

## Supporting Information

### Asymmetric Michael addition of ketones to nitroolefins: Pyrrolidinyl-oxazole-carboxamides as new efficient organocatalysts

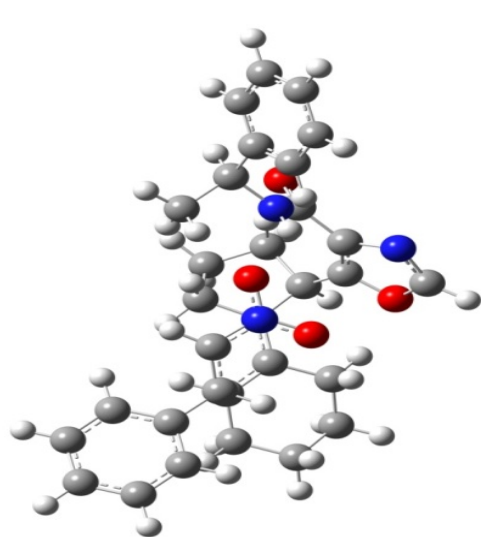
Ahmed Kamal,<sup>\*a,b</sup> Manda Sathish,<sup>a</sup> Vunnam Srinivasulu,<sup>a</sup> Jadala Chetna,<sup>b</sup> Kunta Chandra Shekar,<sup>a</sup> Shalini Nekkanti,<sup>b</sup> Yellaiah Tangella<sup>a</sup> and Nagula Shankaraiah<sup>b</sup>

<sup>a</sup>*Medicinal Chemistry & Pharmacology, CSIR-Indian Institute of Chemical Technology, Hyderabad 500 007, India*

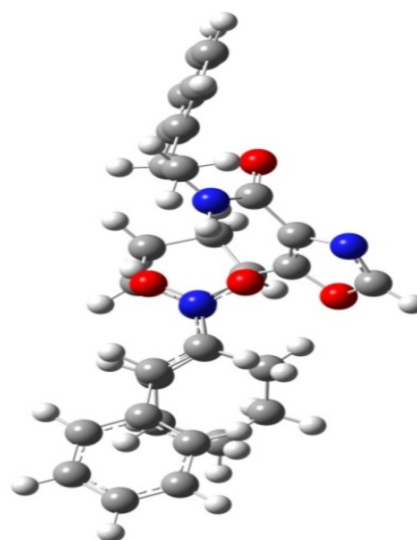
<sup>b</sup>*Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research (NIPER), Hyderabad-500 037, India*

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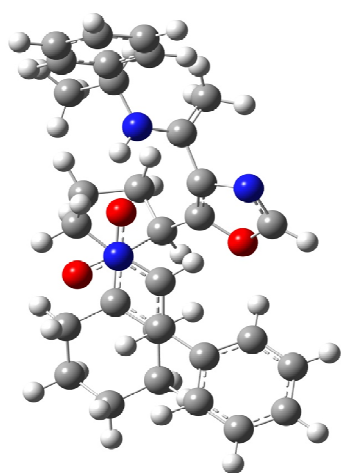
Transition state models	S2
<sup>1</sup> H and <sup>13</sup> C NMR, HRMS and IR spectral data	S3-S40
HPLC Chromatograms	S40-S53



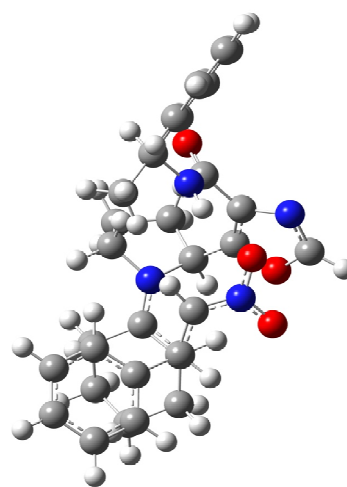
**anti-SRts**



**anti-SSts**

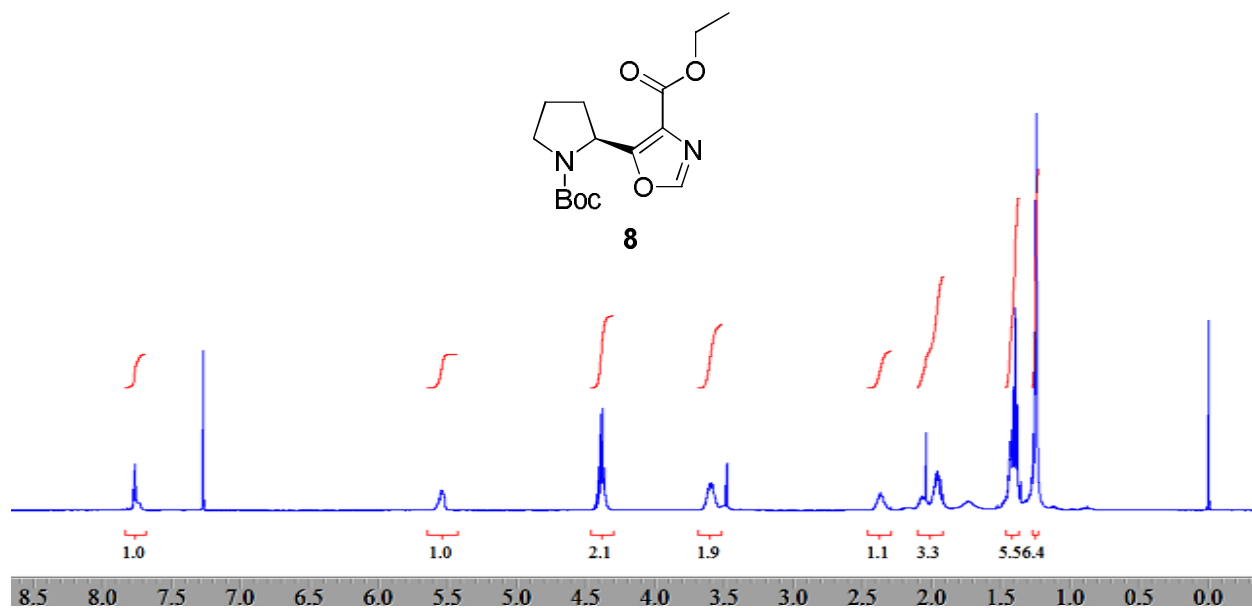


**Syn-RRts**

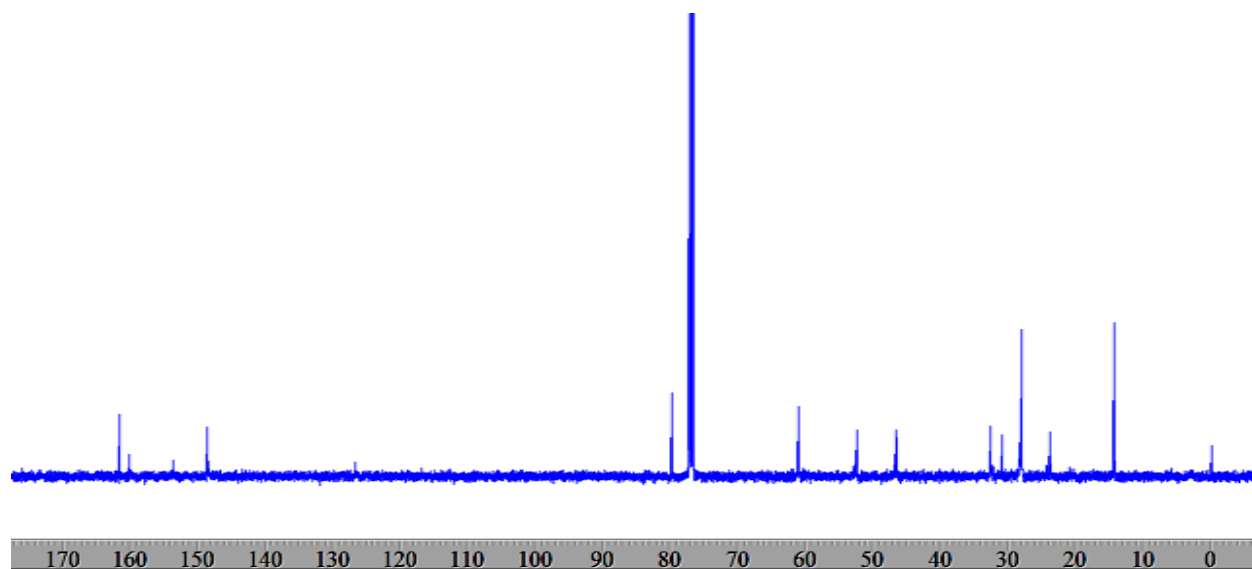


**Syn-RSts**

$^1\text{H}$  NMR spectra of **8**

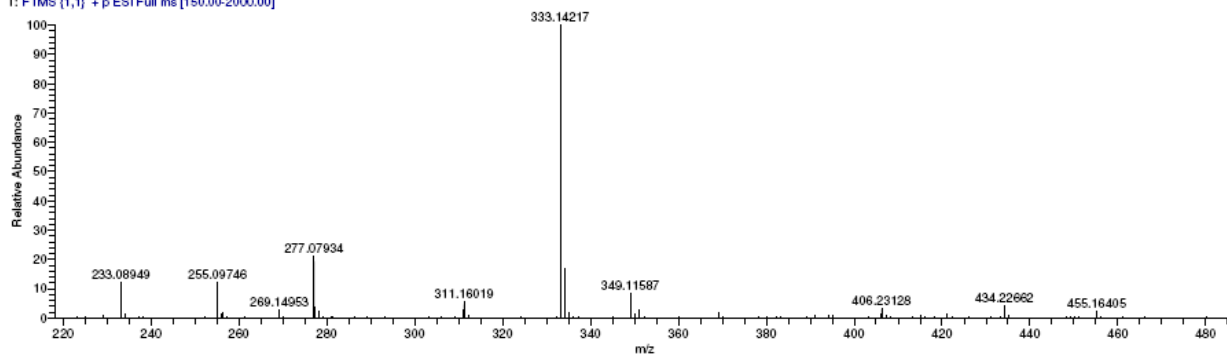


$^{13}\text{C}$  NMR spectra of **8**



## HRMS spectra of **8**

AKL-OXO-ESTR#6-89 RT: 0.02-0.30 AV: 84 SB: 326 0.80-1.90 NL: 8.46E7  
T: FTMS (1,1) + p ESI Full ms [150.00-2000.00]



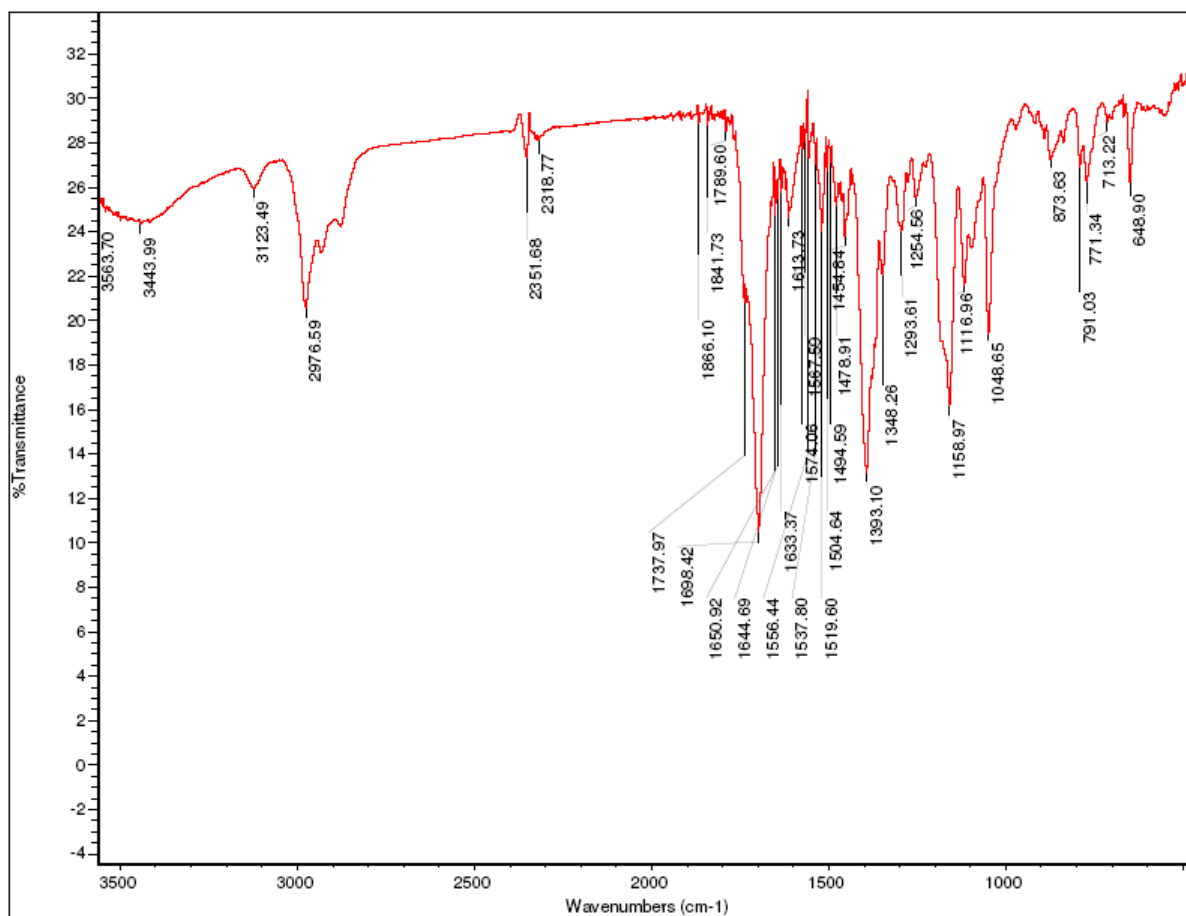
AKL-OXO-ESTR#8-30 RT: 0.03-0.10 AV: 23

T: FTMS (1,1) + p ESI Full ms [150.00-2000.00]

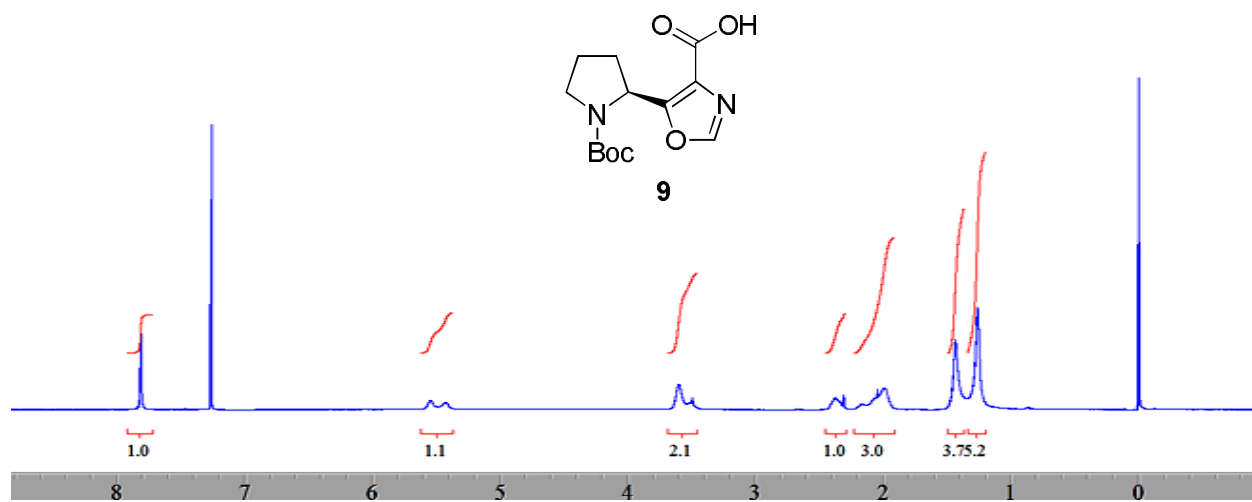
m/z= 303.80-371.90

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
333.14222	8919331.0	100.00	333.14209	0.13	5.5	C <sub>15</sub> H <sub>22</sub> O <sub>5</sub> N <sub>2</sub> Na

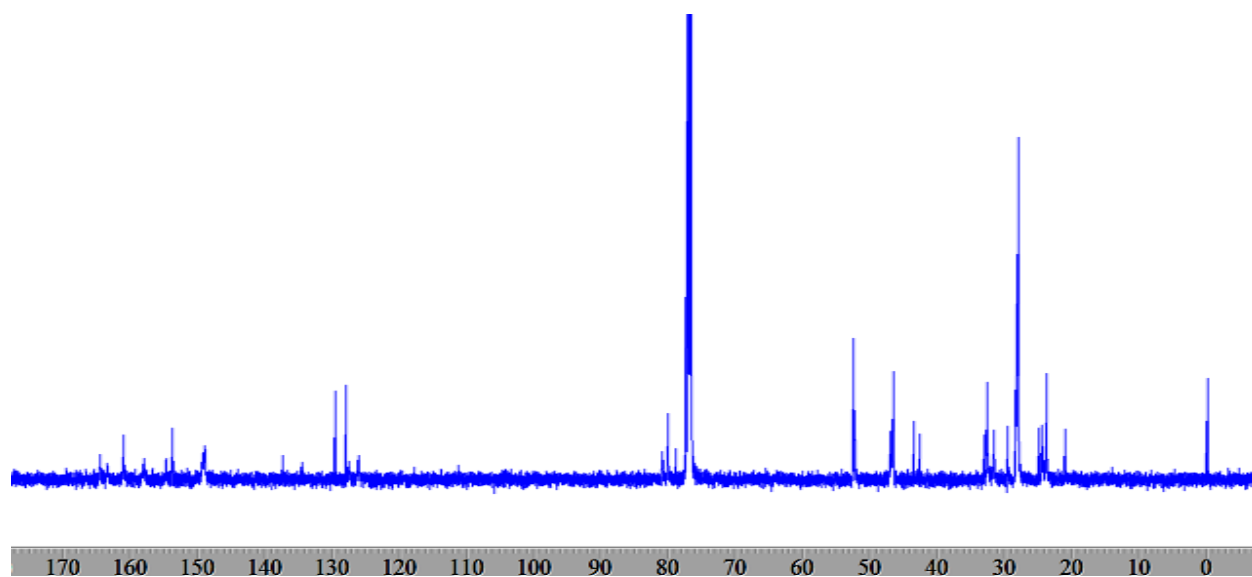
## IR spectra of **8**



$^1\text{H}$  NMR spectra of **9**

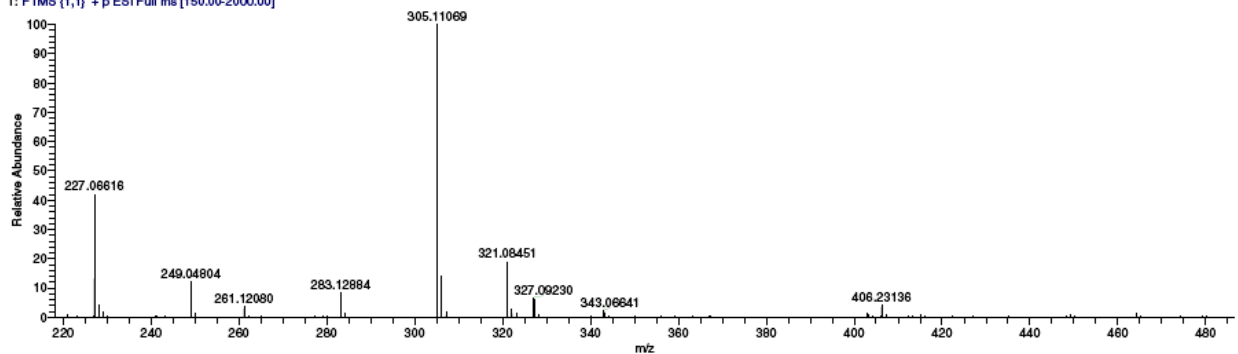


$^{13}\text{C}$  NMR spectra of **9**



## HRMS spectra of 9

AKL-OXO-ACID#8-89 RT: 0.02-0.30 AV: 84 SB: 326 0.80-1.90 NL: 5.71E7  
 T: FTMS (1,1) + p ESI Full ms [150.00-2000.00]

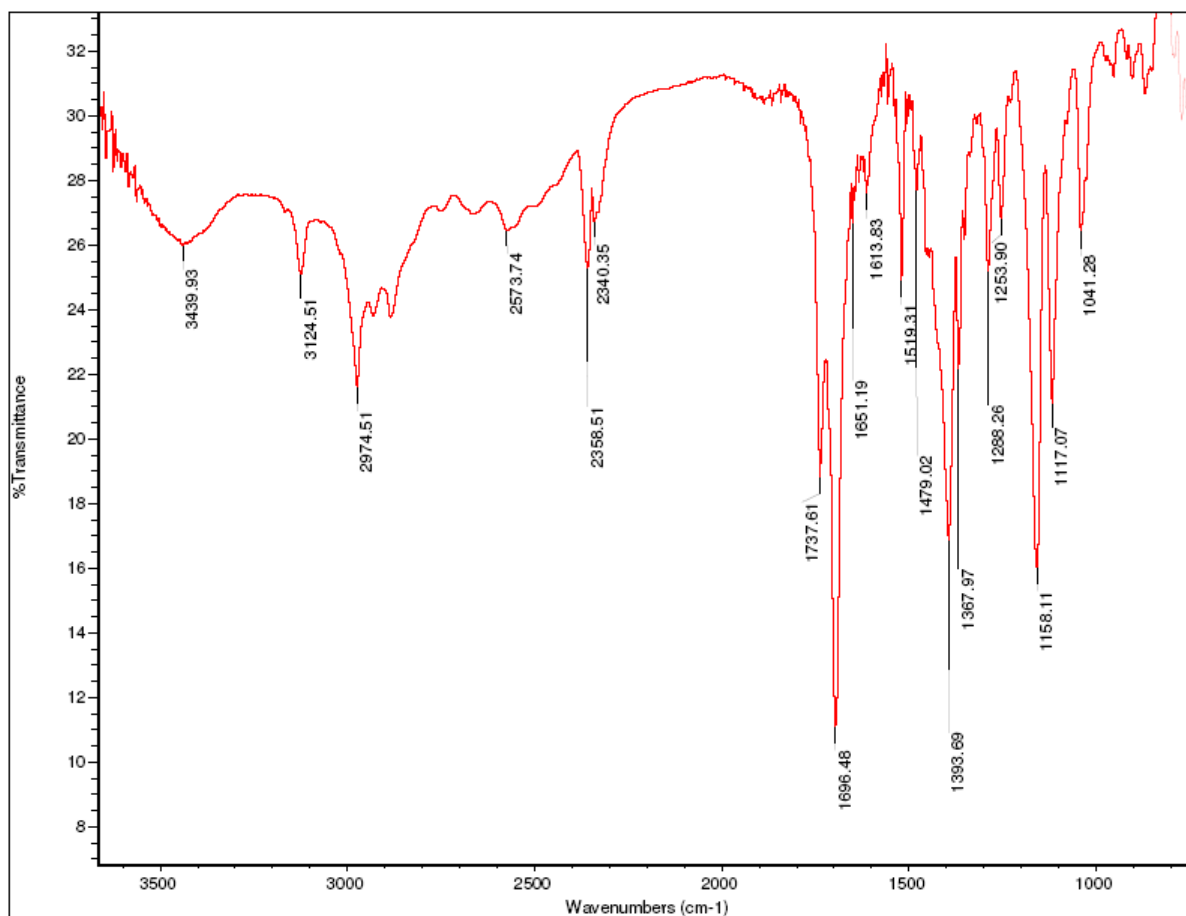


AKL-OXO-ACID#8-30 RT: 0.03-0.10 AV: 23  
 T: FTMS (1,1) + p ESI Full ms [150.00-2000.00]

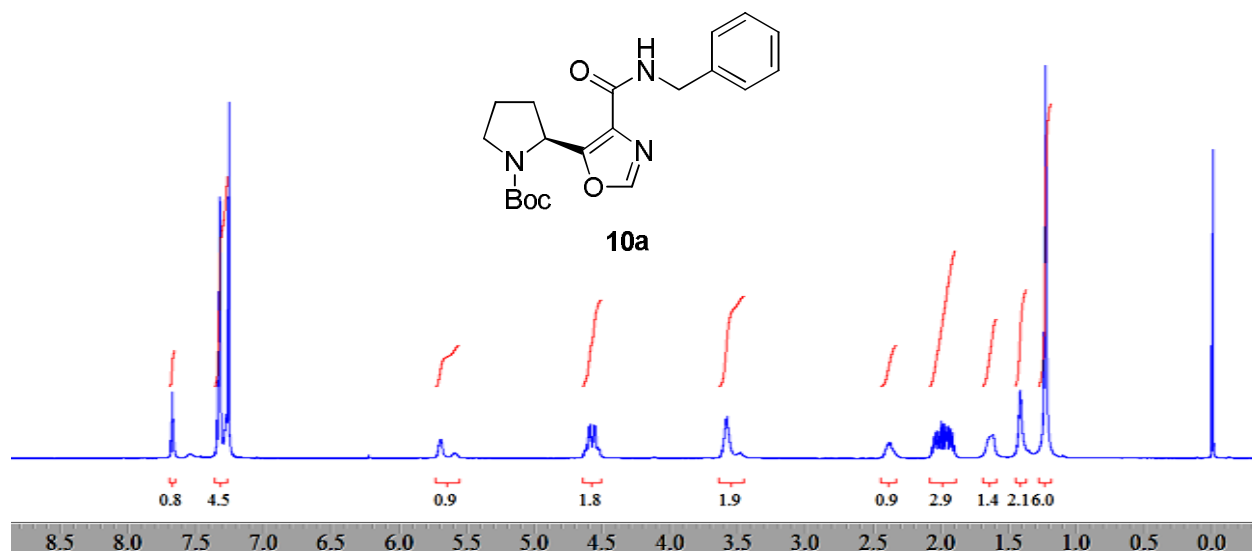
m/z = 295.05-313.78

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
305.11088	2829458.3	100.00	305.11079	0.09	5.5	C <sub>13</sub> H <sub>18</sub> O <sub>5</sub> N <sub>2</sub> Na

