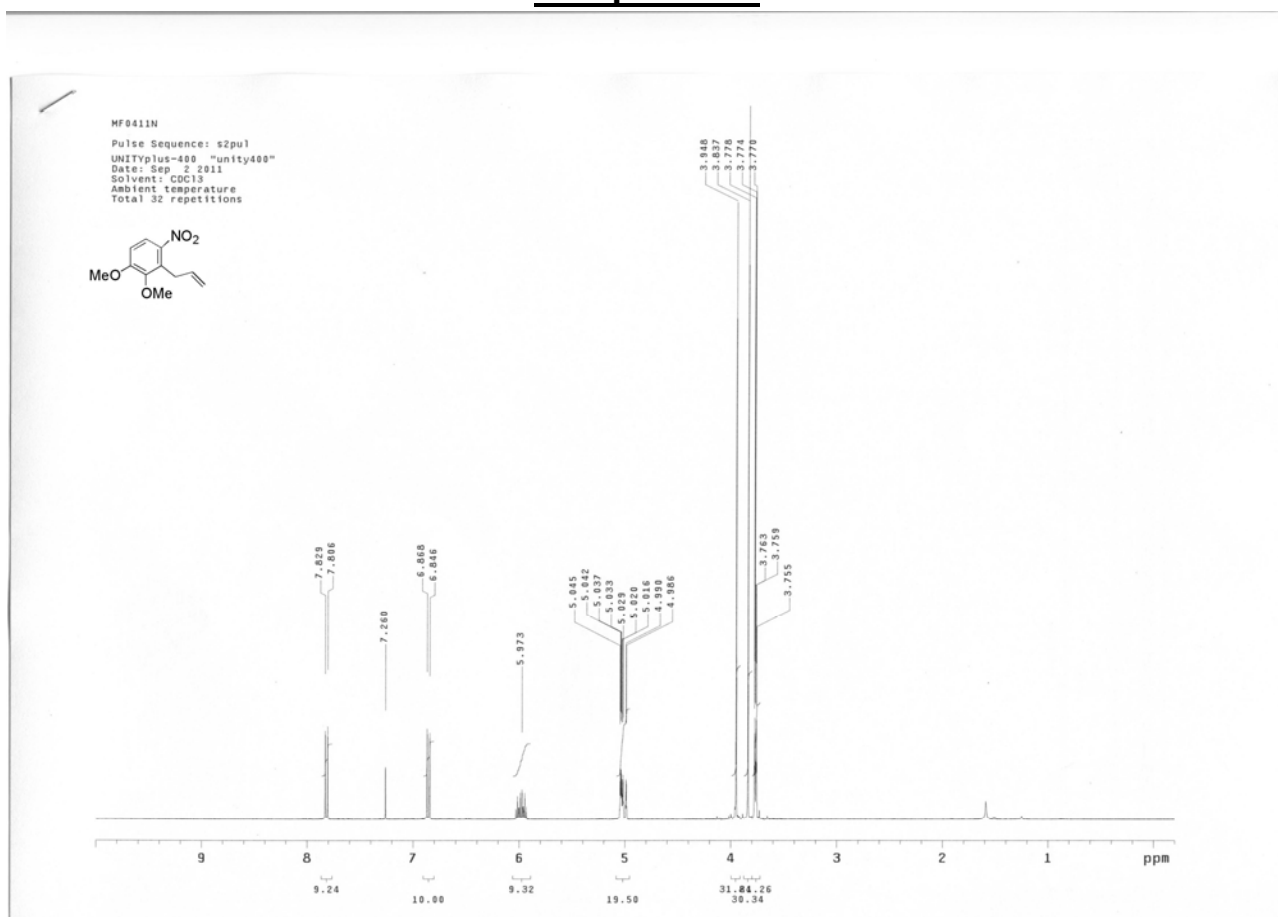


SK1011207

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 Date: Dec 13 2012
 Solvent: CDCl3
 Ambient temperature
 Total 6064 repetitions



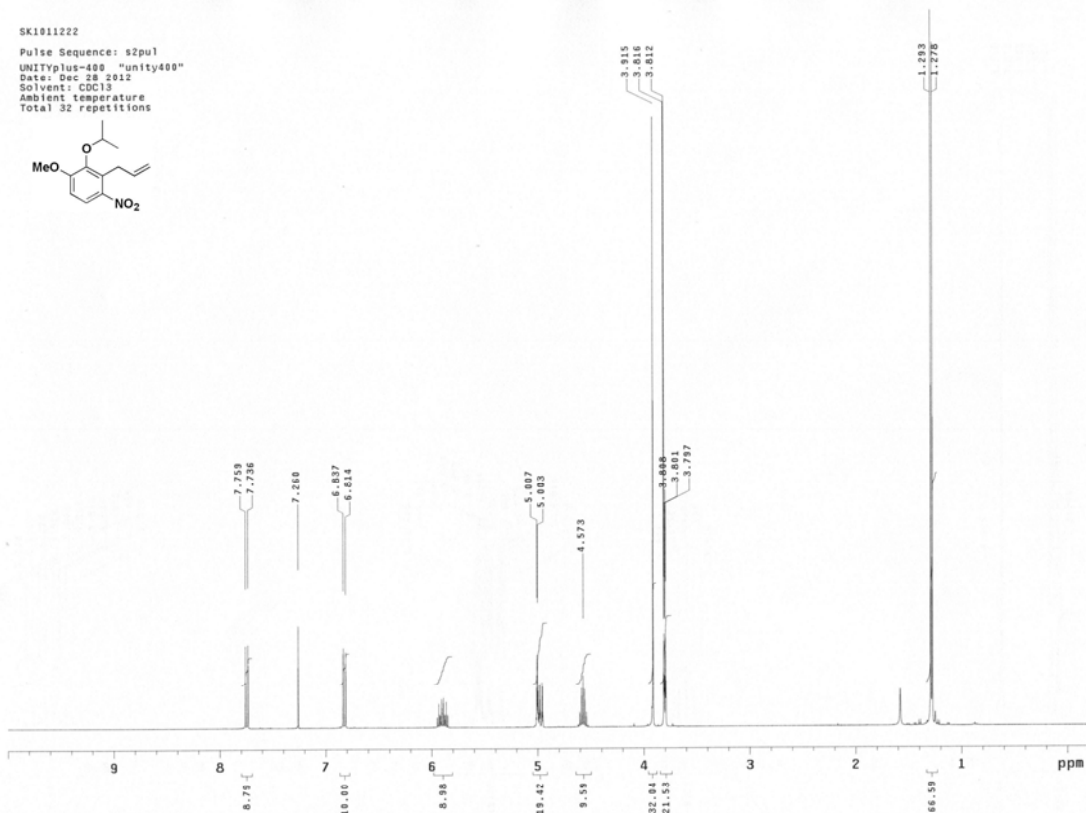
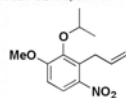
Compound 5a



Compound 5b

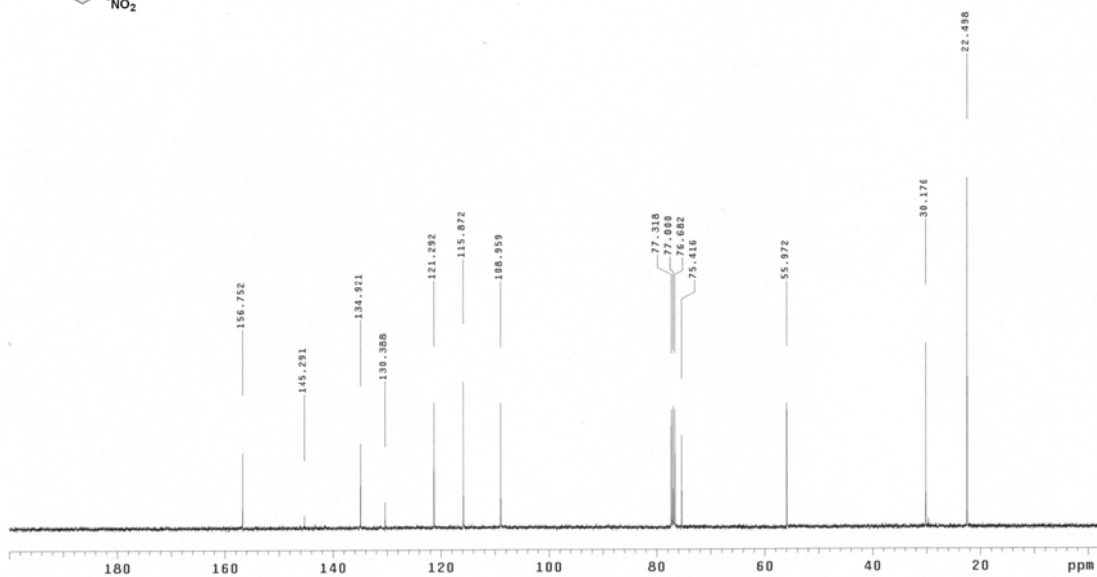
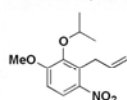
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Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Dec 28 2012
 Solvent: CDCl3
 Ambient temperature
 Total 32 repetitions



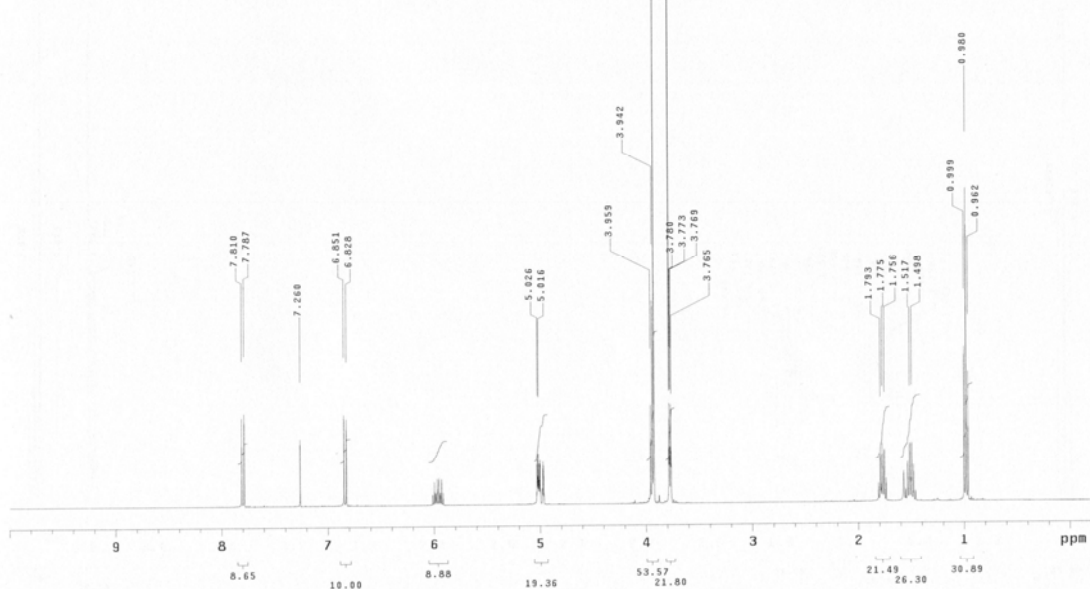
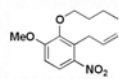
SK1011222

Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Dec 28 2012
 Solvent: CDCl3
 Ambient temperature
 Total 6096 repetitions

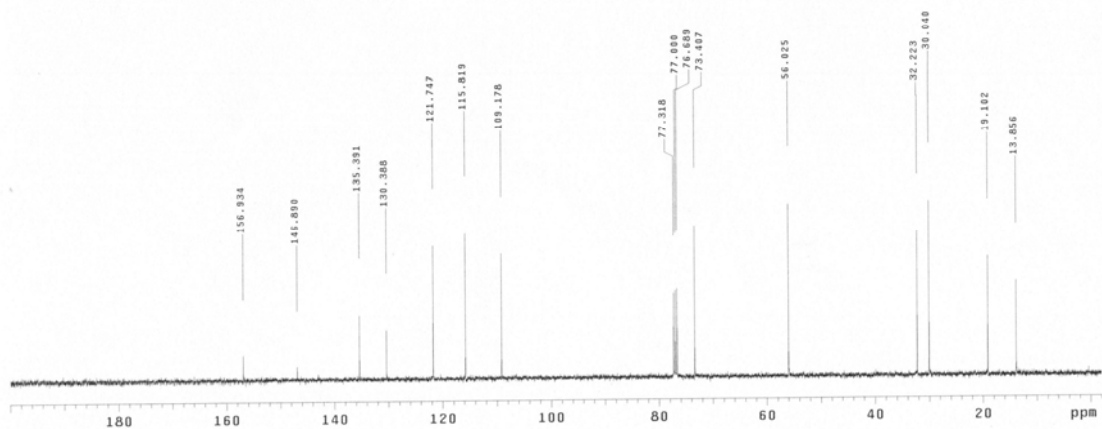
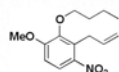


Compound 5c

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 UNITYplus-400 "unity400"
 Date: Oct 29 2012
 Solvent: CDCl3
 Ambient temperature
 Total 64 repetitions



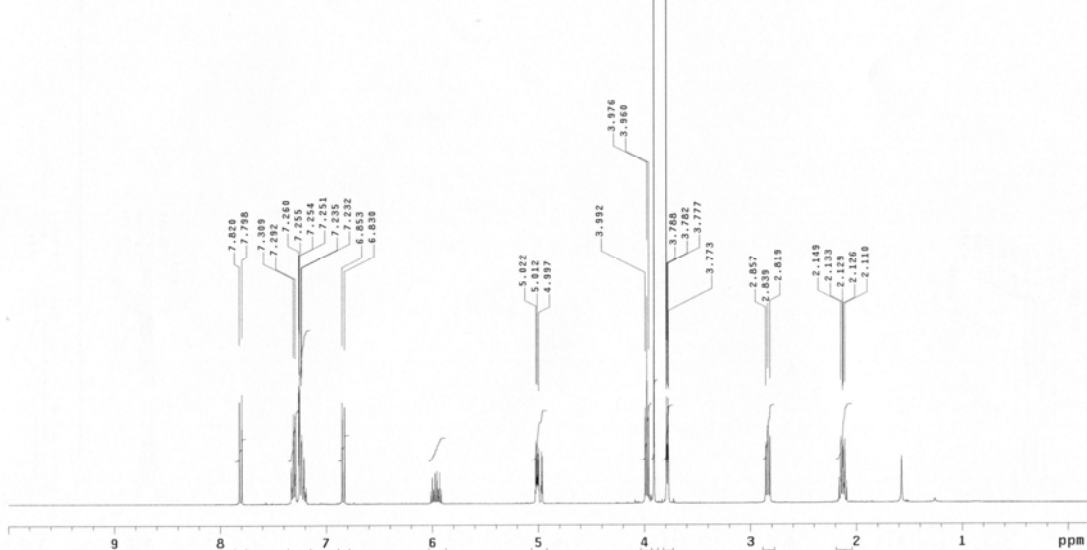
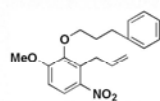
SK1011026
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 UNITYplus-400 "unity400"
 Date: Oct 29 2012
 Solvent: CDCl3
 Ambient temperature
 Total 2256 repetitions



Compound 5d

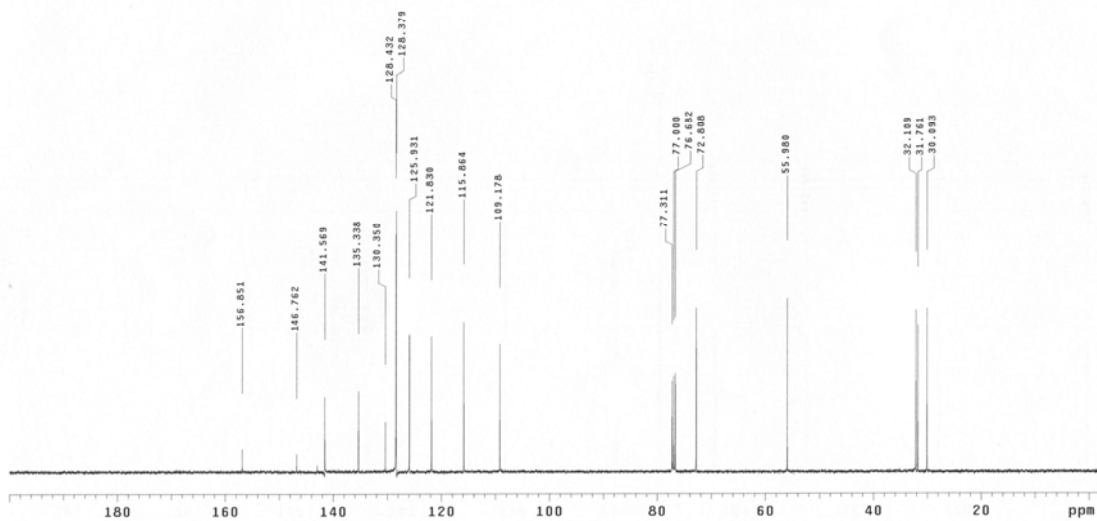
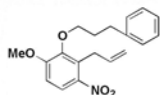
SK1011224

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jan 7 2013
 Solvent: CDCl3
 Ambient temperature
 Total 32 repetitions



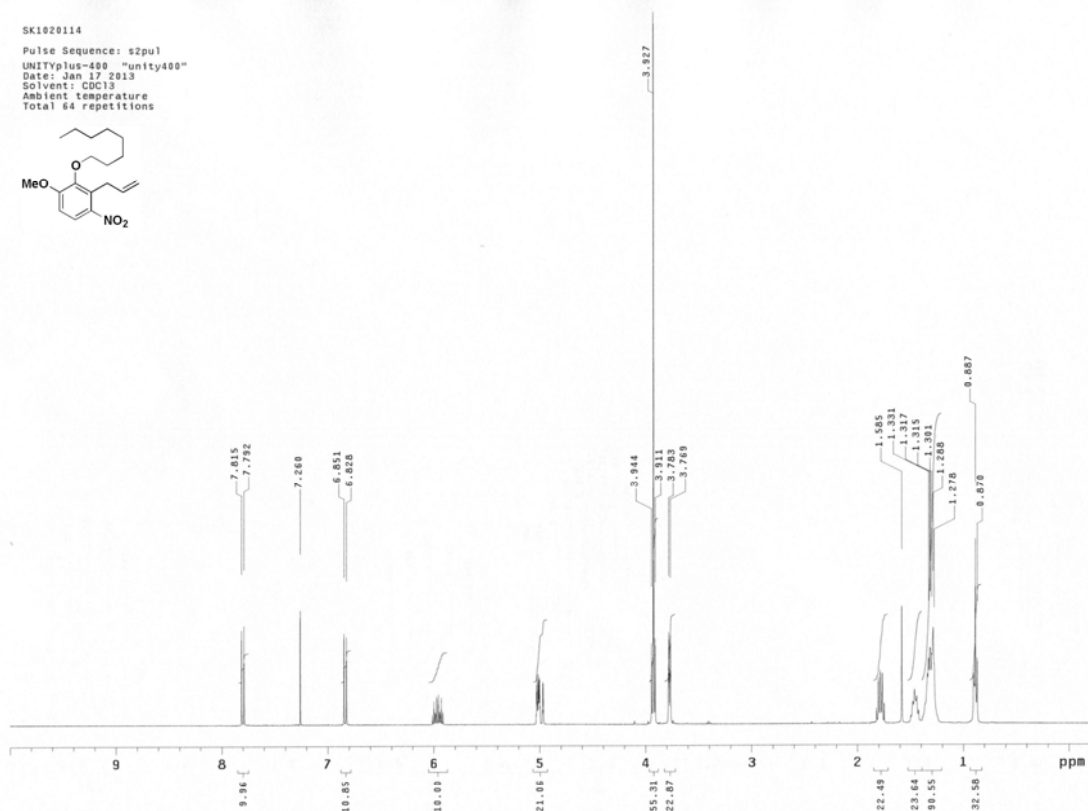
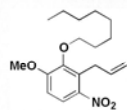
SK1011224

Pulse Sequence: s2pu1
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 Date: Jan 7 2013
 Solvent: CDCl3
 Ambient temperature
 Total 8224 repetitions

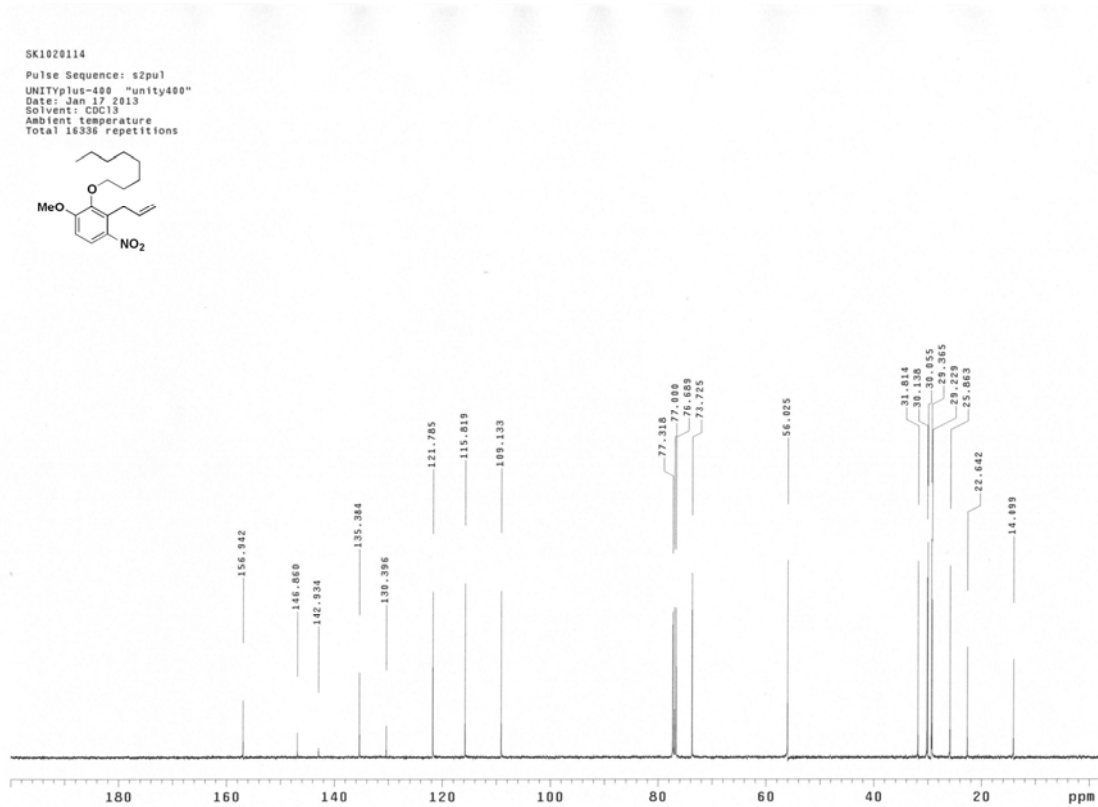
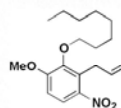


