Supporting Information

Hypervalent Iodine Mediated Chemoselective Iodination of Alkynes

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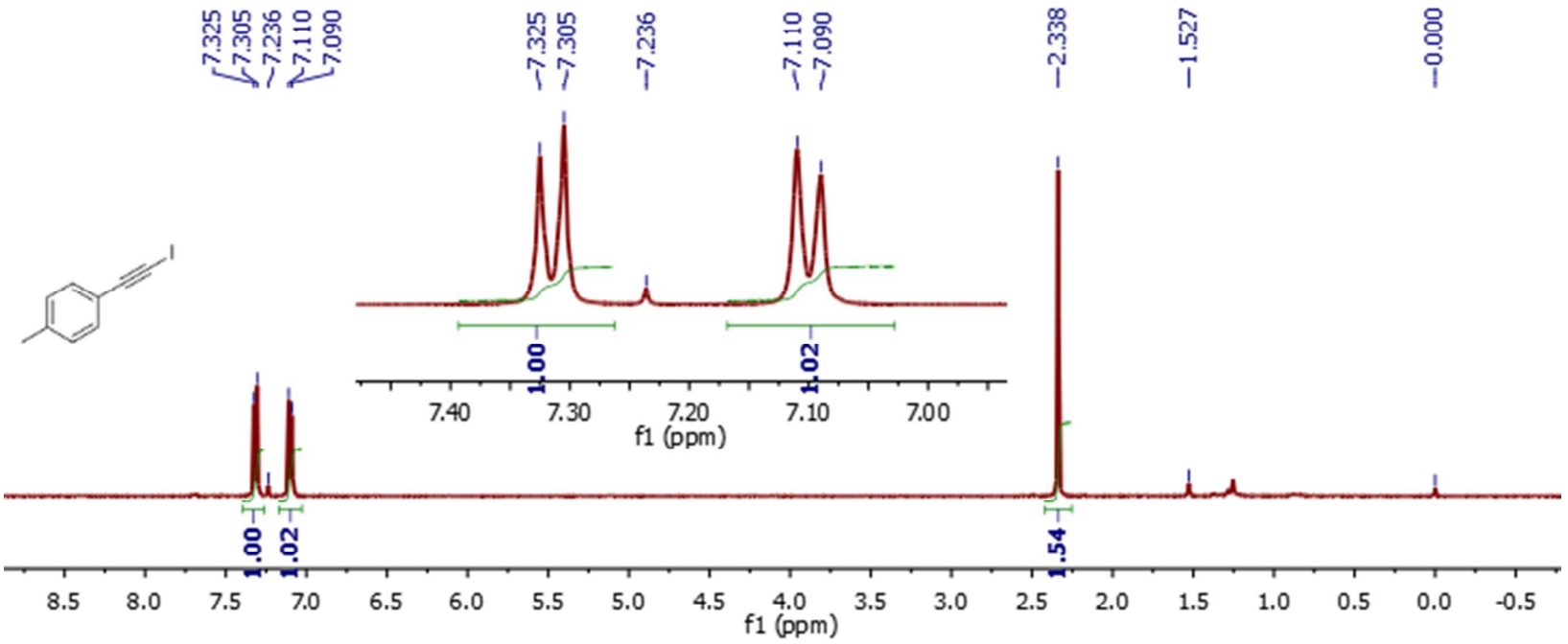
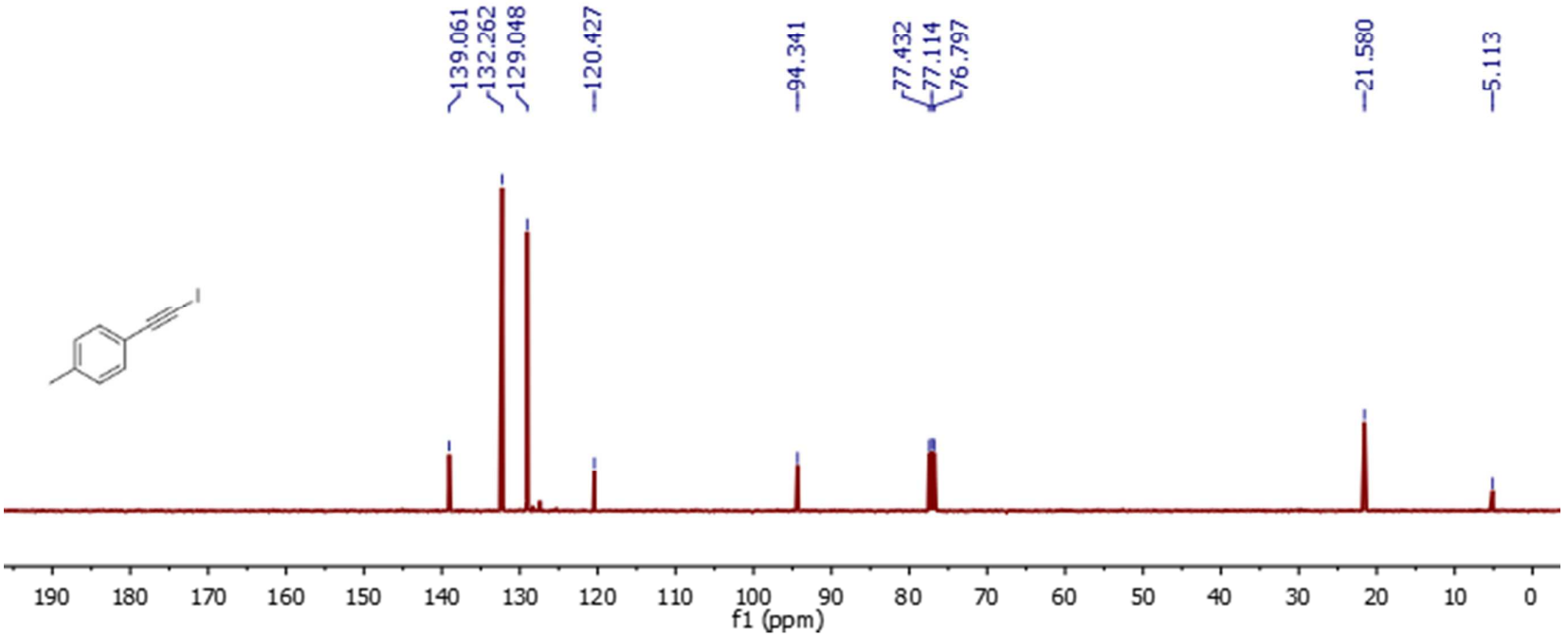
NMR Spectra