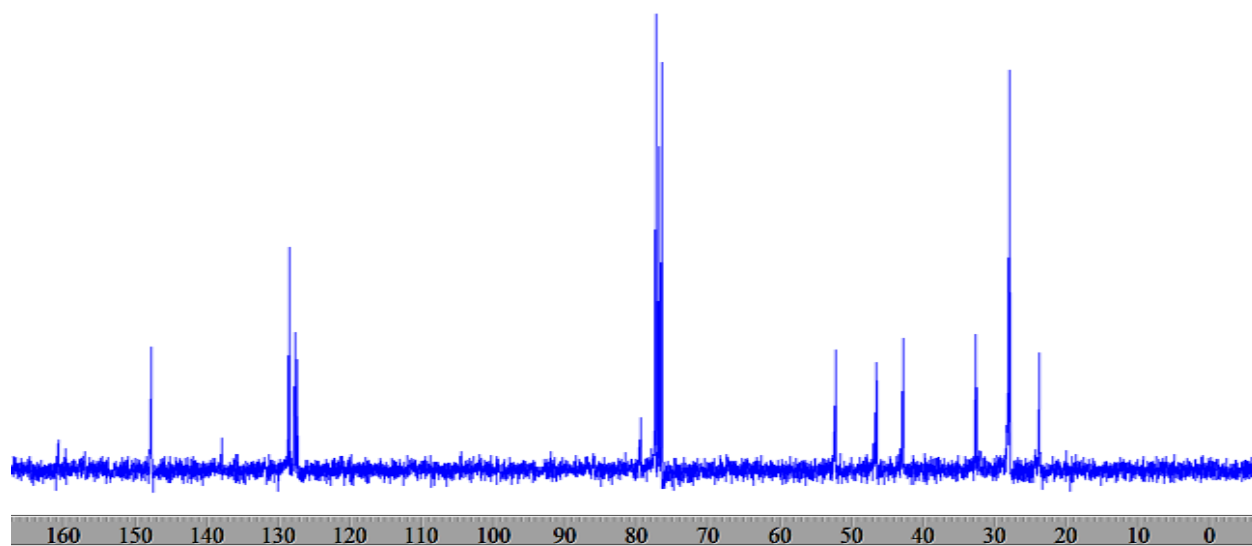
## IR spectra of 9



$^1\text{H}$  NMR spectra of **10a**

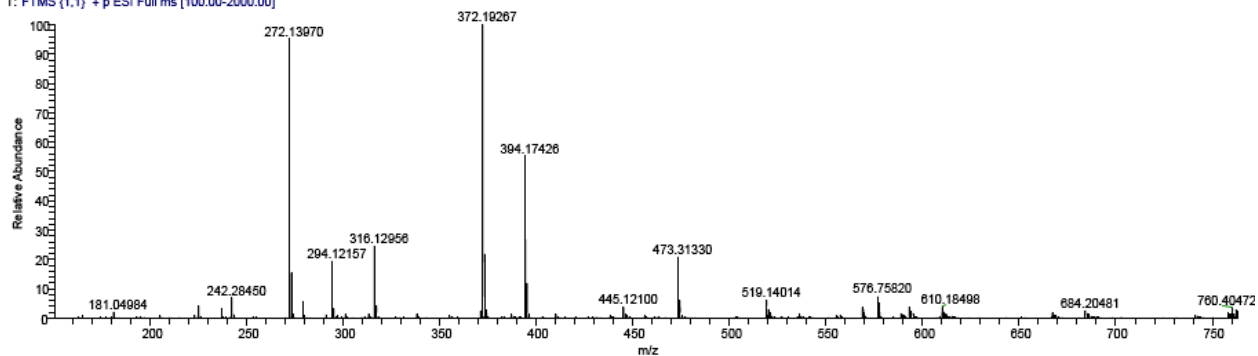


$^{13}\text{C}$  NMR spectra of **10a**



## HRMS spectra of 10a

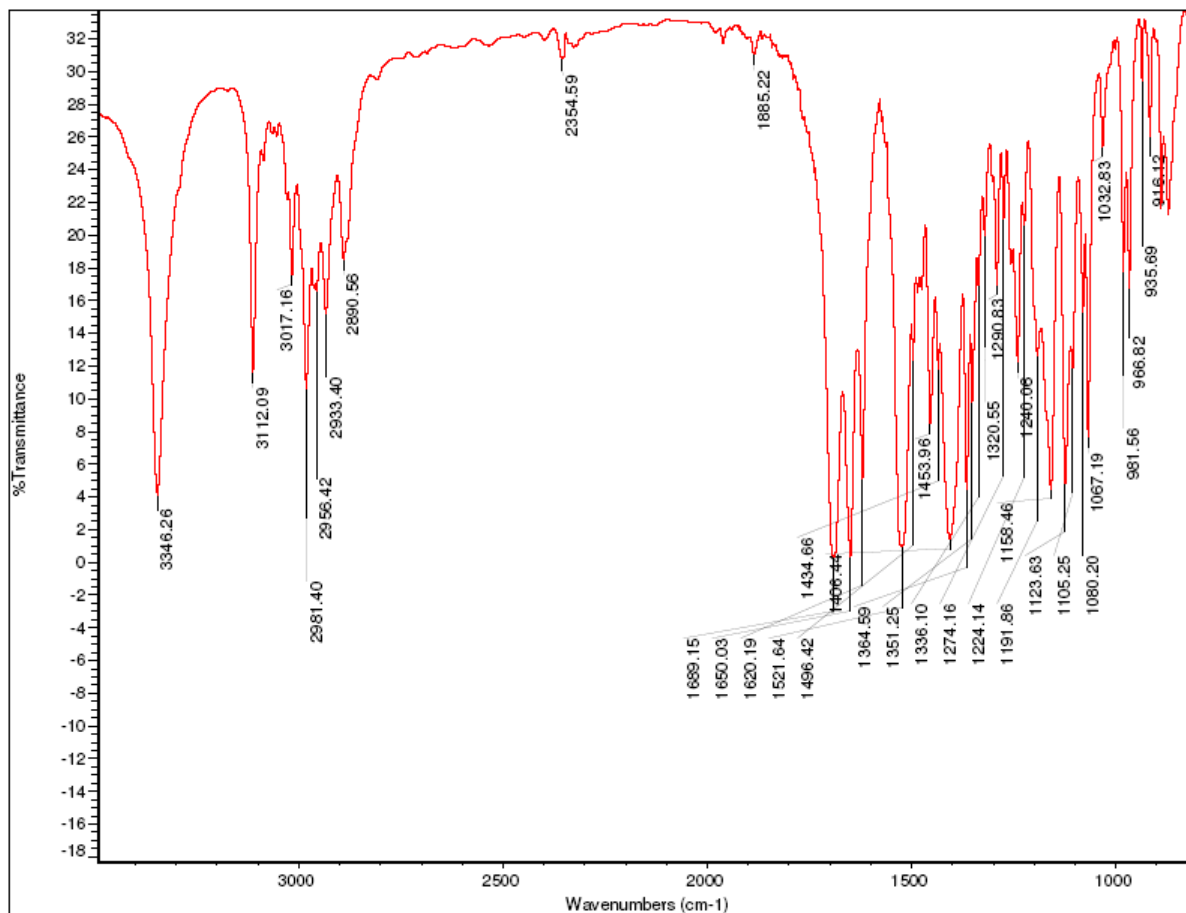
AKL-BOC-BN#2-111 RT: 0.01-0.38 AV: 110 SB: 377 0.73-2.00 NL: 1.52E7  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]



AKL-BOC-BN#8-30 RT: 0.03-0.11 AV: 23  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]

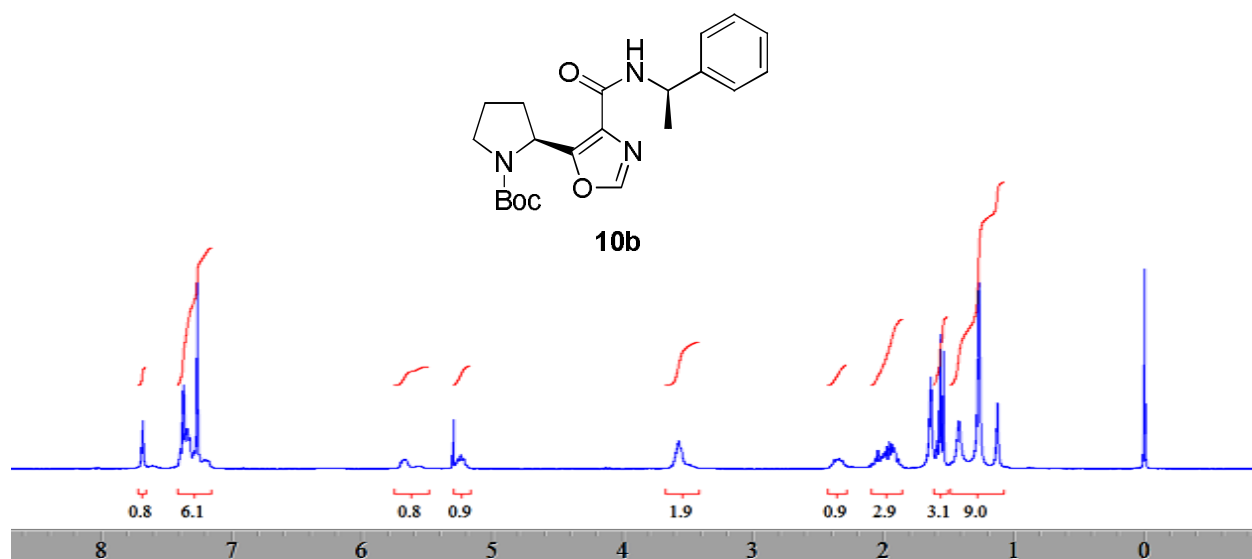
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
272.13966	40724564.0	96.94				
372.19258	42008388.0	100.00	372.19178	2.14	9.5	C <sub>20</sub> H <sub>26</sub> O <sub>4</sub> N <sub>3</sub>

## IR spectra of 10a

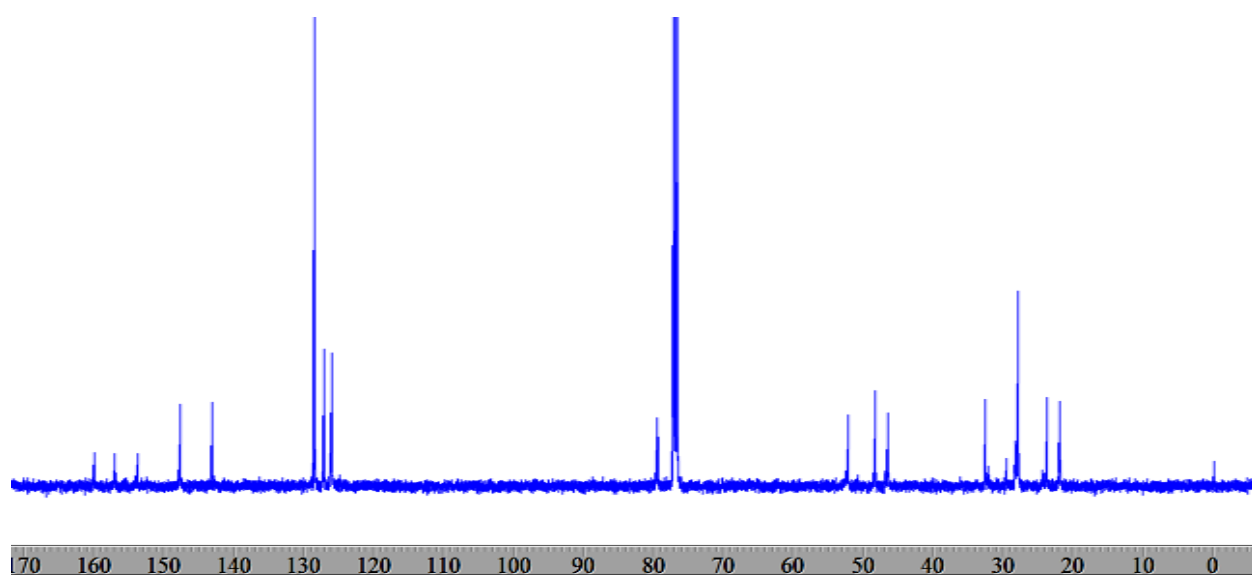




$^1\text{H}$  NMR spectra of **10b**

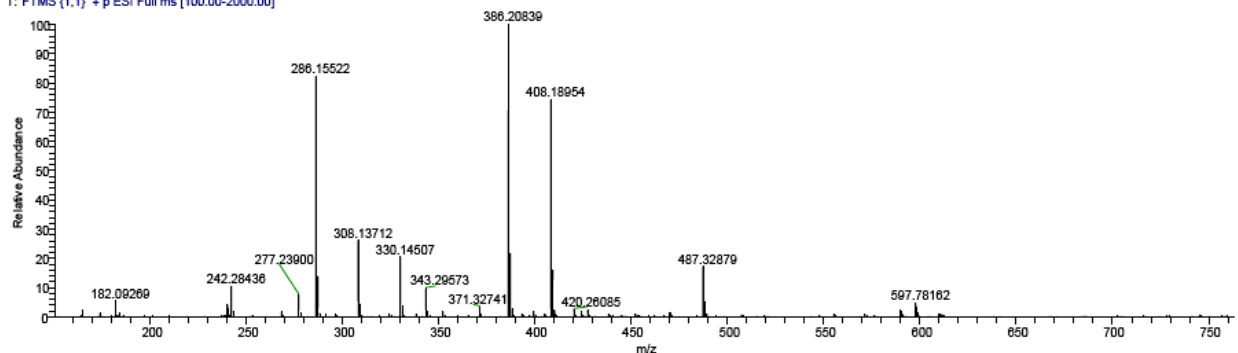


$^{13}\text{C}$  NMR spectra of **10b**



## HRMS spectra of 10b

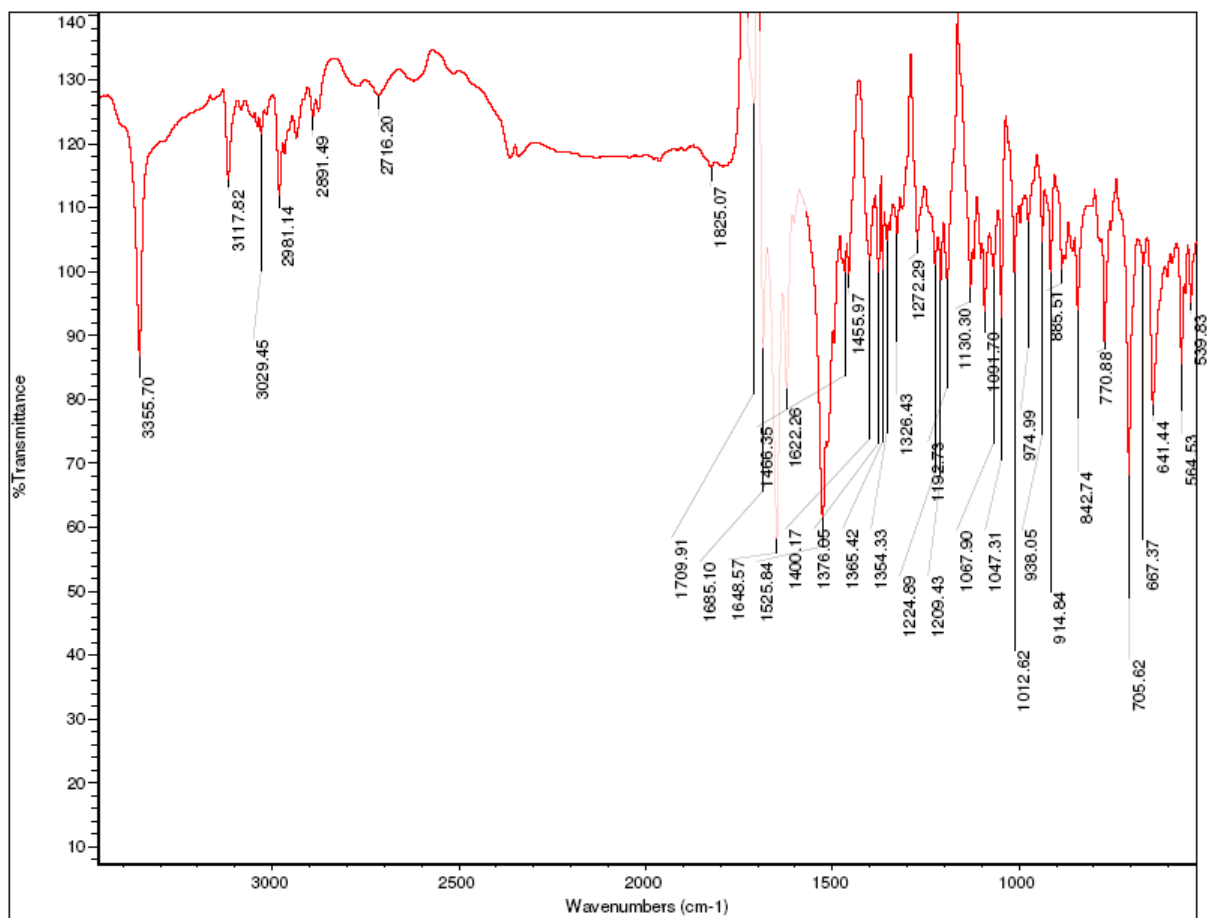
AKL-BOC-R-ME#3-112 RT: 0.01-0.38 AV: 110 SB: 376 0.73-2.00 NL: 1.49E7  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]



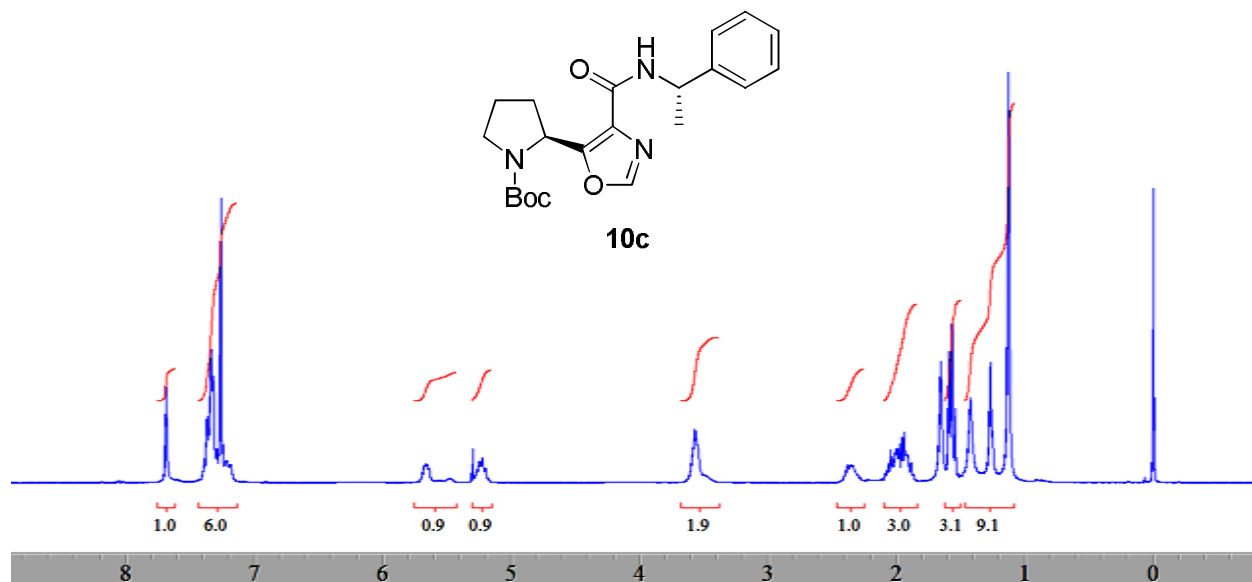
AKL-BOC-R-ME#8-30 RT: 0.03-0.11 AV: 23  
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]  
m/z = 400.97-415.85

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
408.18945	30435216.0	100.00	408.18938	0.17	9.5	C <sub>21</sub> H <sub>27</sub> O <sub>4</sub> N <sub>3</sub> Na
409.19290	6502653.5	21.37				

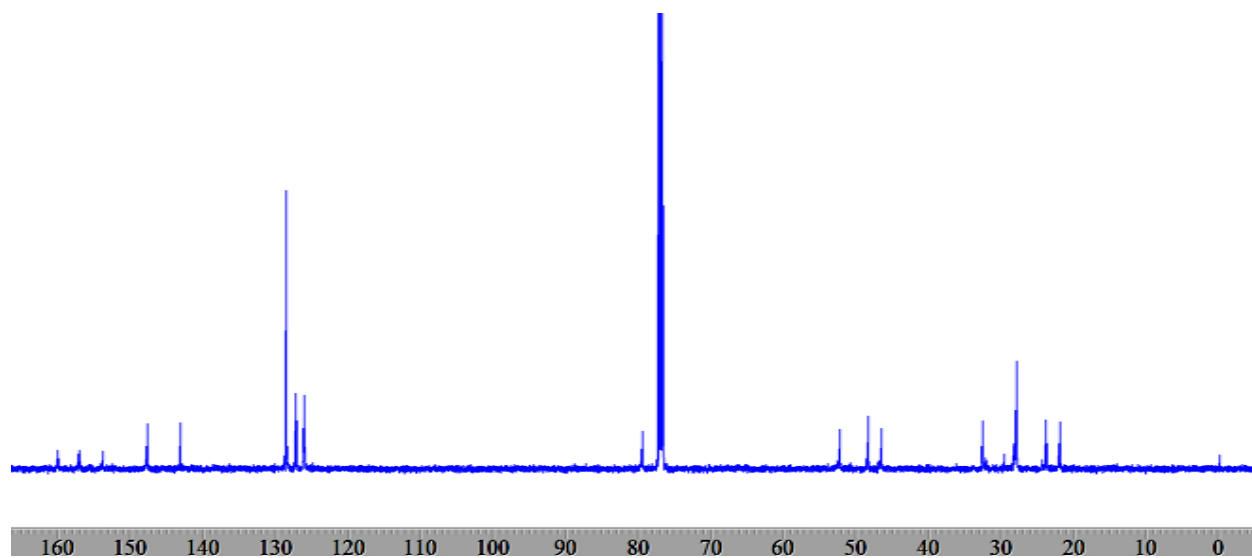
## IR spectra of 10b



$^1\text{H}$  NMR spectra of **10c**

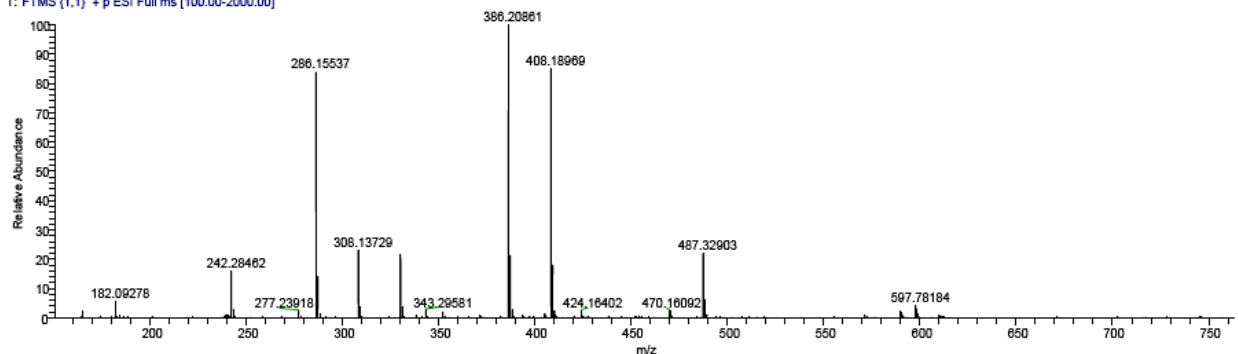


$^{13}\text{C}$  NMR spectra of **10c**



## HRMS spectra of 10c

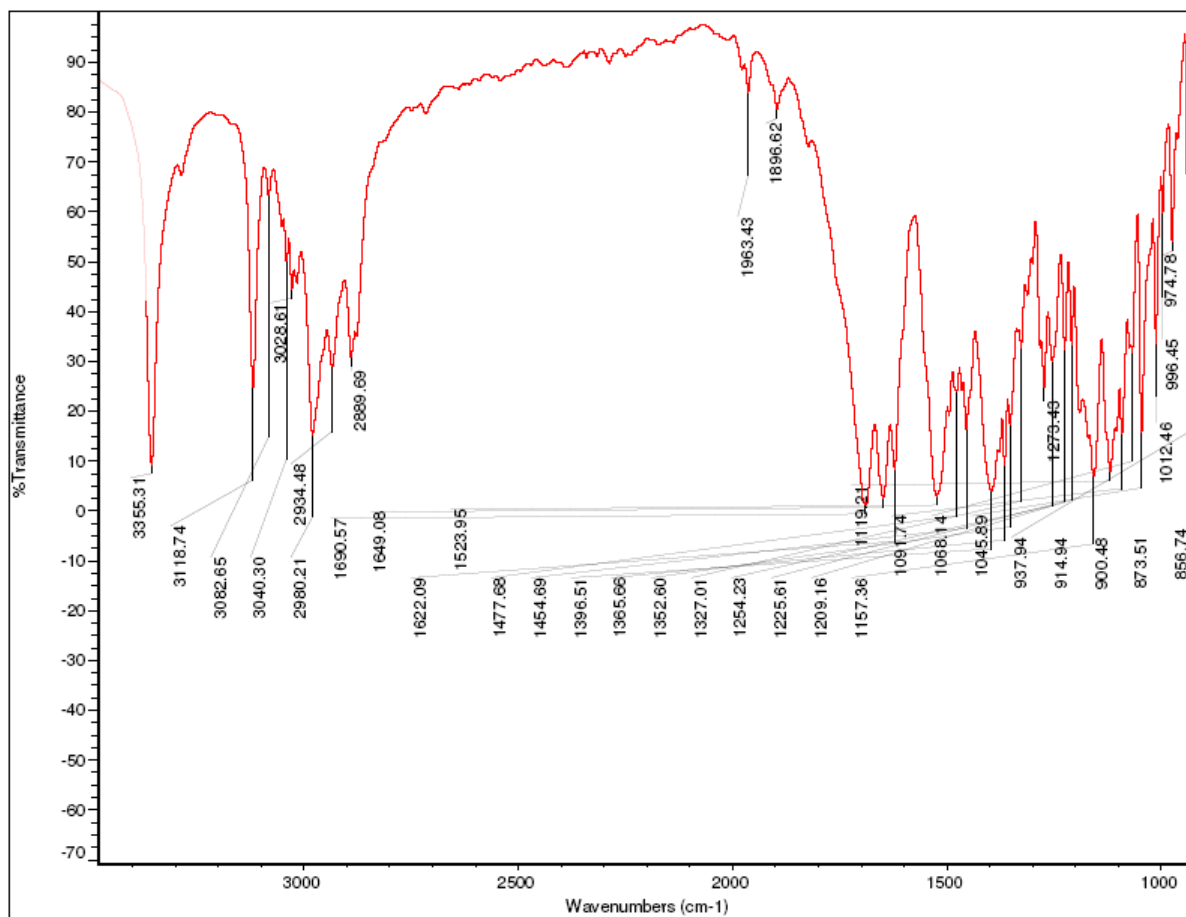
AKL-BOC-S-ME#3-111 RT: 0.02-0.38 AV: 109 SB: 377 0.73-2.00 NL: 8.97E6  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]



