#### **Electronic Supplementary Information**

# Effect of C7-Substitution of 1-Arylsulfonyl-5-(N-hydroxyacrylamide)indolines on the Selectivity Toward Subclass of Histone Deacetlyase.

Hsueh-Yun Lee, \*Li-Ting Wang, \*Yu-Hsuan Li, \*Shiow-Lin Pan, 'Yi-Lin Chen, Che-Ming Teng, and Jing-Ping Liou\*

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HPLC purity data for synthetic compounds	ESI2
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#### **HPLC** purity determination:

The percentage purity of compounds were determined by an Agilent 1100 series HPLC system using C18 column.

Elution conditions: Mobile phase A-Acetonitrile; Mobile phase B-Water containing 0.1% formic acid + 10 mmol NH4OAc. The flow-rate was 0.2 ml/min and the injection volume was 5  $\mu$ l. The system operated at 25 °C. Peaks were detected at 210 nm.

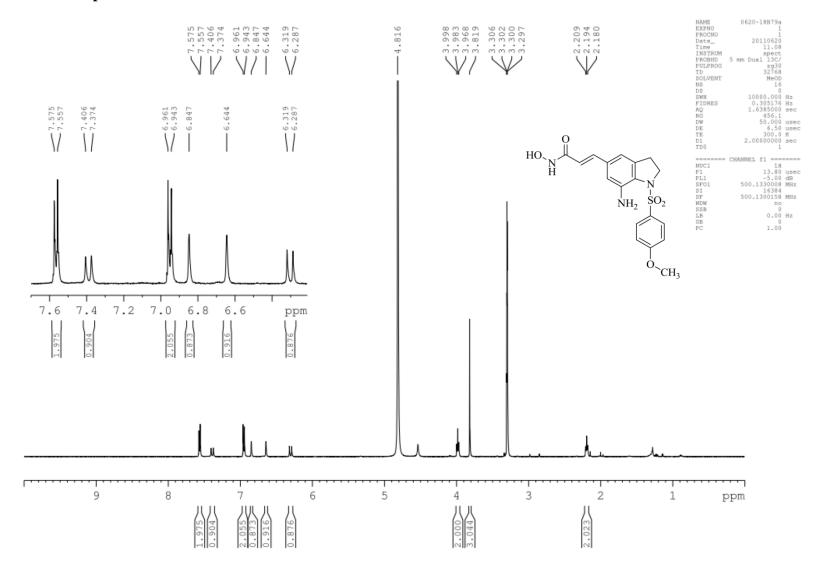
 Table 1. Elution condition

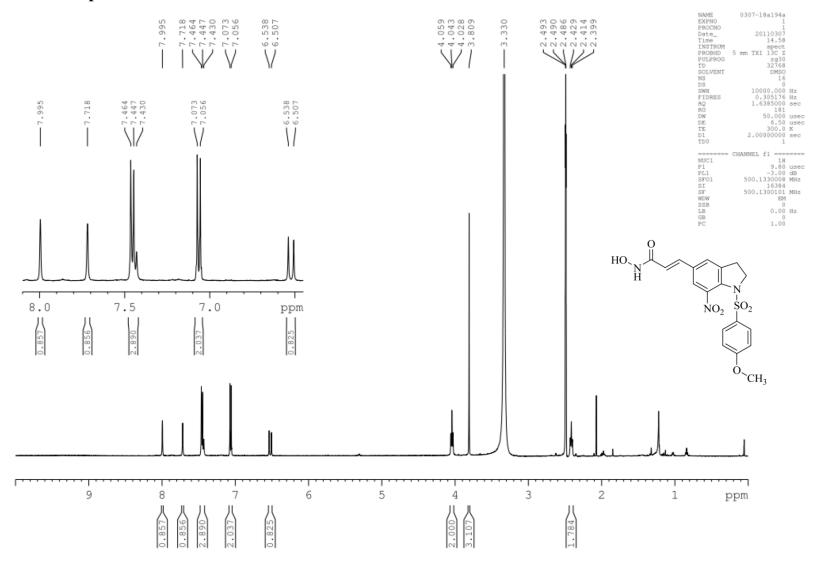
Time (min)	Mobile Phase A (ratio)	Mobile Phase B (ratio)
0	10	90
45	90	10
50	10	90
60	10	90

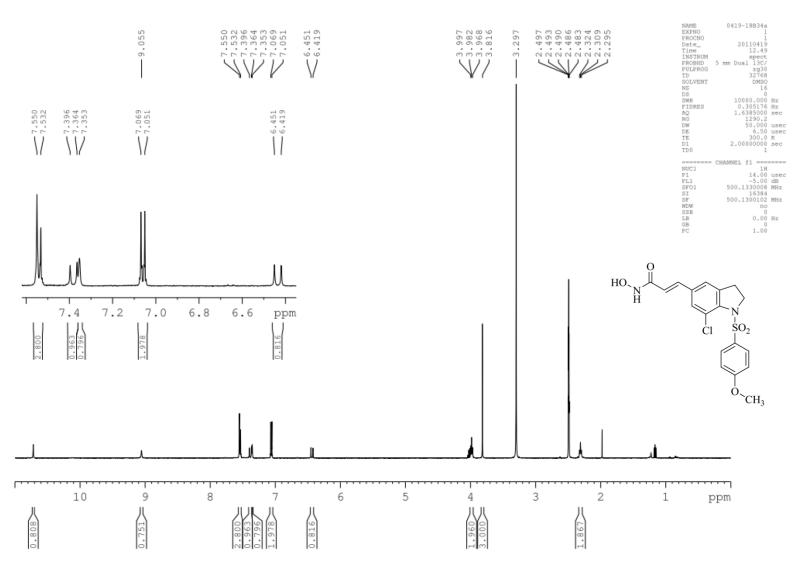
**Table 2**. Purity of synthetic compounds

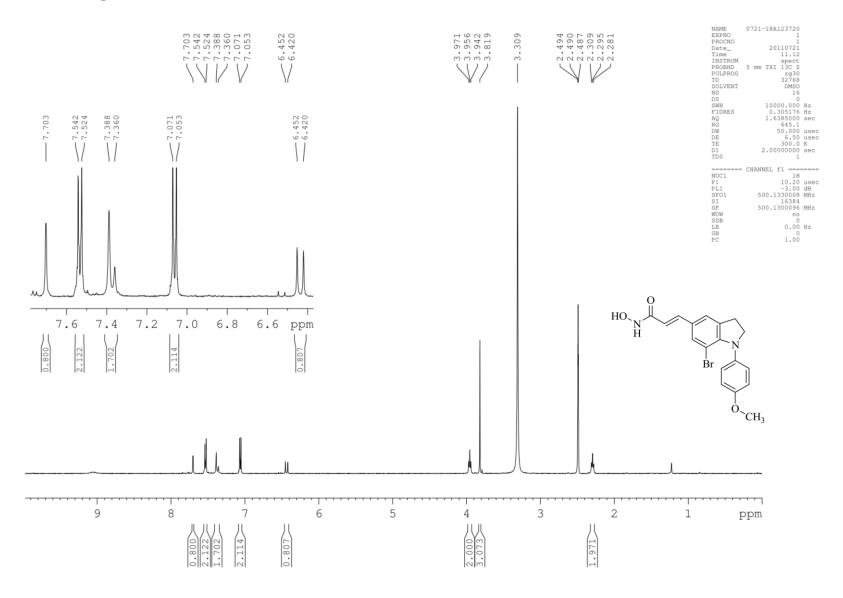
C18 column: Agilent ZORBAX Eclipse XDB-C18 5µm. 4.6 mm × 150 mm column

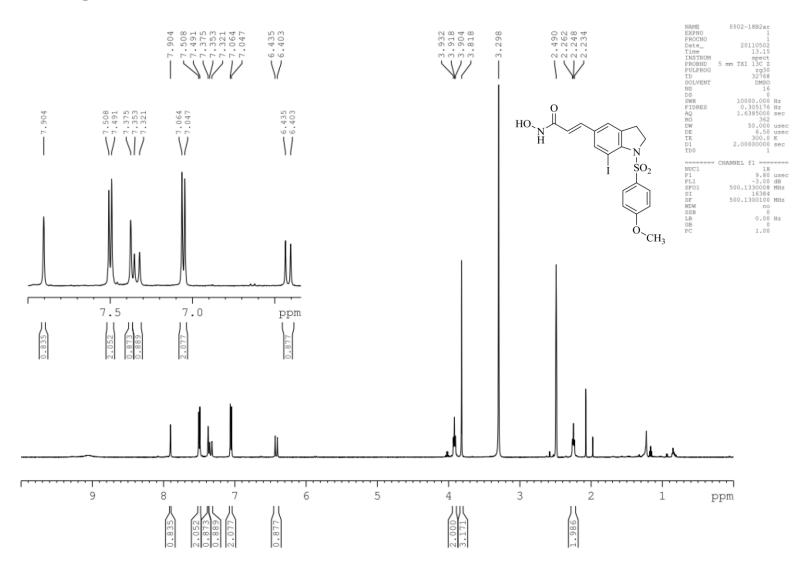
Compounds	Retention time (min)	% Purity
9	20.71	96.52
10	23.26	95.91
11	23.72	95.60
12	24.29	97.54
13	24.89	98.95
17	22.12	94.52