NMR Spectra of Compound 2a

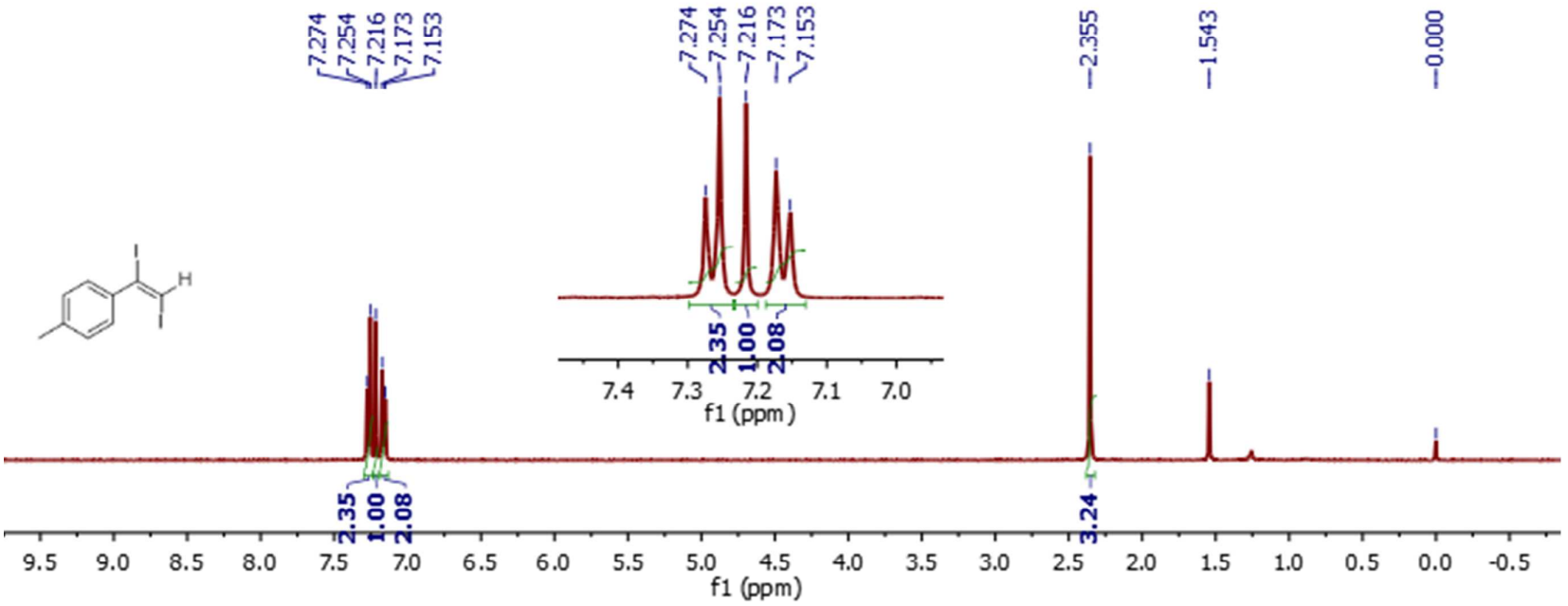


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **2a**

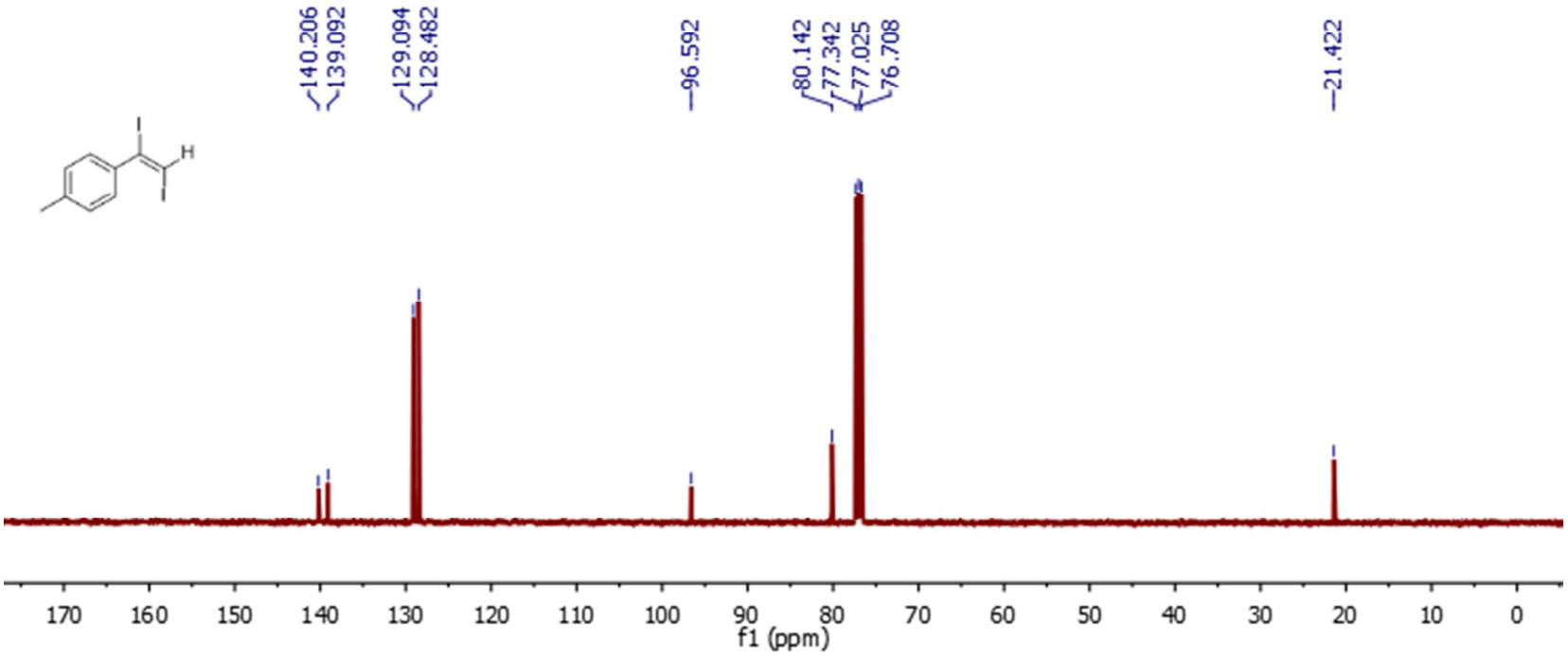


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **2a**

NMR Spectra of Compound 3a

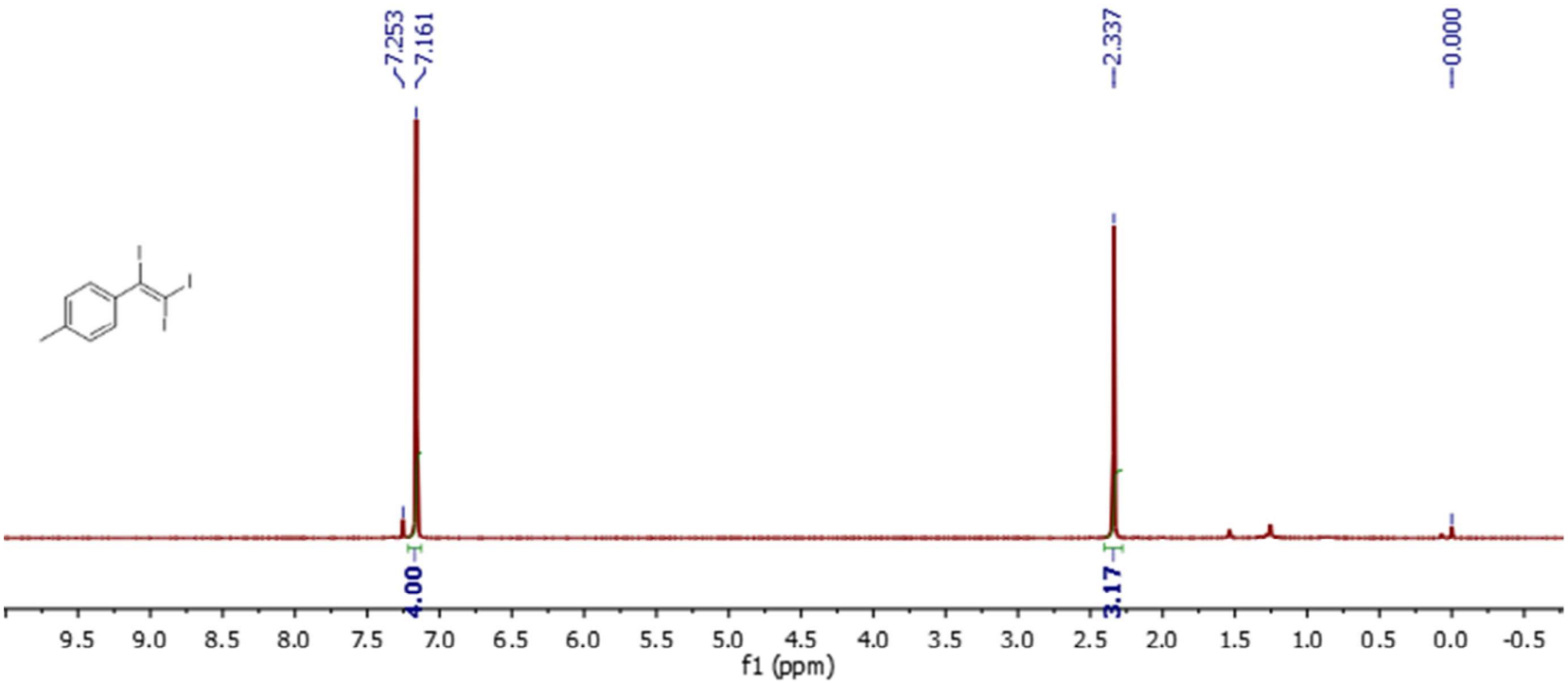


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3a**

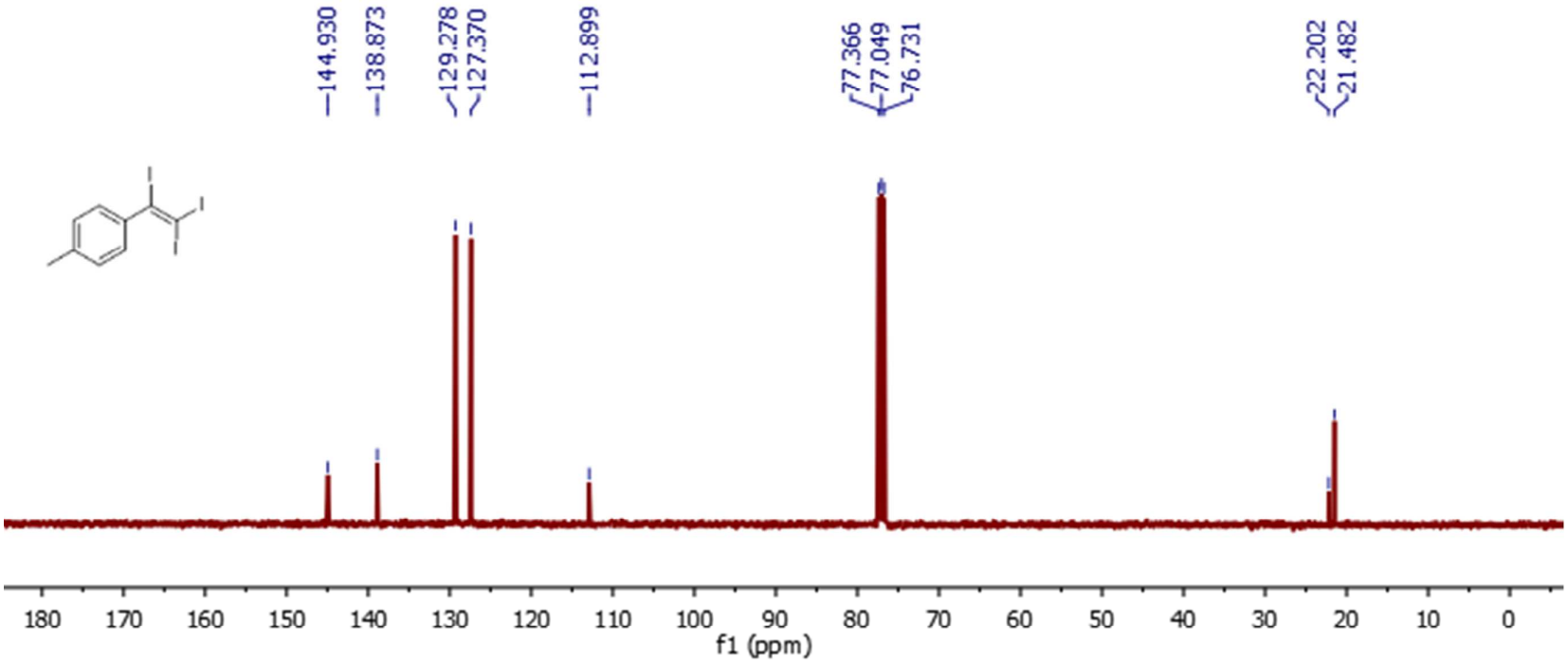


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **3a**

NMR Spectra of Compound 4a

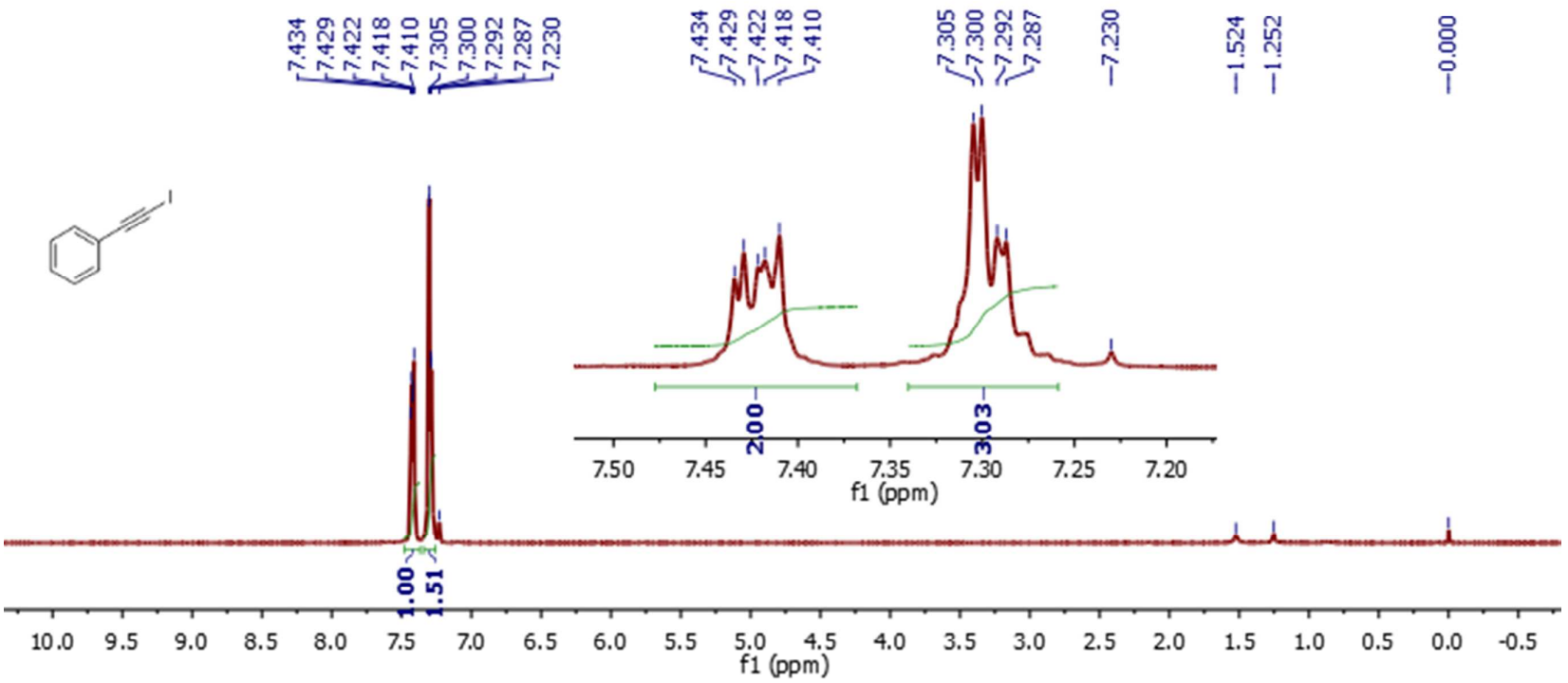


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4a**

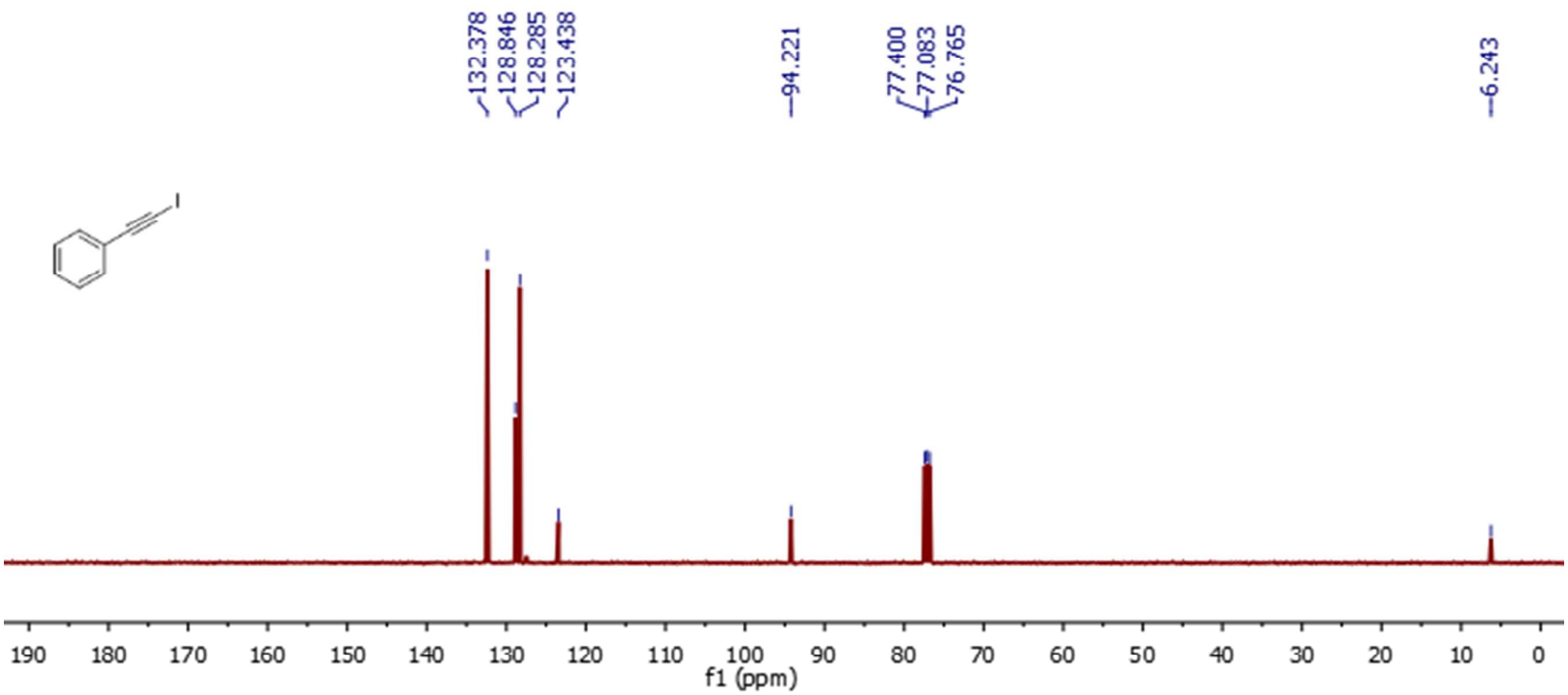


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **4a**

NMR Spectra of Compound 2b

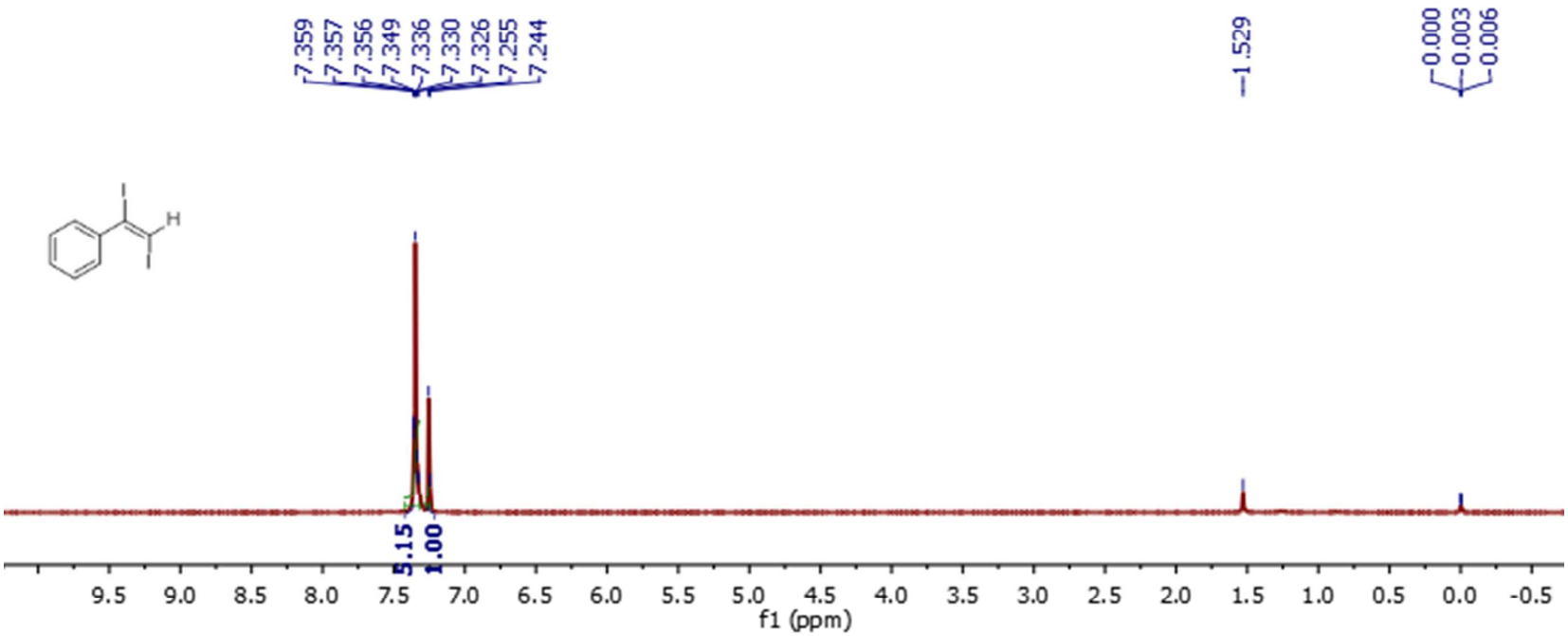


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **2b**

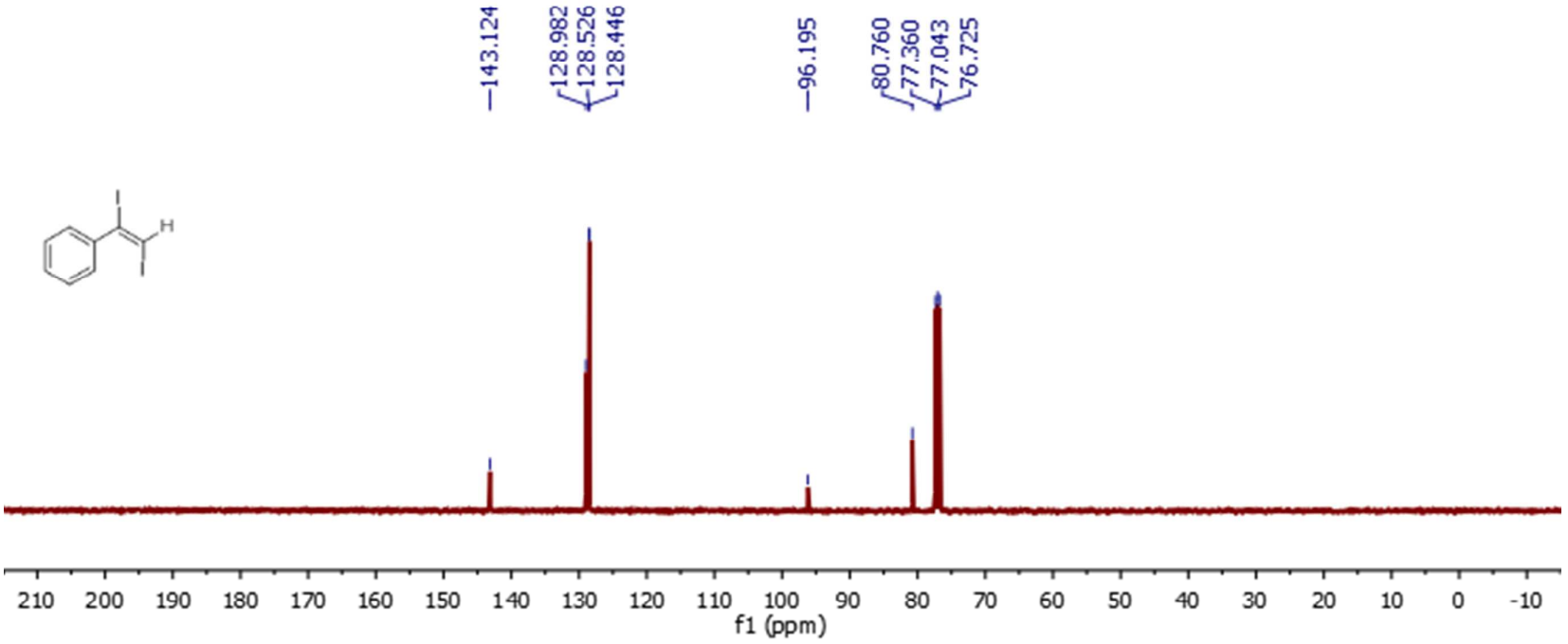


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **2b**

NMR Spectra of Compound 3b

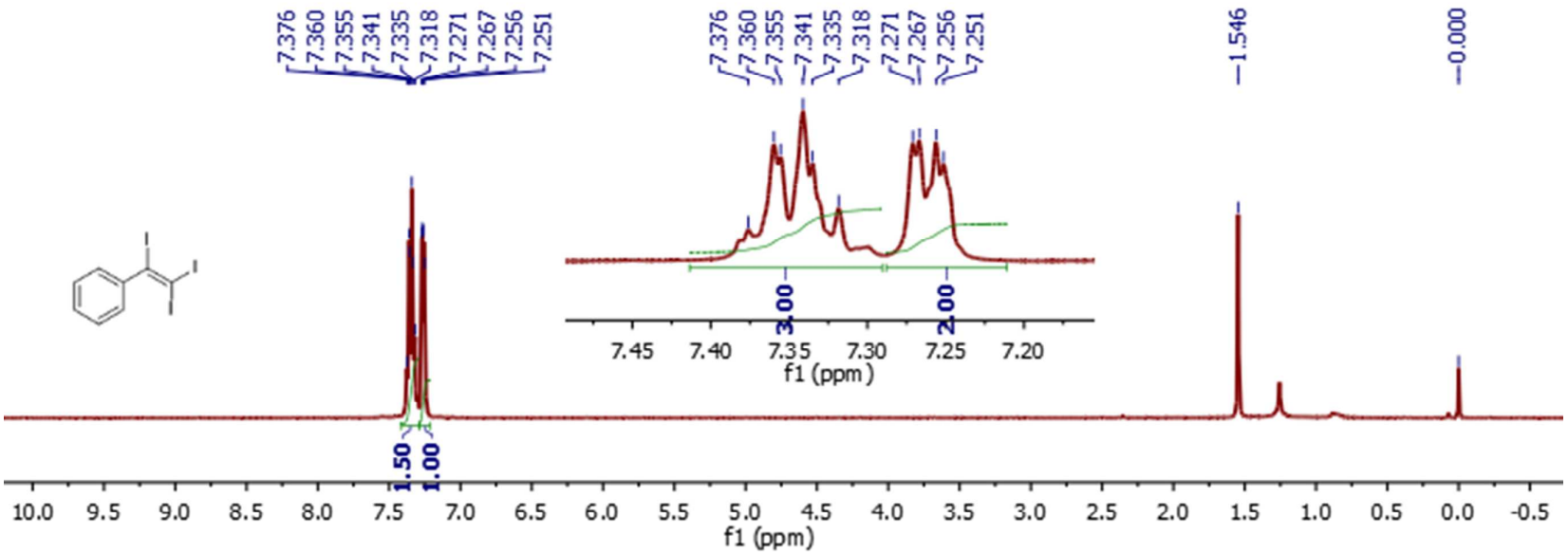


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3b**

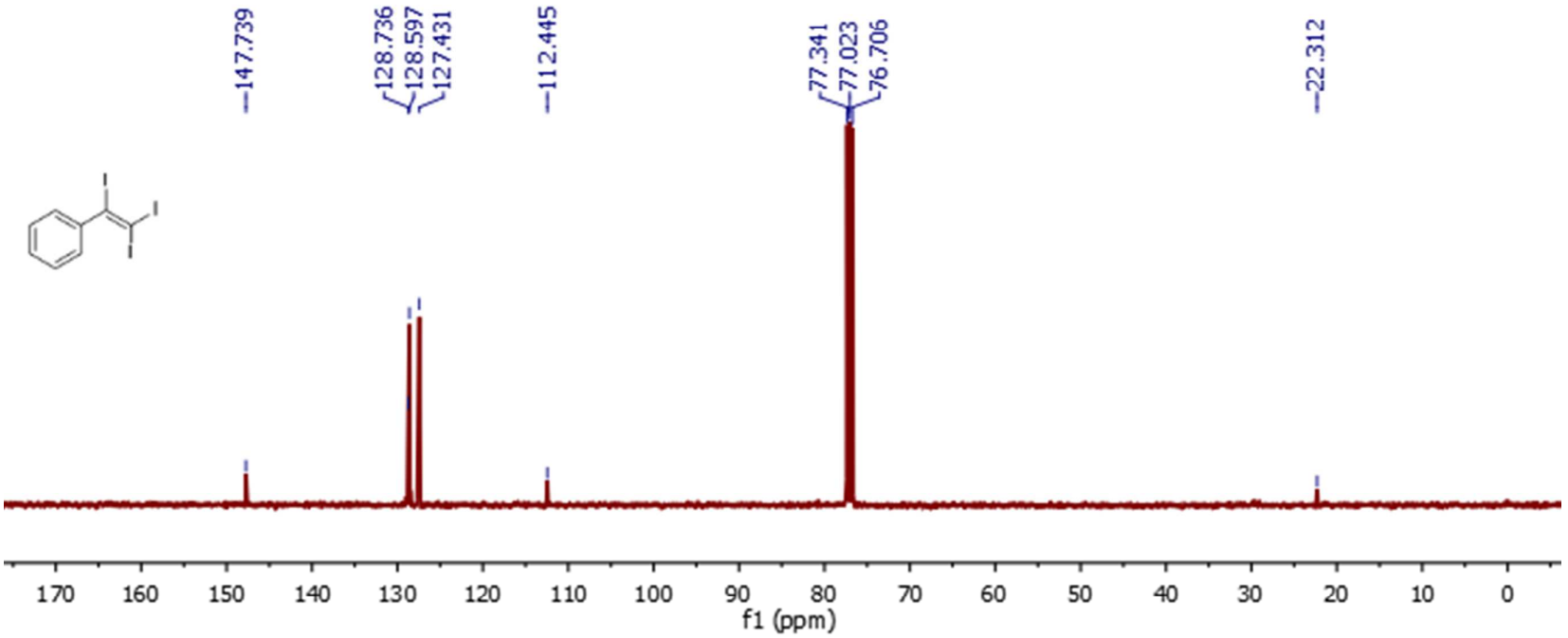


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **3b**

NMR Spectra of Compound 4b

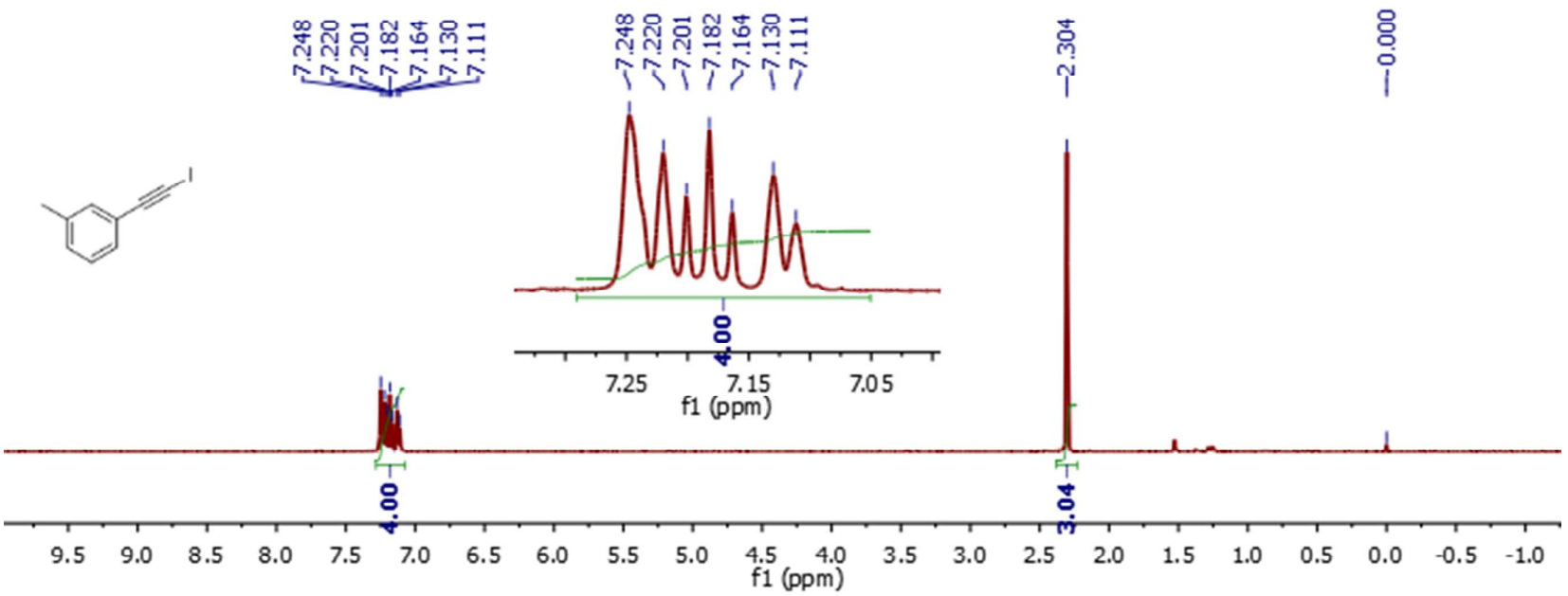


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4b**

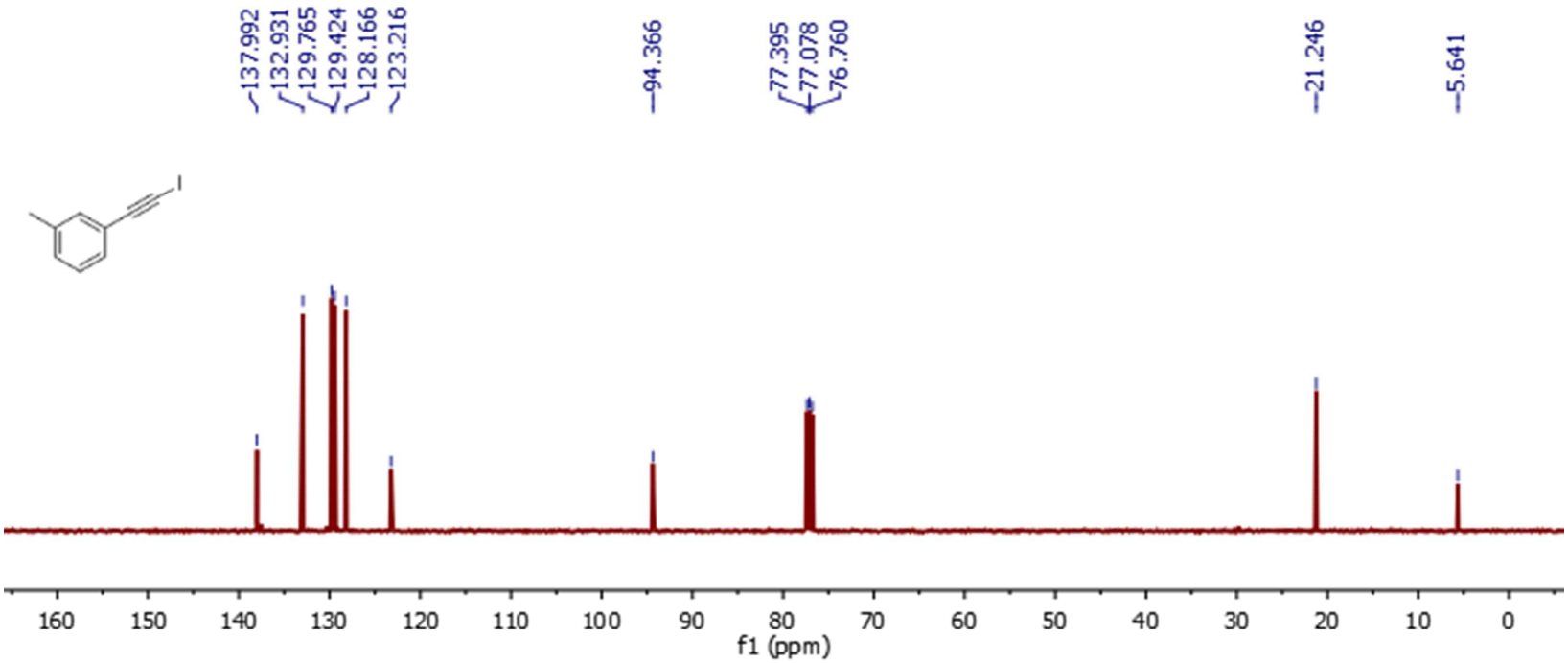


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **4b**

NMR Spectra of Compound 2c

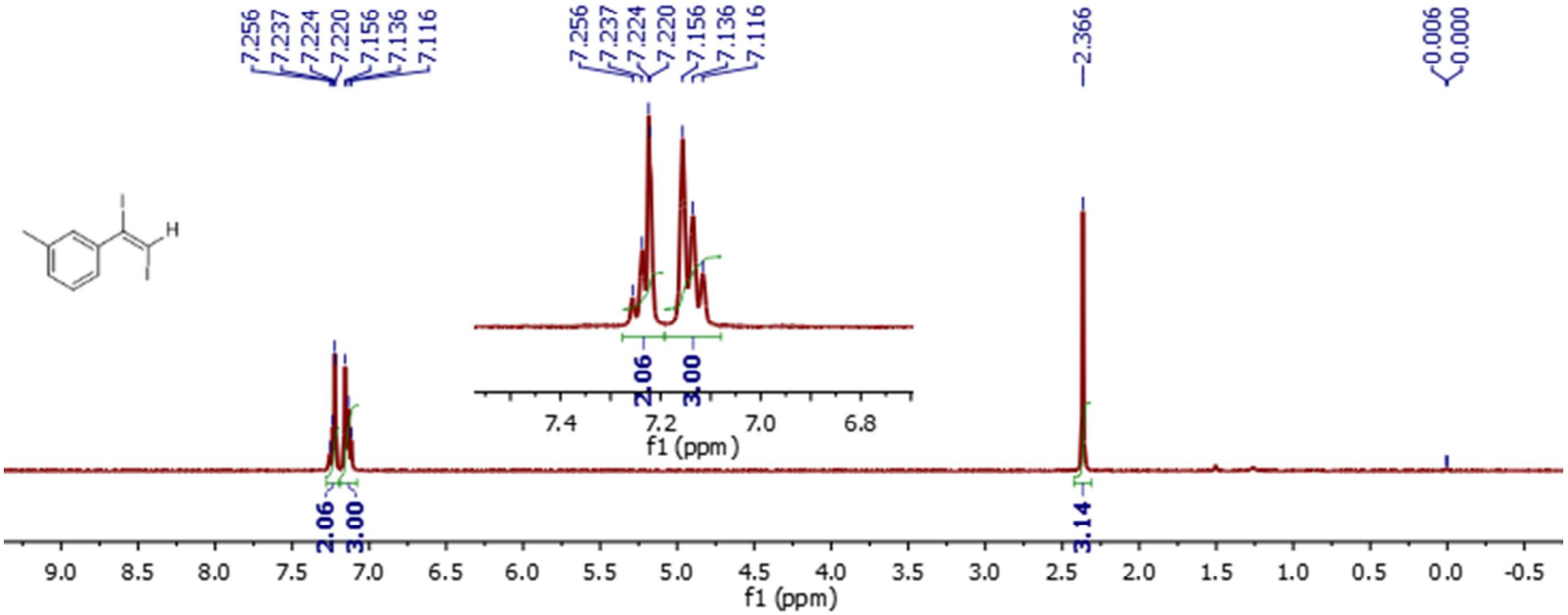


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **2c**

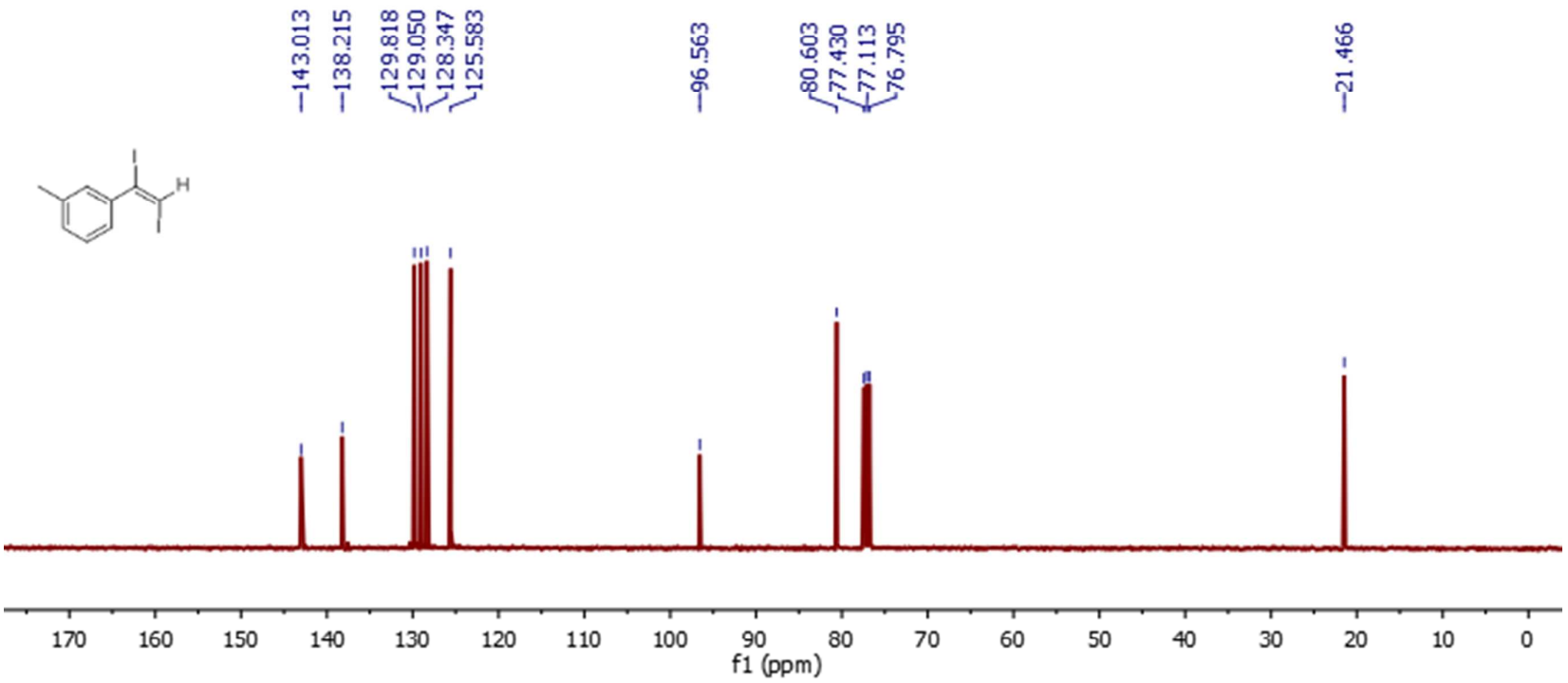


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **2c**

NMR Spectra of Compound 3c

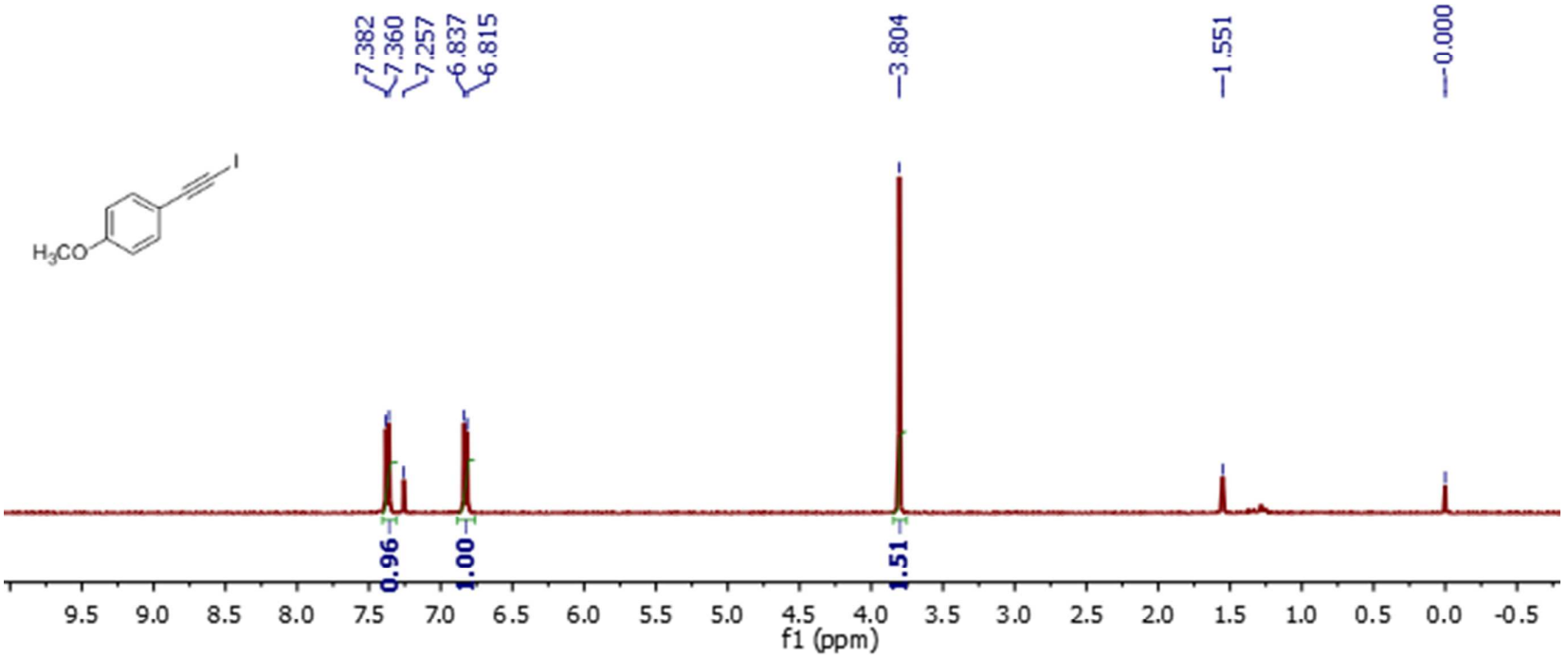


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3c**

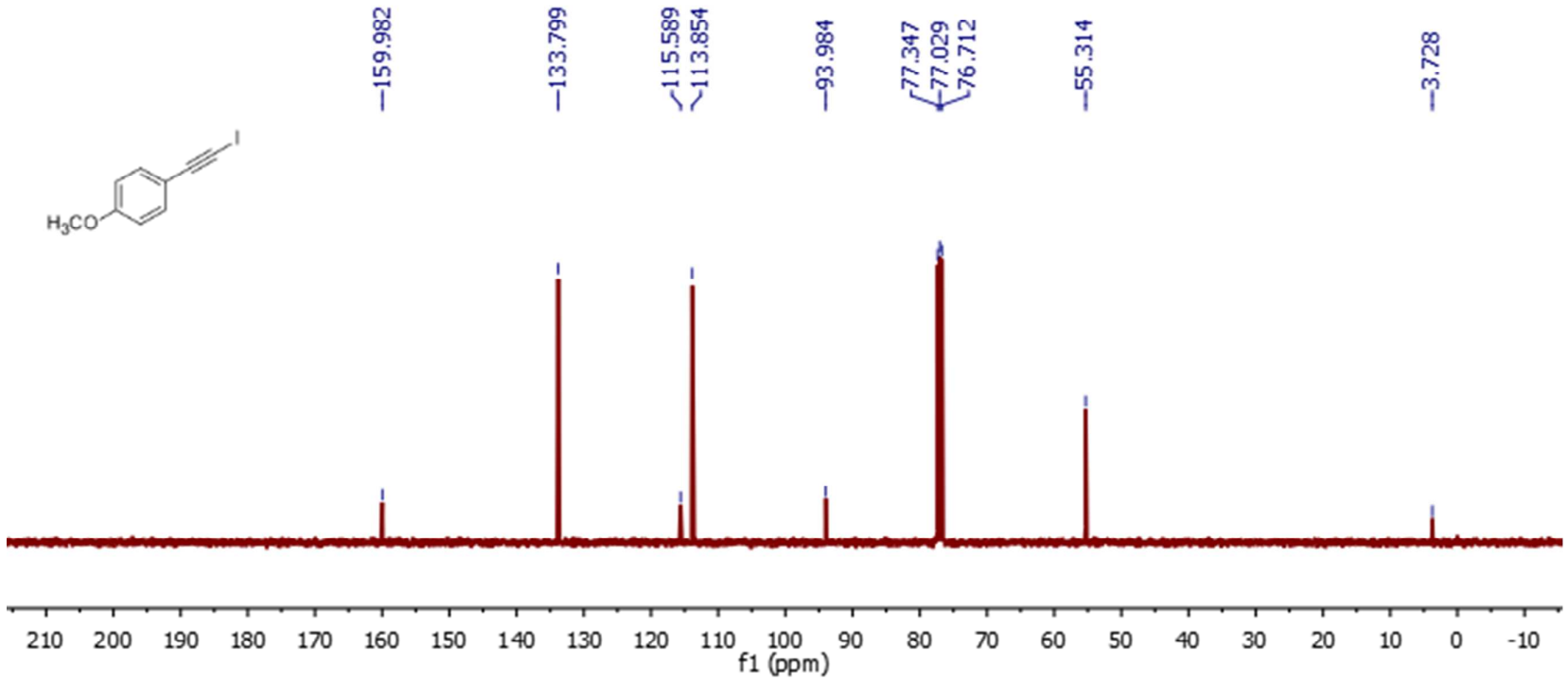


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **3c**

NMR Spectra of Compound 2d