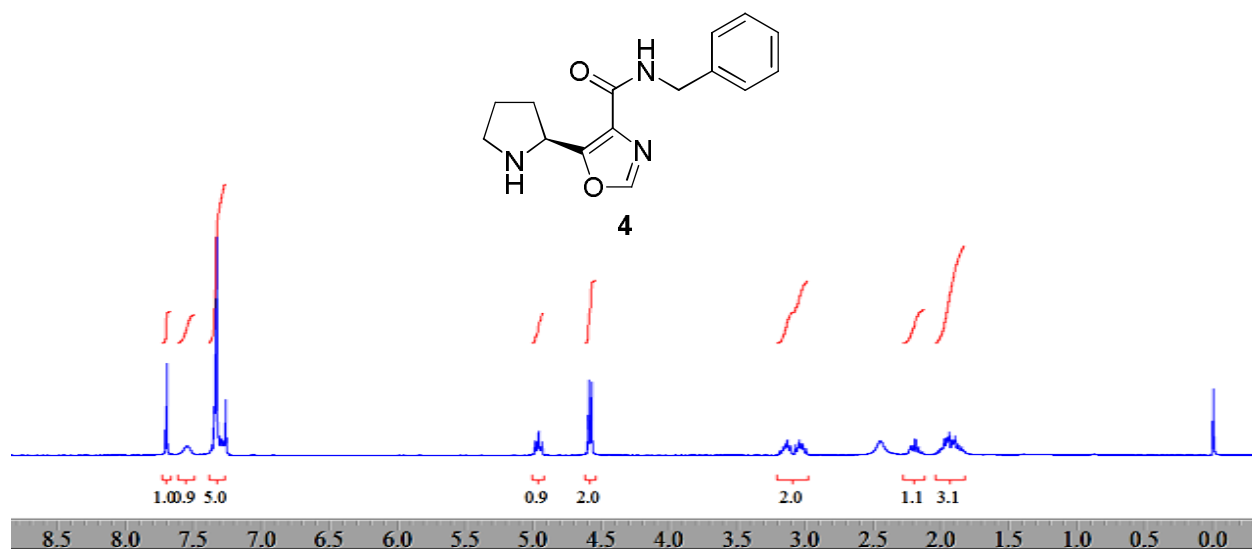
AKL-BOC-S-ME#8-30 RT: 0.03-0.11 AV: 23  
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
386.20855	26210124.0	100.00	386.20743	2.89	9.5	C <sub>21</sub> H <sub>28</sub> O <sub>4</sub> N <sub>3</sub>
408.18961	24608248.0	93.89	408.18938	0.57	9.5	C <sub>21</sub> H <sub>27</sub> O <sub>4</sub> N <sub>3</sub> Na

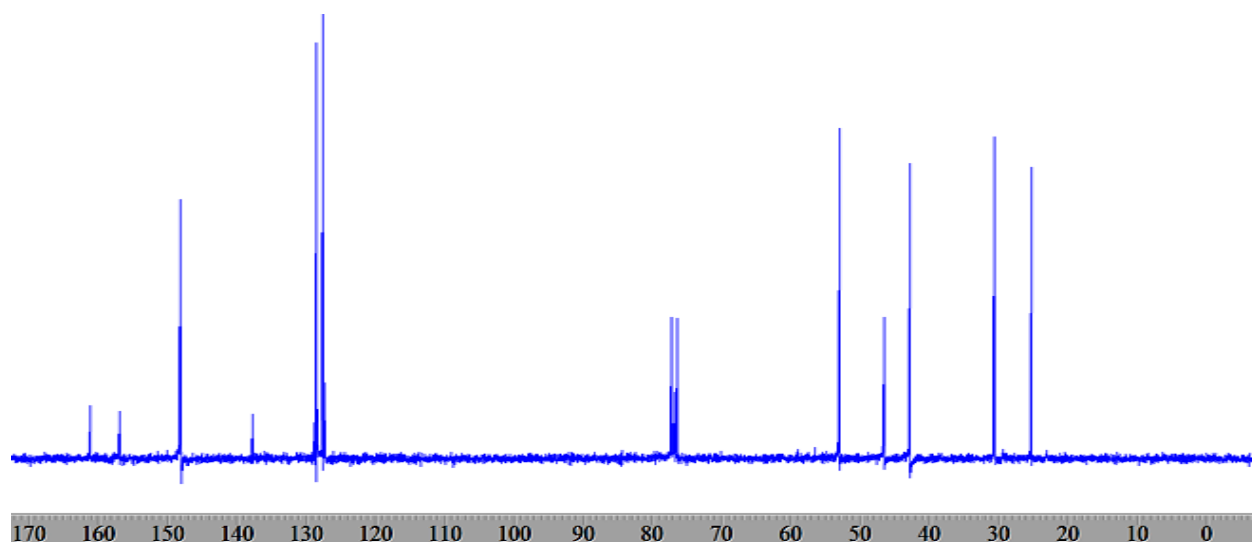
## IR spectra of 10c



$^1\text{H}$  NMR spectra of **4**

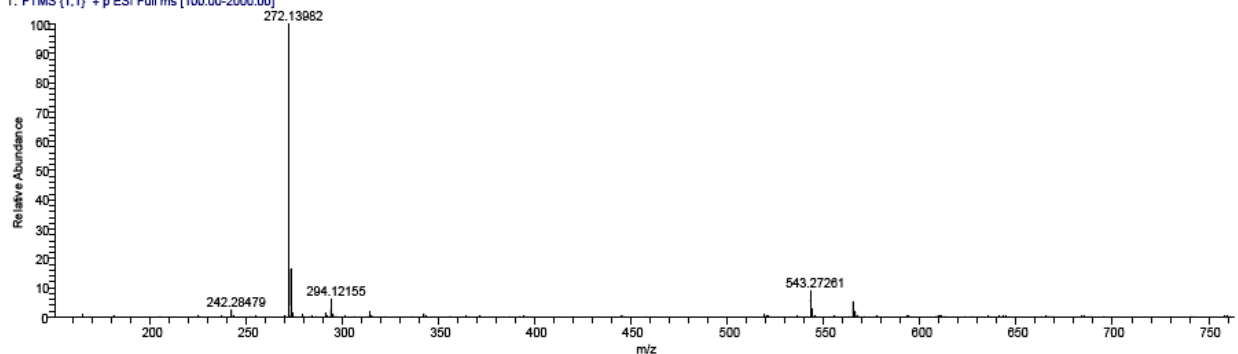


$^{13}\text{C}$  NMR spectra of **4**



## HRMS spectra of 4

AKL-NH-BN#3-112 RT: 0.01-0.38 AV: 110 SB: 377 0.73-2.00 NL: 7.39E7  
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]

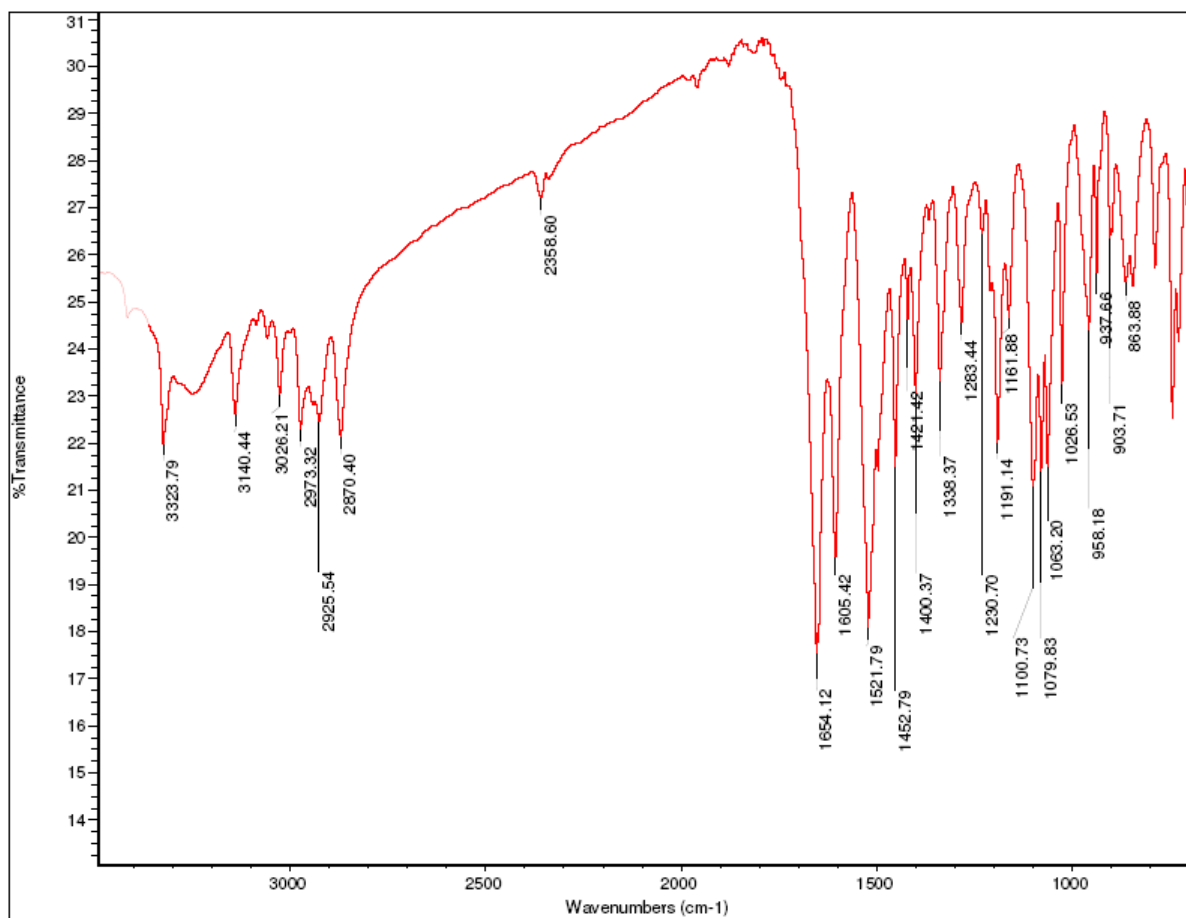


AKL-NH-BN#8-30 RT: 0.03-0.11 AV: 23

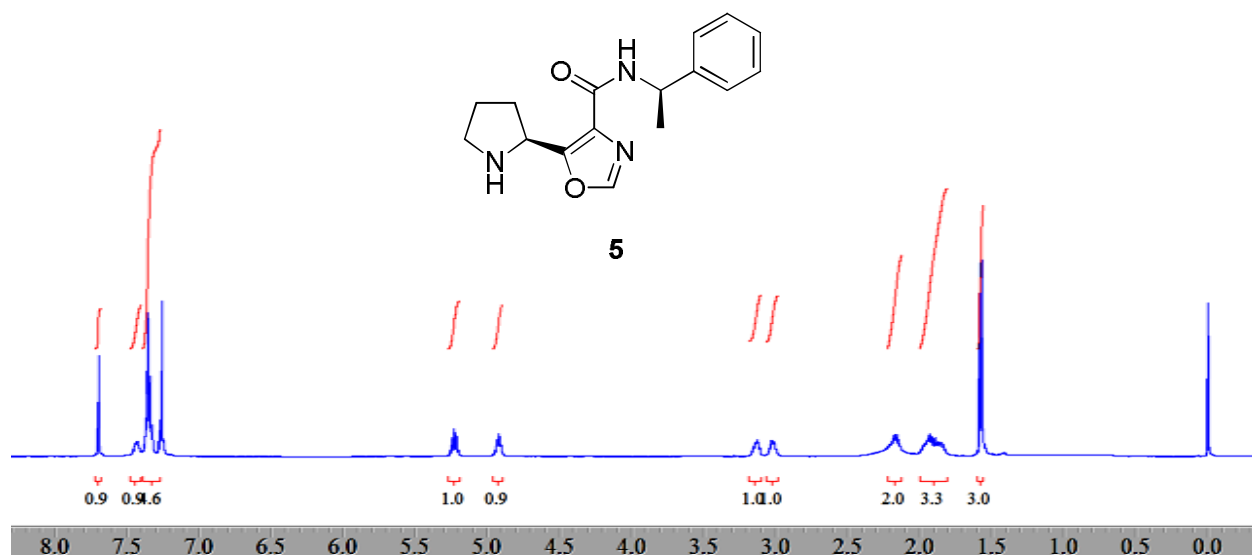
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
272.13975	172969136.0	100.00	272.13935	1.47	8.5	C <sub>15</sub> H <sub>18</sub> O <sub>2</sub> N <sub>3</sub>
273.14269	28560118.0	16.51				

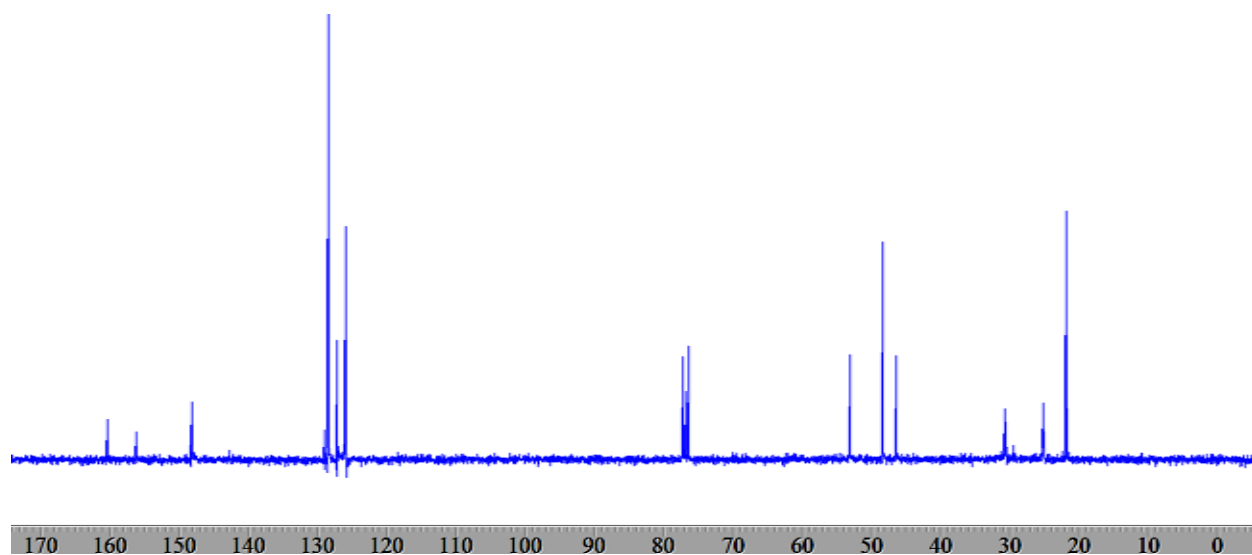
## IR spectra of 4



$^1\text{H}$  NMR spectra of **5**

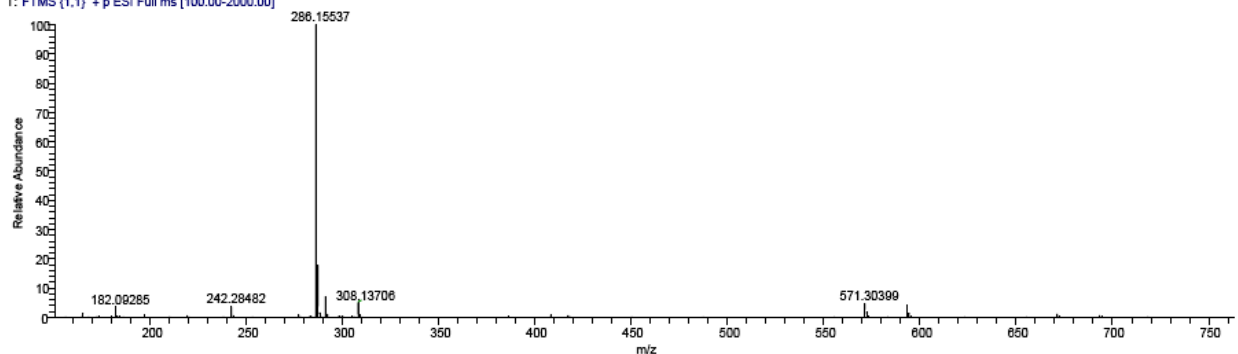


$^{13}\text{C}$  NMR spectra of **5**



## HRMS spectra of 5

AKL-NH-R-ME#2-111 RT: 0.01-0.38 AV: 110 SB: 377 0.73-2.00 NL: 4.07E7  
 T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]

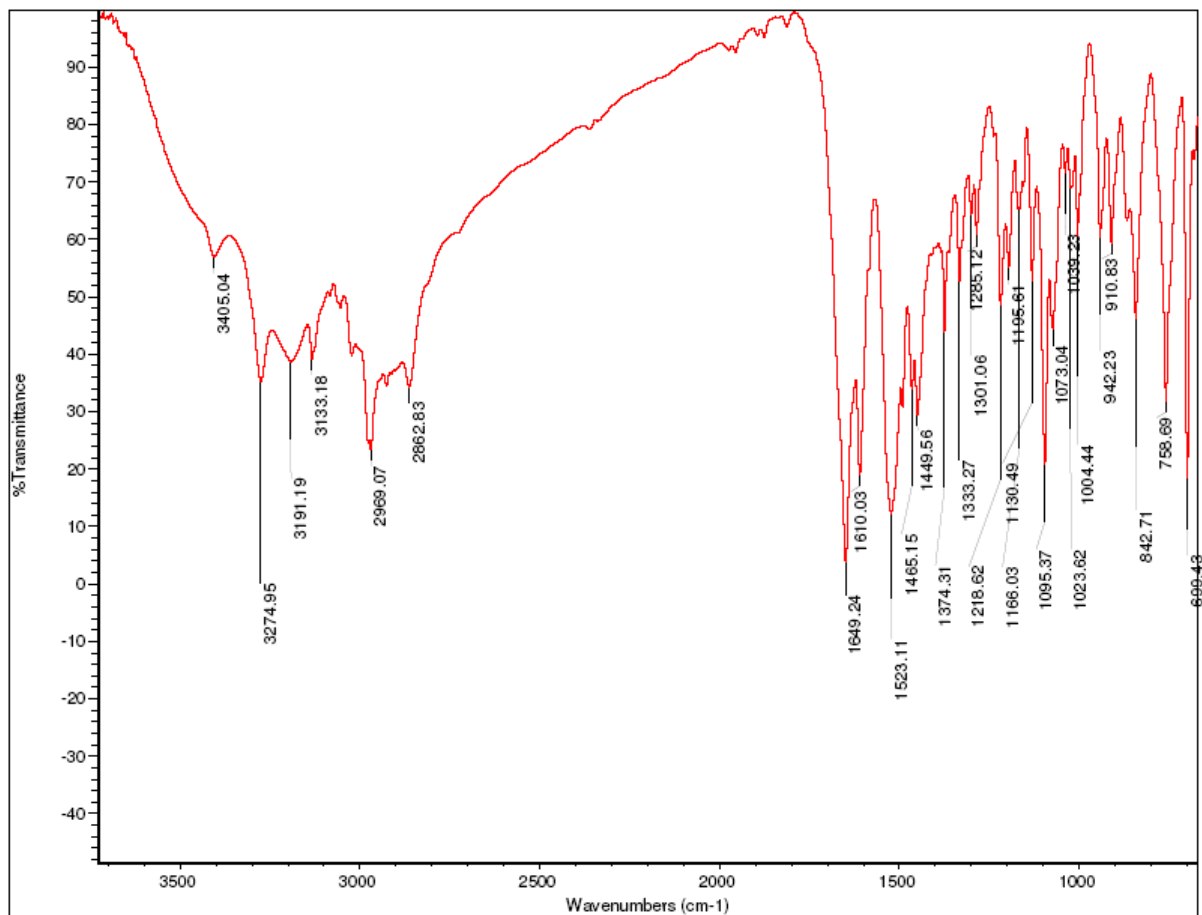


AKL-NH-R-ME#8-30 RT: 0.03-0.11 AV: 23

T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

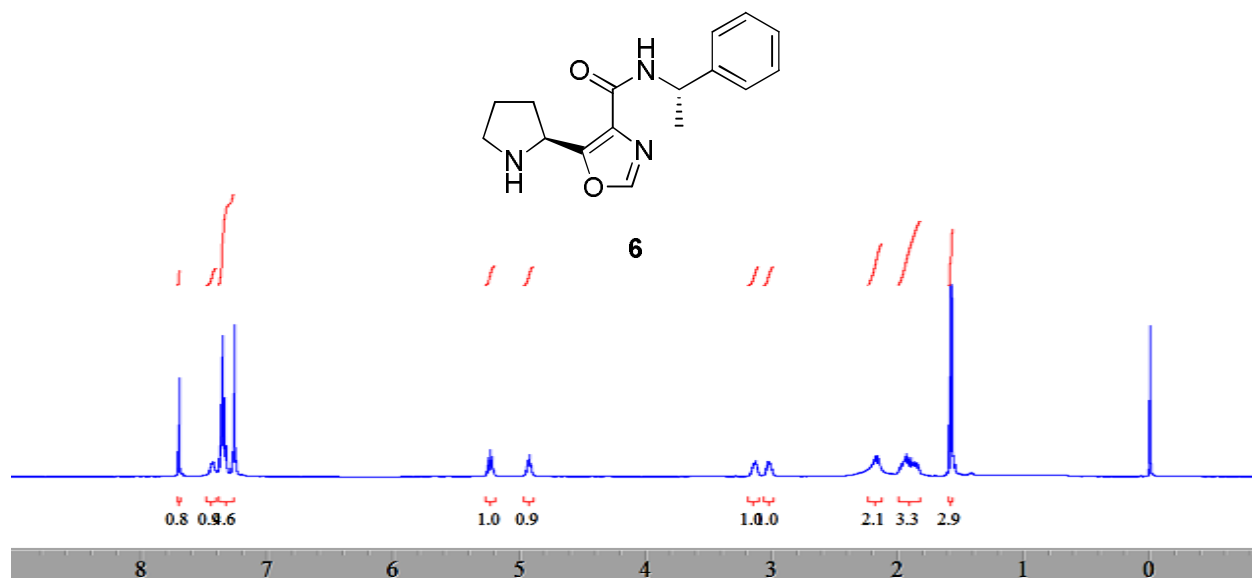
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
286.15532	117799672.0	100.00	286.15500	1.10	8.5	C <sub>16</sub> H <sub>20</sub> O <sub>2</sub> N <sub>3</sub>
287.15826	20997312.0	17.82				

## IR spectra of 5

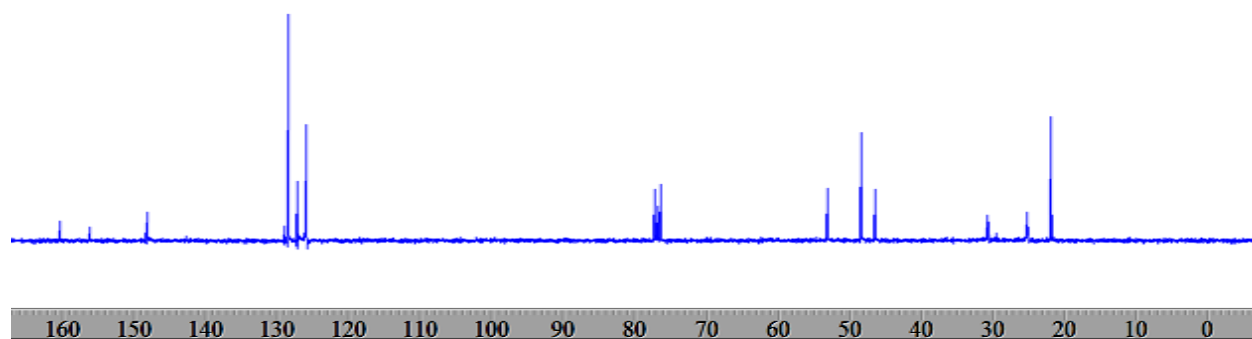




$^1\text{H}$  NMR spectra of **6**

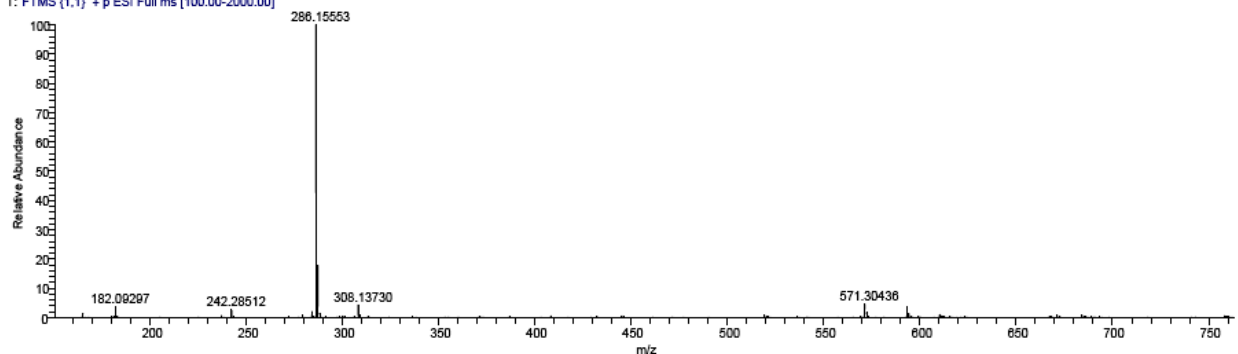


$^{13}\text{C}$  NMR spectra of **6**



## HRMS spectra of 6

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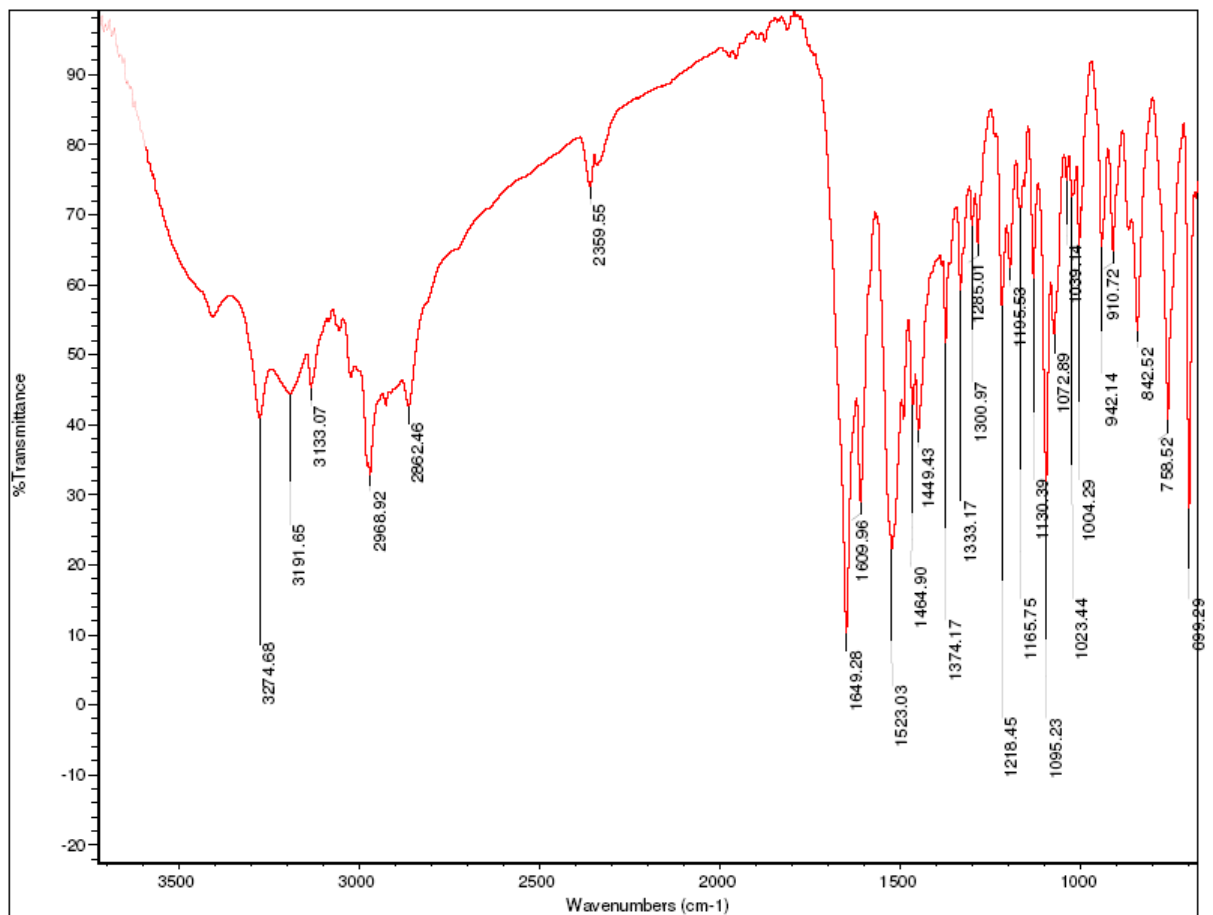