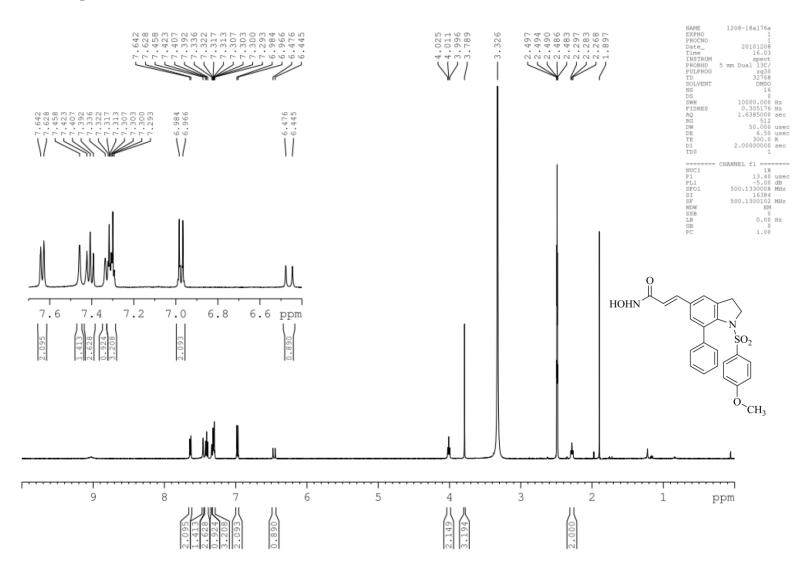


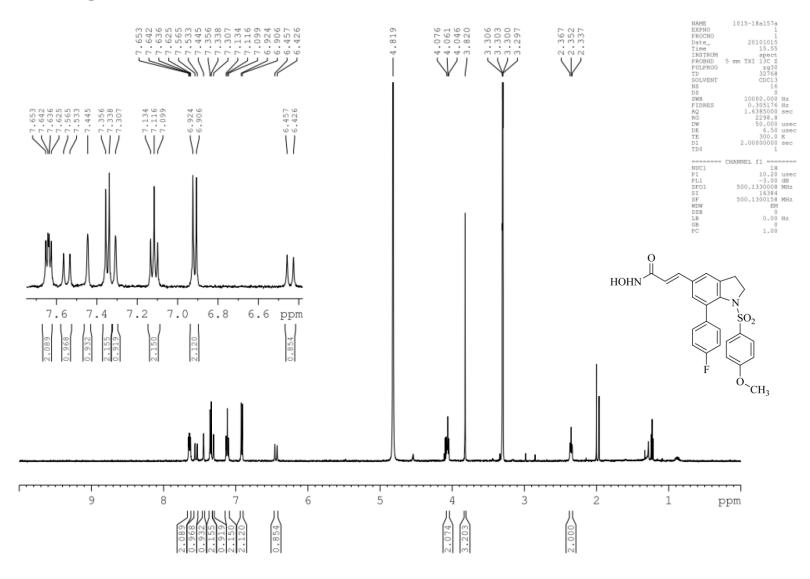


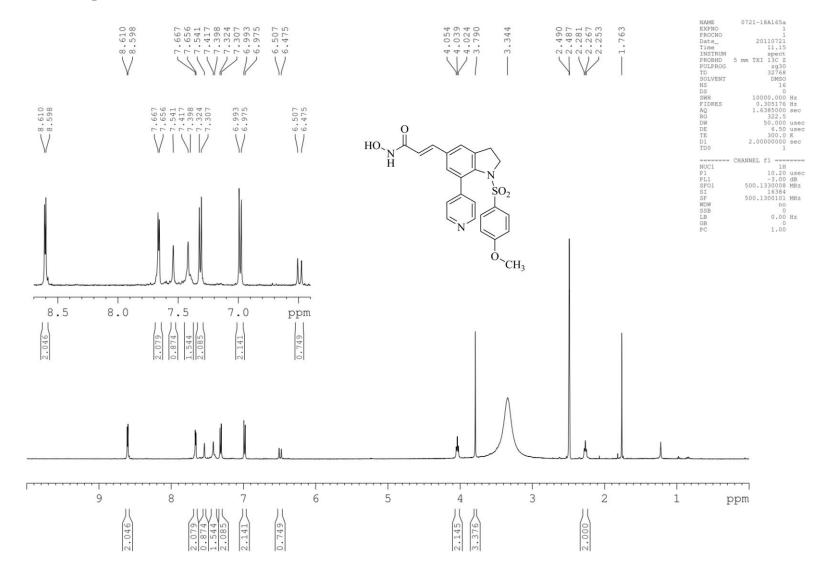


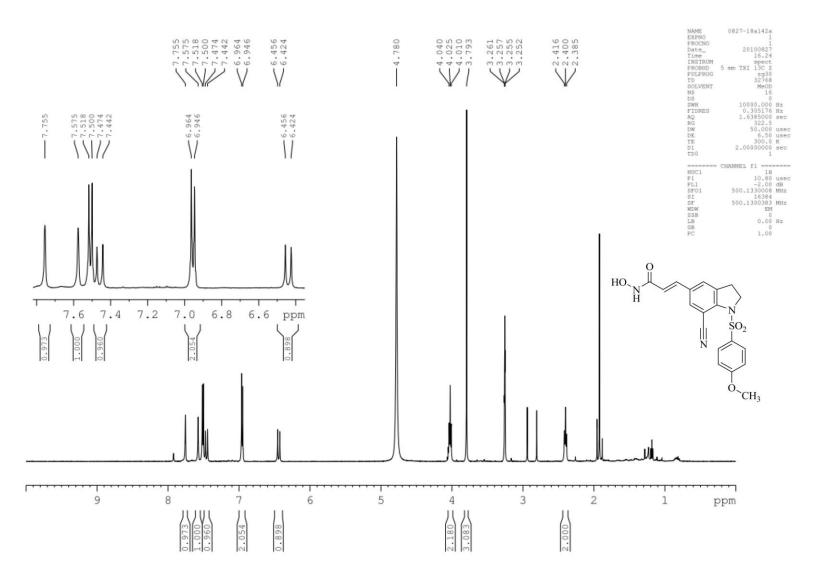


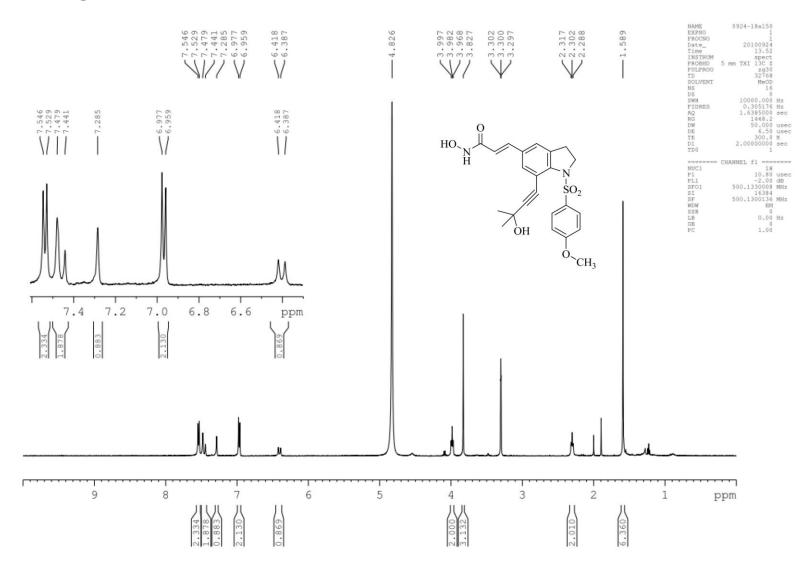


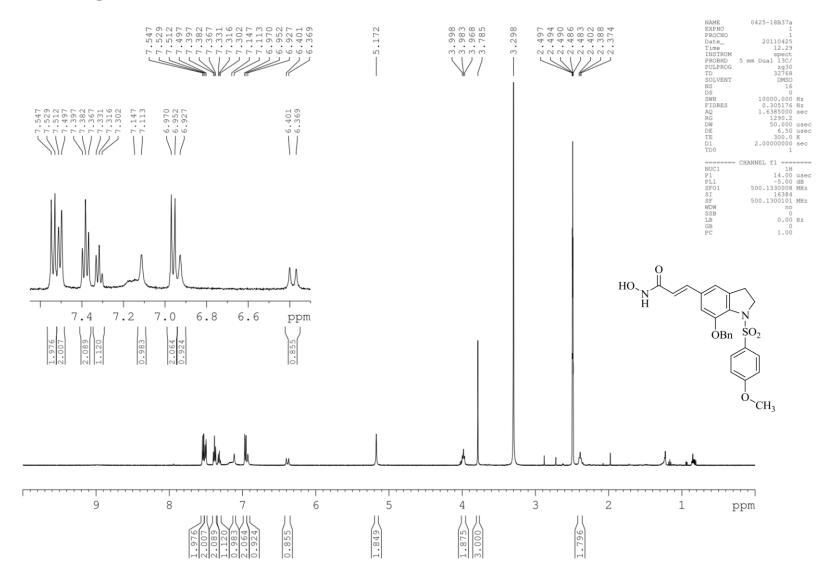


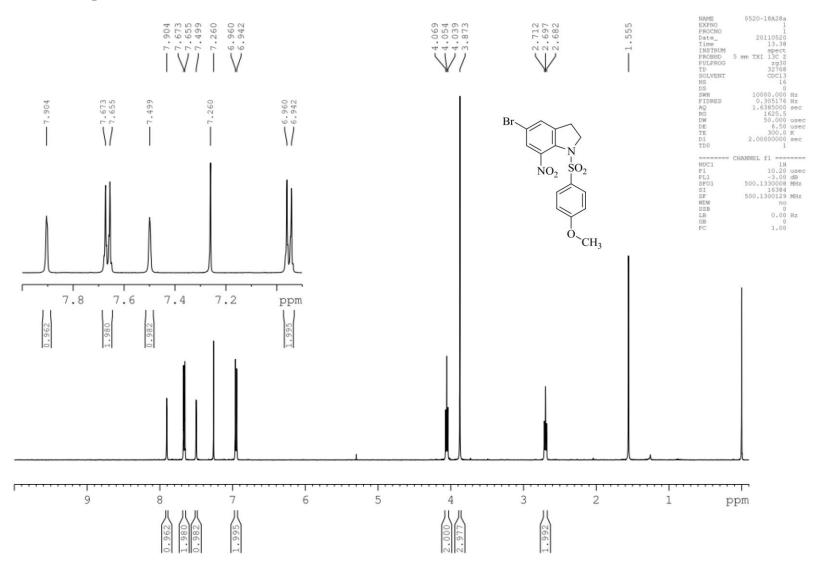


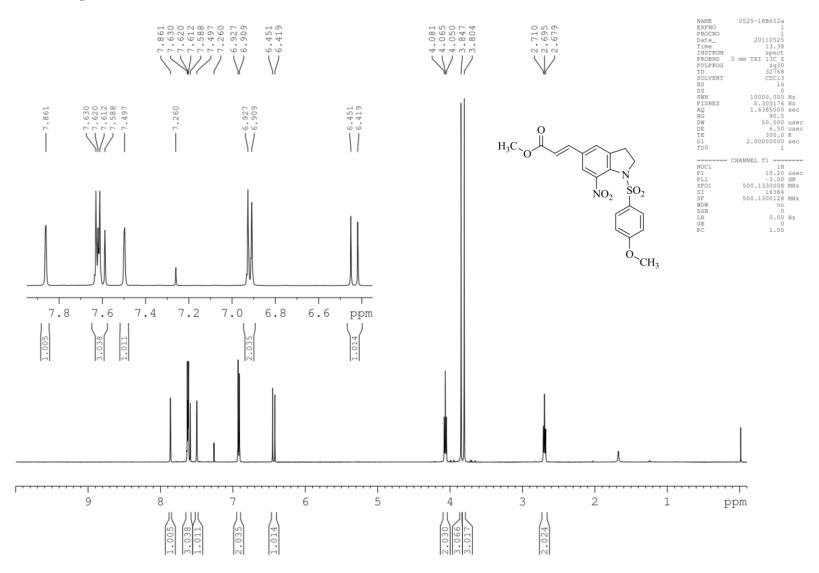


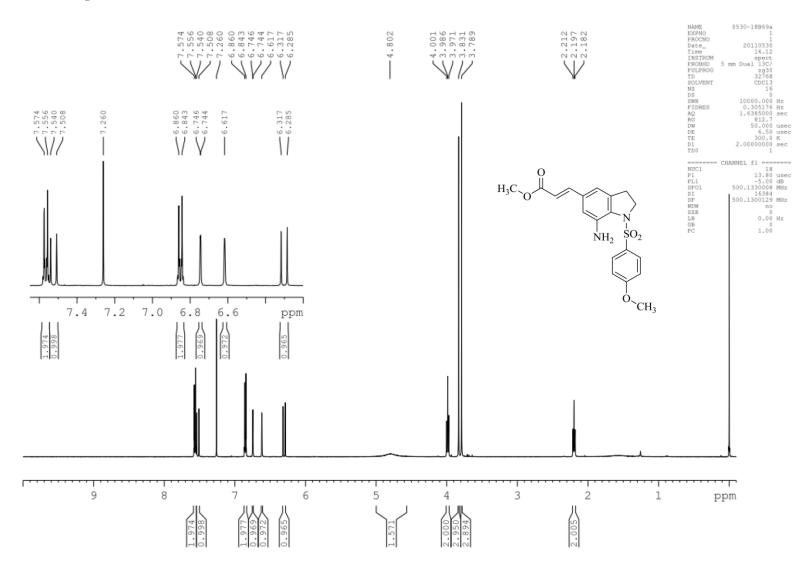


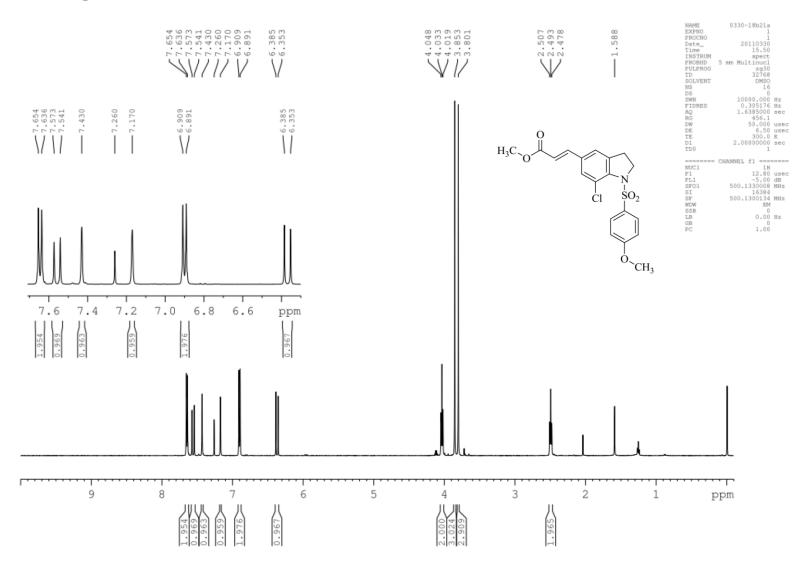


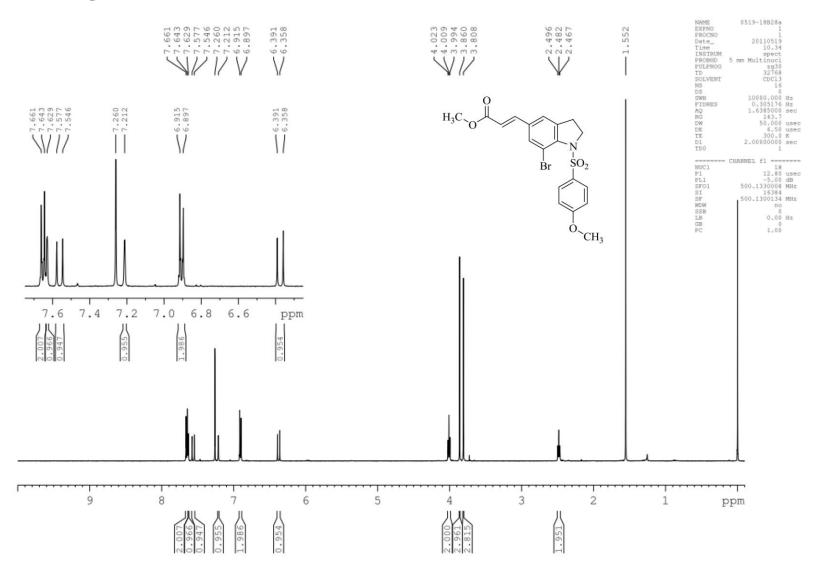