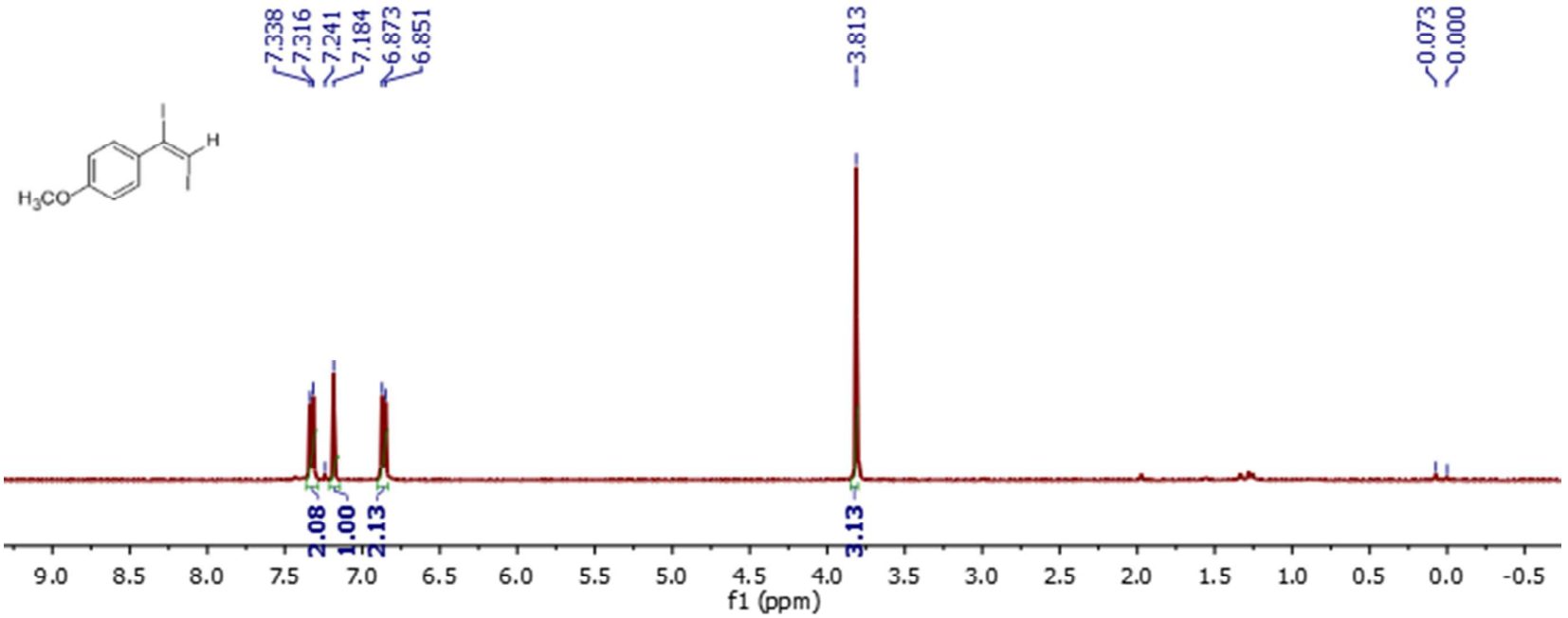


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **2d**

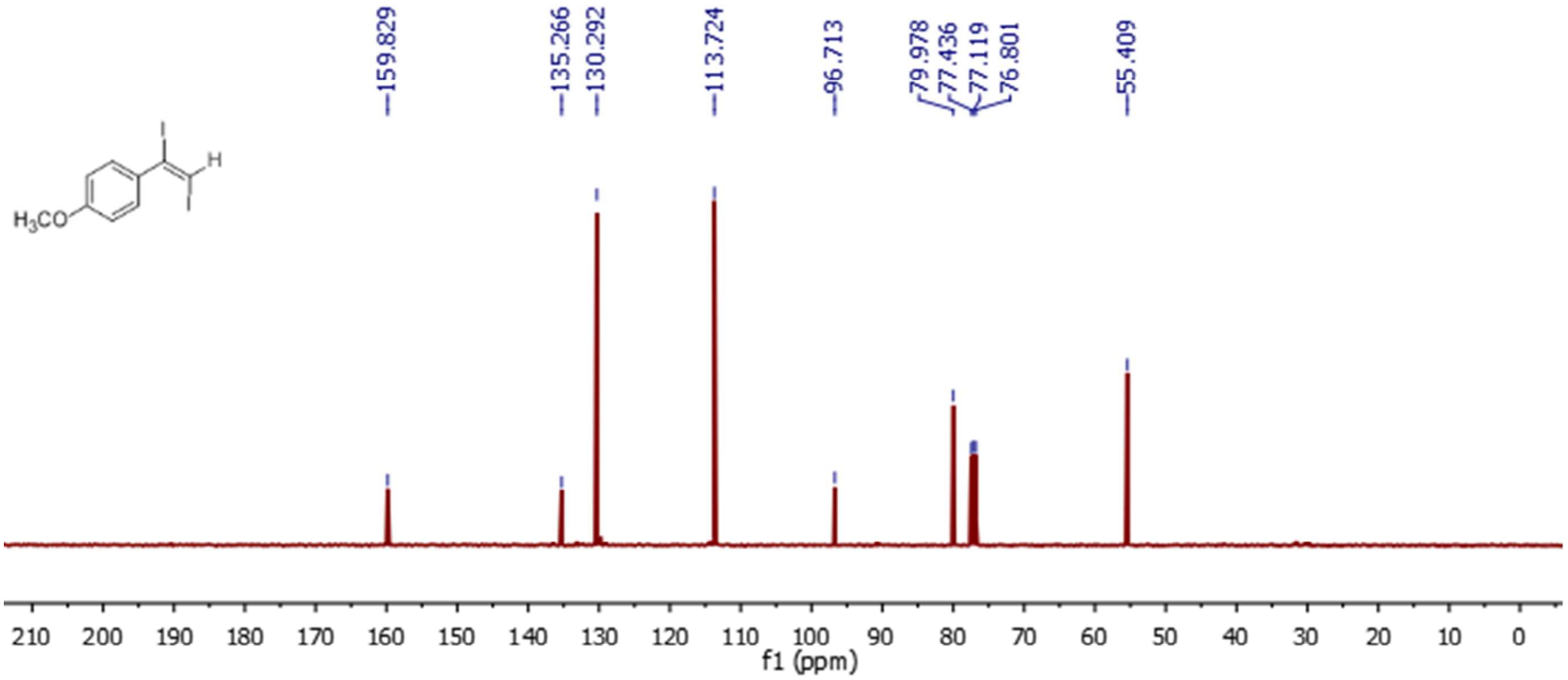


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **2d**

NMR Spectra of Compound 3d

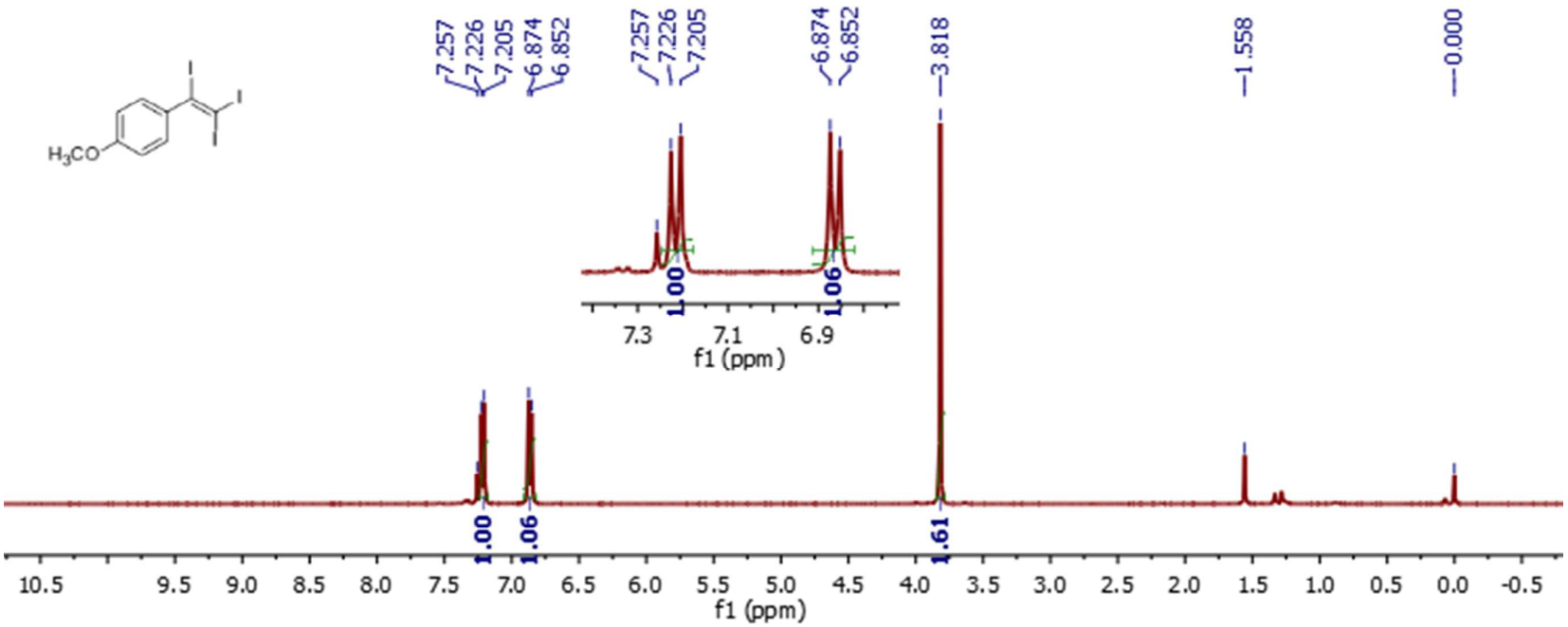


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3d**

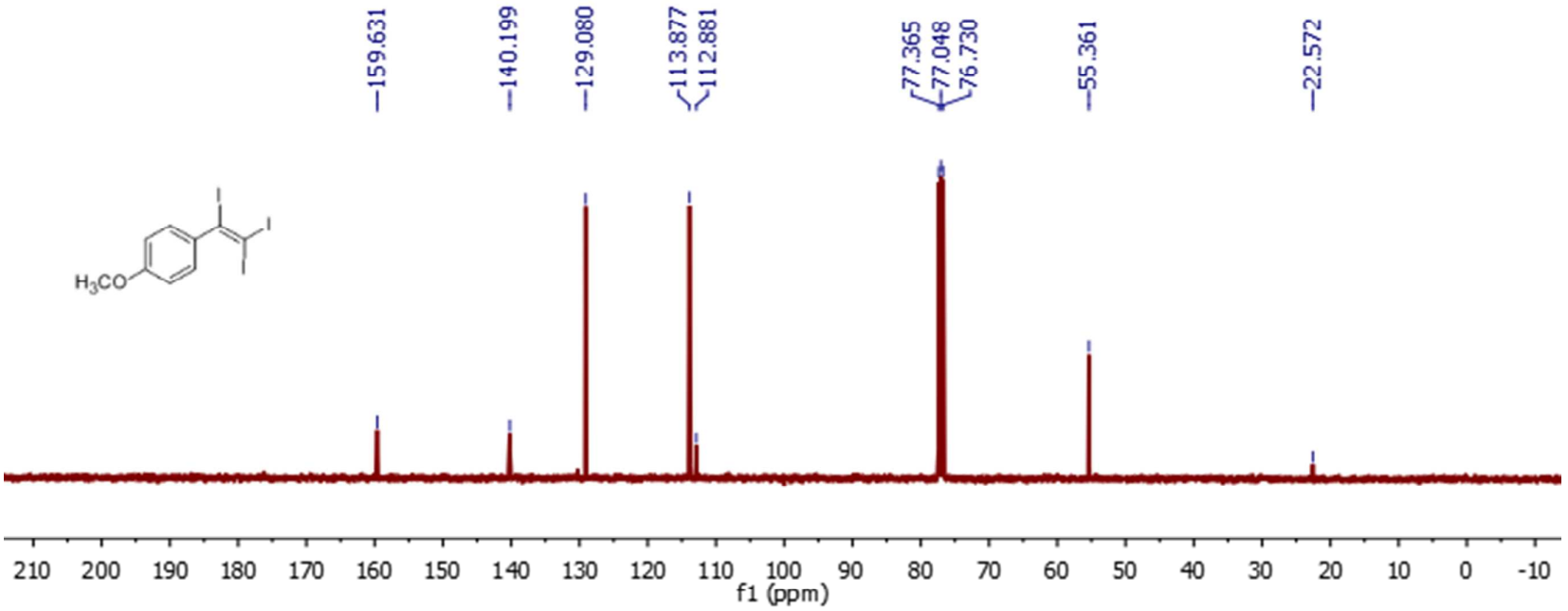


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **3d**

NMR Spectra of Compound 4d

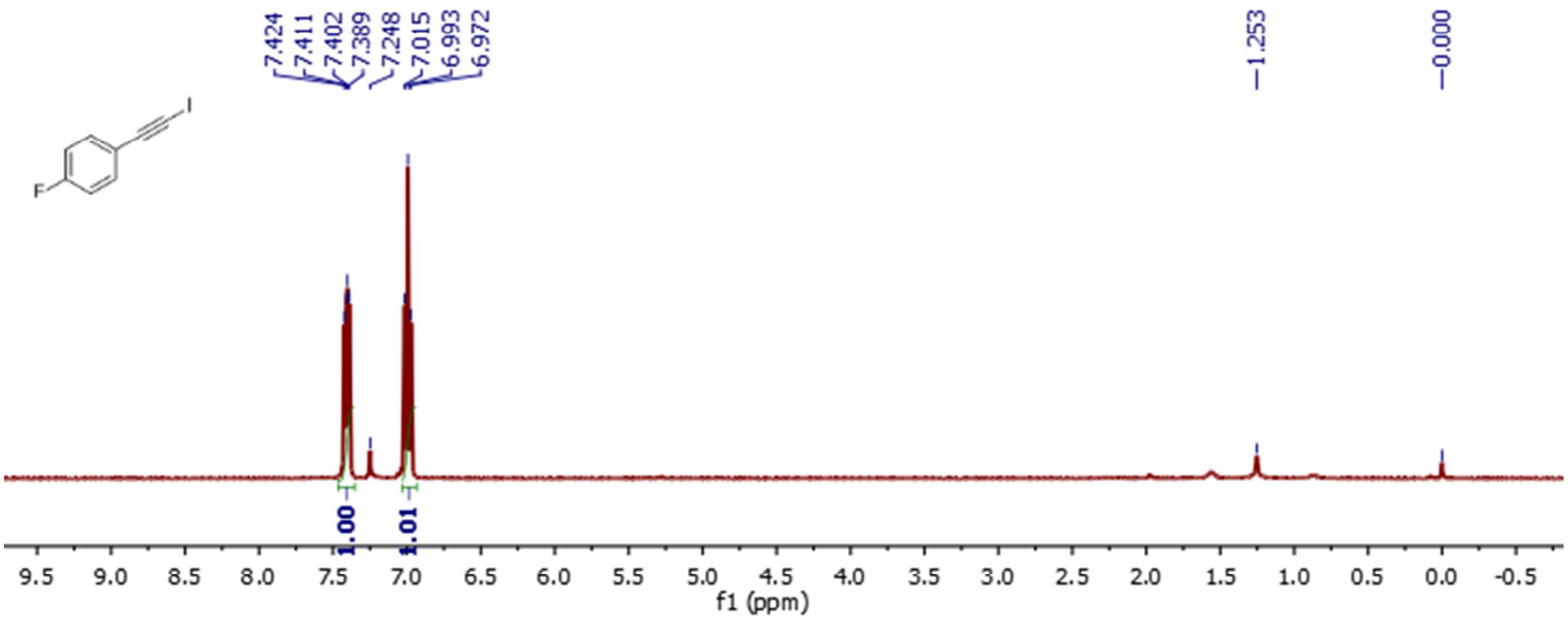


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4d**

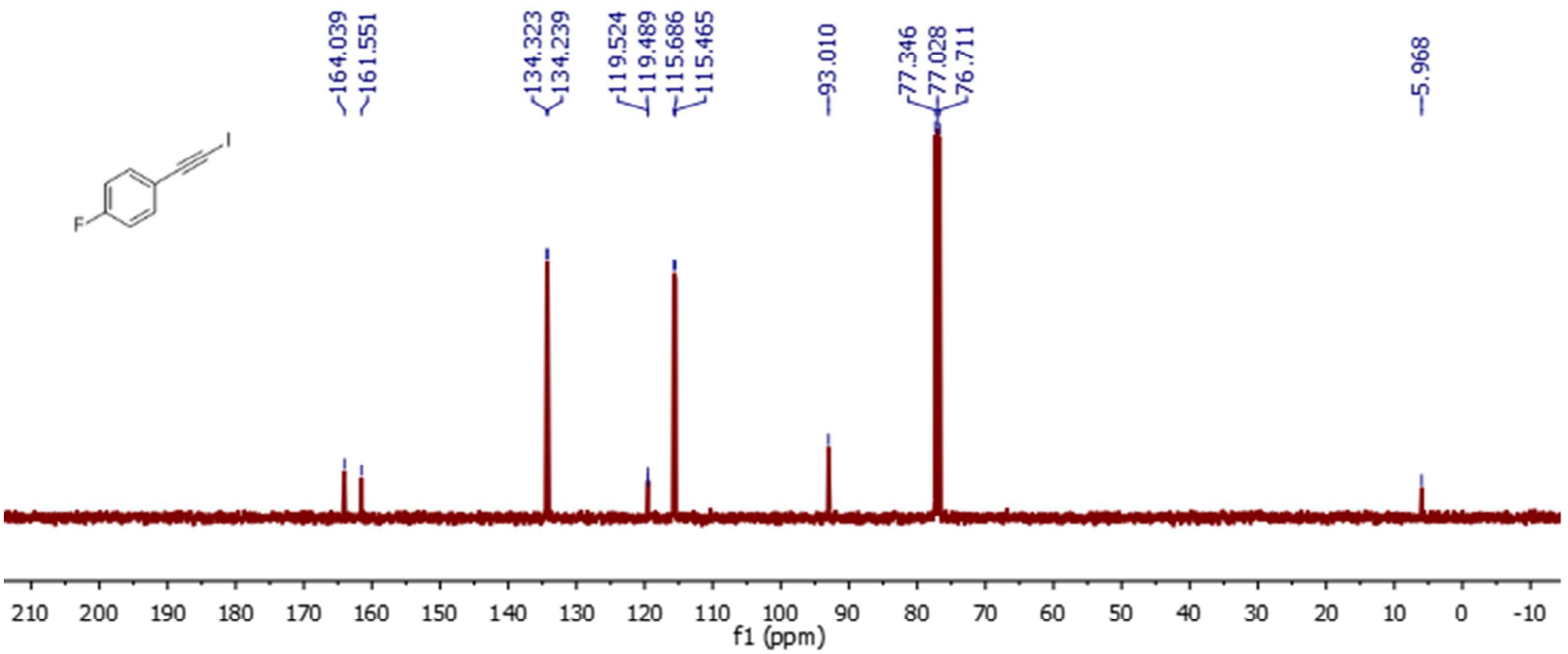


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **4d**

NMR Spectra of Compound 2e

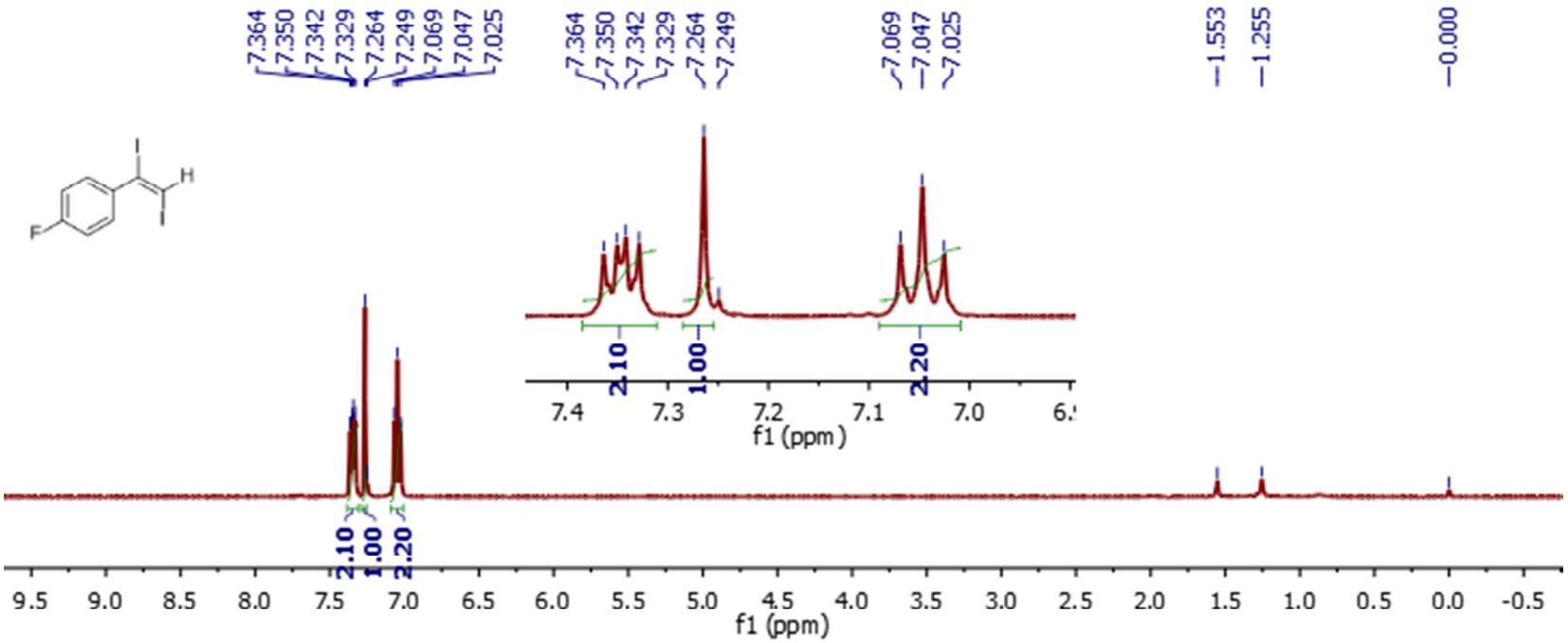


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **2e**

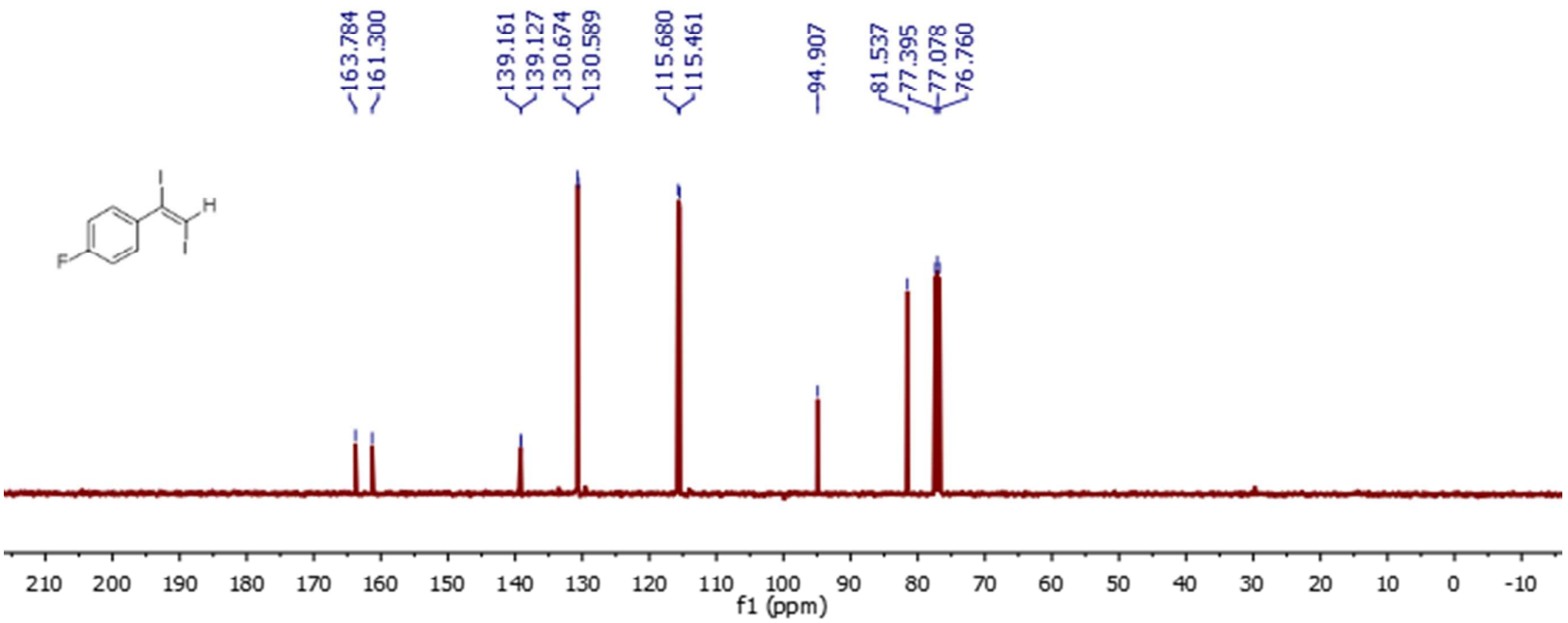


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **2e**

NMR Spectra of Compound 3e

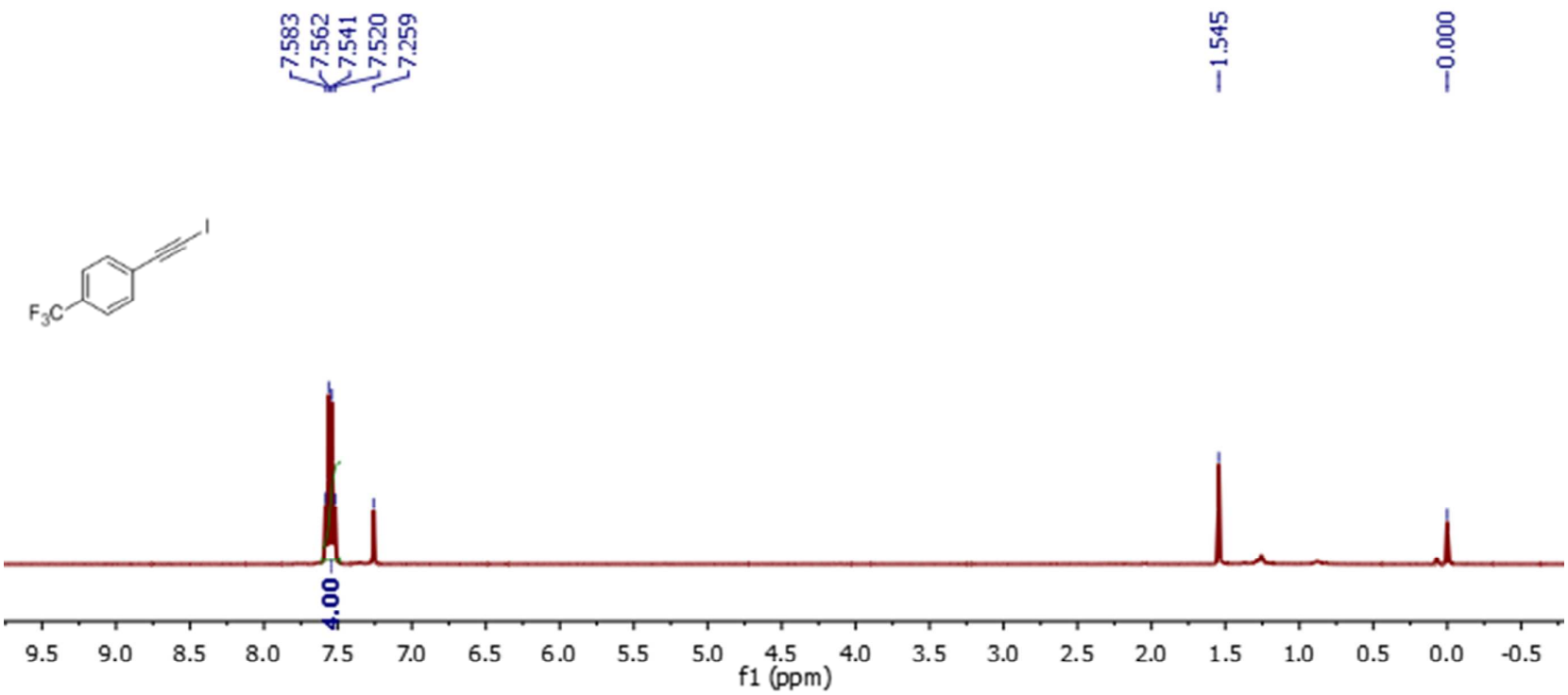


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **3e**

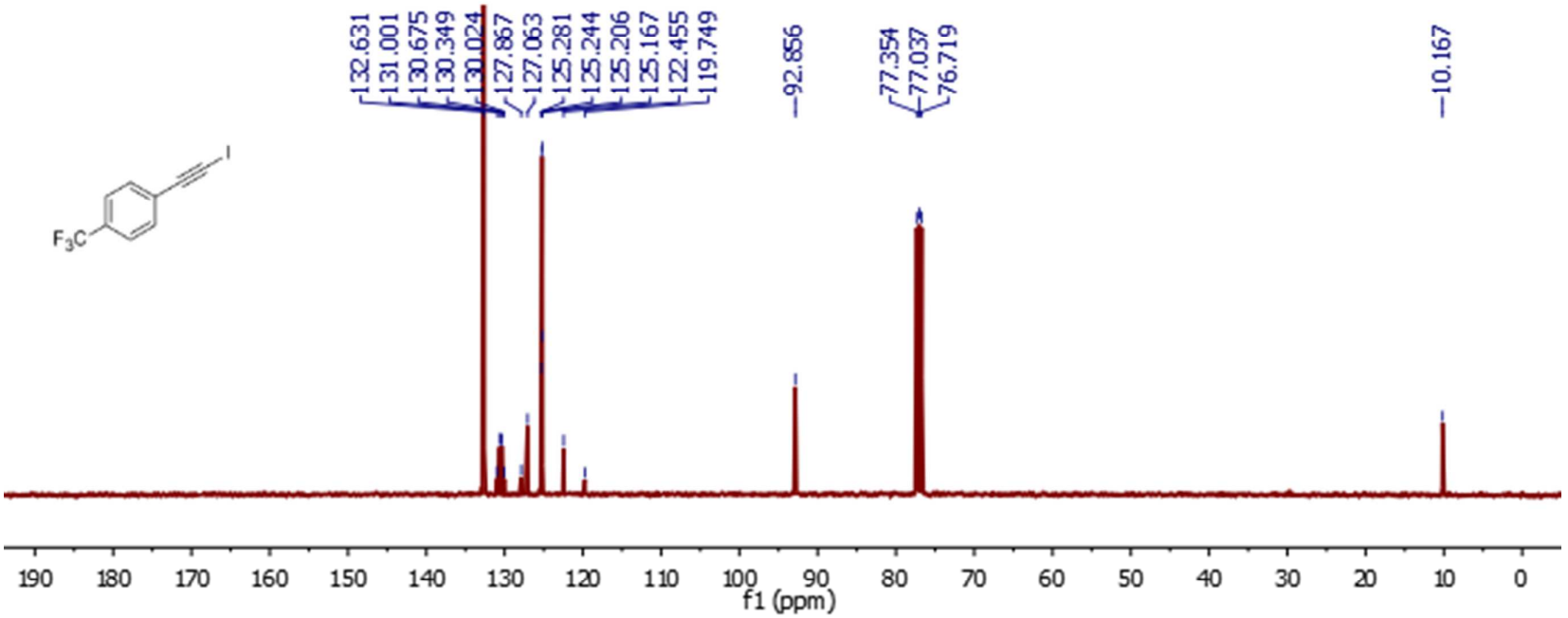


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **3e**

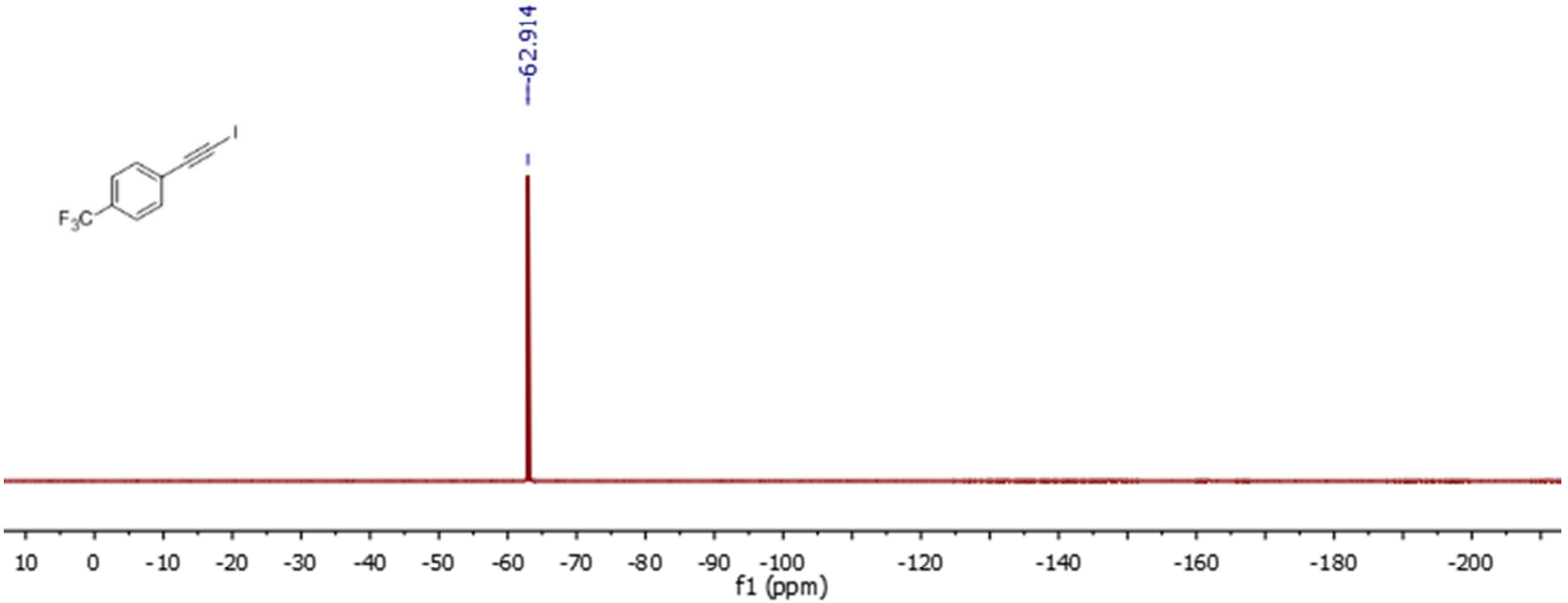
NMR Spectra of Compound 2f



^{1}H NMR (400MHz, $CDCl_3$) spectrum of **3f**

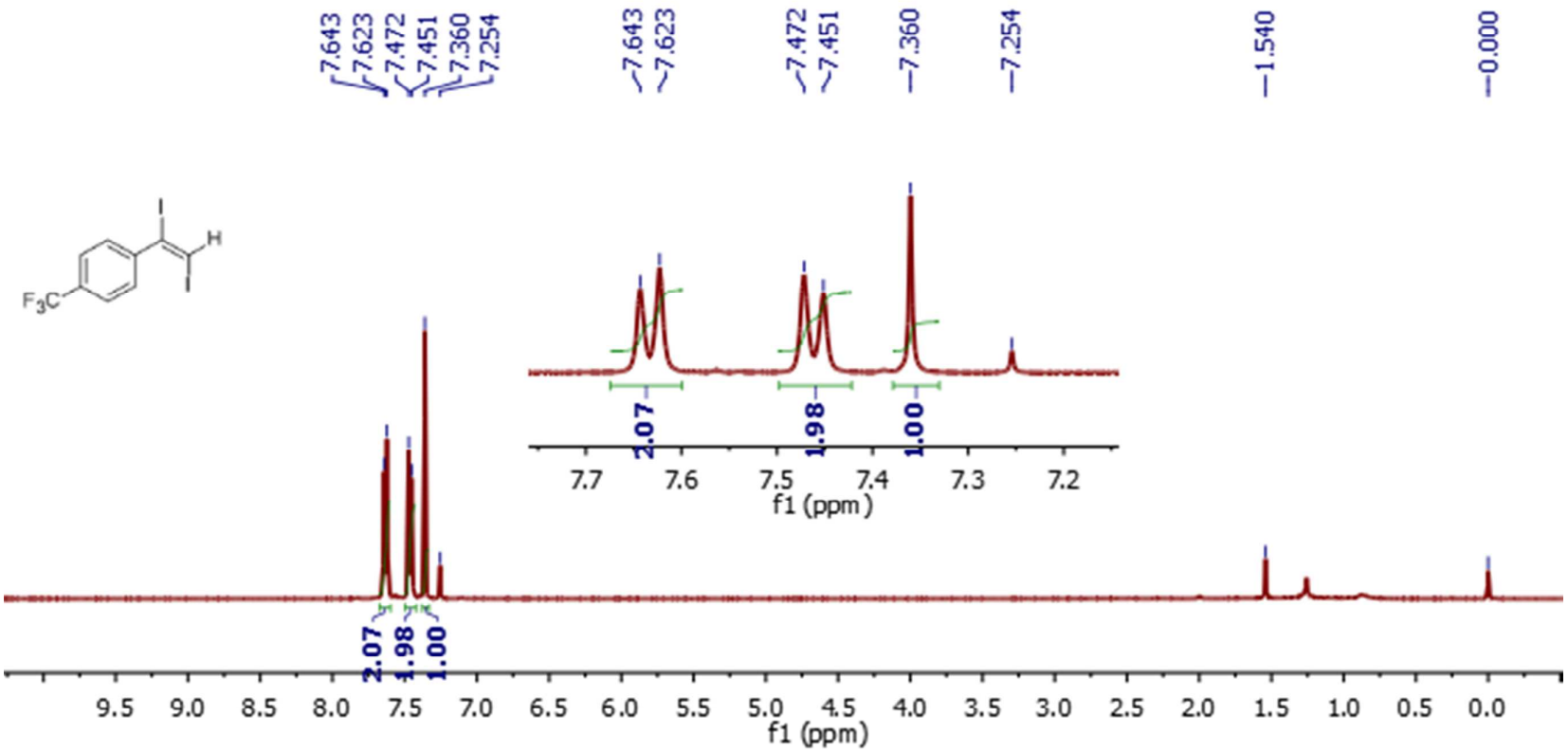


$^{13}C\{^{1}H\}$ NMR (100MHz, $CDCl_3$) spectrum of **2f**

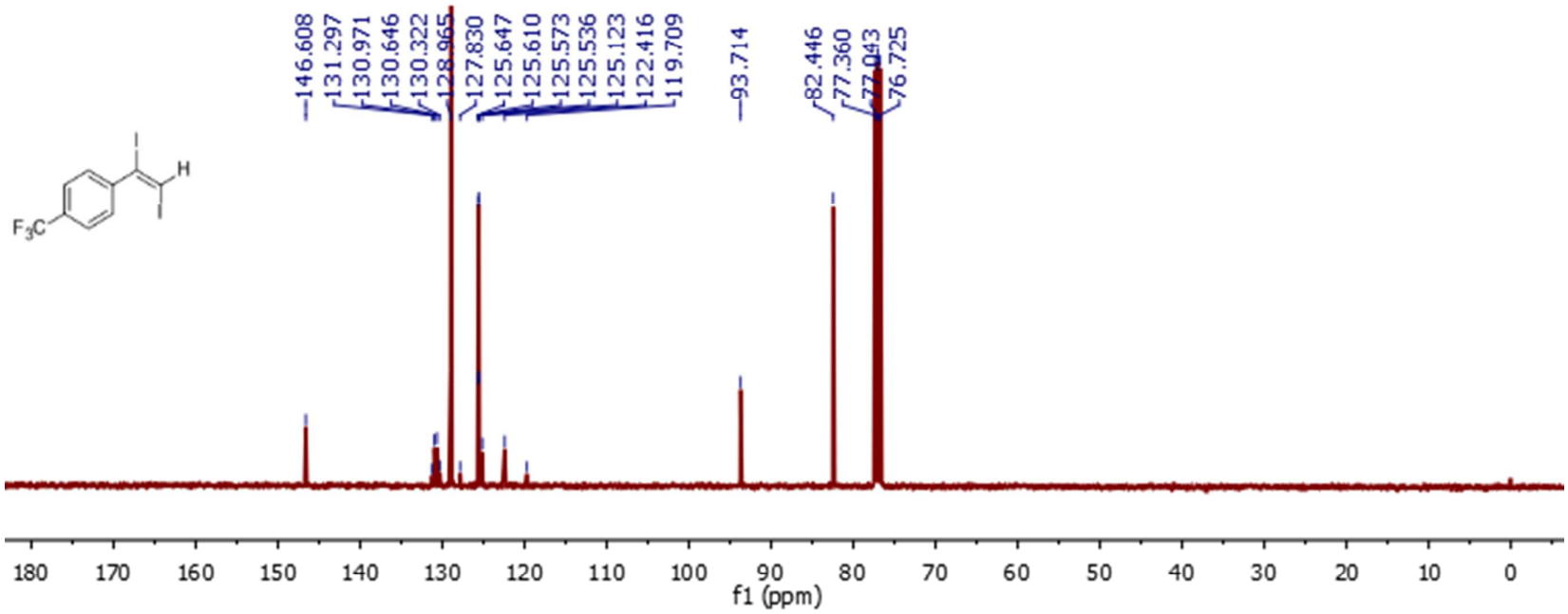


^{19}FNMR (376 MHz, $CDCl_3$) spectrum of **3f**

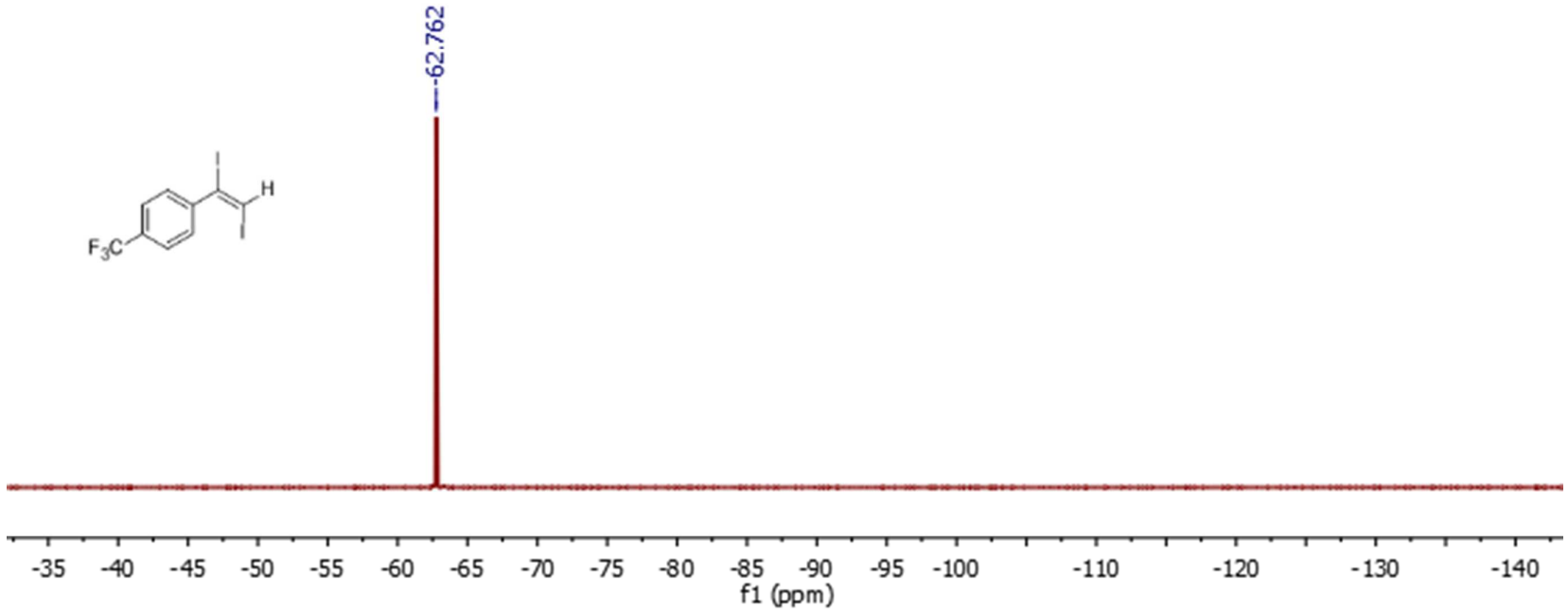
NMR Spectra of Compound 3f



^{1}H NMR (400MHz, $CDCl_3$) spectrum of **3f**

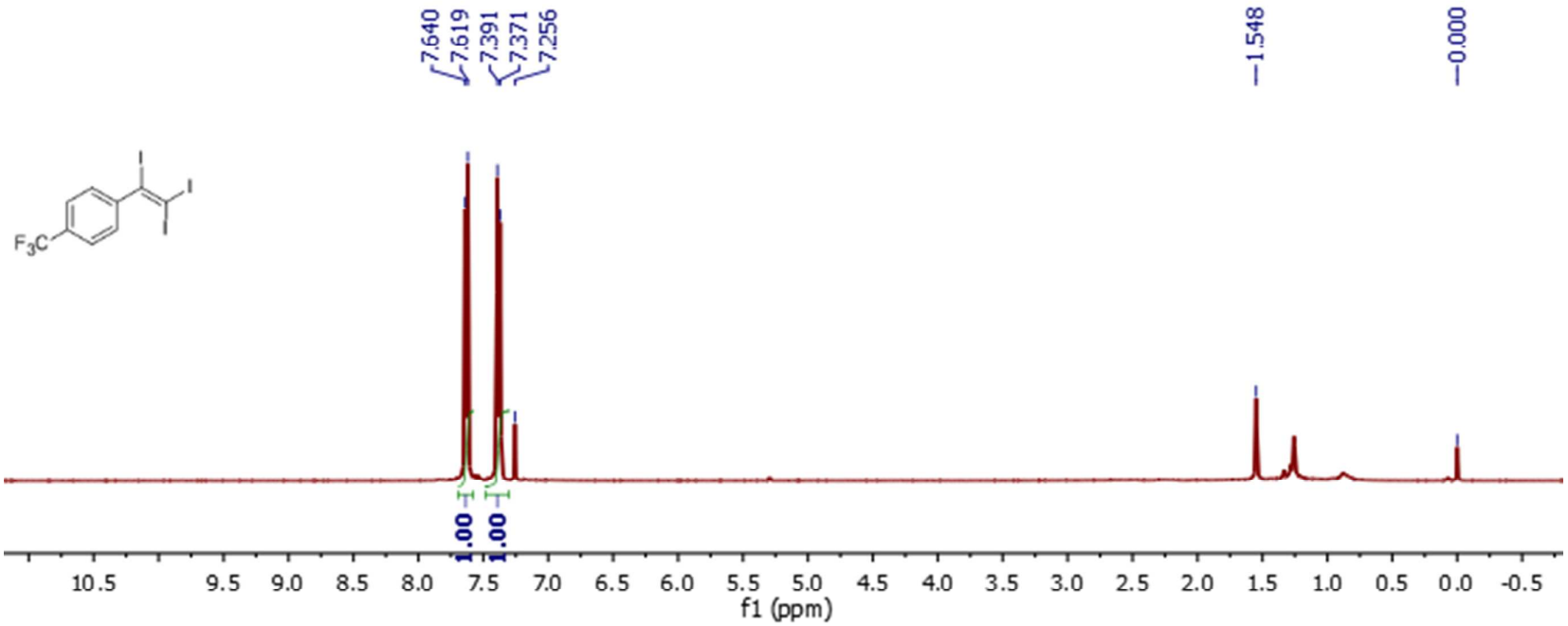


$^{13}C\{^{1}H\}$ NMR (100MHz, $CDCl_3$) spectrum of **3f**



^{19}FNMR (376 MHz, $CDCl_3$) spectrum of **3f**

NMR Spectra of Compound 4f



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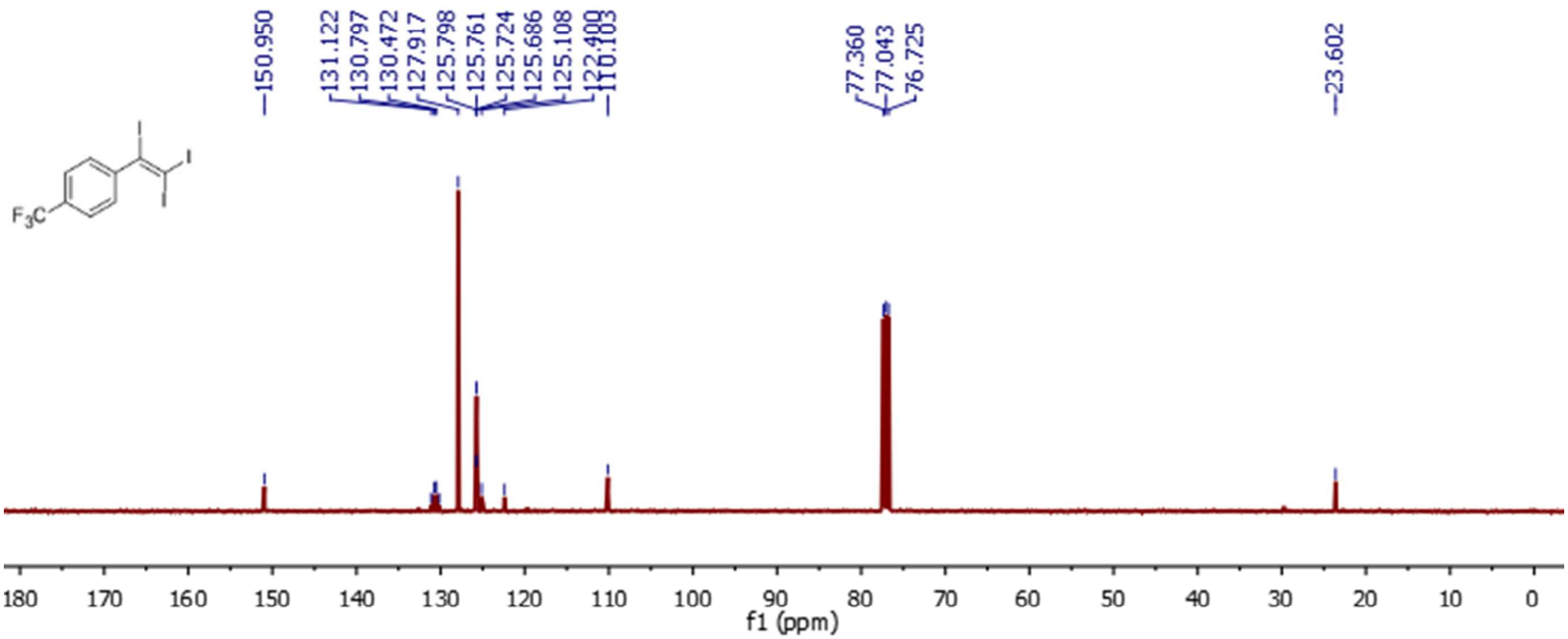
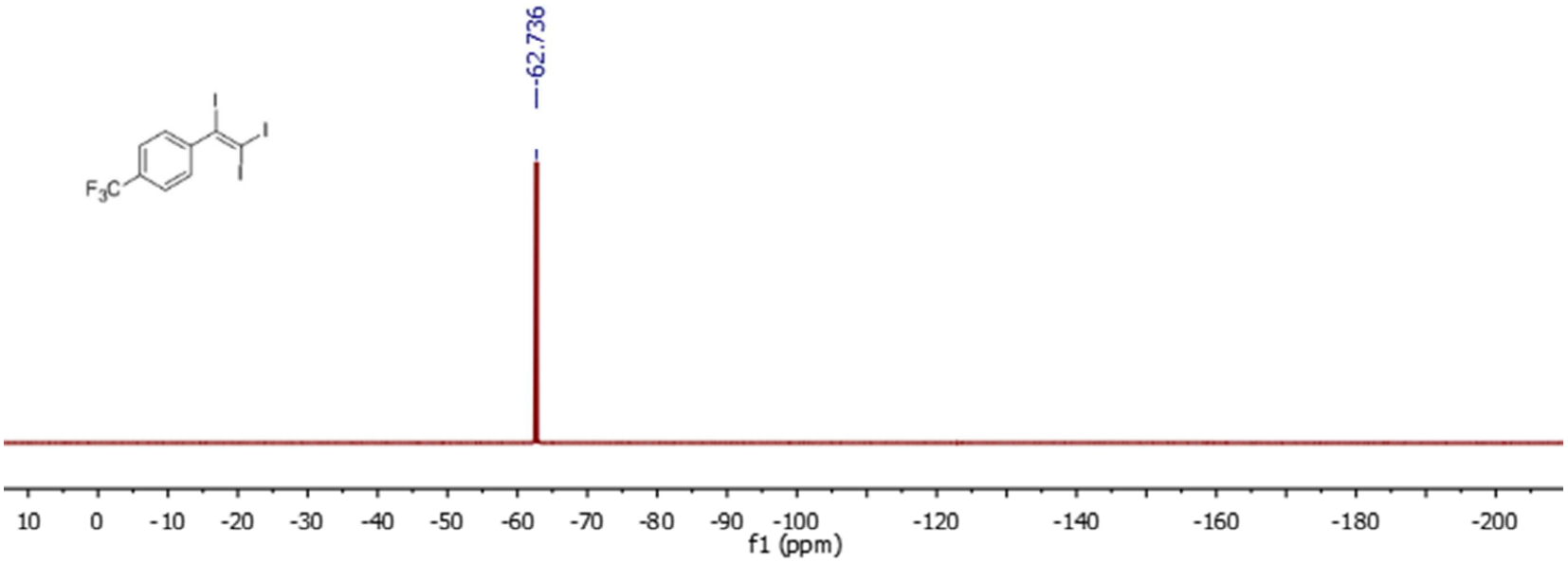
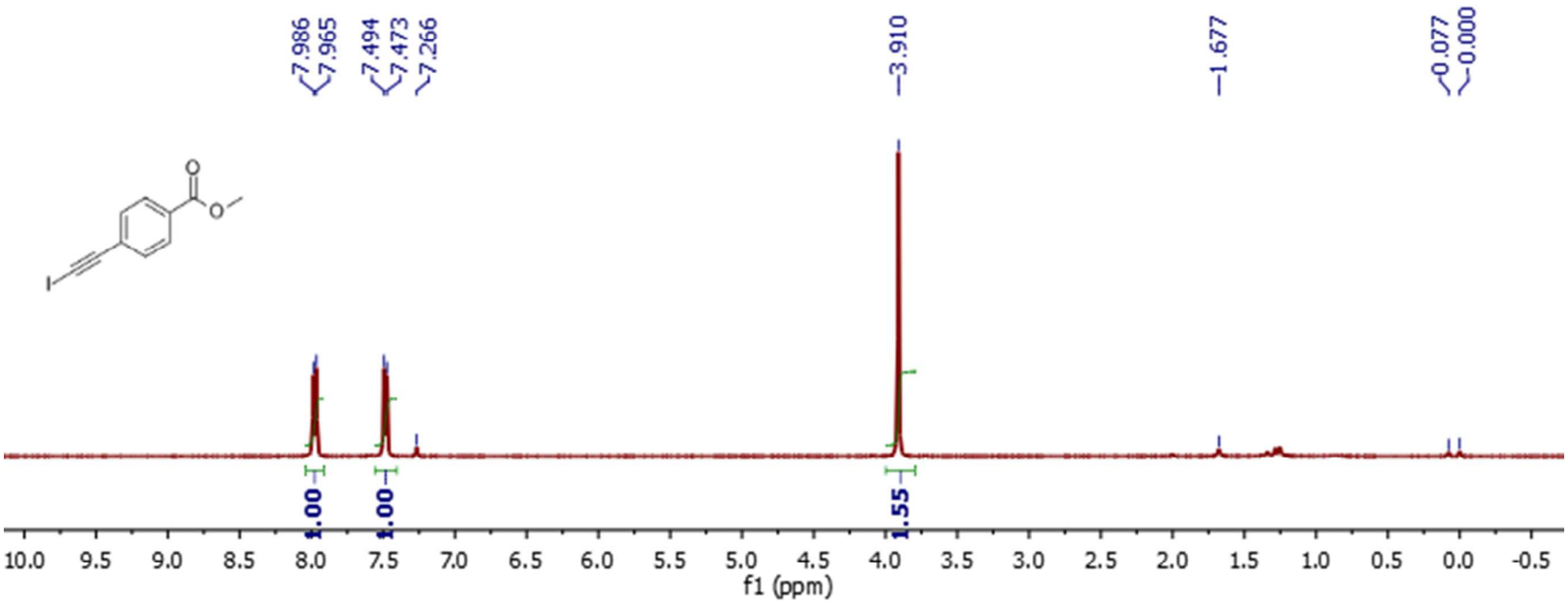