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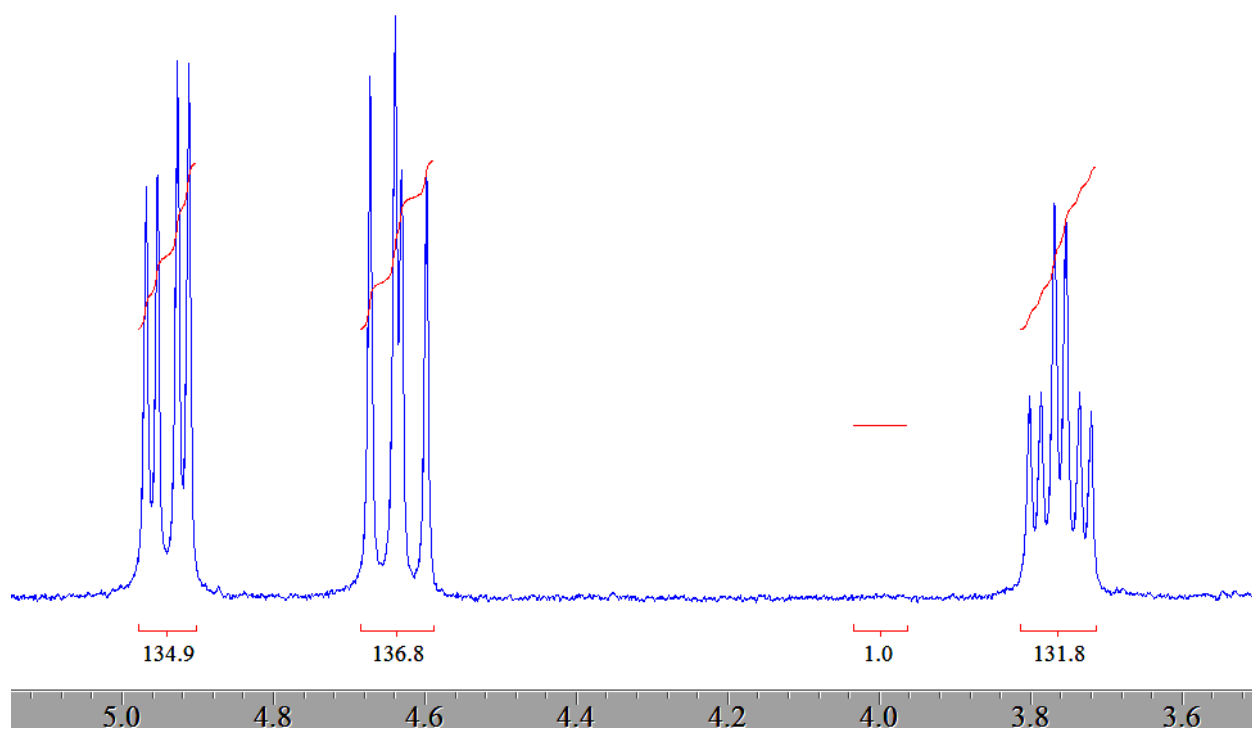
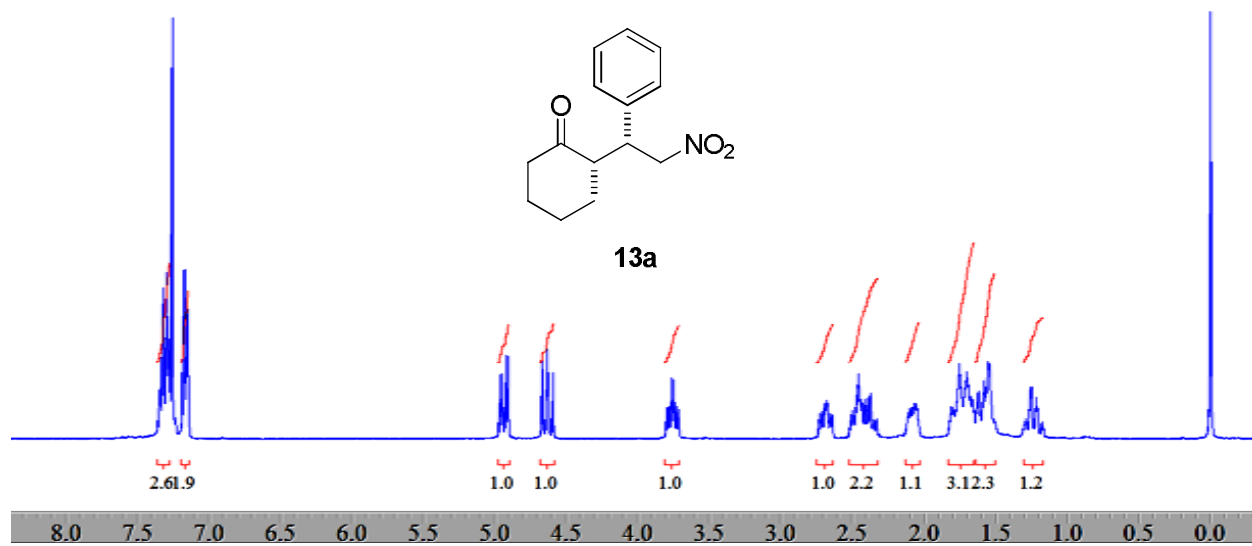
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
286.15551	123481584.0	100.00	286.15500	1.77	8.5	C <sub>16</sub> H <sub>20</sub> O <sub>2</sub> N <sub>3</sub>
287.15843	22120124.0	17.91				

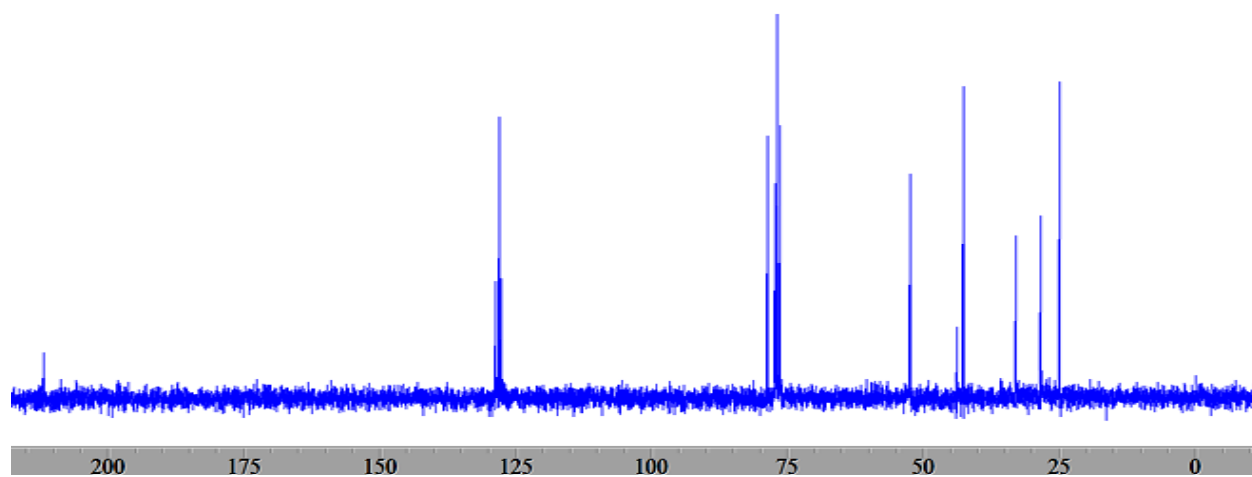
## IR spectra of 6



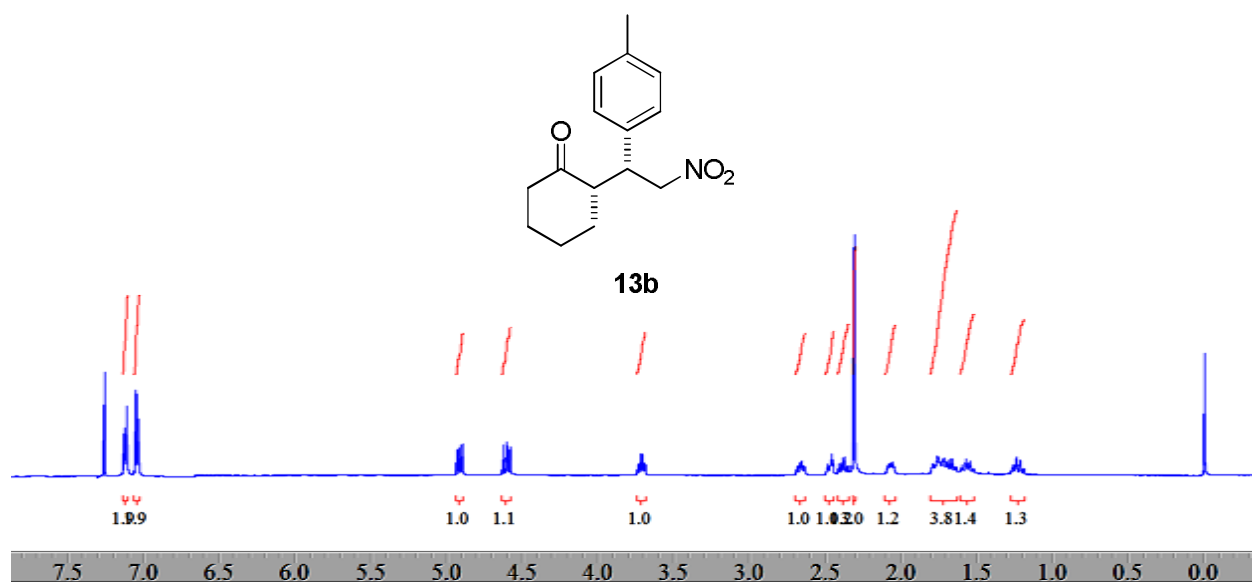
<sup>1</sup>H NMR spectra of **13a**

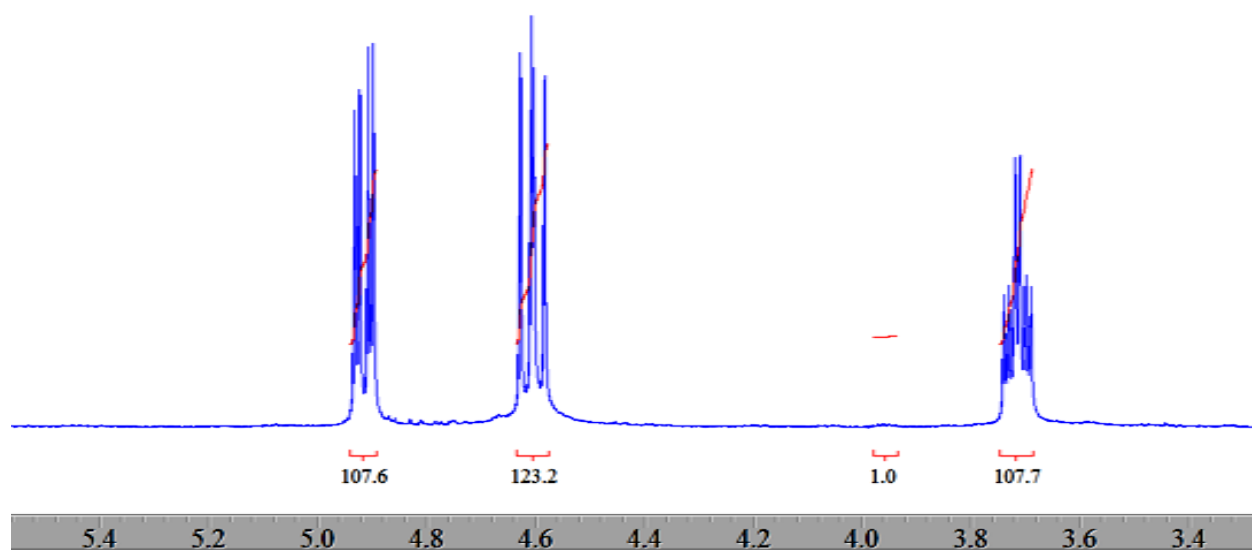


$^{13}\text{C}$  NMR spectra of **13a**

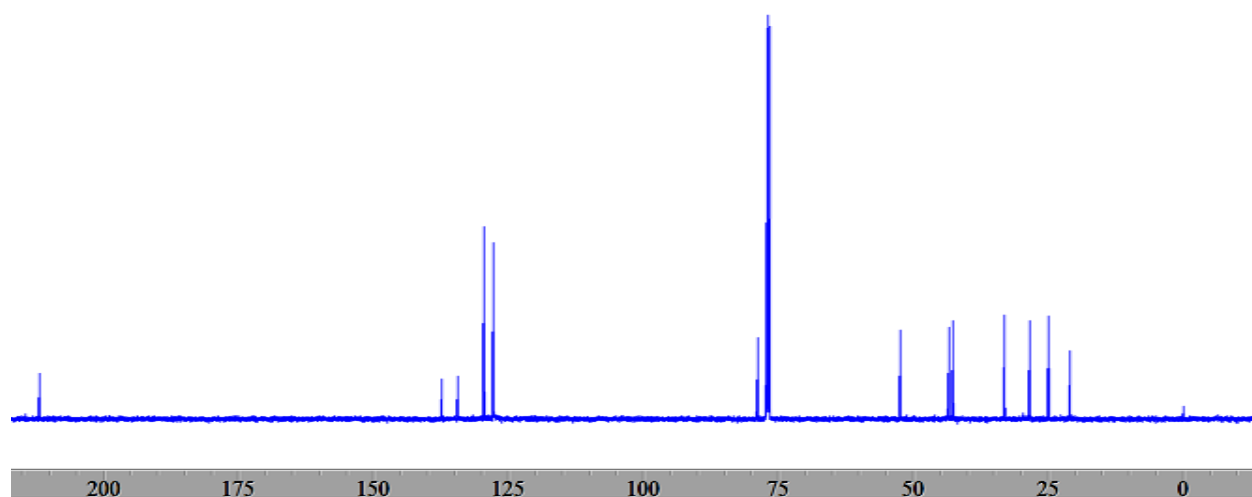


$^1\text{H}$  NMR spectra of **13b**

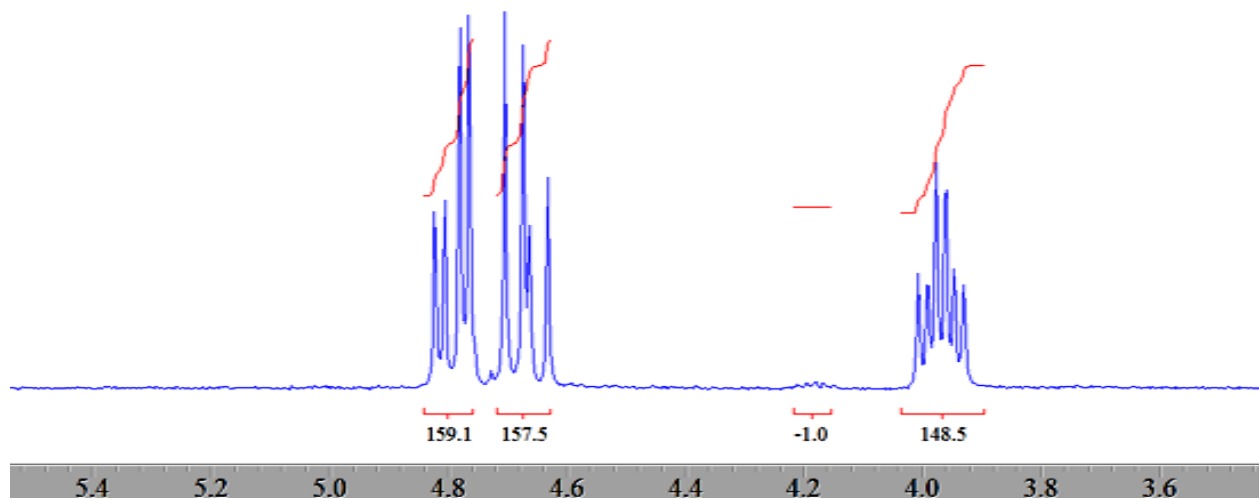
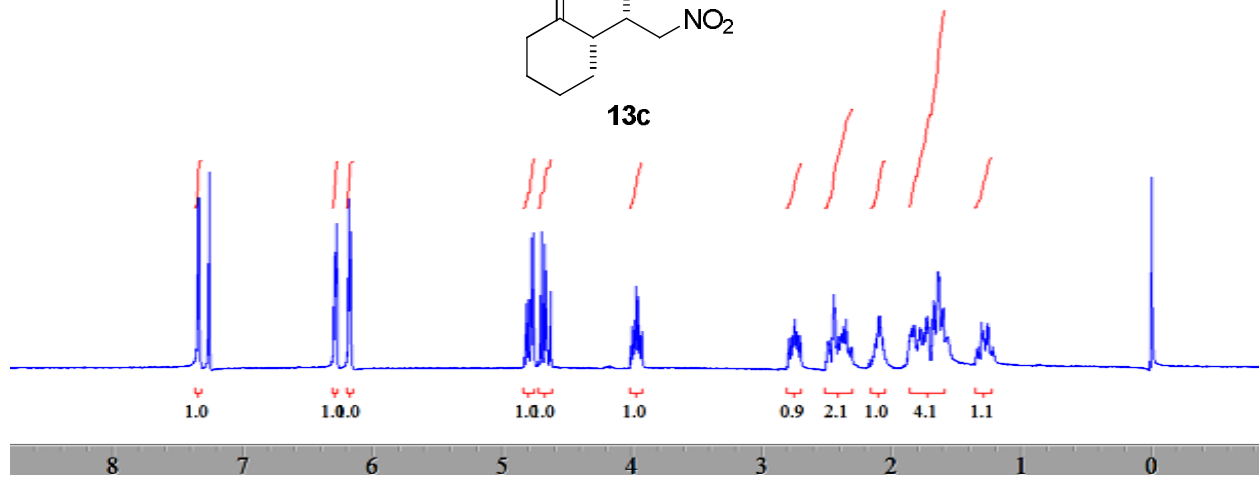
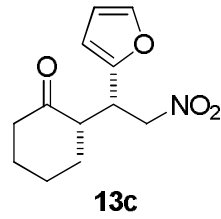




