

Electronic Supporting Information

Construction of the oxaphenalene skeletons of mansonone F derivatives through C-H bond functionalization and their evaluation for anti-proliferative activities

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People's Republic of China*

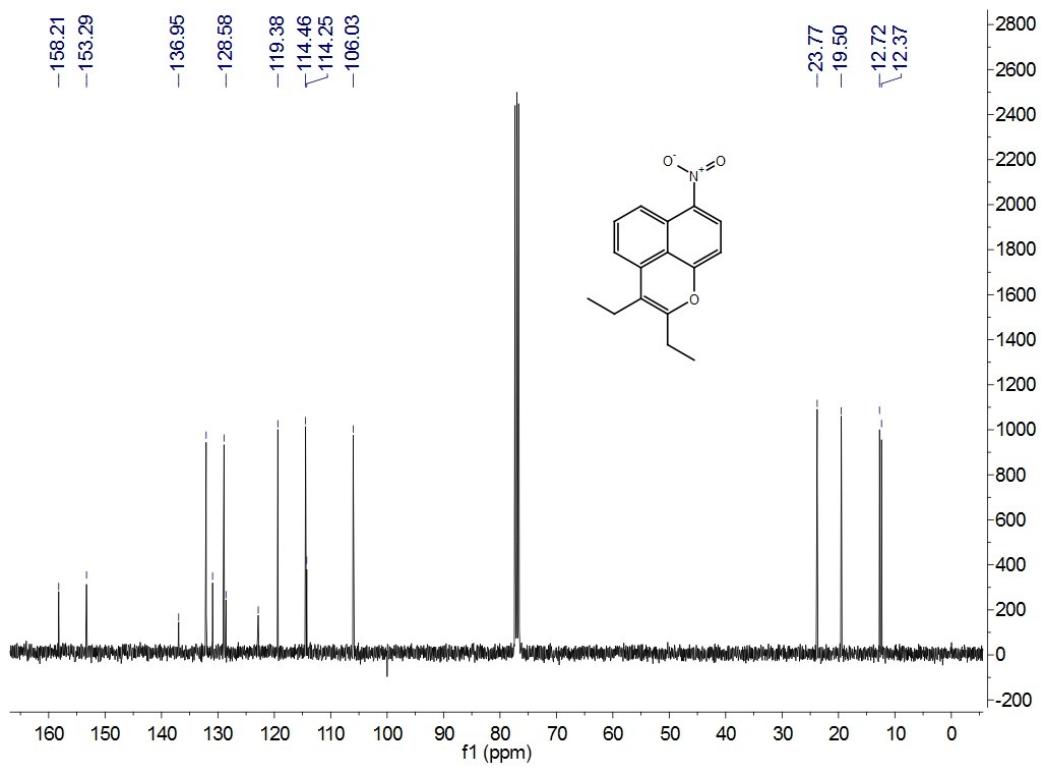
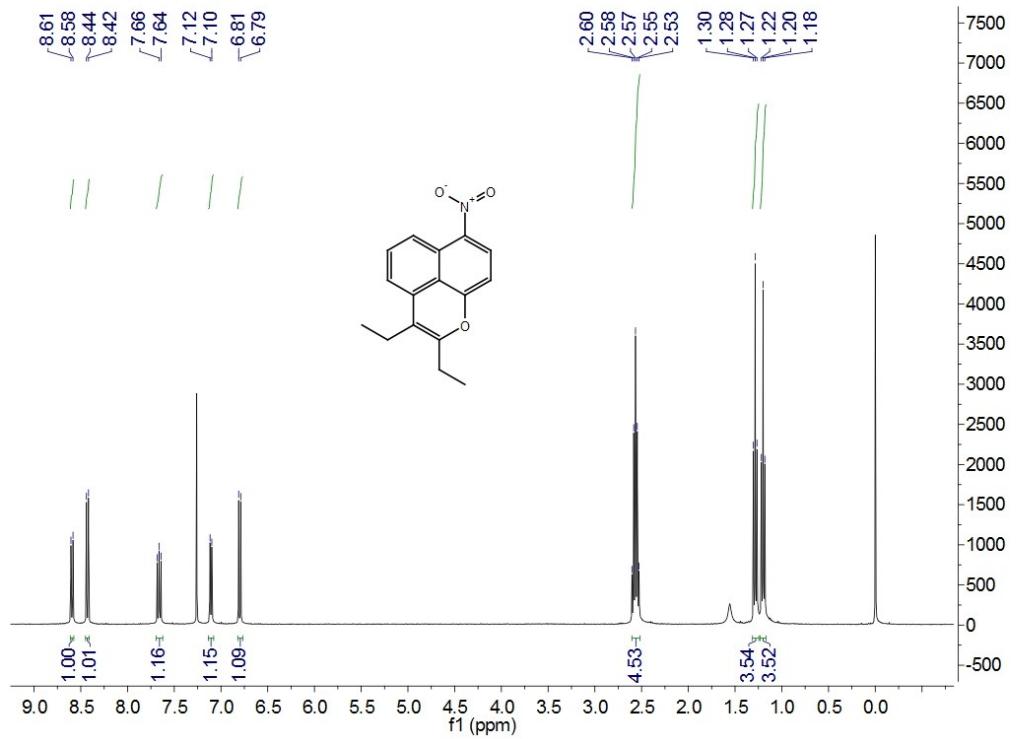
[‡] Contributed equally to this work

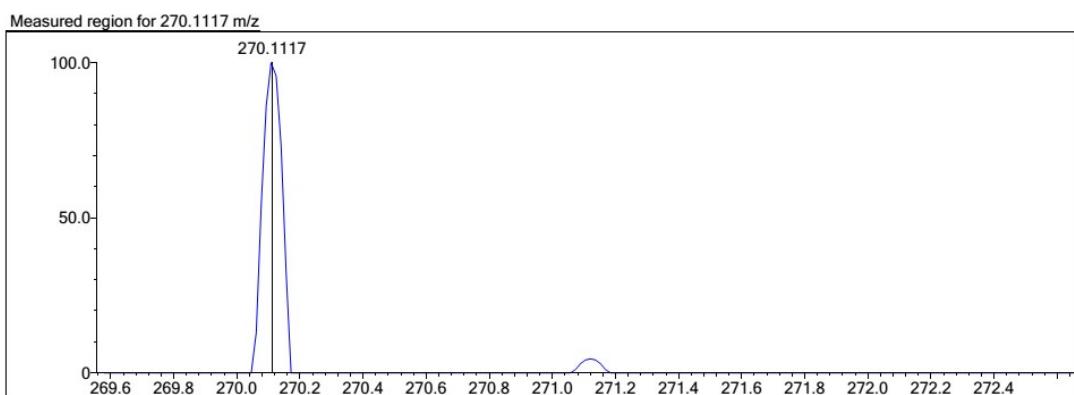
*To whom correspondence should be addressed. Tel.: 8620-39943052,

Fax.: 8620-39943056, e-mail: lsshsl@mail.sysu.edu.cn.

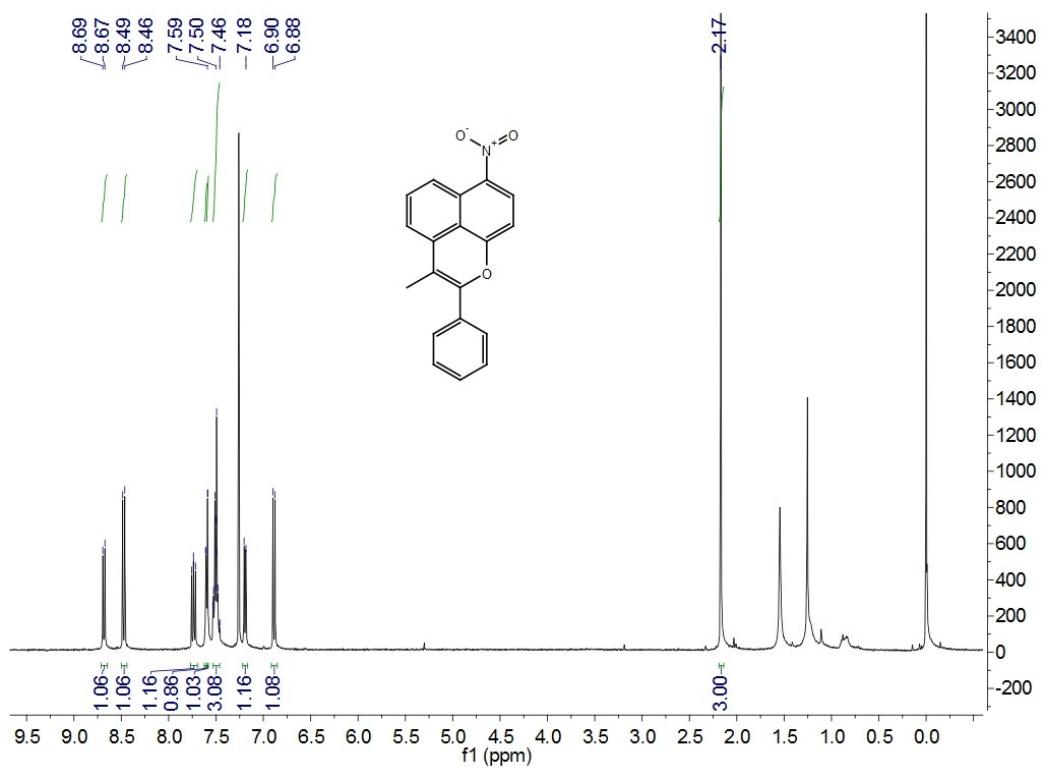
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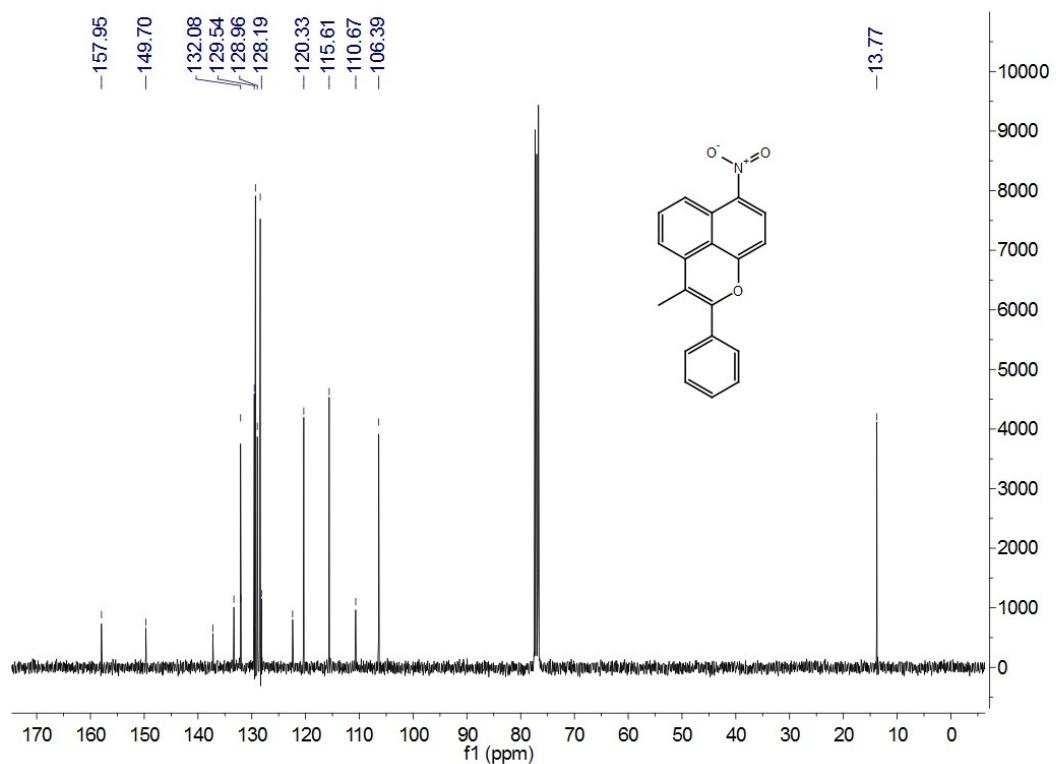