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **4f**

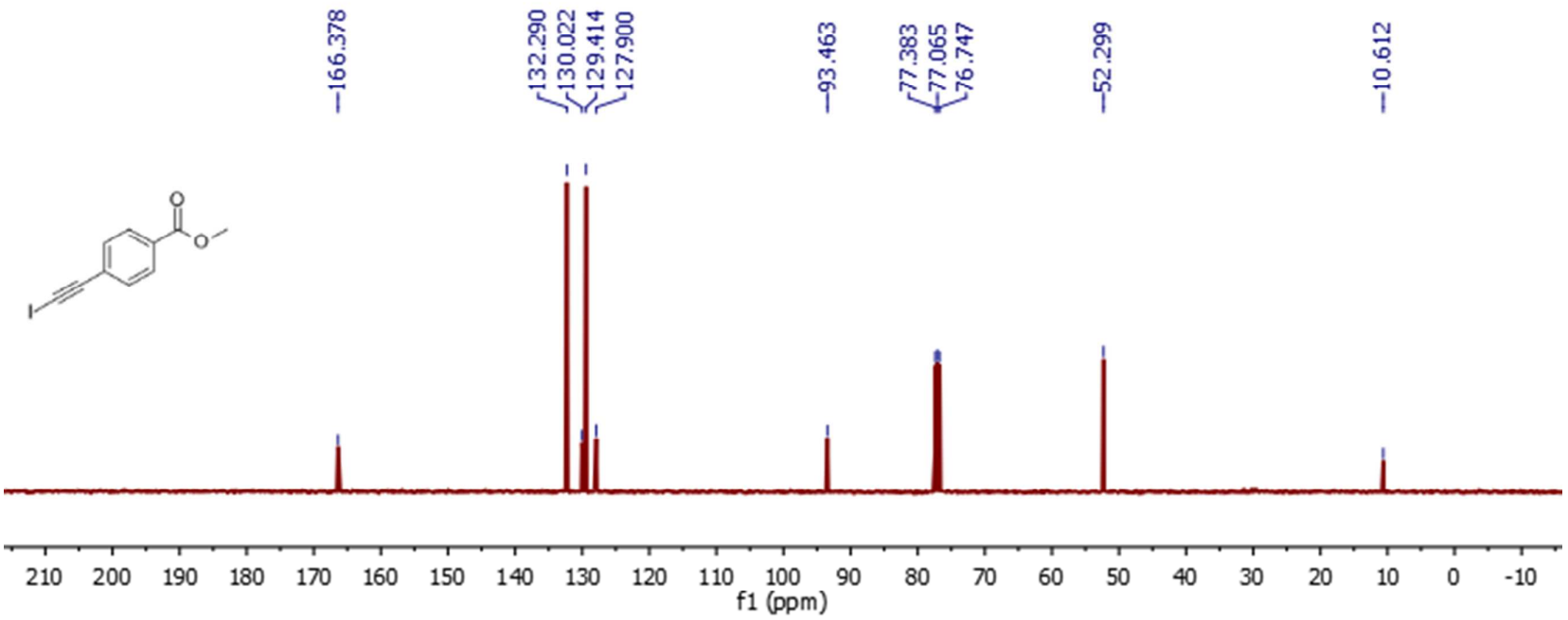


^{19}FNMR (376 MHz, $CDCl_3$) spectrum of **4f**

NMR Spectra of Compound 2g

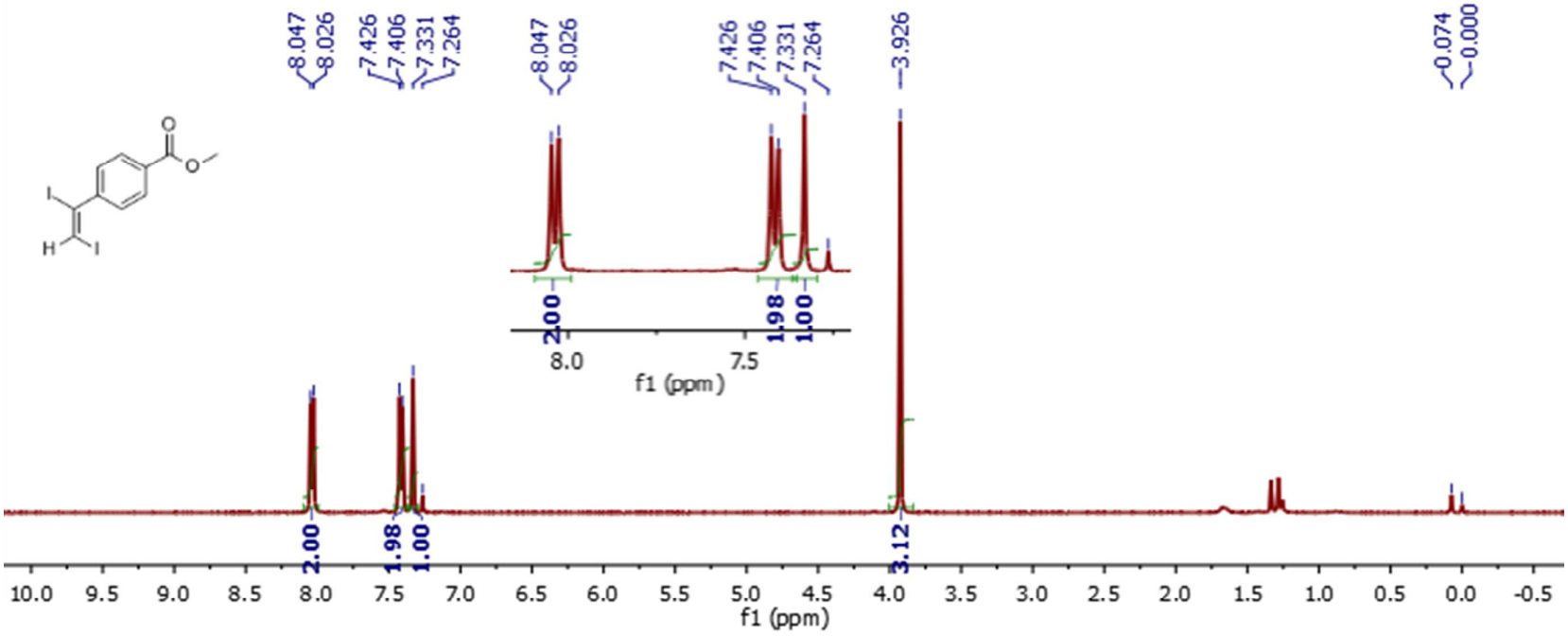


^{1}H NMR (400MHz, $CDCl_3$) spectrum of **2g**

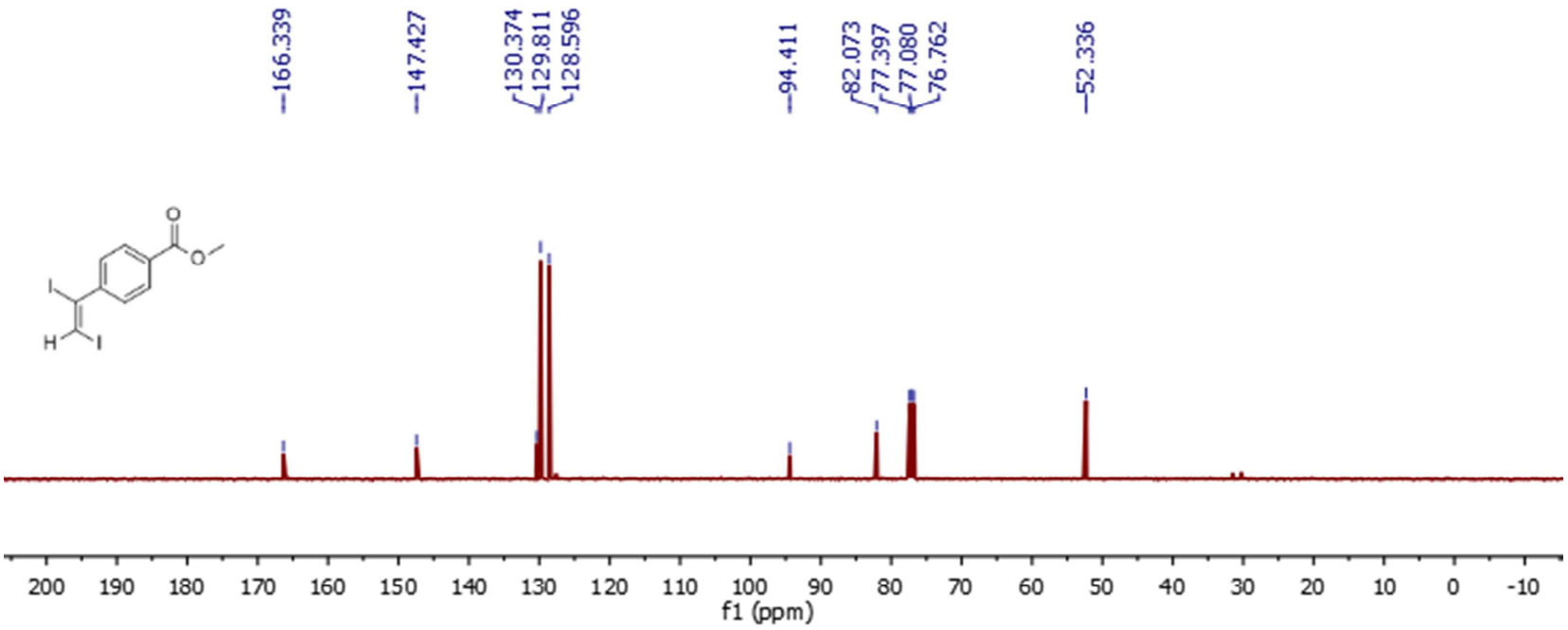


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **2g**

NMR Spectra of Compound 3g

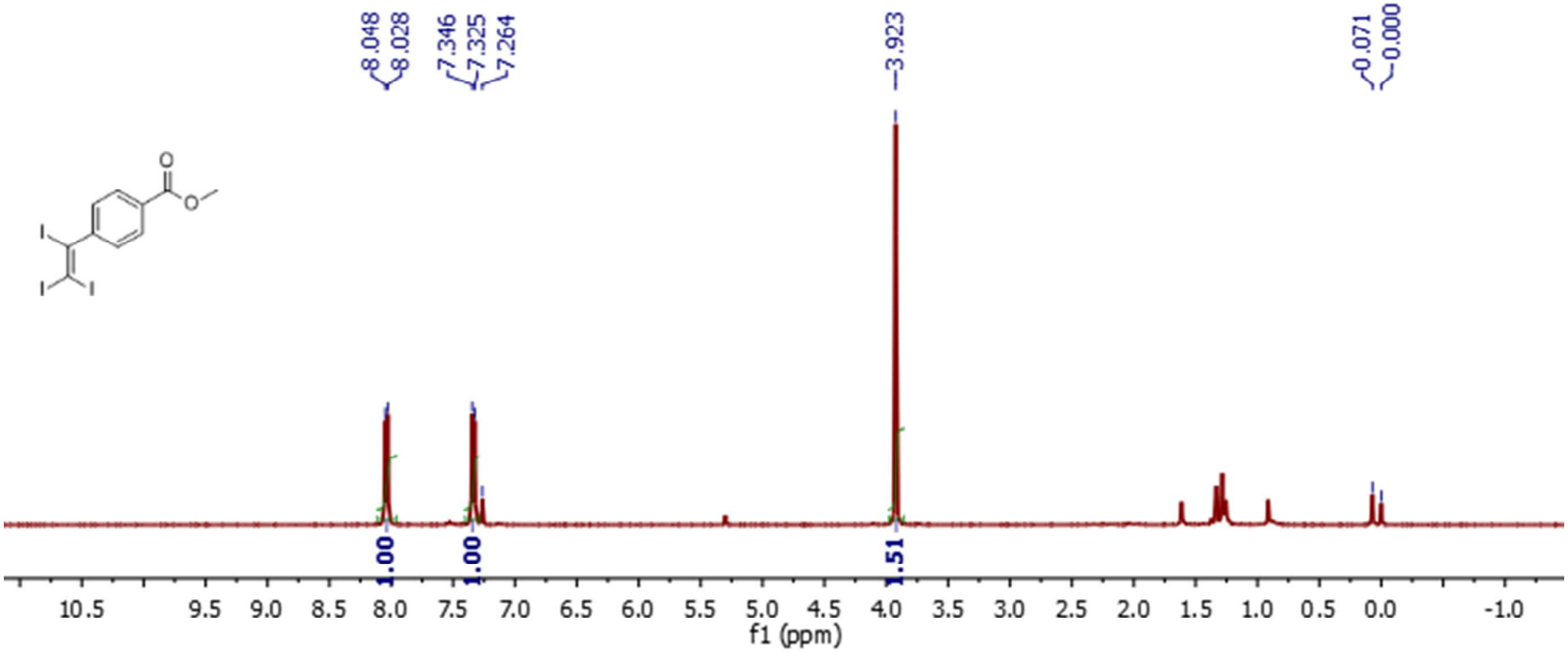


^{1}H NMR (400MHz, $CDCl_3$) spectrum of **3g**

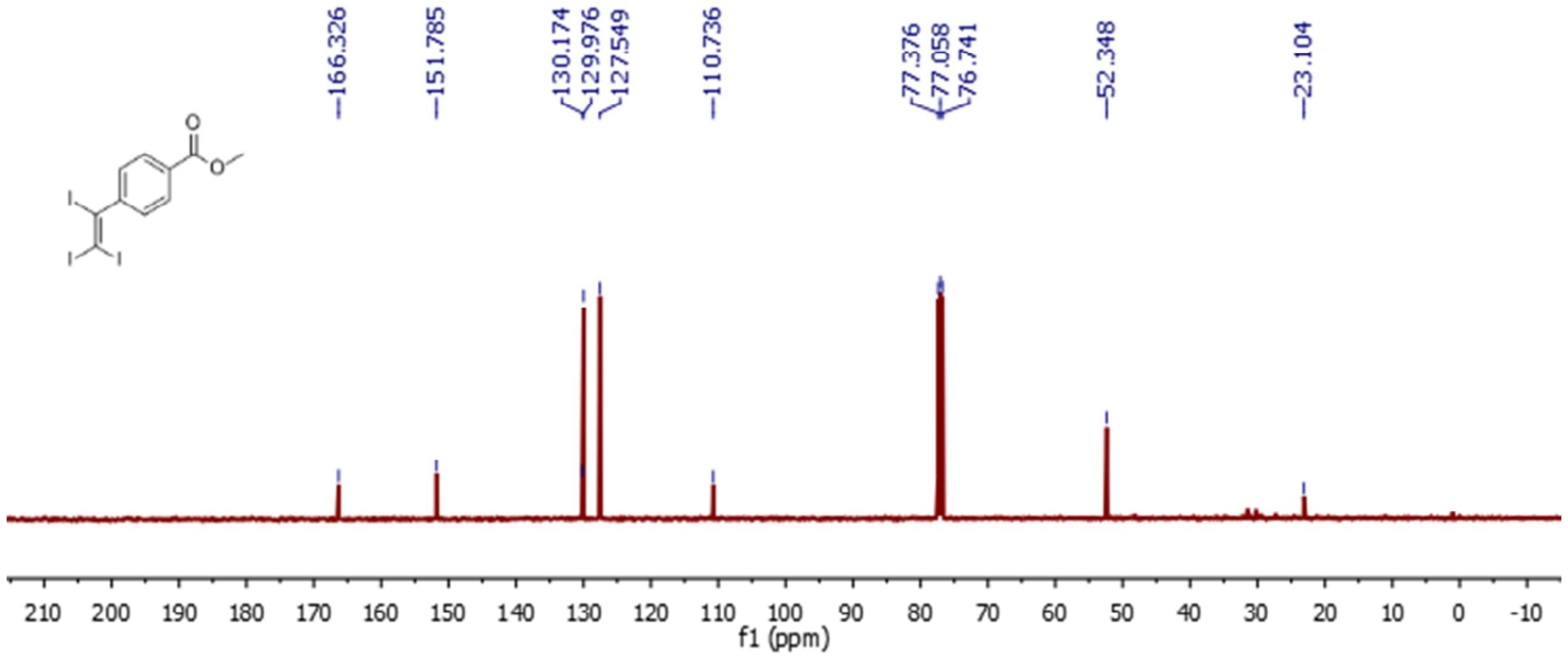


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **3g**

NMR Spectra of Compound 4g

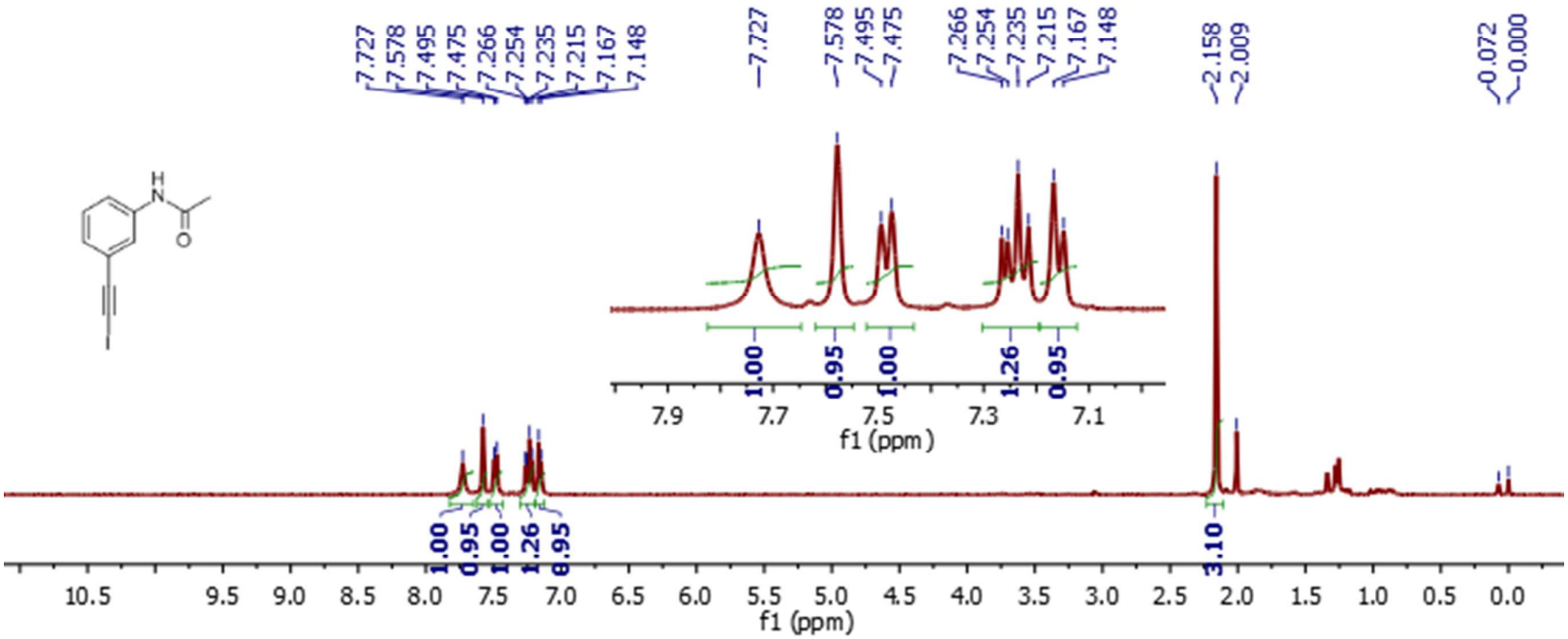


^{1}H NMR (400MHz, $CDCl_3$) spectrum of **4g**

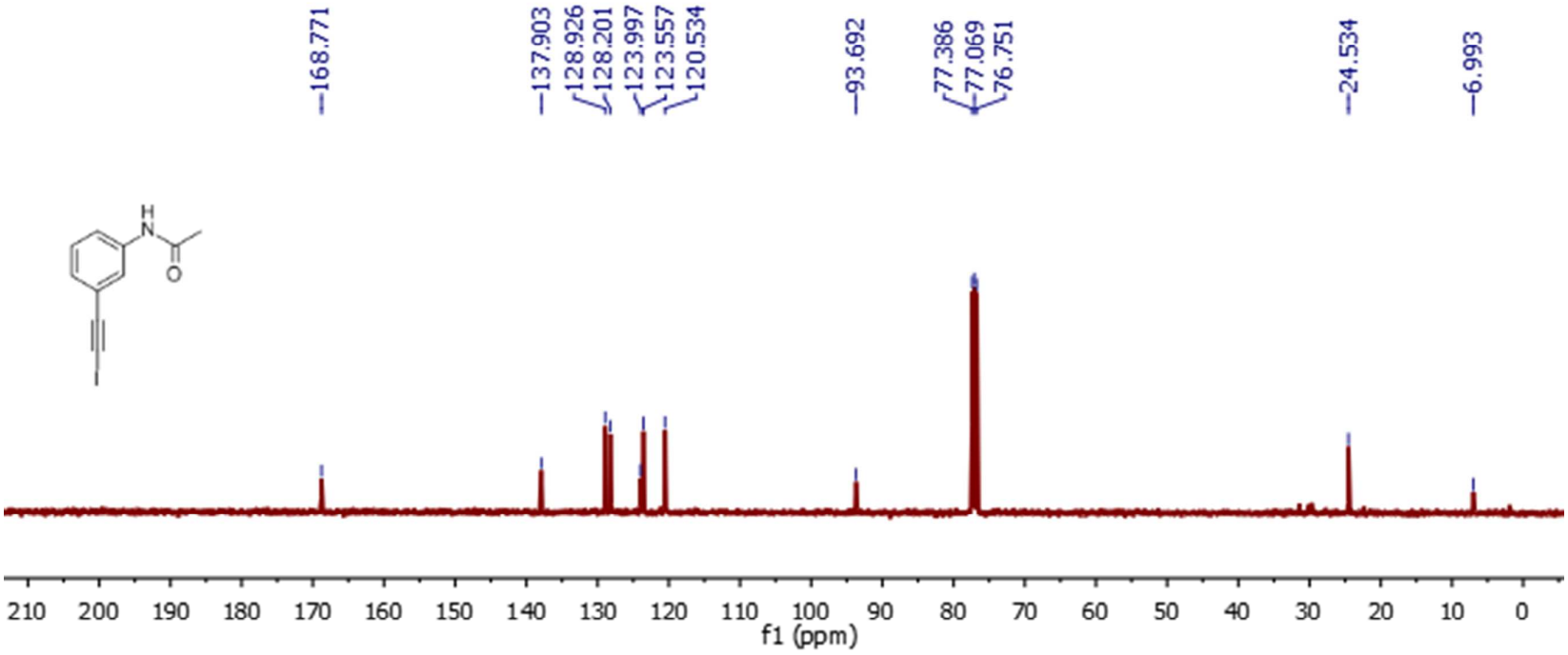


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **4g**

NMR Spectra of Compound 2h

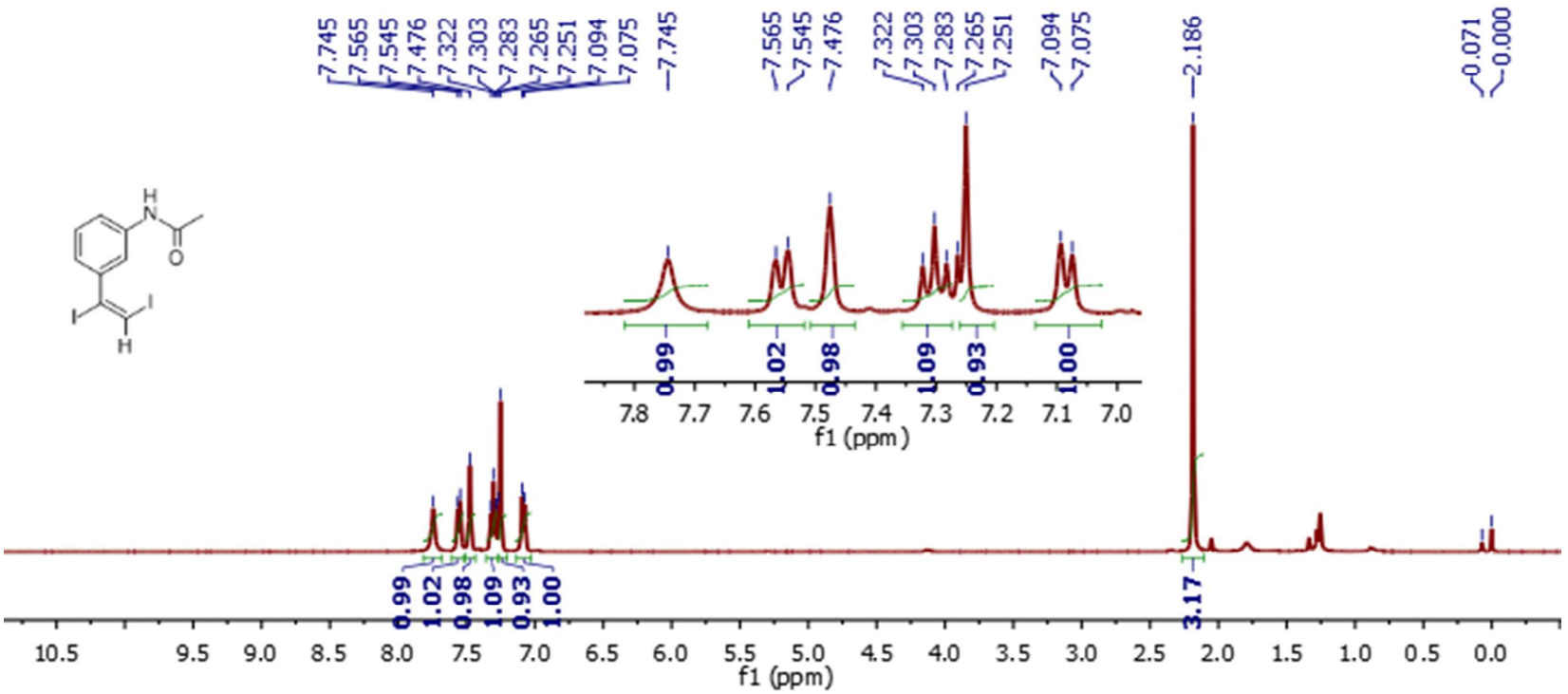


^{1}H NMR (400MHz, $CDCl_3$) spectrum of **2h**

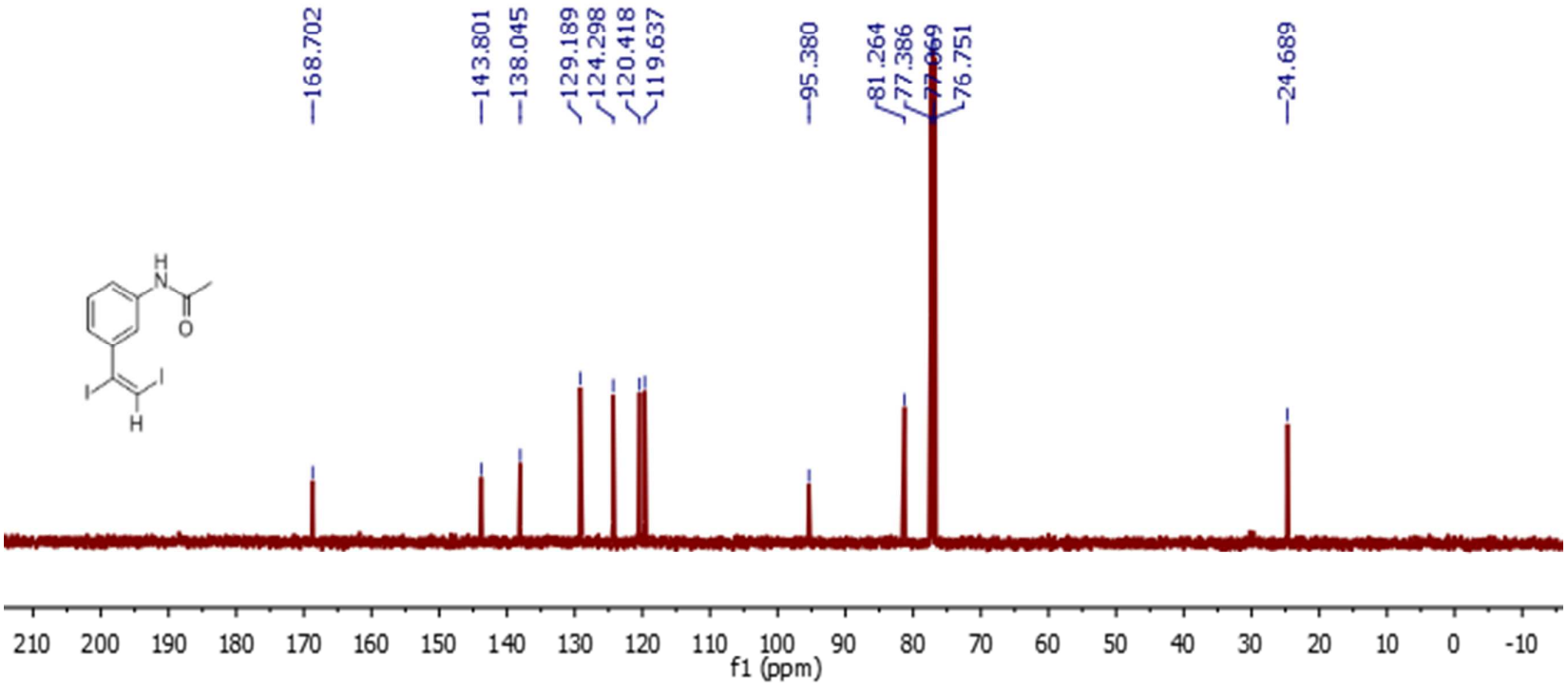


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **2h**

NMR Spectra of Compound 3h

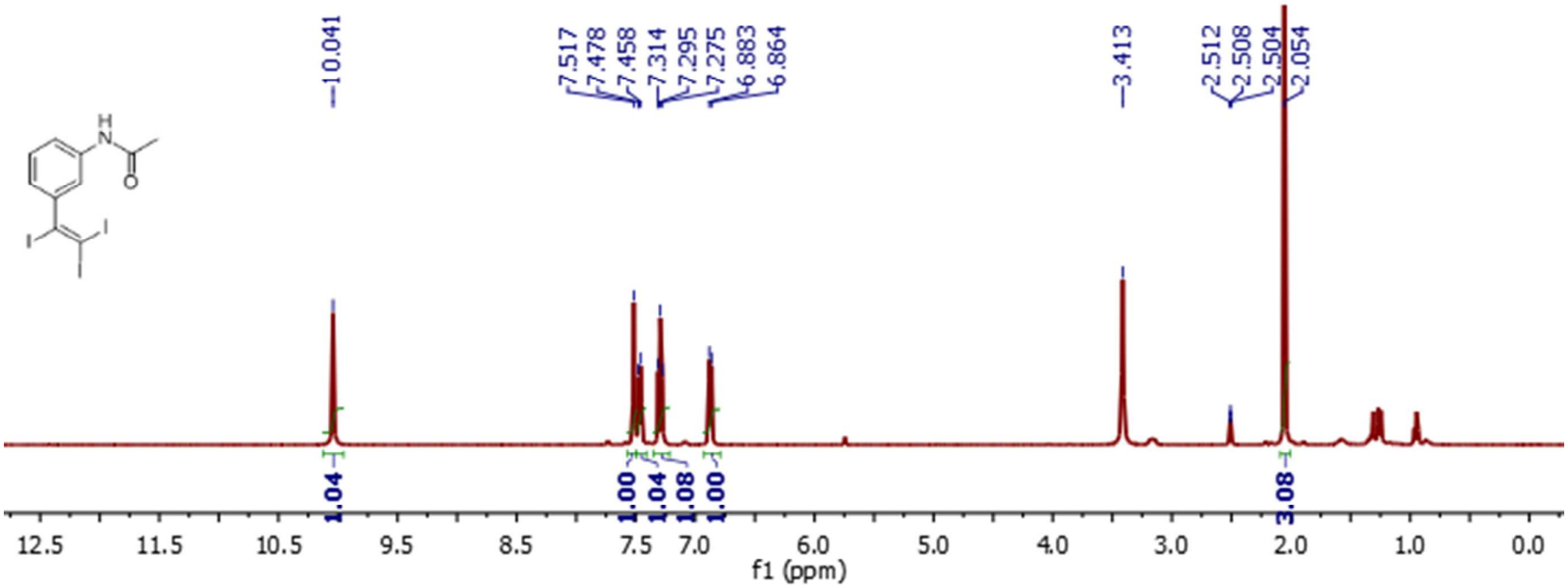


^{1}H NMR (400MHz, $CDCl_3$) spectrum of **3h**

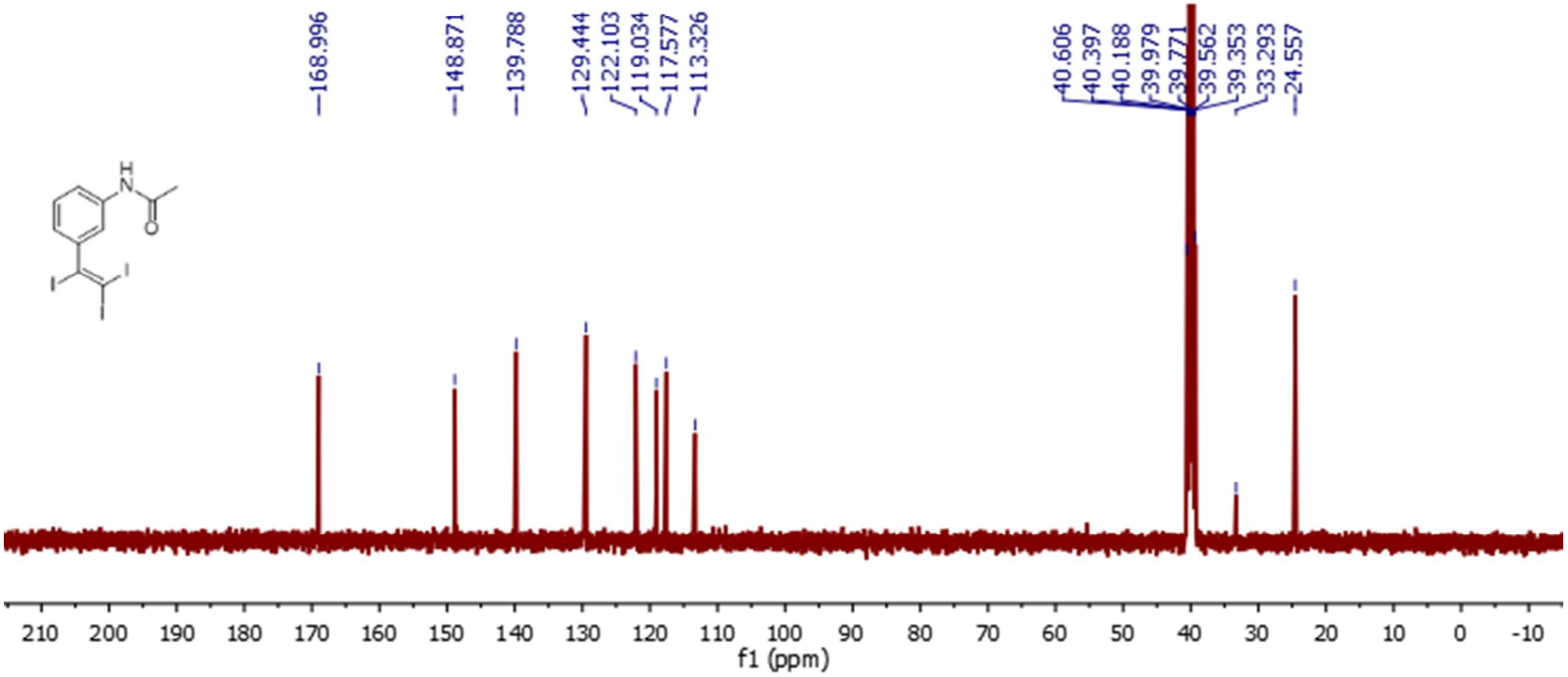


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **3h**

NMR Spectra of Compound 4h

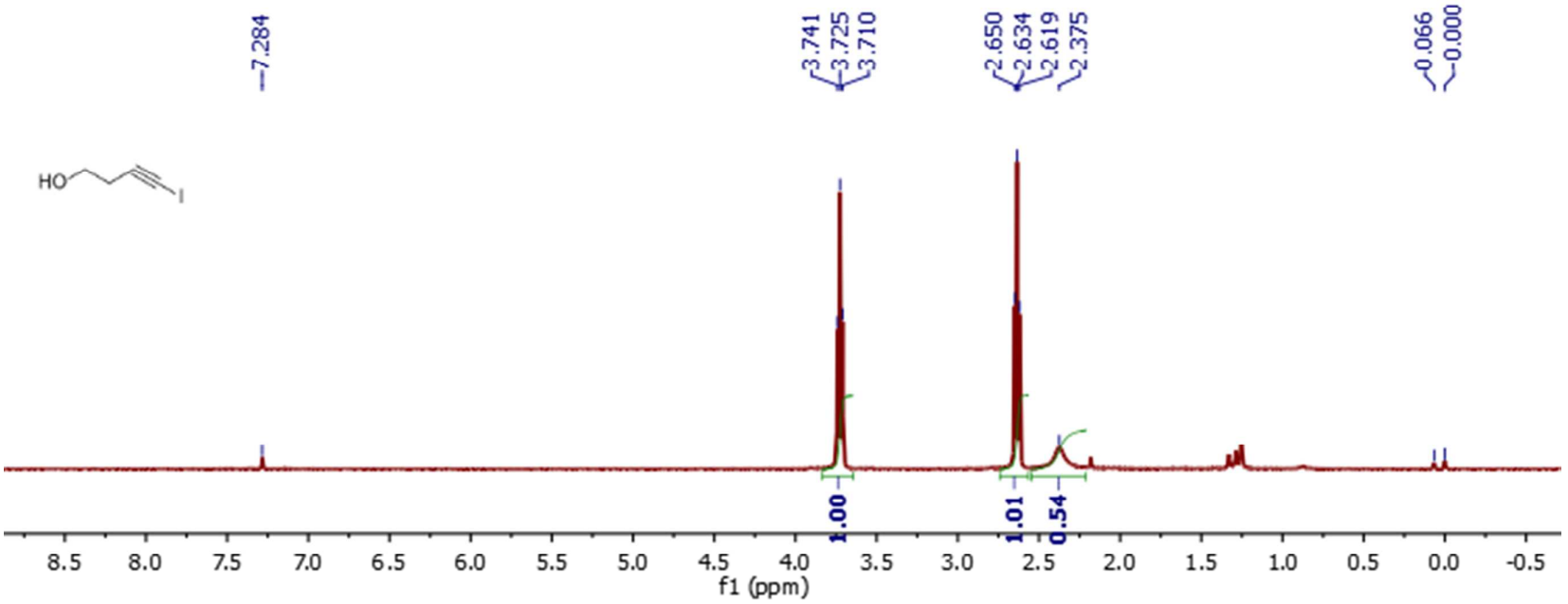


^{1}H NMR (400MHz, DMSO-d_6) spectrum of **4h**

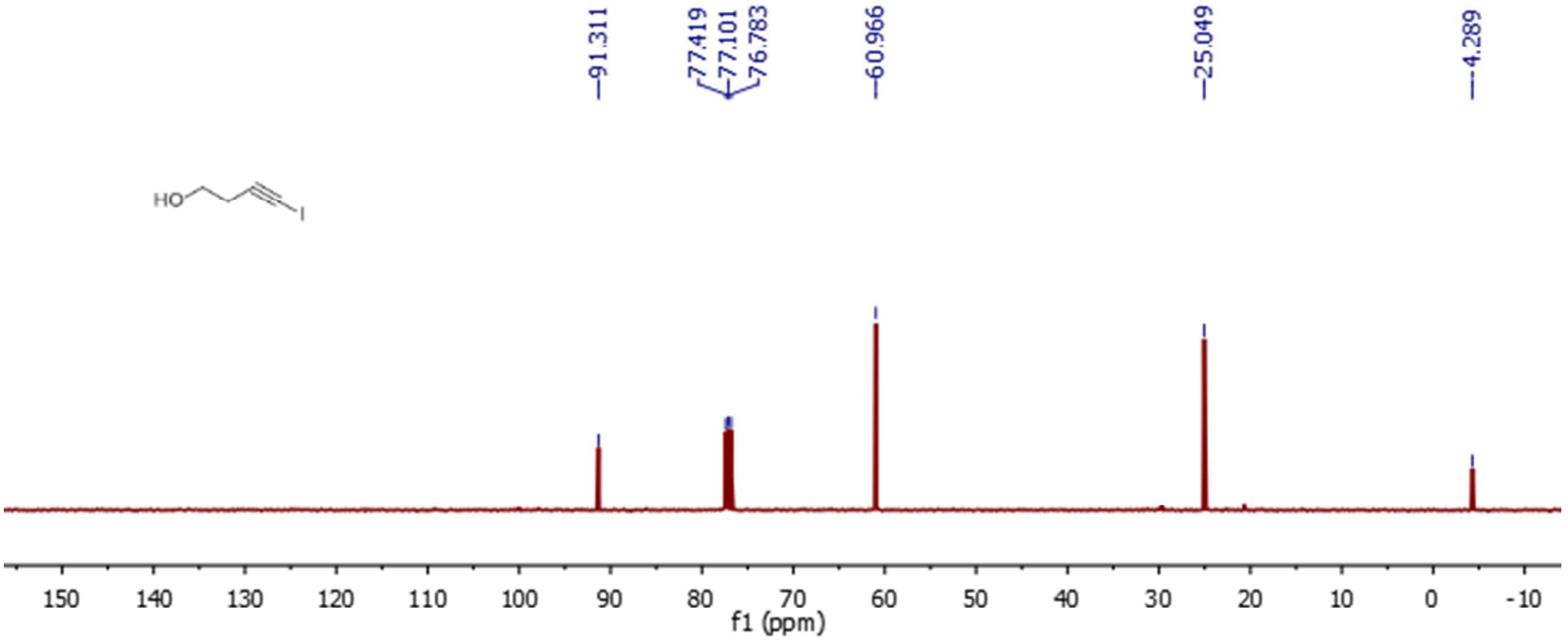


$^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) spectrum of **4h**

NMR Spectra of Compound 2i

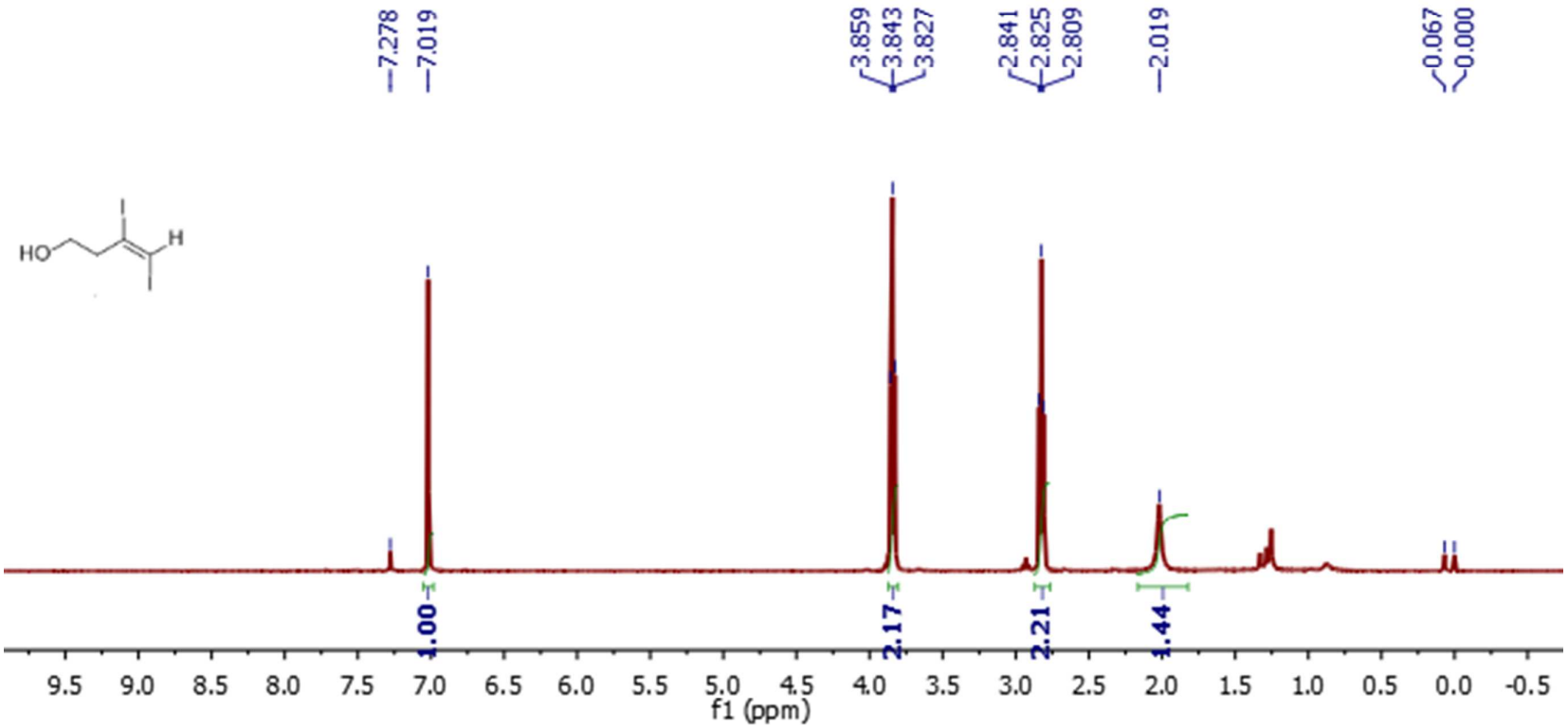


^{1}H NMR (400MHz, $CDCl_3$) spectrum of **2i**

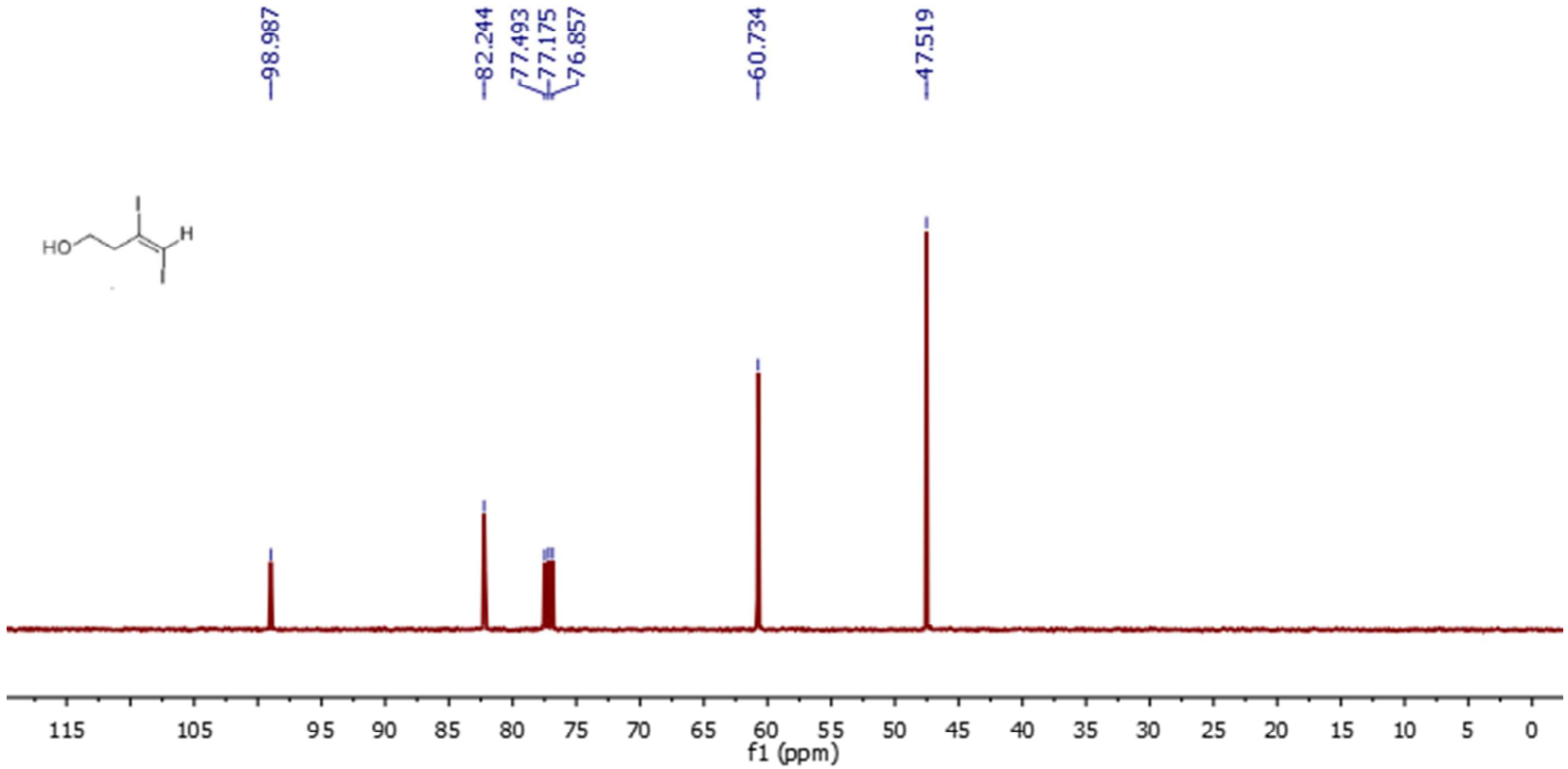


$^{13}C\{^{1}H\}$ NMR (100MHz, $CDCl_3$) spectrum of **4i**

NMR Spectra of Compound 3i

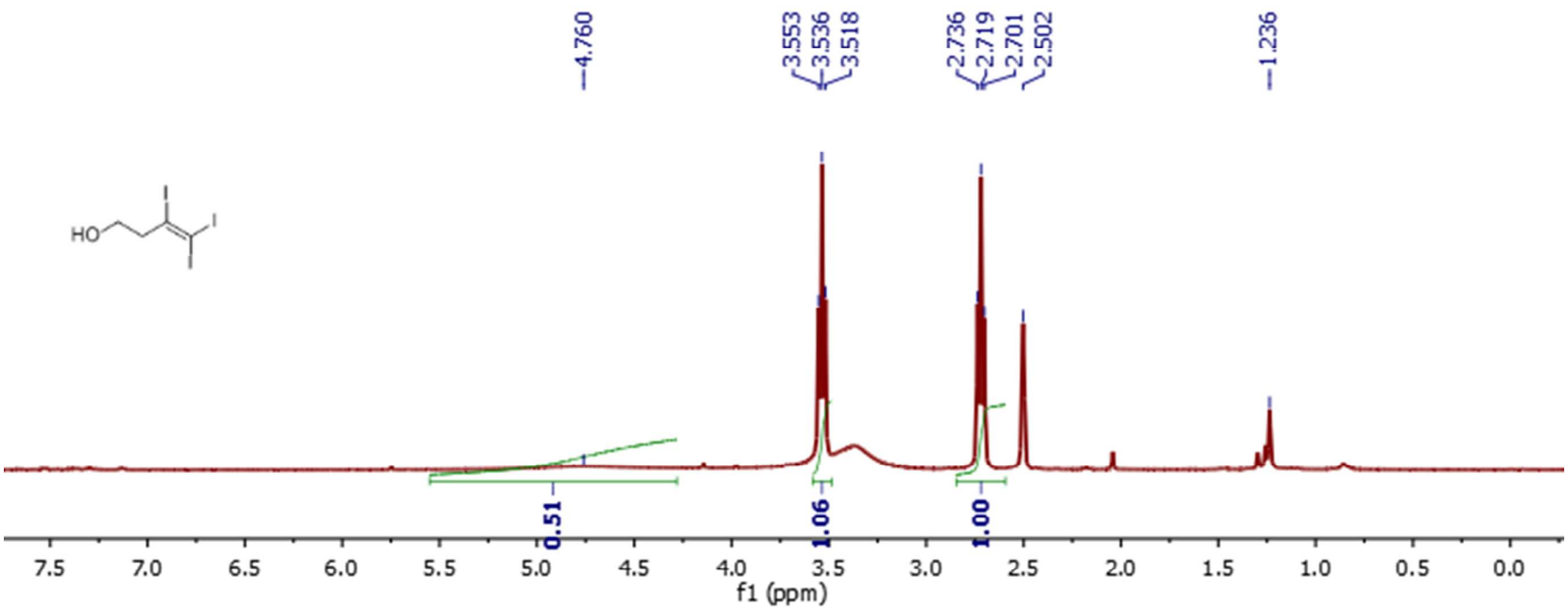


^{1}H NMR (400MHz, $CDCl_3$) spectrum of **3i**

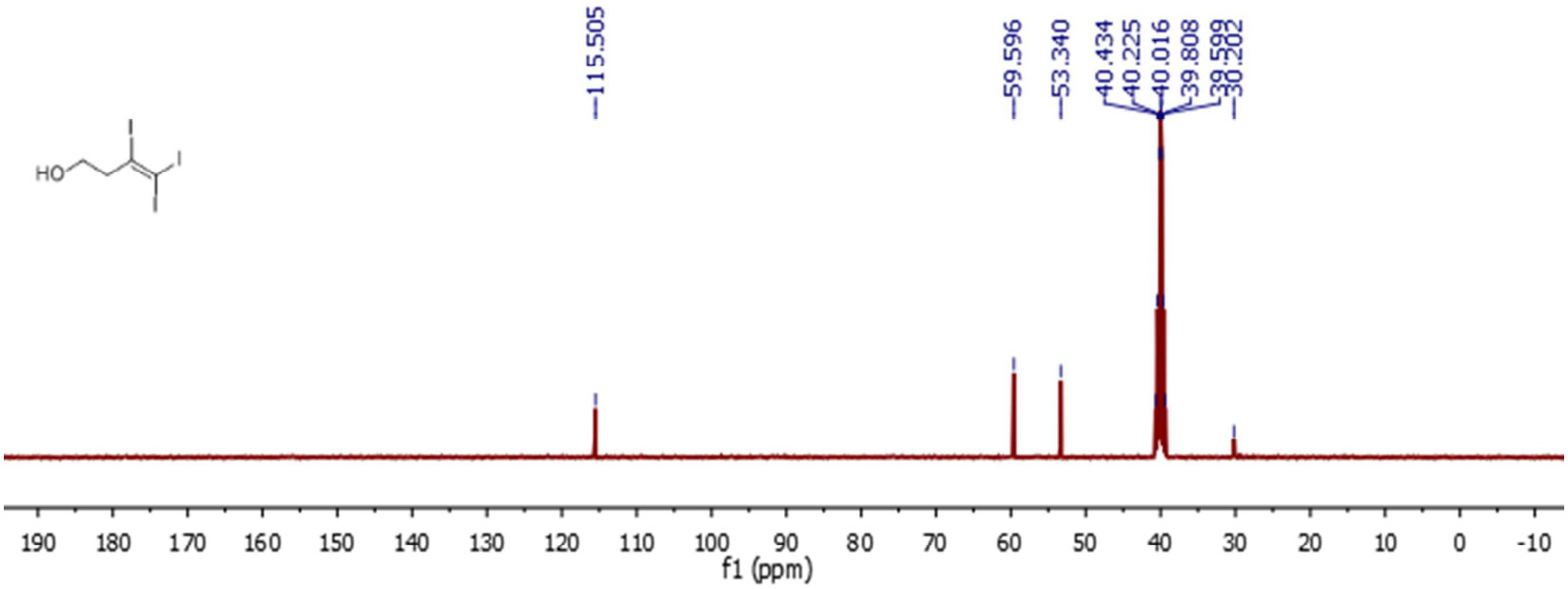


$^{13}C\{^{1}H\}$ NMR (100MHz, $CDCl_3$) spectrum of **3i**

NMR Spectra of Compound 4i

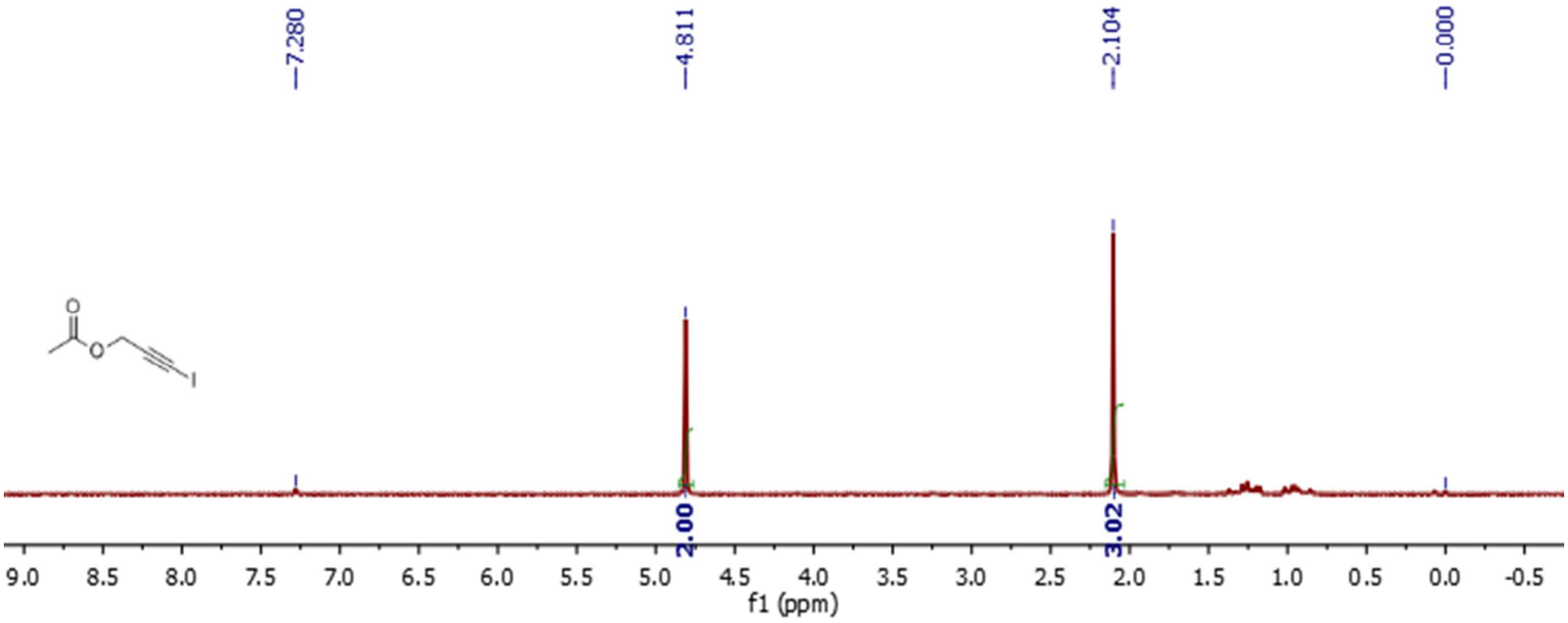


^{1}H NMR (400MHz, DMSO-d_6) spectrum of **4i**

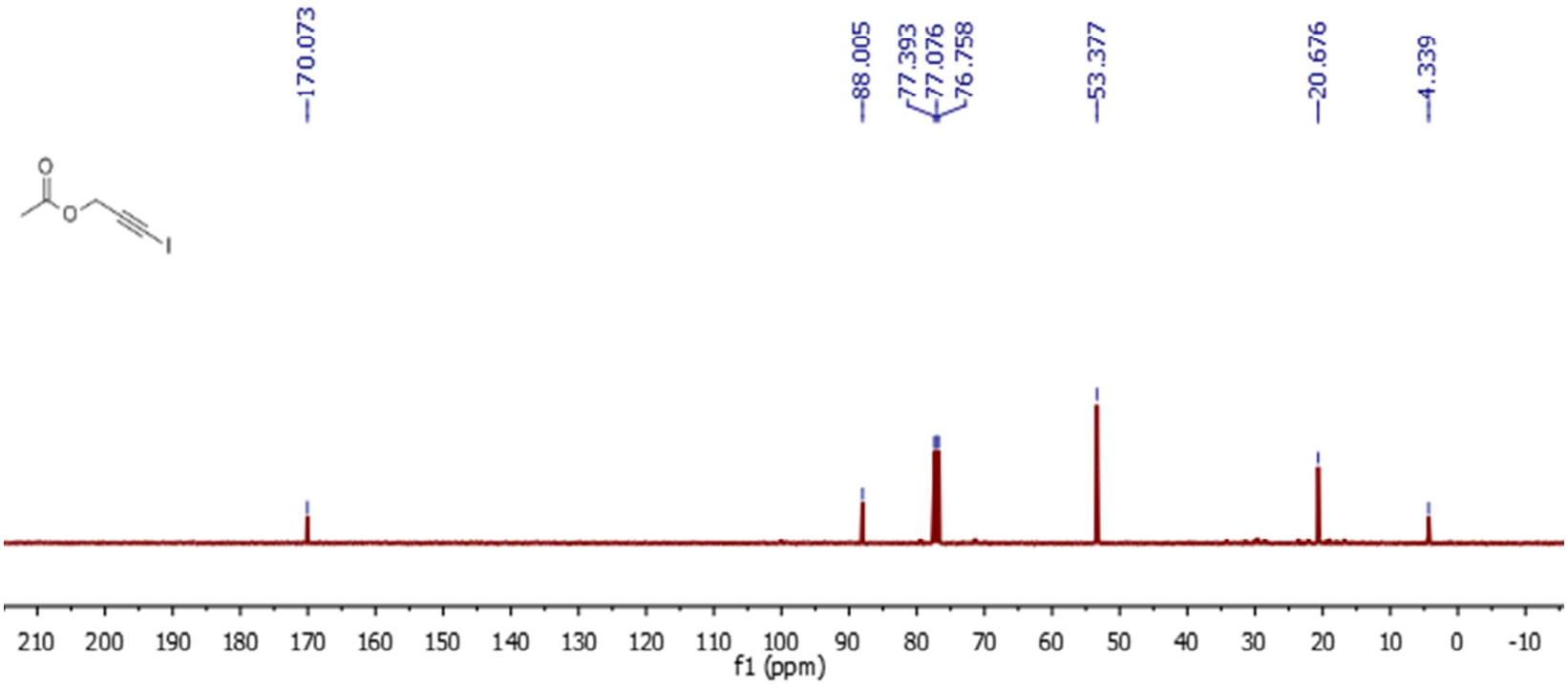


$^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) spectrum of **4i**

NMR Spectra of Compound 2j

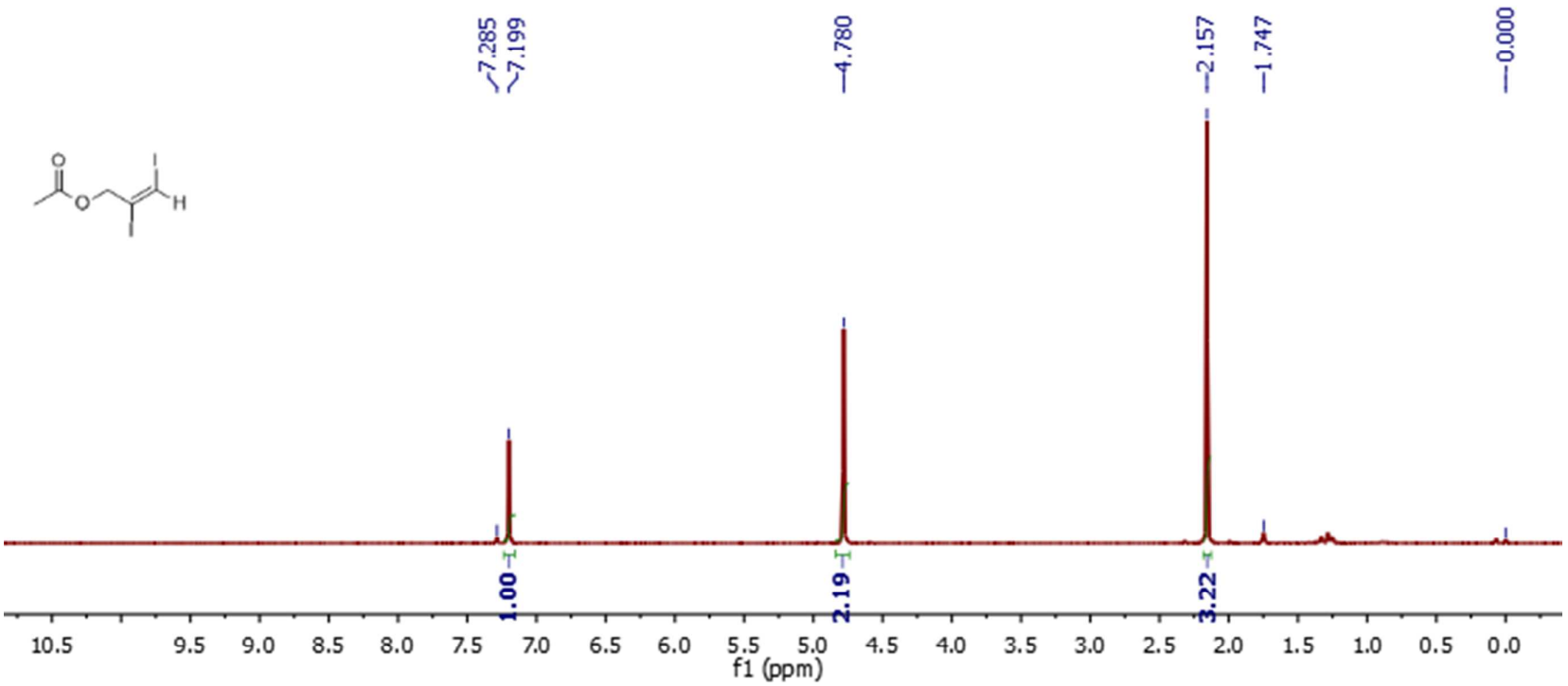


^{1}H NMR (400MHz, $CDCl_3$) spectrum of **2j**