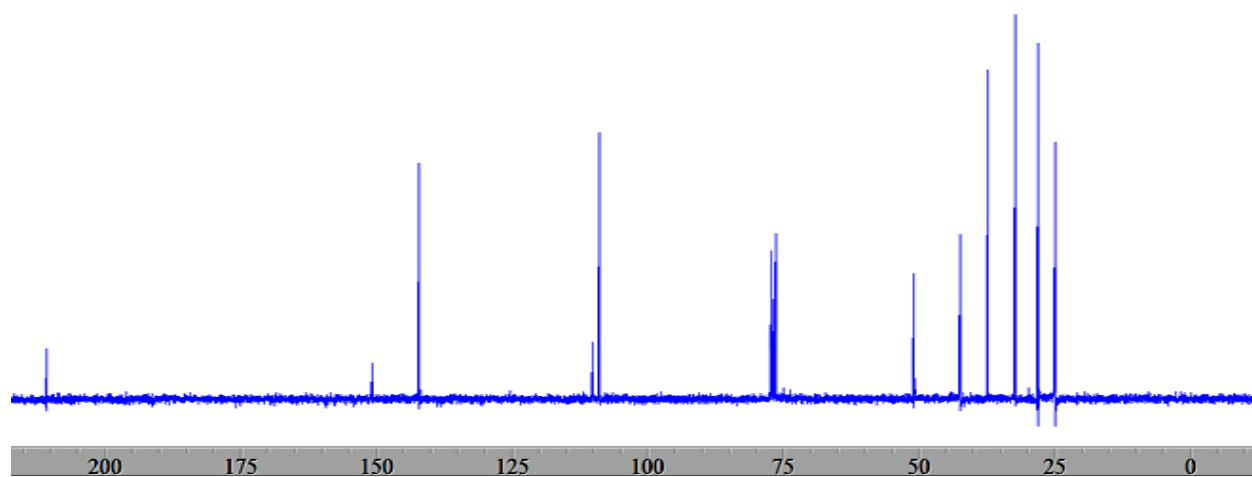
$^{13}\text{C}$  NMR spectra of **13b**



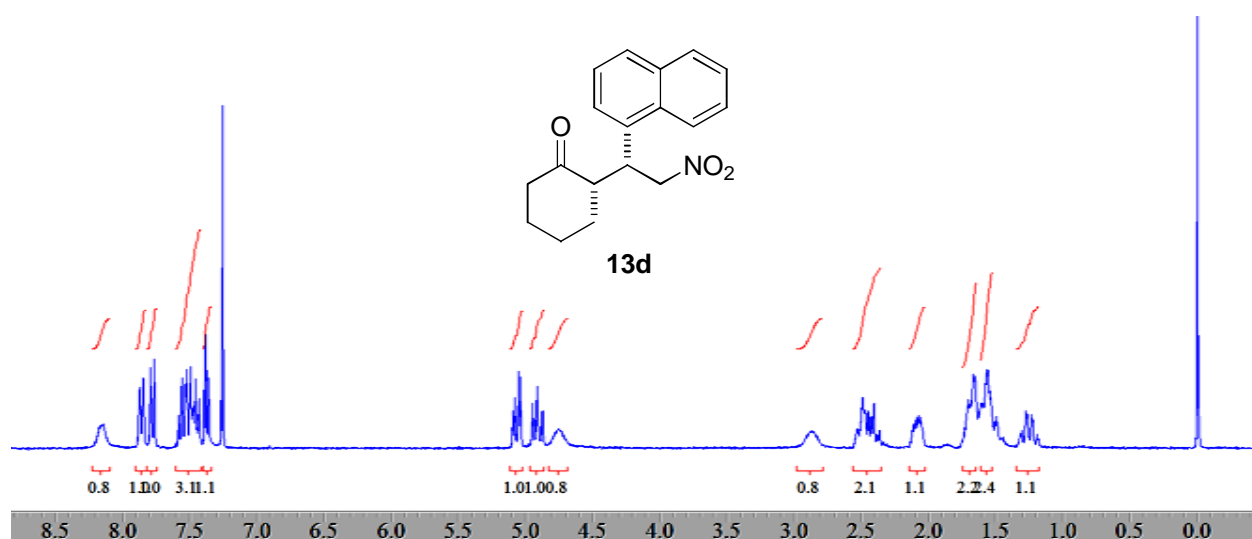
<sup>1</sup>H NMR spectra of **13c**



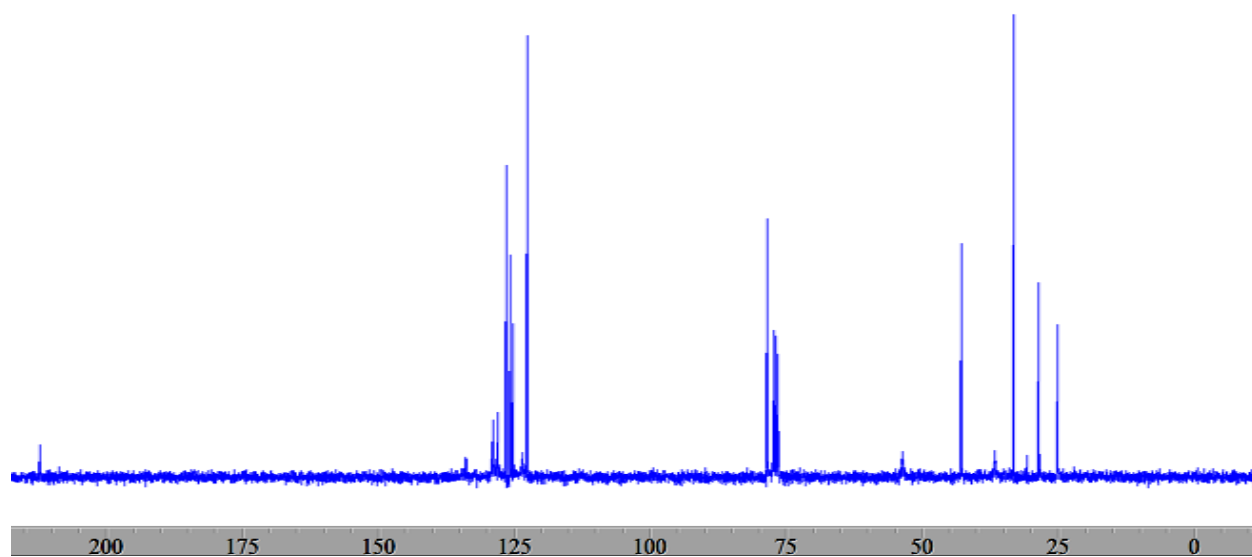
$^{13}\text{C}$  NMR spectra of **13c**



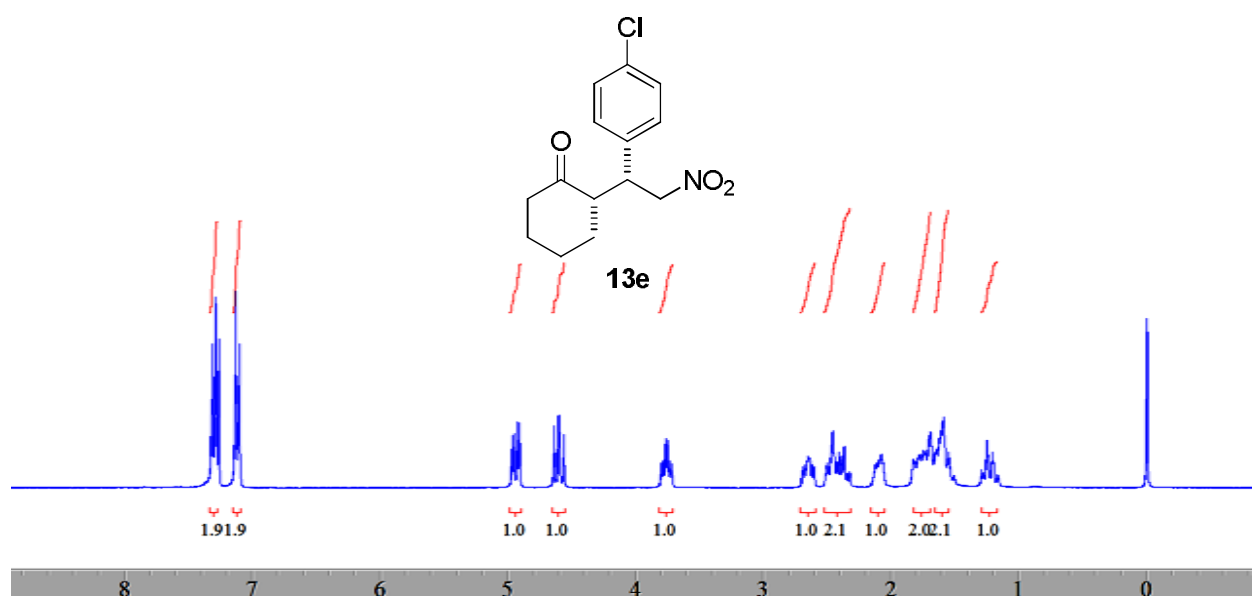
$^1\text{H}$  NMR spectra of **13d**



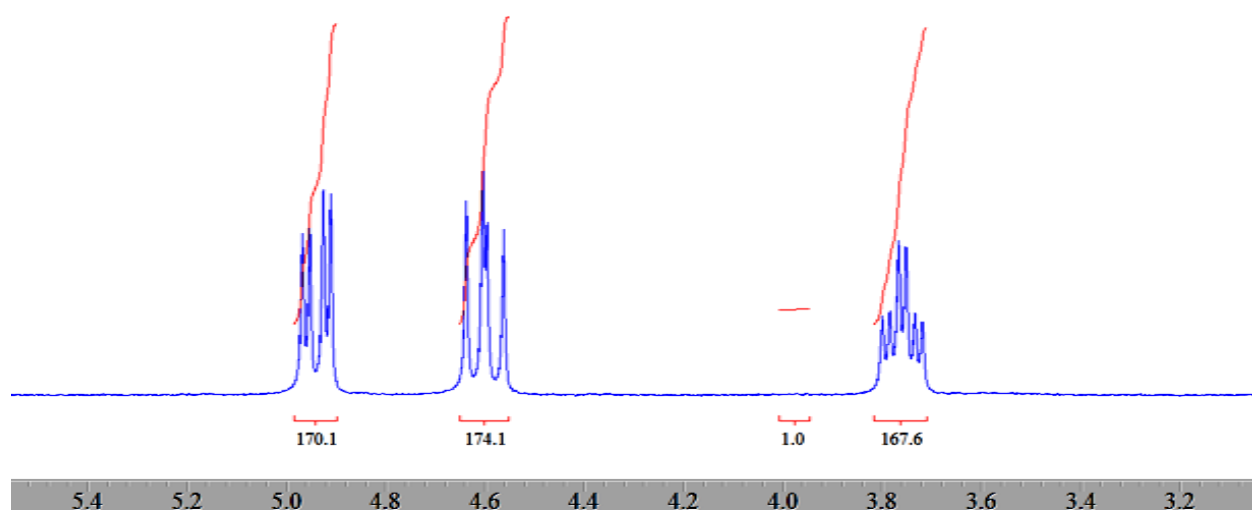
$^{13}\text{C}$  NMR spectra of **13d**



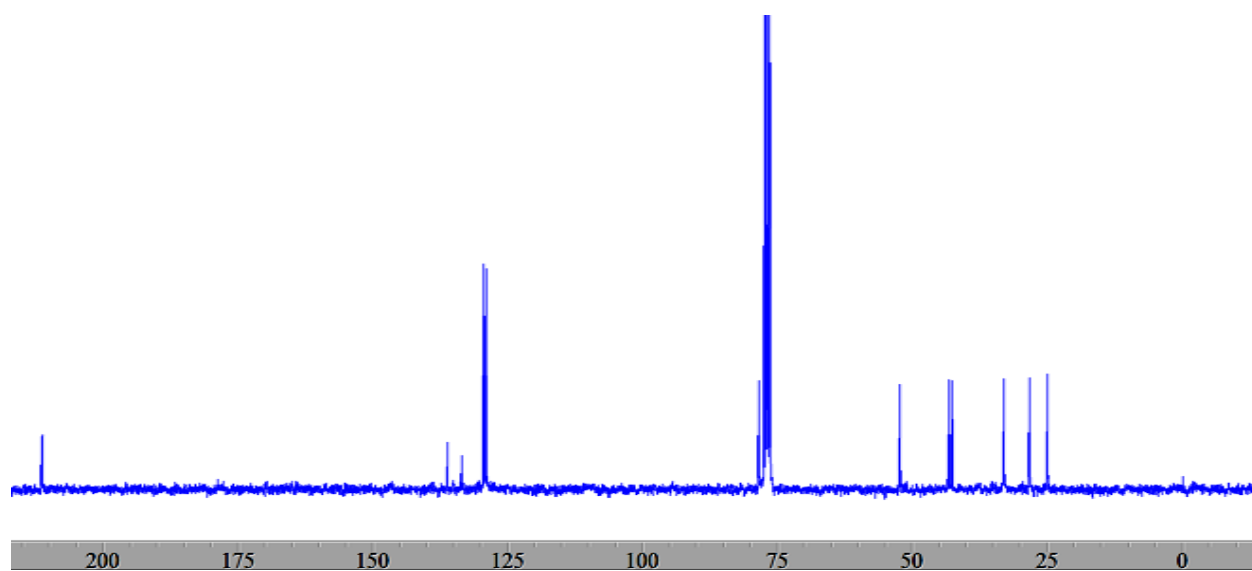
$^1\text{H}$  NMR spectra of **13e**



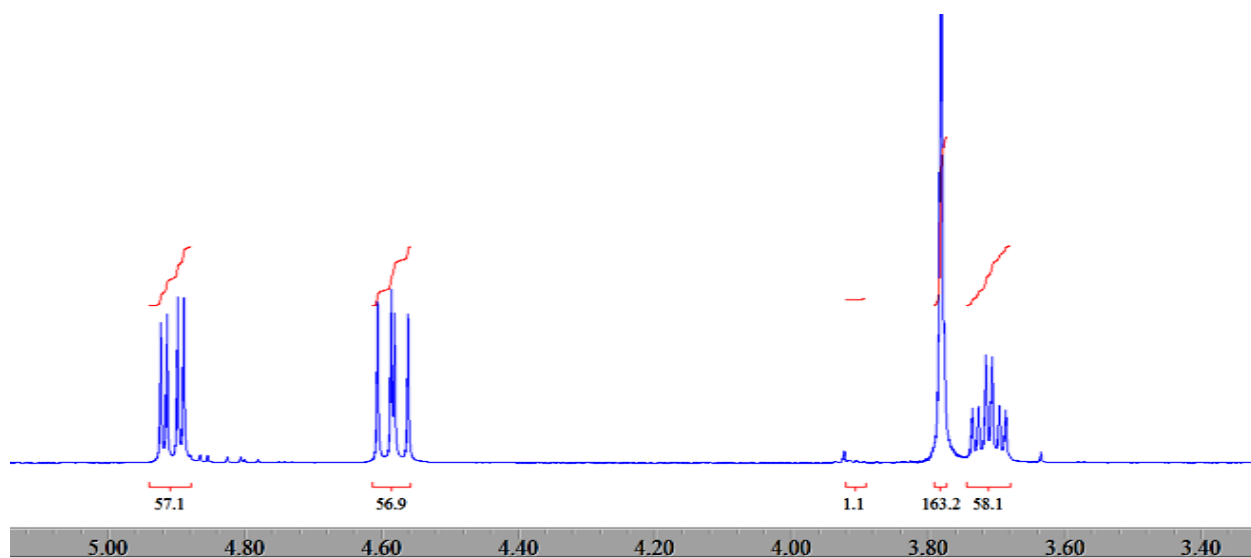
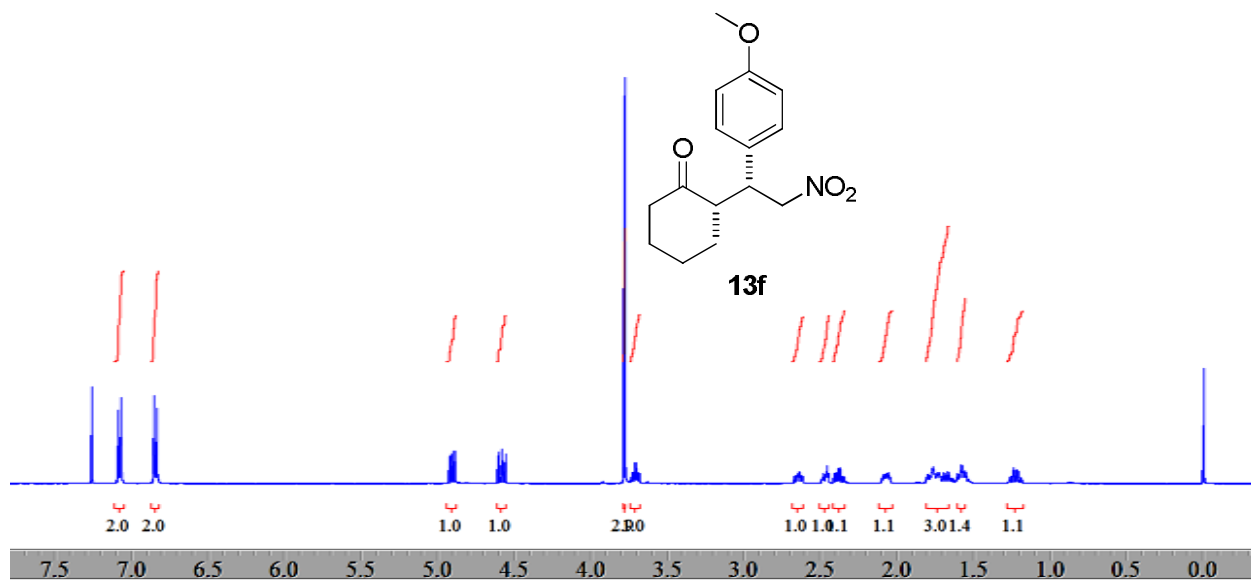




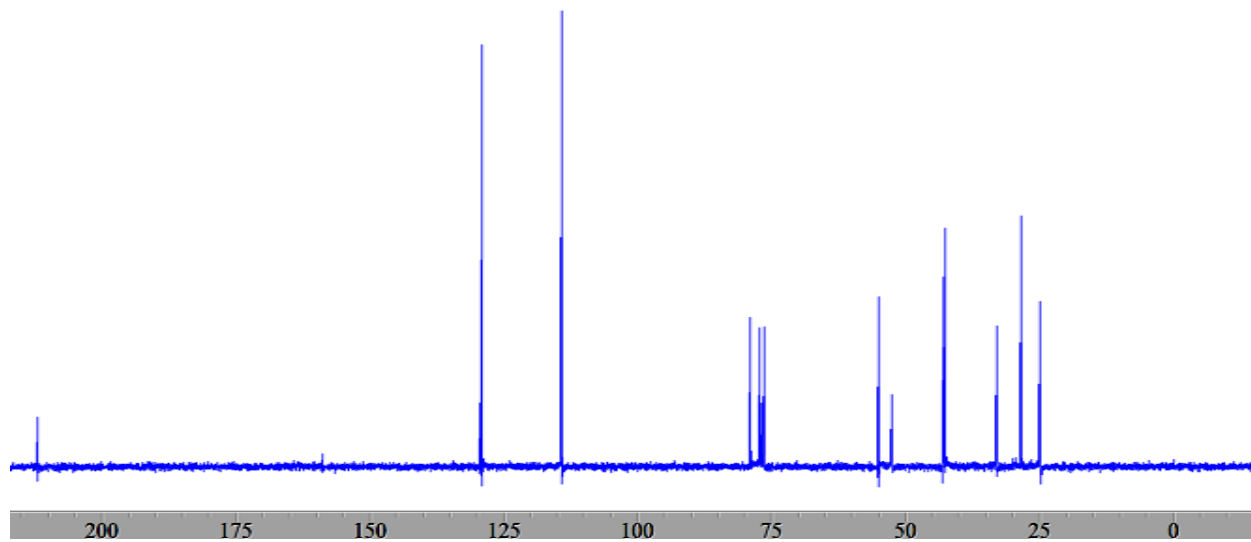
$^{13}\text{C}$  NMR spectra of **13e**



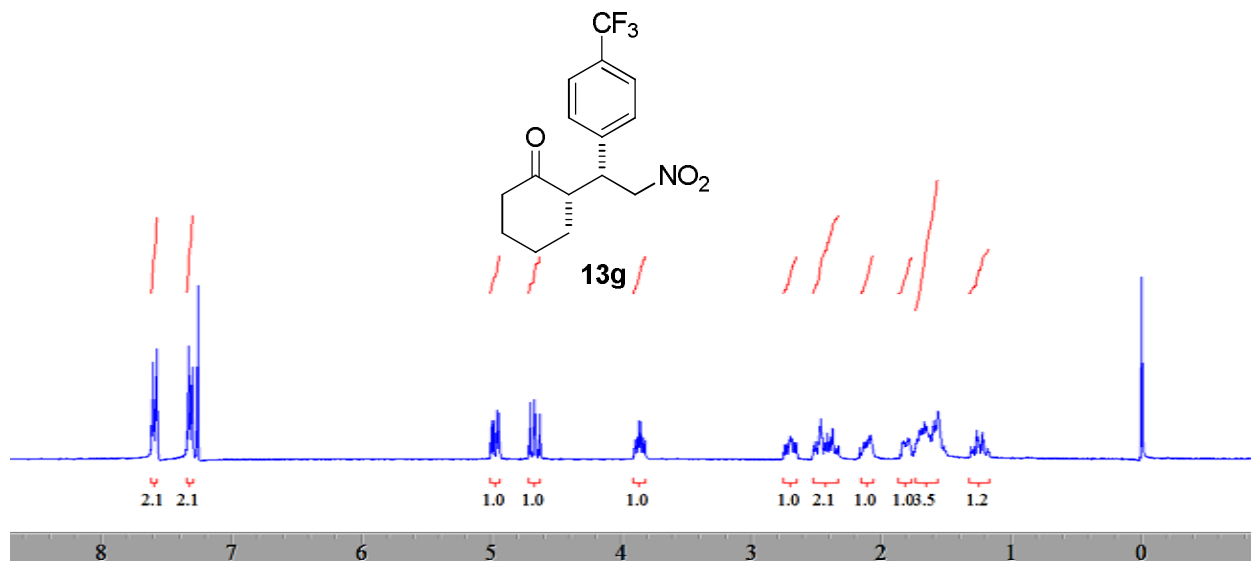
<sup>1</sup>H NMR spectra of **13f**

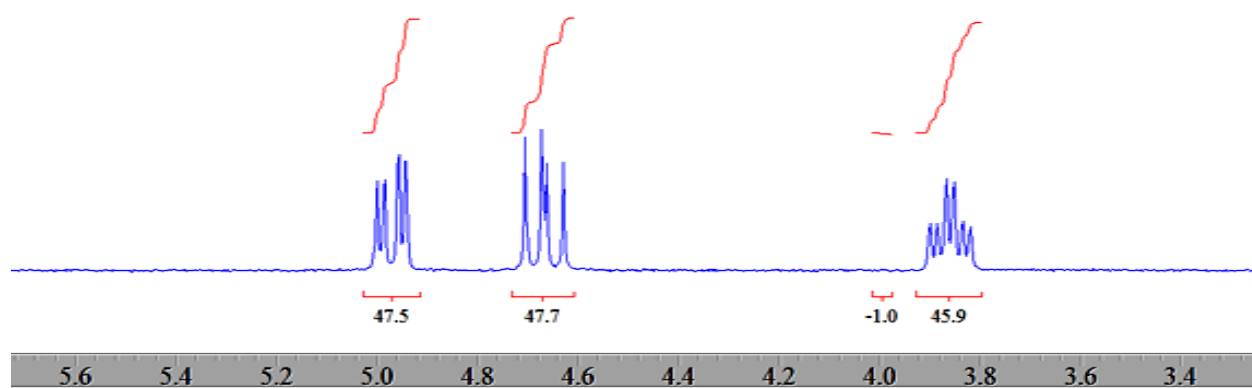


$^{13}\text{C}$  NMR spectra of **13f**

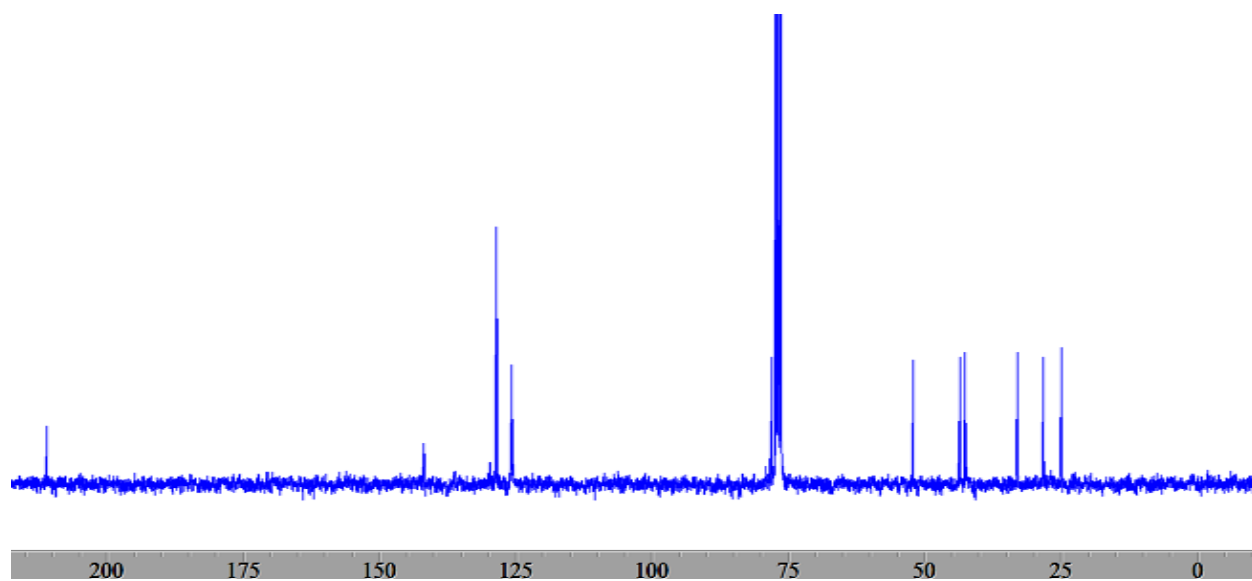


$^1\text{H}$  NMR spectra of **13g**

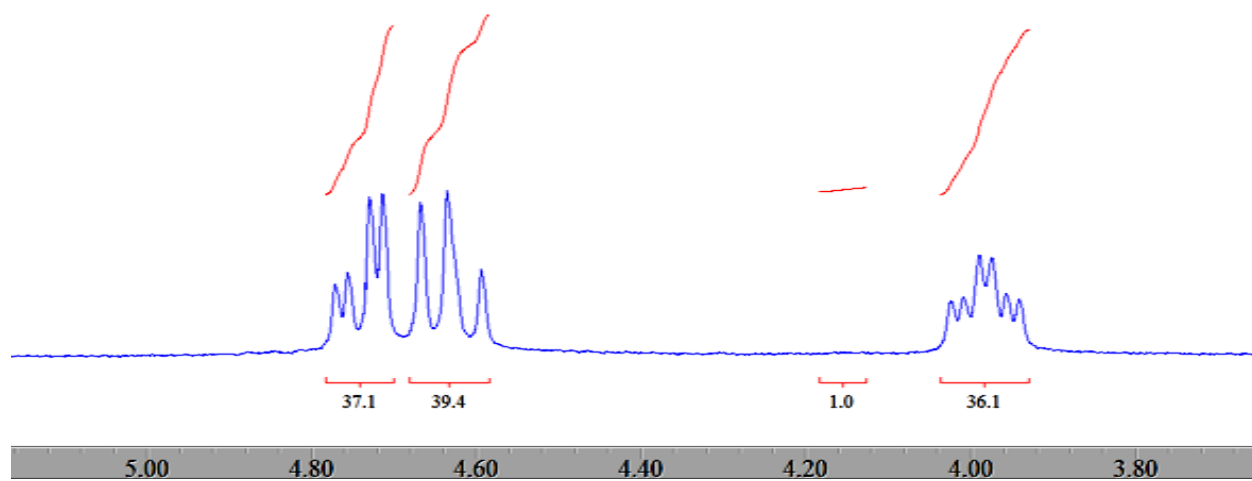
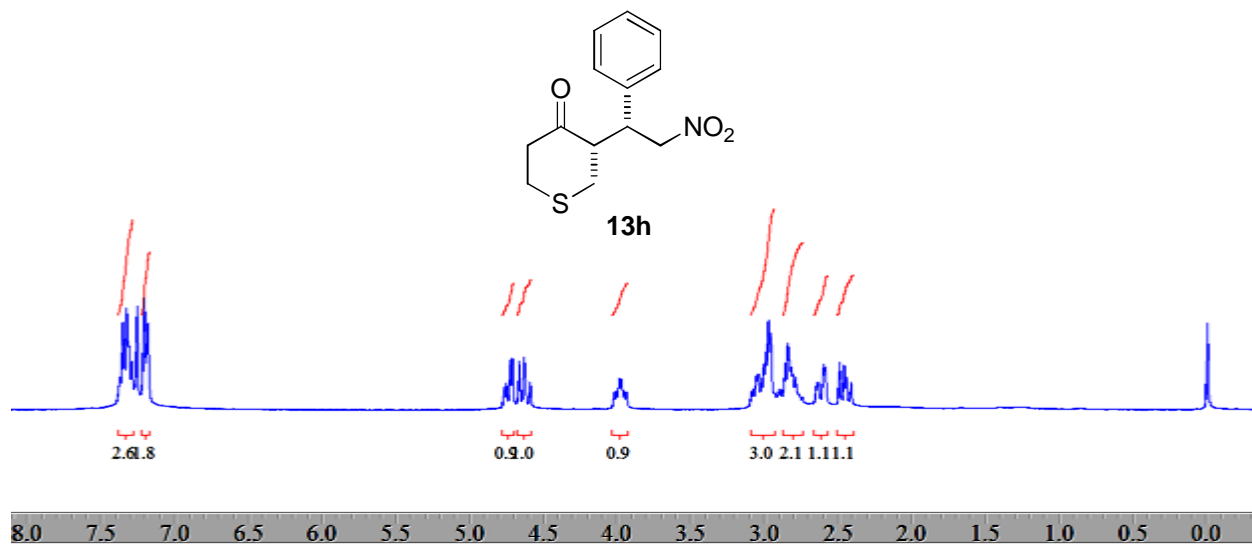