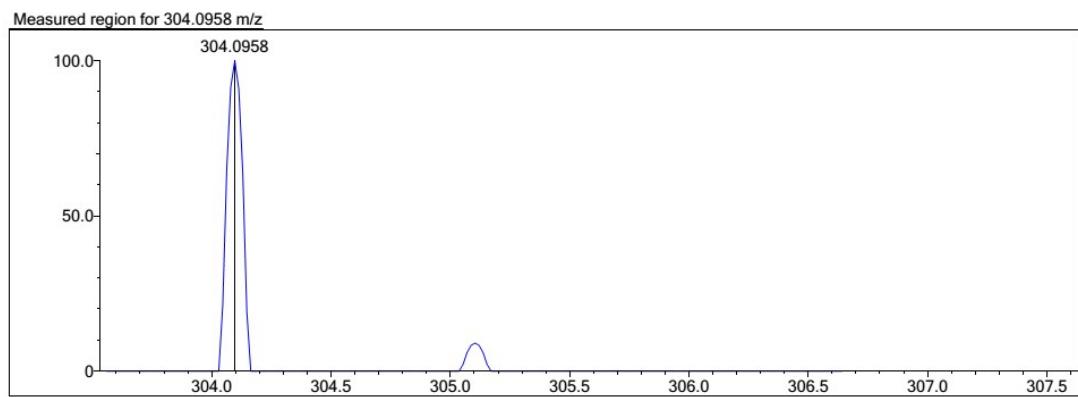
HRMS spectrum of **2a**



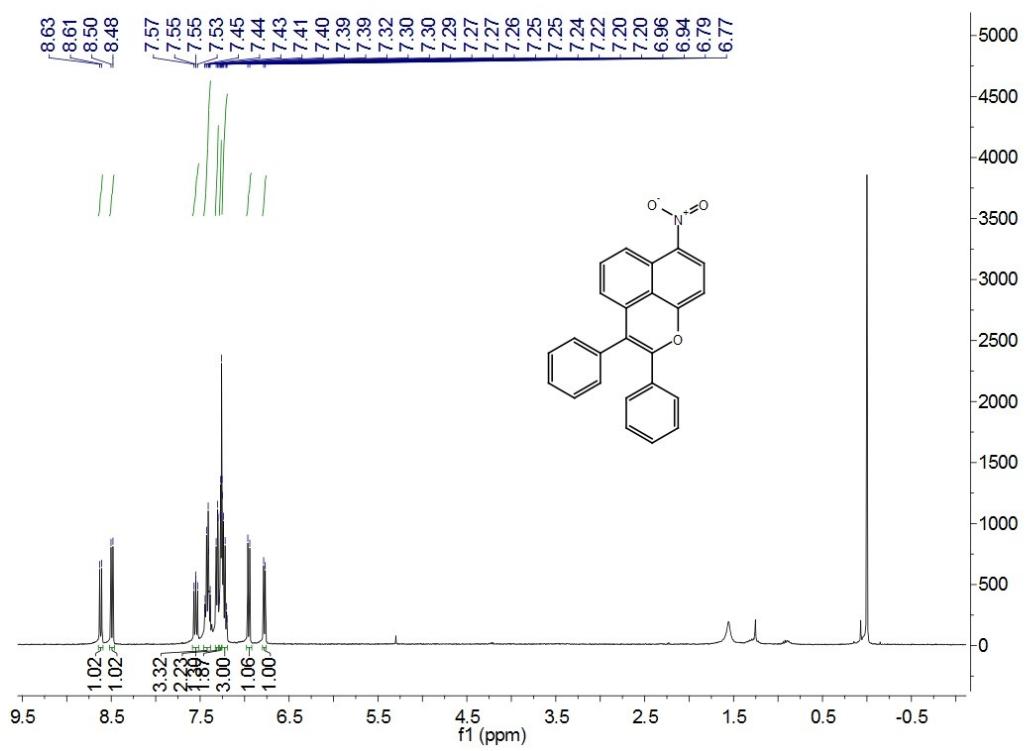
¹H NMR spectra of **2b**



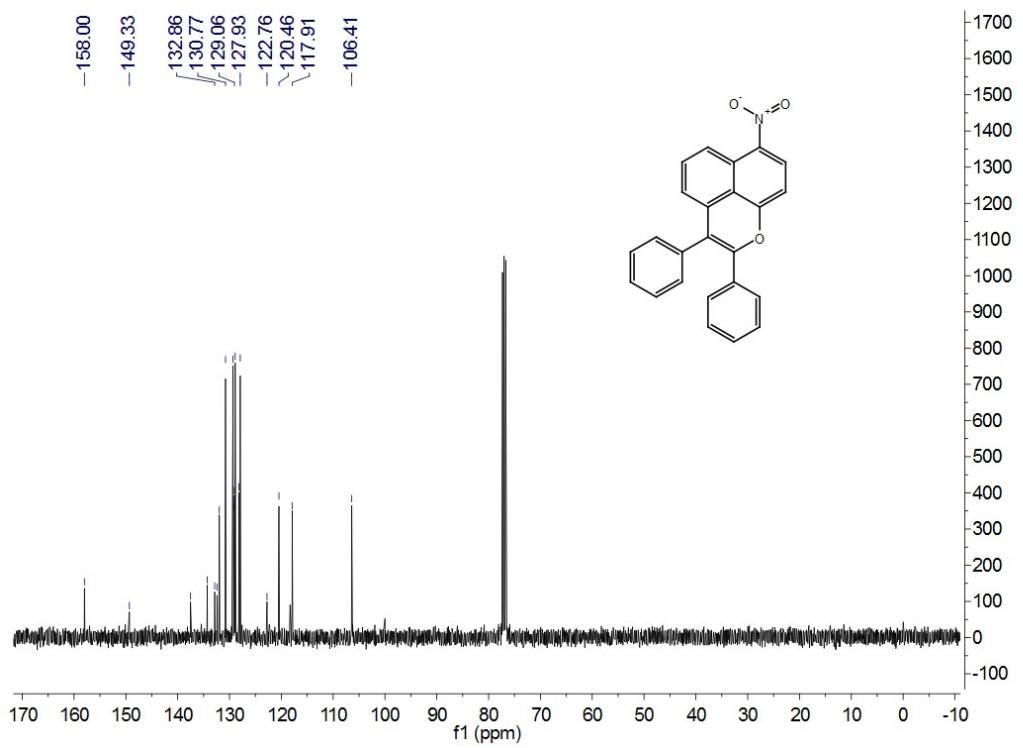
^{13}C NMR spectra of **2b**



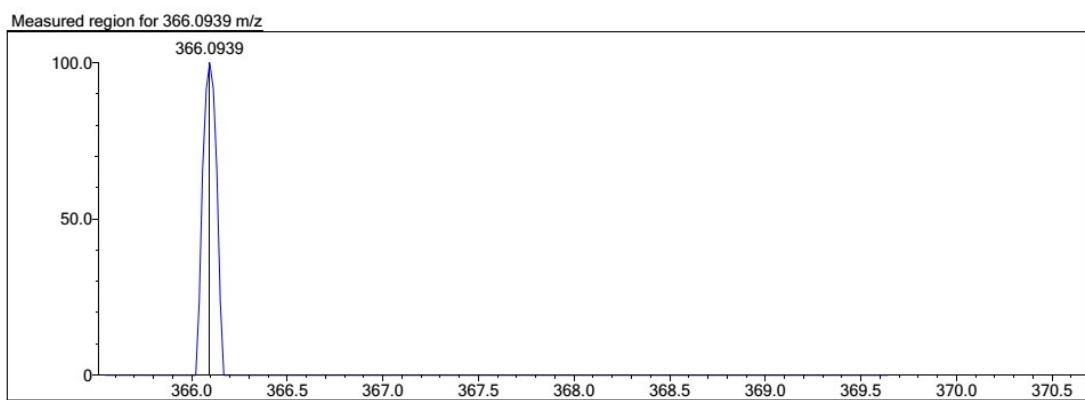
HRMS spectrum of **2b**