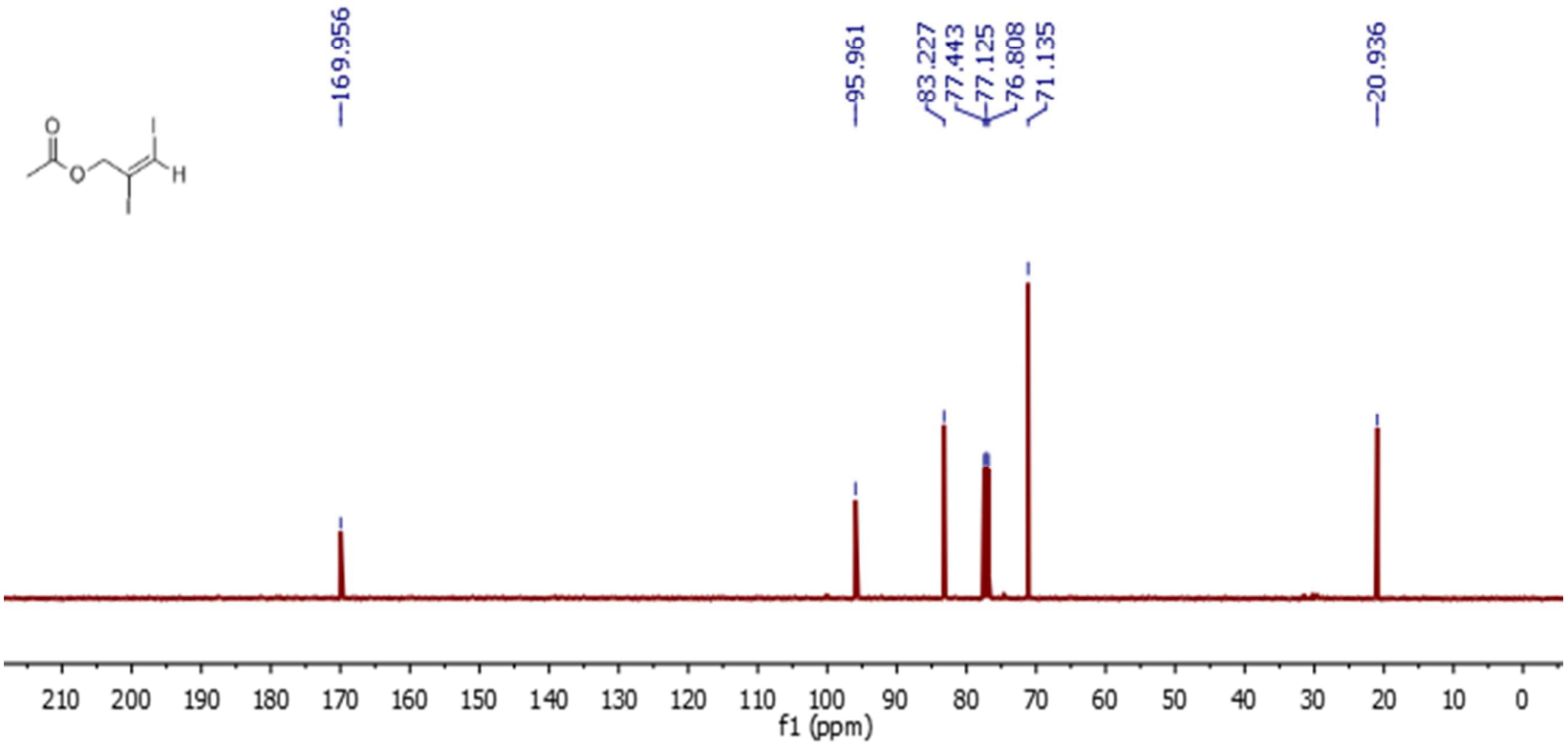


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **2j**

NMR Spectra of Compound 3j

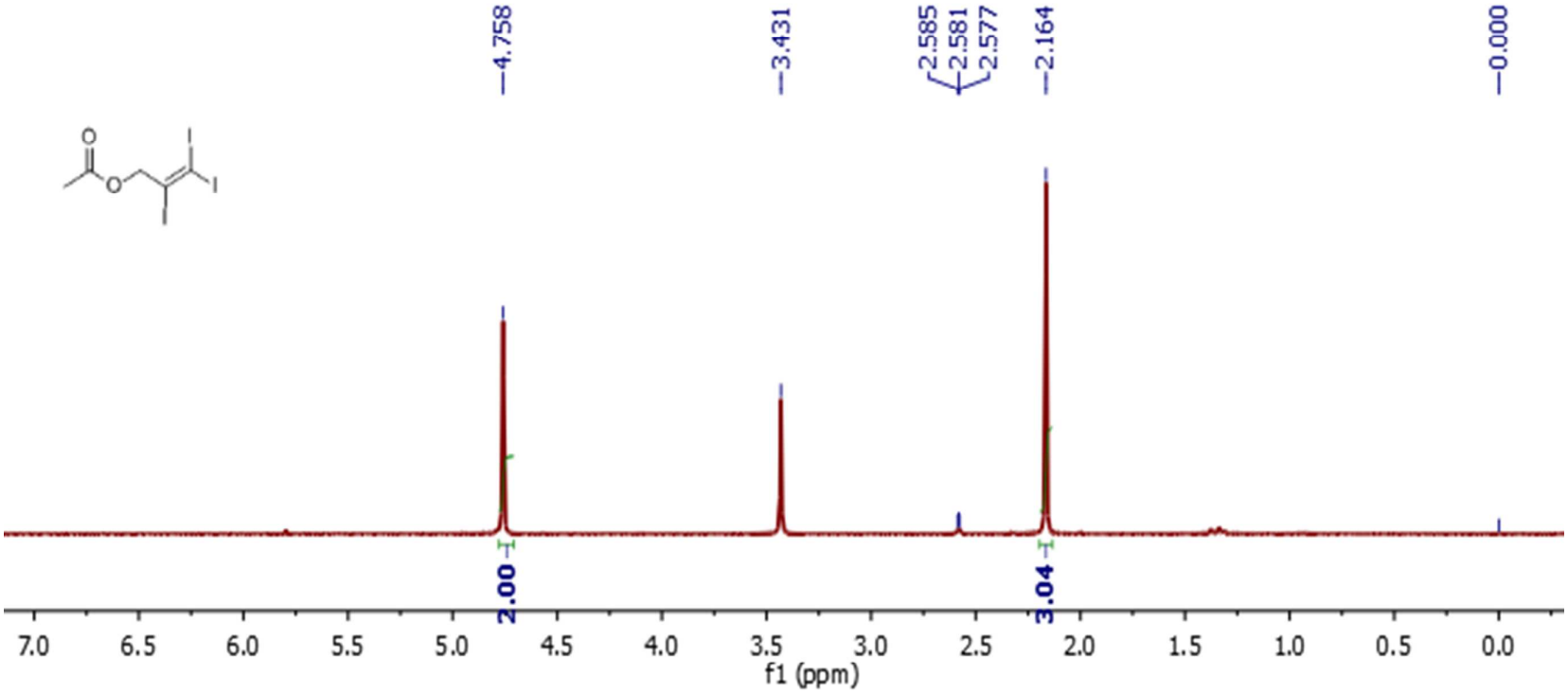


^{1}H NMR (400MHz, $CDCl_3$) spectrum of **3j**

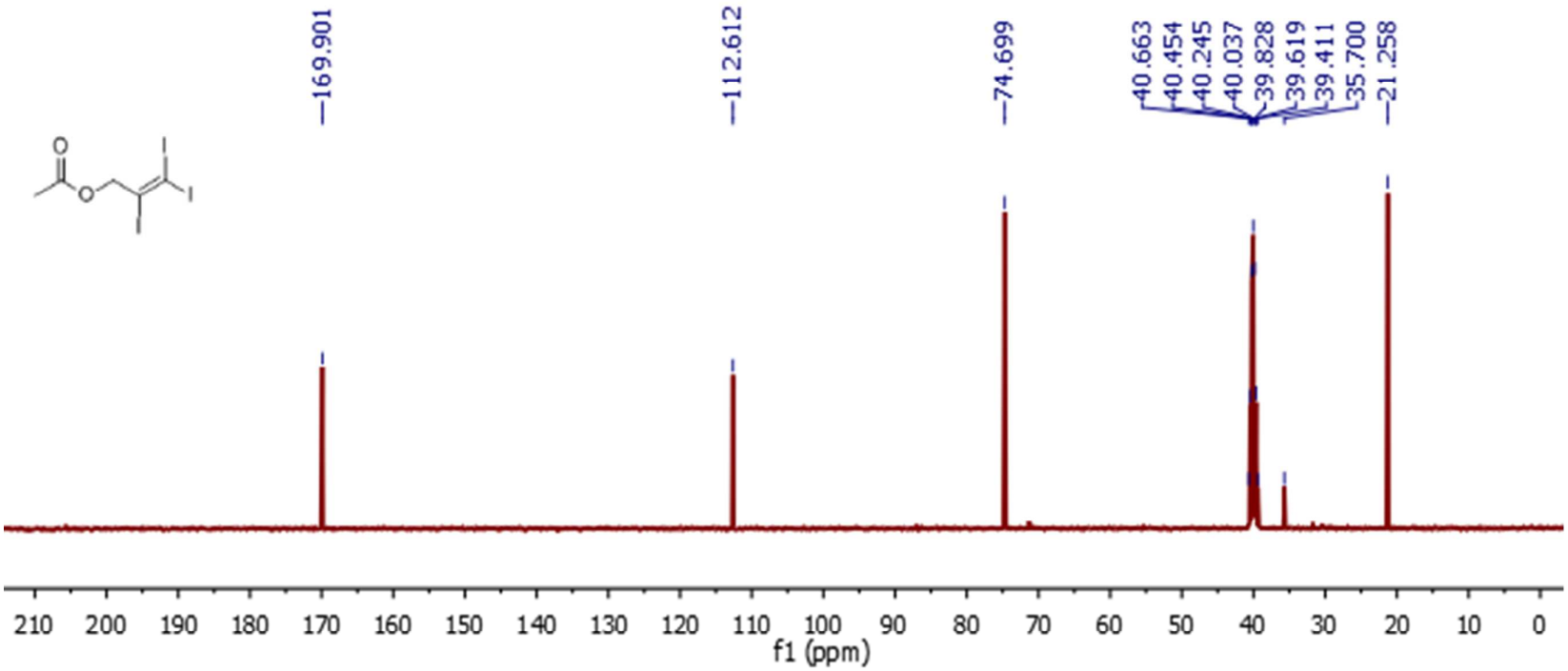


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **3j**

NMR Spectra of Compound 4j

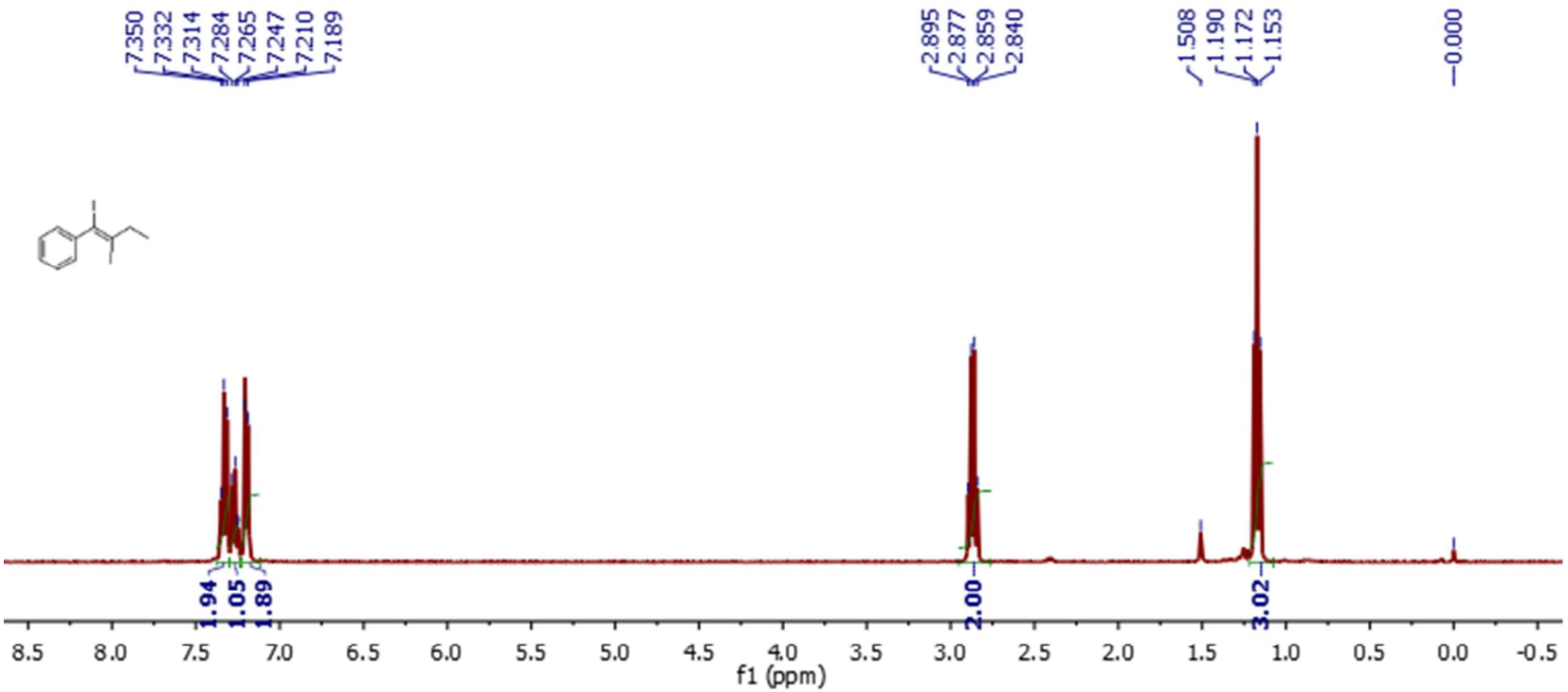


^{1}H NMR (400MHz, $CDCl_3$) spectrum of **4j**

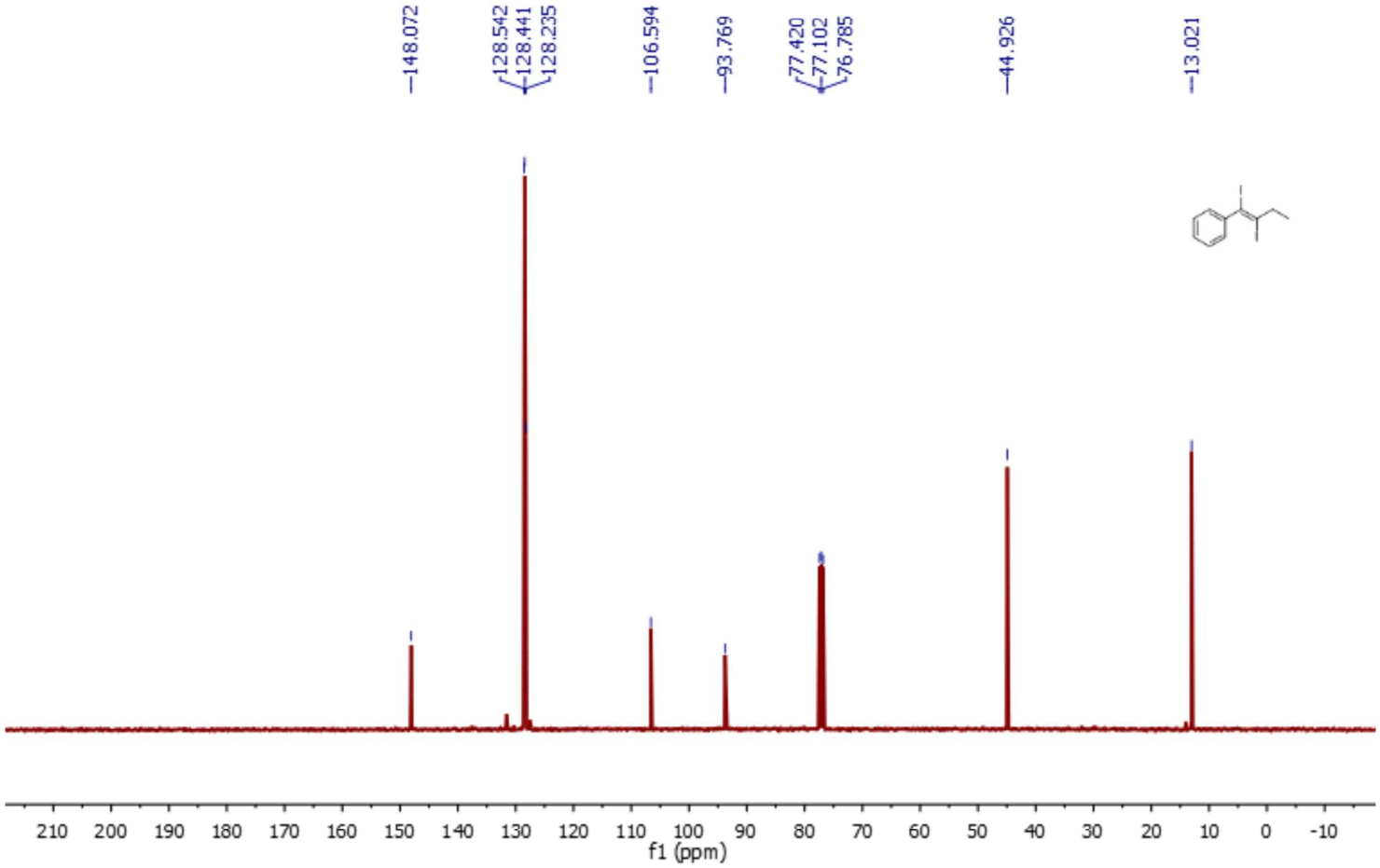


$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **4j**

NMR Spectra of Compound 3k



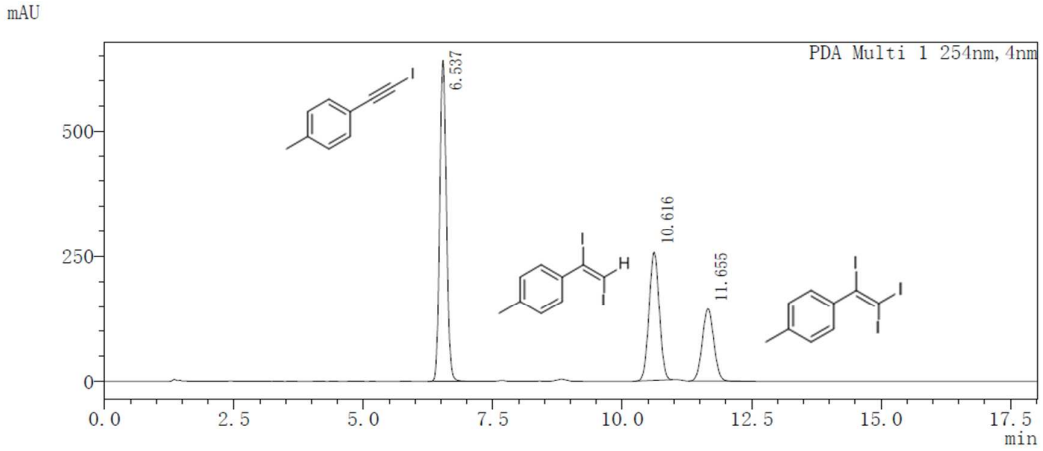
^{1}H NMR (400MHz, $CDCl_3$) spectrum of **3k**



$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) spectrum of **4k**

HPLC Spectra

HPLC Spectrum of **2a, 3a** and **4a**

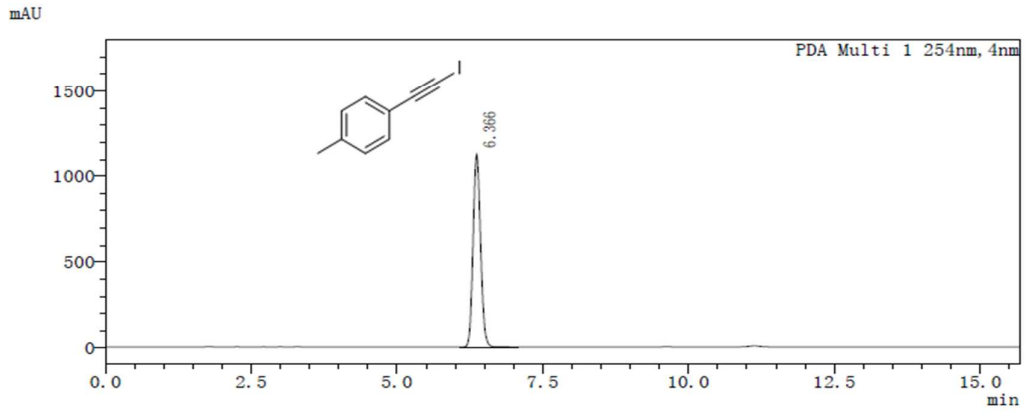


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.537	5736677	642243	49.781		S	
2	10.616	3546464	256588	30.775			
3	11.655	2240616	144750	19.443			
Total		11523757	1043581				

$A_{2a} : A_{3a} : A_{4a} = 2.131 : 1 : 1.472$ (absorbance ratio)

Compound **2a** (furnished by Method **A,** Table 3, entry 1)

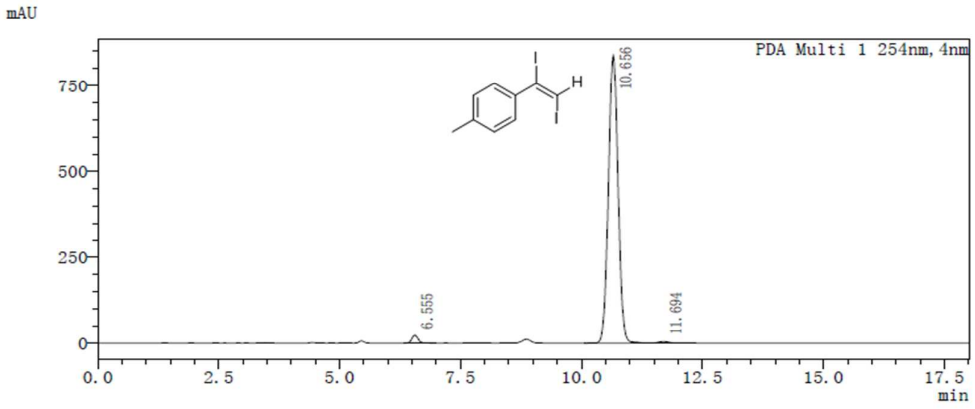


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.366	10139414	1128484	100.000			
Total		10139414	1128484				

2a : **3a** : **4a** = 100 : 0 : 0 (molar ratio)

Compound **3a** (furnished by Method **B**, Table 3, entry 2)

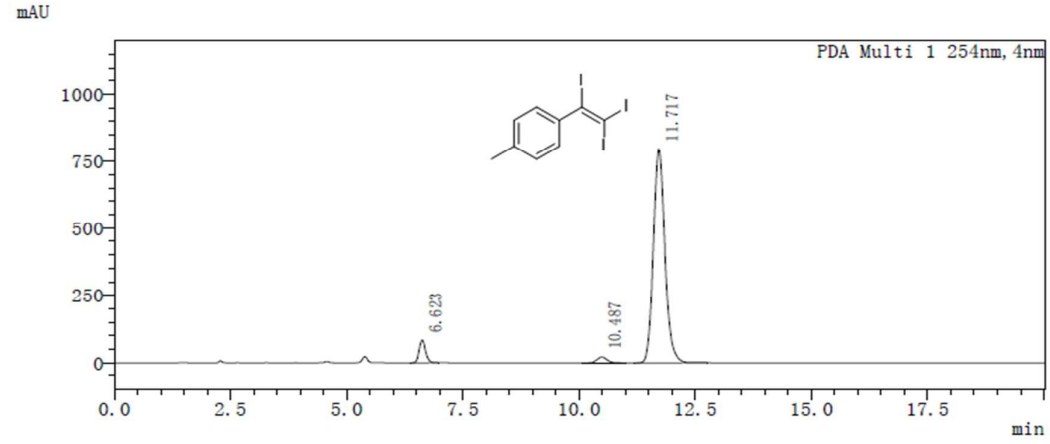


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.555	206794	22875	1.732			
2	10.656	11668850	835900	97.711			
3	11.694	66506	4468	0.557			
Total		11942150	863243				

2a : **3a** : **4a** = 0.8 : 98.8 : 0.4 (molar ratio)

Compound **4a** (furnished by Method **C**, Table 3, entry 3)

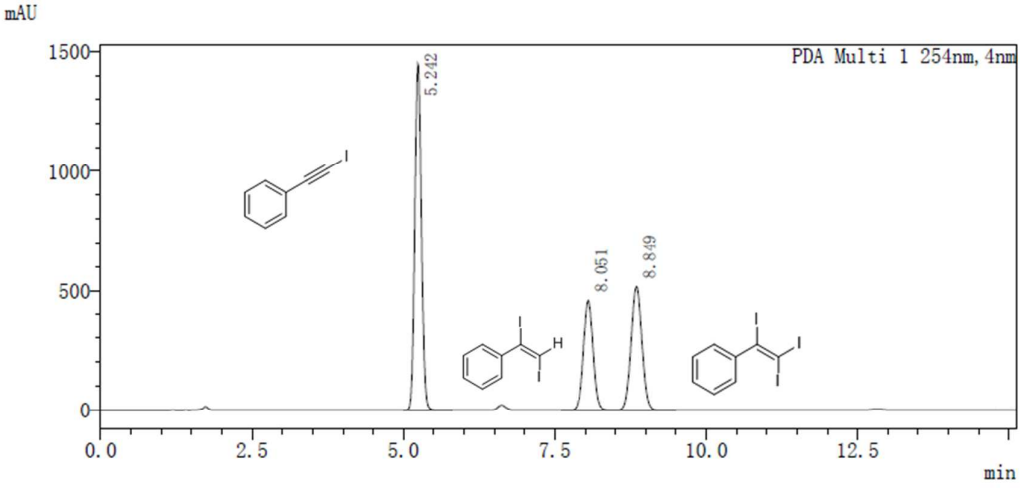


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.623	800127	83411	5.383			
2	10.487	317095	21453	2.133			
3	11.717	13747642	797039	92.484			
Total		14864864	901903				

2a : **3a** : **4a** = 3.7 : 3.2 : 93.1 (molar ratio)

HPLC Spectrum of **2b, 3b** and **4b**

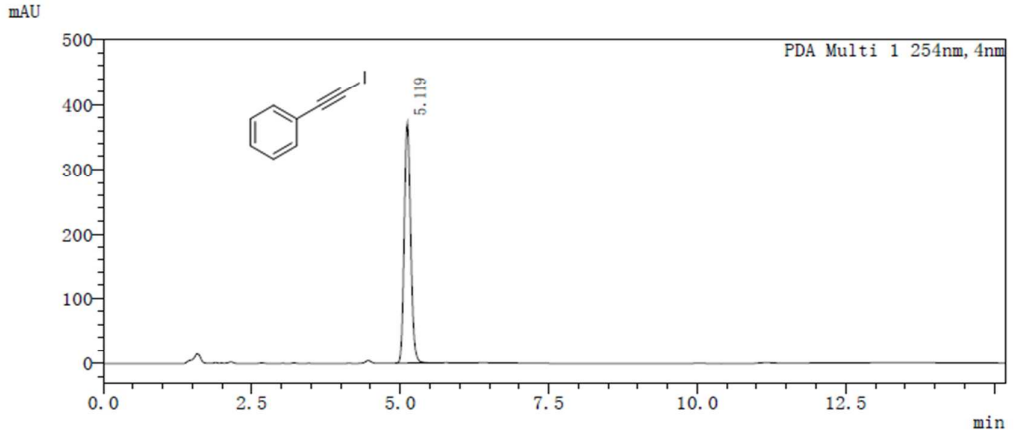


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.242	10959717	1449482	48.713			
2	8.051	5088562	459331	22.617			
3	8.849	6450177	516601	28.669		V	
Total		22498456	2425415				