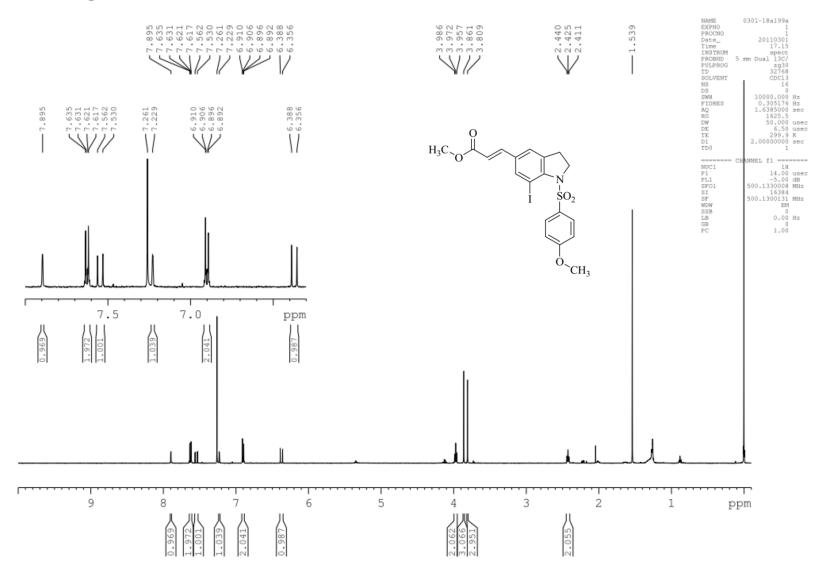


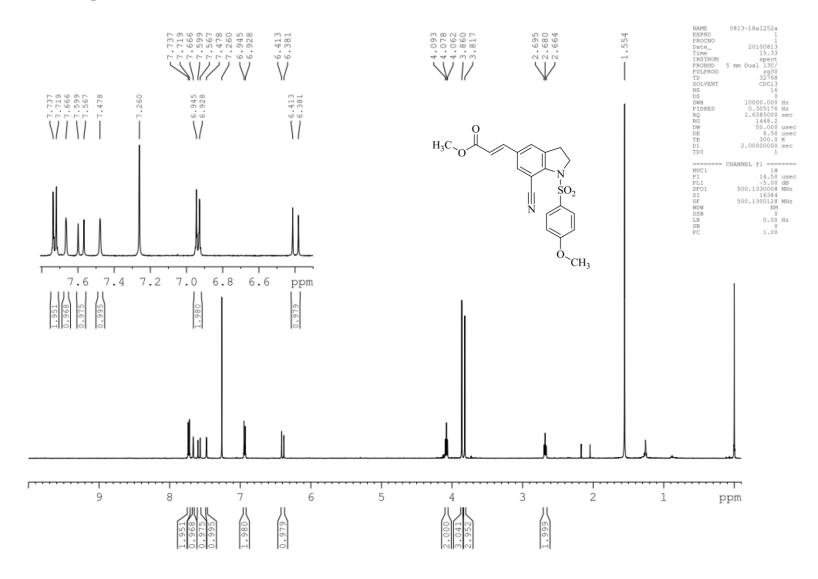


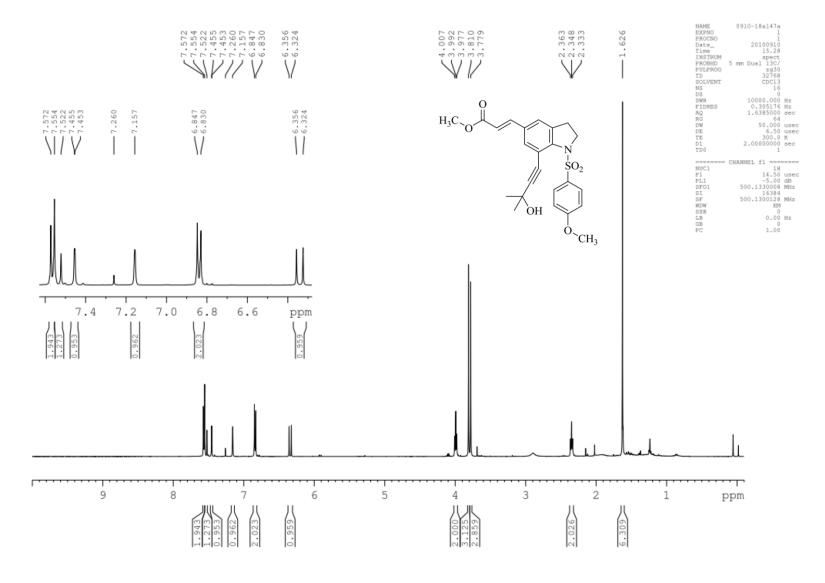


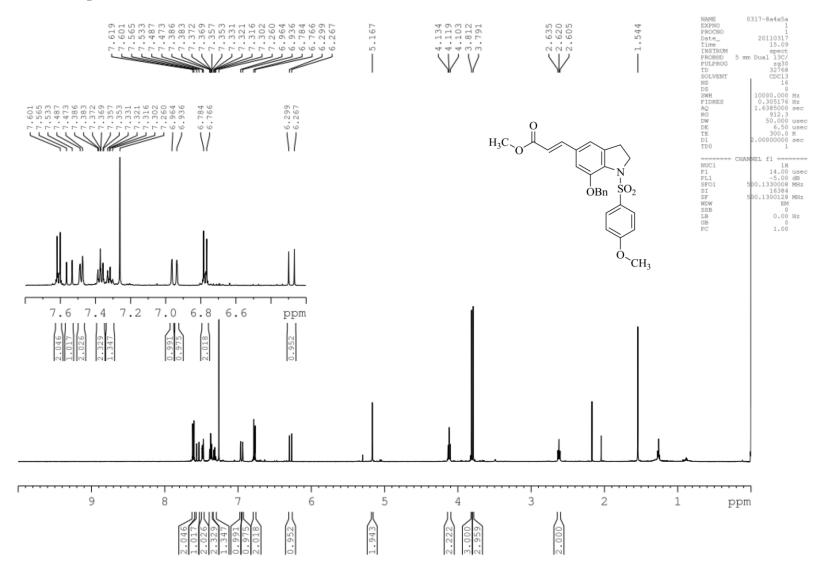


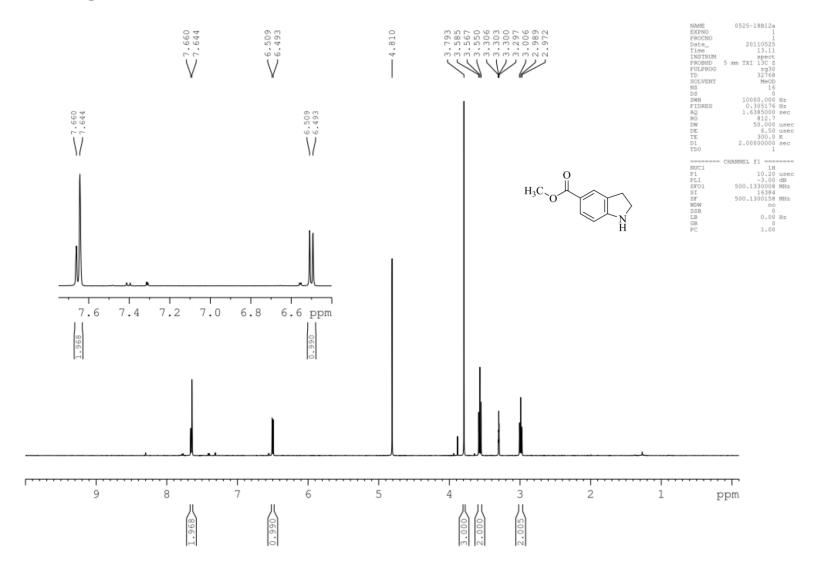


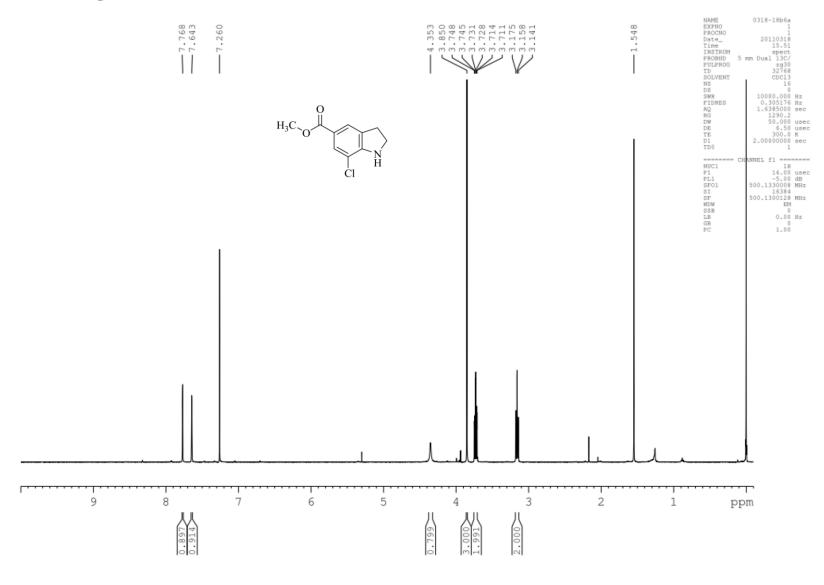


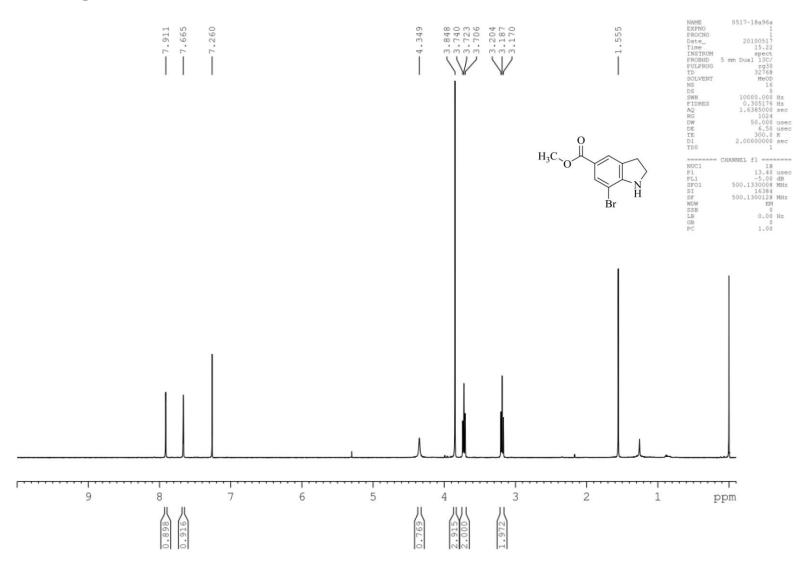


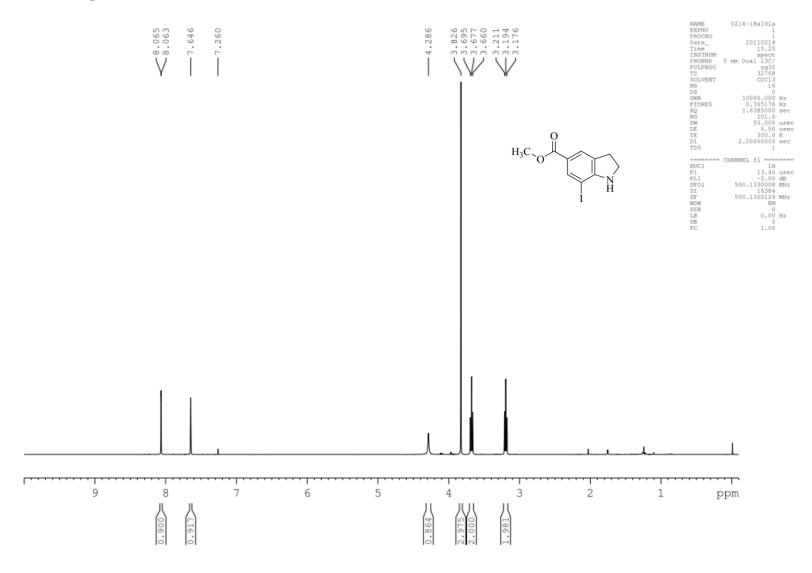


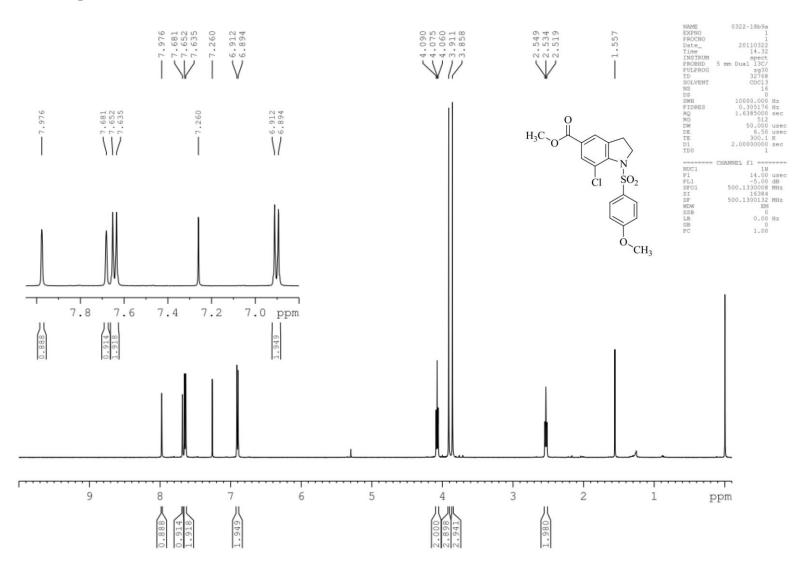


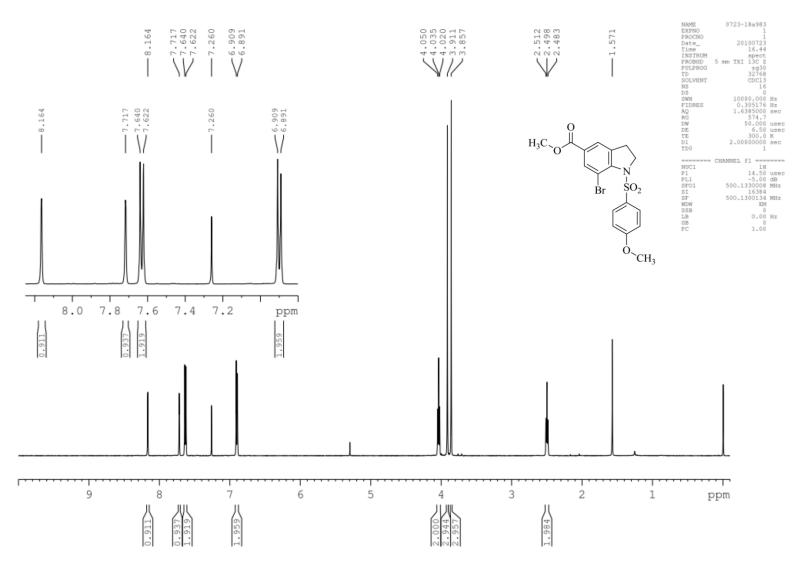