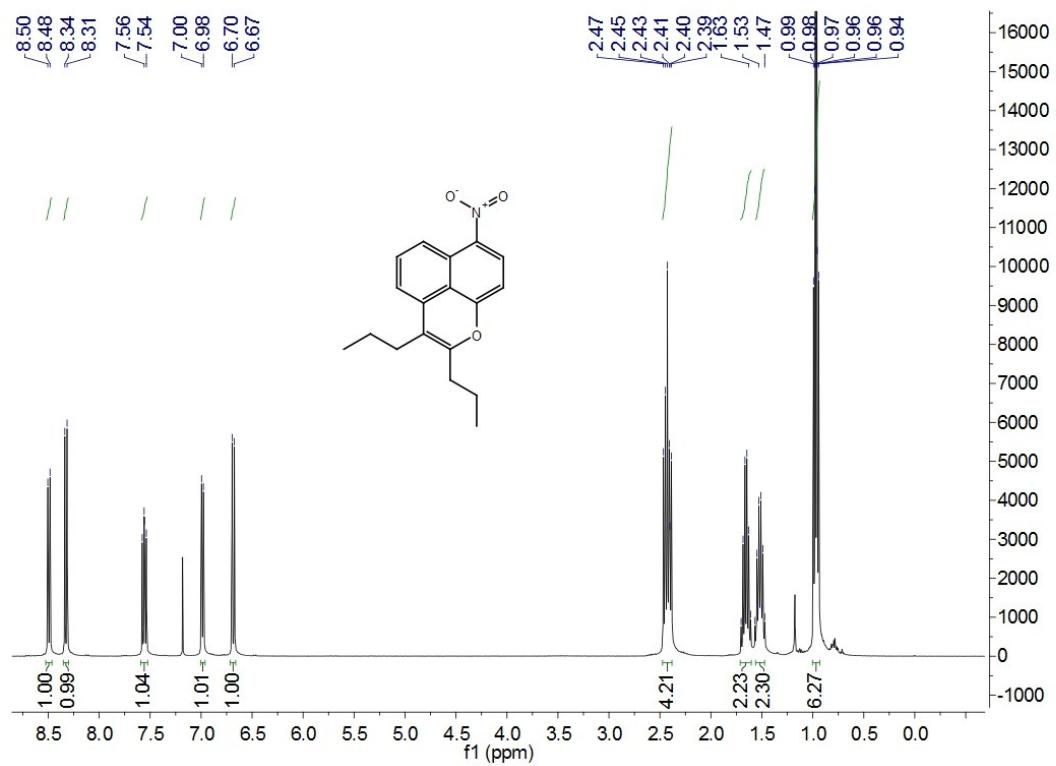
¹H NMR spectra of **2c**



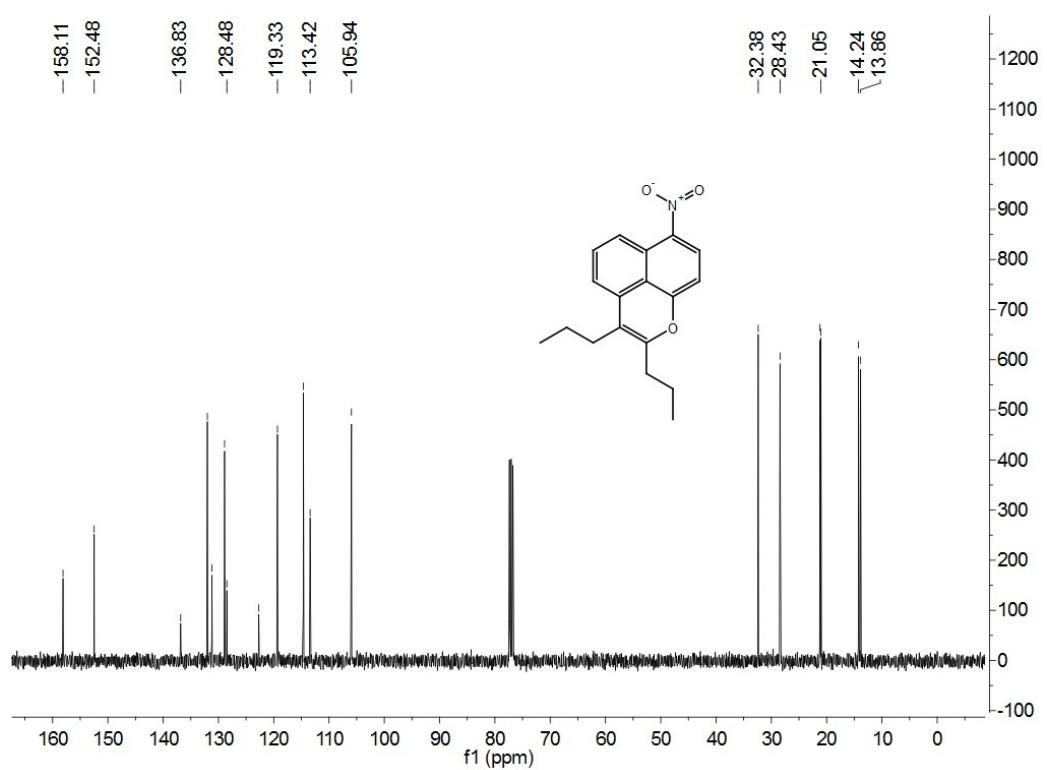
¹³C NMR spectra of **2c**



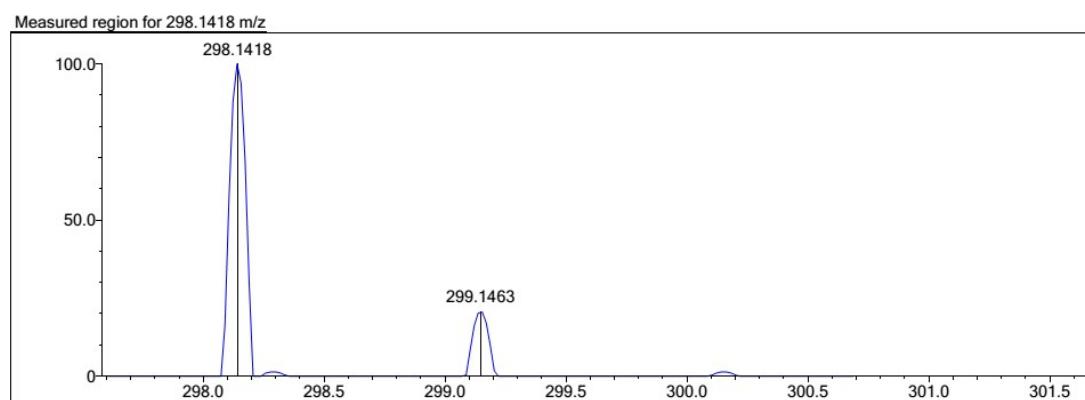
HRMS spectrum of **2c**



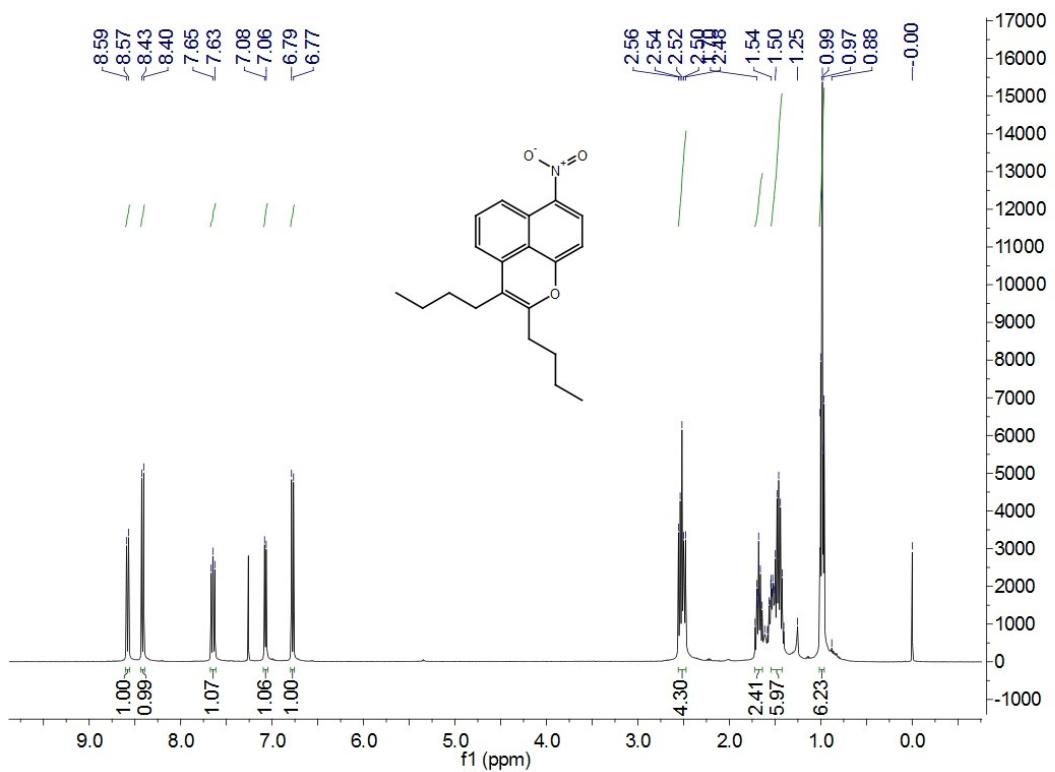
¹H NMR spectra of **2d**