Compound 5e

SK1020114
 Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Jan 17 2013
 Solvent: CDCl3
 Ambient temperature
 Total 64 repetitions

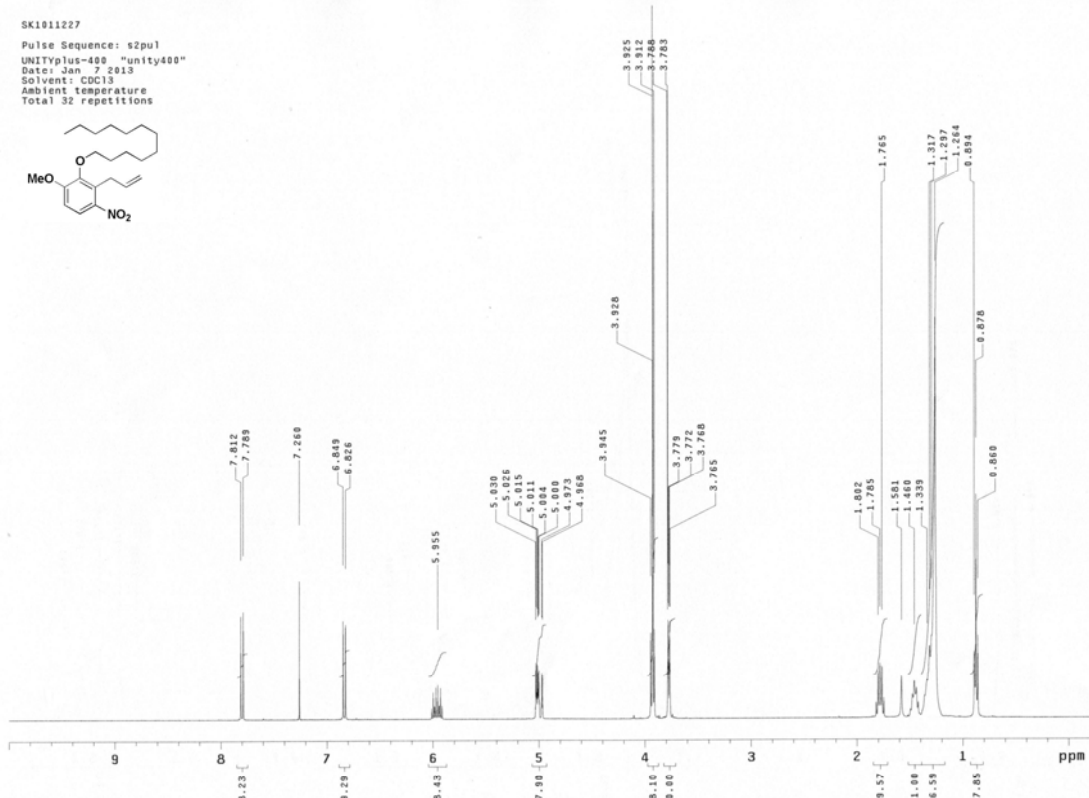
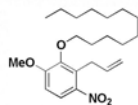


SK1020114
 Pulse Sequence: s2pul
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 Date: Jan 17 2013
 Solvent: CDCl3
 Ambient temperature
 Total 16336 repetitions

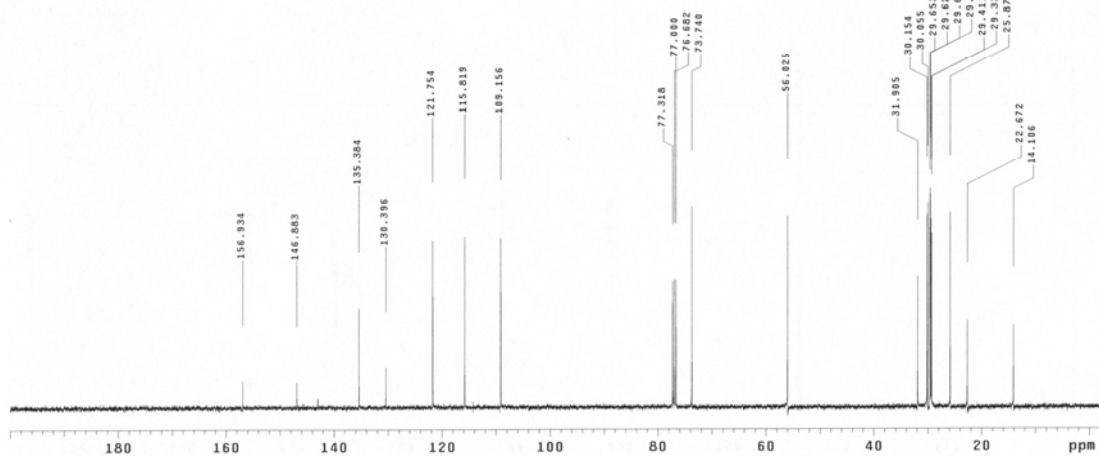
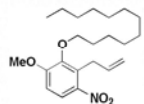


Compound 5f

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 Date: Jan 7 2013
 Solvent: CDCl3
 Ambient temperature
 Total 32 repetitions

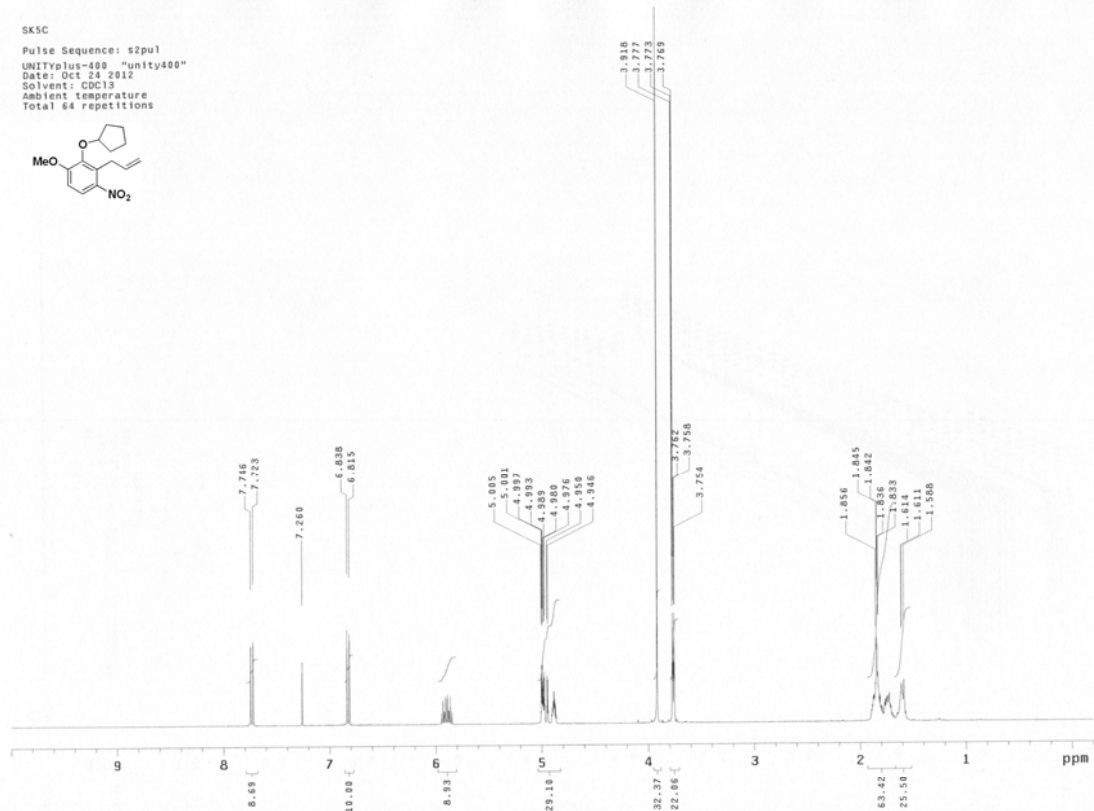
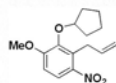


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 Solvent: CDCl3
 Ambient temperature
 Total 4816 repetitions

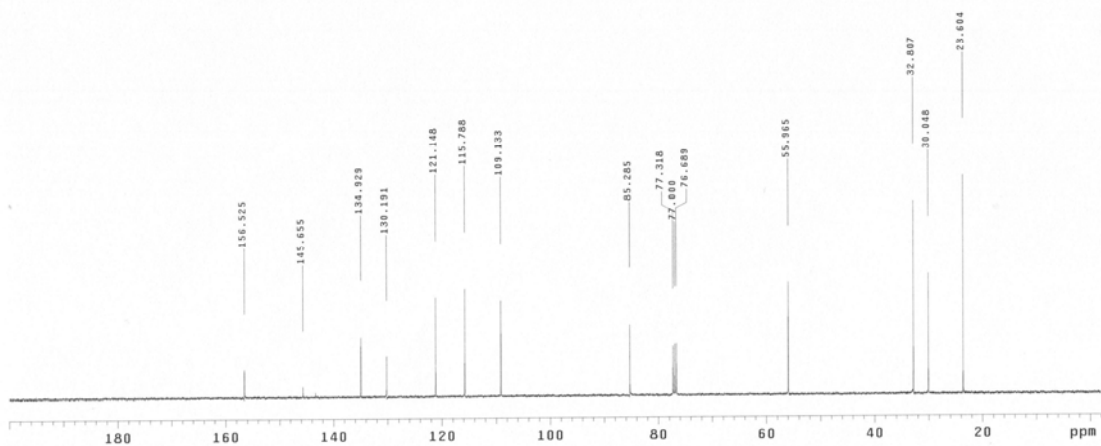
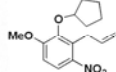


Compound 5g

SKSC
 Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Oct 24 2012
 Solvent: CDCl3
 Ambient temperature
 Total 64 repetitions

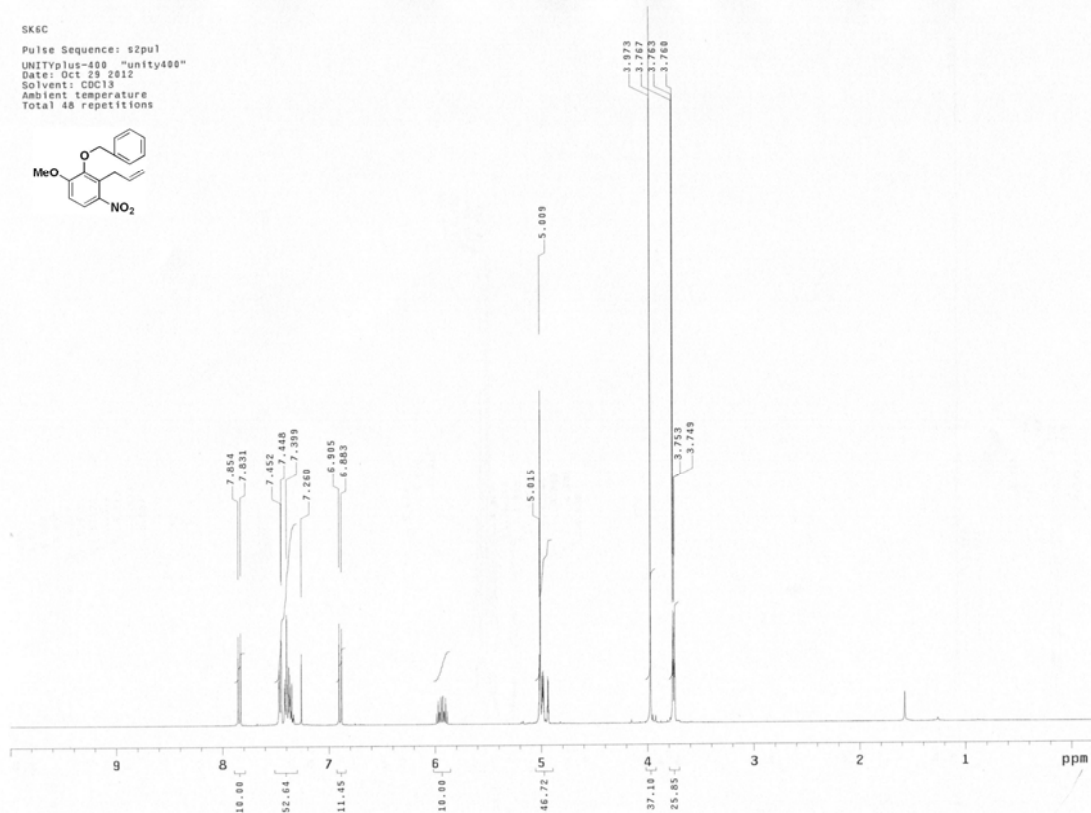
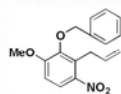


SKSC
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 Date: Oct 24 2012
 Solvent: CDCl3
 Ambient temperature
 Total 3744 repetitions

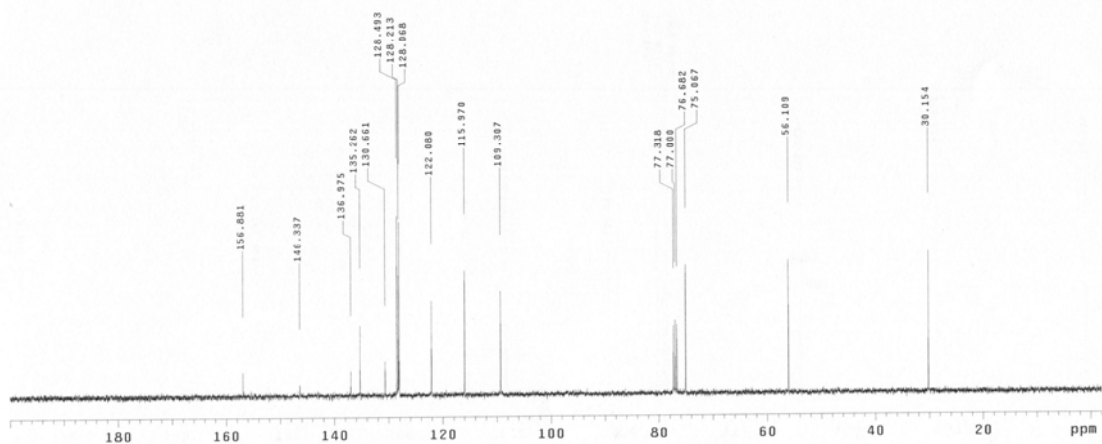
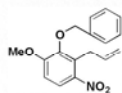


Compound 5h

SK6C
 Pulse Sequence: s2pul
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 Date: Oct 29 2012
 Solvent: CDCl3
 Ambient temperature
 Total 48 repetitions

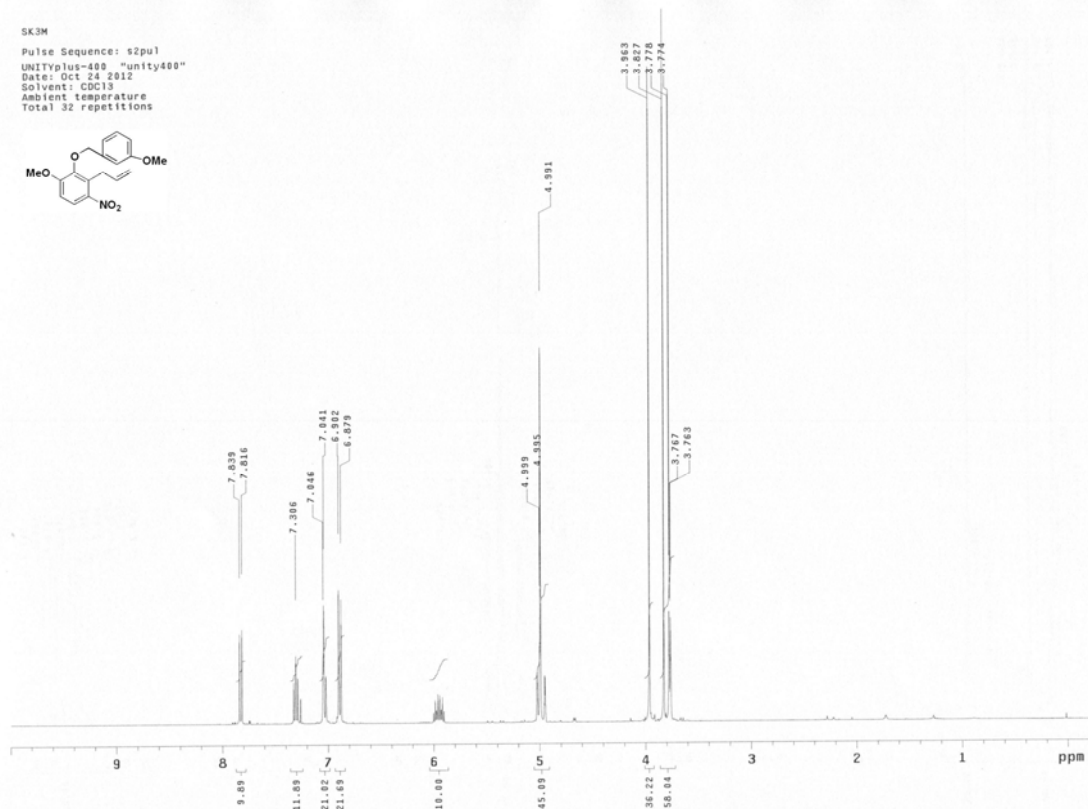
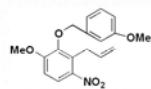


SK6C
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 Date: Oct 29 2012
 Solvent: CDCl3
 Ambient temperature
 Total 128 repetitions

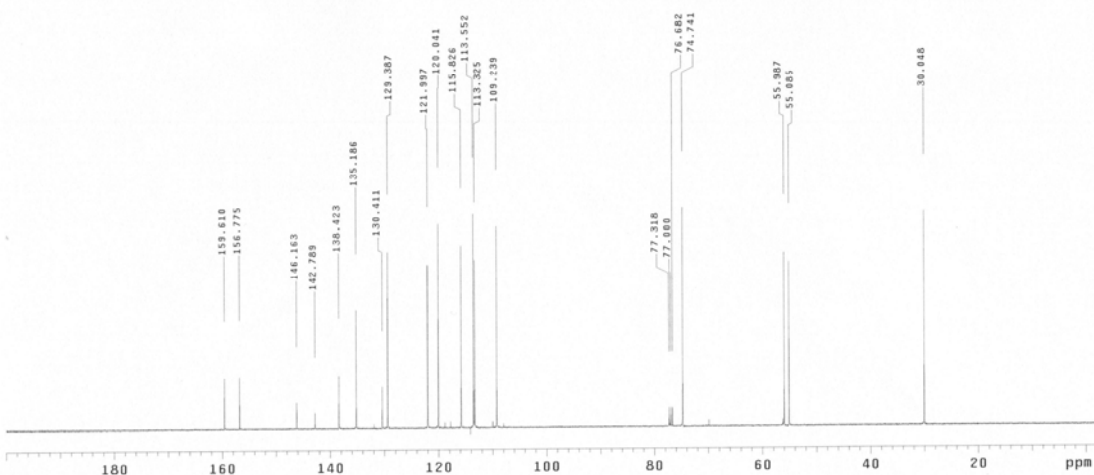
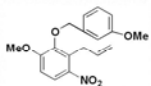


Compound 5i

SK3M
 Pulse Sequence: s2pul
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 Date: Oct 24 2012
 Solvent: CDCl3
 Ambient temperature
 Total 32 repetitions

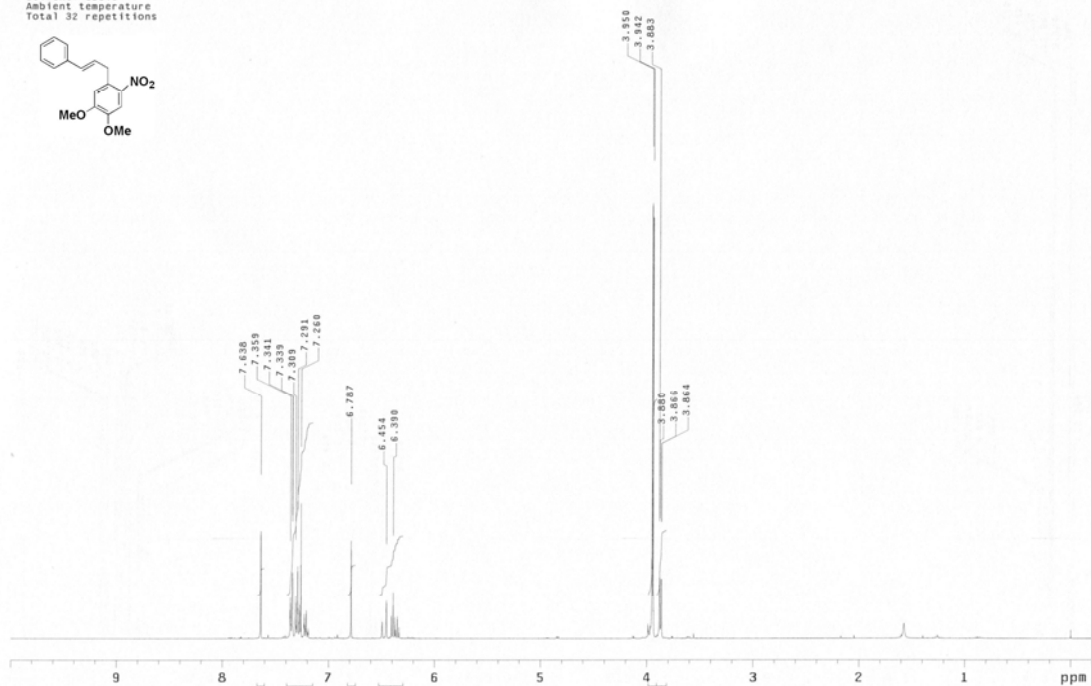
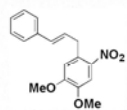


SK3M
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 Date: Oct 24 2012
 Solvent: CDCl3
 Ambient temperature
 Total 6480 repetitions