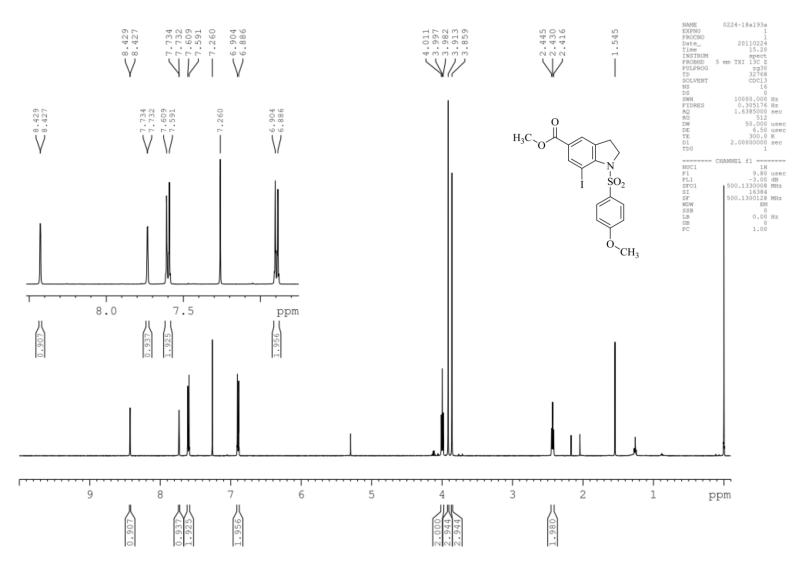


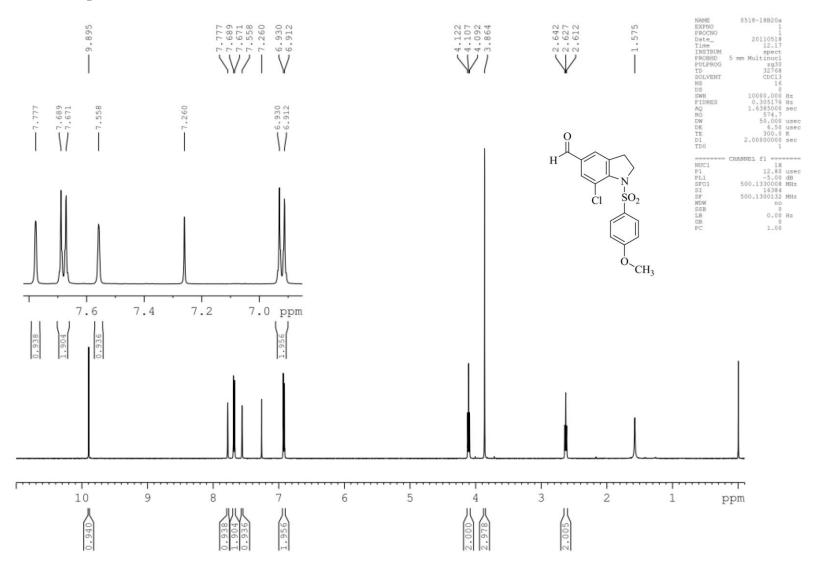


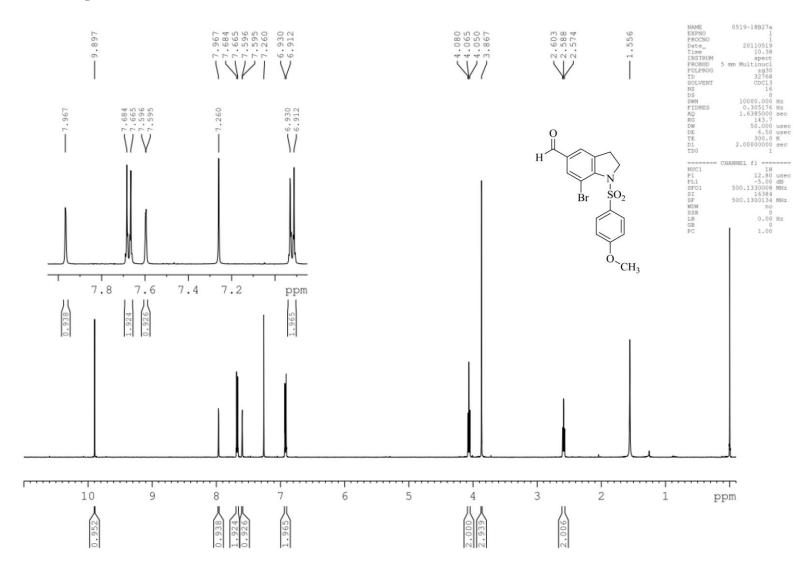




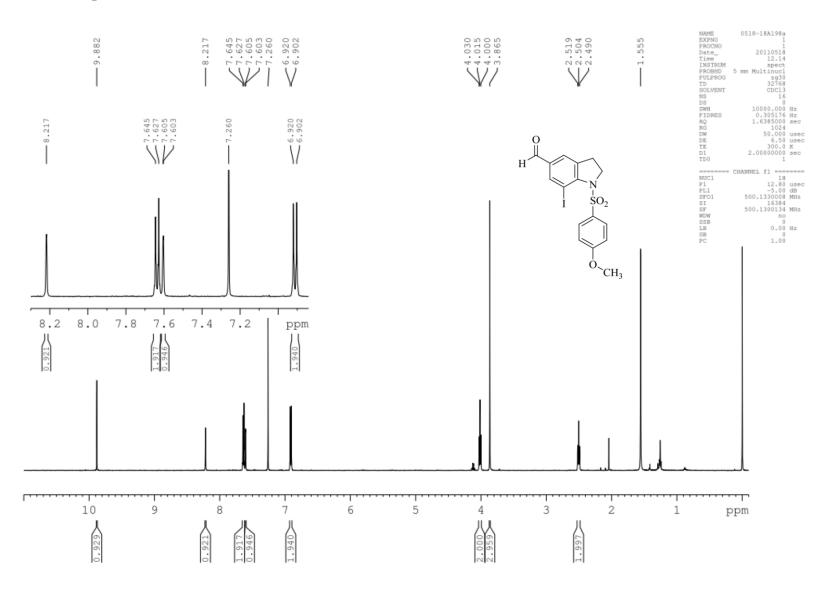


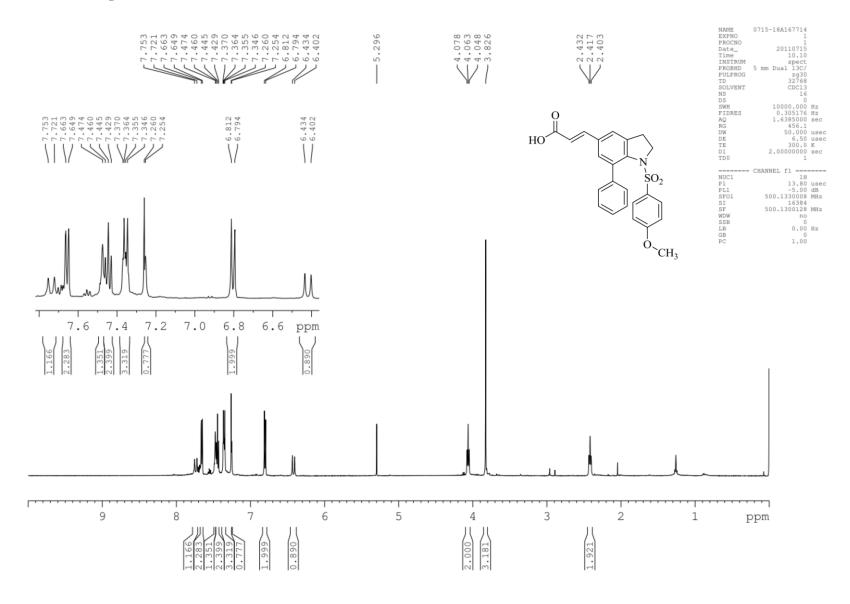


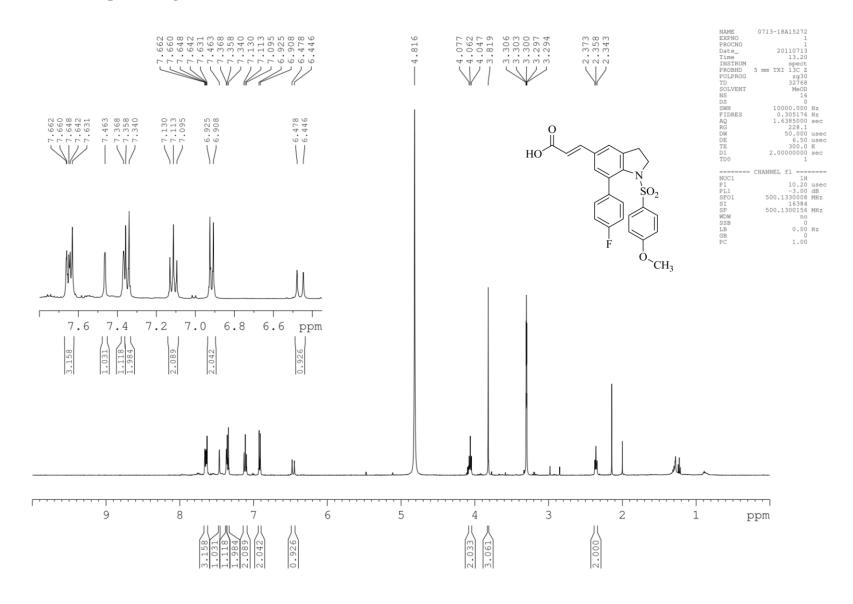


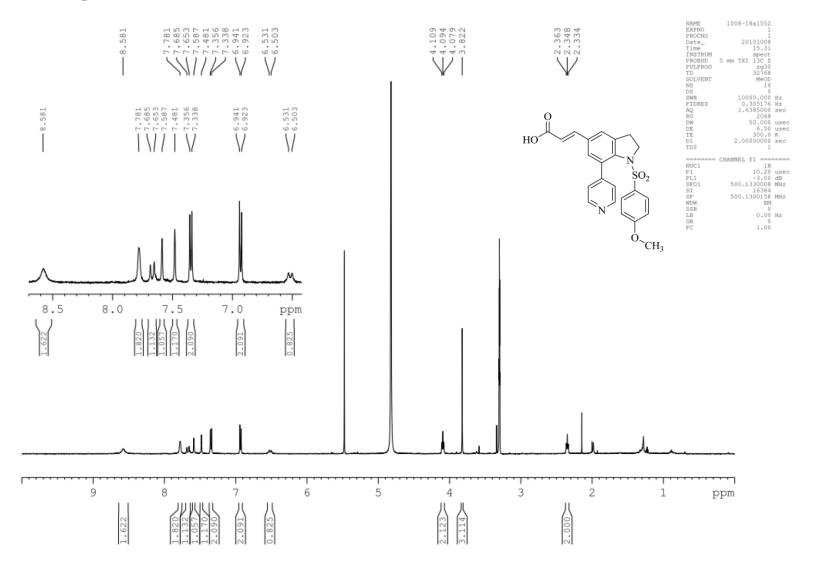


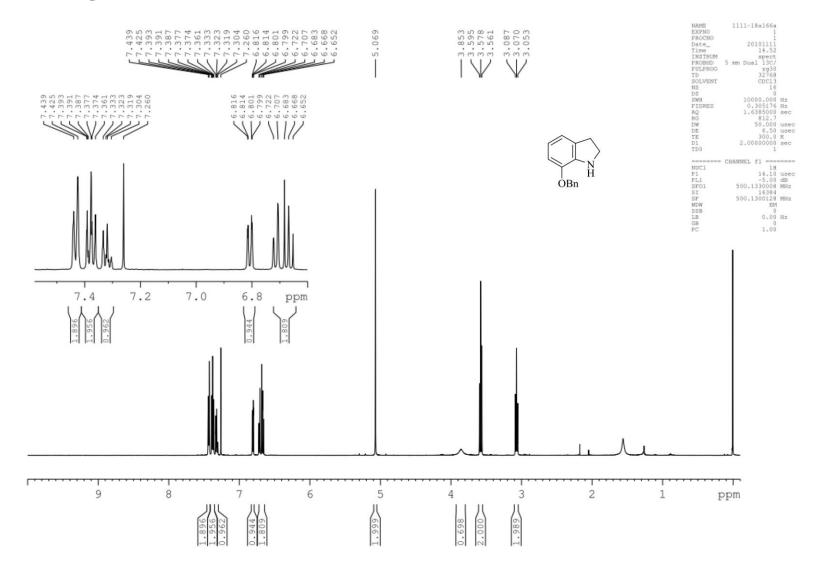
<sup>1</sup>H Spectrum for compound 27e



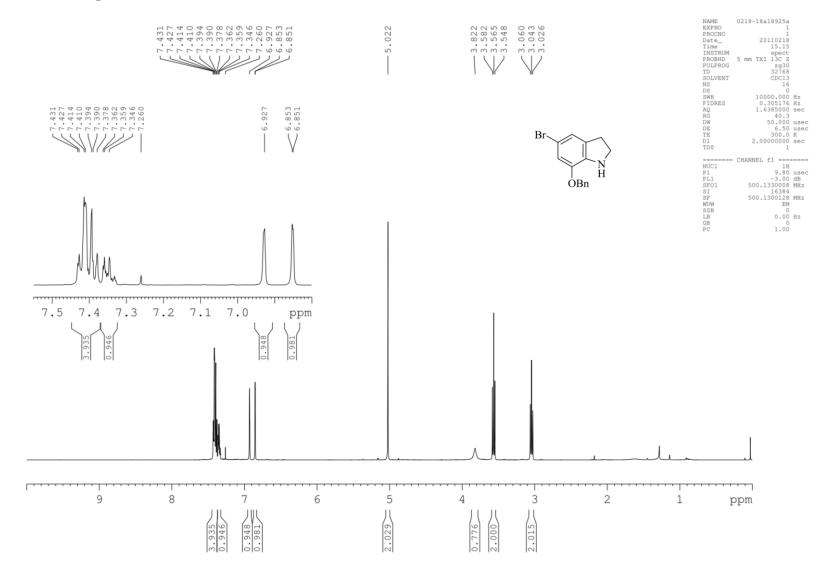