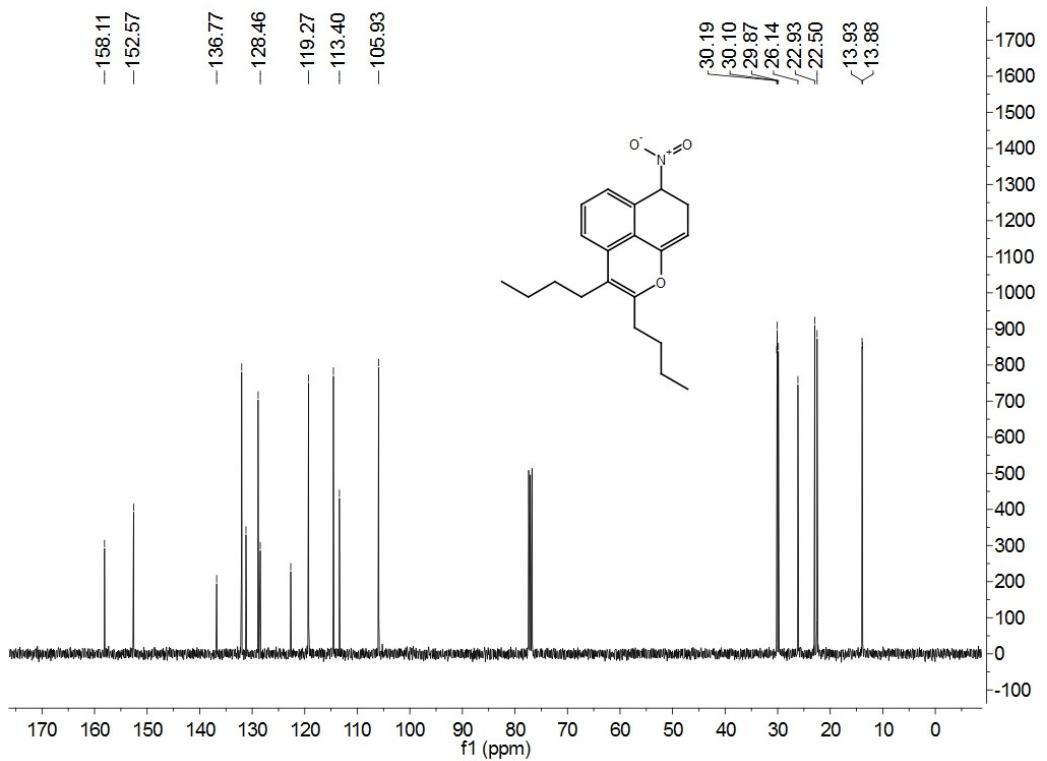
¹³C NMR spectra of **2d**



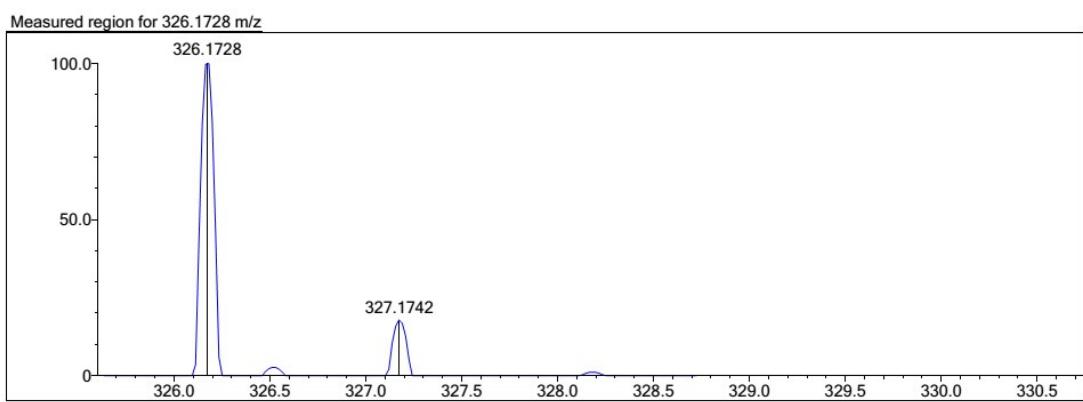
HRMS spectrum of **2d**



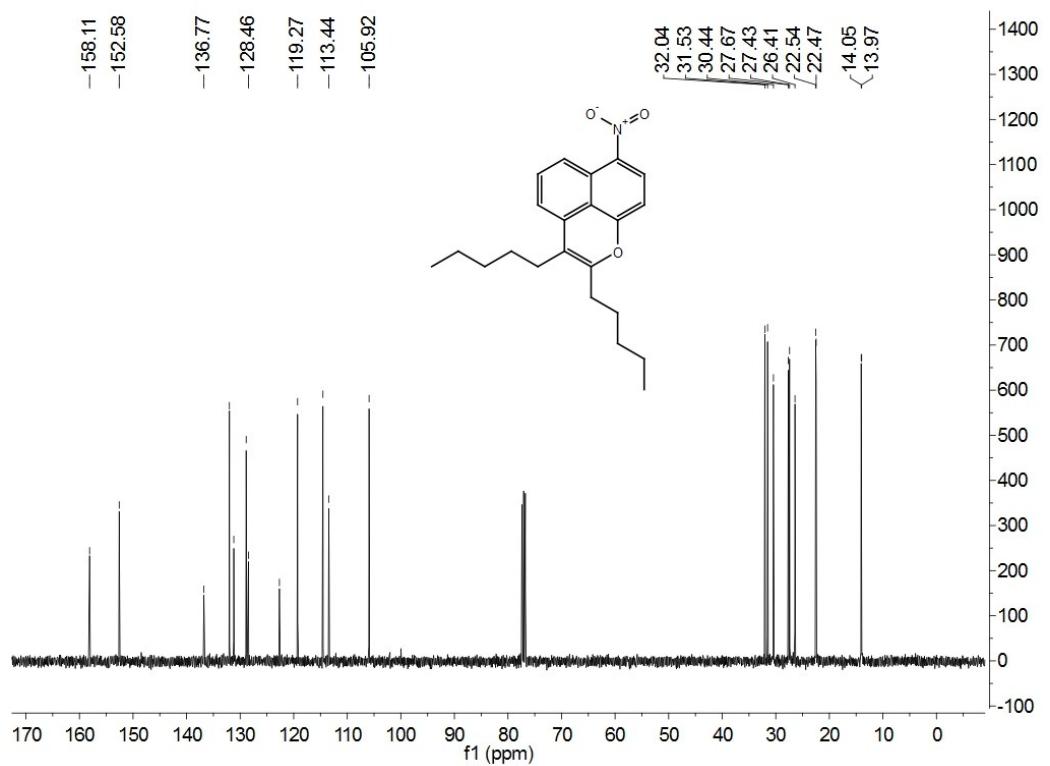
¹H NMR spectra of **2e**



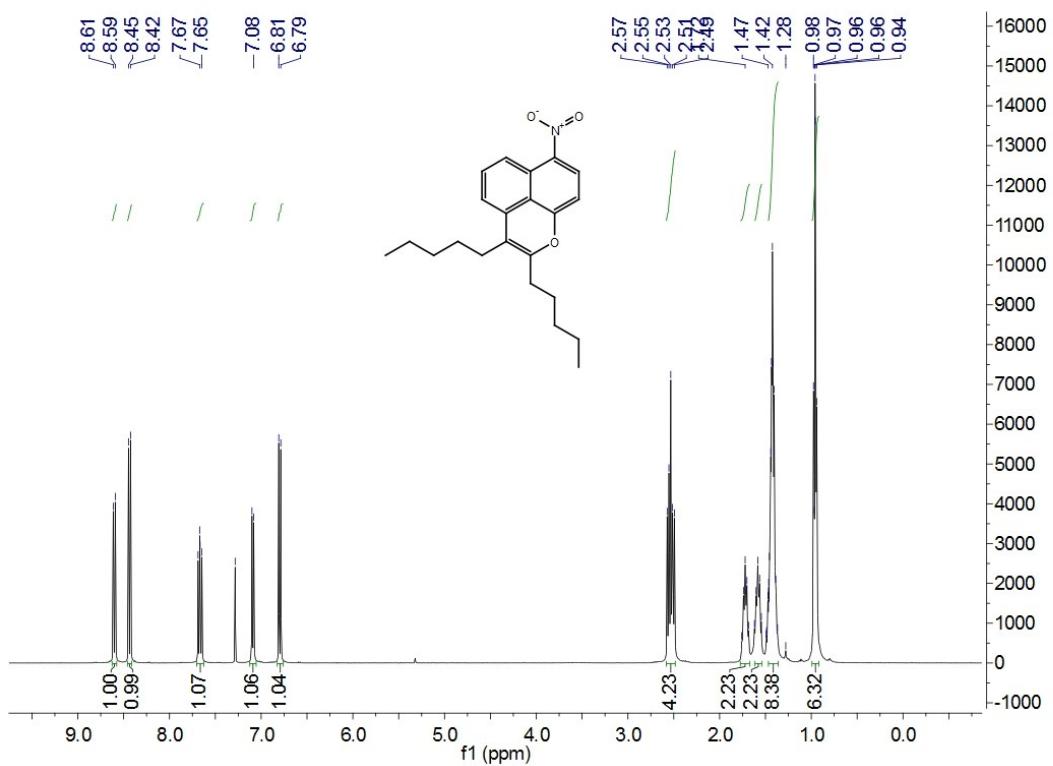
¹³C NMR spectra of **2e**



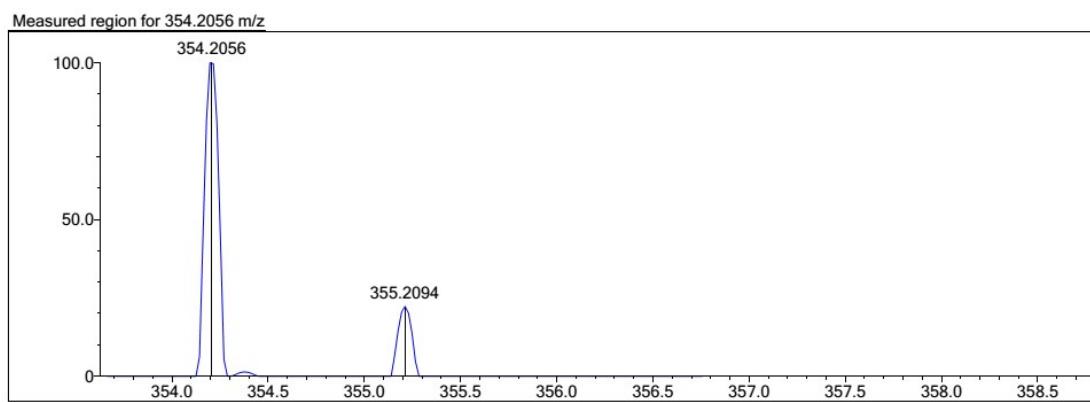