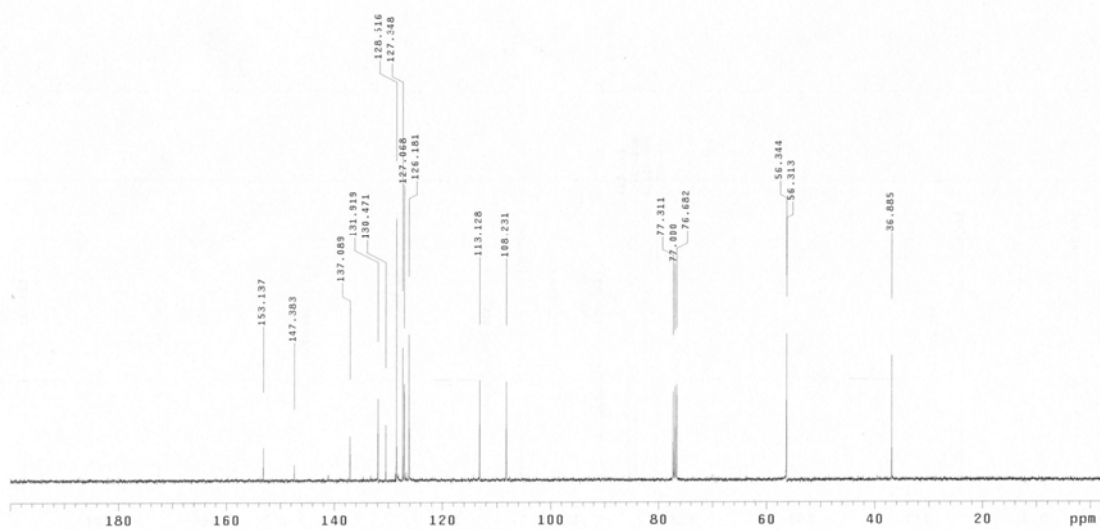
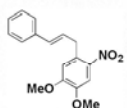


Compound 5j

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 Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Nov 14 2012
 Solvent: CDCl3
 Ambient temperature
 Total 32 repetitions

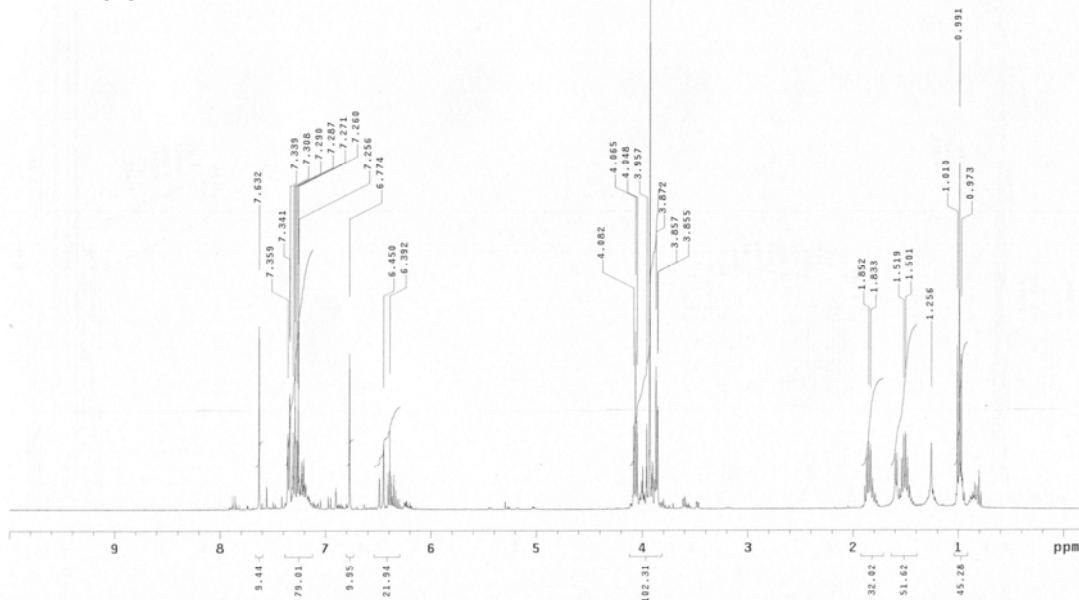
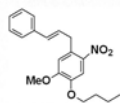


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 Date: Nov 14 2012
 Solvent: CDCl3
 Ambient temperature
 Total 5472 repetitions

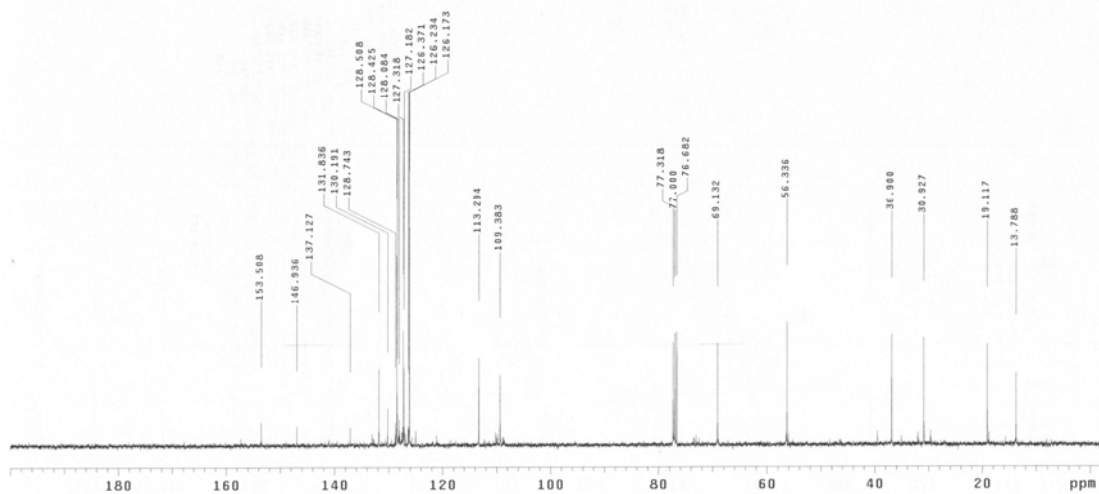
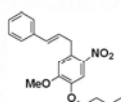


Compound 5k

SK1011115
 Pulse Sequence: s2pul
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 Date: Nov 16 2012
 Solvent: CDCl3
 Ambient temperature
 Total 64 repetitions

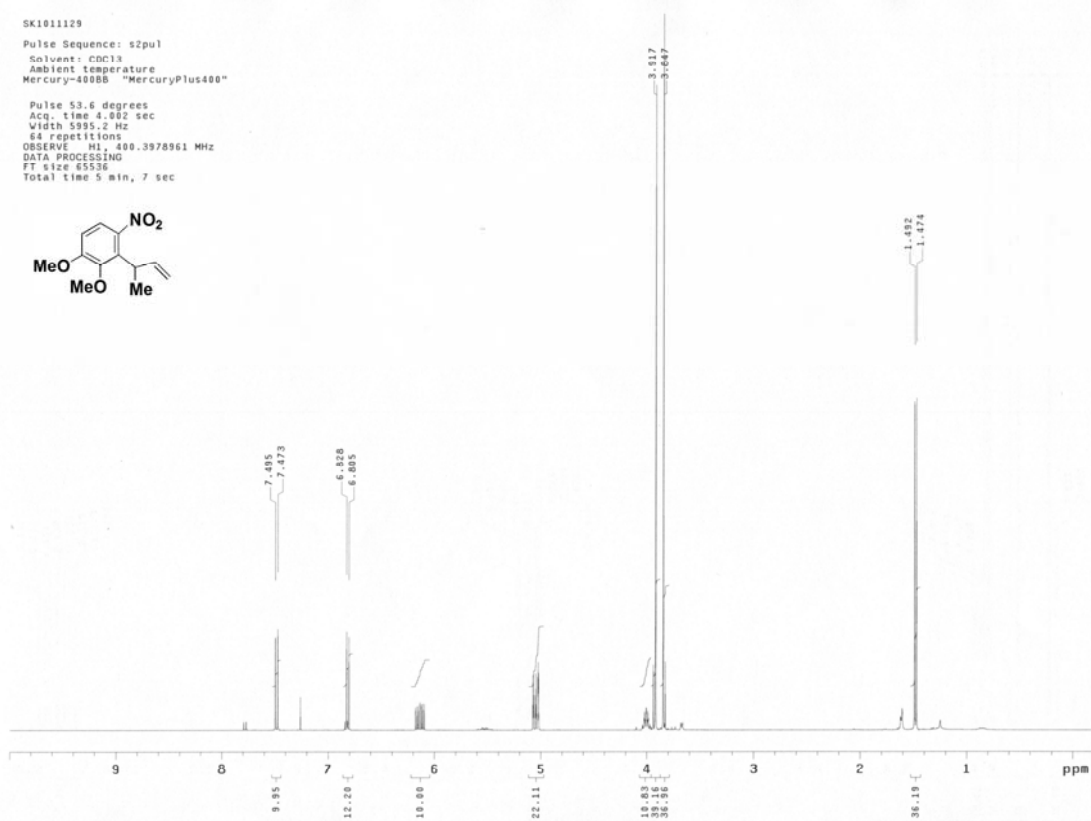
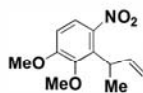


SK1011115
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 Date: Nov 16 2012
 Solvent: CDCl3
 Ambient temperature
 Total 4560 repetitions

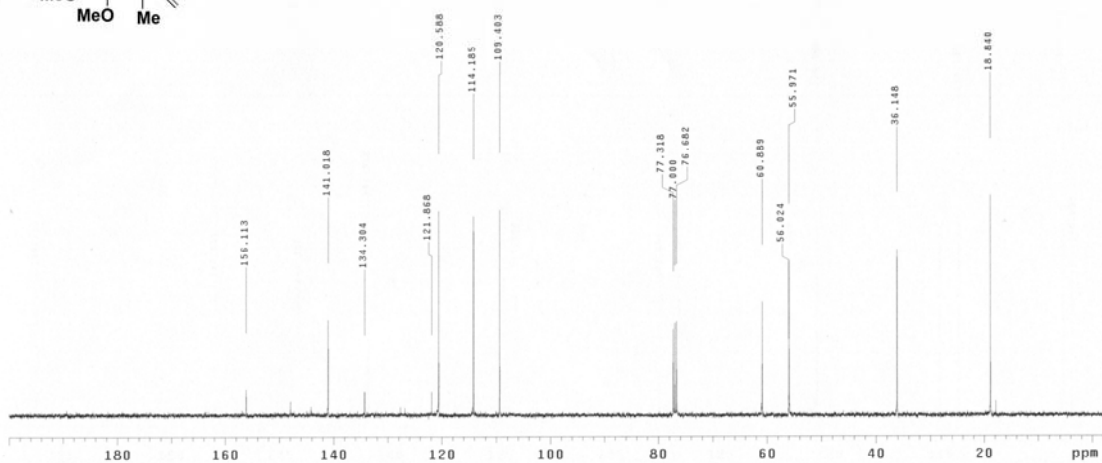
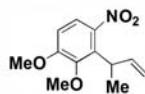


Compound 5l

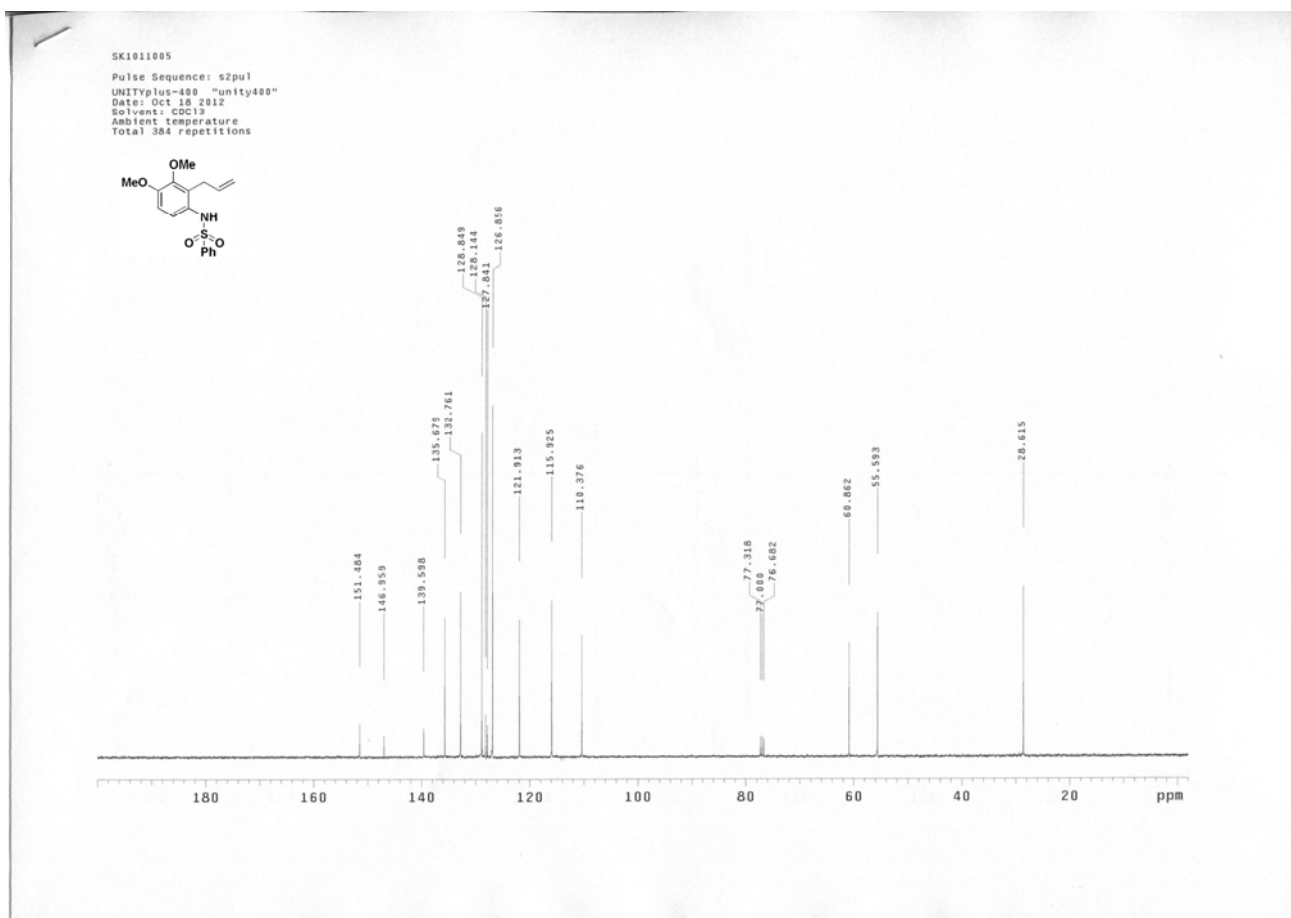
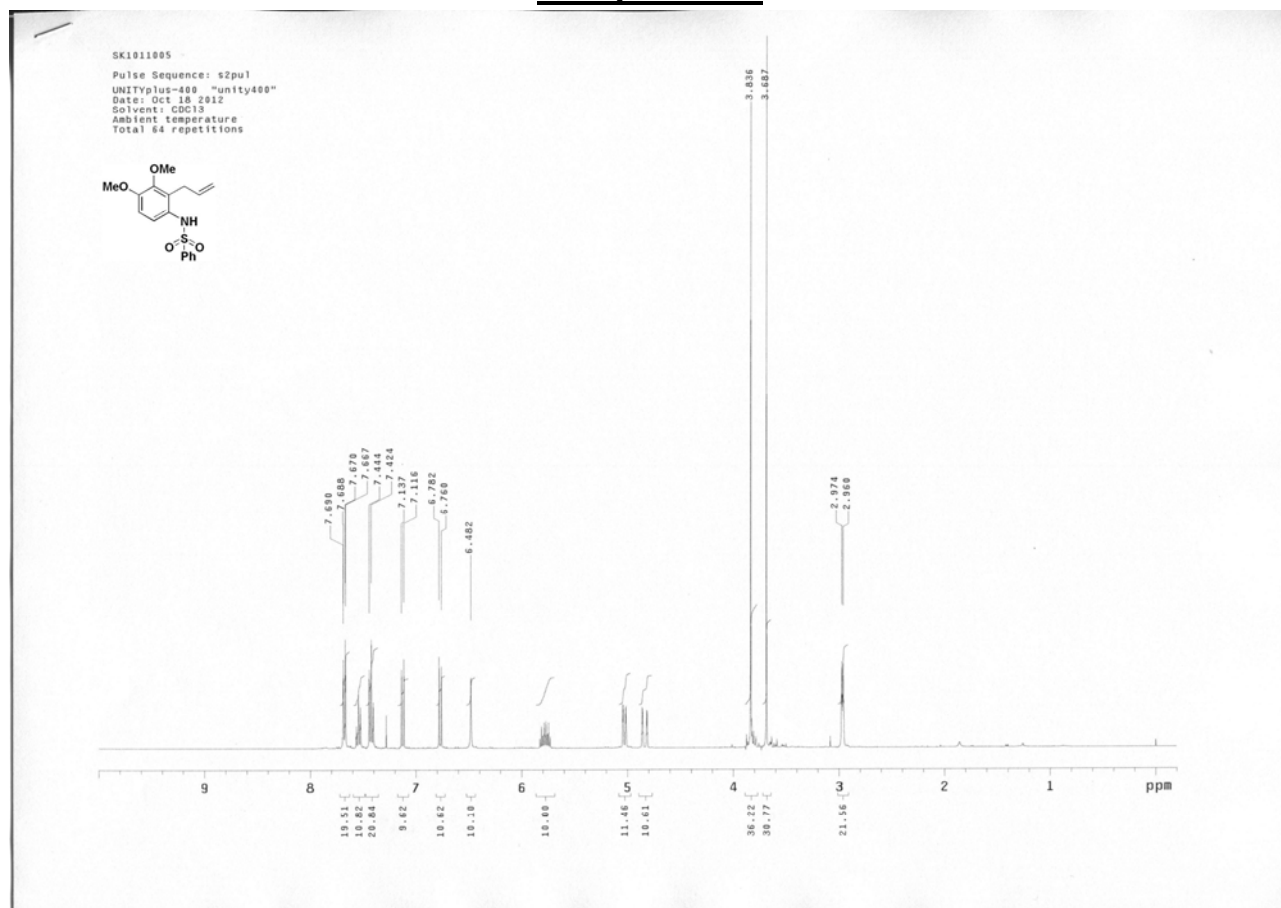
SK1011129
 Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
 Mercury-400BB "MercuryPlus400"
 Power: 0 dB
 Pulse 53.6 degrees
 Acq. time 4.002 sec
 Width 5995.2 Hz
 64 repetitions
 OBSERVE H1, 400.3978961 MHz
 DATA PROCESSING
 FT size 65536
 Total time 5 min, 7 sec



SK1011129
 Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
 Mercury-400BB "MercuryPlus400"
 Power: 0 dB
 Pulse 68.7 degrees
 Acq. time 1.998 sec
 Width 25000.0 Hz
 1232 repetitions
 OBSERVE C13, 100.6801346 MHz
 DECOUPLE H1, 400.3999572 MHz
 Power 38 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 65536
 Total time 21 hr, 51 min, 34 sec



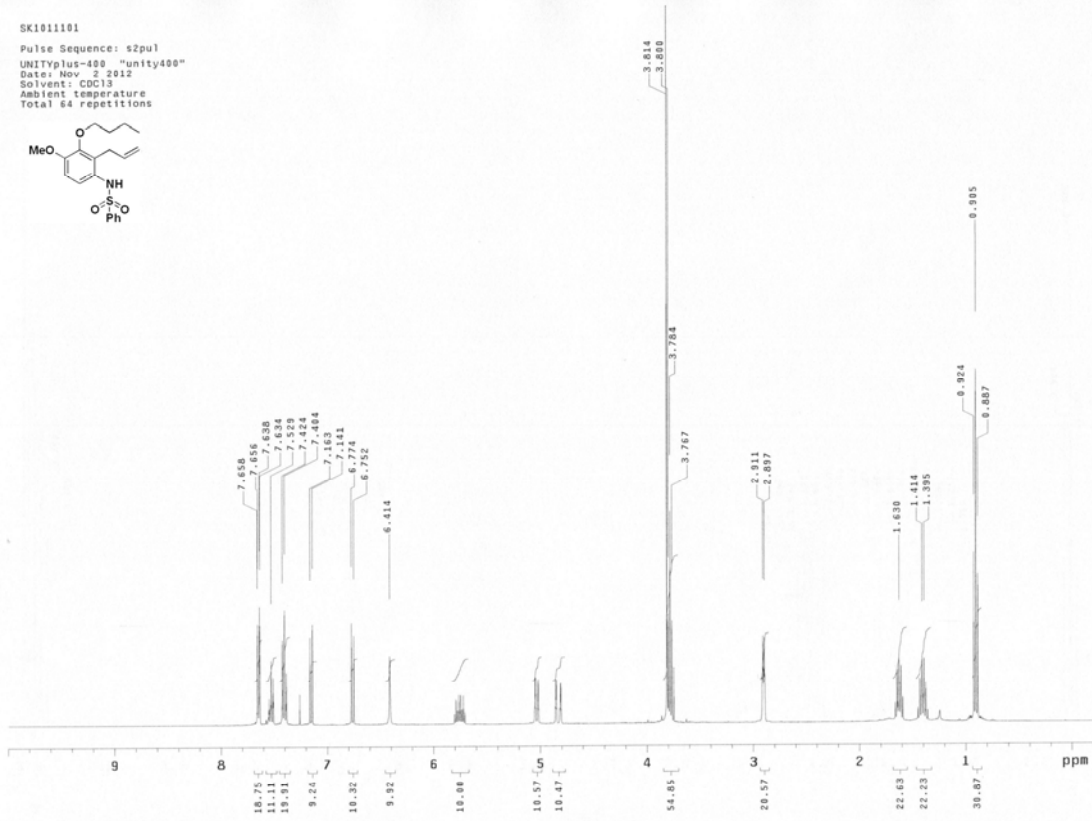
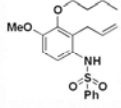
Compound 6a



Compound 6b

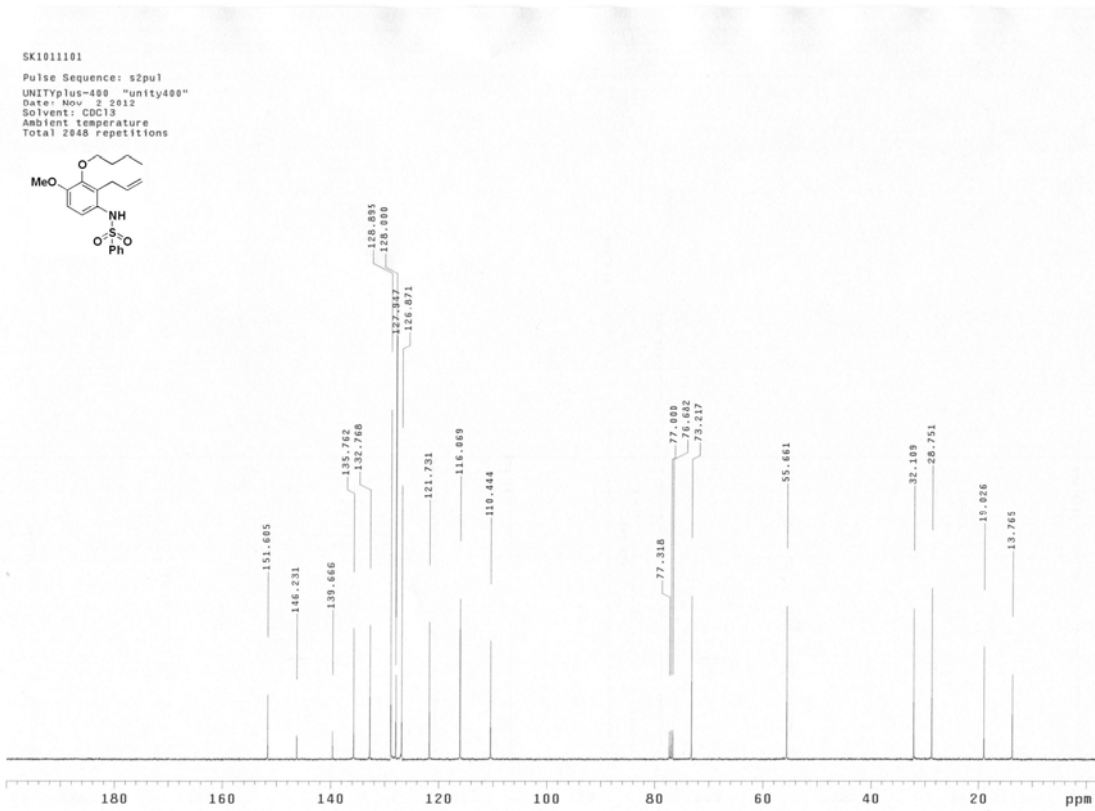
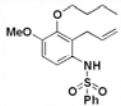
SK1011101