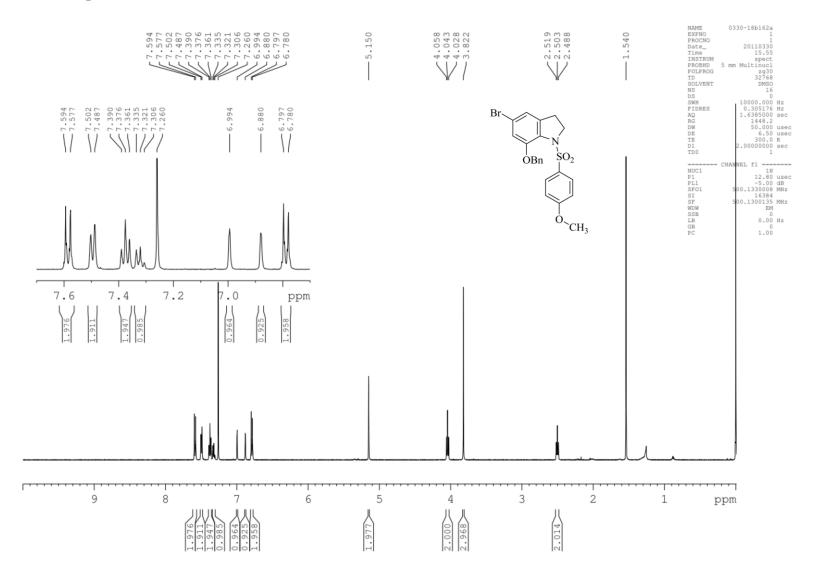




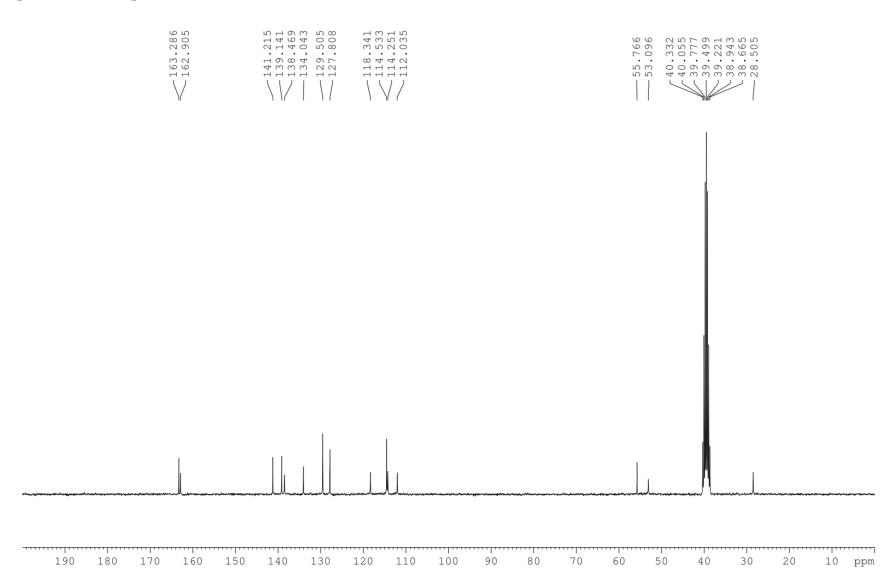
#### <sup>1</sup>H Spectrum for compound 31



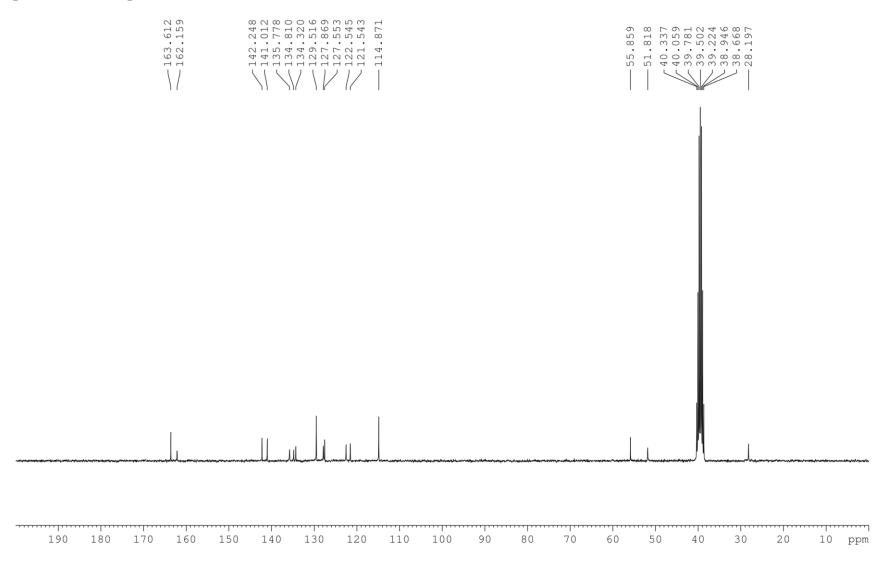
#### <sup>1</sup>H Spectrum for compound 32

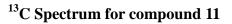


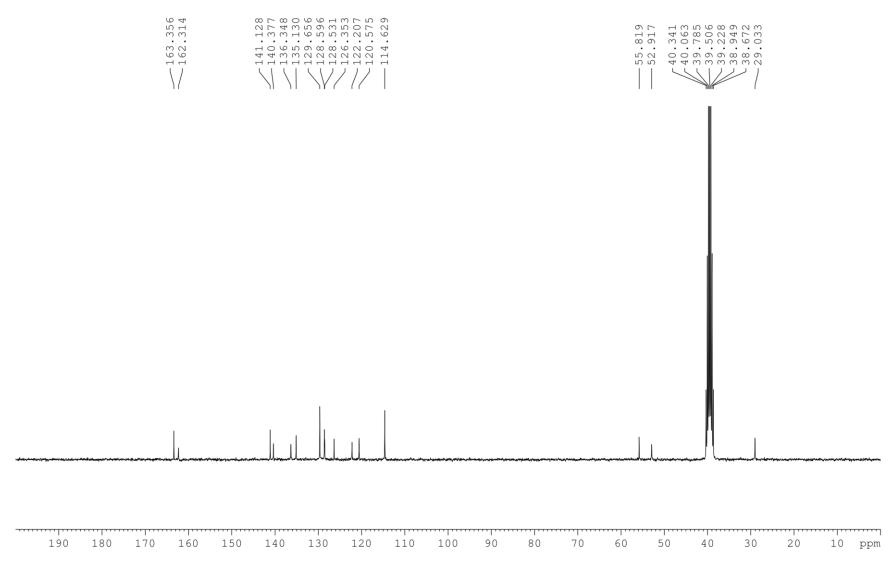
<sup>13</sup>C Spectrum for compound 9

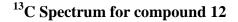


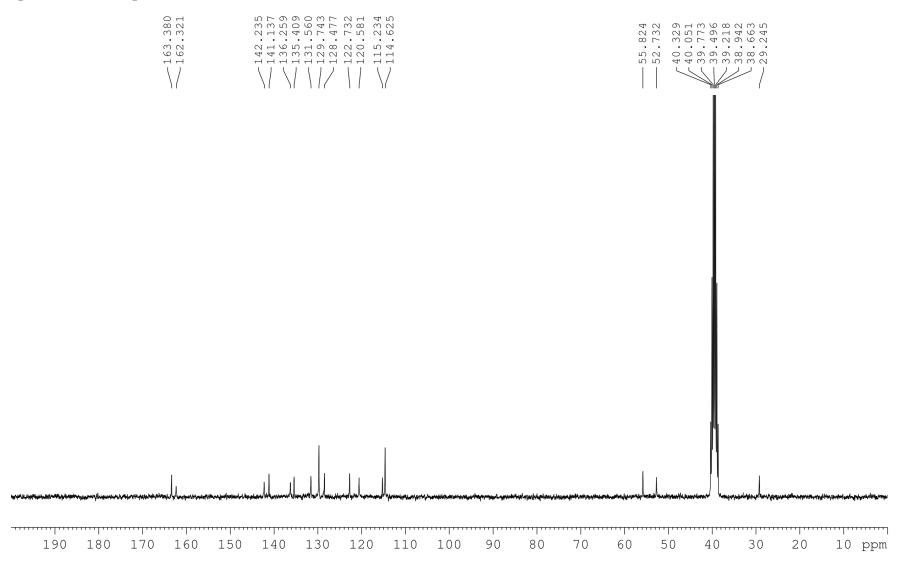
 $^{13}\mathrm{C}$  Spectrum for compound 10