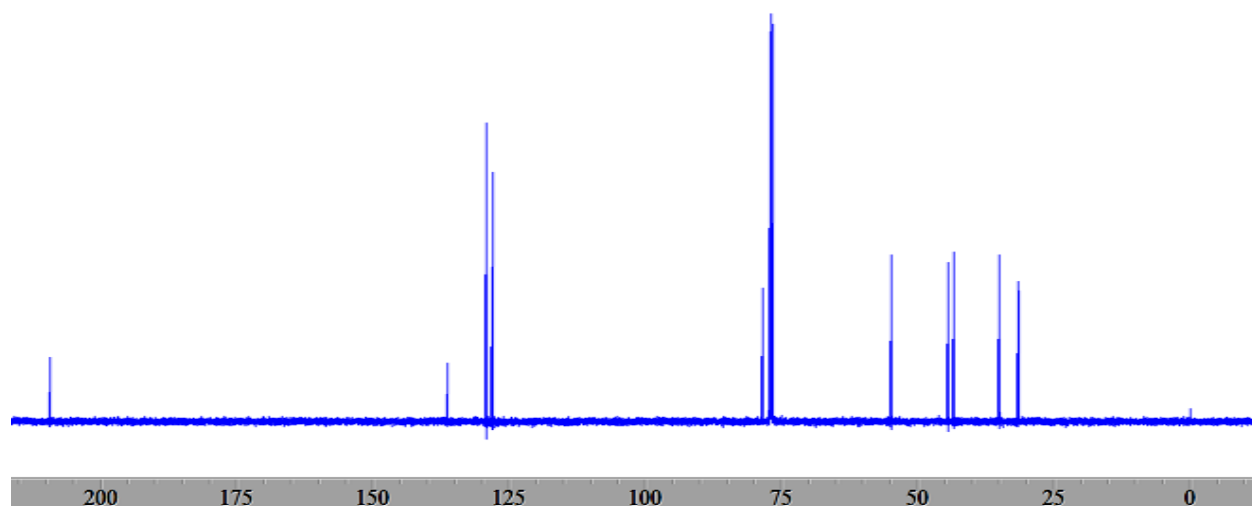
$^{13}\text{C}$  NMR spectra of **13g**



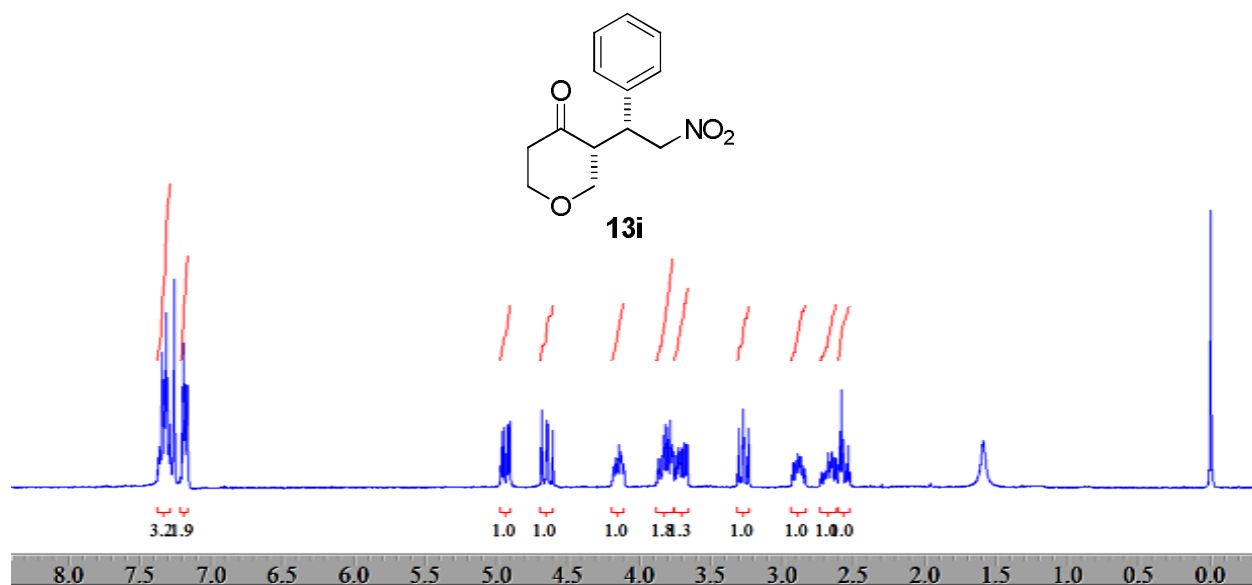
<sup>1</sup>H NMR spectra of **13h**

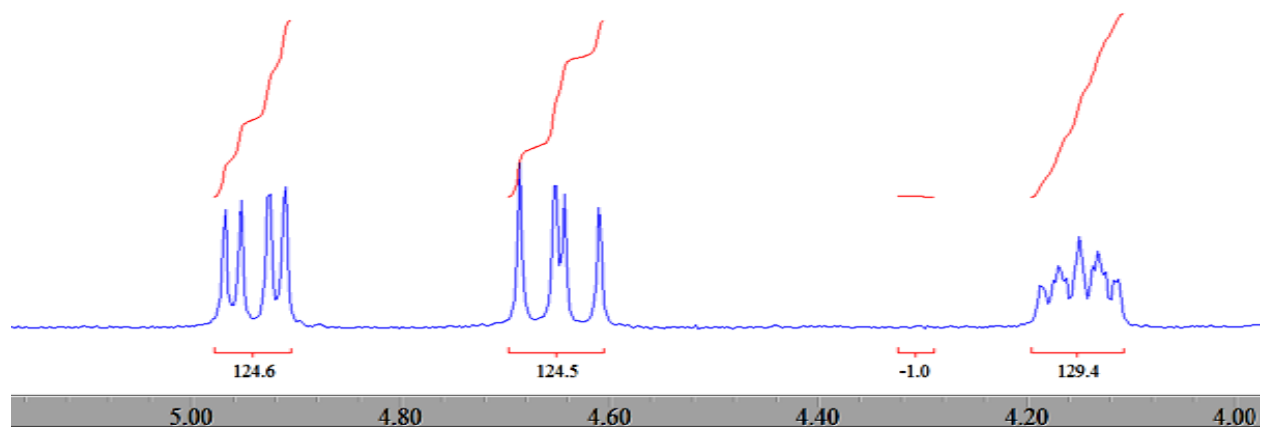


$^{13}\text{C}$  NMR spectra of **13h**

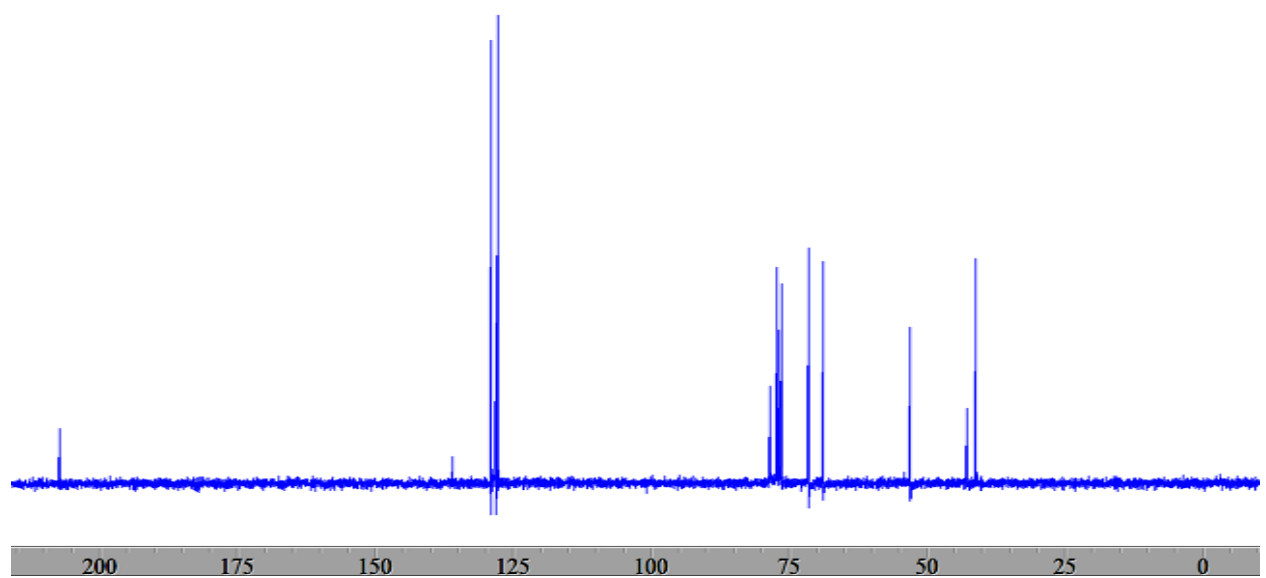


$^1\text{H}$  NMR spectra of **13i**

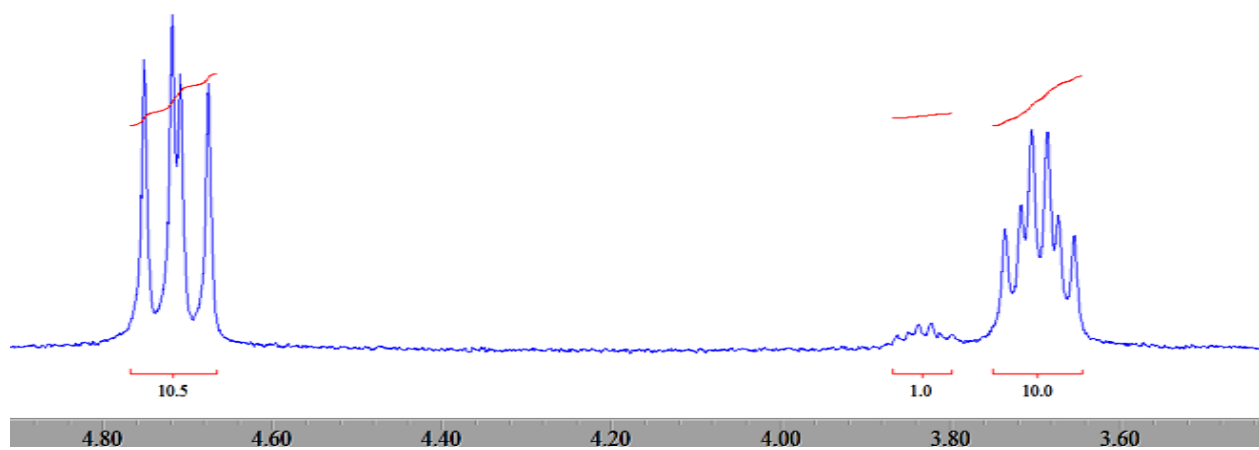
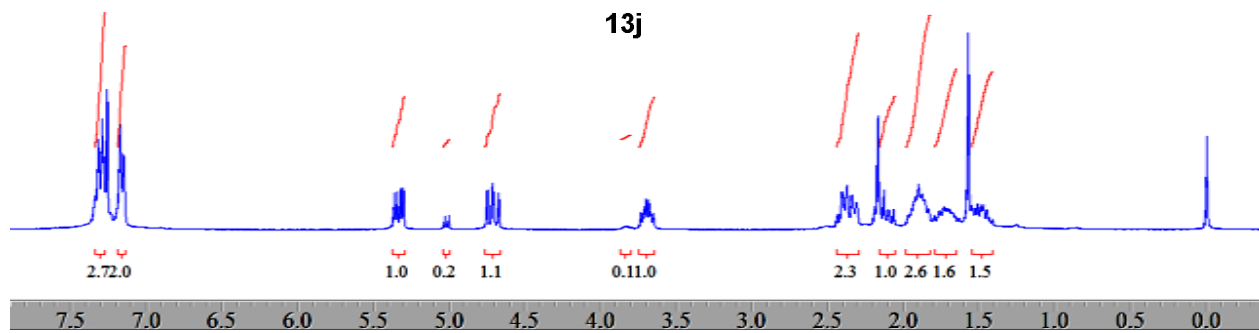
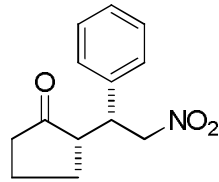




$^{13}\text{C}$  NMR spectra of **13i**

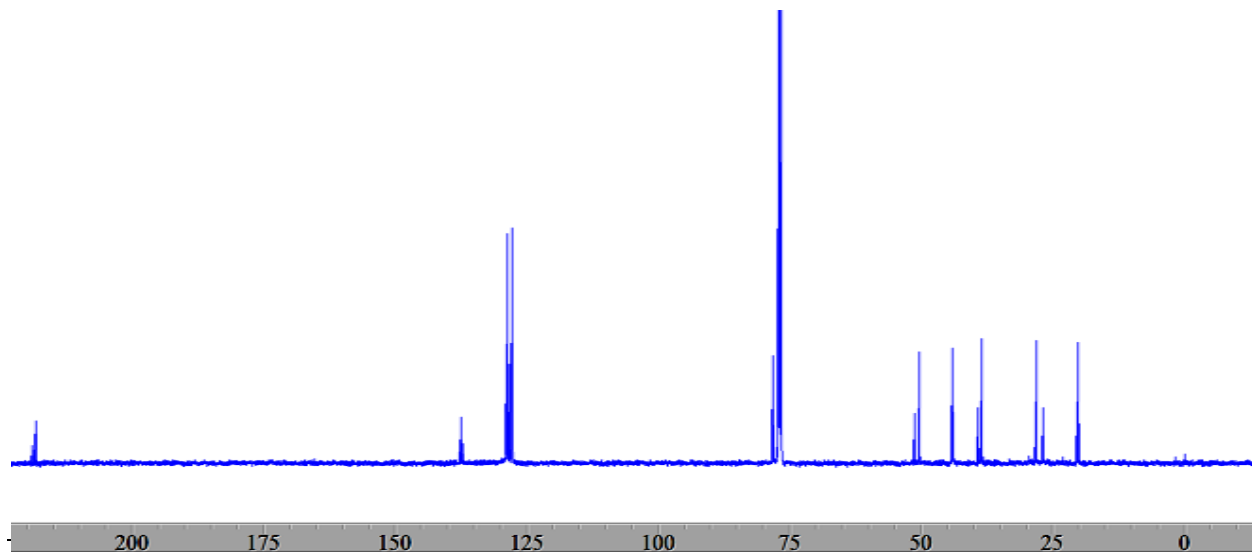


<sup>1</sup>H NMR spectra of **13j**

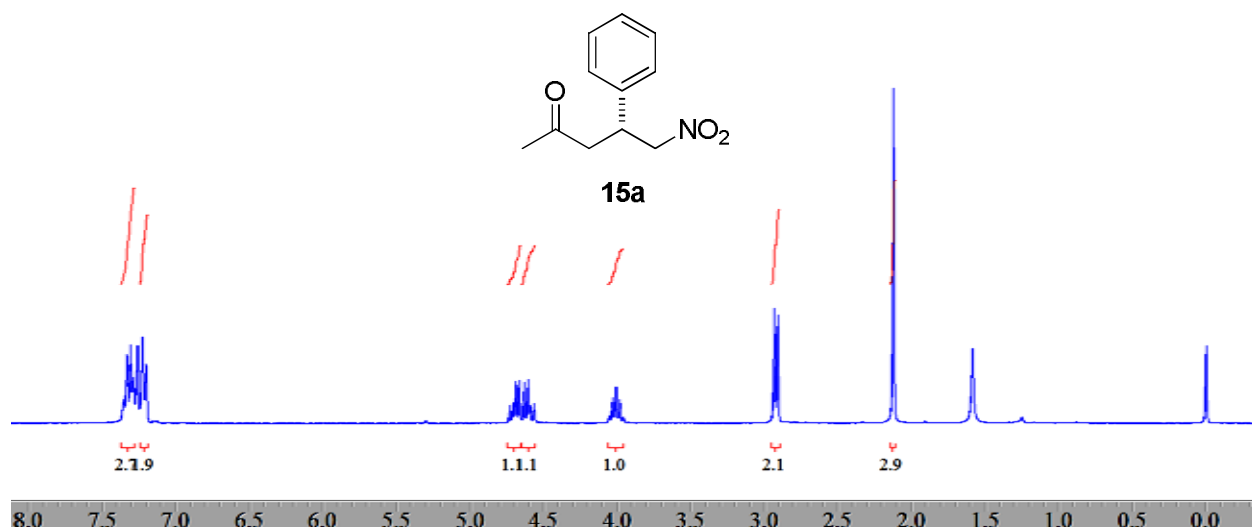




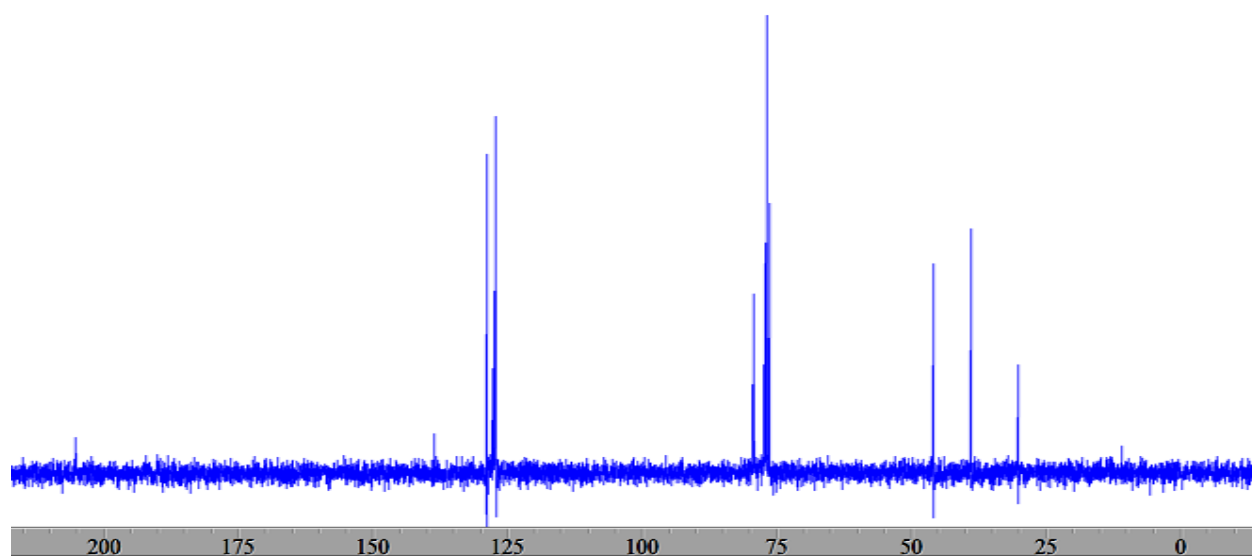
$^1\text{H}$  NMR spectra of **13j**



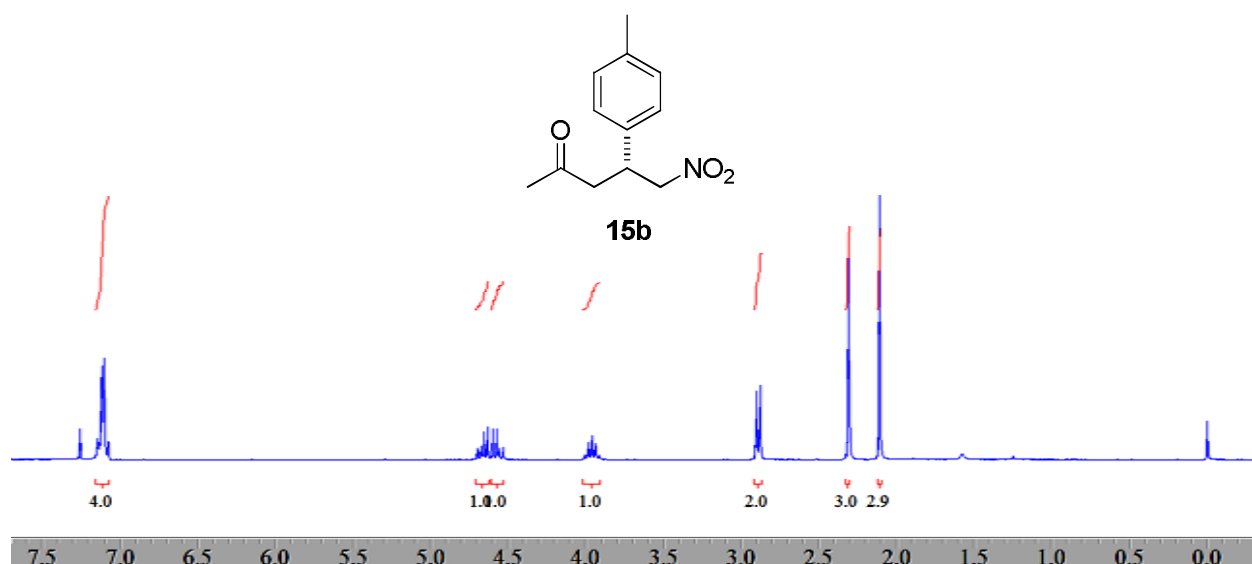
$^1\text{H}$  NMR spectra of **15a**



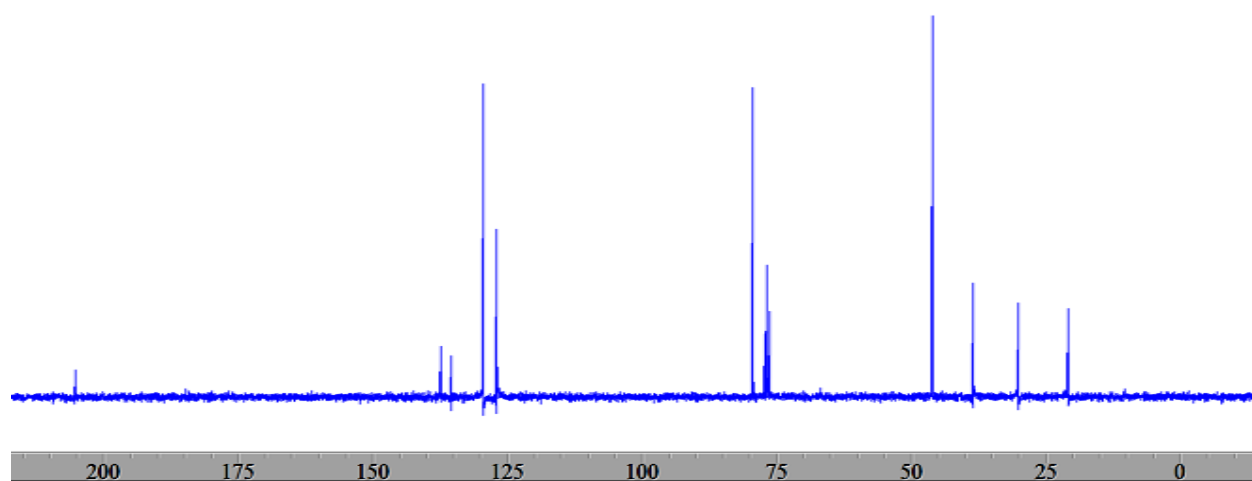
$^{13}\text{C}$  NMR spectra of **15a**



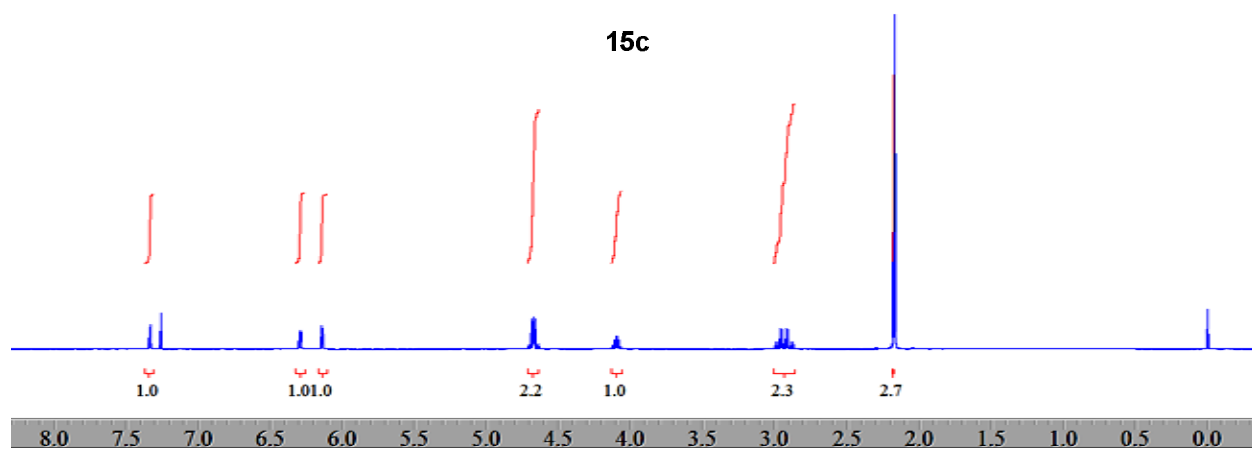
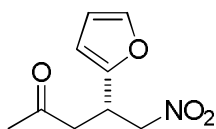
$^1\text{H}$  NMR spectra of **15b**