HRMS spectrum of **2e**



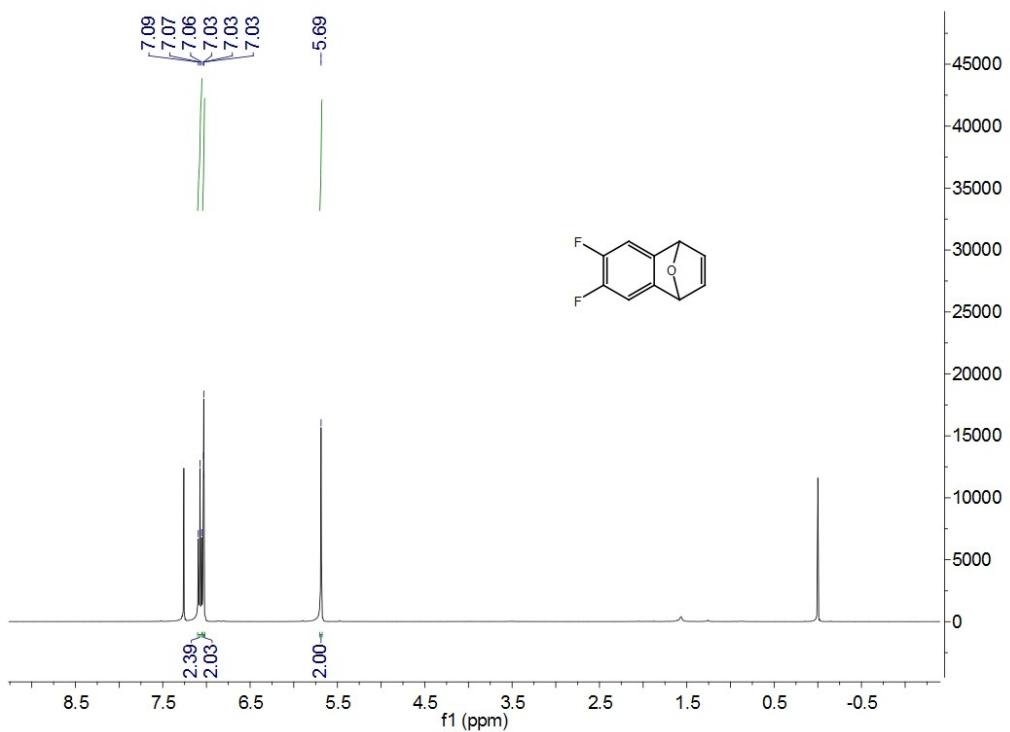
¹H NMR spectra of **2f**



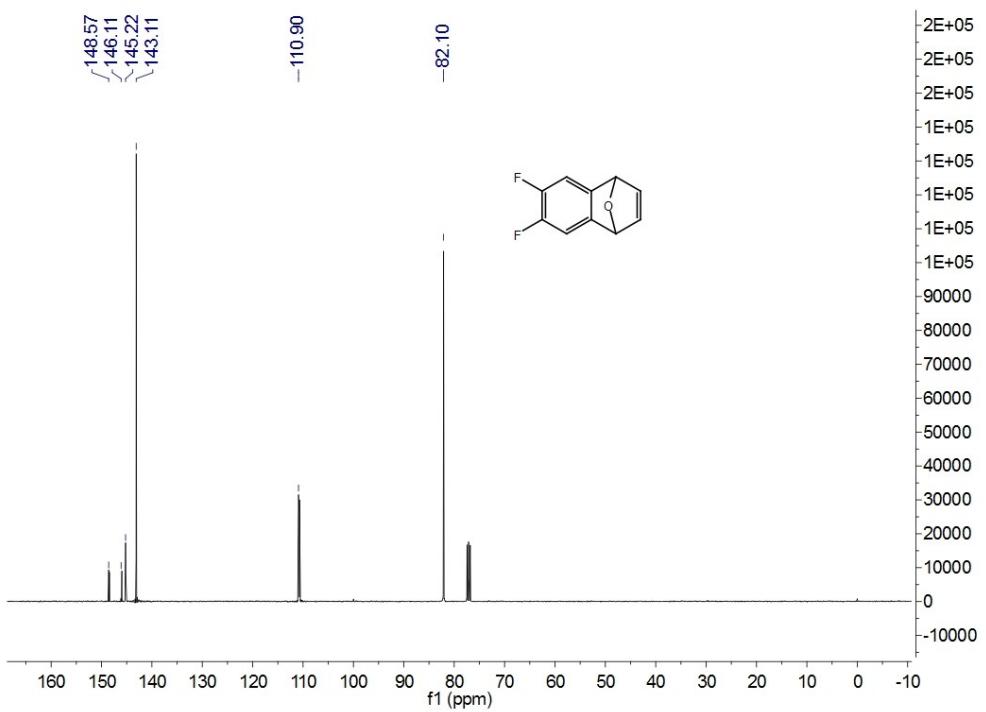
^{13}C NMR spectra of **2f**



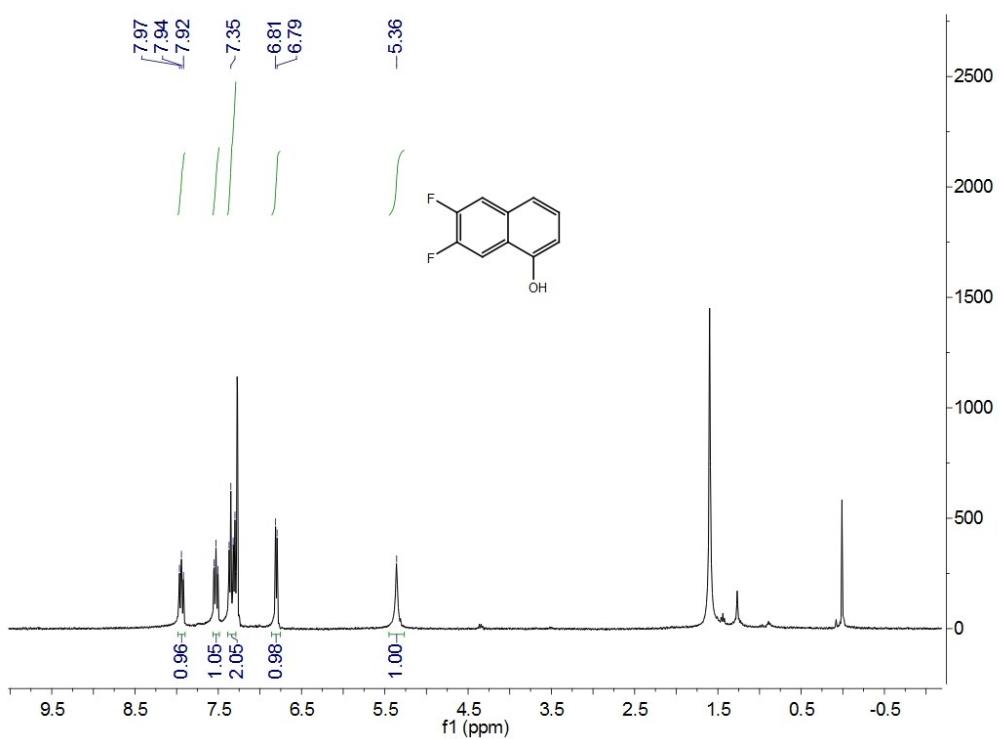
HRMS spectrum of **2f**



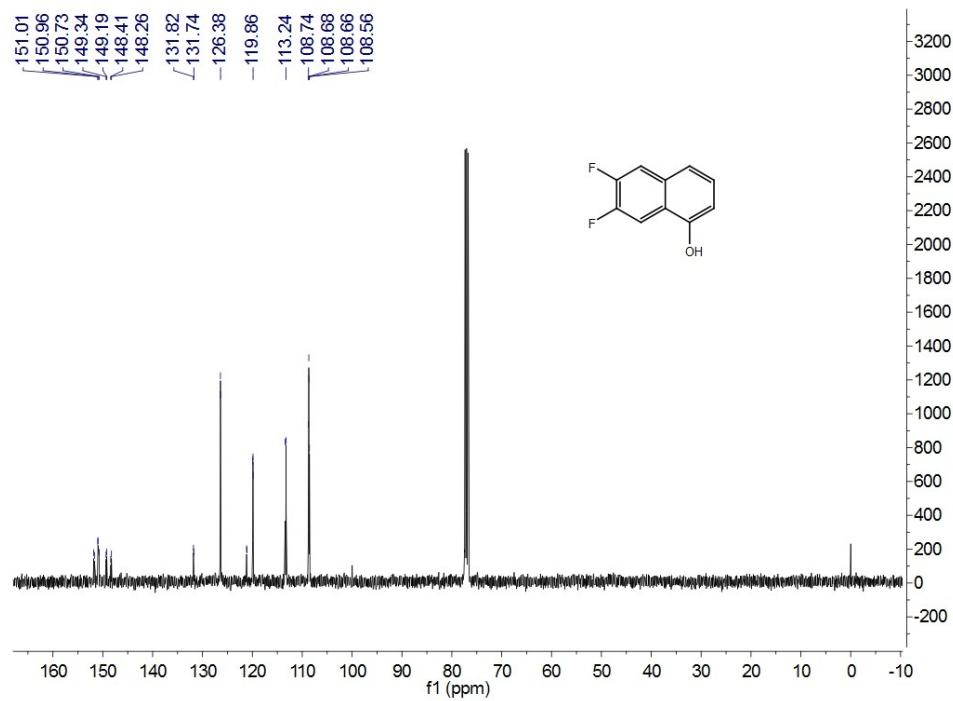