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Nov 2 2012
 Solvent: CDCl3
 Ambient temperature
 Total 64 repetitions



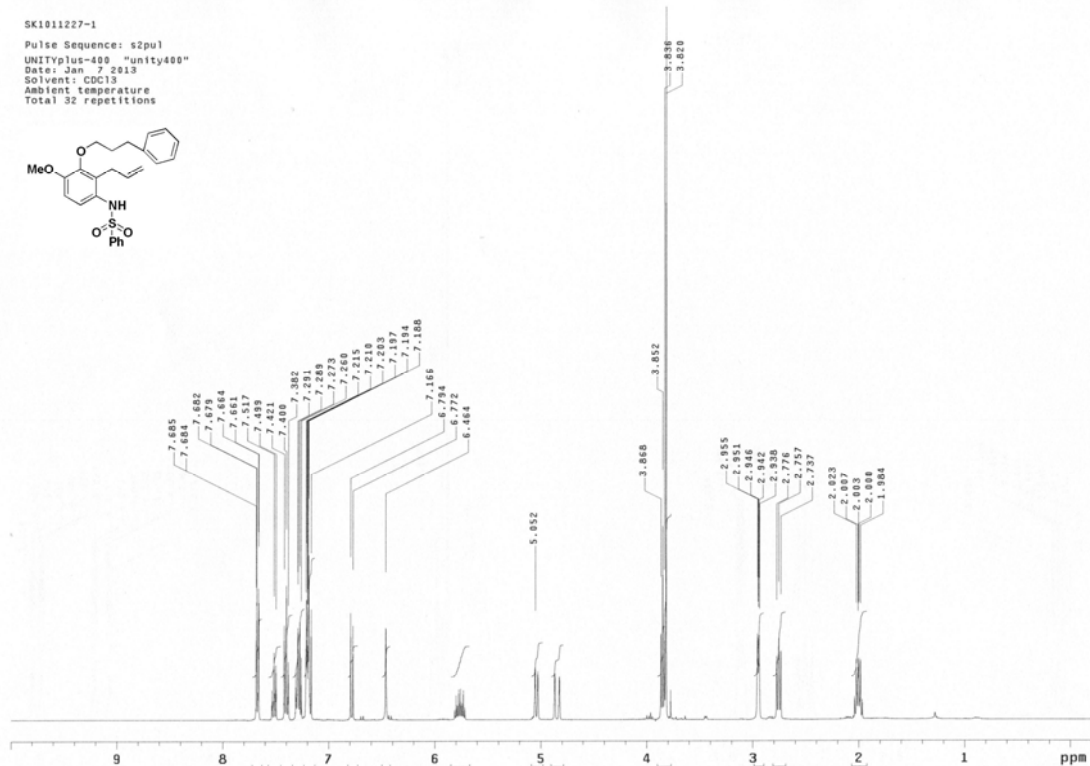
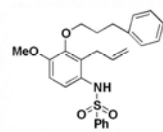
SK1011101

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Nov 2 2012
 Solvent: CDCl3
 Ambient temperature
 Total 2048 repetitions

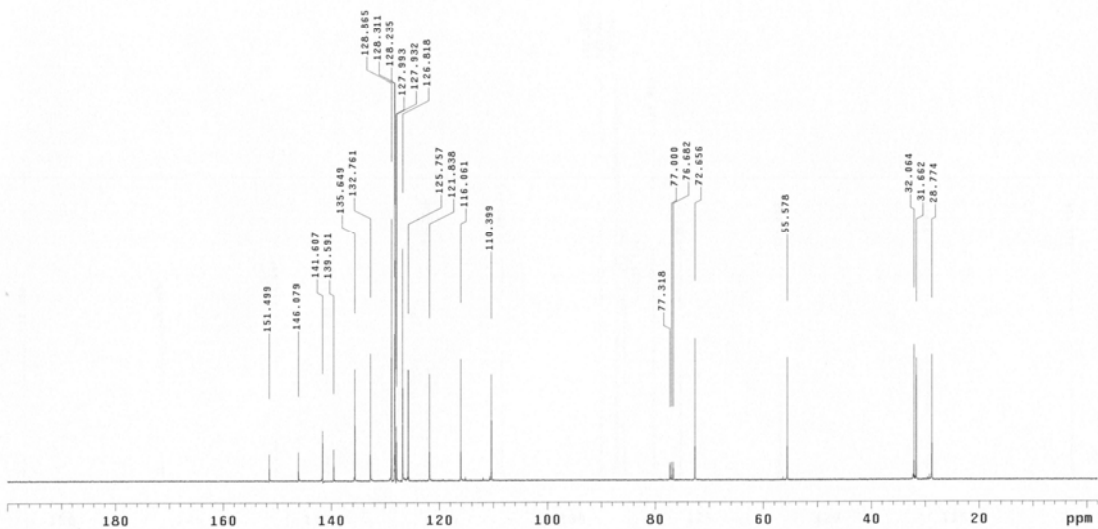
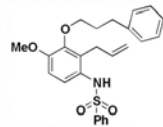


Compound 6c

SK1011227-1
 Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jan 7 2013
 Solvent: CDCl3
 Ambient temperature
 Total 32 repetitions

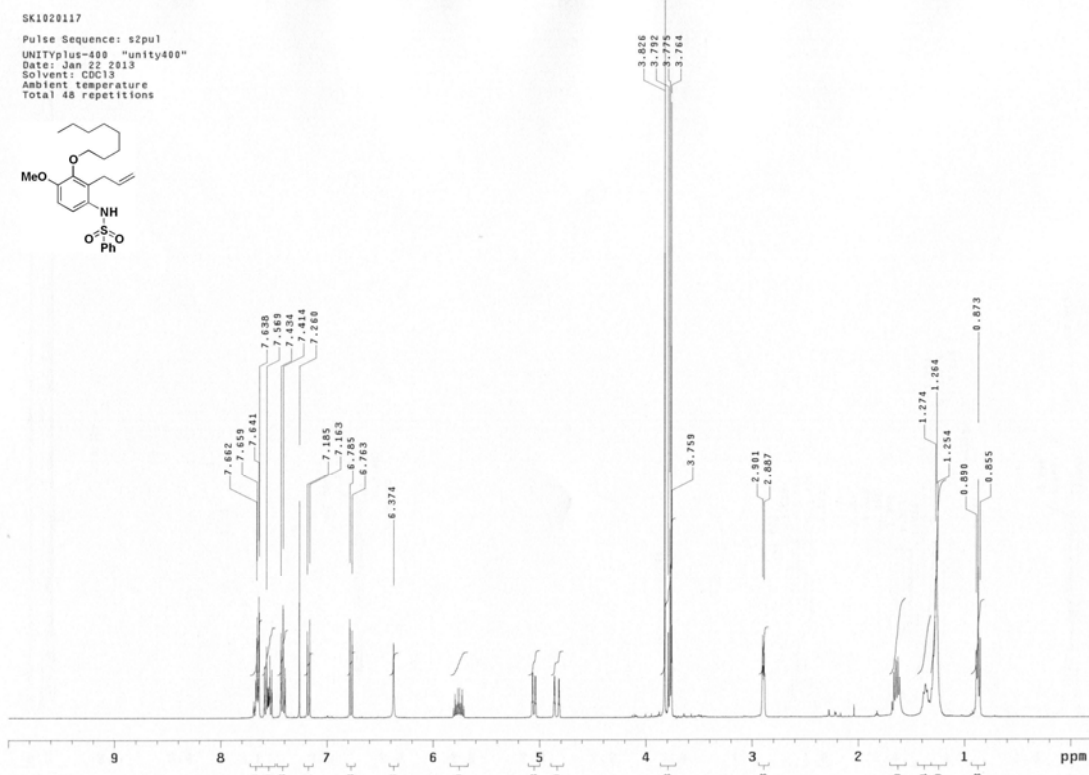
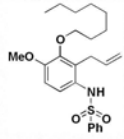


SK1011227-1
 Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jan 7 2013
 Solvent: CDCl3
 Ambient temperature
 Total 2048 repetitions

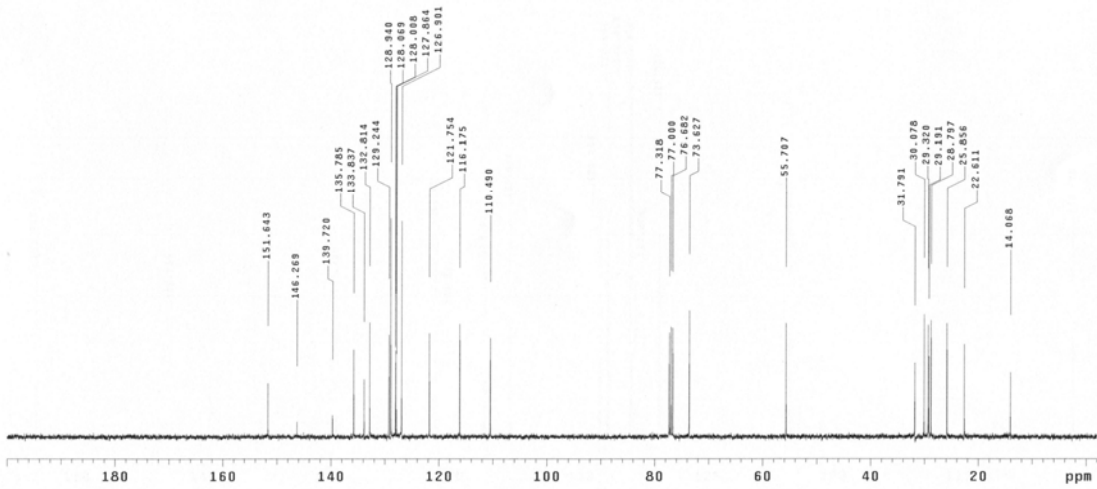
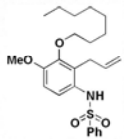


Compound 6d

SK1020117
 Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jan 22 2013
 Solvent: CDCl3
 Ambient temperature
 Total 48 repetitions

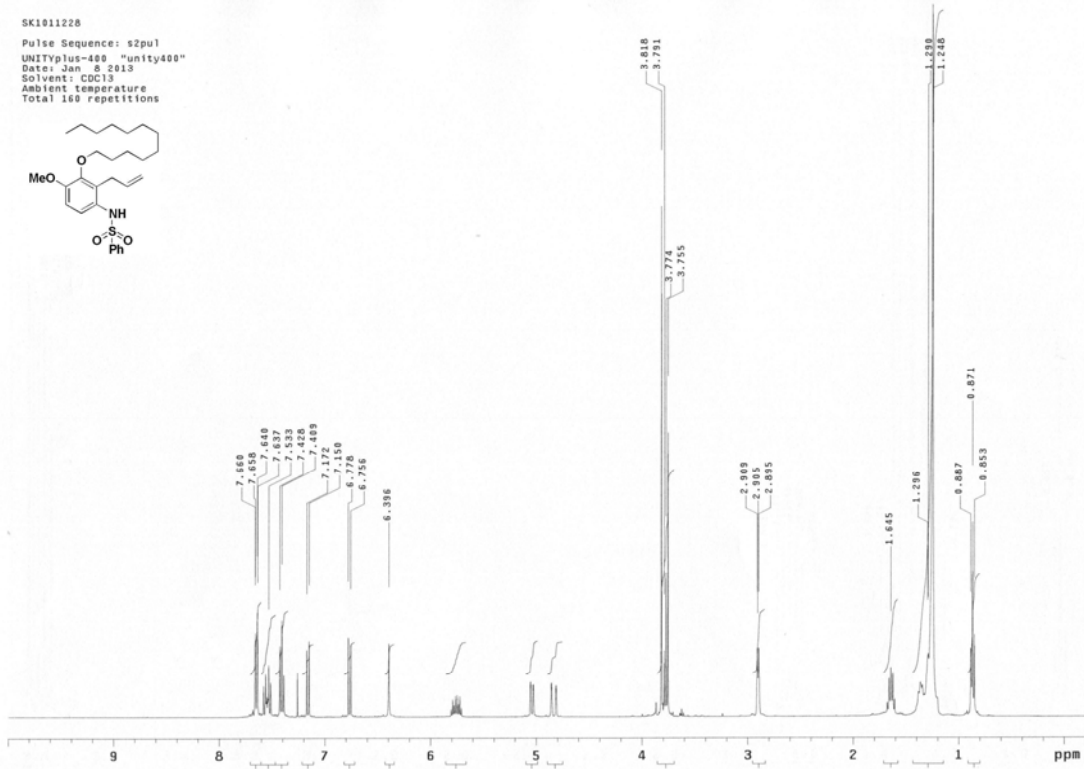
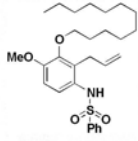


SK1020117
 Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jan 22 2013
 Solvent: CDCl3
 Ambient temperature
 Total 3280 repetitions

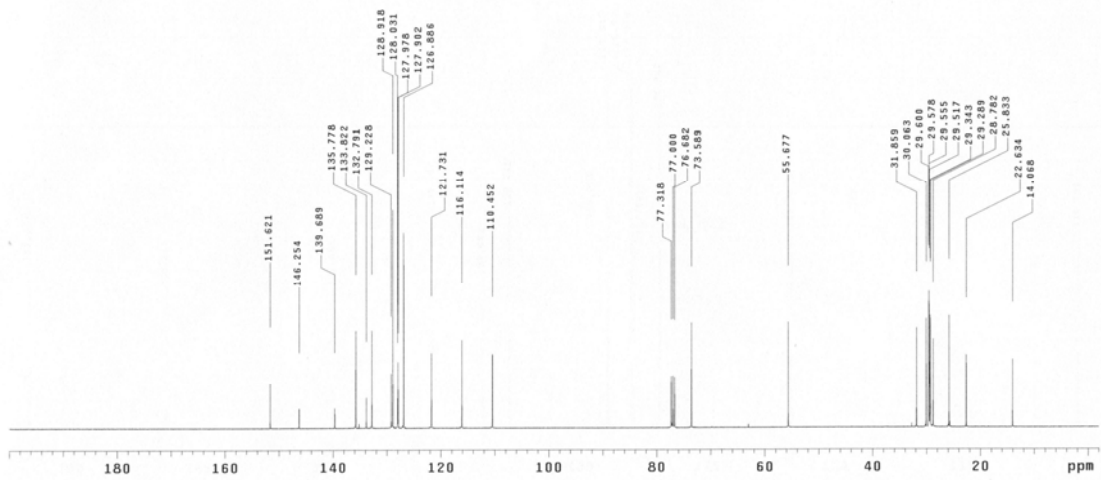
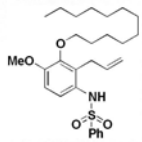


Compound 6e

SK1011228
 Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jan 8 2013
 Solvent: CDCl3
 Ambient temperature
 Total 160 repetitions



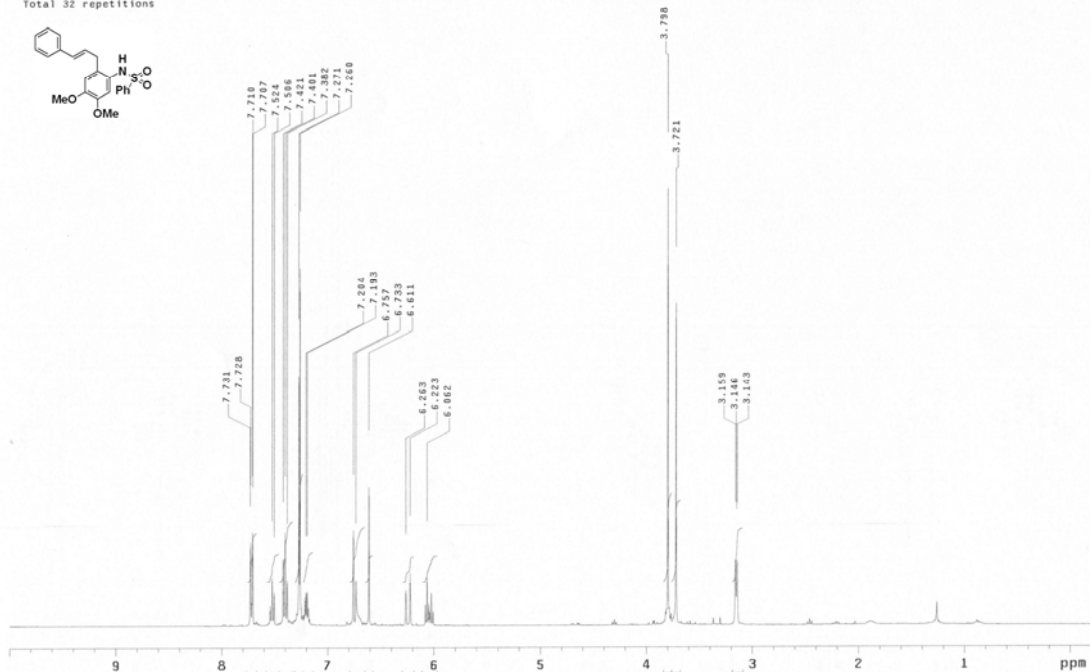
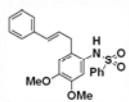
SK1011228
 Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jan 8 2013
 Solvent: CDCl3
 Ambient temperature
 Total 24960 repetitions



Compound 6f

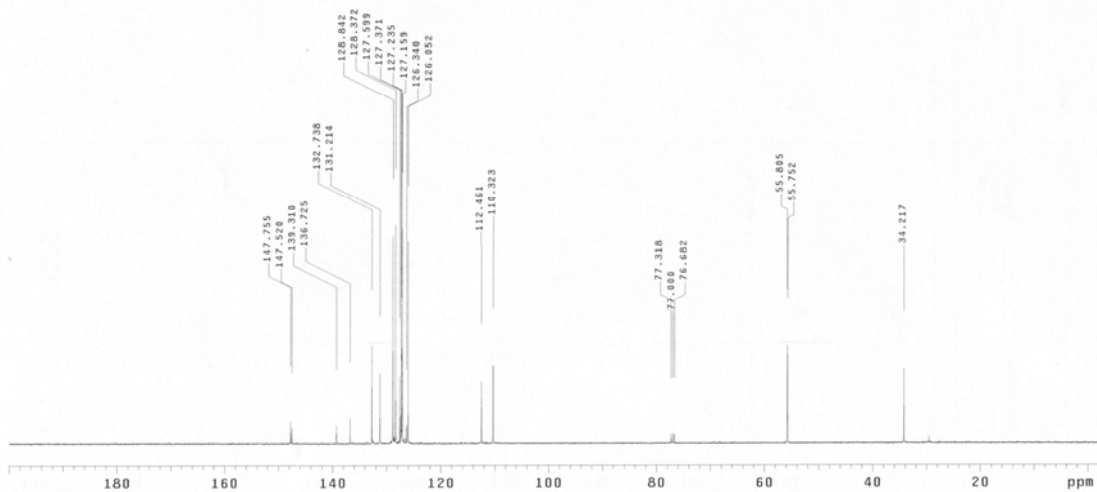
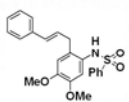
SK1011114

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Nov 16 2012
 Solvent: CDCl3
 Ambient temperature
 Total 32 repetitions



SK1011114

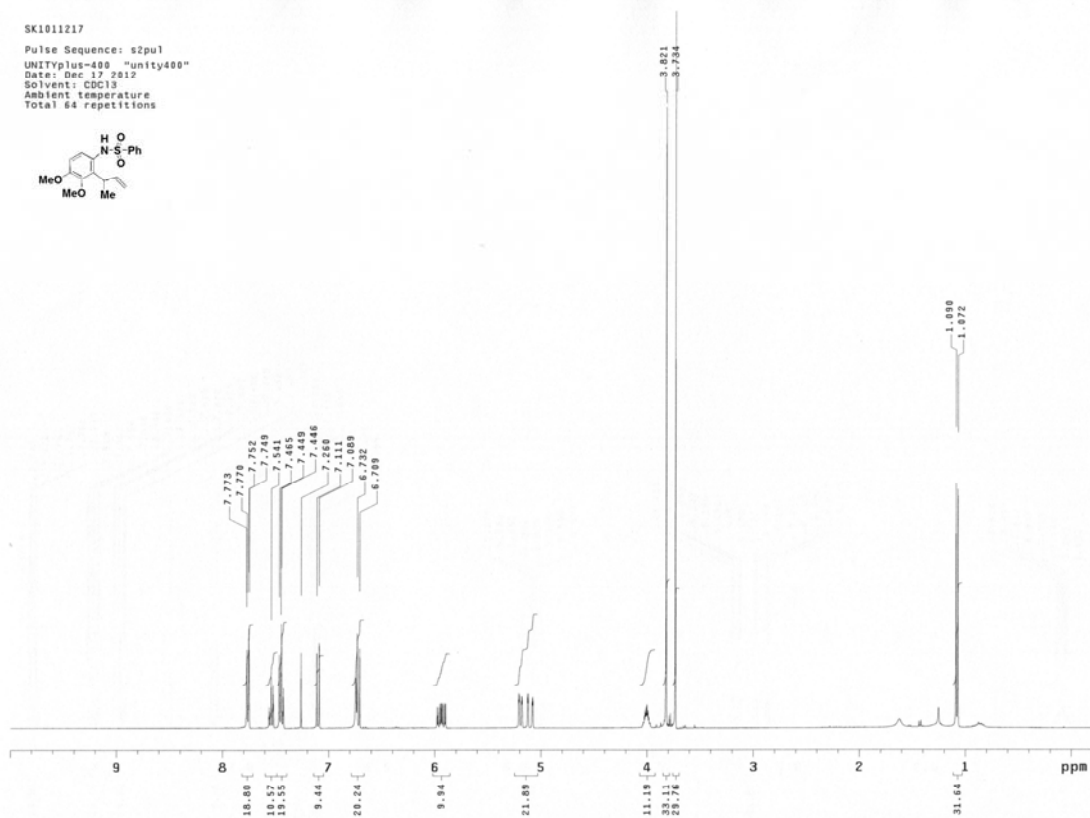
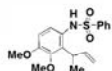
Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Nov 16 2012
 Solvent: CDCl3
 Ambient temperature
 Total 880 repetitions