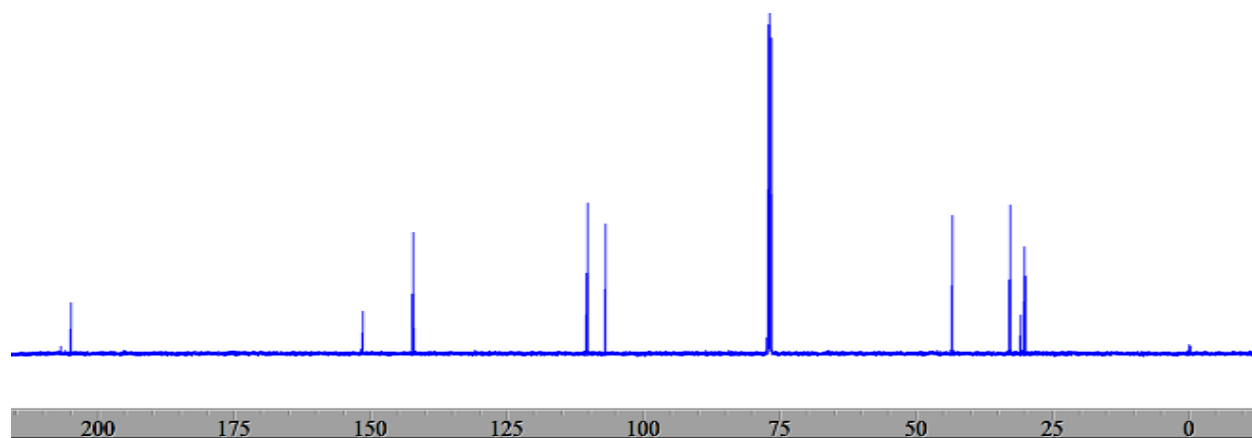
$^{13}\text{C}$  NMR spectra of **15b**



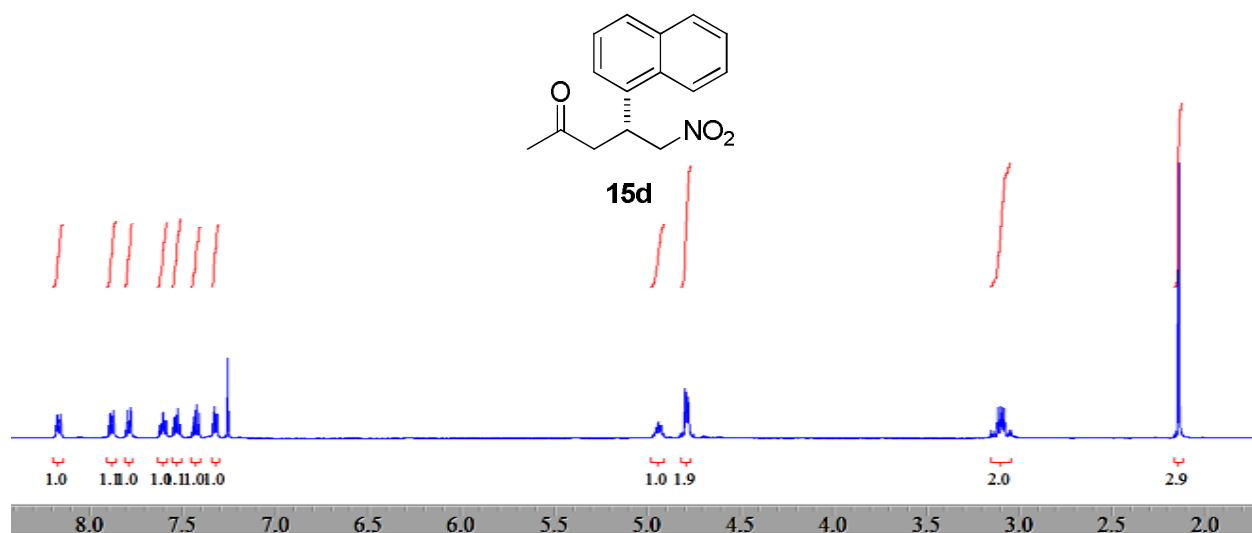
$^1\text{H}$  NMR spectra of **15c**



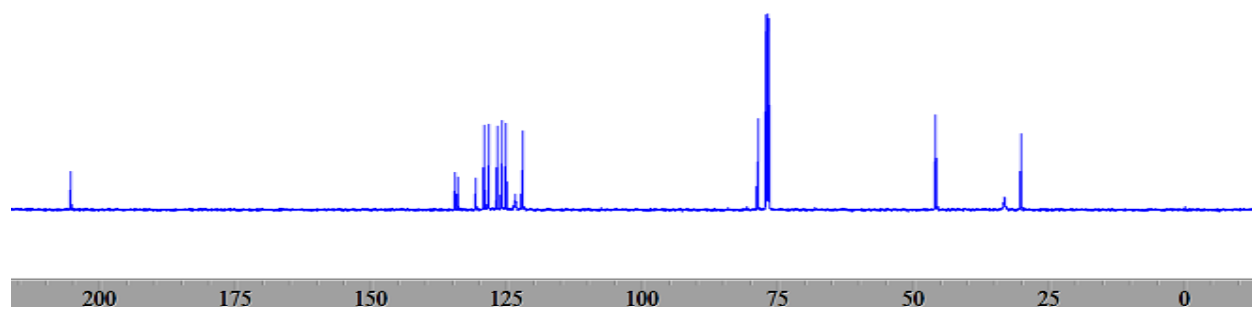
$^{13}\text{C}$  NMR spectra of **15c**



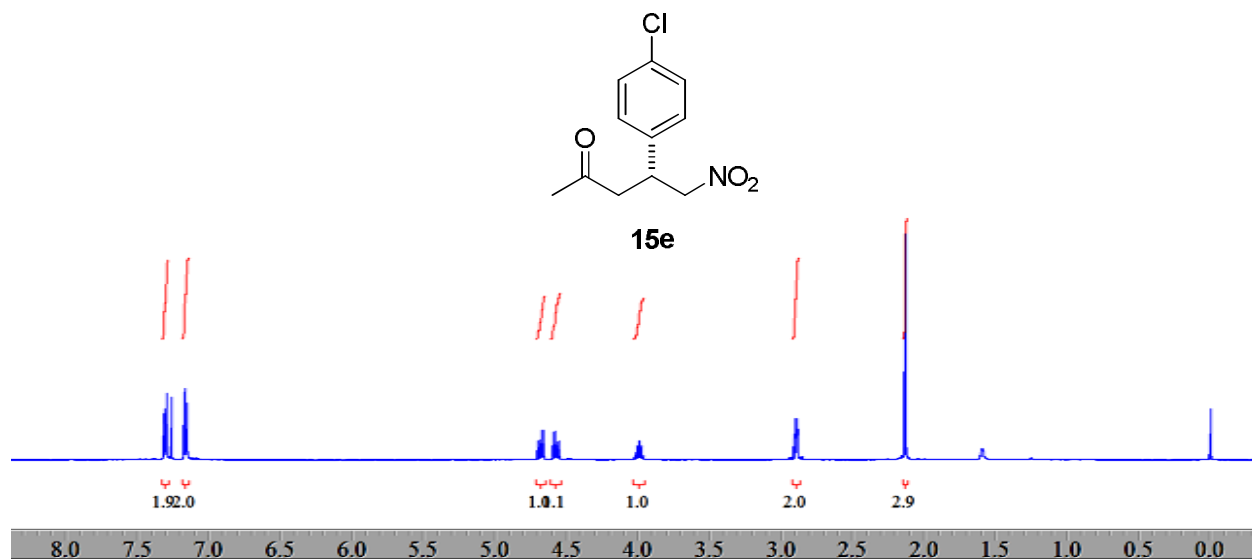
$^1\text{H}$  NMR spectra of **15d**



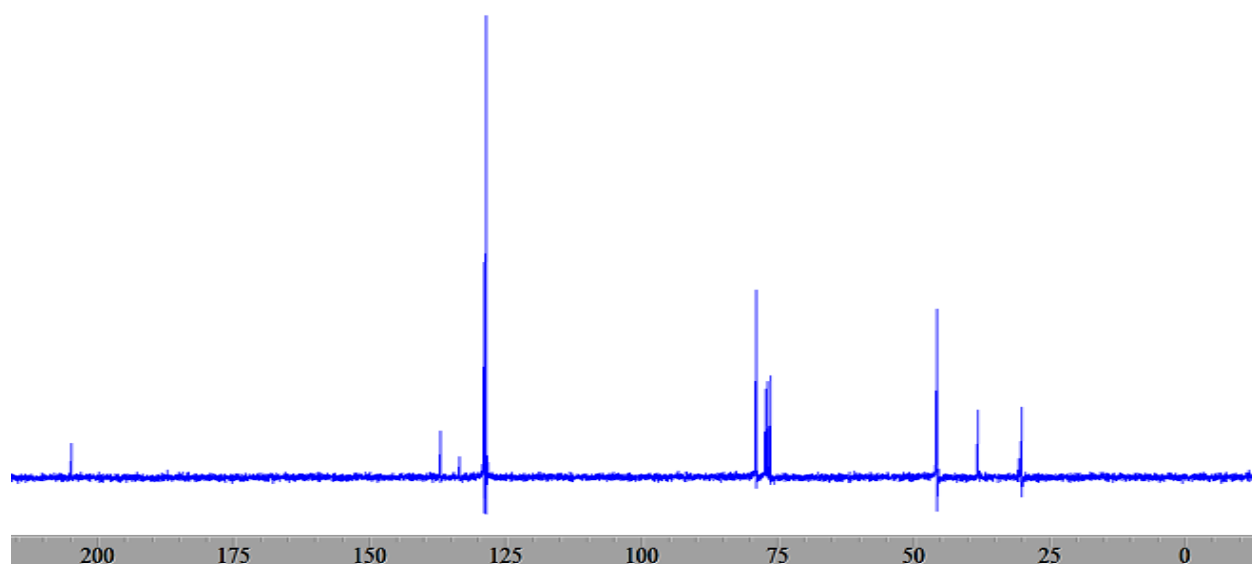
$^{13}\text{C}$  NMR spectra of **15d**



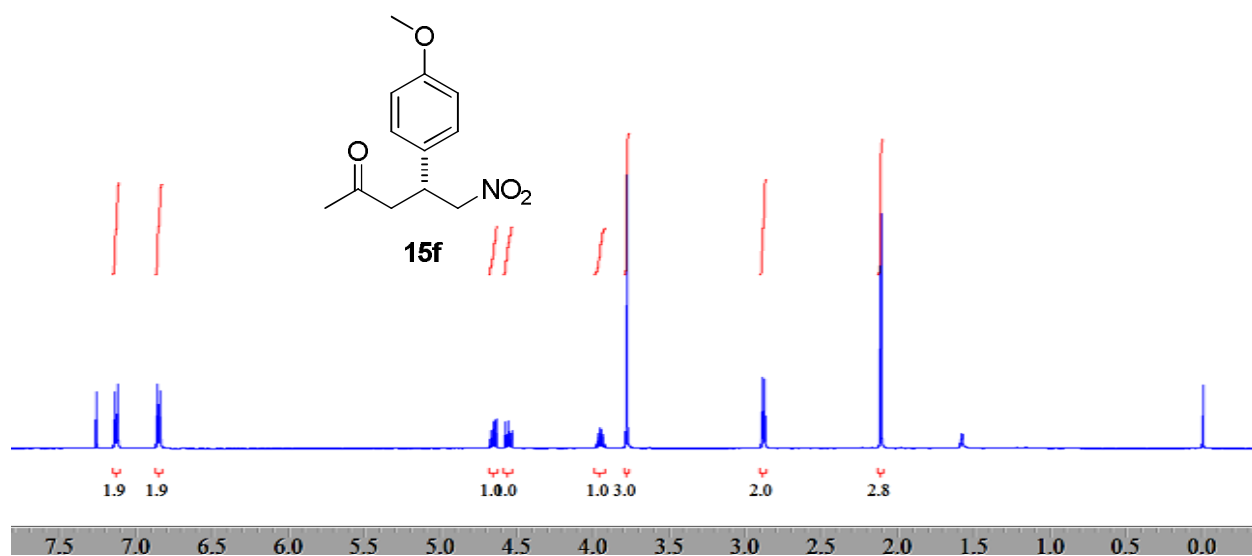
$^1\text{H}$  NMR spectra of **15e**



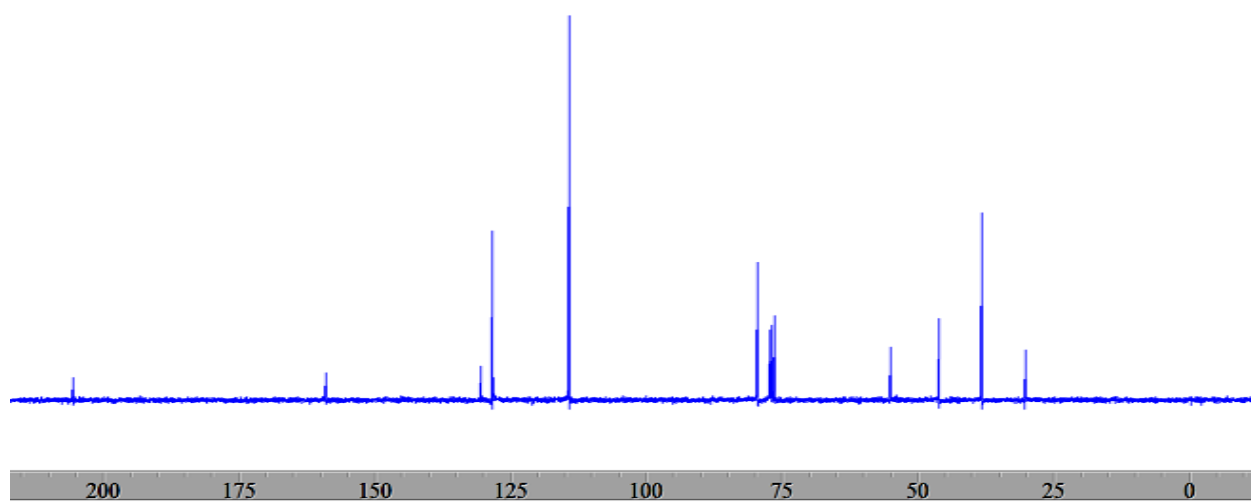
$^{13}\text{C}$  NMR spectra of **15e**



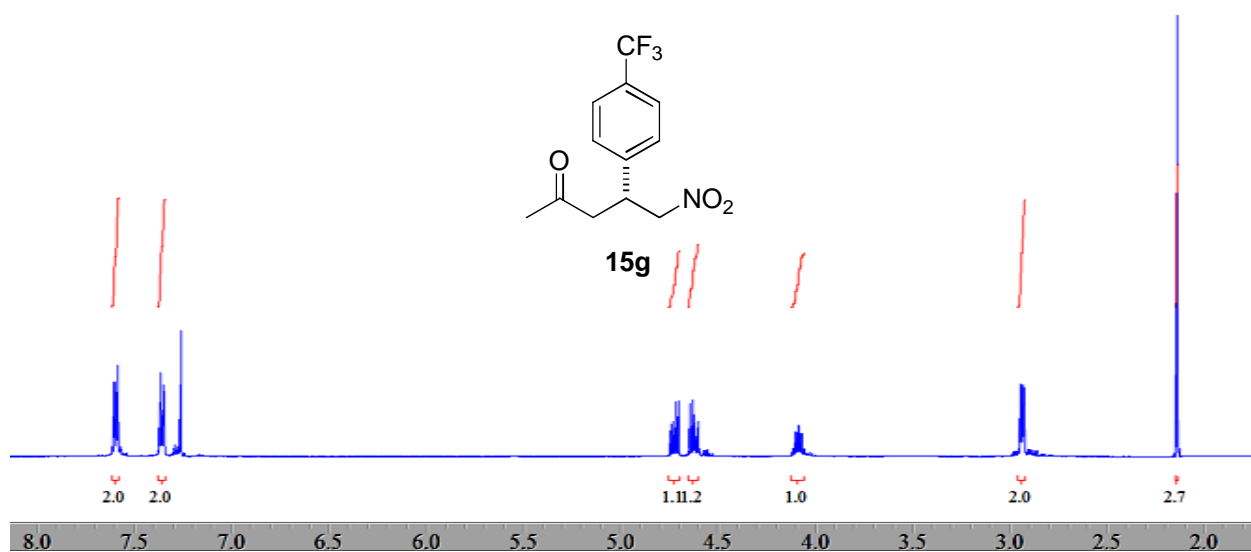
$^1\text{H}$  NMR spectra of **15f**



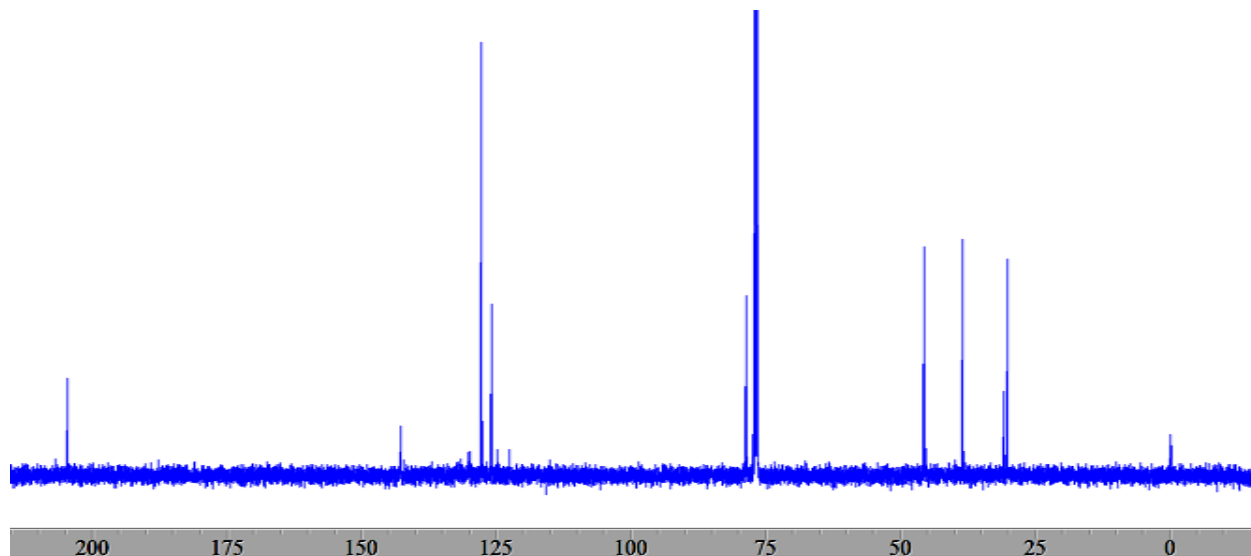
$^{13}\text{C}$  NMR spectra of **15f**



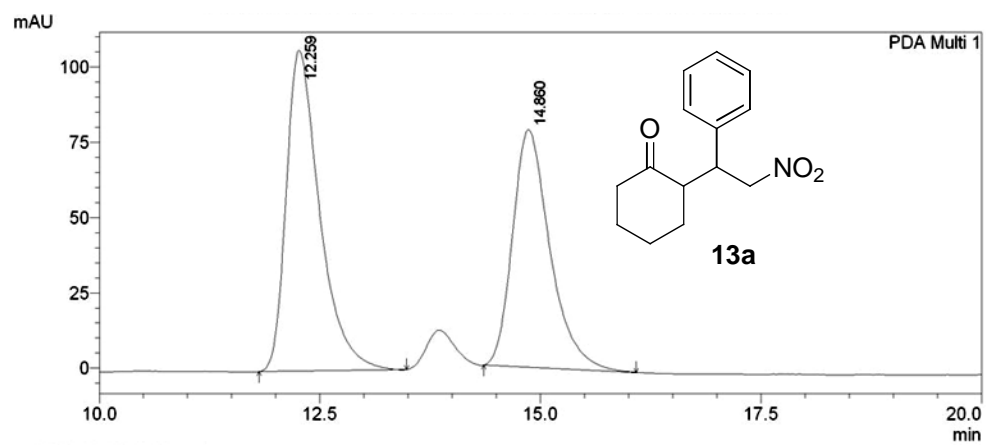
$^1\text{H}$  NMR spectra of **15g**



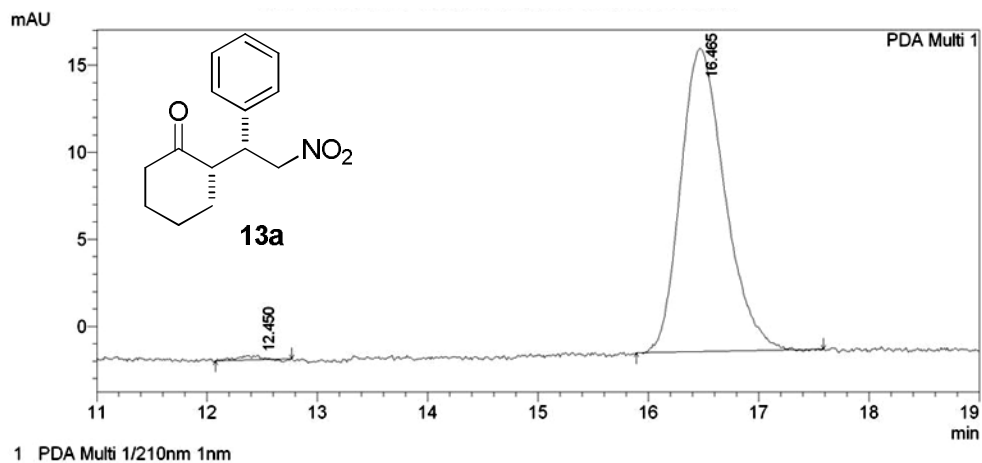
$^{13}\text{C}$  NMR spectra of **15g**



HPLC chromatogram of **13a**



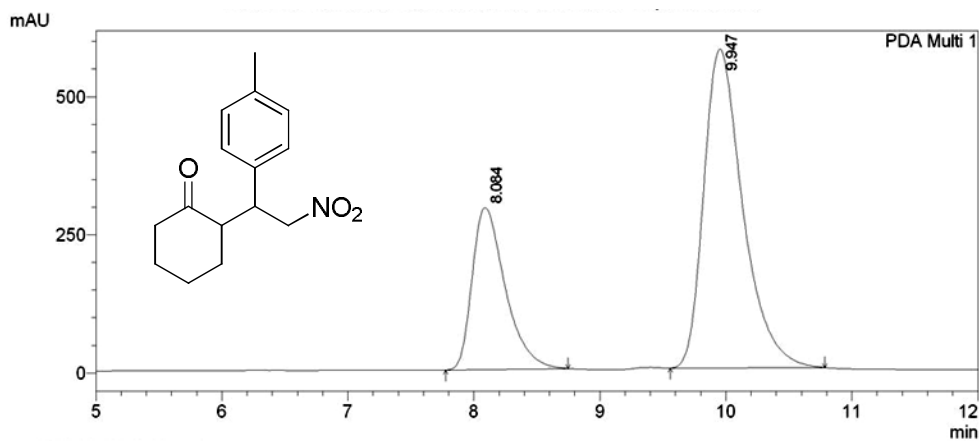


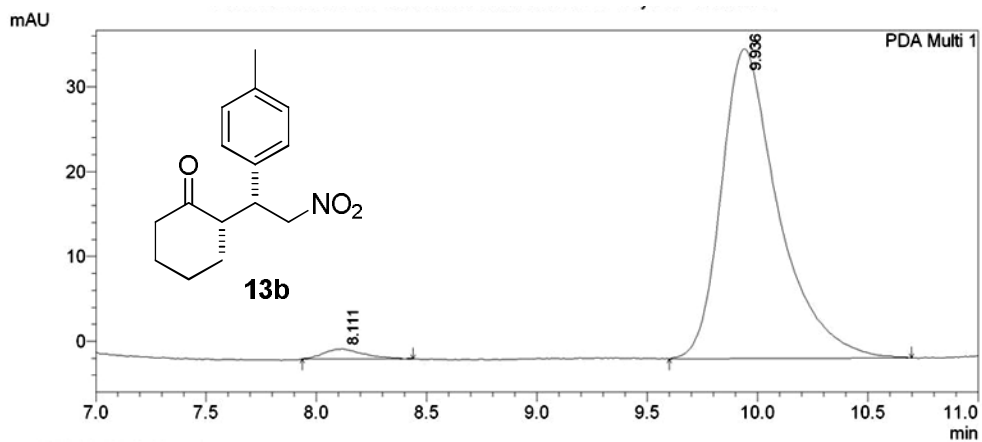


PeakTable

Peak#	Name	Ret. Time	Area	Height	Area %
1	RT:12.450	12.450	3166	255	0.649
2	RT:16.465	16.465	484798	17430	99.351
Total			487964	17685	100.000

### HPLC chromatogram of 13b





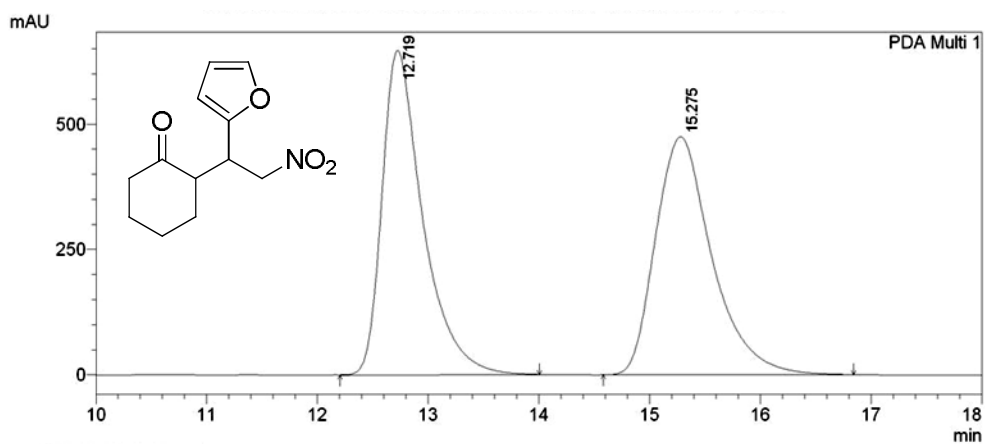
<Results>

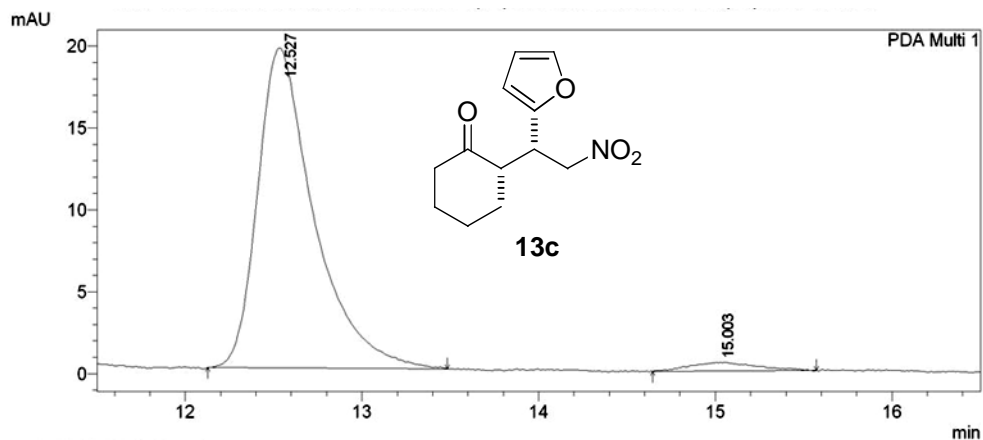
PDA

PeakTable

Peak#	Name	Ret. Time	Area	Height	Area %
1		8.111	14883	1179	2.213
2		9.936	657654	36536	97.787
Total			672537	37715	100.000

### HPLC chromatogram of 13c





<Results>

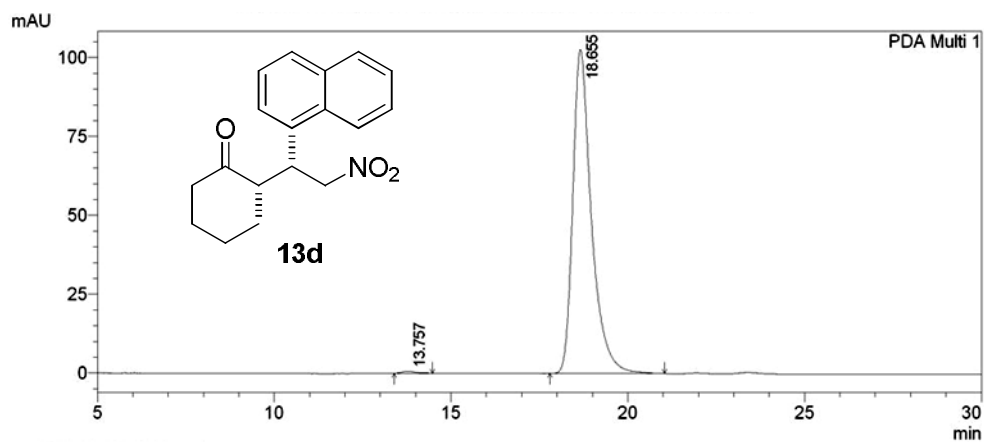
PDA

PeakTable

PDA Ch1 210nm 4nm

Peak#	Name	Ret. Time	Area	Height	Area %
1		12.527	434299	19529	96.976
2		15.003	13542	523	3.024
Total			447841	20052	100.000

### HPLC chromatogram of 13d



<Results>

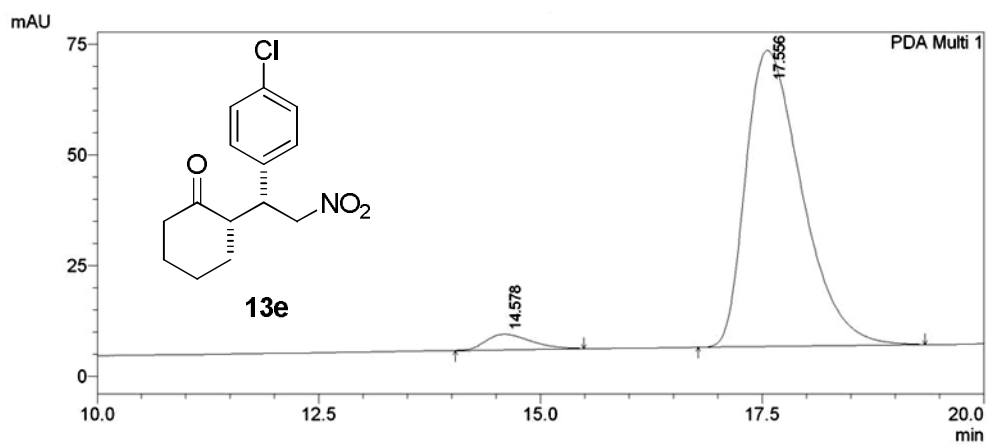
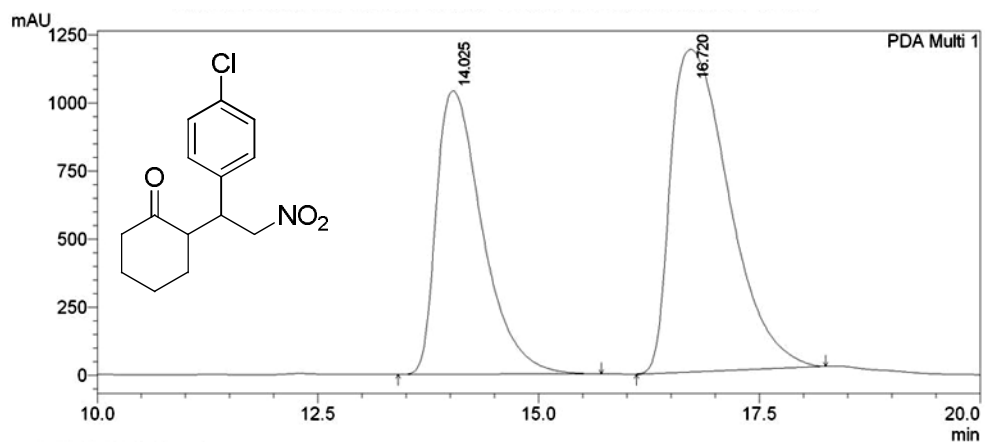
PDA

PeakTable

PDA Ch1 220nm 4nm

Peak#	Name	Ret. Time	Area	Height	Area %
1		13.757	15997	652	0.423
2		18.655	3767220	102698	99.577
Total			3783217	103350	100.000