¹H NMR spectra of **9**



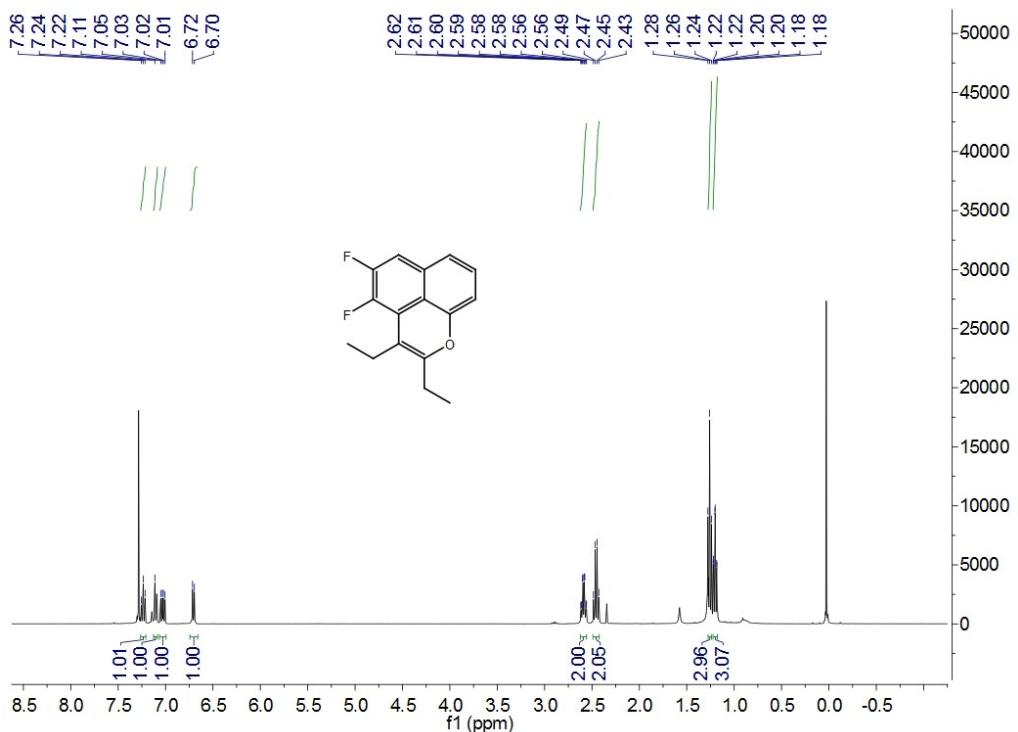
¹³C NMR spectra of **9**



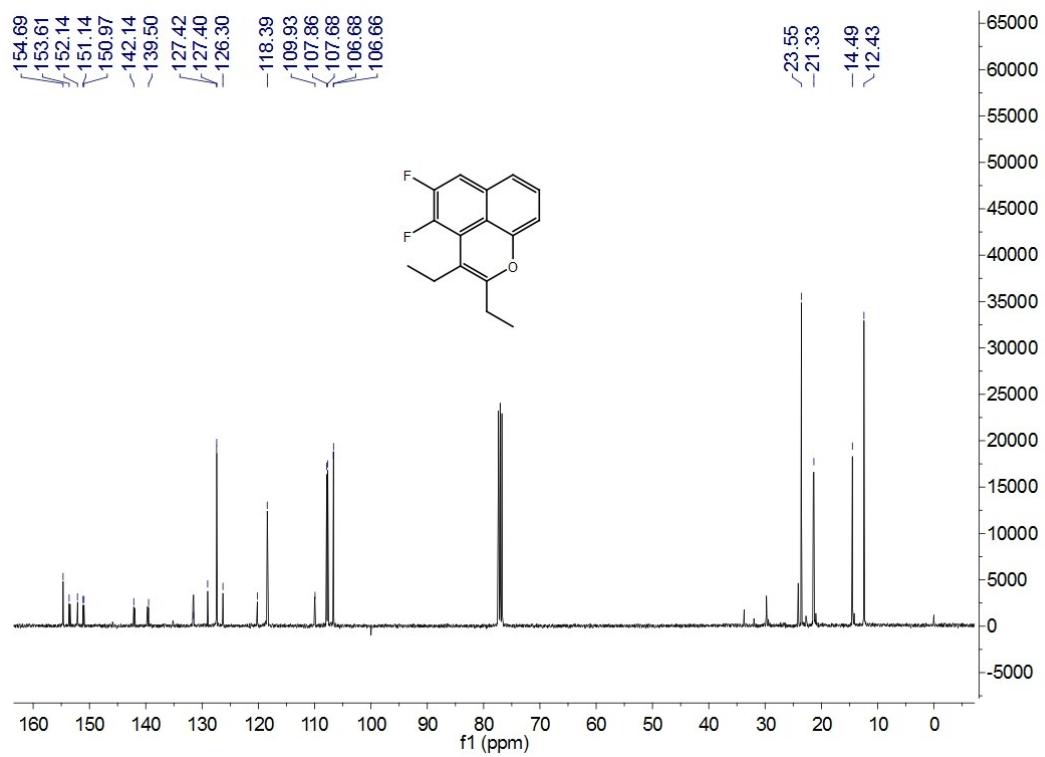
¹H NMR spectra of **10**



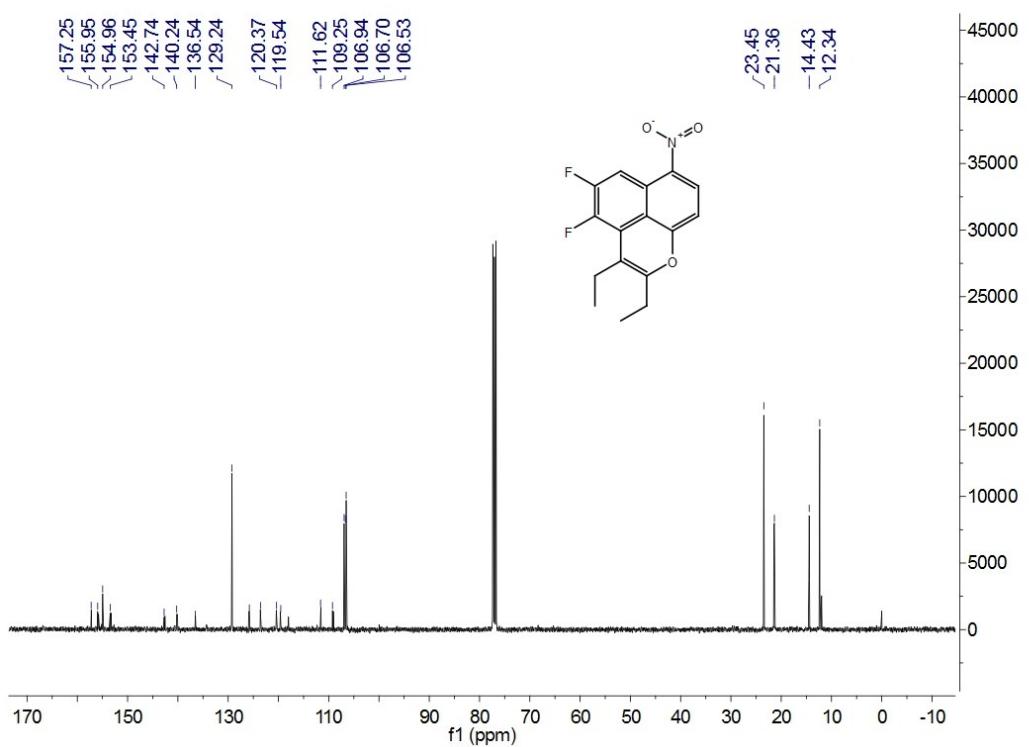
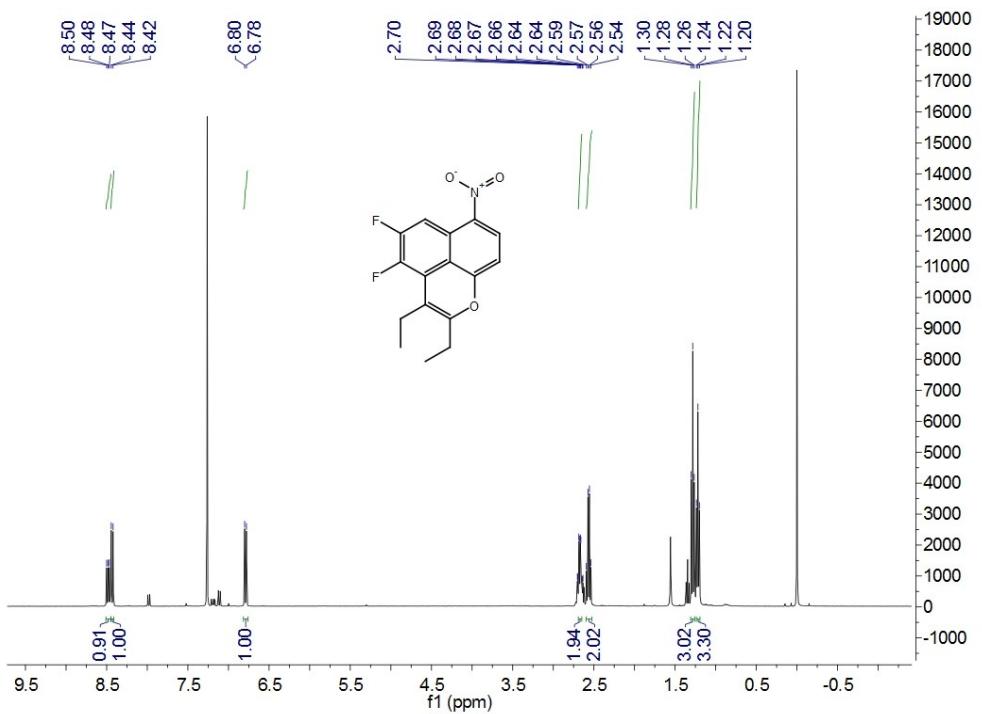
¹³C NMR spectra of **10**