Compound 6g

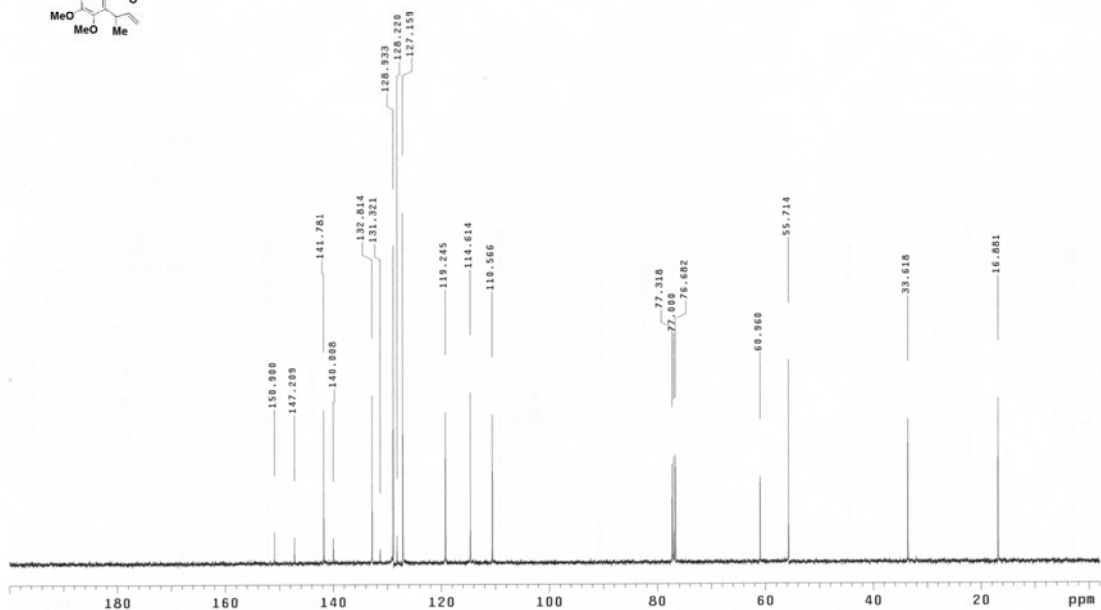
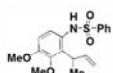
SK1011217

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Dec 17 2012
 Solvent: CDCl3
 Ambient temperature
 Total 64 repetitions



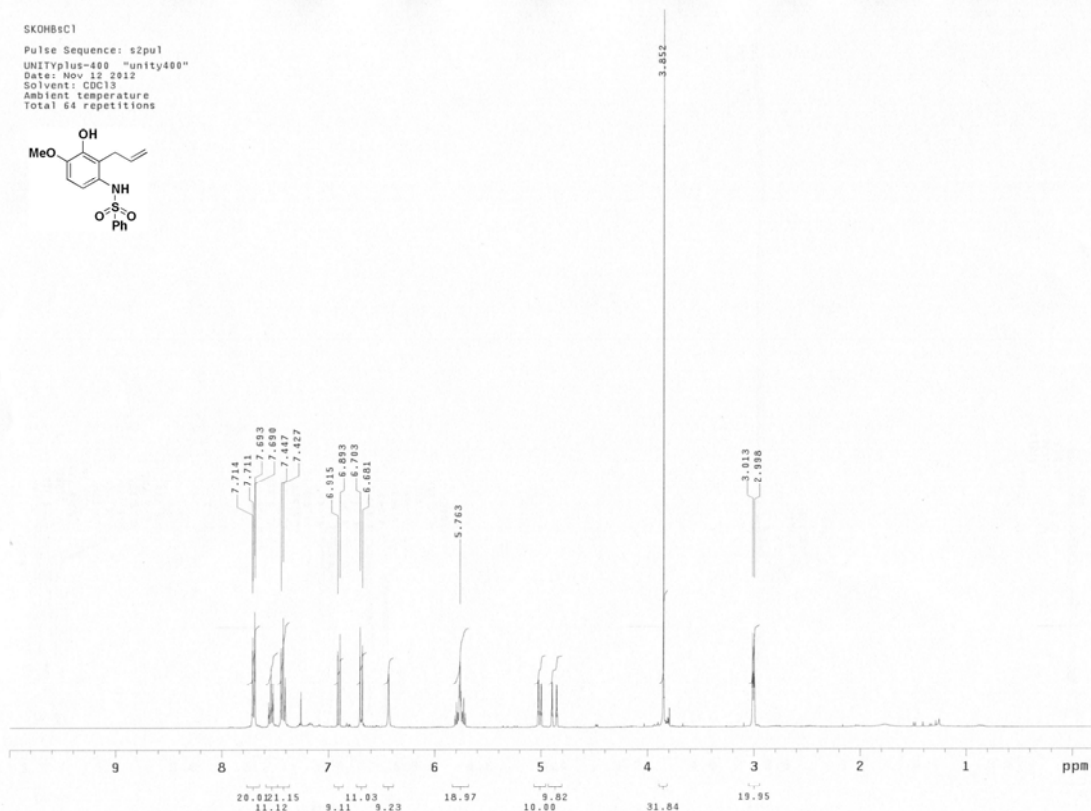
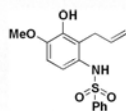
SK1011217

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Dec 17 2012
 Solvent: CDCl3
 Ambient temperature
 Total 4080 repetitions

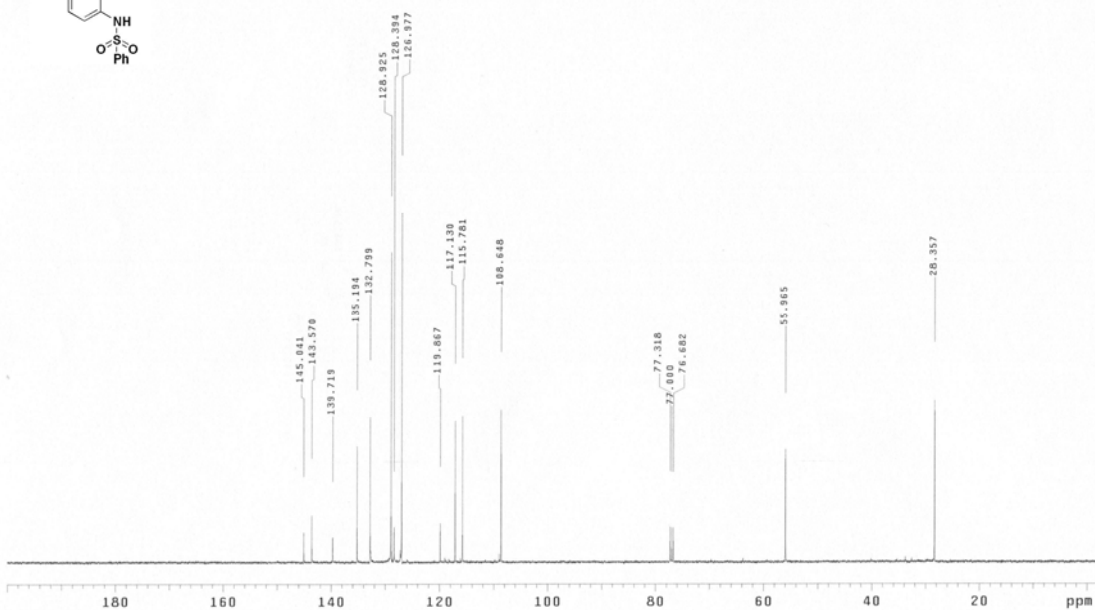
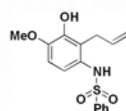


Compound 6h

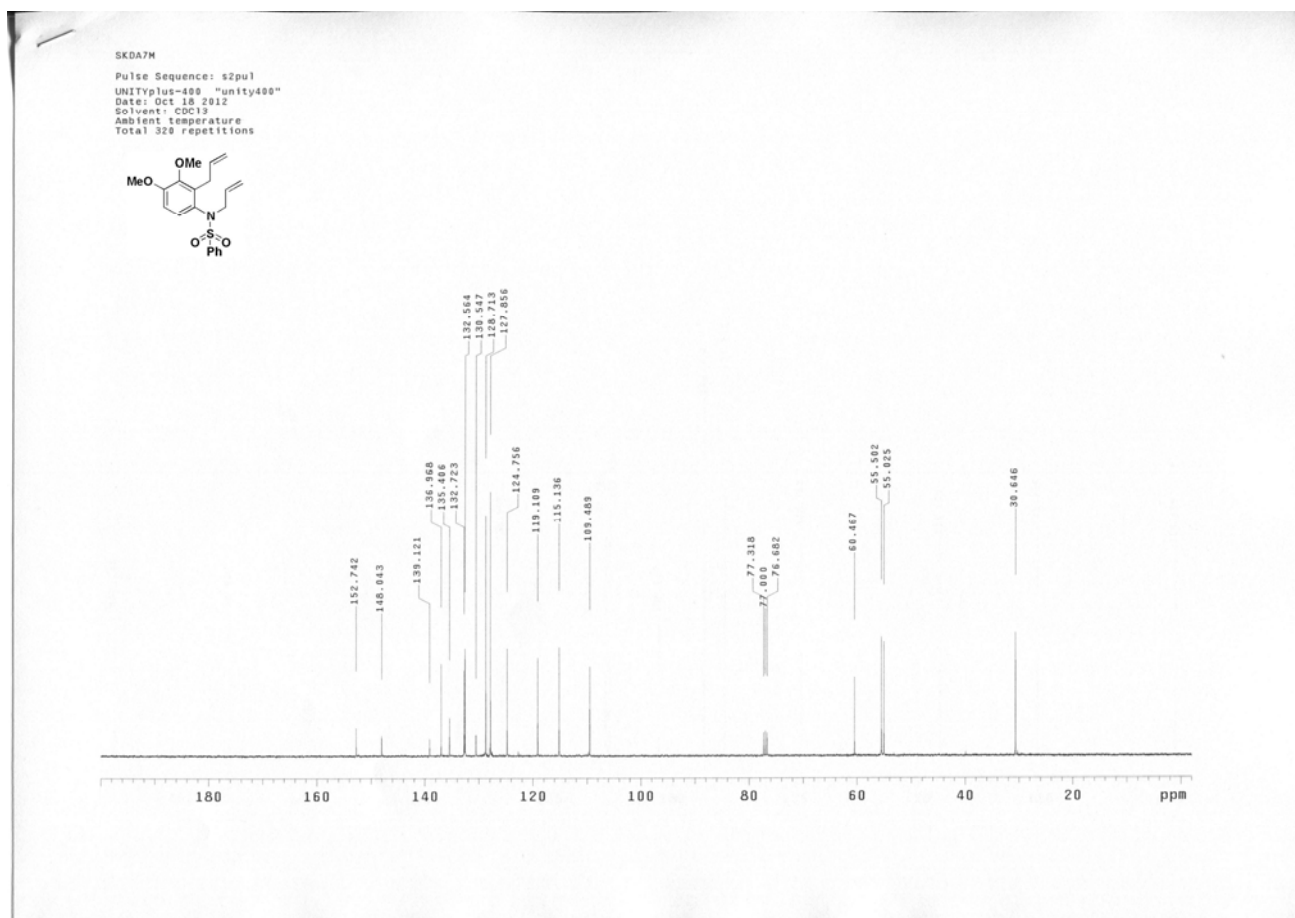
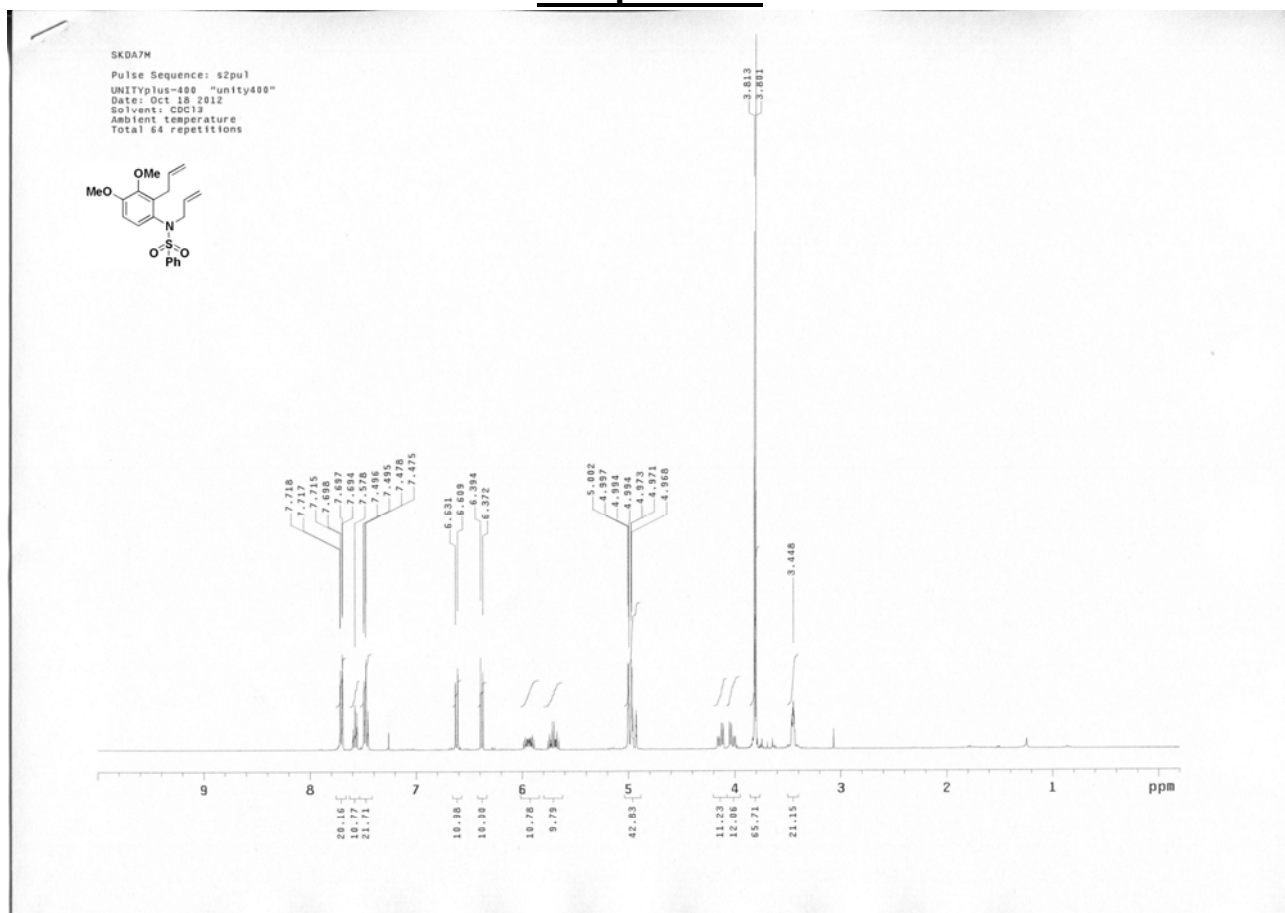
SKOH8c1
 Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Nov 12 2012
 Solvent: CDCl3
 Ambient temperature
 Total 64 repetitions



SKOH8c1
 Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Nov 12 2012
 Solvent: CDCl3
 Ambient temperature
 Total 1680 repetitions

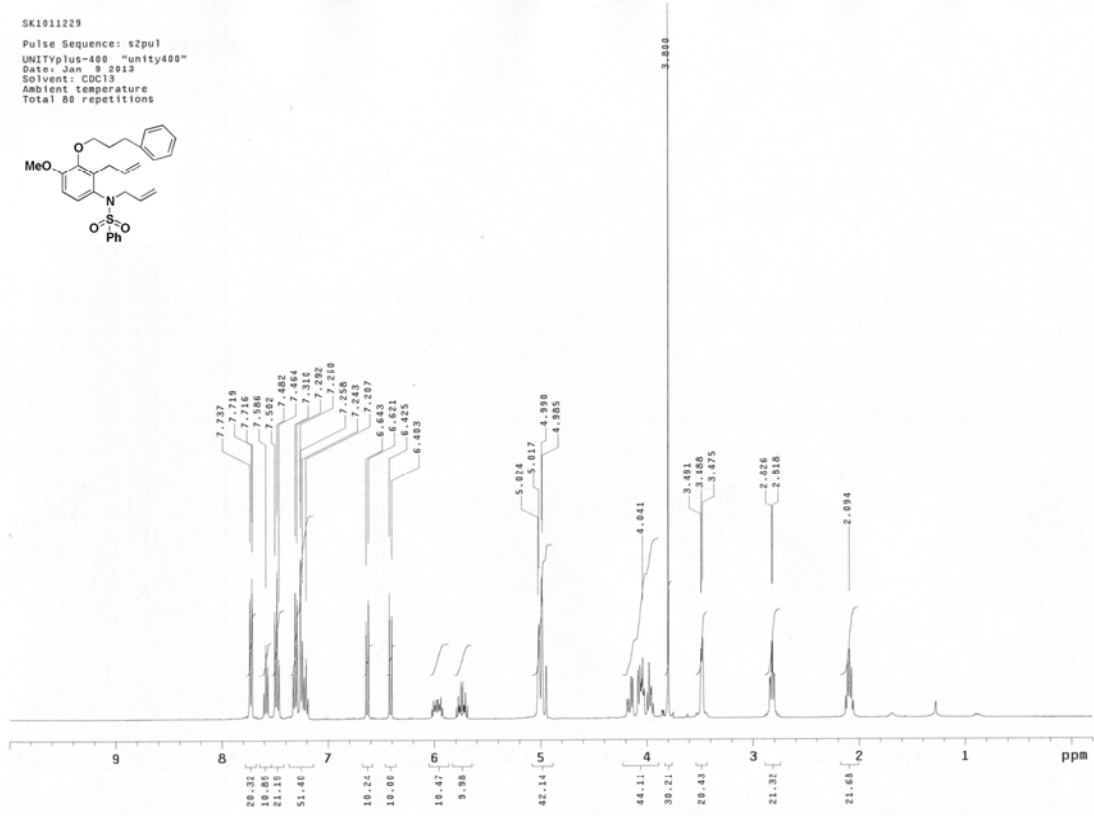
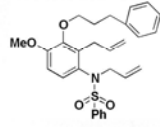


Compound 7a

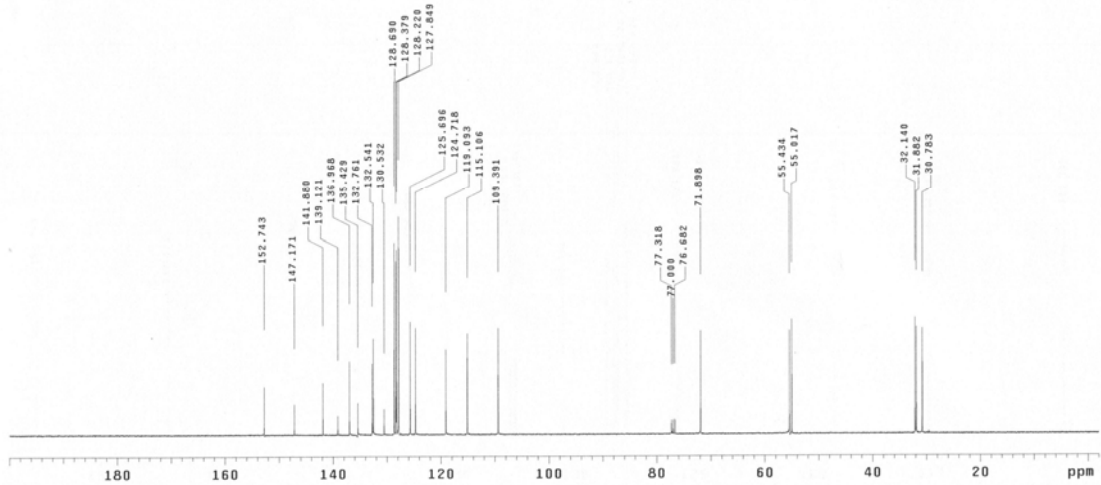
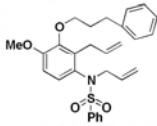


Compound 7c

SK1011229
 Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Jan 9 2013
 Solvent: CDCl3
 Ambient temperature
 Total 80 repetitions

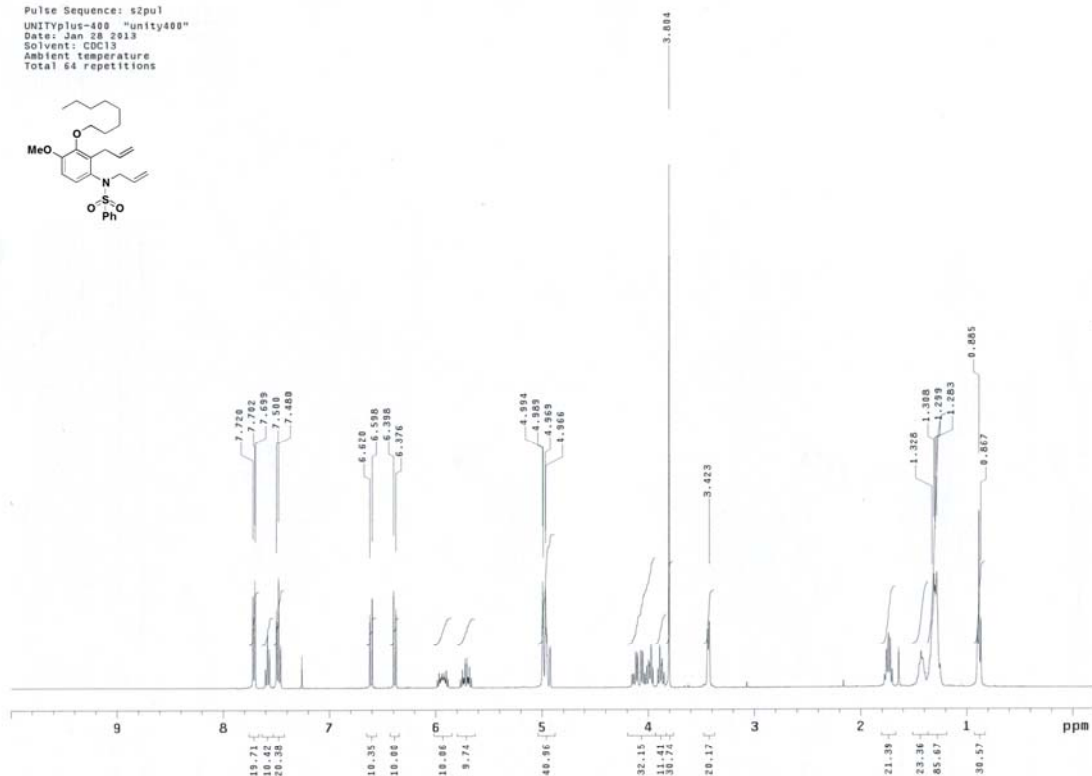
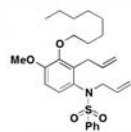