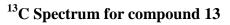


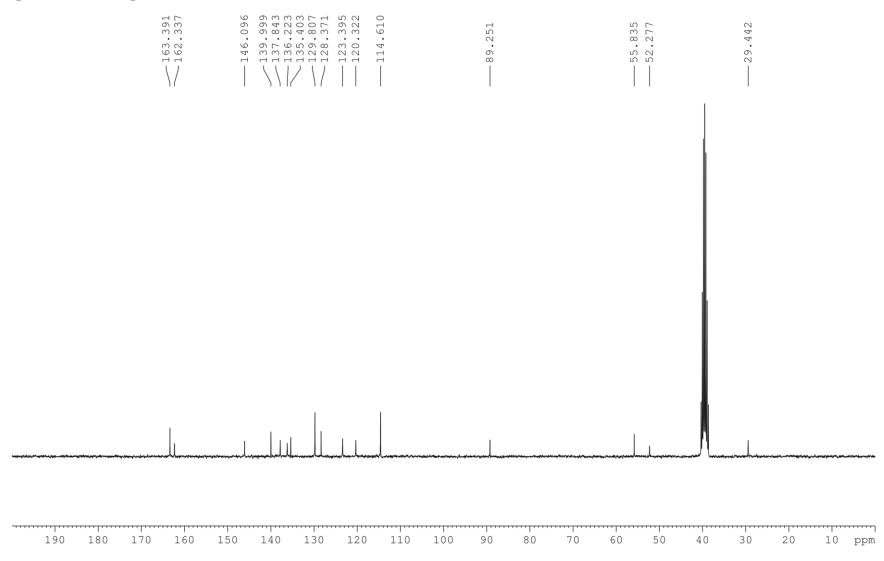




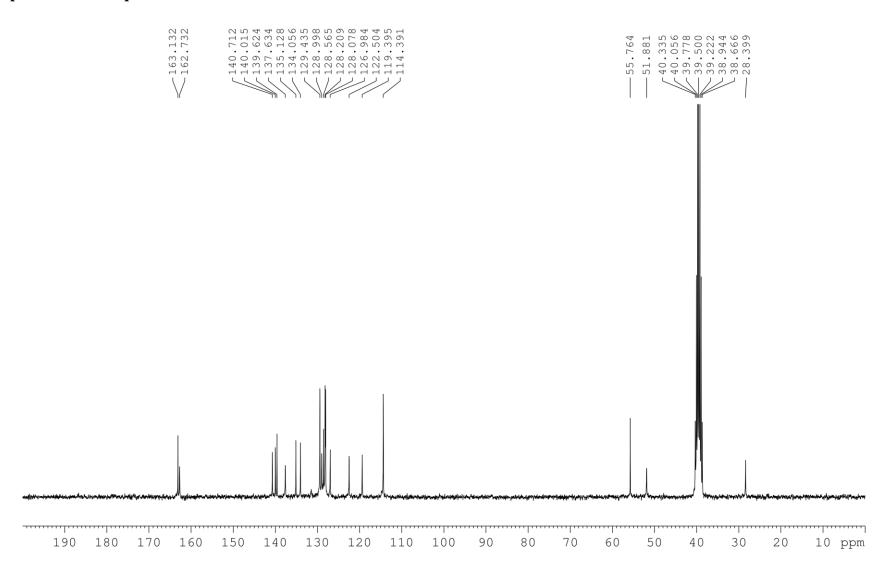




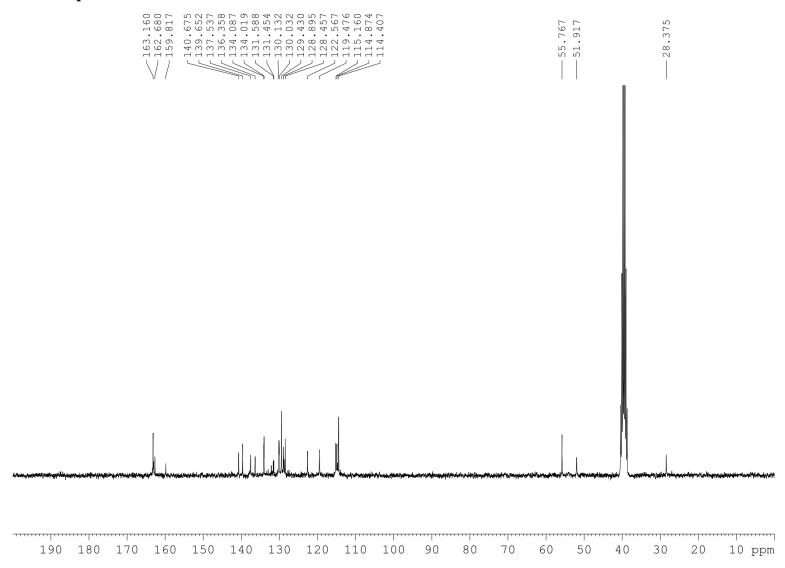




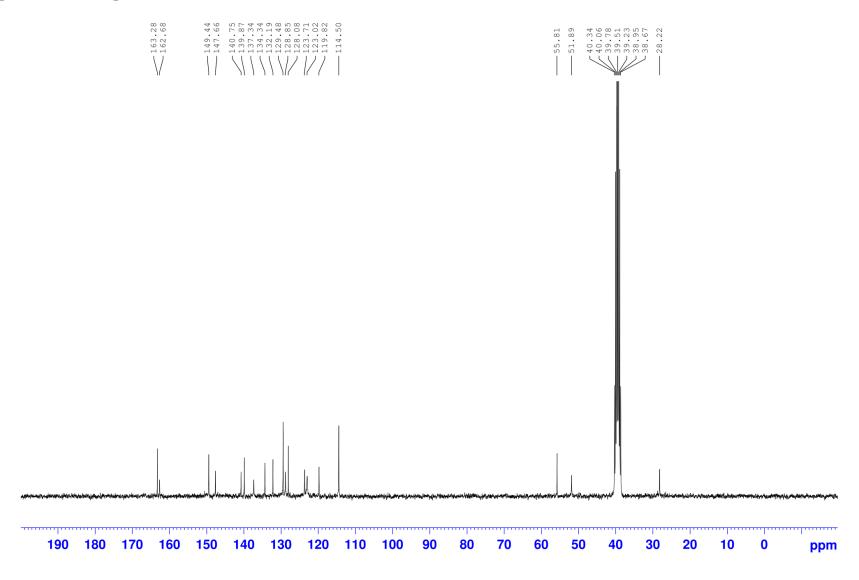
<sup>13</sup>C Spectrum for compound 14



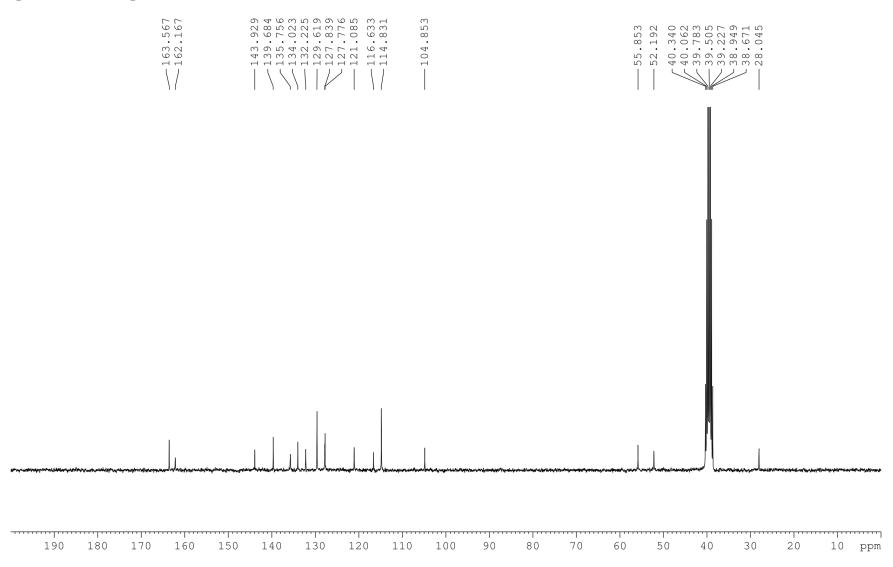
<sup>13</sup>C Spectrum for compound 15



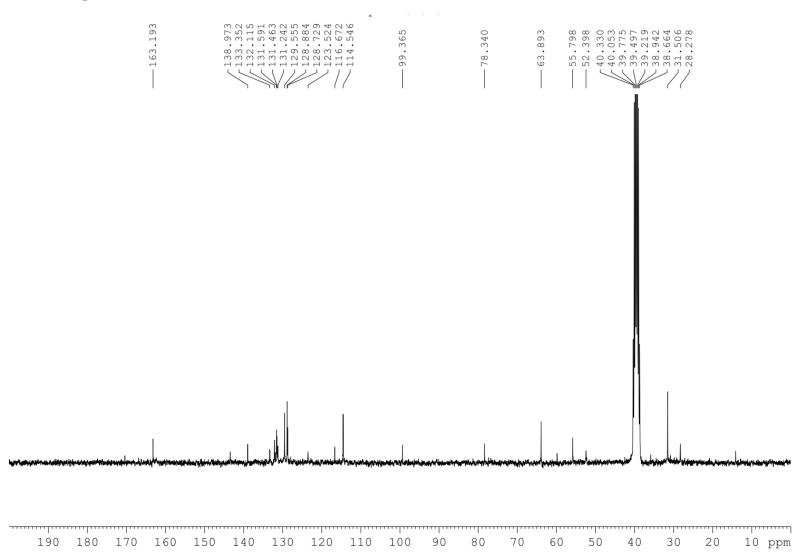
<sup>13</sup>C Spectrum for compound 16



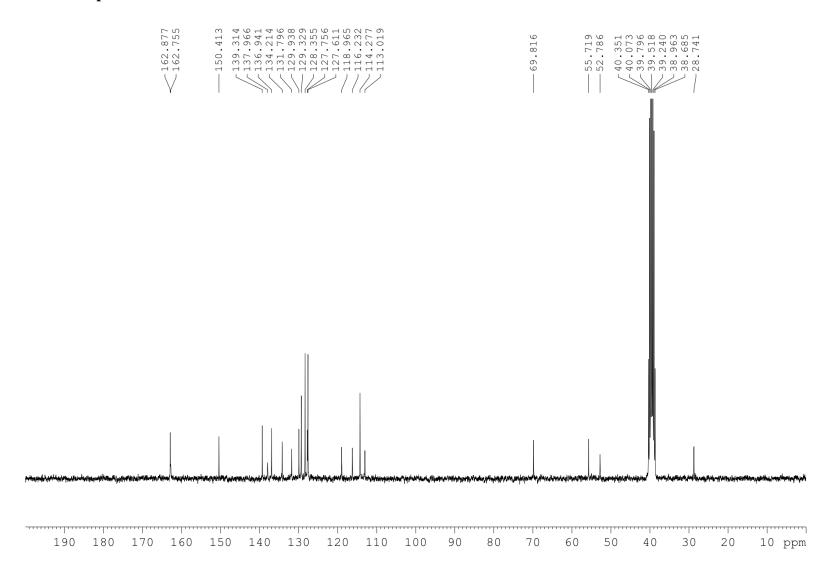
 $^{13}\mathrm{C}$  Spectrum for compound 17



<sup>13</sup>C Spectrum for compound 18

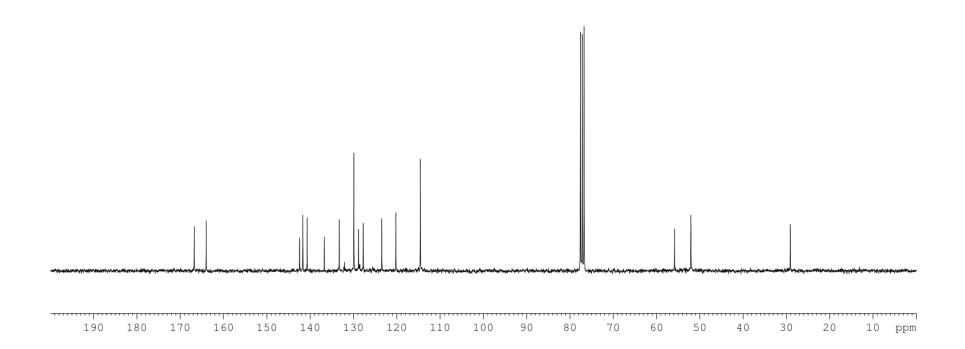


<sup>13</sup>C Spectrum for compound 19



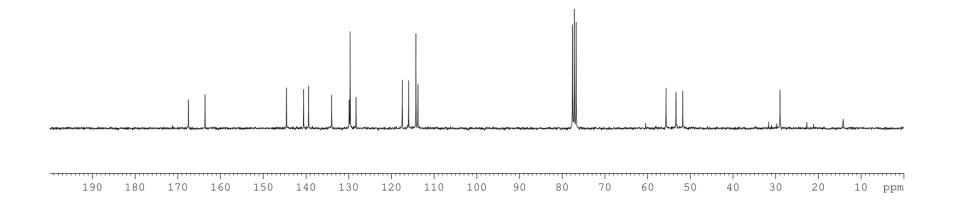
# $^{13}\mathrm{C}$ Spectrum for compound 22a





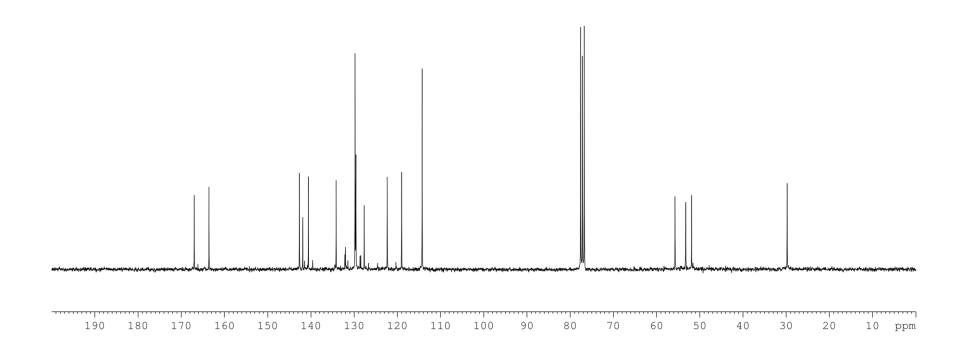
# <sup>13</sup>C Spectrum for compound 22b