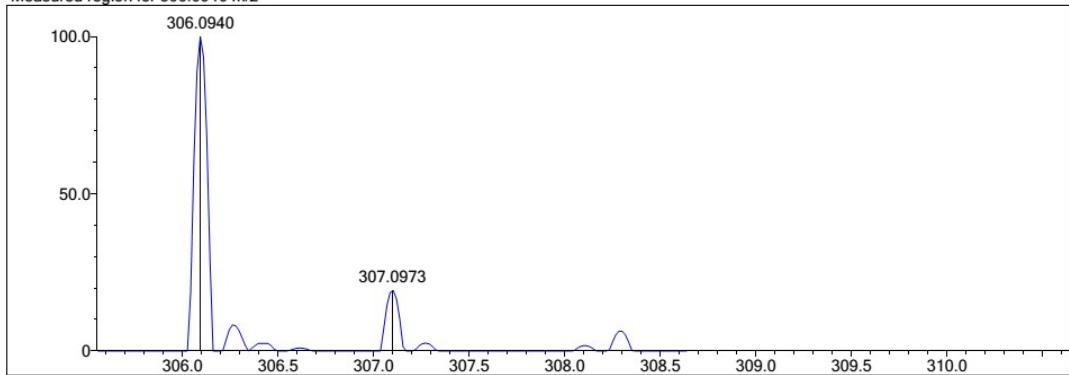
¹H NMR spectra of 11



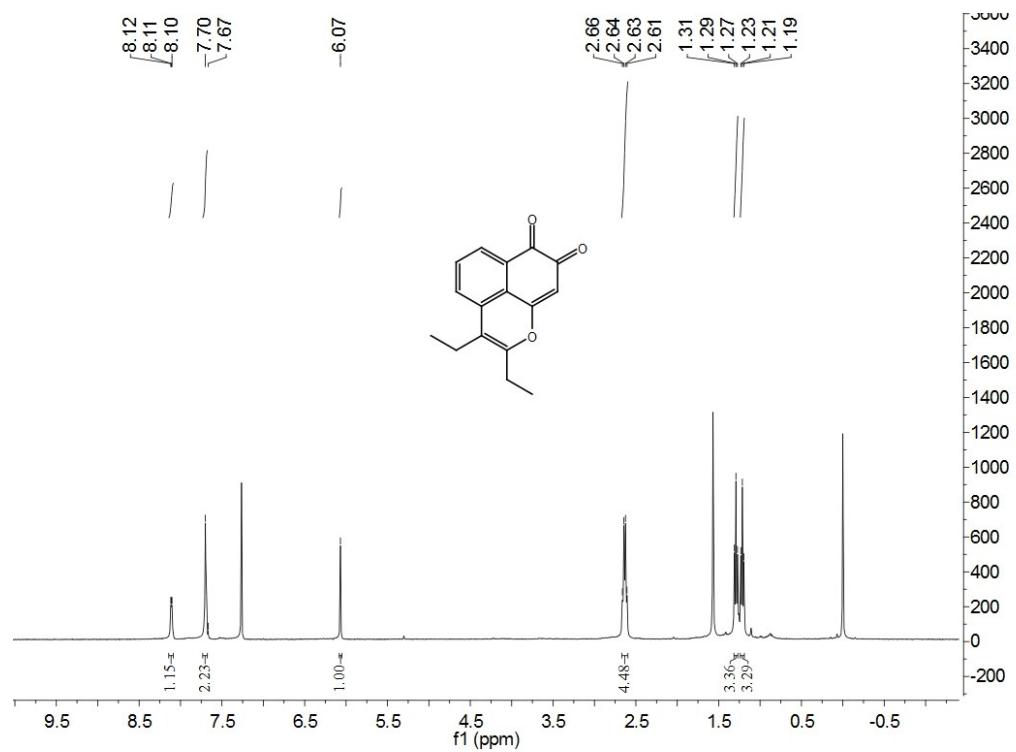
¹³C NMR spectra of 11



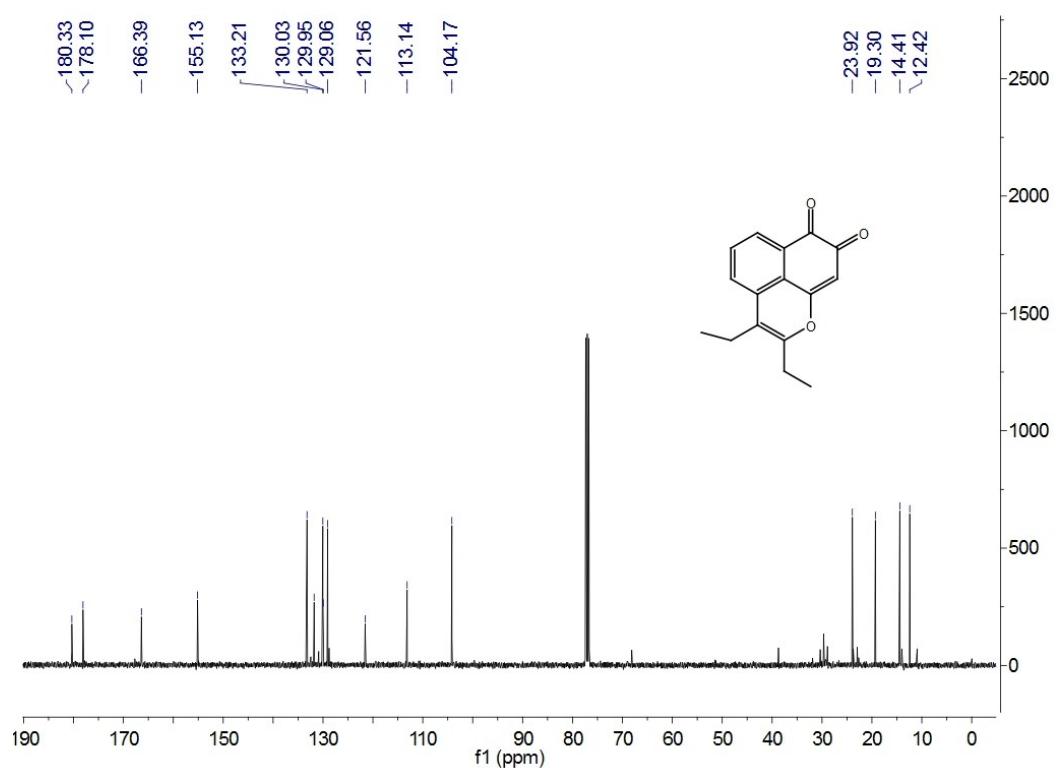
Measured region for 306.0940 m/z



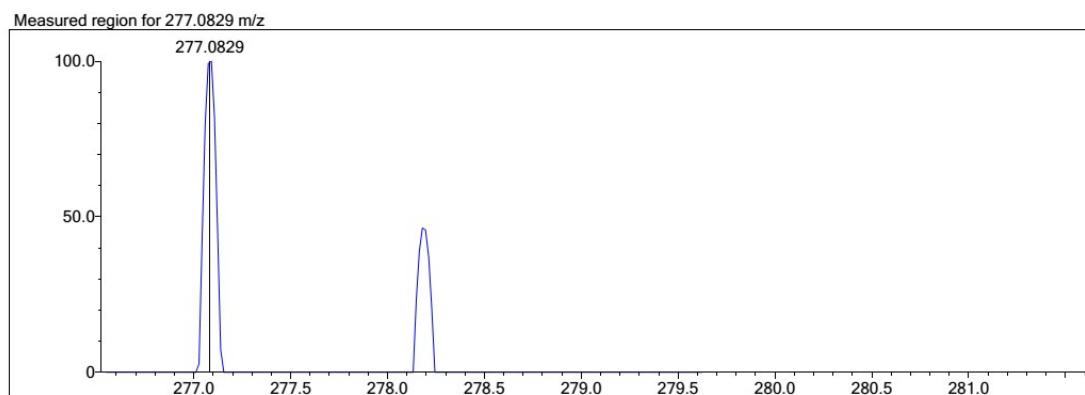
HRMS spectrum of **12**



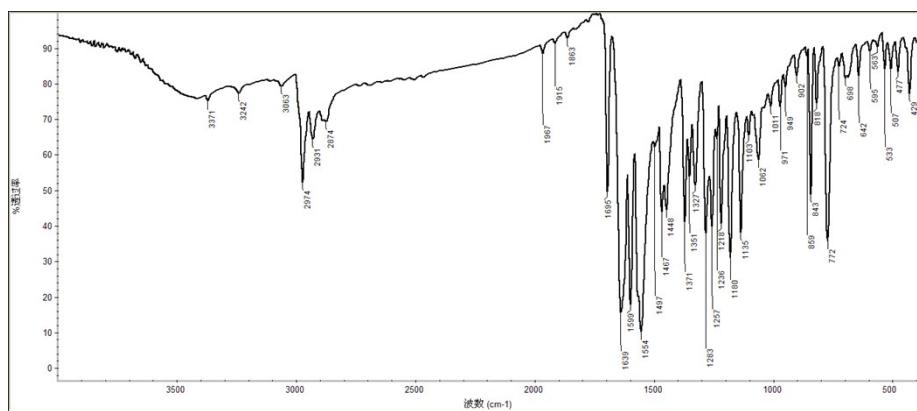
¹H NMR spectra of **3a**



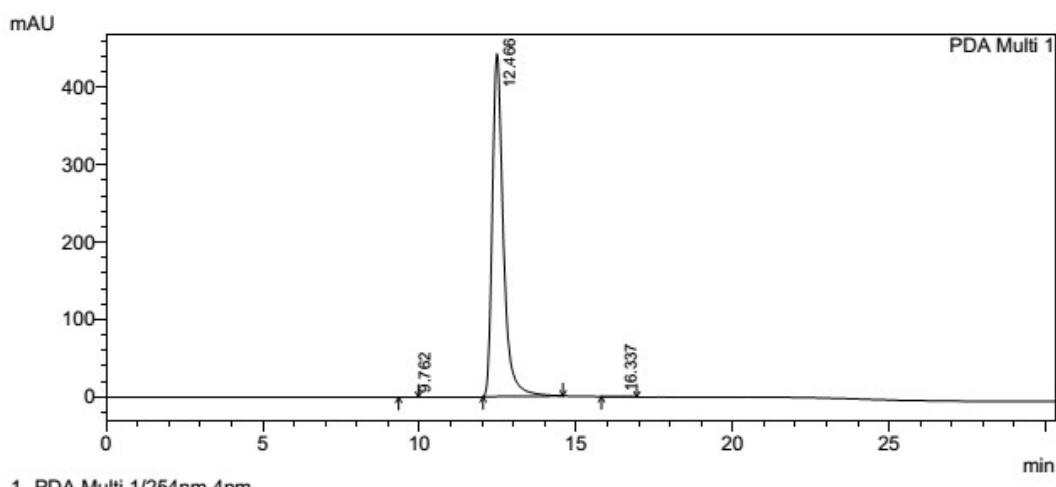
^{13}C NMR spectra of **3a**