SK1011229
 Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Jan 9 2013
 Solvent: CDCl3
 Ambient temperature
 Total 1200 repetitions

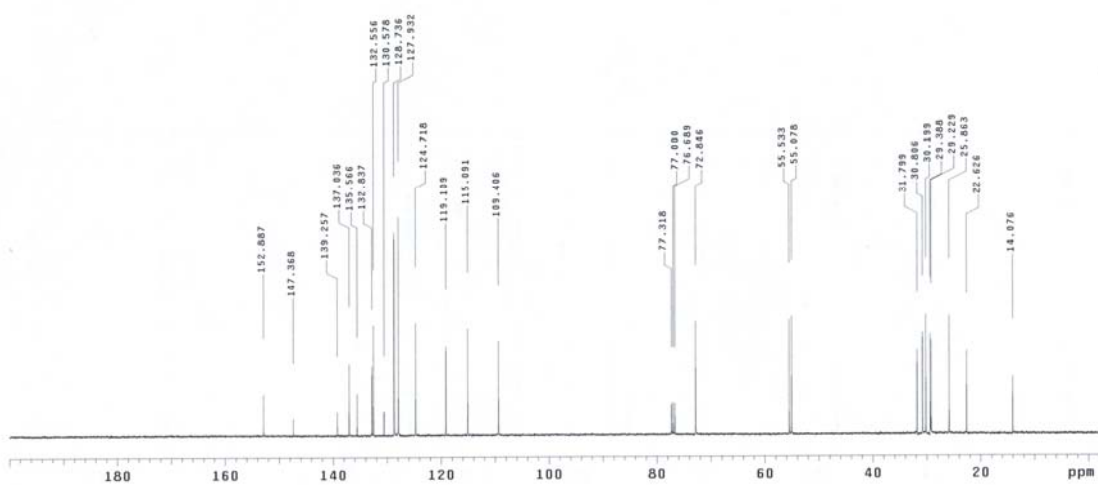
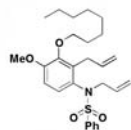


Compound 7d

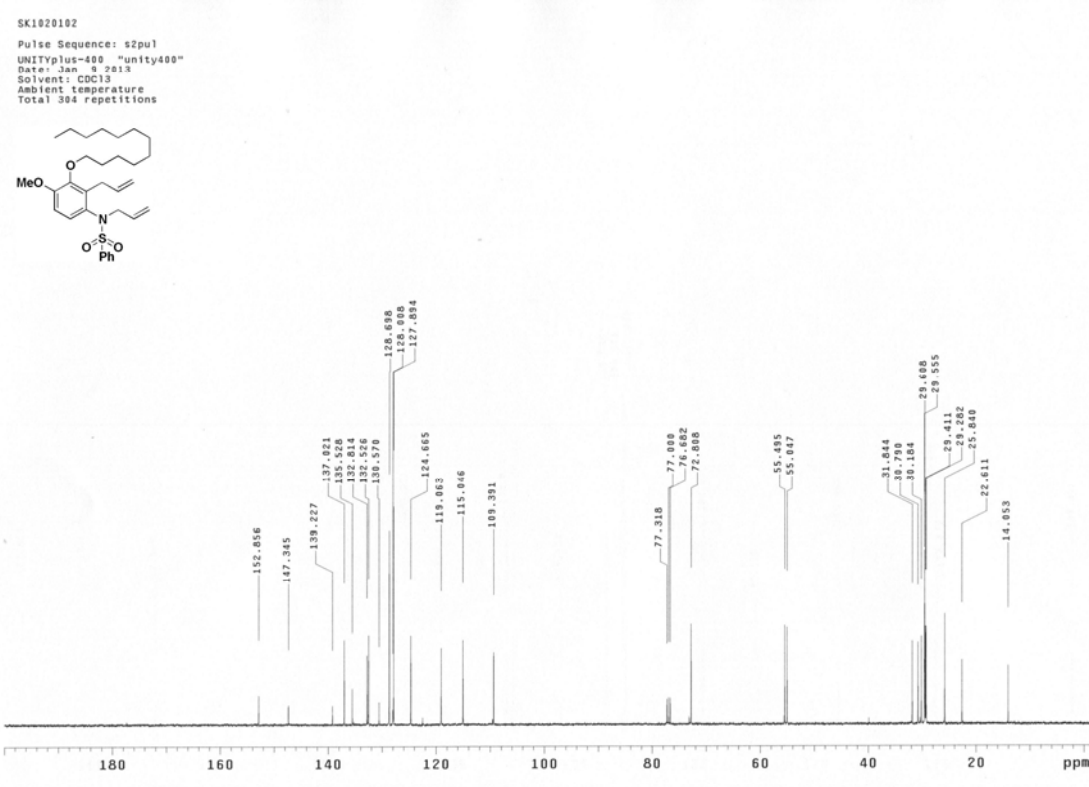
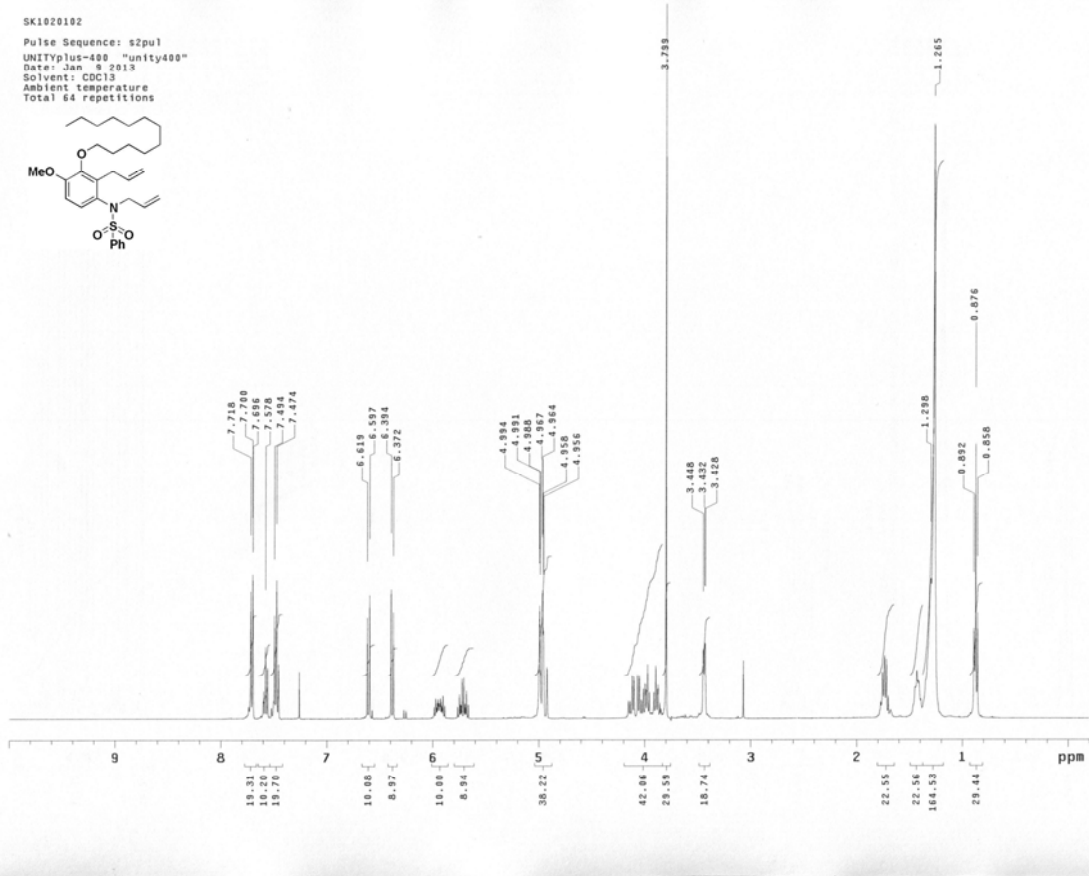
SK1020118
 Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Jan 28 2013
 Solvent: CDCl3
 Ambient temperature
 Total 54 repetitions



SK1020118
 Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Jan 28 2013
 Solvent: CDCl3
 Ambient temperature
 Total 1392 repetitions



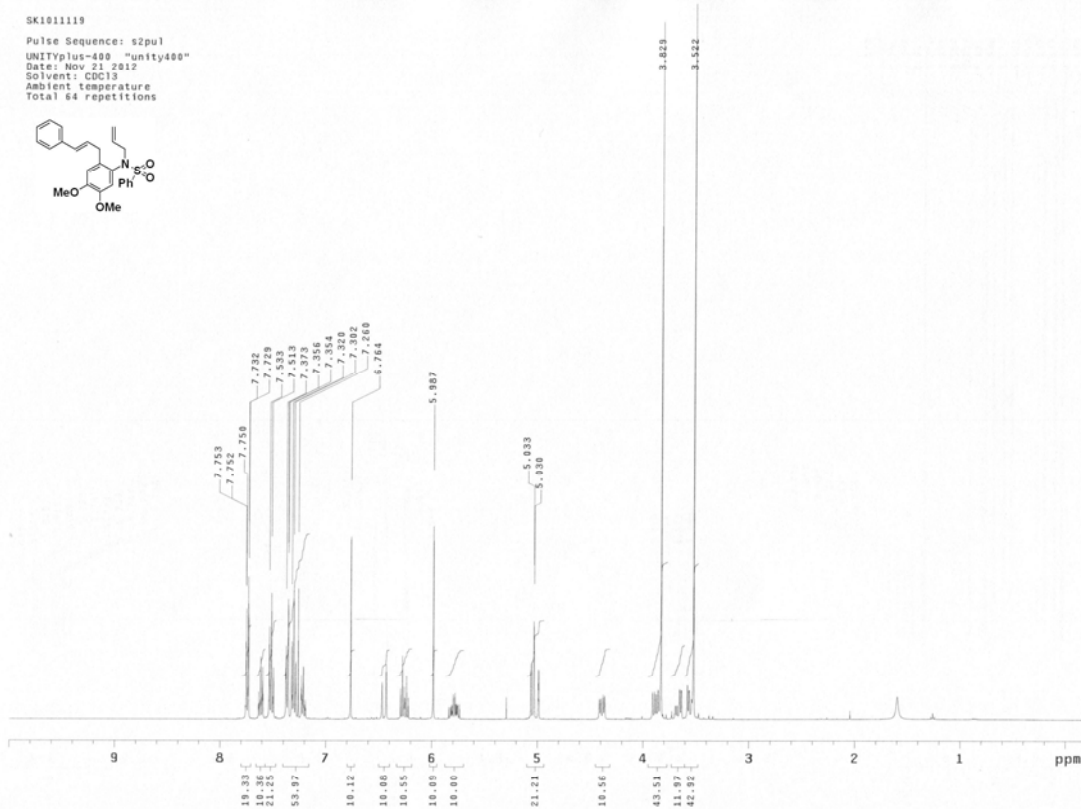
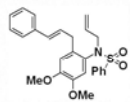
Compound 7e



Compound 7f

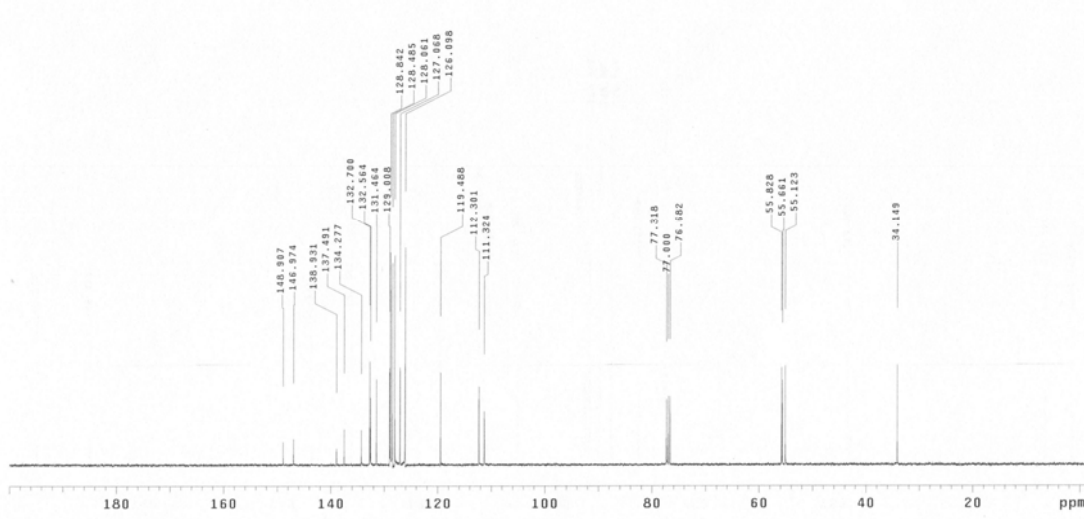
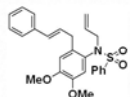
SK1011119

Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Nov 21 2012
 Solvent: CDCl3
 Ambient temperature
 Total 64 repetitions



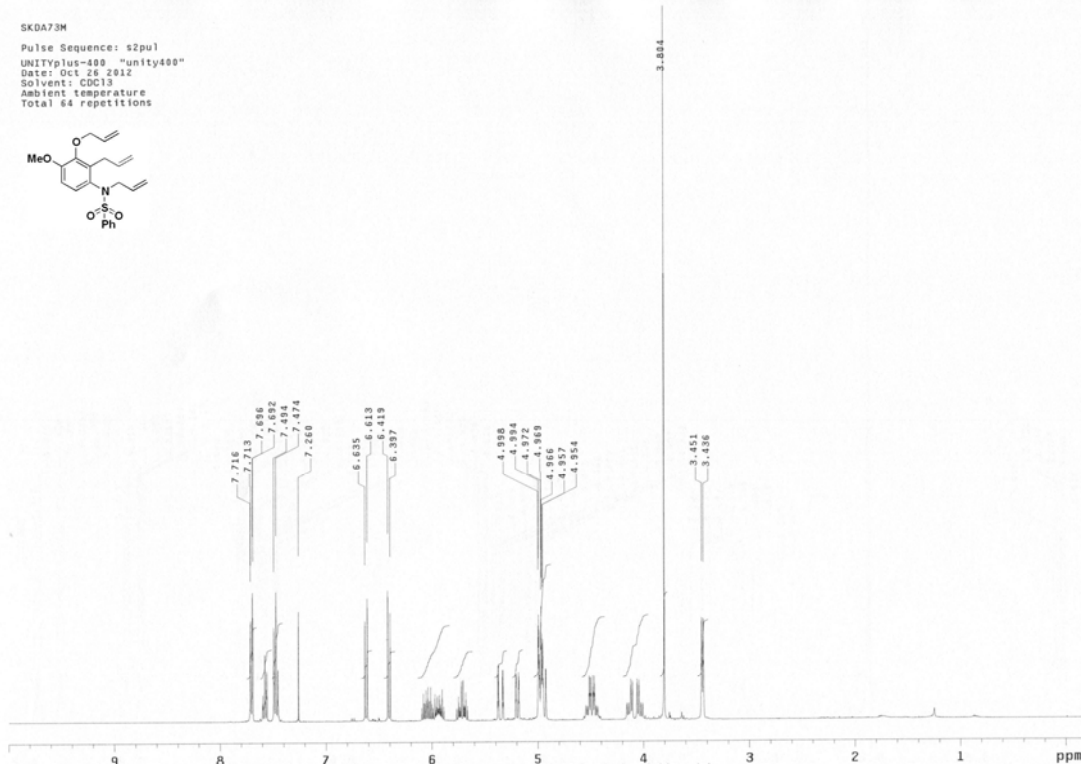
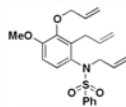
SK1011119

Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Nov 21 2012
 Solvent: CDCl3
 Ambient temperature
 Total 4526 repetitions

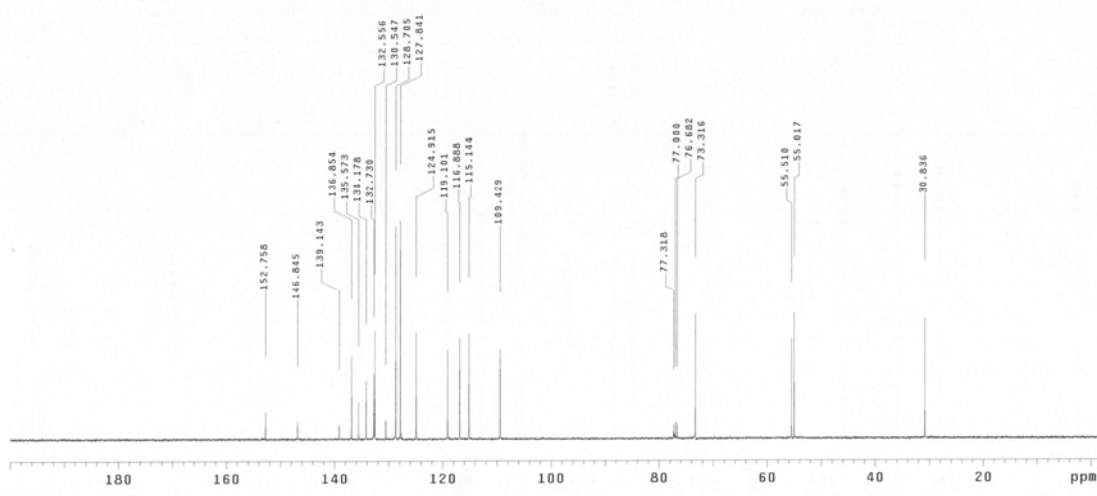
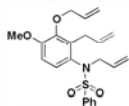


Compound 7i

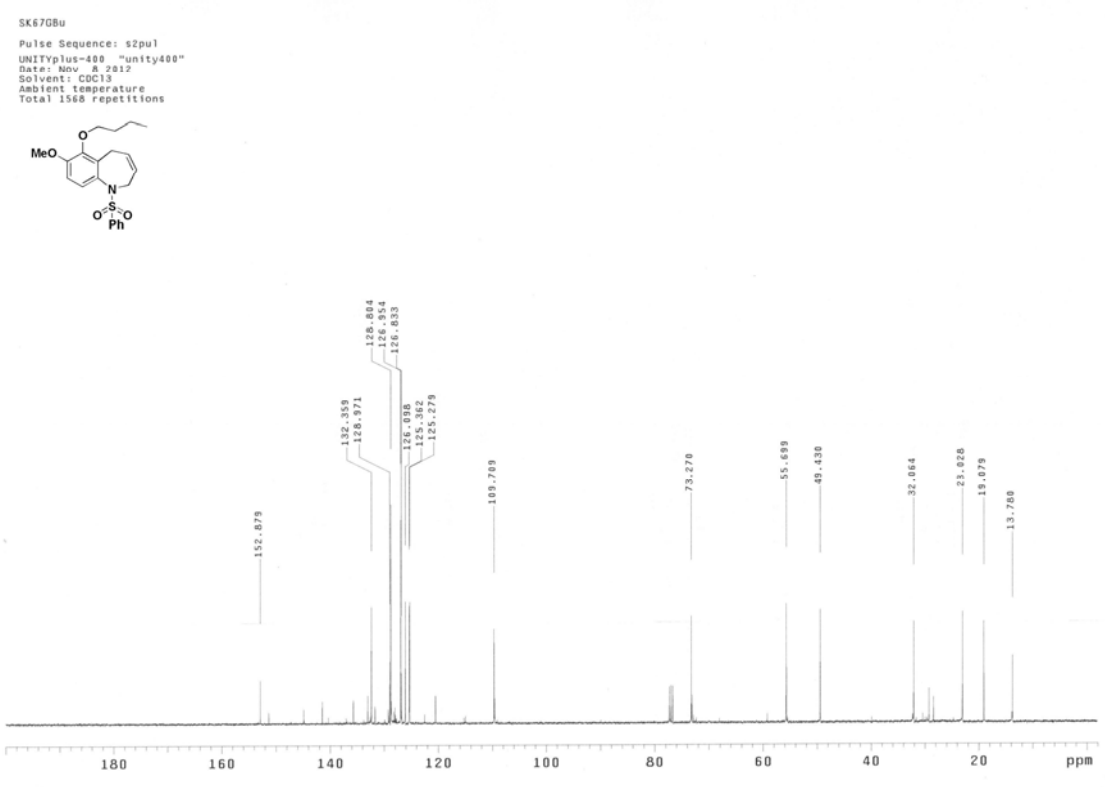
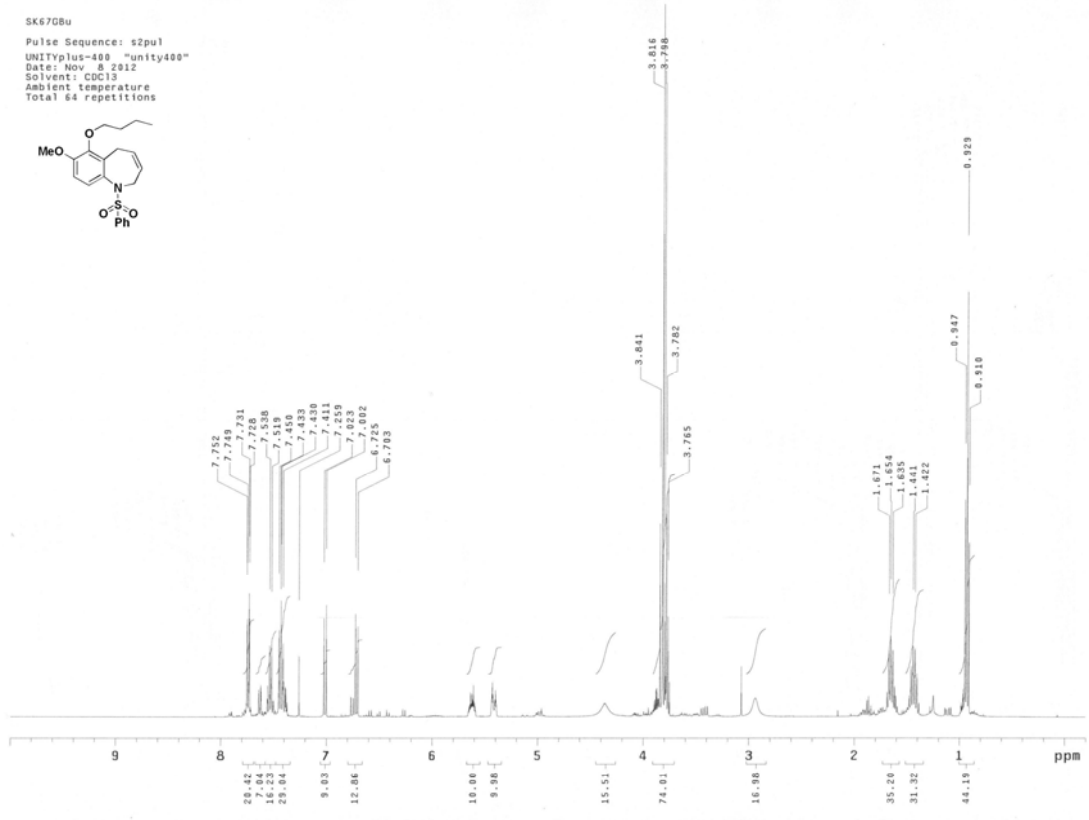
SKDA73M
 Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Oct 26 2012
 Solvent: CDCl3
 Ambient temperature
 Total 64 repetitions