$A_{\mathbf{2b}} : A_{\mathbf{3b}} : A_{\mathbf{4b}} = 1.948 : 1 : 1.599$ (absorbance ratio)

Compound **2b** (furnished by Method **A**, Table 3, entry 4)

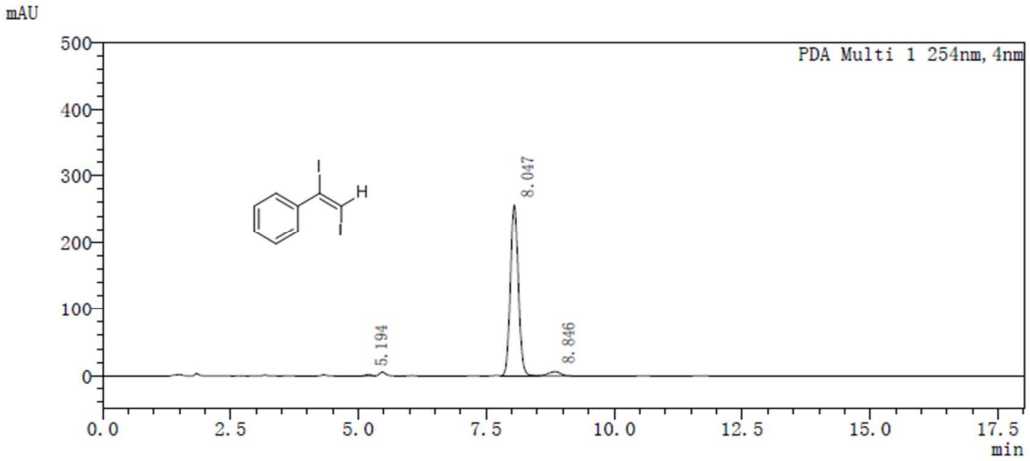


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.119	2778997	371312	100.000			
Total		2778997	371312				

2b : **3b** : **4b** = 100 : 0 : 0 (molar ratio)

Compound **3**b (furnished by Method **B**, Table 3, entry 5)

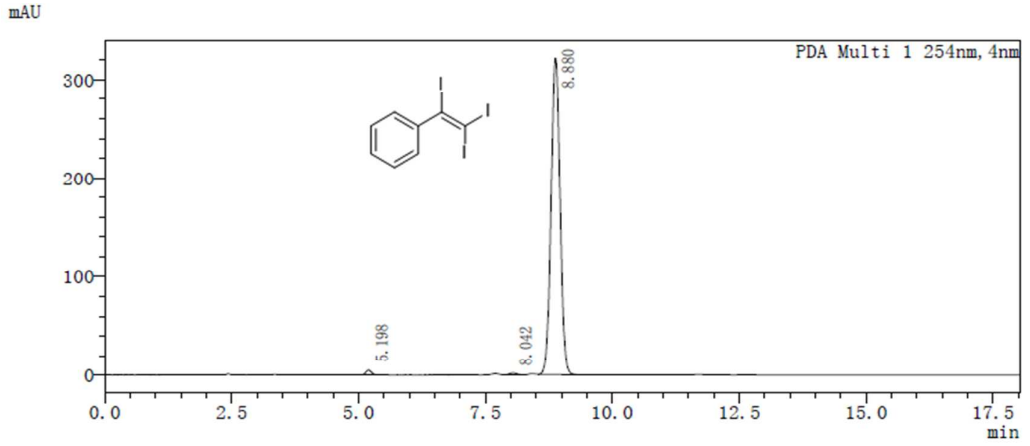


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.194	13638	1958	0.472			
2	8.047	2775382	255523	96.092			
3	8.846	99242	6153	3.436		V	
Total		2888261	263634				

2b : **3b** : **4b** = 0.2 : 97.6 : 2.2 (molar ratio)

Compound **4**b (furnished by Method **C**, Table 3, entry 6)

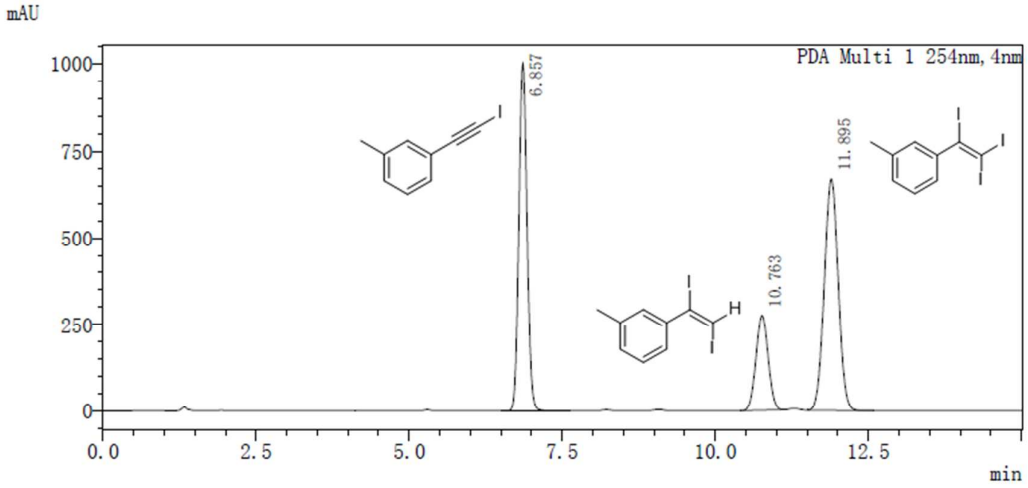


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.198	37093	4948	0.924			
2	8.042	17878	1810	0.446			
3	8.880	3957680	321149	98.630			
Total		4012651	327907				

2b : **3b** : **4b** = 0.8 : 0.7 : 98.5 (molar ratio)

HPLC Spectrum of **2c, 3c** and **4c**

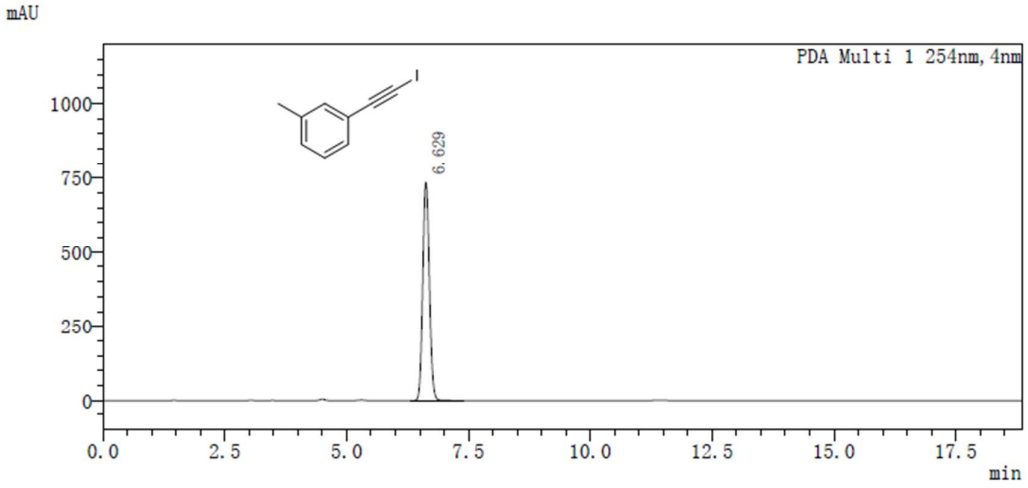


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.857	9329805	1000285	39.292			
2	10.763	3823989	274428	16.105			
3	11.895	10590704	668707	44.603			
Total		23744498	1943419				

$A_{2c} : A_{3c} : A_{4c} = 2.296 : 1 : 1.542$ (absorbance ratio)

Compound **2c** (furnished by Method **A**, Table 3, entry 7)

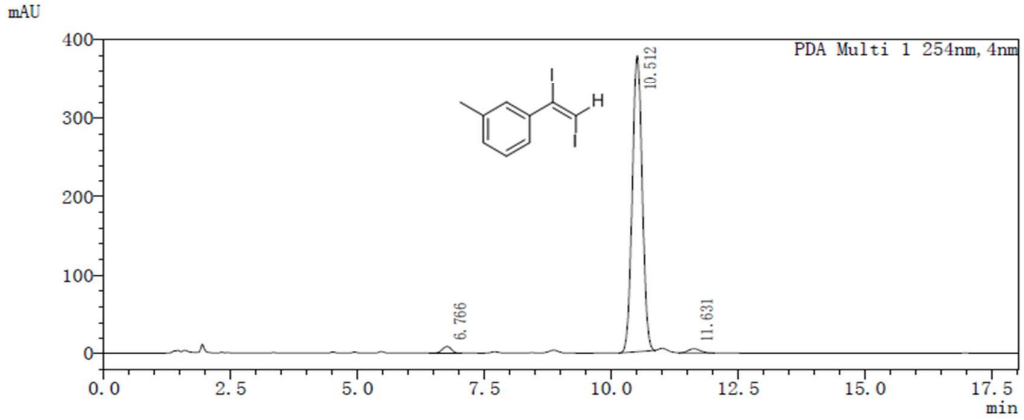


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.629	6859818	734695	100.000			
Total		6859818	734695				

2c : **3c** : **4c** = 100 : 0 : 0 (molar ratio)

Compound **3c** (furnished by Method **B**, Table 3, entry 8)

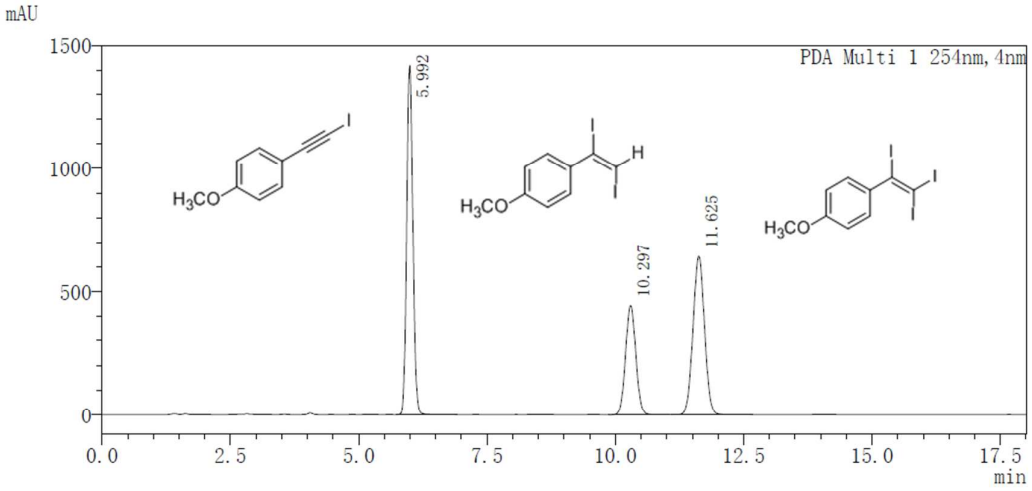


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.766	104111	8320	1.939			
2	10.512	5179806	377541	96.471			
3	11.631	85394	5165	1.590			
Total		5369311	391025				

2c : **3c** : **4c** = 0.9 : 98.1 : 1.0 (molar ratio)

HPLC Spectrum of **2d, 3d** and **4d**

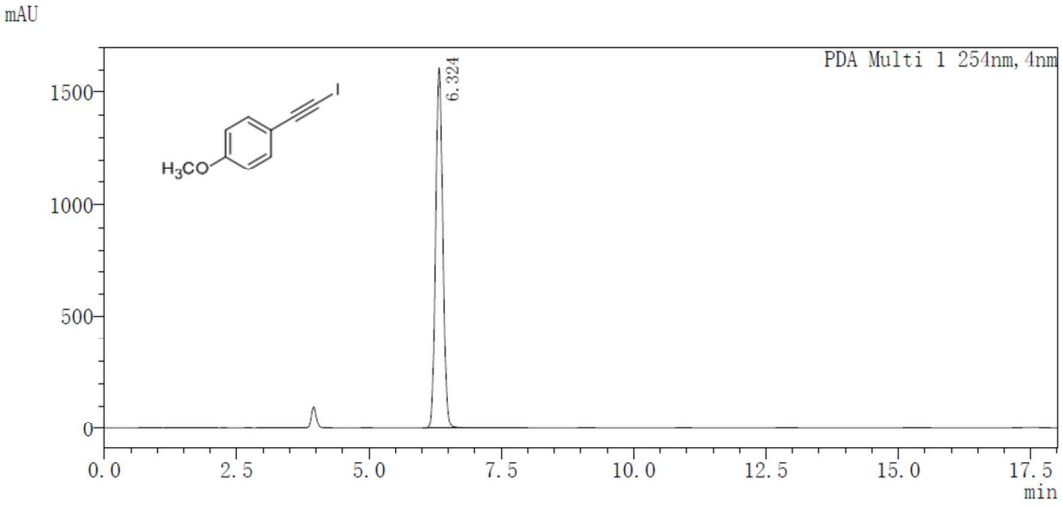


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.992	11877777	1420050	42.277			
2	10.297	6170063	444408	21.961			
3	11.625	10047068	642542	35.761			
Total		28094909	2507000				

$A_{2d} : A_{3d} : A_{4d} = 1.725 : 1 : 1.216$ (absorbance ratio)

Compound **2d** (furnished by Method **A**, Table 3, entry 9)

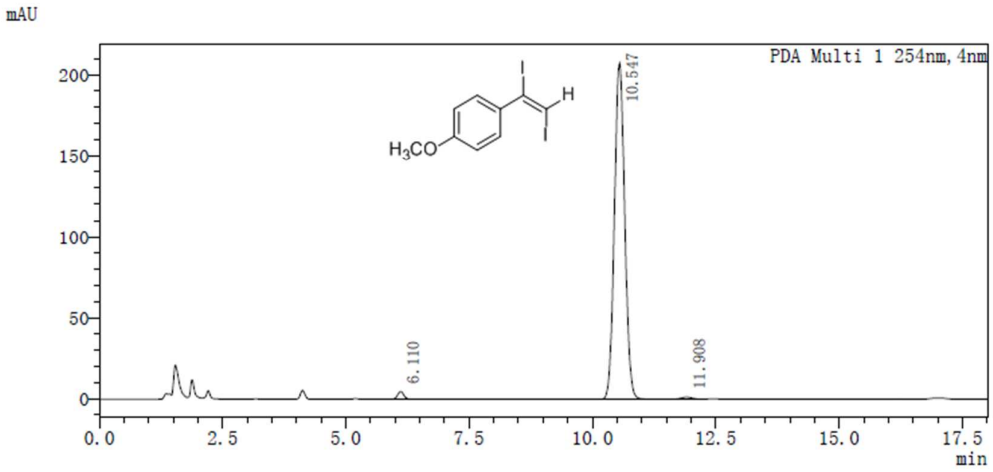


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.324	15126997	1611508	100.000			
Total		15126997	1611508				

2d : **3d** : **4d** = 100 : 0 : 0 (molar ratio)

Compound **3d** (furnished by Method **B**, Table 3, entry 10)

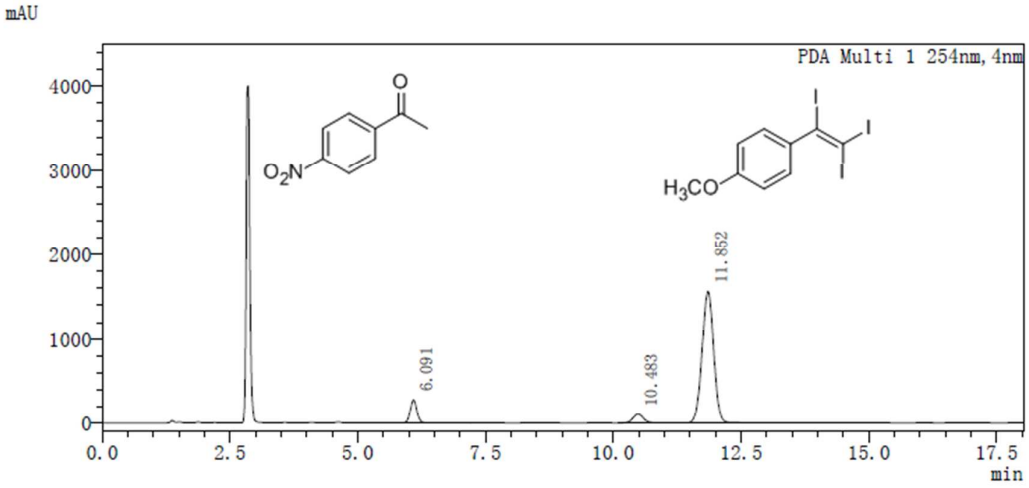


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.110	40986	4710	1.337			
2	10.547	3005227	207234	98.059			
3	11.908	18497	1206	0.604			
Total		3064710	213150				

2d : **3d** : **4d** = 0.8 : 98.7 : 0.5 (molar ratio)

Compound **4d** (furnished by Method **C**, Table 3, entry 11)

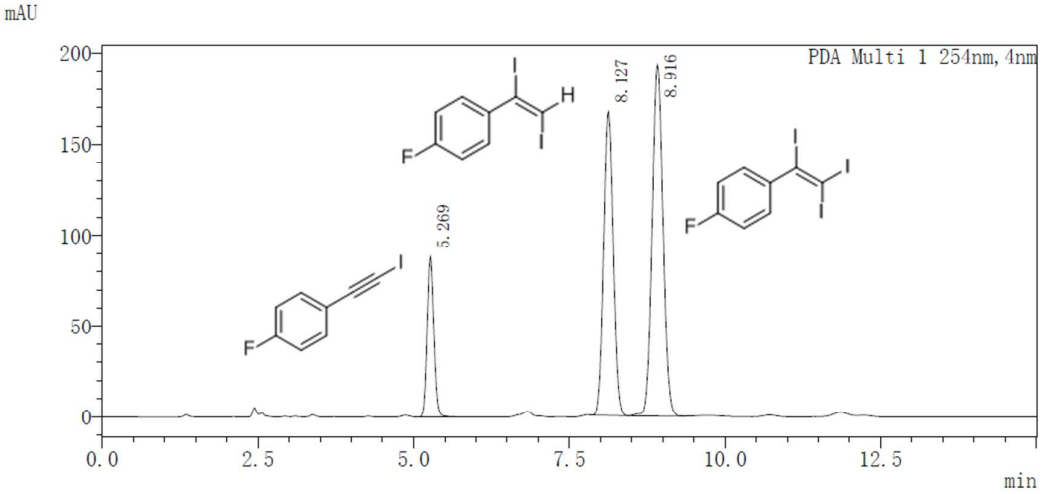


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.091	2517508	279788	8.702			
2	10.483	1498748	106185	5.180			
3	11.852	24915578	1564358	86.118			
Total		28931835	1950332				

2d : **3d** : **4d** = 6.2 : 6.4 : 87.4 (molar ratio)

HPLC Spectrum of **2e, 3e** and **4e**

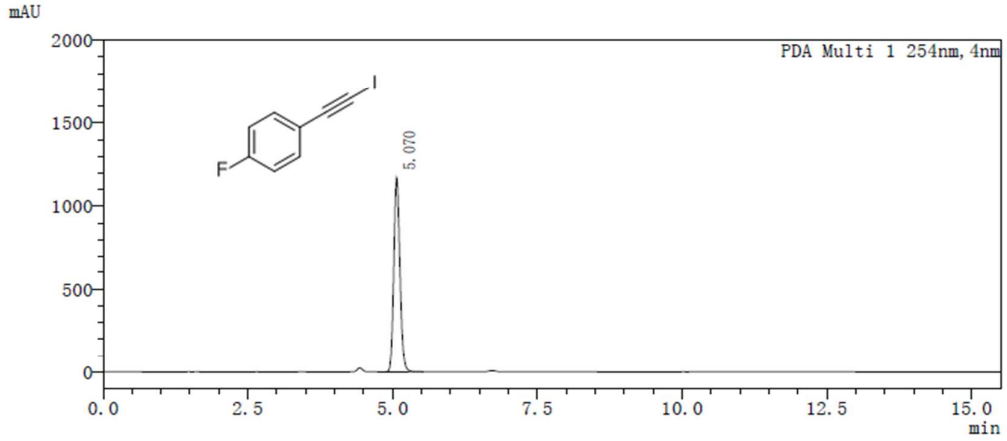


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.269	655581	88047	13.635			
2	8.127	1796264	166902	37.360			
3	8.916	2356152	193128	49.005			
Total		4807997	448077				

A_{2e} : A_{3e} : A_{4e} = 1 : 1.508 : 2.339 (absorbance ratio)

Compound **2e** (furnished by Method **A**, Table 3, entry 12)

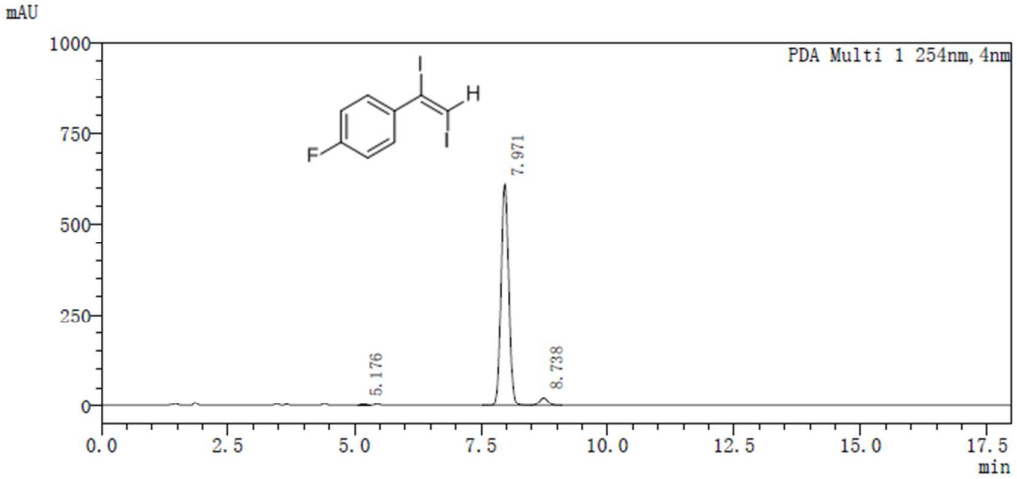


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.070	8728520	1174118	100.000			
Total		8728520	1174118				

2e : **3e** : **4e** = 100 : 0 : 0 (molar ratio)

Compound **3e** (furnished by Method **B**, Table 3, entry 13)

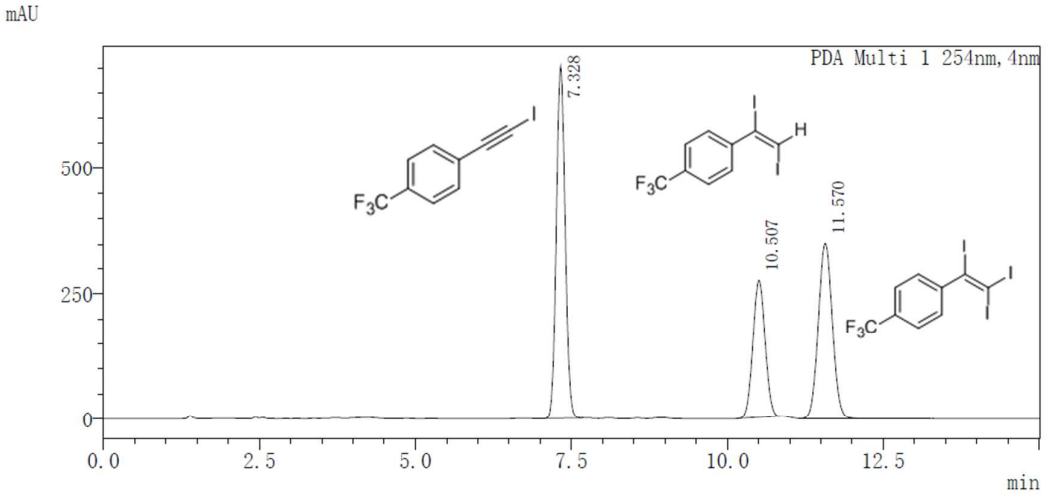


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.176	28756	4227	0.425			
2	7.971	6476352	609630	95.752			
3	8.738	258567	21866	3.823			
Total		6763675	635723				

2e : **3e** : **4e** = 0.6 : 96.9 : 2.5 (molar ratio)

HPLC Spectrum of **2f, 3f** and **4f**

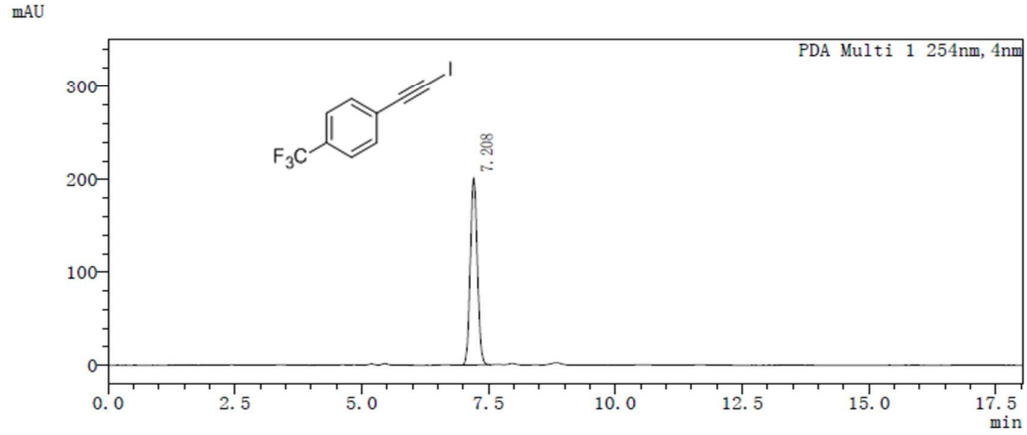


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	7.328	6904087	704560	42.784			
2	10.507	3748180	274523	23.227			
3	11.570	5484979	351717	33.990			
Total		16137247	1330801				

$A_{2f} : A_{3f} : A_{4f} = 2.991 : 1 : 1.725$ (absorbance ratio)

Compound **2f** (furnished by Method **A**, Table 3, entry 14)

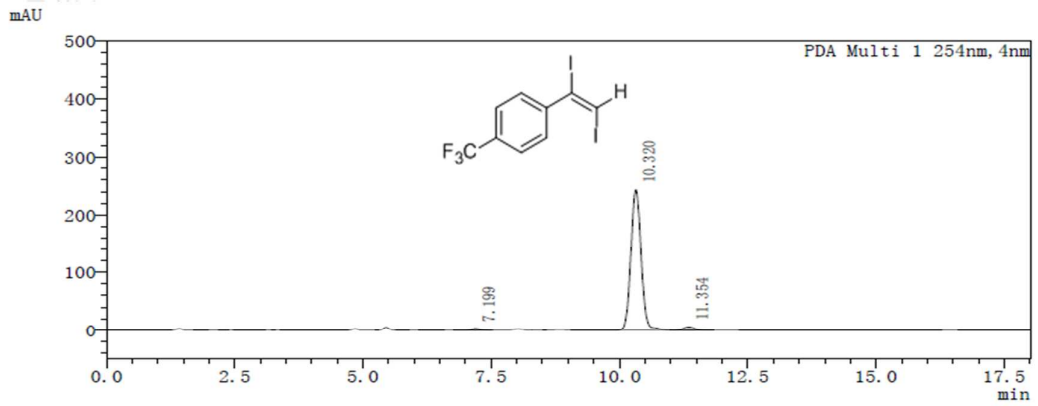


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	7.208	1942945	199968	100.000			
Total		1942945	199968				

2f : **3f** : **4f** = 100 : 0 : 0 (molar ratio)

Compound **3f** (furnished by Method **B**, Table 3, entry 15)

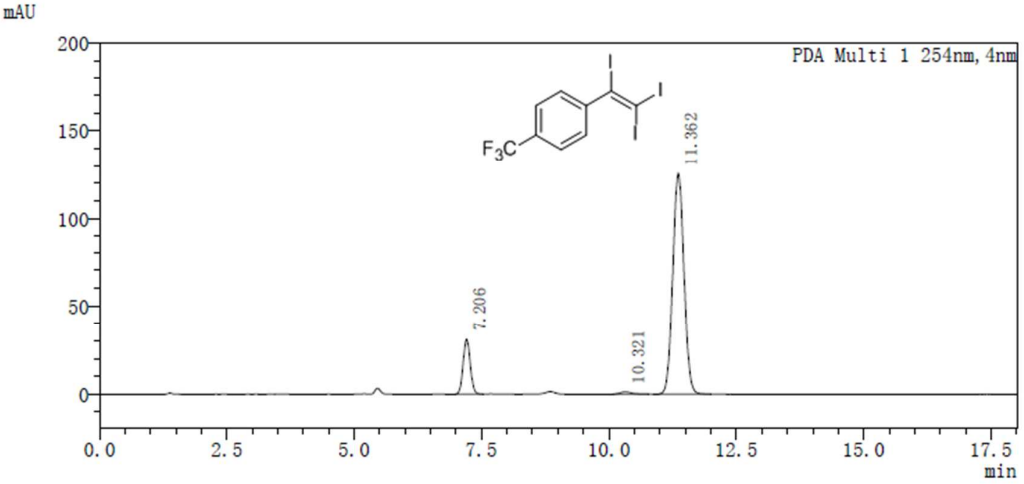


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	7.199	29876	3098	0.857			
2	10.320	3371576	242965	96.679			
3	11.354	85937	5652	2.464			
Total		3487390	251715				

2f : **3f** : **4f** = 0.3 : 98.3 : 1.4 (molar ratio)

Compound **4f** (furnished by Method **C**, Table 3, entry 16)

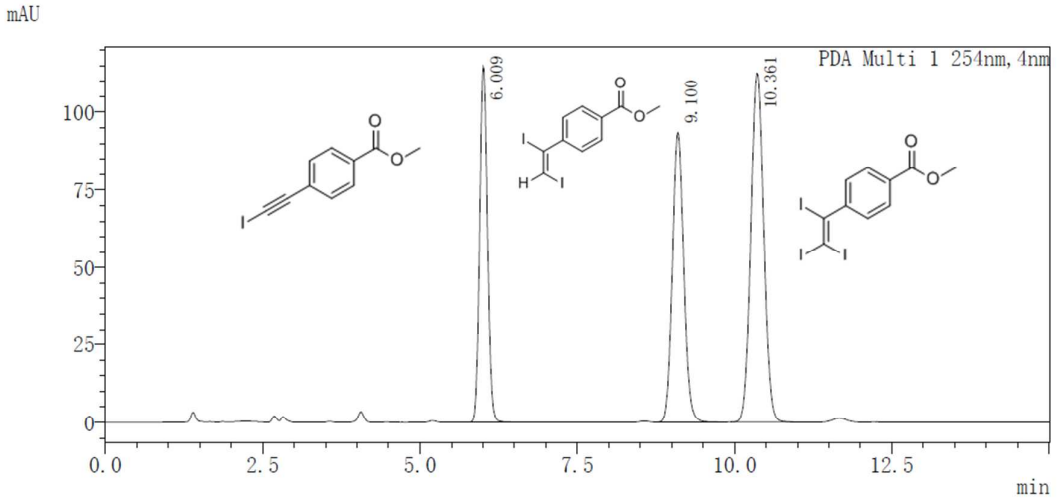


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	7.206	299644	30745	13.413			
2	10.321	19329	1292	0.865			
3	11.362	1915082	125382	85.722			
Total		2234055	157418				

2f : **3f** : **4f** = 8.1 : 1.6 : 90.3 (molar ratio)

HPLC Spectrum of **2g, 3g** and **4g**

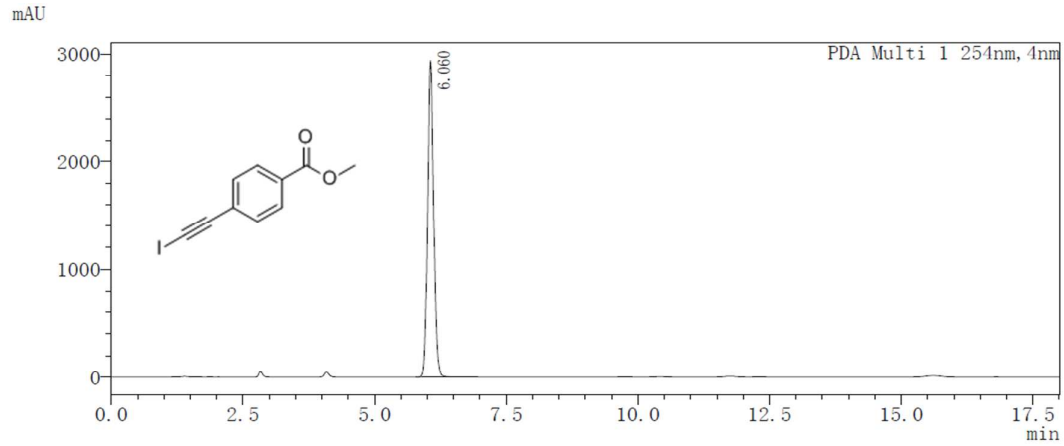


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.009	983950	114710	26.135			
2	9.100	1177552	93464	31.278			
3	10.361	1603317	112606	42.587			
Total		3764819	320780				

$A_{2g} : A_{3g} : A_{4g} = 1.042 : 1 : 1.340$ (absorbance ratio)

Compound **2g** (furnished by Method **A**, Table 3, entry 17)

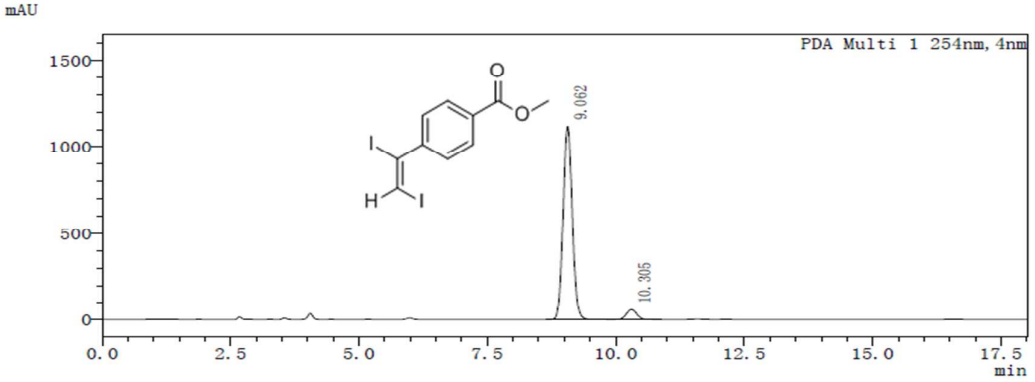


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.060	23187253	2945788	100.000			
Total		23187253	2945788				

2g : **3g** : **4g** = 100 : 0 : 0 (molar ratio)

Compound **3g** (furnished by Method **B**, Table 3, entry 18)

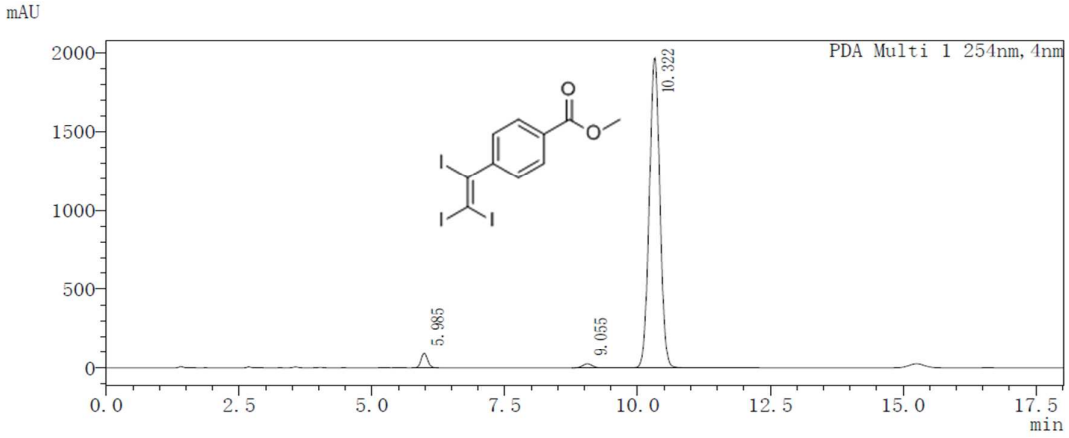


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	9.062	13975430	1117611	94.446			
2	10.305	821854	58354	5.554			
Total		14797285	1175964				

2g : **3g** : **4g** = 0 : 95.8 : 4.2 (molar ratio)

Compound **4g** (furnished by Method **C**, Table 3, entry 19)

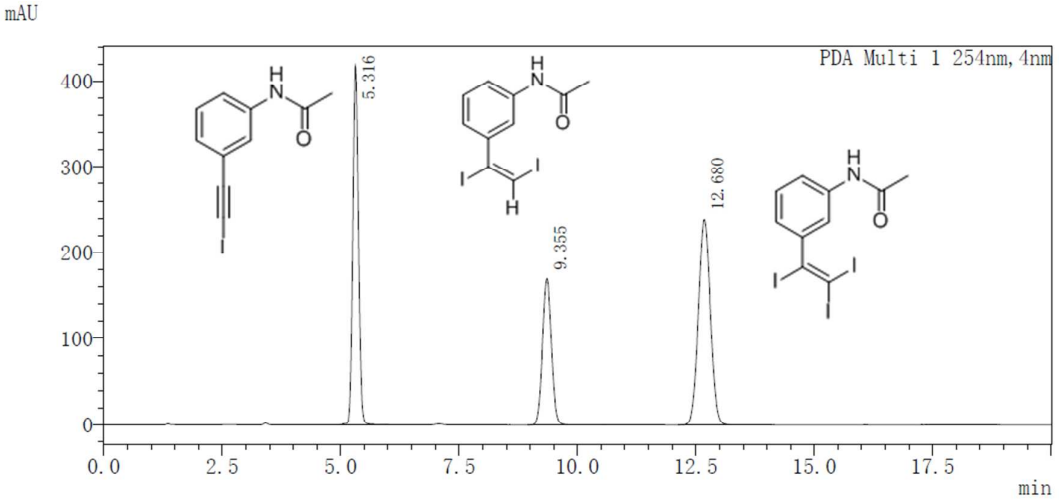


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.985	756323	89895	2.665			
2	9.055	301216	24678	1.061			
3	10.322	27319229	1968659	96.273			
Total		28376769	2083232				

2g : **3g** : **4g** = 3.4 : 1.4 : 95.2 (molar ratio)

HPLC Spectrum of **2h, 3h** and **4h**

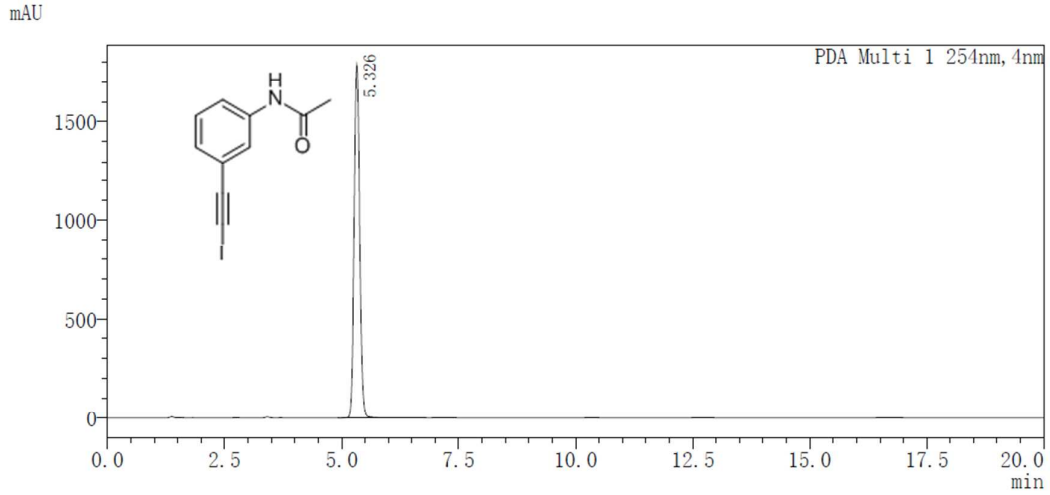


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.316	3452185	417664	34.895			
2	9.355	2232802	169649	22.569			
3	12.680	4208194	238881	42.536			
Total		9893182	826194				

$A_{\mathbf{2h}}$: $A_{\mathbf{3h}}$: $A_{\mathbf{4h}}$ = 1.493 : 1: 1.284 (absorbance ratio)

Compound **2h** (furnished by Method **A**, Table 3, entry 20)