2 2	7 8 8 1 L 7 4 K 4 K 8			
8 4	0 4 & & & U U U L	9 1 0	T 4 K	7
9	らりのののの 4ののと	$\infty \otimes \infty$	വവയ	$\infty$
		7	730	0
N 7	4000000 7540			•
9	4400000 1111	677	J 20 Cl	$\infty$
$\vdash$	$\dashv$ $\dashv$ $\dashv$ $\dashv$ $\dashv$ $\dashv$ $\dashv$ $\dashv$		$\Omega$ $\Omega$	2
			\	



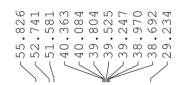
#### <sup>13</sup>C Spectrum for compound 22c

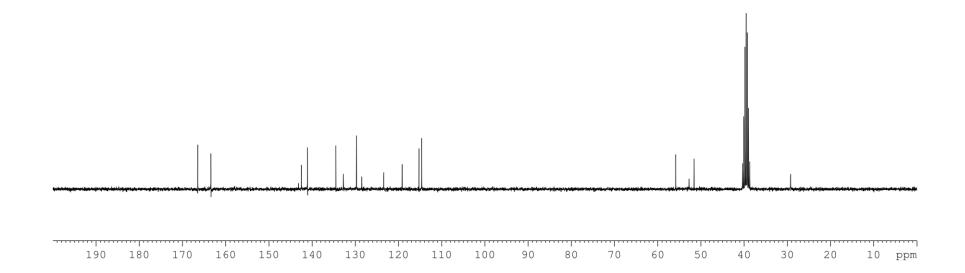


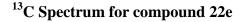


#### <sup>13</sup>C Spectrum for compound 22d

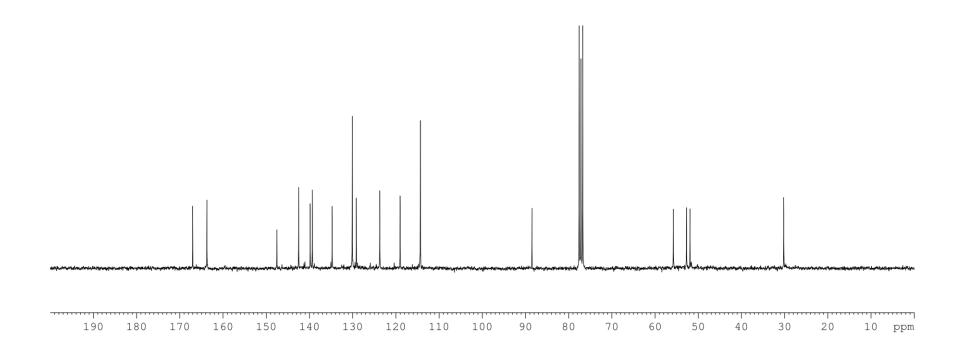






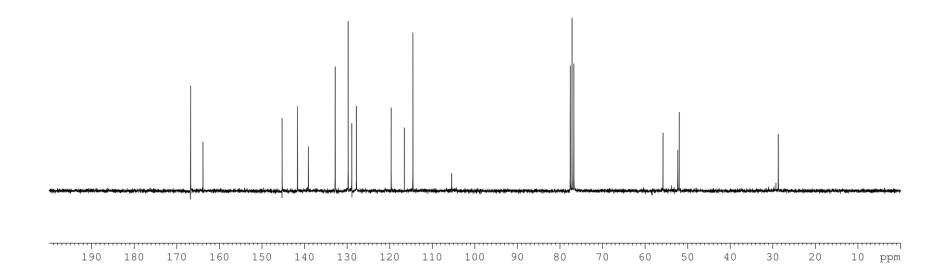






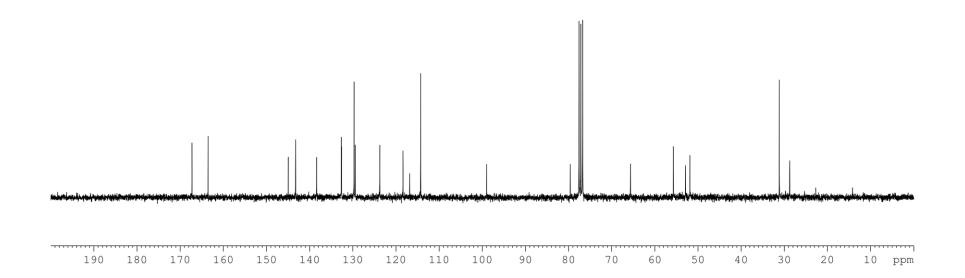
# <sup>13</sup>C Spectrum for compound 22i

00	0 0 4 1 2 7 0 9 8 4	9			
2		4	1 7 0	2 1 3	$\infty$
N 2	700070000	4	0 W	7 17 88	0
		•	7 1	L W 0	9
9 8	5102087 094	2			•
9 9	4400000 1111	0	0 1 1	1 2 2	$\infty$
$\vdash$	$\neg$	$\vdash$		2 2 2	$\sim$
				\ \/	



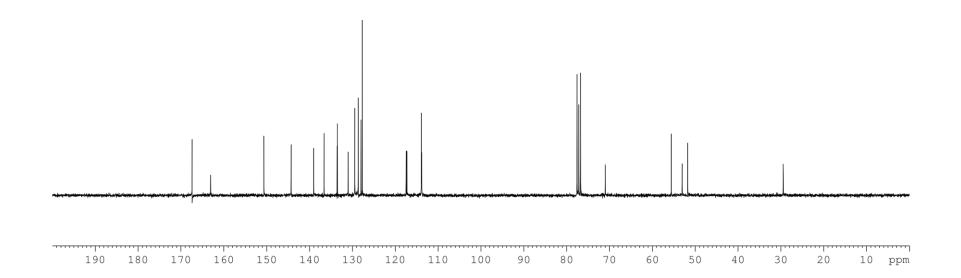
# <sup>13</sup>C Spectrum for compound 22j

0) [	0 0 4 0 6 9 9 9 9 9 9 9					
2 2	2121800113012	$\vdash$	4861	9	780	$\infty \sim$
2	0200047002	2	2 8 2 4	2	0 8	7
		0	7 1 2 2	9	00 00	7
D 0	4 M & Z Z D D D M & D 4	•		•		
9	44888222111	$\infty$	0770	2	1 2 2	$\sim$ $\sim$
$\vdash$		0	$\Gamma$	9	222	$\sim$ $\sim$
	\ \\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\					\ /



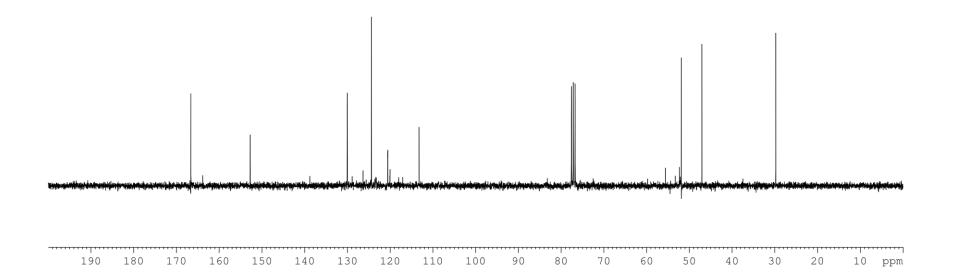
#### <sup>13</sup>C Spectrum for compound 22k





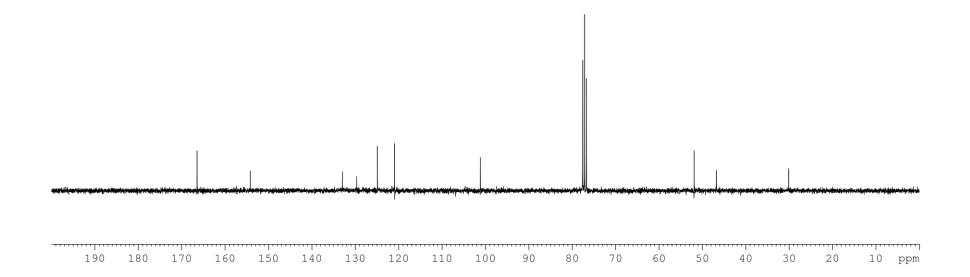
# $^{13}\mathrm{C}$ Spectrum for compound 25c

0	$\sim$	7 2 0 0	0				
$\sim$	4	0 22 0	$\sim$	2 W 4	$\sim$	2	$\sim$
9	_	223	$\sim$	0 O M	$\infty$	9	_
•	•		•	7 1	$\infty$	0	_
9	$\sim$	0 4 0 0	$\sim$		•	•	•
9	2	N N N	$\leftarrow$	677	$\leftarrow$	_	9
$\leftarrow$	$\vdash$	$\vdash$ $\vdash$ $\vdash$ $\vdash$	$\vdash$		2	4	$\sim$



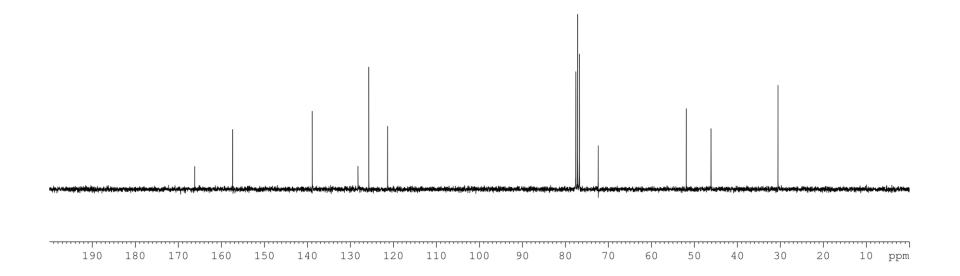
# $^{13}\mathrm{C}$ Spectrum for compound 25d

$\bigcirc$ I	√ t	4	O			
_	9	5	$\infty$	0000	0 0	$\sim$
4	$\leftarrow$	0000	$\leftarrow$	798	7 7	0
•			•	7 1 2	0 1	$\vdash$
9	4	26 40	$\leftarrow$			
9	2	M M M M	0	7 7 9	9	0
$\vdash$	$\leftarrow$	$\vdash$ $\vdash$ $\vdash$	$\leftarrow$		5 4	$\sim$



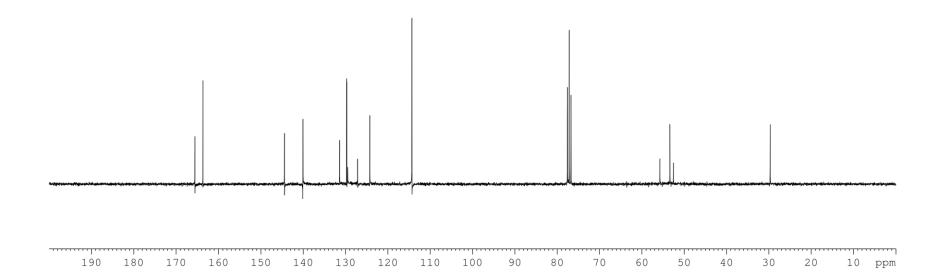
# <sup>13</sup>C Spectrum for compound 25e

0	_		7 0 1					
0	9	9 6	N O M	0 2	$\infty \circ$	2	$\sim$	4
$\sim$	$\sim$	00 0	$N \vdash W$	ω ω	J W L	$\infty$	4	9
•	•	•		7 7	3 J F	$\infty$	$\vdash$	2
9	7	00 00	$\sim 10^{\circ}$			•	•	
9	2	w ~	$N \cap N$	L L	0 0	$\vdash$	9	0
$\leftarrow$	$\vdash$	← ←	$\dashv$ $\leftarrow$		-   -	2	4	$\sim$
			\		//			



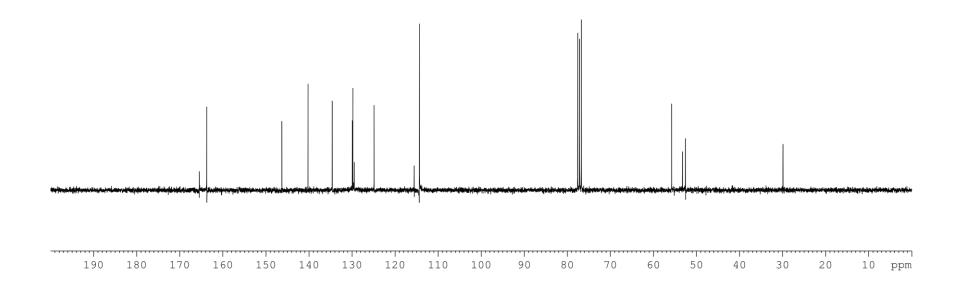
# <sup>13</sup>C Spectrum for compound 26c

0) (/		$\infty$			
5	0 0 0 0 0 0 0	$\leftarrow$	2 2 2	E 4 9	2
9	4 0 8 7 9 4 1 2	$\sim$	∞ v m	4 7 2	$\infty$
		•	7 1	5 3 7	9
3 2	4 0 1 0 0 0 0 7 4	4			
9	4 4 6 8 8 8 8 8 8	$\leftarrow$	7 7 9	2 2 2	0
$\vdash$	$\vdash$ $\vdash$ $\vdash$ $\vdash$ $\vdash$ $\vdash$ $\vdash$	$\leftarrow$	7 7 7	2 2 2	$\sim$
\ /					