SKDA73M
 Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Oct 26 2012
 Solvent: CDCl3
 Ambient temperature
 Total 368 repetitions

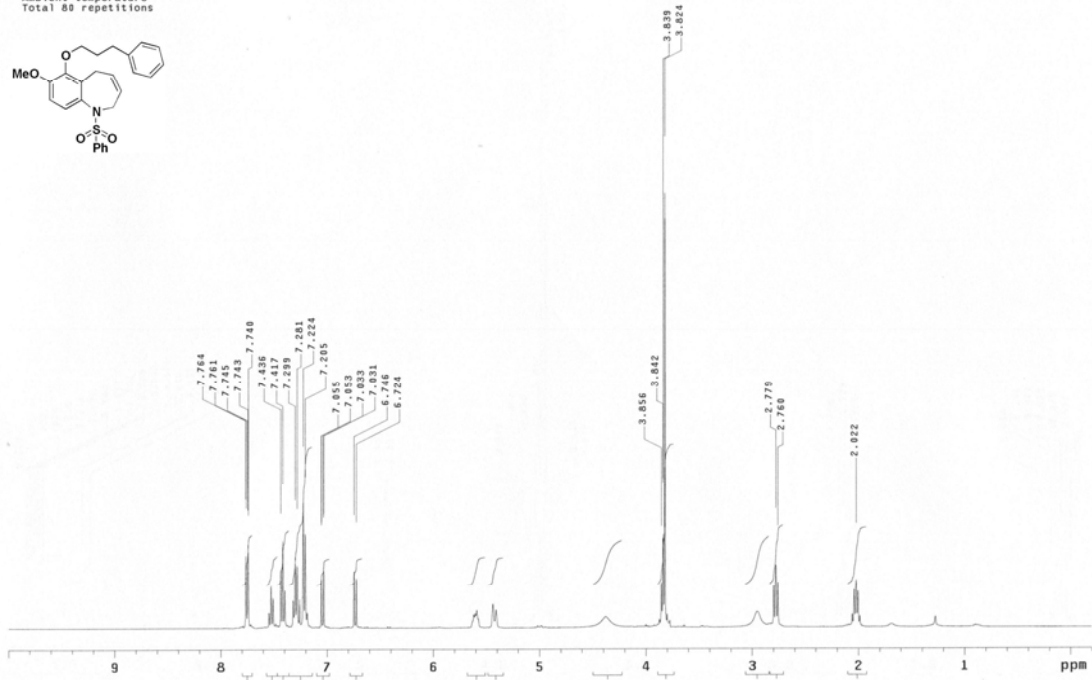
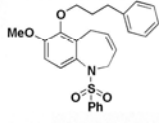


Compound 8b

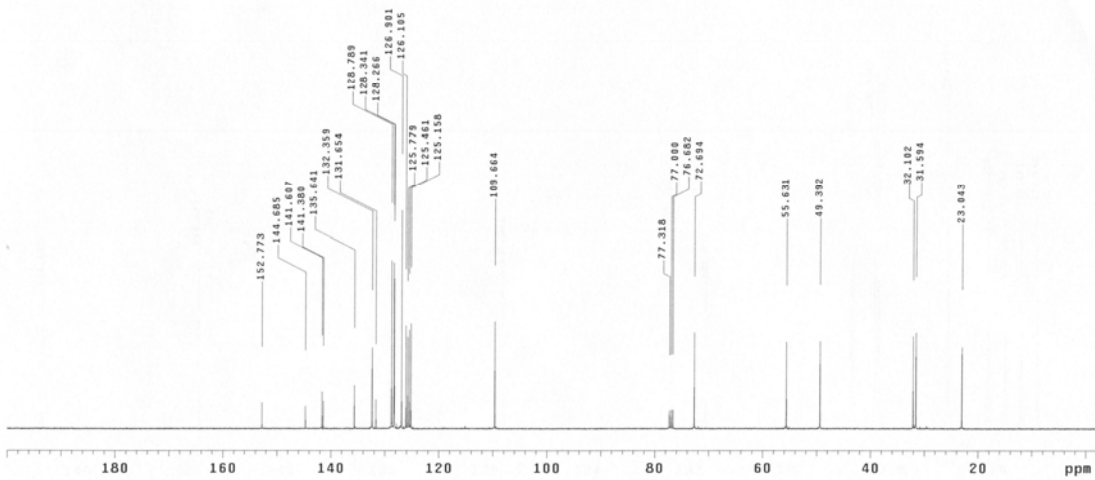
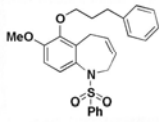


Compound 8c

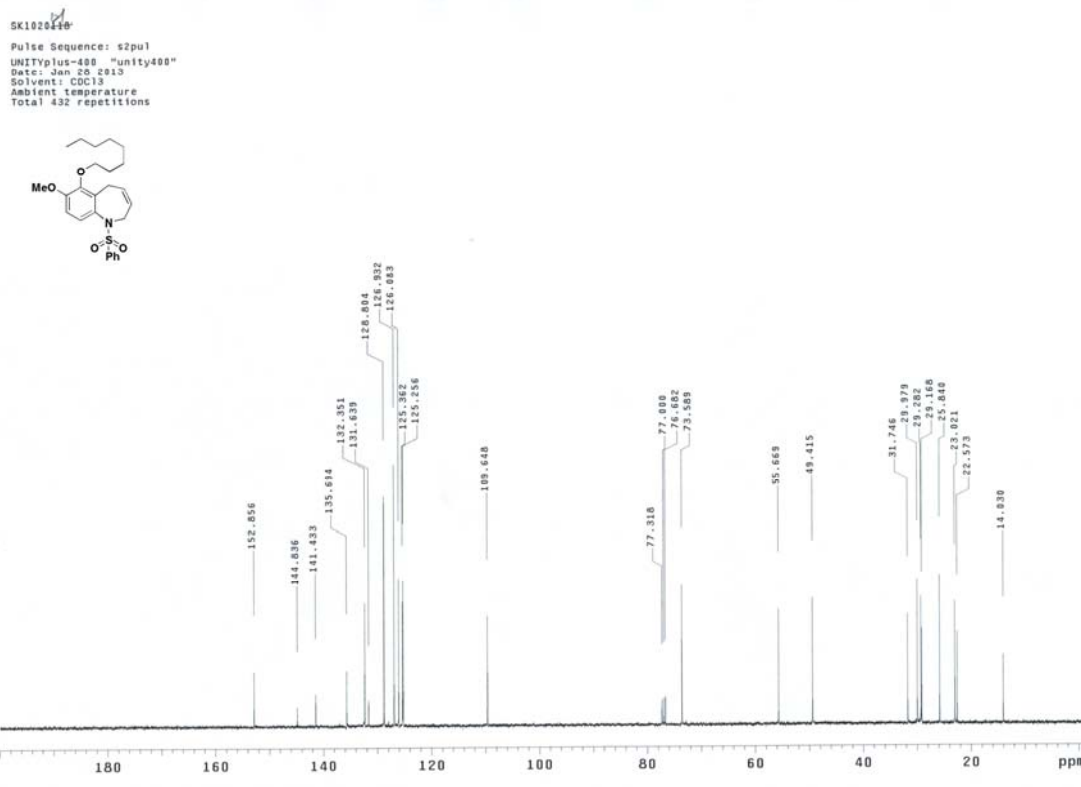
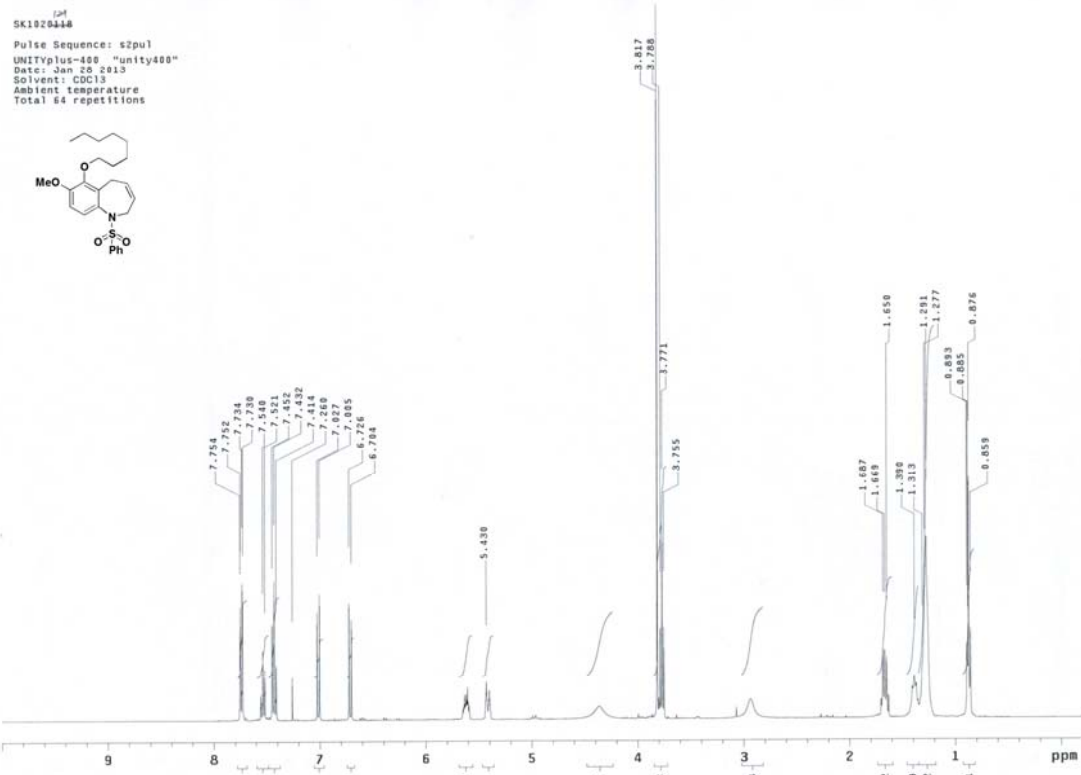
SK1020101
 Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jan 9 2013
 Solvent: CDCl3
 Ambient temperature
 Total 80 repetitions



SK1020101
 Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jan 9 2013
 Solvent: CDCl3
 Ambient temperature
 Total 2016 repetitions

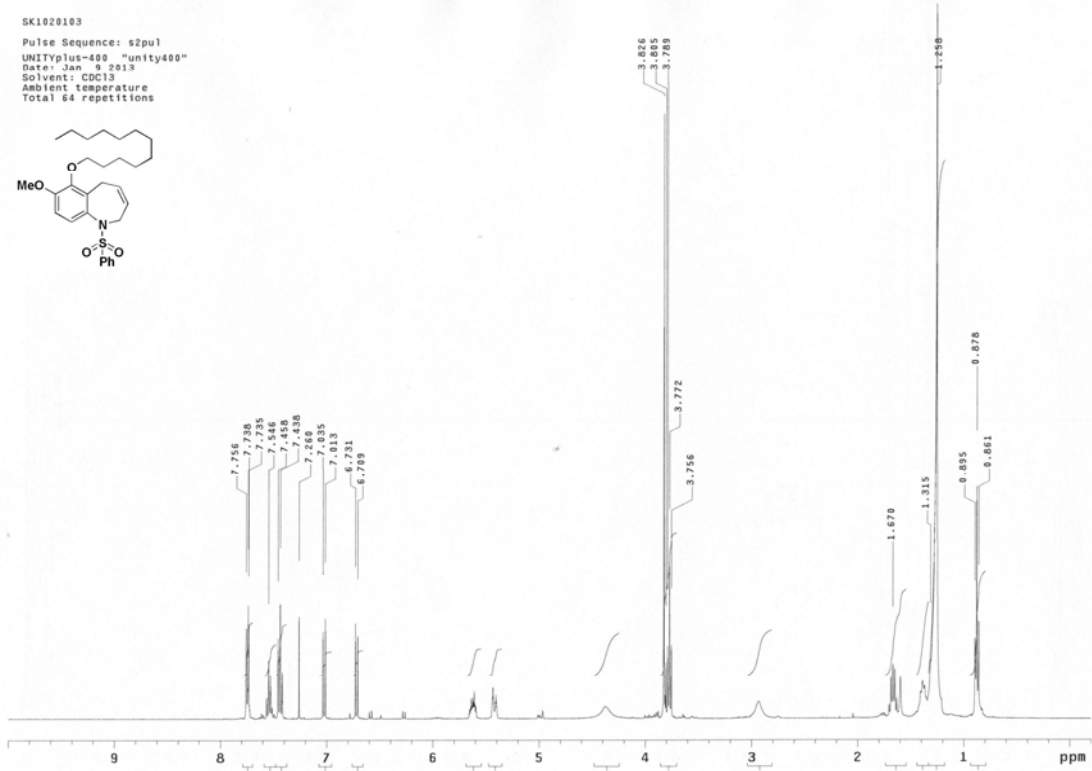
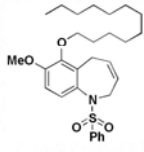


Compound 8d

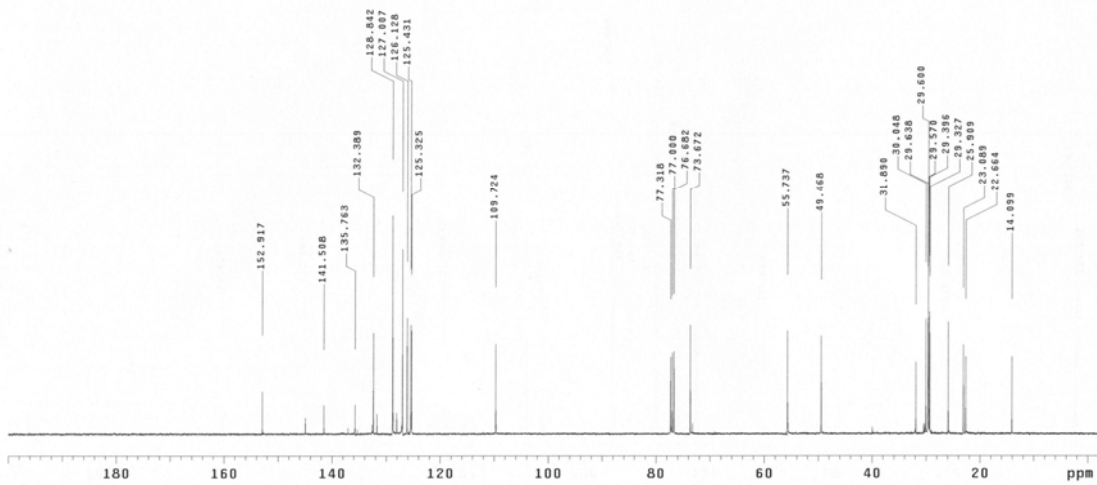
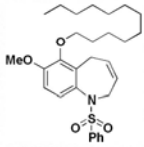


Compound 8e

SK1020103
 Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jan 8 2013
 Solvent: CDCl3
 Ambient temperature
 Total 64 repetitions



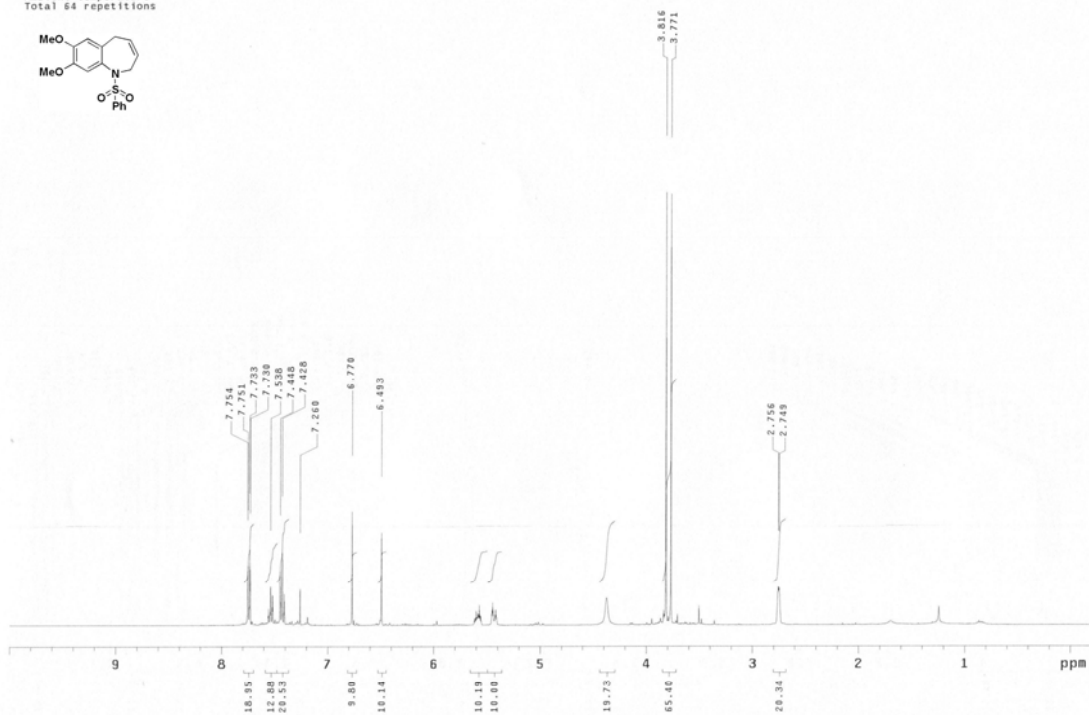
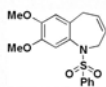
SK1020103
 Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Jan 8 2013
 Solvent: CDCl3
 Ambient temperature
 Total 14176 repetitions



Compound 8f

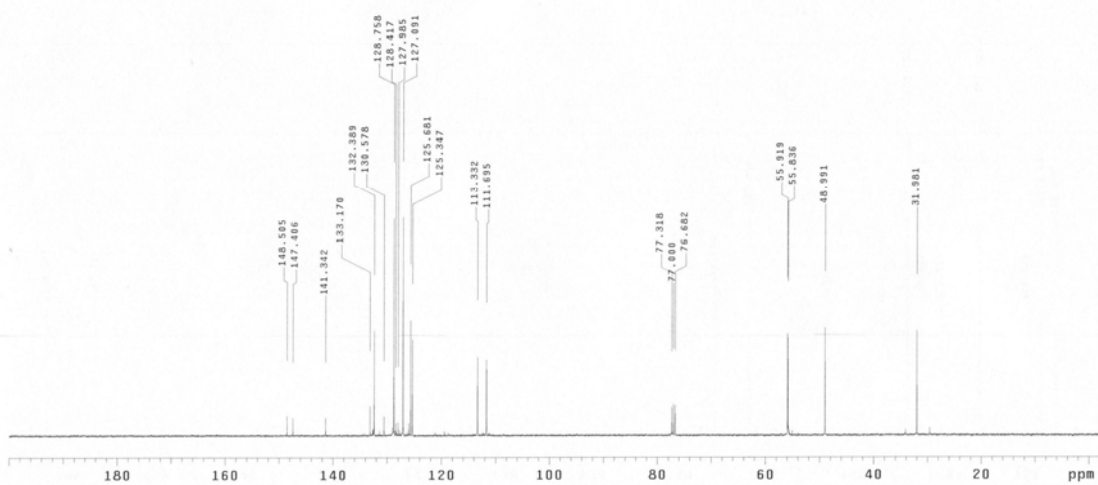
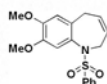
SK1011122

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Nov 22 2012
 Solvent: CDCl3
 Ambient temperature
 Total 64 repetitions



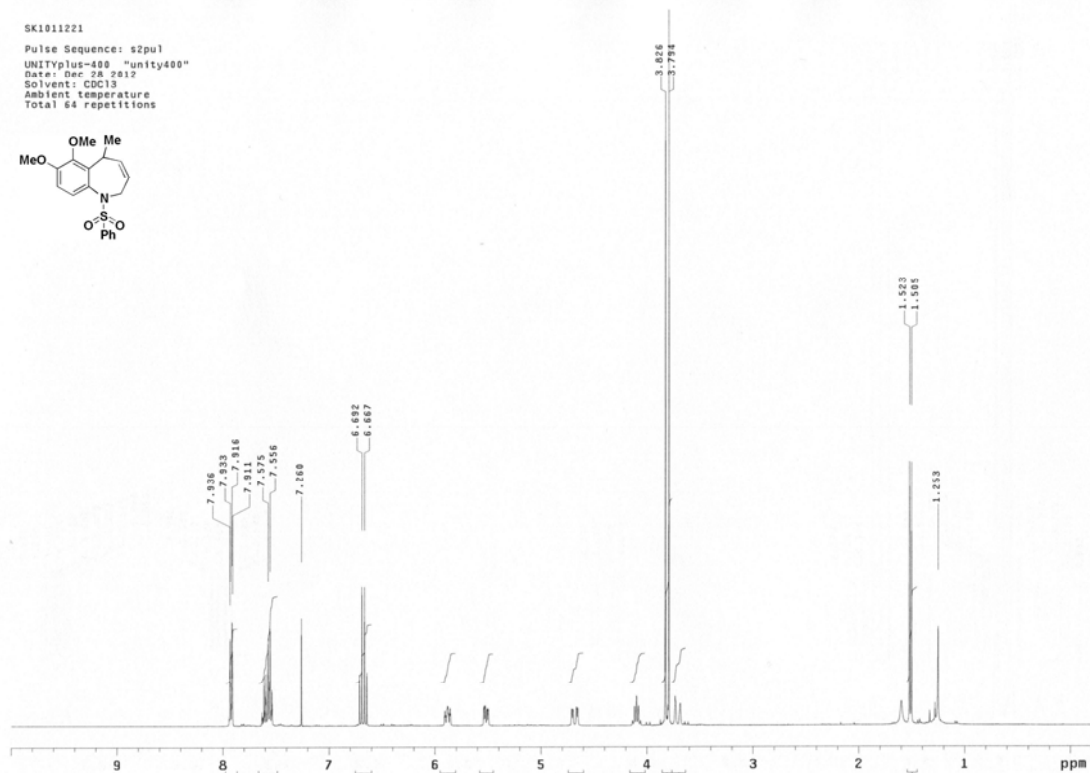
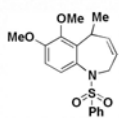
SK1011122

Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Nov 22 2012
 Solvent: CDCl3
 Ambient temperature
 Total 1024 repetitions

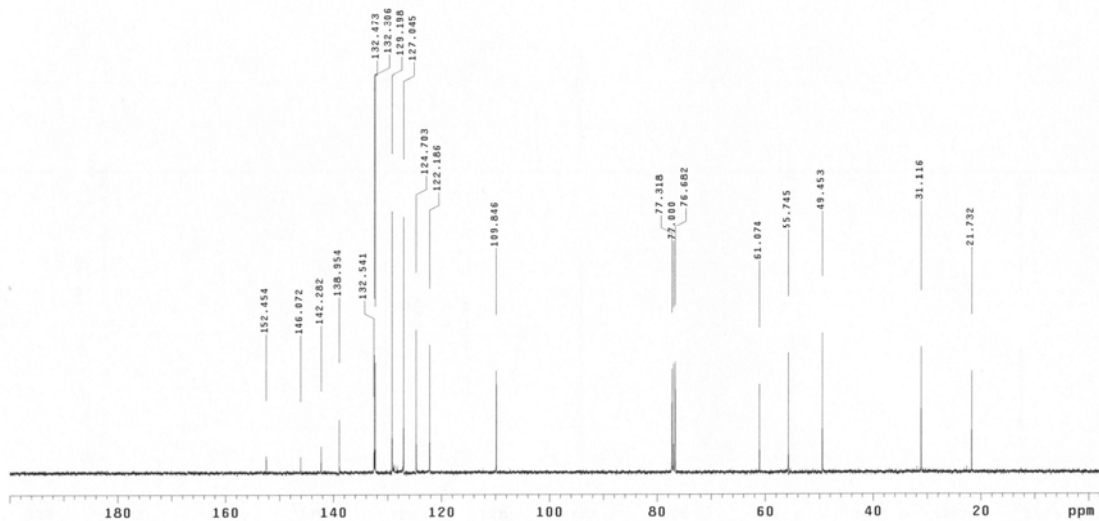
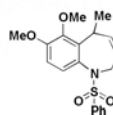


Compound 8g

SK1011221
 Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Dec 28 2012
 Solvent: CDCl3
 Ambient temperature
 Total 64 repetitions

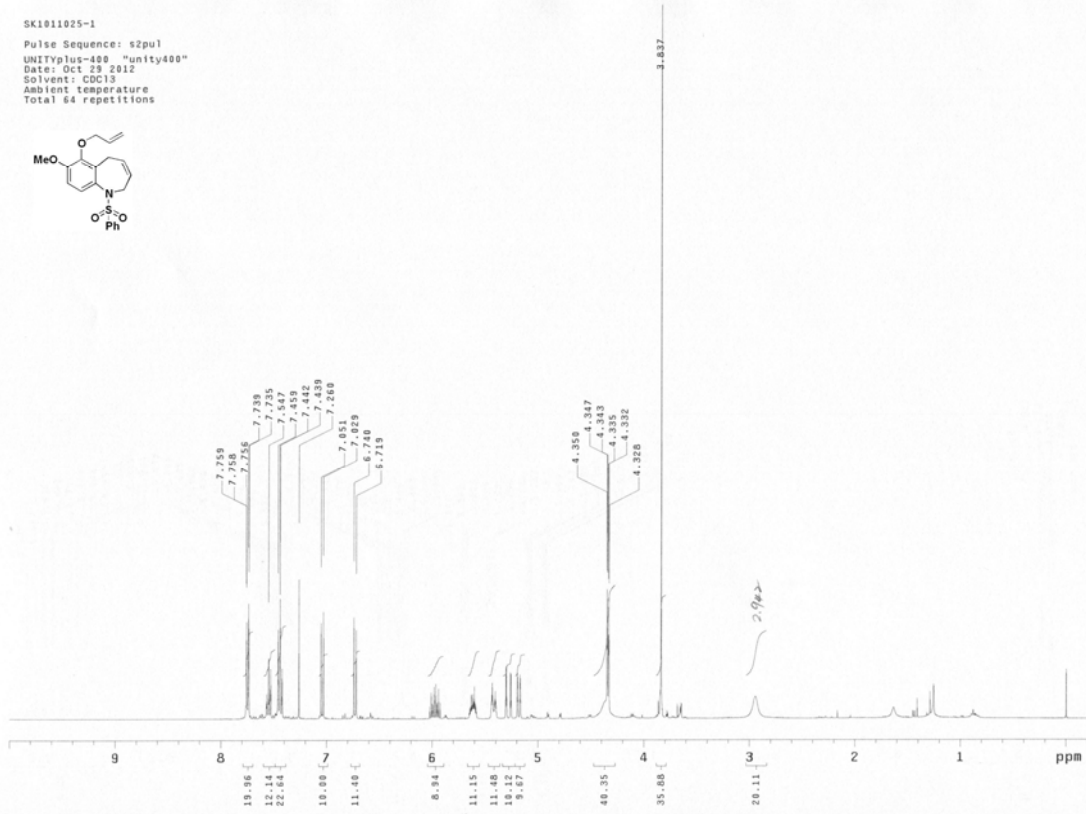
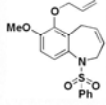


SK1011221
 Pulse Sequence: s2pu1
 UNITYplus-400 "unity400"
 Date: Dec 28 2012
 Solvent: CDCl3
 Ambient temperature
 Total 5040 repetitions

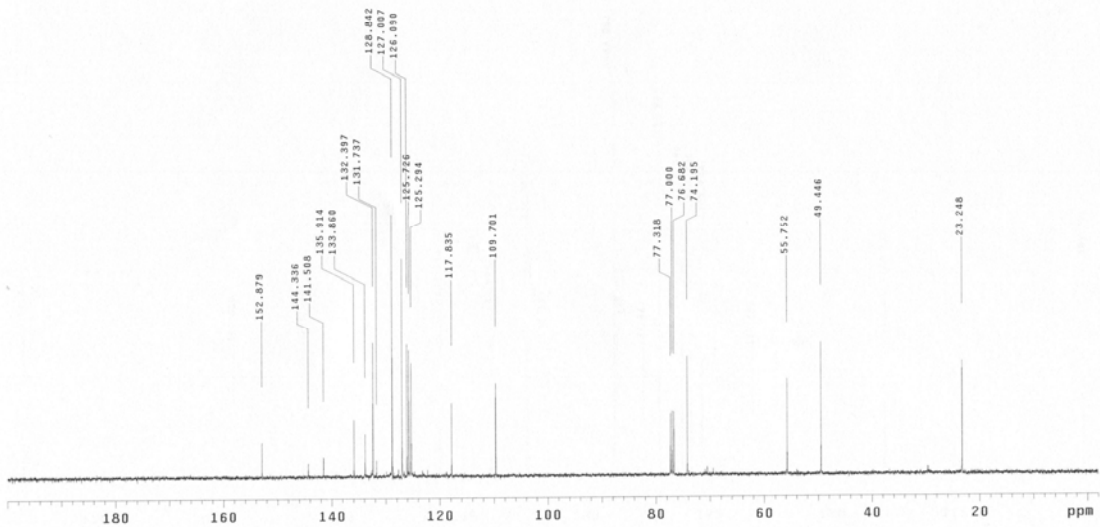
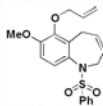


Compound 8h

SK1011025-1
 Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Oct 29 2012
 Solvent: CDCl3
 Ambient temperature
 Total 64 repetitions

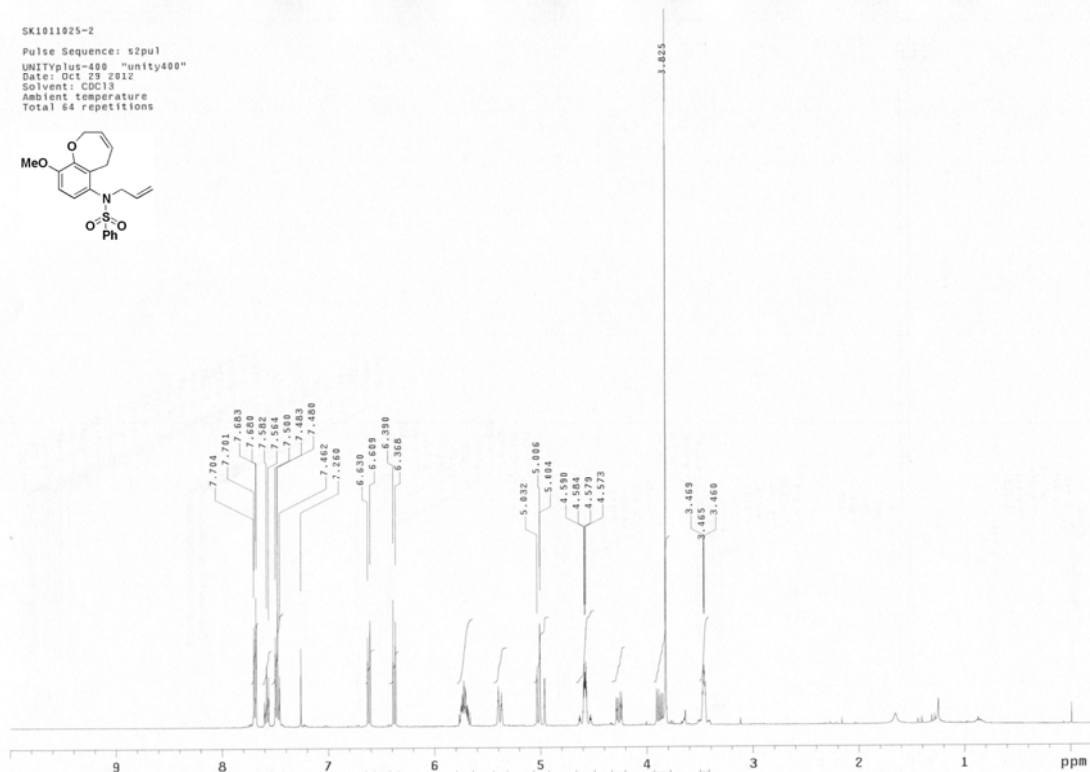
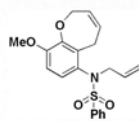


SK1011025-1
 Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Oct 29 2012
 Solvent: CDCl3
 Ambient temperature
 Total 2112 repetitions

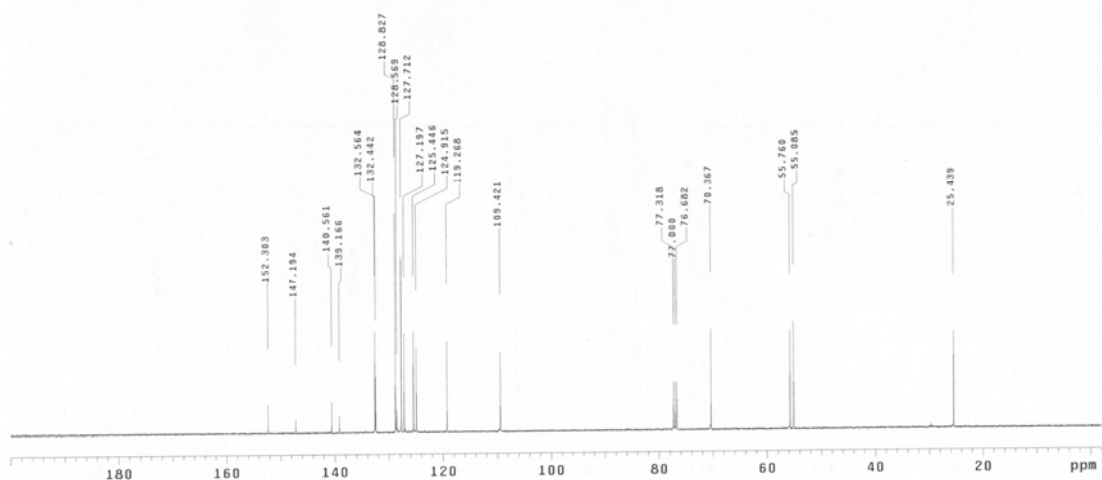
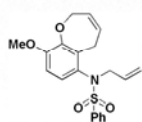


Compound 9

SK1011025-2
 Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Oct 29 2012
 Solvent: CDCl3
 Ambient temperature
 Total 64 repetitions



SK1011025-2
 Pulse Sequence: s2pul
 UNITYplus-400 "unity400"
 Date: Oct 29 2012
 Solvent: CDCl3
 Ambient temperature
 Total 3000 repetitions



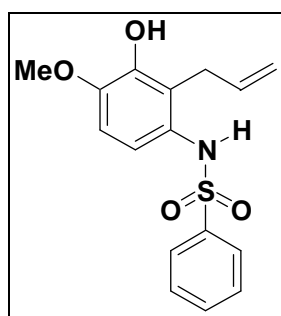
X-ray crystal data of compound 4h

Table 1. Crystal data and structure refinement for mo_130201lt_0m.

Identification code	mo_130201lt_0m	
Empirical formula	C ₁₆ H ₁₈ N O ₄ S	
Formula weight	320.37	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P b c a	
Unit cell dimensions	a = 14.0992(8) Å	α = 90°.
	b = 14.5823(9) Å	β = 90°.
	c = 15.0416(9) Å	γ = 90°.
Volume	3092.5(3) Å ³	
Z	8	
Density (calculated)	1.376 Mg/m ³	
Absorption coefficient	0.227 mm ⁻¹	
F(000)	1352	
Crystal size	0.3 x 0.27 x 0.25 mm ³	
Theta range for data collection	2.42 to 28.27°.	
Index ranges	-18 ≤ h ≤ 18, -8 ≤ k ≤ 19, -20 ≤ l ≤ 20	
Reflections collected	27580	
Independent reflections	3824 [R(int) = 0.0153]	
Completeness to theta = 28.27°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9804 and 0.8816	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3824 / 0 / 199	
Goodness-of-fit on F ²	1.064	
Final R indices [I > 2σ(I)]	R1 = 0.0399, wR2 = 0.1129	
R indices (all data)	R1 = 0.0439, wR2 = 0.1182	
Largest diff. peak and hole	0.788 and -0.822 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for mo_130201t_0m. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	5831(1)	1072(1)	5807(1)	14(1)
N(1)	5962(1)	-22(1)	6010(1)	15(1)
O(1)	8314(1)	-918(1)	8190(1)	21(1)
O(2)	6988(1)	-1226(1)	9396(1)	22(1)
O(3)	6684(1)	1533(1)	6071(1)	18(1)
O(4)	5527(1)	1122(1)	4888(1)	18(1)
C(1)	7386(1)	-747(1)	7969(1)	16(1)
C(2)	6665(1)	-908(1)	8595(1)	16(1)
C(3)	5724(1)	-759(1)	8373(1)	18(1)
C(4)	5503(1)	-452(1)	7520(1)	16(1)
C(5)	6218(1)	-299(1)	6904(1)	14(1)
C(6)	7180(1)	-436(1)	7116(1)	14(1)
C(7)	7969(1)	-296(1)	6447(1)	16(1)
C(8)	8249(1)	-1182(1)	6003(1)	19(1)
C(9)	8309(1)	-1294(1)	5132(1)	30(1)
C(10)	6286(1)	-1542(1)	10011(1)	24(1)
C(11)	4908(1)	1484(1)	6490(1)	16(1)
C(12)	5144(1)	1939(1)	7276(1)	20(1)
C(13)	4421(1)	2234(1)	7835(1)	24(1)
C(14)	3479(1)	2076(1)	7608(1)	26(1)
C(15)	3253(1)	1617(1)	6828(1)	26(1)
C(16)	3965(1)	1315(1)	6259(1)	21(1)

Table 3. Bond lengths [\AA] and angles [$^\circ$] for mo_1302011t_0m.

S(1)-O(3)	1.4329(11)
S(1)-O(4)	1.4505(11)
S(1)-N(1)	1.6351(13)
S(1)-C(11)	1.7632(15)
N(1)-C(5)	1.4501(18)
N(1)-H(1A)	0.8800
O(1)-C(1)	1.3716(17)
O(1)-H(1B)	0.8700
O(2)-C(2)	1.3696(18)
O(2)-C(10)	1.4308(18)
C(1)-C(6)	1.3920(19)
C(1)-C(2)	1.405(2)
C(2)-C(3)	1.385(2)
C(3)-C(4)	1.395(2)
C(3)-H(3B)	0.9500
C(4)-C(5)	1.386(2)
C(4)-H(4B)	0.9735
C(5)-C(6)	1.4077(19)
C(6)-C(7)	1.5137(19)
C(7)-C(8)	1.506(2)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.323(2)
C(8)-H(8A)	0.9500
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-C(12)	1.395(2)
C(11)-C(16)	1.396(2)
C(12)-C(13)	1.390(2)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.391(3)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.388(3)

C(14)-H(14A)	0.9500
C(15)-C(16)	1.391(2)
C(15)-H(15A)	0.9500
C(16)-H(16A)	0.9500
O(3)-S(1)-O(4)	119.27(7)
O(3)-S(1)-N(1)	108.14(7)
O(4)-S(1)-N(1)	105.08(6)
O(3)-S(1)-C(11)	107.34(7)
O(4)-S(1)-C(11)	108.67(7)
N(1)-S(1)-C(11)	107.89(7)
C(5)-N(1)-S(1)	118.26(10)
C(5)-N(1)-H(1A)	120.9
S(1)-N(1)-H(1A)	120.9
C(1)-O(1)-H(1B)	108.0
C(2)-O(2)-C(10)	116.67(12)
O(1)-C(1)-C(6)	118.80(13)
O(1)-C(1)-C(2)	119.84(13)
C(6)-C(1)-C(2)	121.35(13)
O(2)-C(2)-C(3)	125.64(13)
O(2)-C(2)-C(1)	113.91(13)
C(3)-C(2)-C(1)	120.44(14)
C(2)-C(3)-C(4)	119.01(13)
C(2)-C(3)-H(3B)	120.5
C(4)-C(3)-H(3B)	120.5
C(5)-C(4)-C(3)	120.27(13)
C(5)-C(4)-H(4B)	119.9
C(3)-C(4)-H(4B)	119.8
C(4)-C(5)-C(6)	121.79(13)
C(4)-C(5)-N(1)	118.92(13)
C(6)-C(5)-N(1)	119.25(12)
C(1)-C(6)-C(5)	117.13(13)
C(1)-C(6)-C(7)	120.21(12)
C(5)-C(6)-C(7)	122.61(13)
C(8)-C(7)-C(6)	111.88(12)
C(8)-C(7)-H(7A)	109.2
C(6)-C(7)-H(7A)	109.2
C(8)-C(7)-H(7B)	109.2
C(6)-C(7)-H(7B)	109.2

H(7A)-C(7)-H(7B)	107.9
C(9)-C(8)-C(7)	124.22(15)
C(9)-C(8)-H(8A)	117.9
C(7)-C(8)-H(8A)	117.9
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
O(2)-C(10)-H(10A)	109.5
O(2)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
O(2)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(12)-C(11)-C(16)	121.45(14)
C(12)-C(11)-S(1)	118.63(12)
C(16)-C(11)-S(1)	119.85(12)
C(13)-C(12)-C(11)	119.03(15)
C(13)-C(12)-H(12A)	120.5
C(11)-C(12)-H(12A)	120.5
C(12)-C(13)-C(14)	120.05(16)
C(12)-C(13)-H(13A)	120.0
C(14)-C(13)-H(13A)	120.0
C(15)-C(14)-C(13)	120.41(15)
C(15)-C(14)-H(14A)	119.8
C(13)-C(14)-H(14A)	119.8
C(14)-C(15)-C(16)	120.46(16)
C(14)-C(15)-H(15A)	119.8
C(16)-C(15)-H(15A)	119.8
C(15)-C(16)-C(11)	118.59(16)
C(15)-C(16)-H(16A)	120.7
C(11)-C(16)-H(16A)	120.7

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for mo_130201lt_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
S(1)	13(1)	15(1)	14(1)	0(1)	0(1)	0(1)
N(1)	16(1)	14(1)	14(1)	-1(1)	-2(1)	0(1)
O(1)	12(1)	32(1)	19(1)	7(1)	-2(1)	0(1)
O(2)	18(1)	32(1)	14(1)	5(1)	-1(1)	-4(1)
O(3)	15(1)	18(1)	20(1)	-1(1)	-1(1)	-3(1)
O(4)	19(1)	21(1)	14(1)	2(1)	-1(1)	0(1)
C(1)	12(1)	18(1)	17(1)	0(1)	-1(1)	-1(1)
C(2)	17(1)	19(1)	14(1)	0(1)	-1(1)	-3(1)
C(3)	14(1)	22(1)	17(1)	0(1)	2(1)	-2(1)
C(4)	12(1)	18(1)	19(1)	-1(1)	0(1)	0(1)
C(5)	13(1)	14(1)	15(1)	0(1)	-1(1)	-1(1)
C(6)	13(1)	14(1)	16(1)	0(1)	1(1)	-1(1)
C(7)	12(1)	18(1)	17(1)	2(1)	2(1)	0(1)
C(8)	15(1)	20(1)	23(1)	3(1)	2(1)	2(1)
C(9)	36(1)	28(1)	26(1)	-2(1)	2(1)	2(1)
C(10)	23(1)	33(1)	16(1)	3(1)	1(1)	-11(1)
C(11)	16(1)	15(1)	18(1)	3(1)	2(1)	2(1)
C(12)	23(1)	18(1)	20(1)	0(1)	2(1)	0(1)
C(13)	33(1)	20(1)	20(1)	0(1)	7(1)	2(1)
C(14)	28(1)	22(1)	26(1)	7(1)	11(1)	8(1)
C(15)	17(1)	30(1)	30(1)	6(1)	4(1)	3(1)
C(16)	17(1)	23(1)	23(1)	1(1)	1(1)	1(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for mo_1302011t_0m.

	x	y	z	U(eq)
H(1A)	5880	-432	5588	18
H(3B)	5236	-864	8797	21
H(7A)	7758	147	5989	19
H(7B)	8528	-32	6752	19
H(8A)	8392	-1692	6372	23
H(9A)	8509	-1924	5001	45
H(9B)	8774	-863	4888	45
H(9C)	7688	-1180	4861	45
H(10A)	6597	-1757	10555	36
H(10B)	5927	-2047	9744	36
H(10C)	5853	-1038	10156	36
H(12A)	5789	2045	7426	24
H(13A)	4571	2543	8373	29
H(14A)	2987	2283	7990	31
H(15A)	2607	1509	6681	31
H(16A)	3813	1000	5725	25
H(4B)	4843	-367	7349	50
H(1B)	8329	-1096	8742	50