### HPLC chromatogram of **13e**



**<Results>**

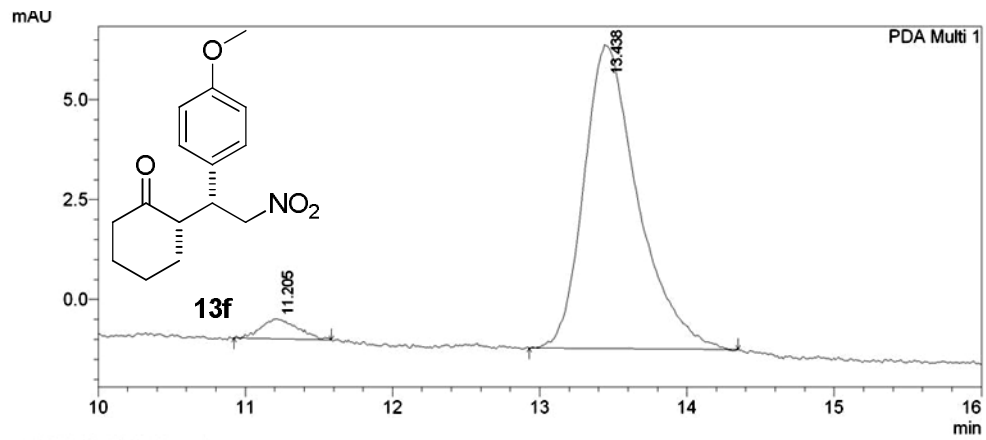
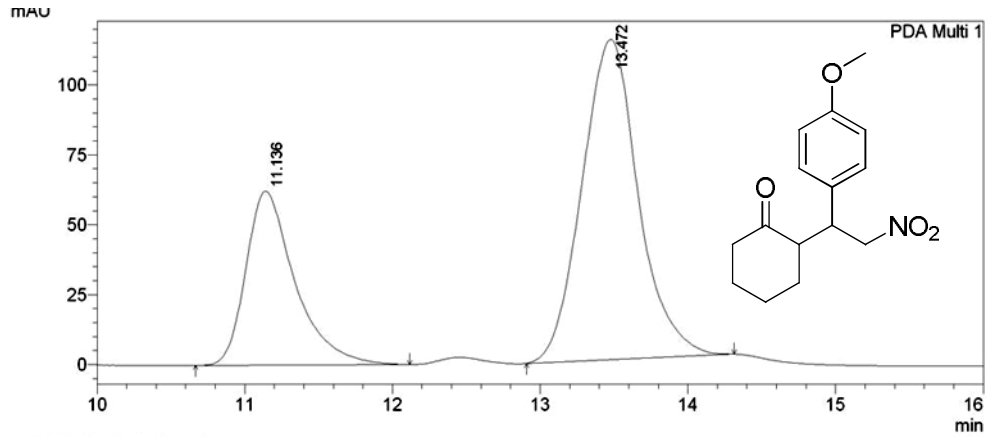
PDA

PeakTable

PDA Ch1 254nm 4nm

Peak#	Name	Ret. Time	Area	Height	Area %
1		14.578	121939	3488	3.967
2		17.556	2951532	66880	96.033
Total			3073471	70368	100.000

# HPLC chromatogram of 13f



1 PDA Multi 1/210nm 4nm

## <Results>

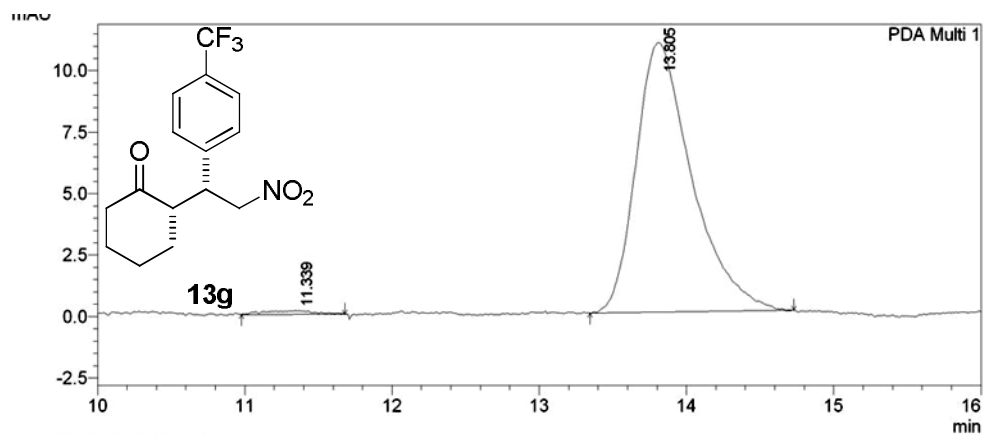
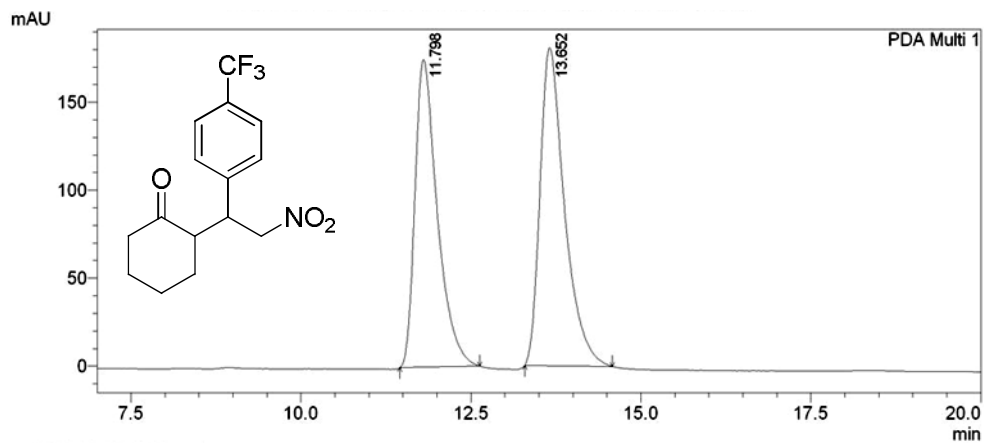
PDA

PeakTable

PDA Ch1 210nm 4nm

Peak#	Name	Ret. Time	Area	Height	Area %
1		11.205	8512	499	4.213
2		13.438	193543	7606	95.787
Total			202056	8104	100.000

## HPLC chromatogram of 13g



1 PDA Multi 1/210nm 4nm

### <Results>

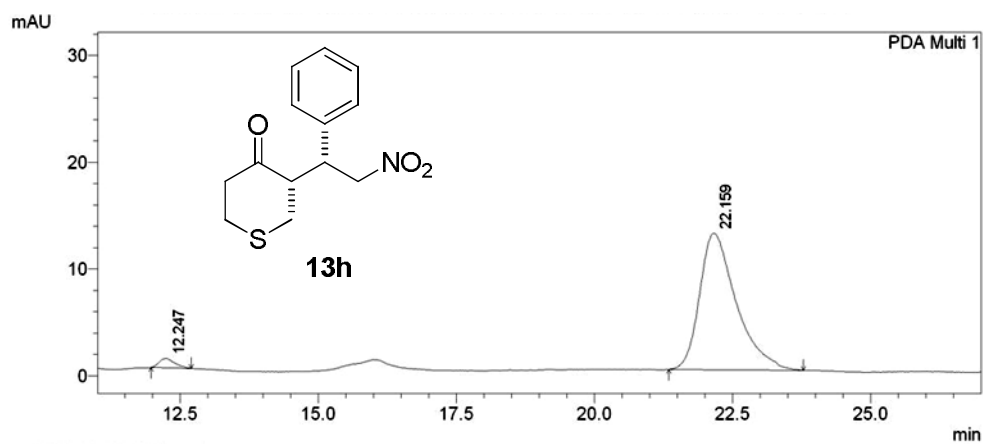
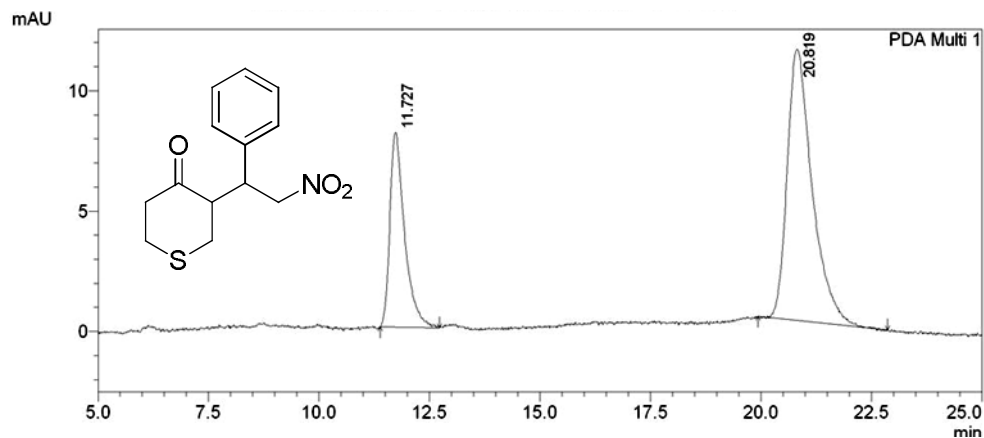
PDA

PeakTable

PDA Ch1 210nm 4nm

Peak#	Name	Ret. Time	Area	Height	Area %
1		11.339	3584	152	1.224
2		13.805	289261	10957	98.776
Total			292846	11109	100.000

## HPLC chromatogram of 13h



1 PDA Multi 1/254nm 4nm

### <Results>

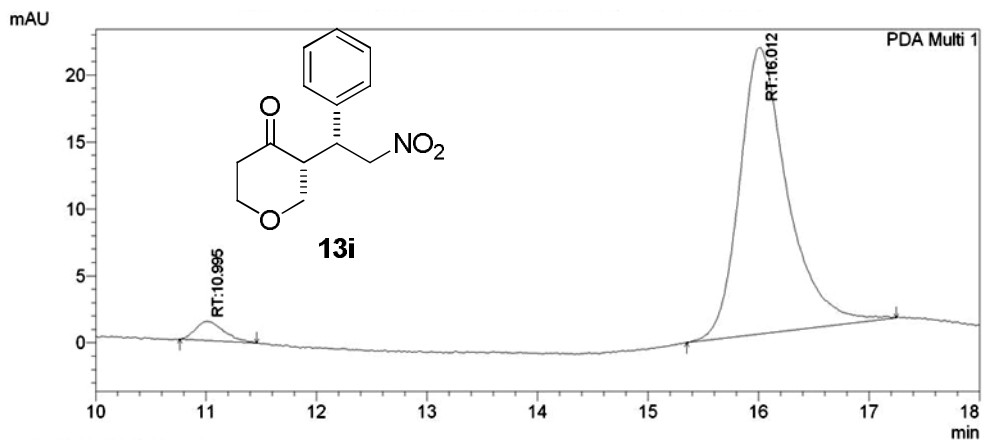
PDA

PeakTable

PDA Ch1 254nm 4nm

Peak#	Name	Ret. Time	Area	Height	Area %
1		12.247	16999	883	2.795
2		22.159	591209	12806	97.205
Total			608208	13689	100.000

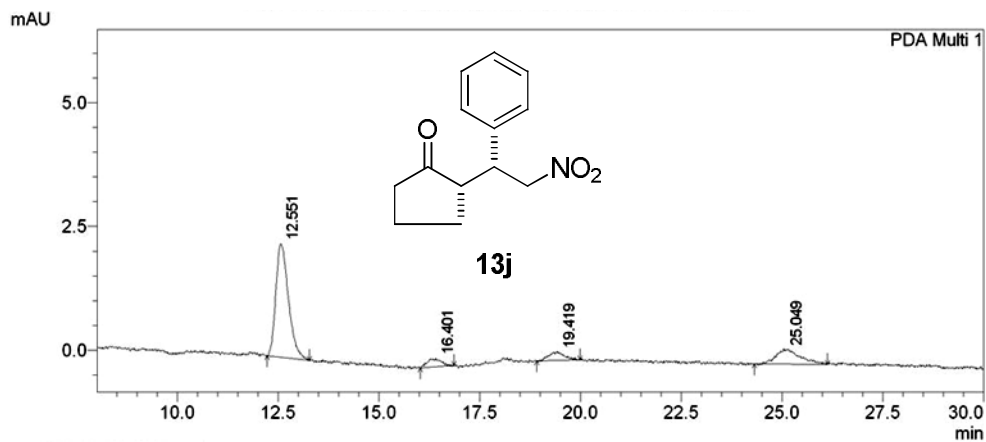
### HPLC chromatogram of **13i**



PeakTable

Peak#	Name	Ret. Time	Area	Height	Area %
1	RT:10.995	10.995	25388	1430	3.779
2	RT:16.012	16.012	646435	21379	96.221
Total			671823	22809	100.000

### HPLC chromatogram of **13j**



<Results>

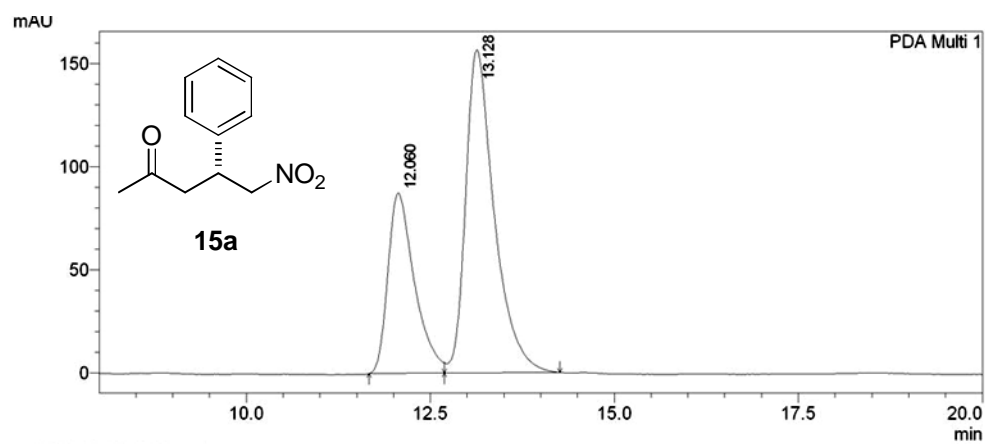
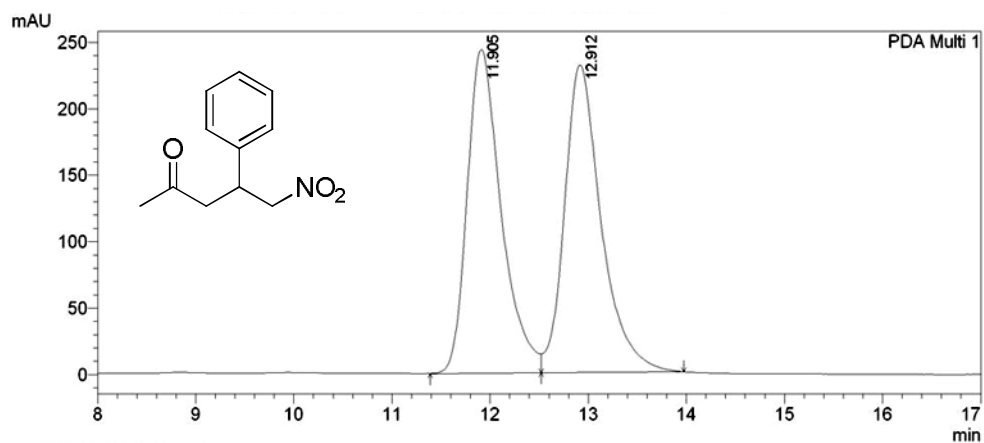
PDA

PeakTable

Peak#	Name	Ret. Time	Area	Height	Area %
1		12.551	49929	2284	70.398
2		16.401	4012	172	5.656
3		19.419	4728	191	6.666
4		25.049	12255	307	17.280
Total			70923	2954	100.000



### HPLC chromatogram of **15a**



1 PDA Multi 1/210nm 4nm

#### <Results>

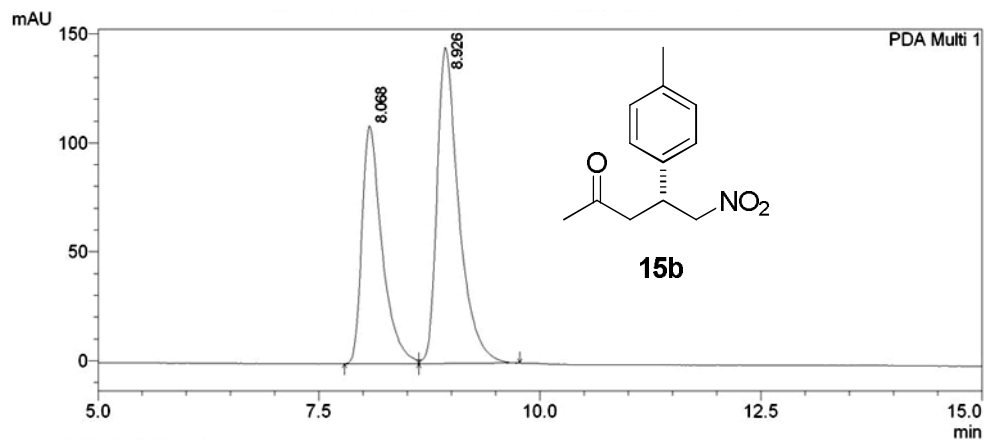
PDA

PeakTable

PDA Ch1 210nm 4nm

Peak#	Name	Ret. Time	Area	Height	Area %
1		12.060	2195786	87476	34.049
2		13.128	4253199	156817	65.951
Total			6448986	244293	100.000

### HPLC chromatogram of **15b**



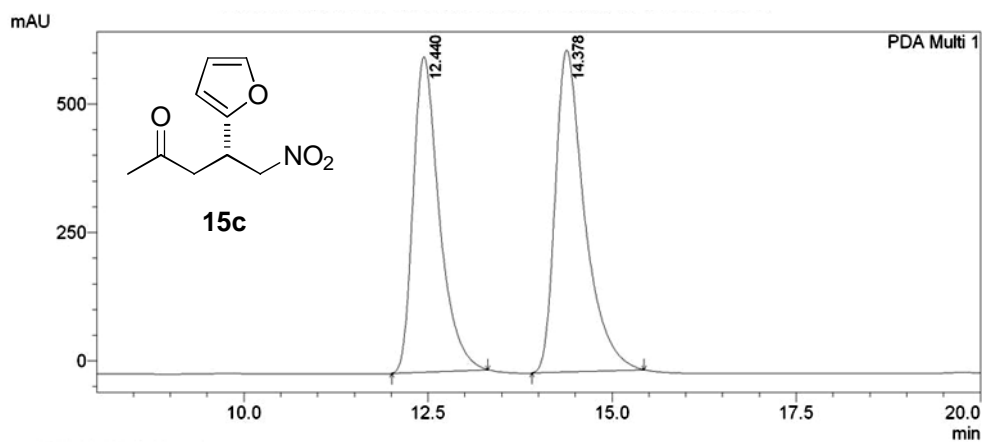
**<Results>**

PDA

PeakTable

Peak#	Name	Ret. Time	Area	Height	Area %
1		8.068	1731104	109168	40.974
2		8.926	2493798	144962	59.026
Total			4224902	254130	100.000

### HPLC chromatogram of **15c**



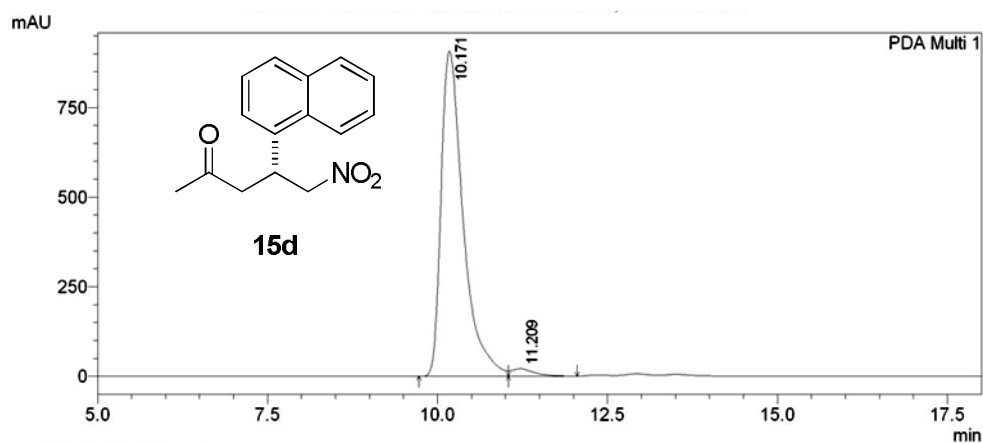
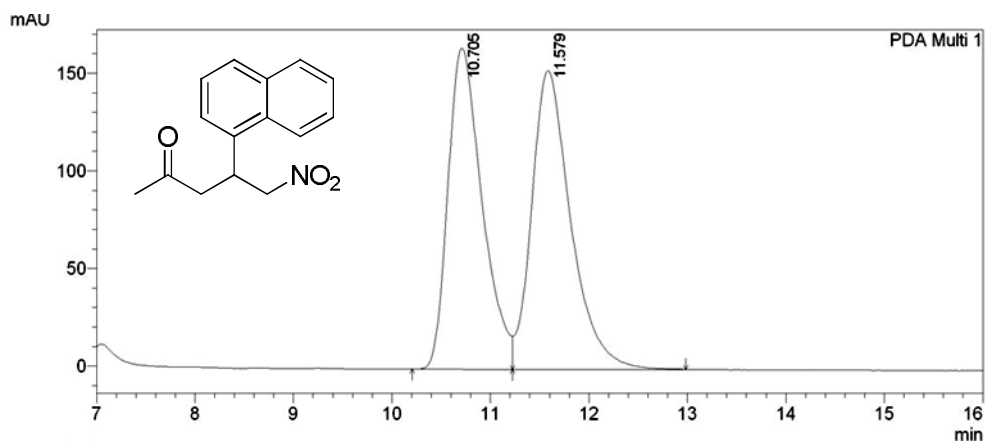
**<Results>**

PDA

PeakTable

Peak#	Name	Ret. Time	Area	Height	Area %
1		12.440	15179118	613327	46.632
2		14.378	17371713	626528	53.368
Total			32550832	1239854	100.000

## HPLC chromatogram of **15d**



1 PDA Multi 1/220nm 4nm

### <Results>

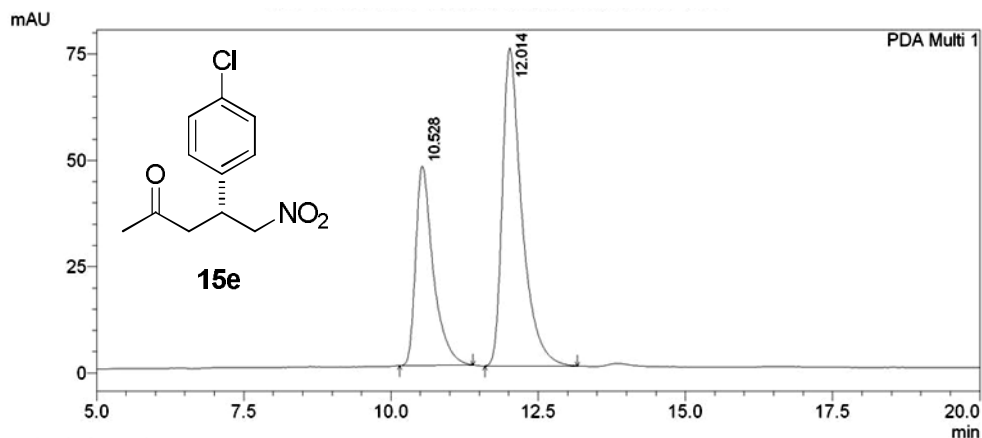
PDA

PeakTable

PDA Ch1 220nm 4nm

Peak#	Name	Ret. Time	Area	Height	Area %
1		10.171	20462248	906683	97.704
2		11.209	480799	20937	2.296
Total			20943048	927620	100.000

### HPLC chromatogram of 15e



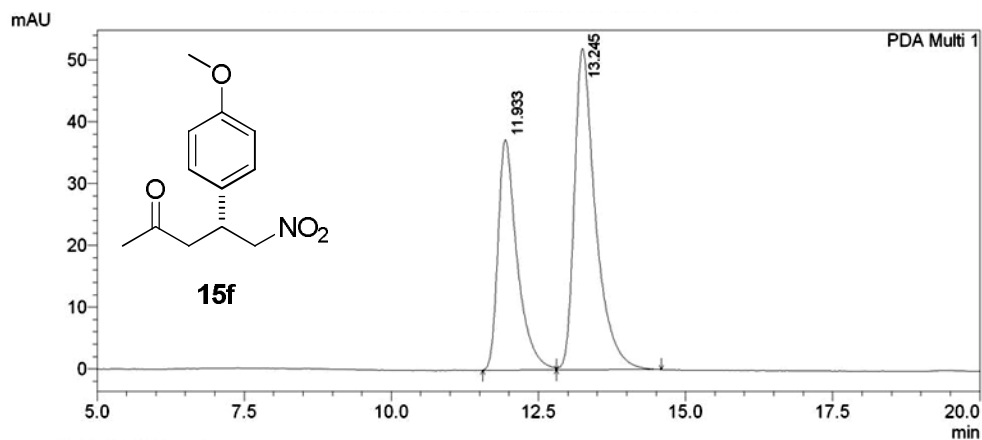
**<Results>**

PDA

PeakTable

Peak#	Name	Ret. Time	Area	Height	Area %
1		10.528	966509	46830	35.892
2		12.014	1726330	74745	64.108
Total			2692839	121575	100.000

### HPLC chromatogram of 15f



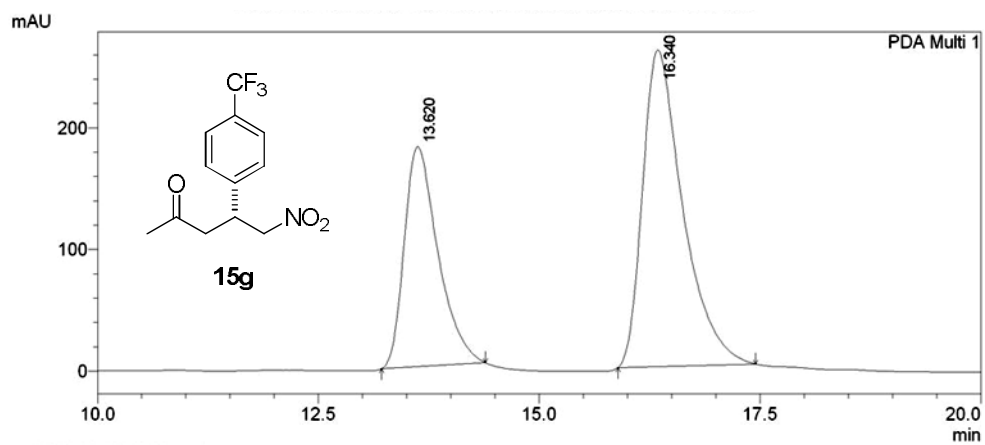
**<Results>**

PDA

PeakTable

Peak#	Name	Ret. Time	Area	Height	Area %
1		11.933	843849	37324	39.299
2		13.245	1303399	52017	60.701
Total			2147248	89341	100.000

# HPLC chromatogram of 15g



## Results>

DA

PDA Ch1 210nm 4nm

PeakTable

Peak#	Name	Ret. Time	Area	Height	Area %
1		13.620	4804870	180827	36.760
2		16.340	8266018	259964	63.240
Total			13070888	440791	100.000