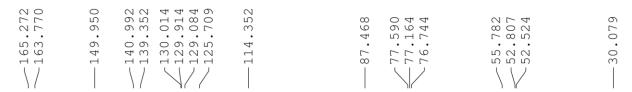


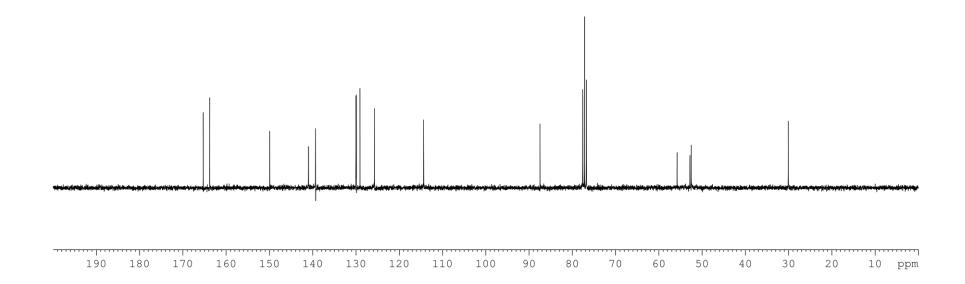
# <sup>13</sup>C Spectrum for compound 26d

7 4	0	1 4 5 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	$\infty$ $\Omega$			
M	0	7 7 8 0 8 7	2 2	0 7 0	0 1 2	9
4 7	$\sim$	250748	3 2	8 5 4	5 2 7	$\vdash$
	•			7 1	7 2 7	0
N 0	9	040004	4			
9	4	4 8 8 8 8 8 8	$\vdash$	7 7 9	N W 2	9
$\vdash$	$\vdash$	$\vdash$ $\vdash$ $\vdash$ $\vdash$ $\vdash$ $\vdash$ $\vdash$	$\vdash$	7 7 7	222	$\sim$
\ /			\ /			



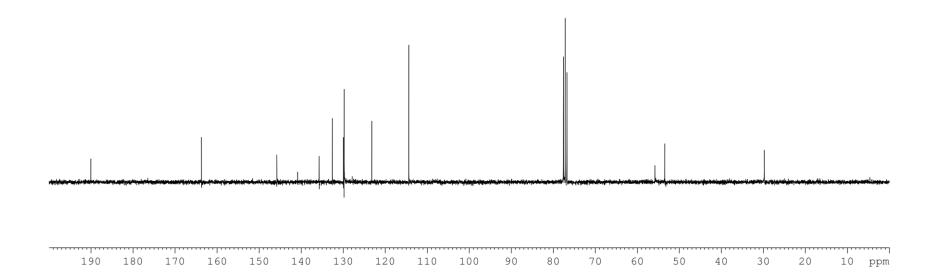
#### <sup>13</sup>C Spectrum for compound 26e





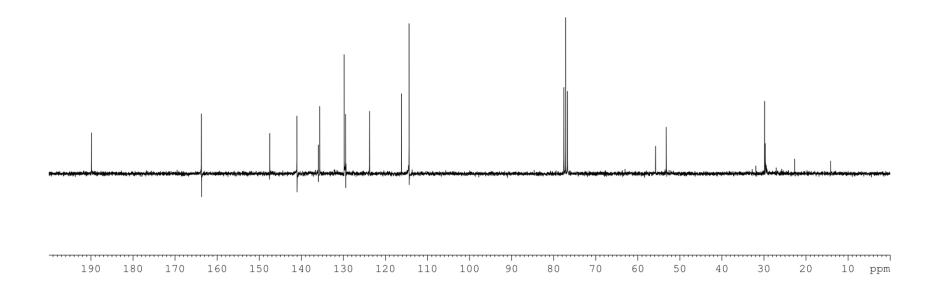
# <sup>13</sup>C Spectrum for compound 27c

2	0	0 0 1 7 0 7 8 7	4			
N	2	8 4 8 7 5 7 7 6	0	000	0 0	$\sim$
0	_	18790181	$\sim$	7 9 8	0	9
•	•		•	7 1	8 4	7
0	$\sim$	0 0 0 0 0 0 0 C W	4			•
9	9	4 4 8 8 8 8 8 8	$\vdash$	7 7 9	N 01	0
$\vdash$	$\vdash$	$\dashv$ $\dashv$ $\dashv$ $\dashv$ $\dashv$ $\dashv$ $\dashv$	$\leftarrow$		$\Omega$	$\sim$
					\ /	



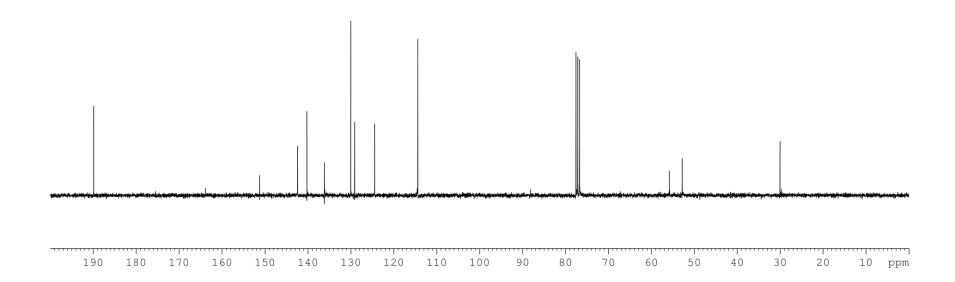
#### <sup>13</sup>C Spectrum for compound 27d

4	_	2	40278	L 0			
0	9	$\vdash$	418319	~ 1	0 1 0	√ ∞	2
0	_	2	069847	$\rightarrow$	D D D	7 4	2
•	•	•			7 1	7 7	$\infty$
0	$\sim$	_	$\omega$ $\omega$ $\omega$ $\omega$	9			
$\infty$	9	4	4000000	$\vdash$	7 7 9	N 22	9
$\leftarrow$	$\leftarrow$	$\vdash$	$\dashv$ $\dashv$ $\dashv$ $\dashv$ $\dashv$	$\vdash$	777	2 2	$\sim$
			$  \vee \vee  $	\ /		\ /	

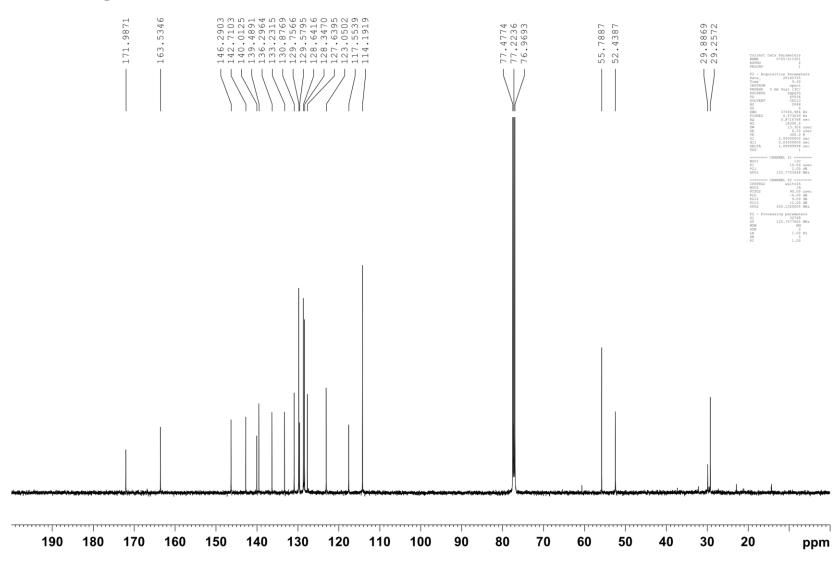


<sup>13</sup>C Spectrum for compound 27e

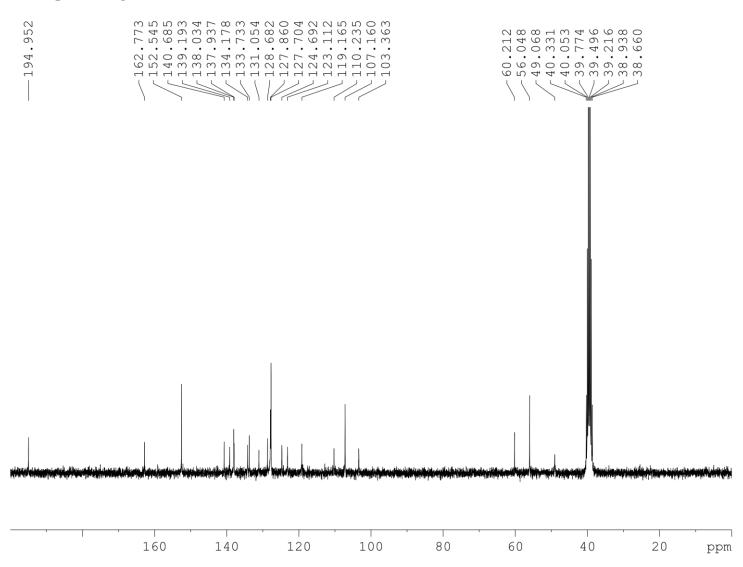
00	$\sim$	9	7 8 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	4				
$\infty$	9	2	73 631	1 0	$\vdash$	8 1 6	0 0	9
$\infty$	$\infty$	8	42101	4 4	4	707	0 0	$\sim$
•		•			$\leftarrow$	7 1	∞ ∞	0
0	$\sim$	$\leftarrow$	00 00	4 4	•			
$\infty$	9	2	4 4 M M Z	7 7	$\infty$	0 1 1	2 2	0
$\vdash$	$\leftarrow$	$\leftarrow$	$\neg$ $\neg$ $\neg$ $\neg$ $\neg$	$\vdash$	$\infty$	7 7 7	2 2	$\sim$
			\				\	



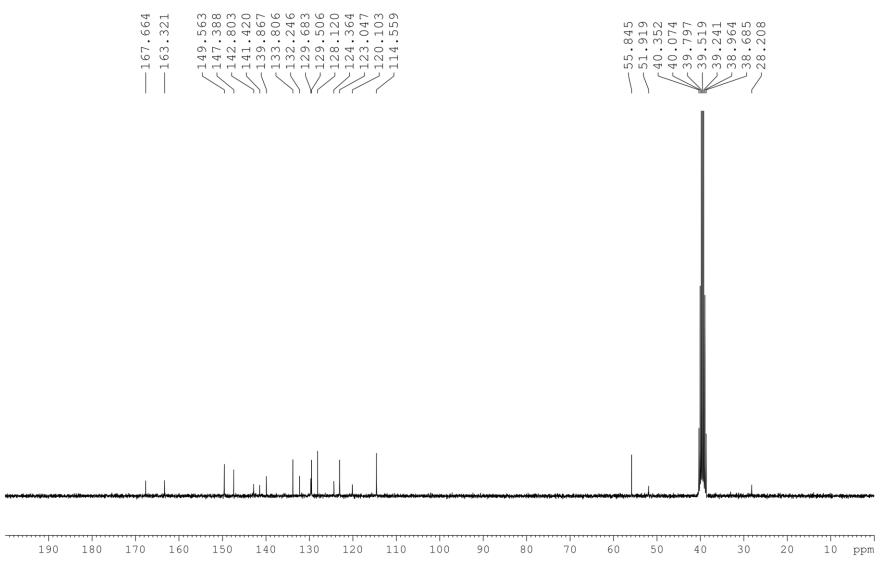
<sup>13</sup>C Spectrum for compound 28f



<sup>13</sup>C Spectrum for compound 28g

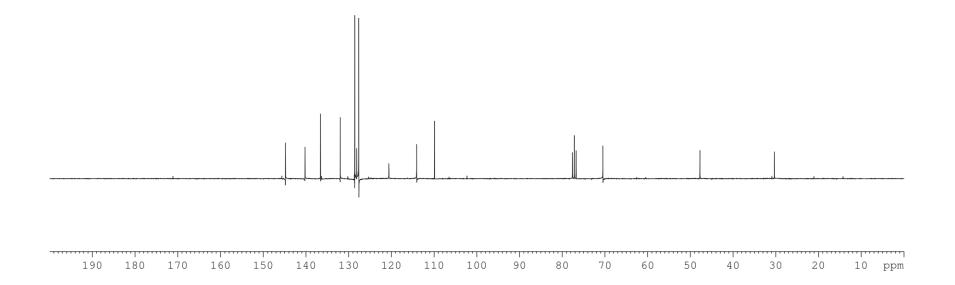


<sup>13</sup>C Spectrum for compound 28h



#### <sup>13</sup>C Spectrum for compound 31





# <sup>13</sup>C Spectrum for compound 32

_	0	500140001180			
2	9	W 4 L U O O W O U O W L	0 8 7 6	$\vdash$ $\sim$	0
$\vdash$	2	4 8 9 4 5 9 0 7 9 5 1 9	L 70 C1 W	0 4	4
•	•		2 1 2	9	9
$\sim$	$\vdash$	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0			
9	2	4 8 8 8 8 8 8 8 8 8 8 8 8 8 8	1 6 7	N 22	9
$\vdash$	$\vdash$	$\neg \neg $		2 2	2