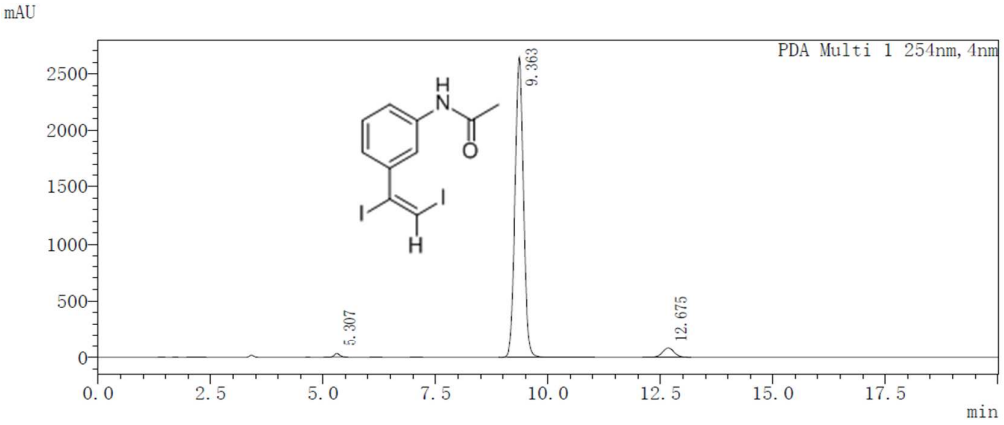


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.326	14711138	1789563	100.000			
Total		14711138	1789563				

2h : **3h** : **4h** = 100 : 0 : 0 (molar ratio)

Compound **3h** (furnished by Method **B**, Table 3, entry 21)

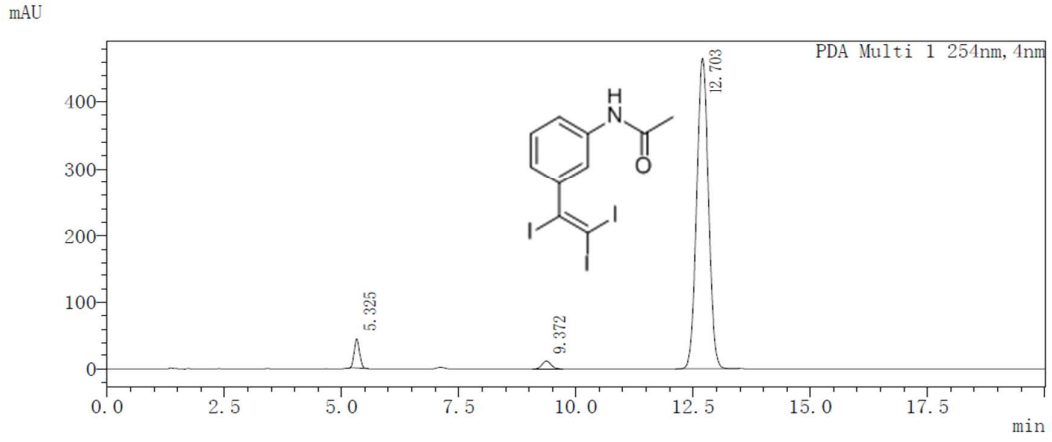


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.307	242175	30805	0.670			
2	9.363	34502379	2643242	95.503			
3	12.675	1382511	79392	3.827			
Total		36127065	2753440				

2h : **3h** : **4h** = 0.5 : 96.5 : 3.0 (molar ratio)

Compound **4h** (furnished by Method **C**, Table 3, entry 22)

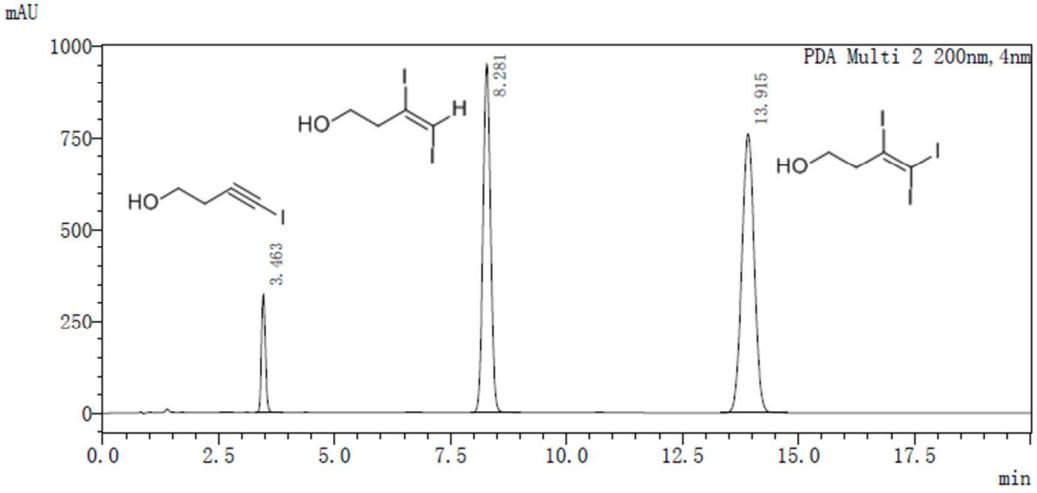


PDA Ch1 254nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	5.325	352200	44784	4.066			
2	9.372	149618	11489	1.727			
3	12.703	8161039	465290	94.207			
Total		8662857	521564				

2h : **3h** : **4h** = 3.5 : 2.2 : 94.3 (molar ratio)

HPLC Spectrum of **2i, 3i** and **4i**

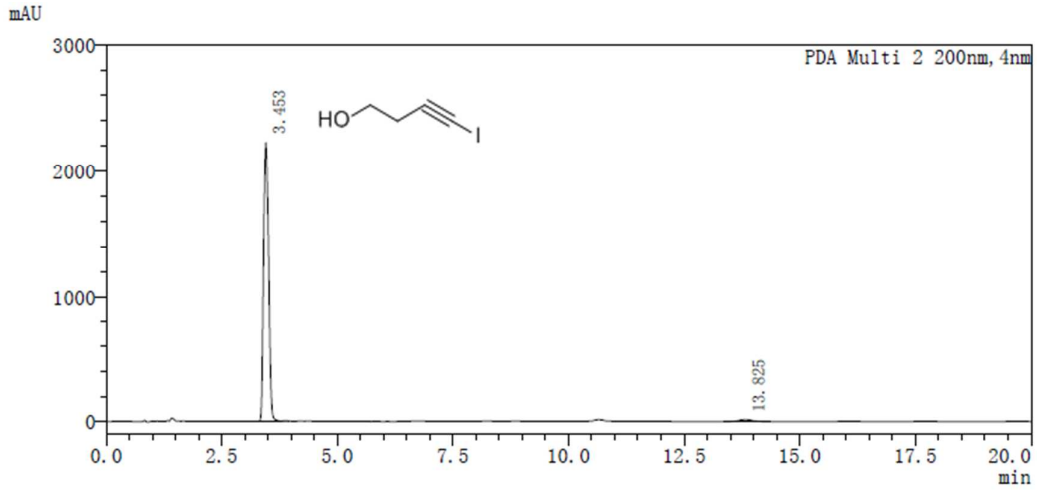


PDA Ch2 200nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	3.463	1913755	320704	7.164			
2	8.281	10725230	950474	40.148			
3	13.915	14075108	760998	52.688			
Total		26714093	2032176				

A_{2i} : A_{3i} : A_{4i} = 1 : 6.023: 9.014 (absorbance ratio)

Compound **2i** (furnished by Method **A**, Table 3, entry 23)

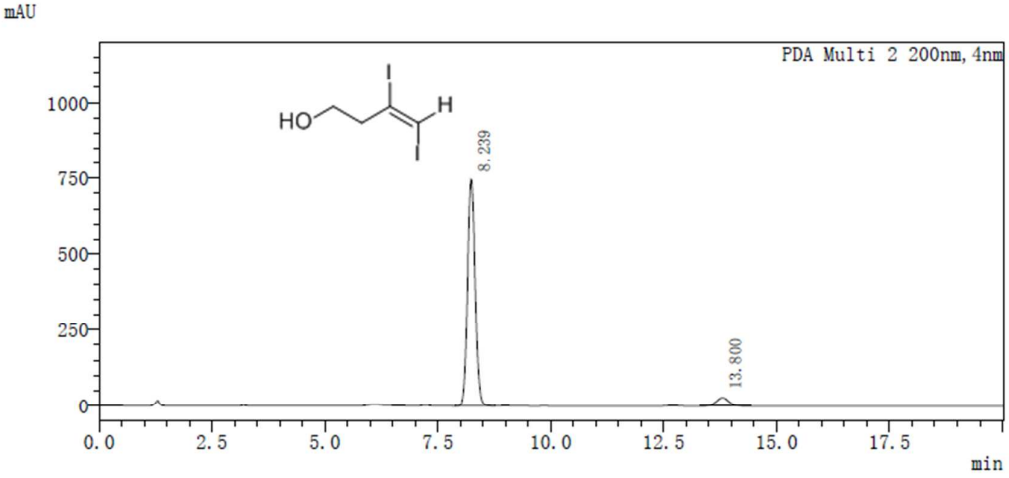


PDA Ch2 200nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	3.453	17063569	2227252	98.260			
2	13.825	302143	16069	1.740			
Total		17365713	2243321				

2i : **3i** : **4i** = 99.8 : 0 : 0.2 (molar ratio)

Compound **3i** (furnished by Method **B**, Table 3, entry 24)

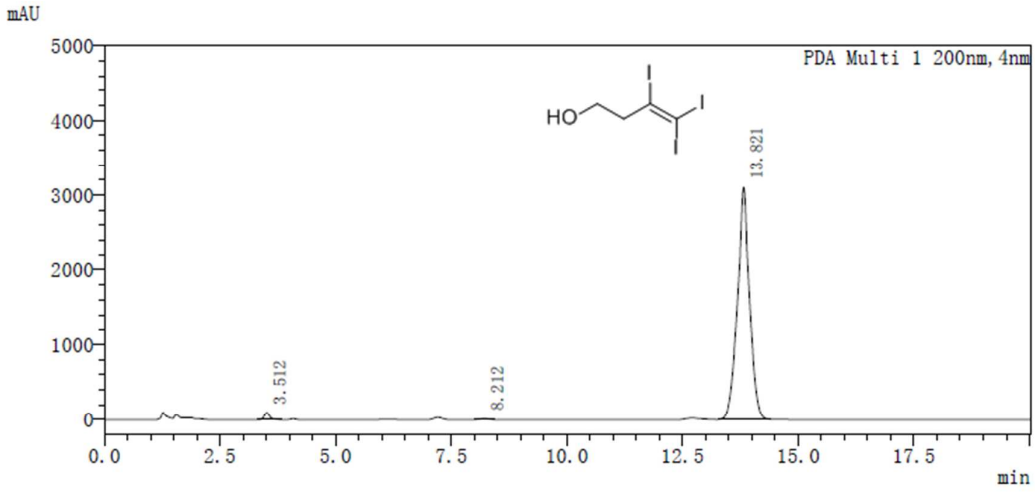


PDA Ch2 200nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	8.239	8739380	746313	94.213			
2	13.800	536841	28014	5.787			
Total		9276221	774326				

2i : **3i** : **4i** = 0 : 96.1 : 3.9 (molar ratio)

Compound **4i** (furnished by Method **C**, Table 3, entry 25)

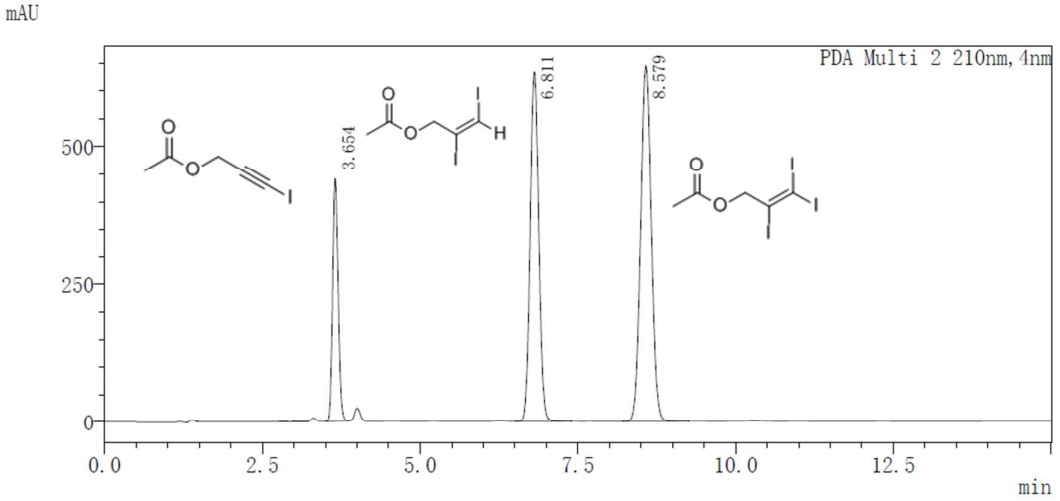


PDA Ch1 200nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	3.512	781475	94861	1.368			
2	8.212	126114	10170	0.221			
3	13.821	56225202	3093908	98.411			
Total		57132791	3198940				

2i : **3i** : **4i** = 11.1 : 0.3 : 88.6 (molar ratio)

HPLC Spectrum of **2j, 3j** and **4j**

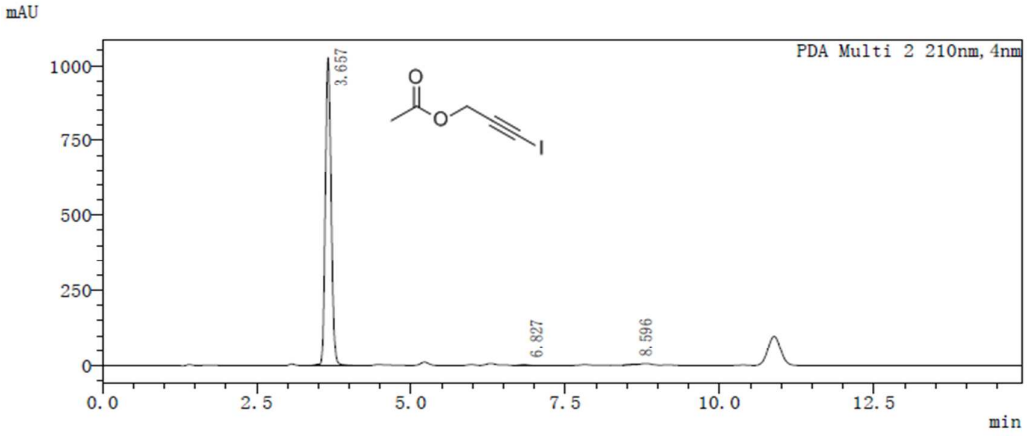


PDA Ch2 210nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	3.654	2698377	440050	16.556			
2	6.811	6020576	634086	36.939			
3	8.579	7579897	644876	46.506			
Total		16298850	1719013				

A_{2j} : A_{3j} : A_{4j} = 1 : 6.040: 14.023 (absorbance ratio)

Compound **2j** (furnished by Method **A**, Table 3, entry 26)

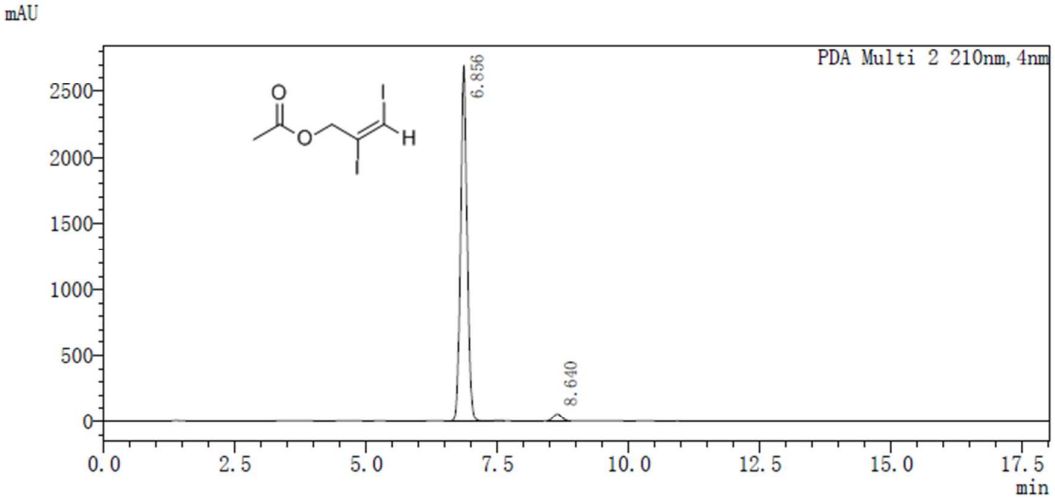


PDA Ch2 210nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	3.657	6694074	1026286	99.533			
2	6.827	22029	2320	0.328			
3	8.596	9404	1062	0.140			
Total		6725508	1029668				

2j : **3j** : **4j** = 99.94 : 0.05 : 0.01 (molar ratio)

Compound **3j** (furnished by Method **B**, Table 3, entry 27)

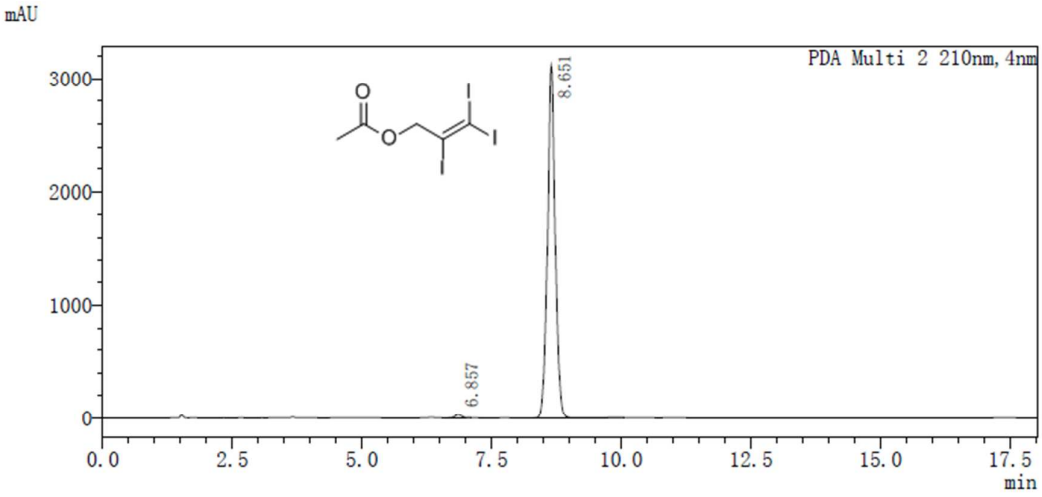


PDA Ch2 210nm

峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.856	23208051	2698932	97.336			
2	8.640	635184	55851	2.664			
Total		23843235	2754783				

2j : **3j** : **4j** = 0 : 98.8 : 1.2 (molar ratio)

Compound **4j** (furnished by Method **C**, Table 3, entry 28)

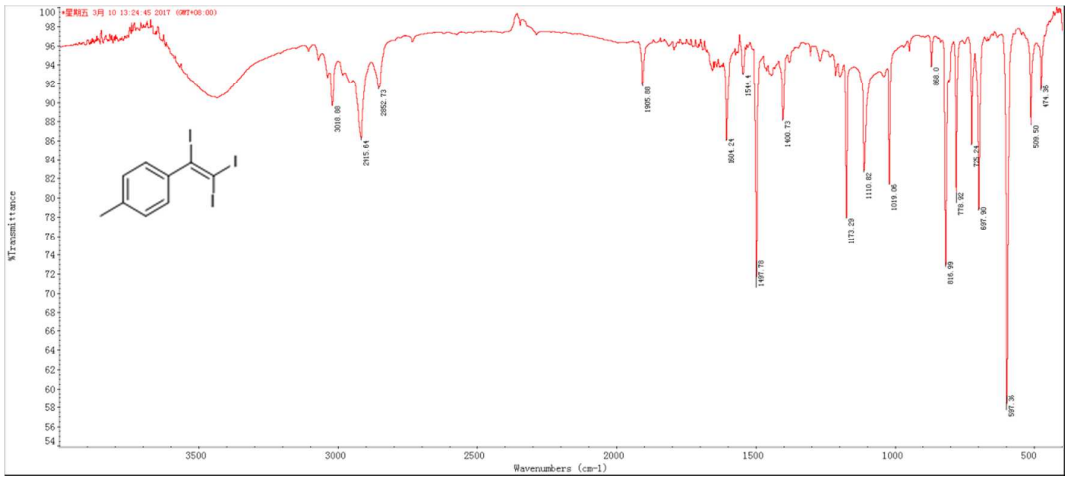


PDA Ch2 210nm

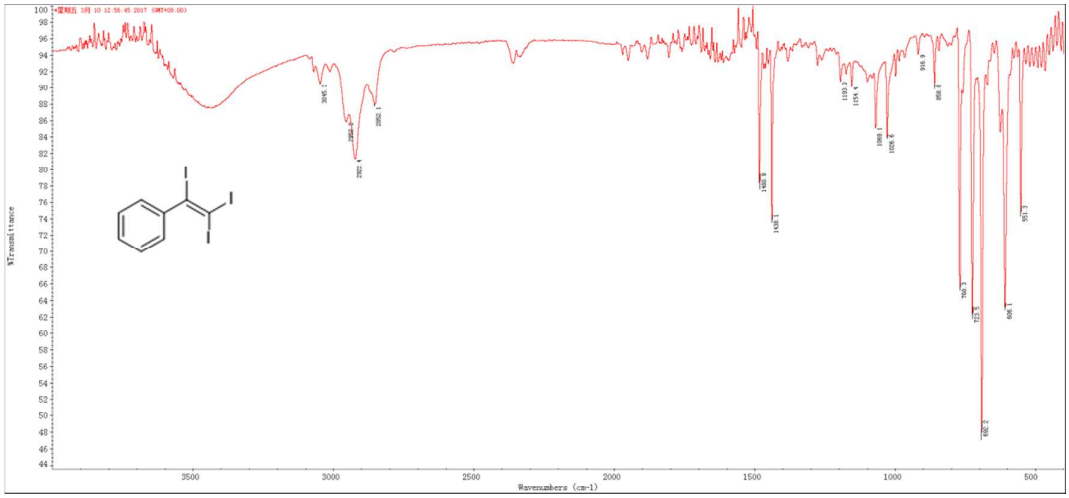
峰号	保留时间	面积	高度	浓度	浓度单位	标记	化合物名
1	6.857	277195	29318	0.854			
2	8.651	32168833	3117291	99.146		S	
Total		32446029	3146610				

2j : **3j** : **4j** = 0 : 2.0 : 98.0 (molar ratio)

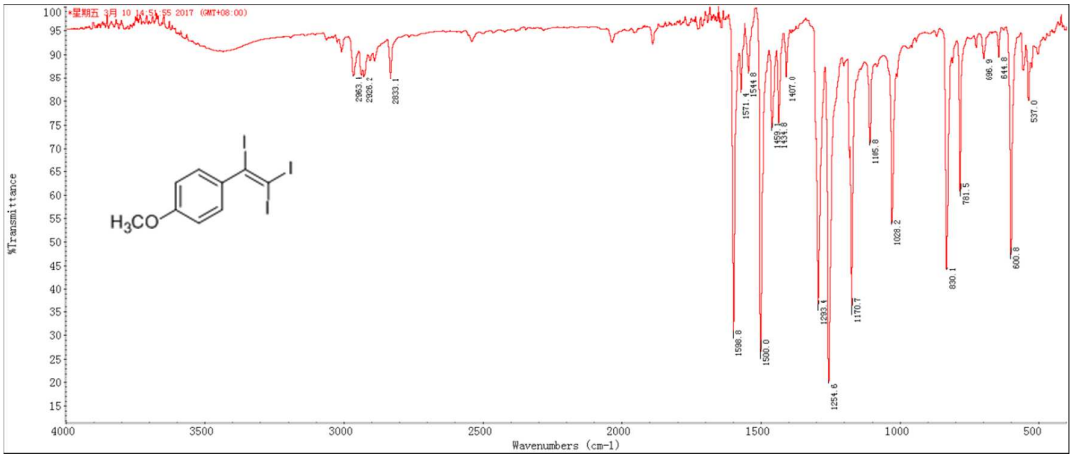
IR Spectra



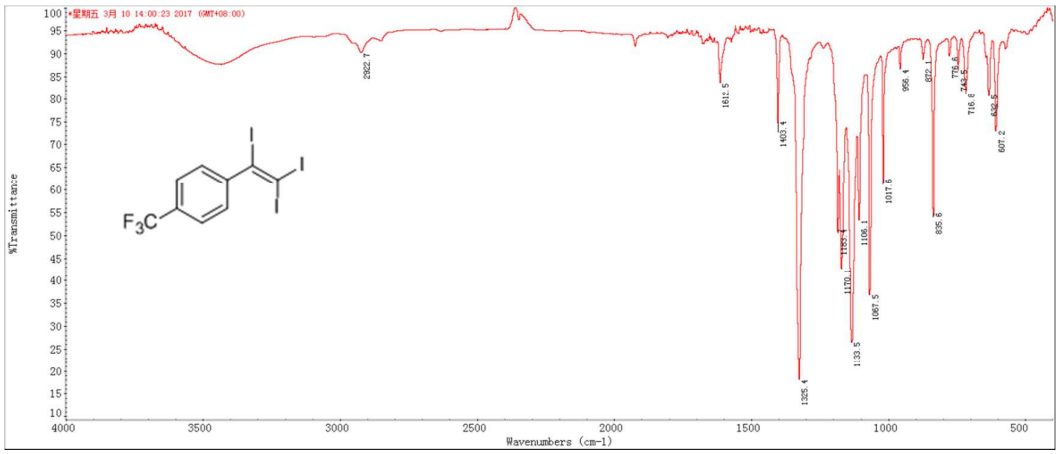
IR spectrum of **4a**



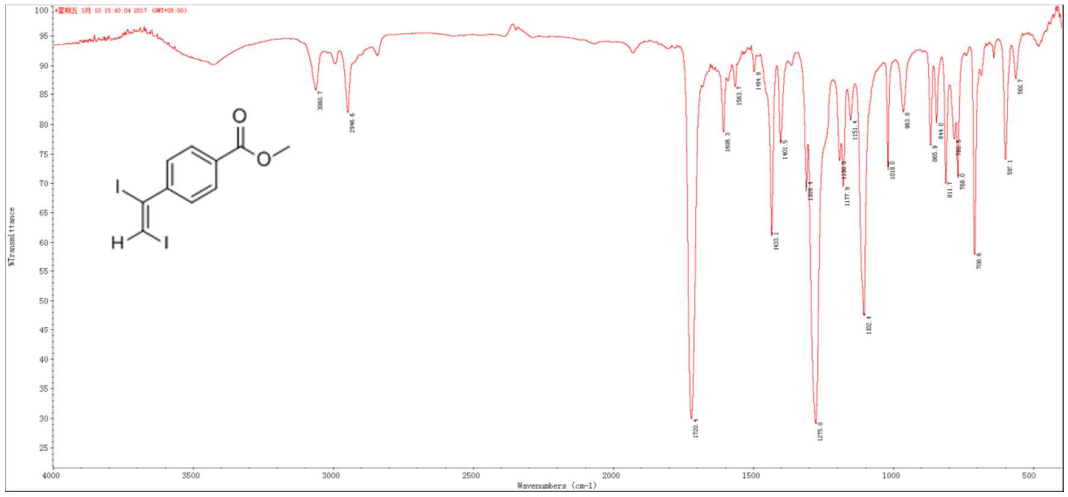
IR spectrum of **4b**



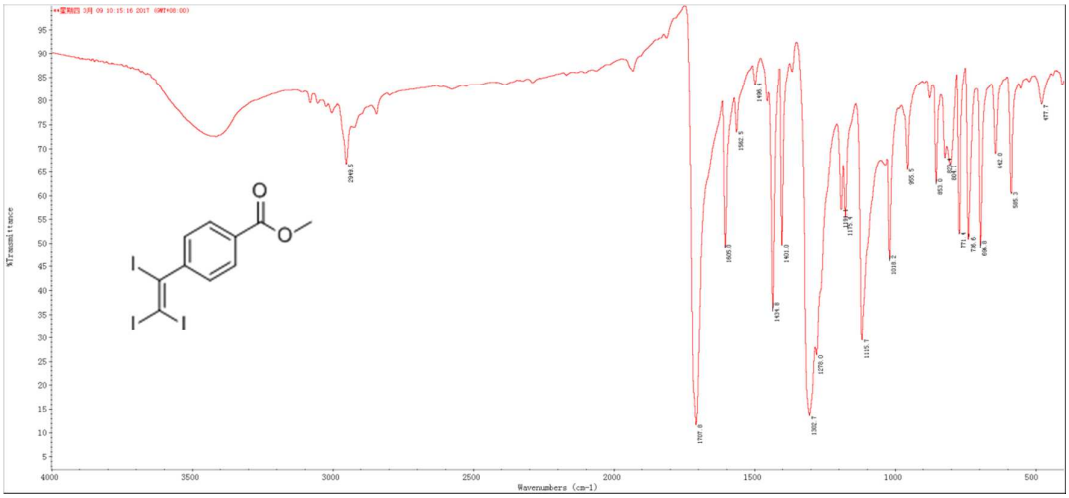
IR spectrum of **4d**



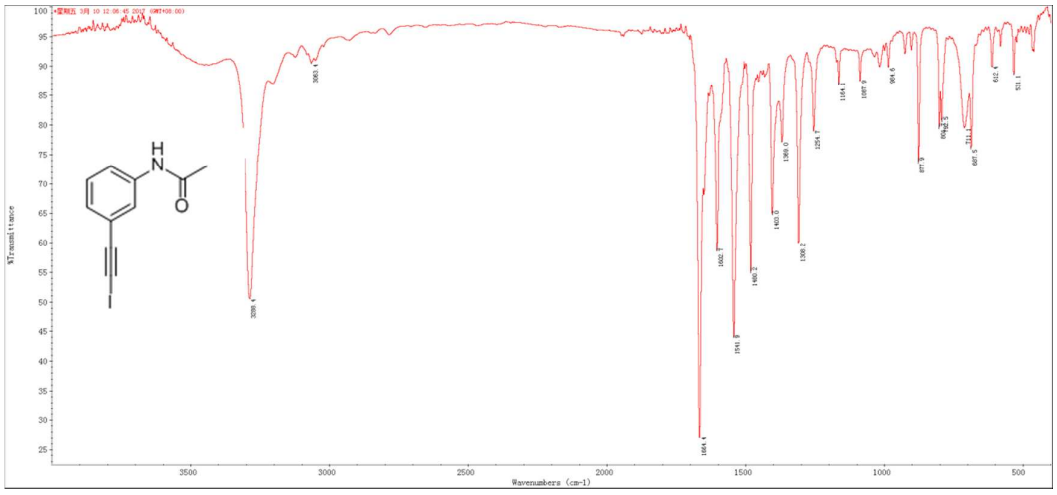
IR spectrum of **4f**



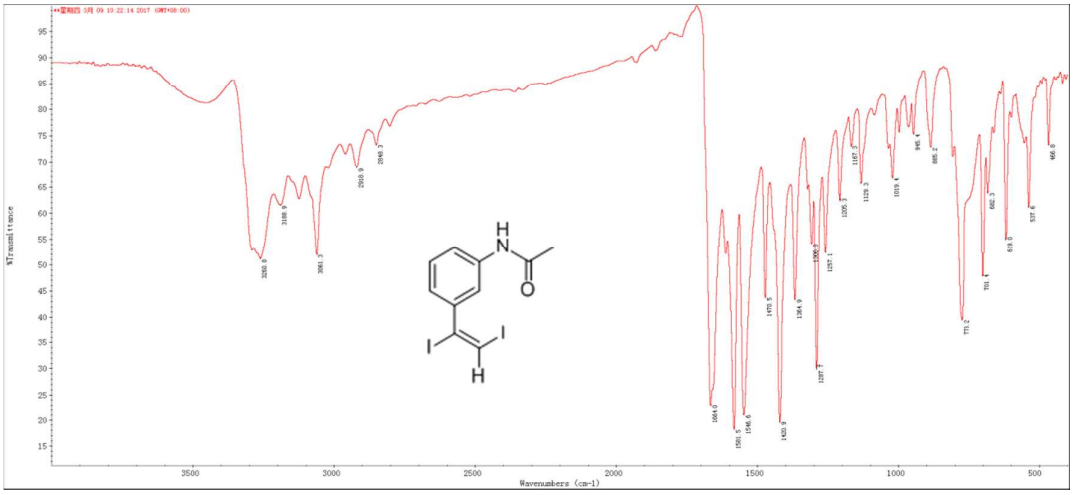
IR spectrum of **3g**



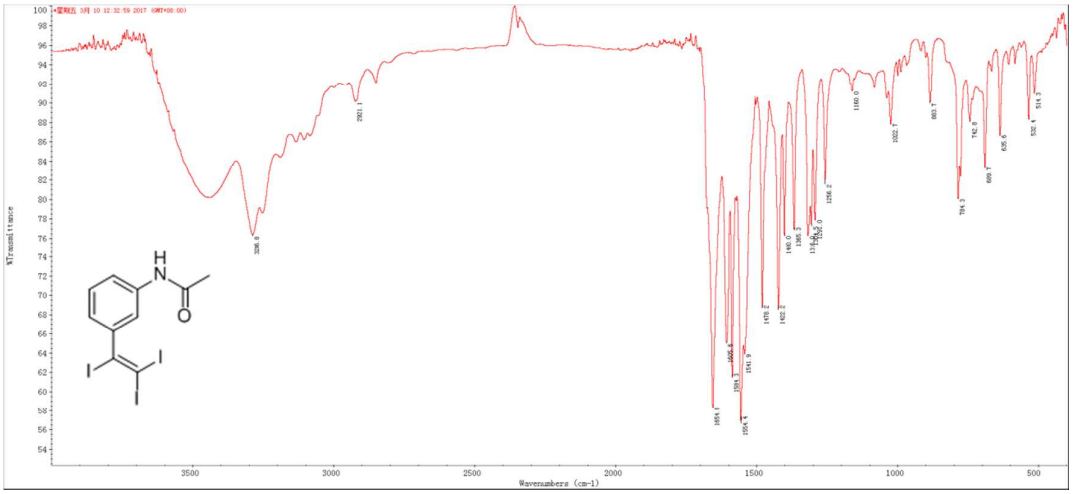
IR spectrum of **4g**



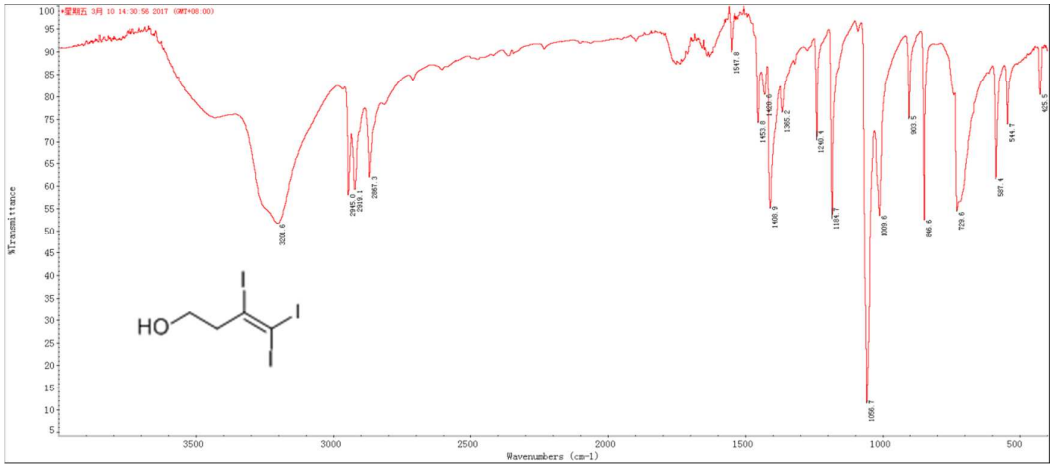
IR spectrum of **2h**



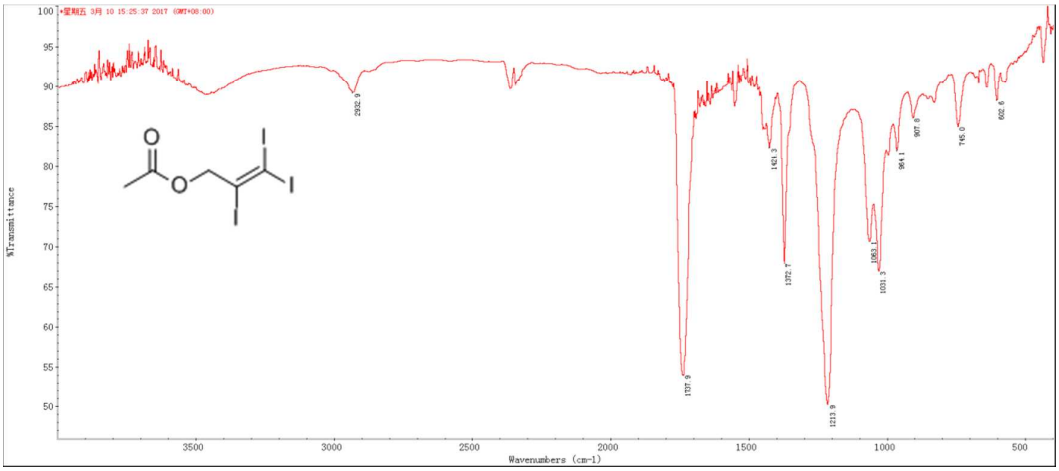
IR spectrum of **3h**



IR spectrum of **4h**



IR spectrum of **4i**

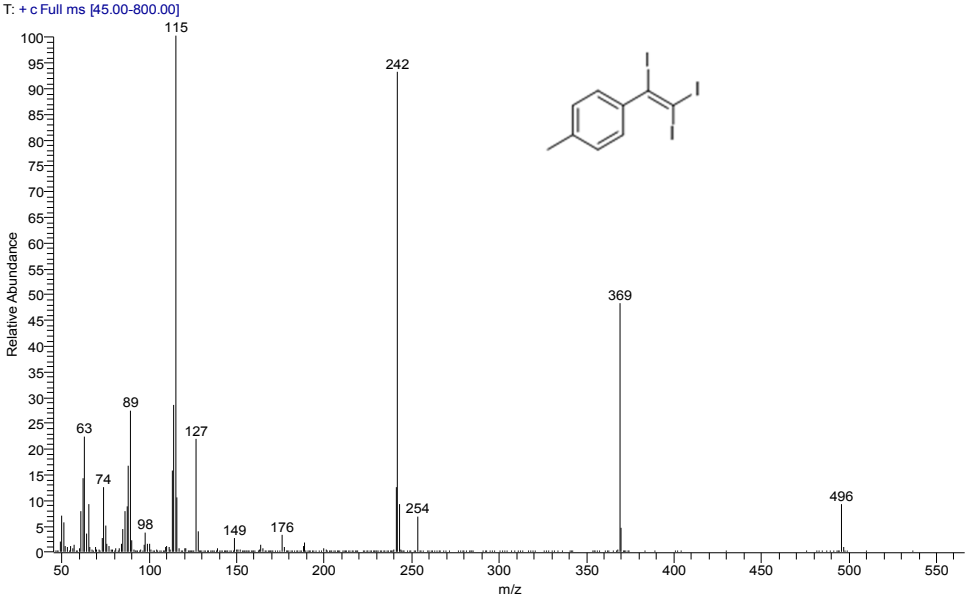


IR spectrum of **4j**

MS Spectra

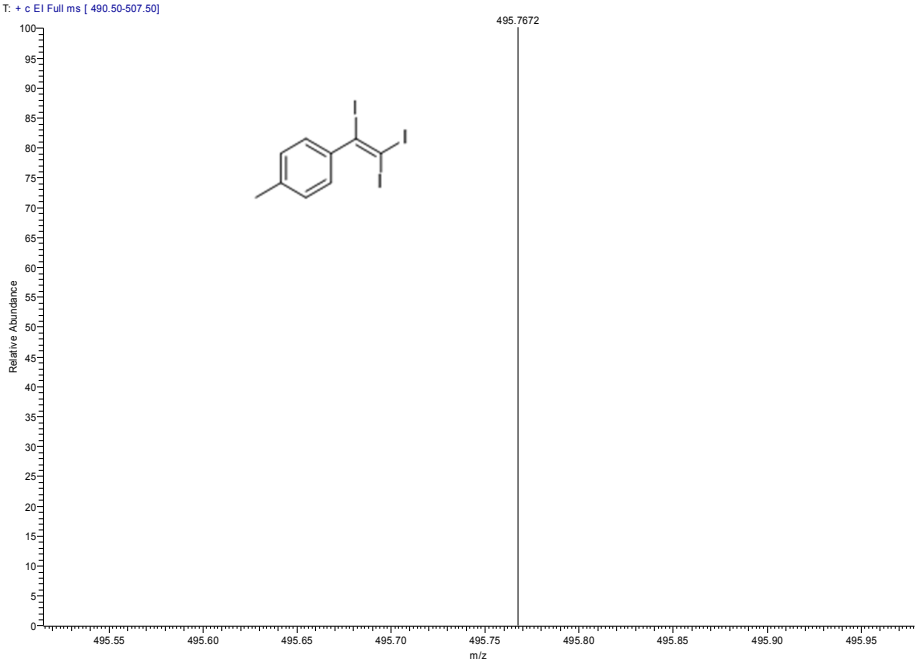
Instrument:DSQ(Thermo)
Ionization Method:EI
D:\DSQ\DATA-LR\17\041405 4/14/2017 10:11:39 AM 20161213-60

041405 #6 RT: 0.17 AV: 1 NL: 1.95E6
T: + c Full ms [45.00-800.00]



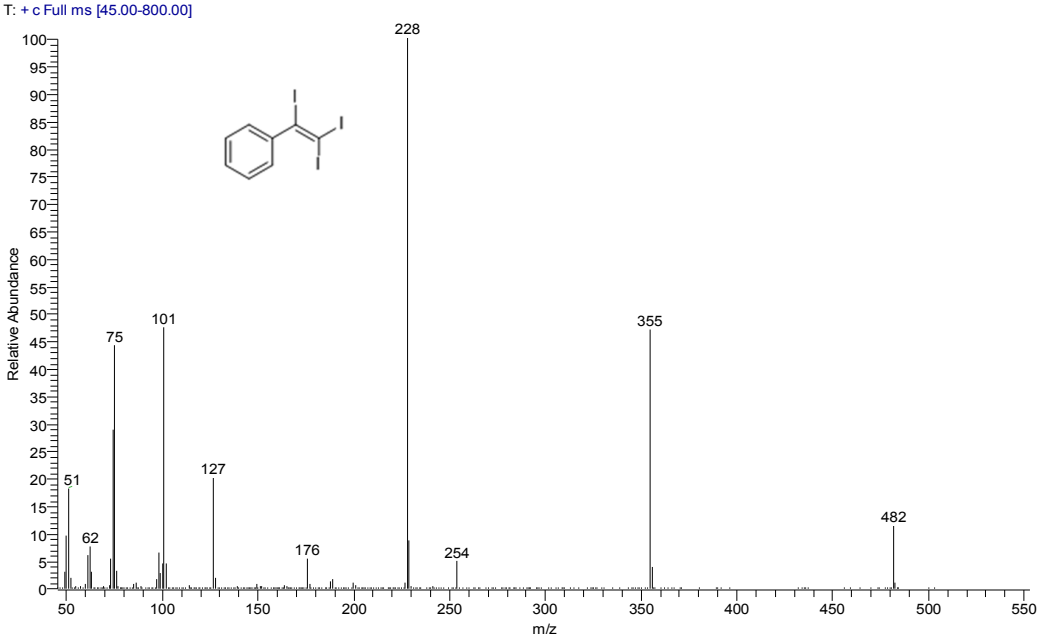
Instrument:MAT 95XP(Thermo)
D:\DATA-HR\17\041706-20161213-60-c1 4/17/2017 2:35:38 PM 20161213-60

041706-20161213-60-c1 #3 RT: 0.14 AV: 1 NL: 5.19E4
T: + c EI Full ms [490.50-507.50]



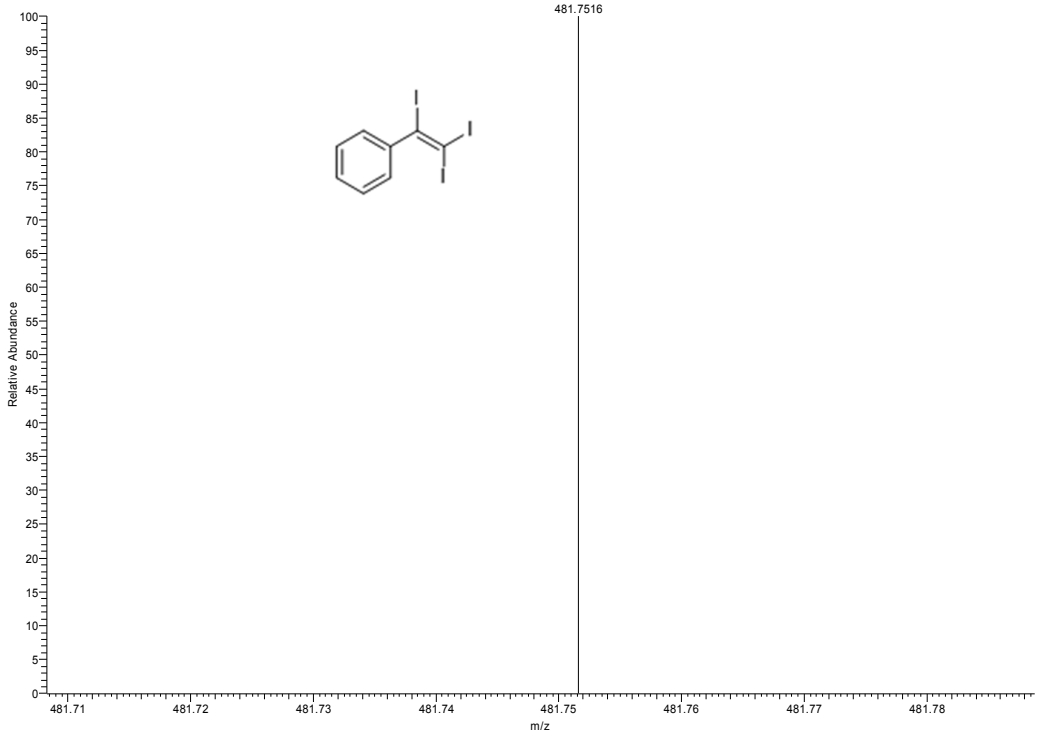
Instrument:DSQ(Thermo)
Ionization Method:EI
D:\DSQ\DATA-LR\17\041404 4/14/2017 10:04:43 AM 20170301-48

041404 #7 RT: 0.20 AV: 1 NL: 5.78E6
T: + c Full ms [45.00-800.00]



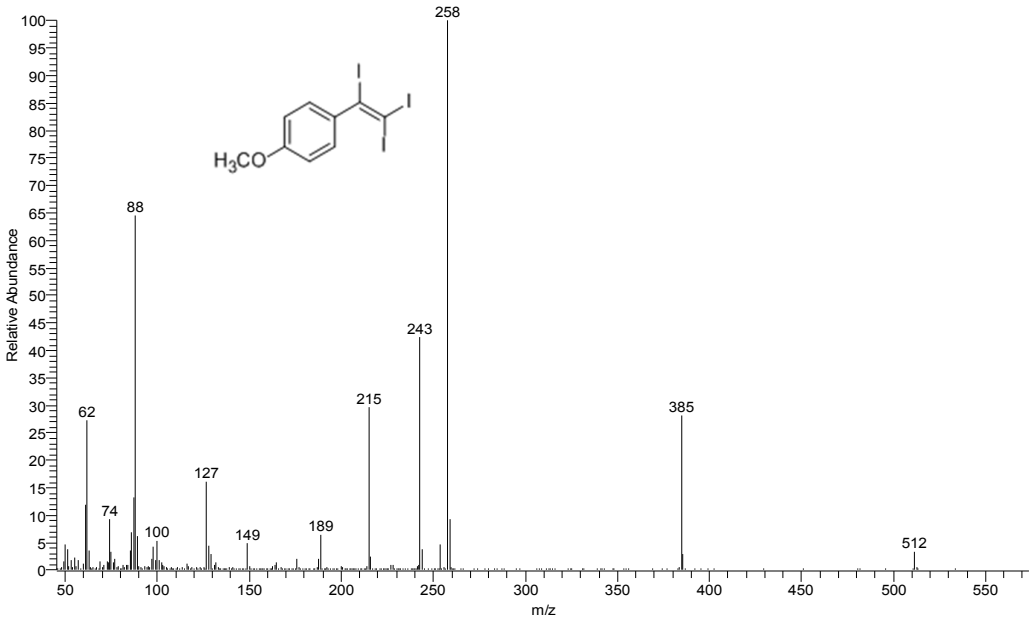
Instrument:MAT 95XP(Thermo)
D:\DATA-HR\17\041707-20170301-48-c2 4/17/2017 2:41:51 PM 20170301-48

041707-20170301-48-c2 #5 RT: 0.19 AV: 1 NL: 1.18E5
T: + c EI Full ms [478.50-495.50]



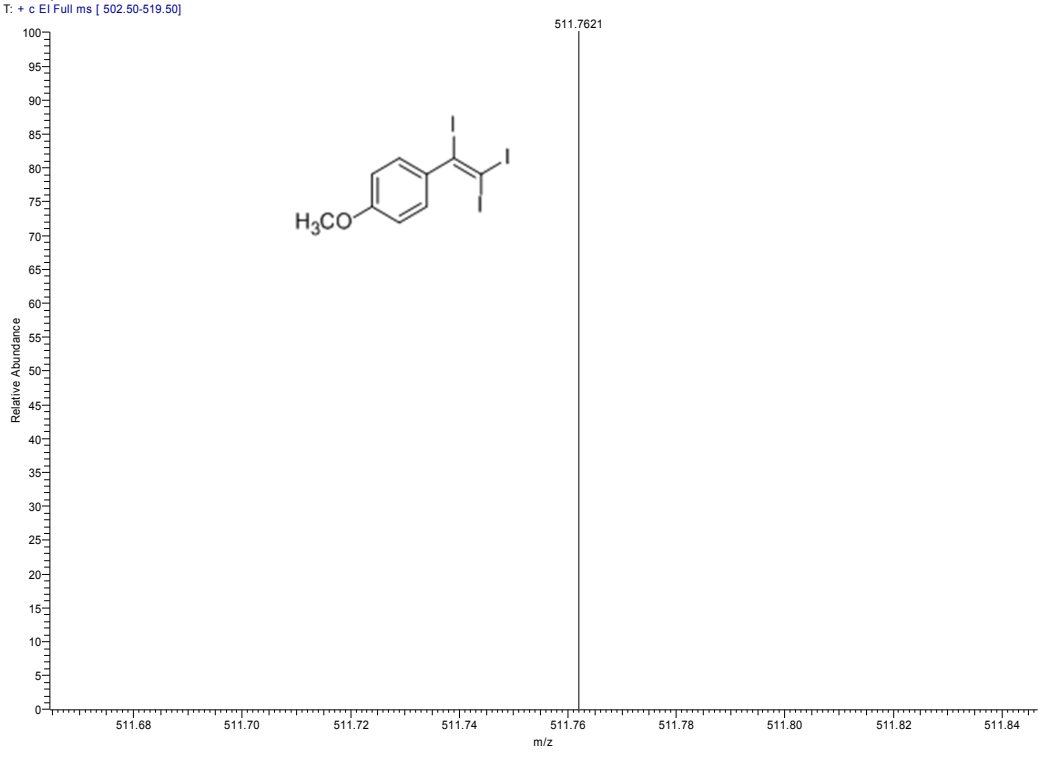
Instrument:DSQ(Thermo)
Ionization Method:EI
D:\DSQ\DATA-LR\17\041406 4/14/2017 10:17:08 AM hj-20170321A

041406 #4 RT: 0.12 AV: 1 NL: 9.21E5
T: + c Full ms [45.00-800.00]



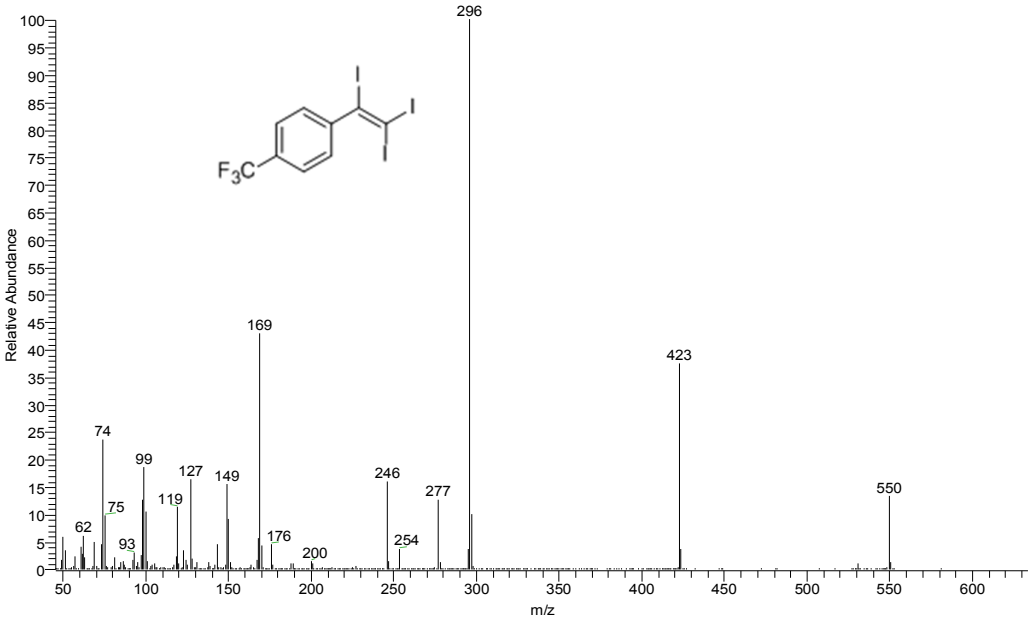
Instrument:MAT 95XP(Thermo)
D:\DATA-HR\17\041705-hj--20170321a-c1 4/17/2017 2:29:55 PM hj-20170321A

041705-hj--20170321a-c1 #9 RT: 0.35 AV: 1 NL: 3.08E4
T: + c EI Full ms [502.50-519.50]



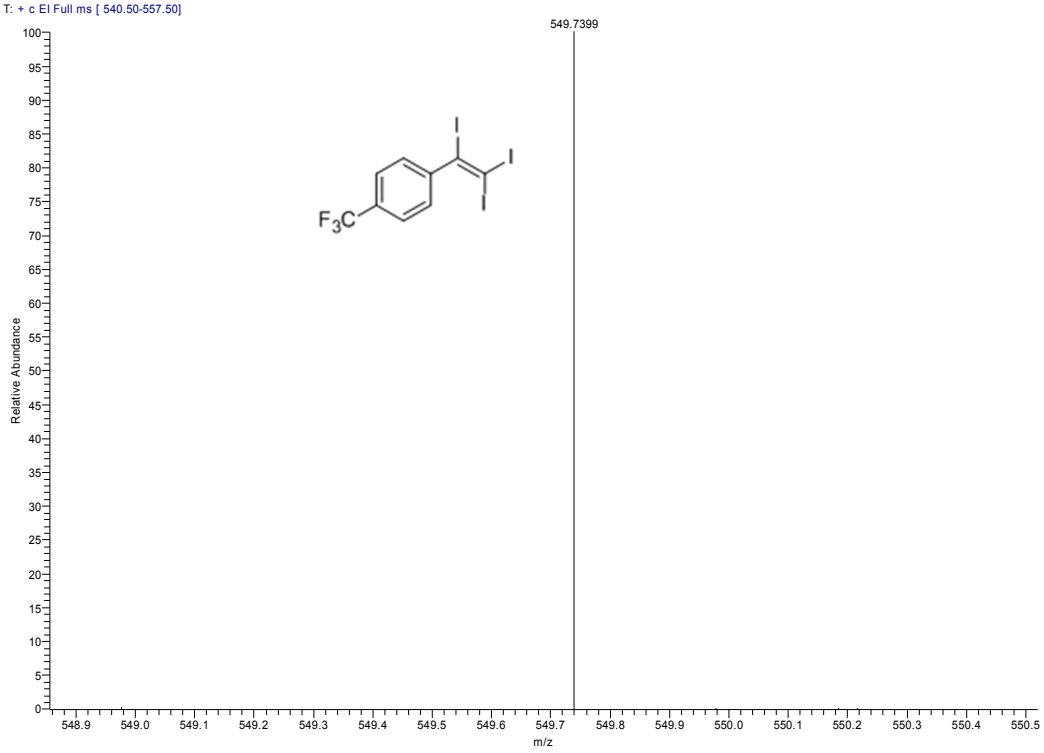
Instrument:DSQ(Thermo)
Ionization Method:EI
D:\DSQ\DATA-LR\17\041408 4/14/2017 10:34:32 AM 20170216-16

041408 #5 RT: 0.14 AV: 1 NL: 1.05E7
T: + c Full ms [45.00-800.00]



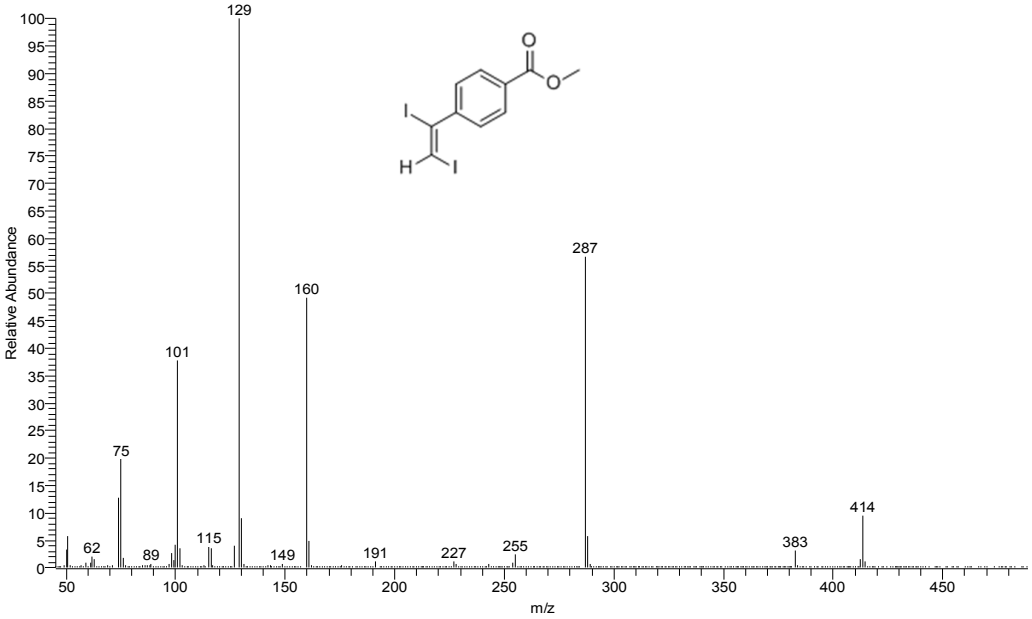
Instrument:MAT 95XP(Thermo)
D:\DATA-HR\17\041703-20170216-16-c1 4/17/2017 2:20:29 PM 20170216-16

041703-20170216-16-c1 #10 RT: 0.40 AV: 1 NL: 1.48E6
T: + c EI Full ms [540.50-557.50]



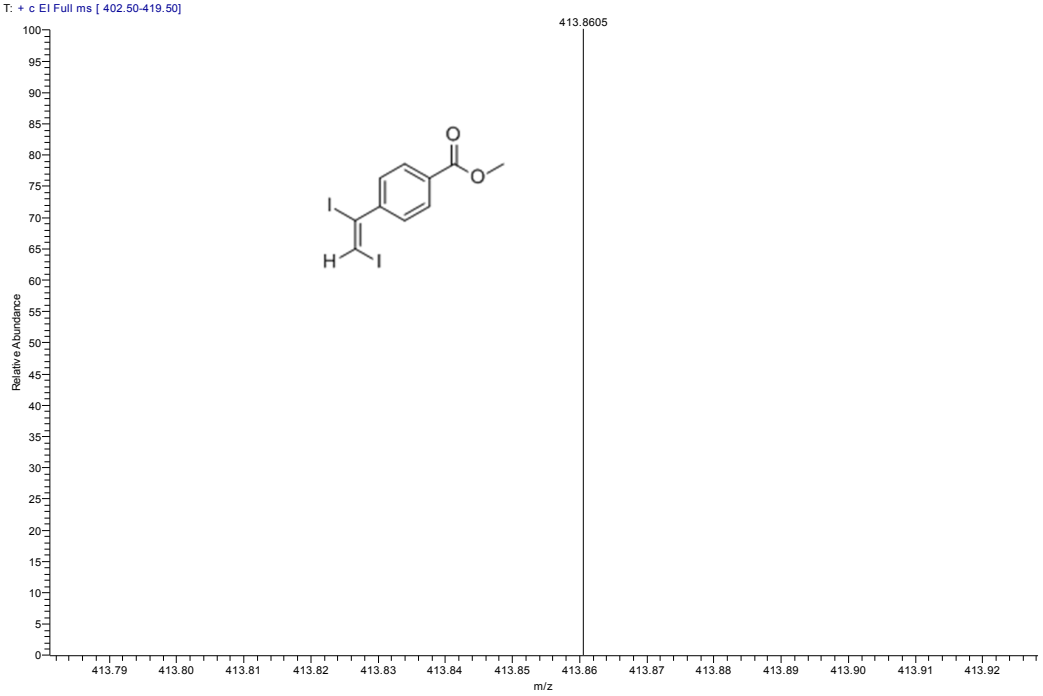
Instrument:DSQ(Thermo)
Ionization Method:EI
D:\DSQ\DATA-LR\17\042603 4/26/2017 4:17:06 PM 20170221-30

042603 #28 RT: 0.64 AV: 1 NL: 1.10E8
T: + c Full ms [45.00-700.00]



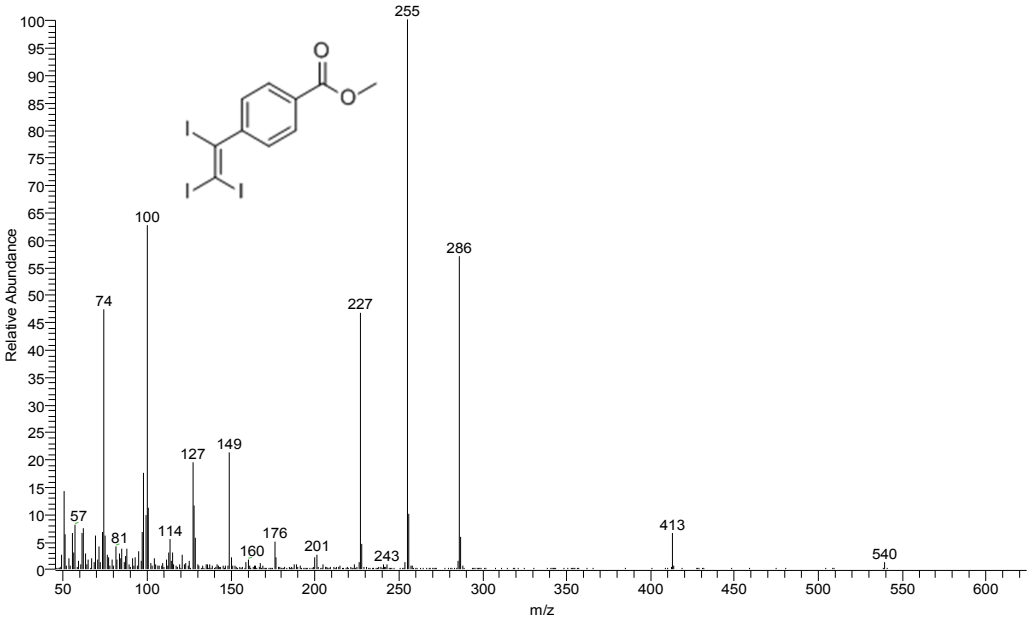
Instrument:MAT 95XP(Thermo)
D:\DATA-HR\17\042701-20170221-30-c1 4/27/2017 9:53:08 AM 20170221-30

042701-20170221-30-c1 #4 RT: 0.17 AV: 1 NL: 9.99E4
T: + c EI Full ms [402.50-419.50]



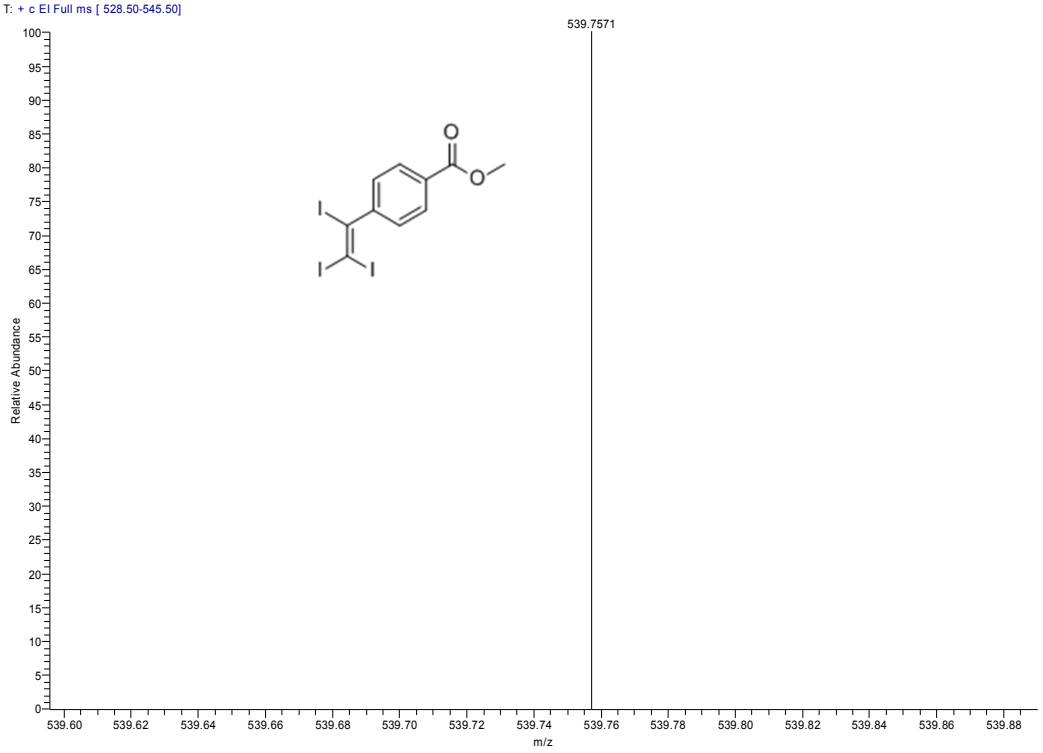
Instrument:DSQ(Thermo)
Ionization Method:EI
D:\DSQ\DATA-LR\17\041407 4/14/2017 10:29:38 AM 20170224-39

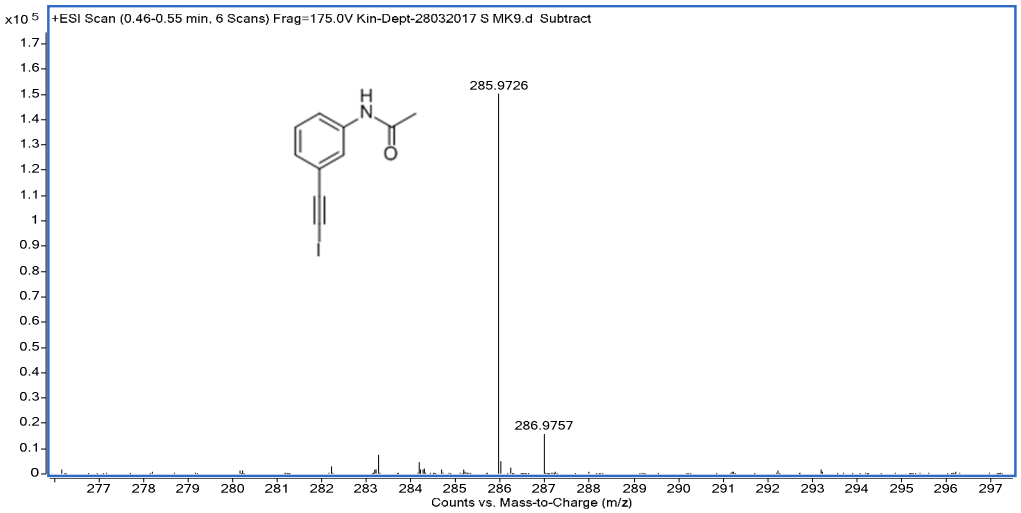
041407 #10 RT: 0.27 AV: 1 NL: 3.76E5
T: + c Full ms [45.00-800.00]

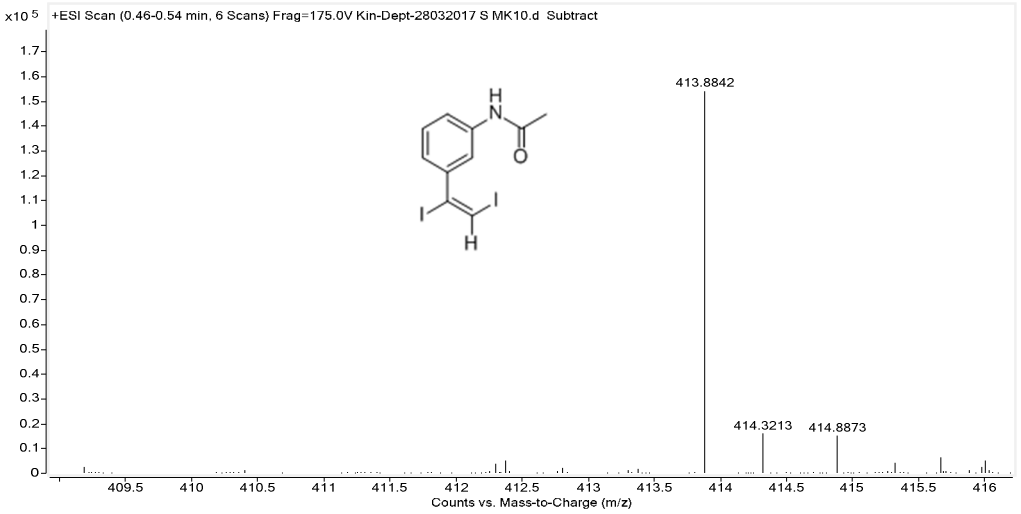


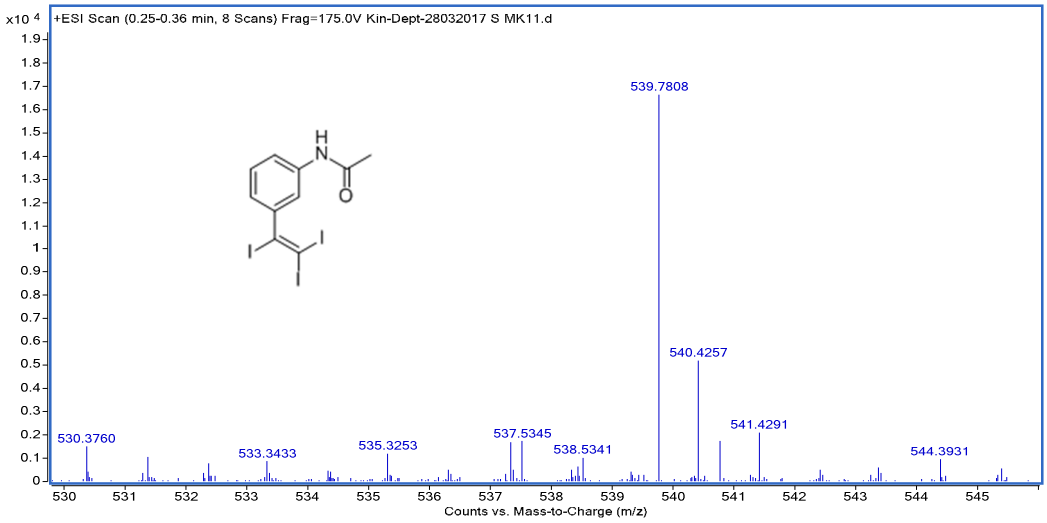
Instrument:MAT 95XP(Thermo)
D:\DATA-HR\17\041704-20170224-39-c1 4/17/2017 2:25:16 PM 20170224-39

041704-20170224-39-c1 #20 RT: 0.75 AV: 1 NL: 1.97E4
T: + c EI Full ms [528.50-545.50]



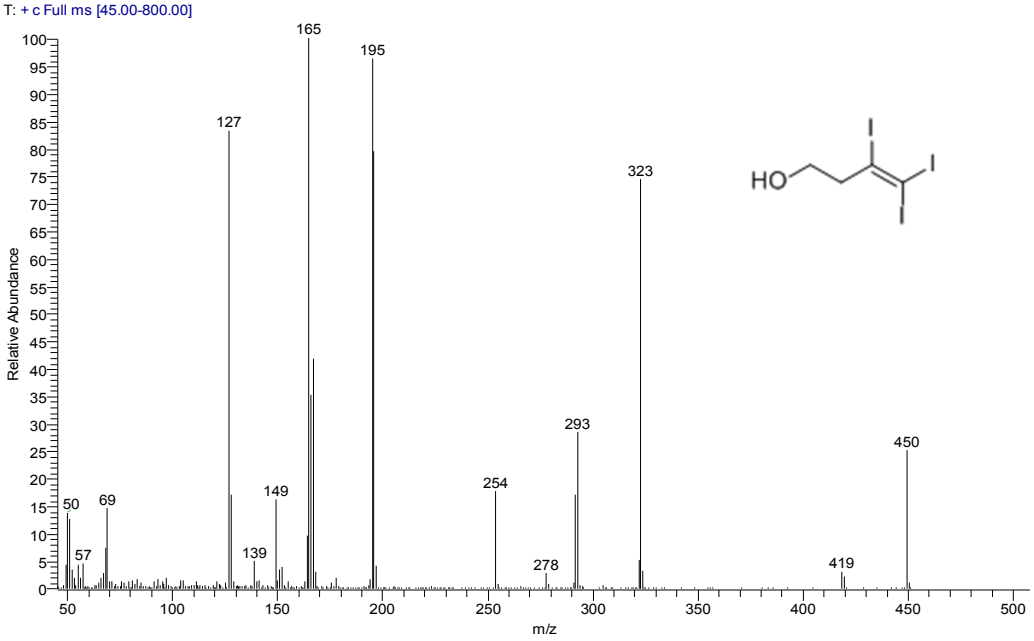

x10 5
+ESI Scan (0.46-0.55 min, 6 Scans) Frag=175.0V Kin-Dept-28032017 S MK9.d Subtract
285.9726
286.9757
Counts vs. Mass-to-Charge (m/z)


x10 5
+ESI Scan (0.46-0.54 min, 6 Scans) Frag=175.0V Kin-Dept-28032017 S MK10.d Subtract
413.8842
414.3213
414.8873
Counts vs. Mass-to-Charge (m/z)


x10 4
+ESI Scan (0.25-0.36 min, 8 Scans) Frag=175.0V Kin-Dept-28032017 S MK11.d
539.7808
540.4257
541.4291
530.3760
533.3433
535.3253
537.5345
538.5341
544.3931
Counts vs. Mass-to-Charge (m/z)

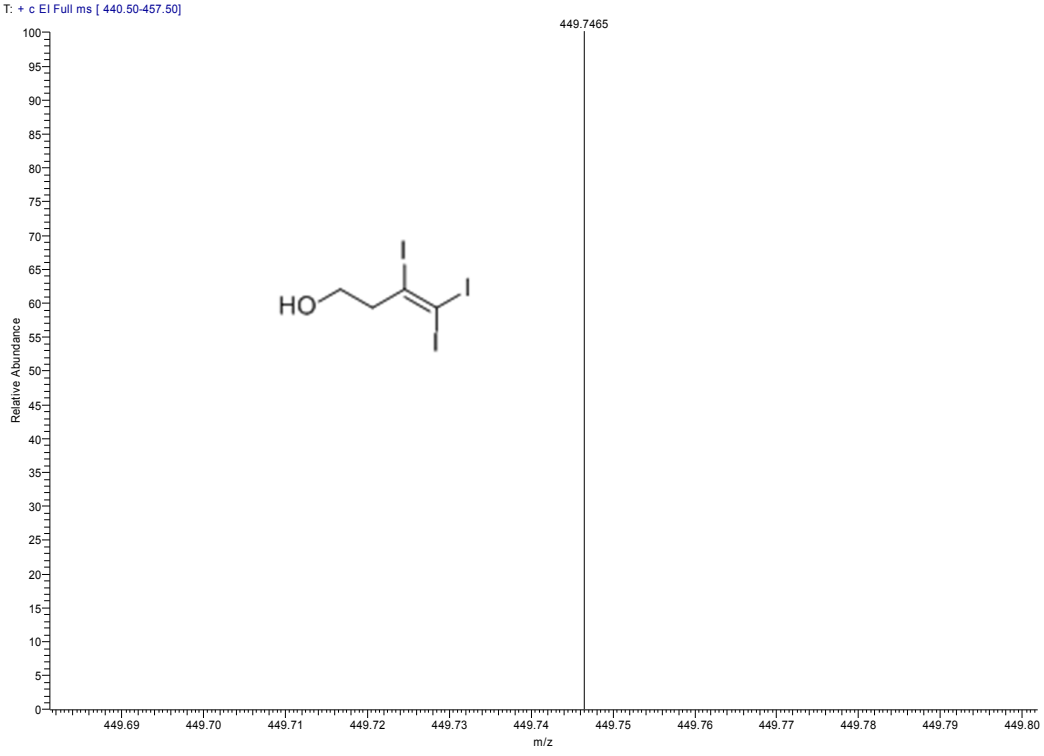
Instrument:DSQ(Thermo)
Ionization Method:EI
D:\DSQ\DATA-LR\17\041403 4/14/2017 9:57:09 AM 20170303-52

041403 #6 RT: 0.17 AV: 1 NL: 4.71E5
T: + c Full ms [45.00-800.00]



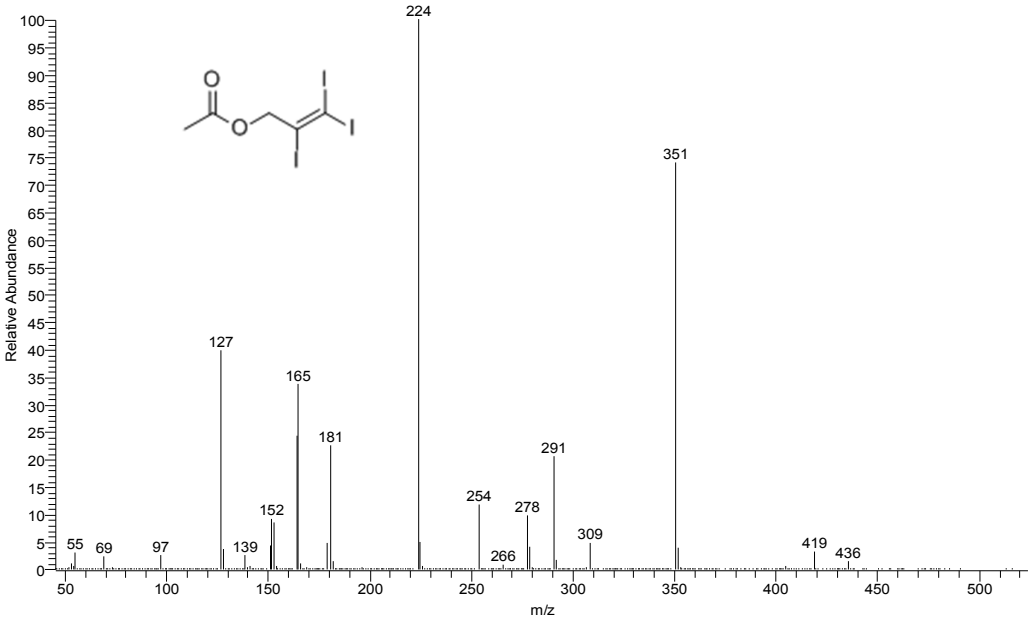
Instrument:MAT 95XP(Thermo)
D:\DATA-HR\17\041708-20170303-52-c1 4/17/2017 2:47:17 PM 20170303-52

041708-20170303-52-c1 #9 RT: 0.37 AV: 1 NL: 5.81E4
T: + c EI Full ms [440.50-457.50]



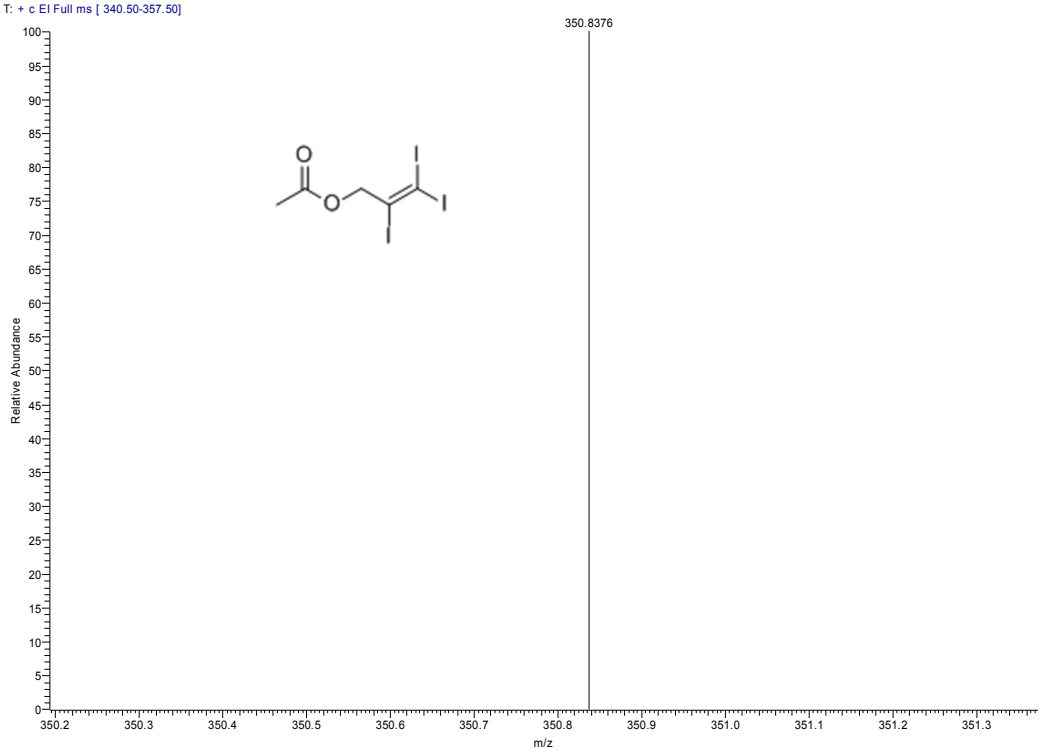
Instrument:DSQ(Thermo)
Ionization Method:EI
D:\DSQ\DATA-LR\17\042602 4/26/2017 4:05:45 PM 20170221-29

042602 #46 RT: 1.04 AV: 1 NL: 6.02E7
T: + c Full ms [45.00-700.00]



Instrument:MAT 95XP(Thermo)
D:\DATA-HR\17\050301-20170221-29-c1 5/3/2017 11:37:15 AM 20170221-29

050301-20170221-29-c1 #1 RT: 0.06 AV: 1 NL: 2.07E4
T: + c EI Full ms [340.50-357.50]



The Plausible Reaction Pathways