HRMS spectrum of **3a**

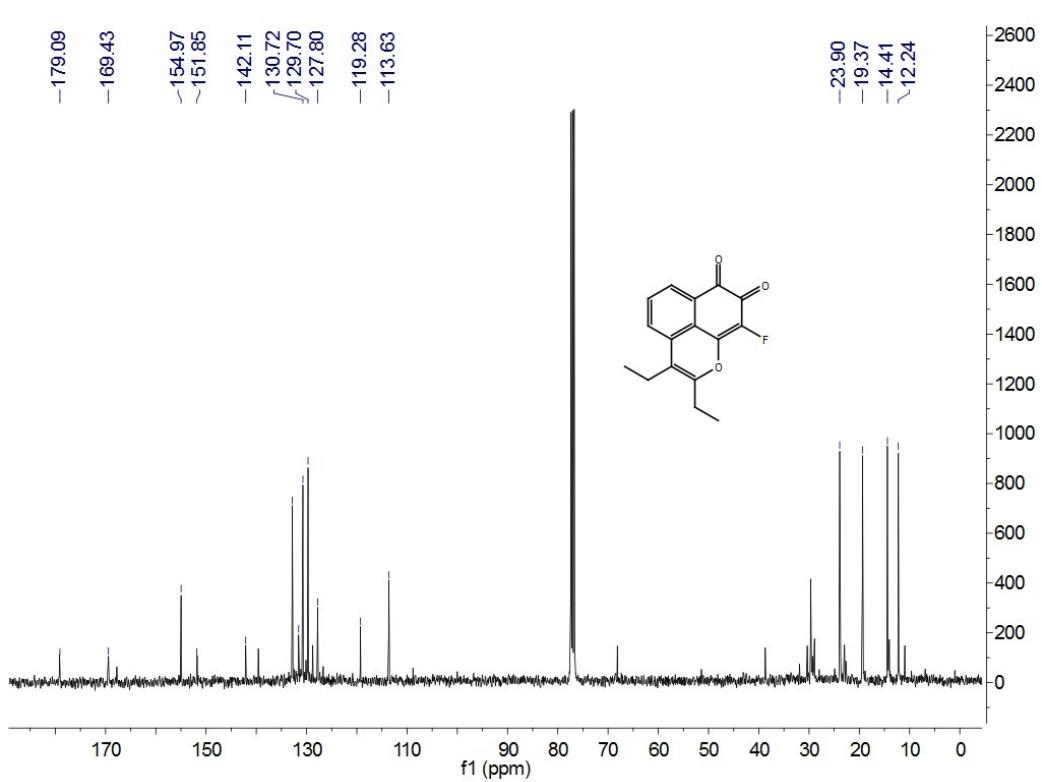
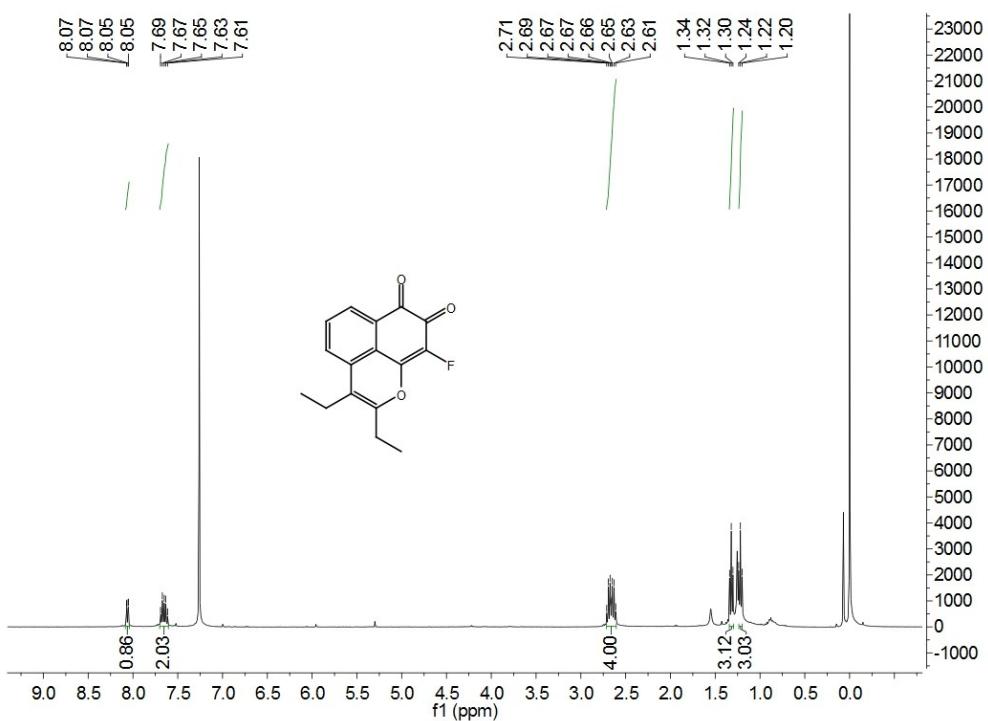


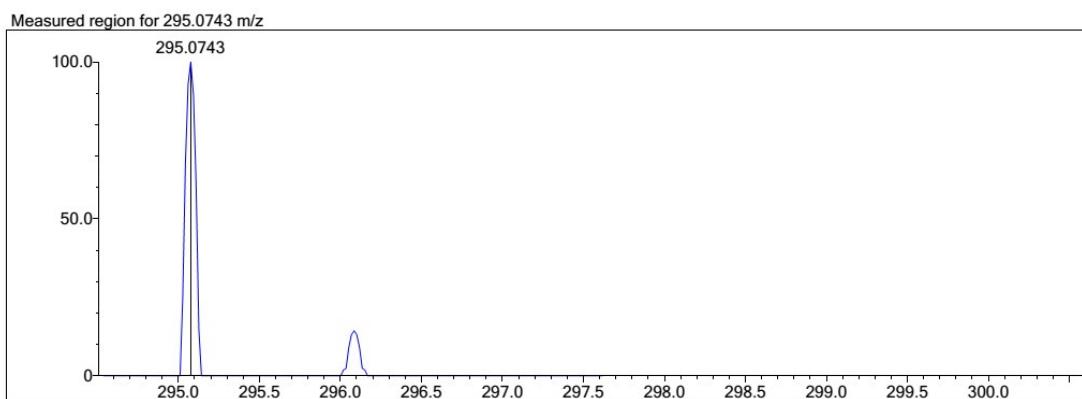
IR spectra of **3a**



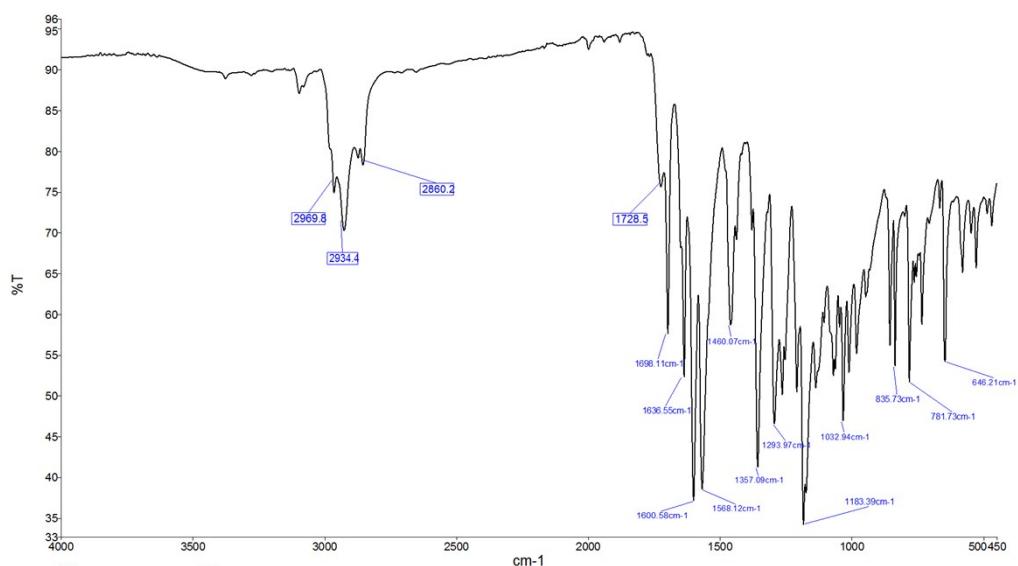
PeakTable					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.762	394	178	0.004	0.040
2	12.466	10783235	443562	99.925	99.881
3	16.337	7689	352	0.071	0.079
Total		10791318	444092	100.000	100.000

HPLC profile of **3a**

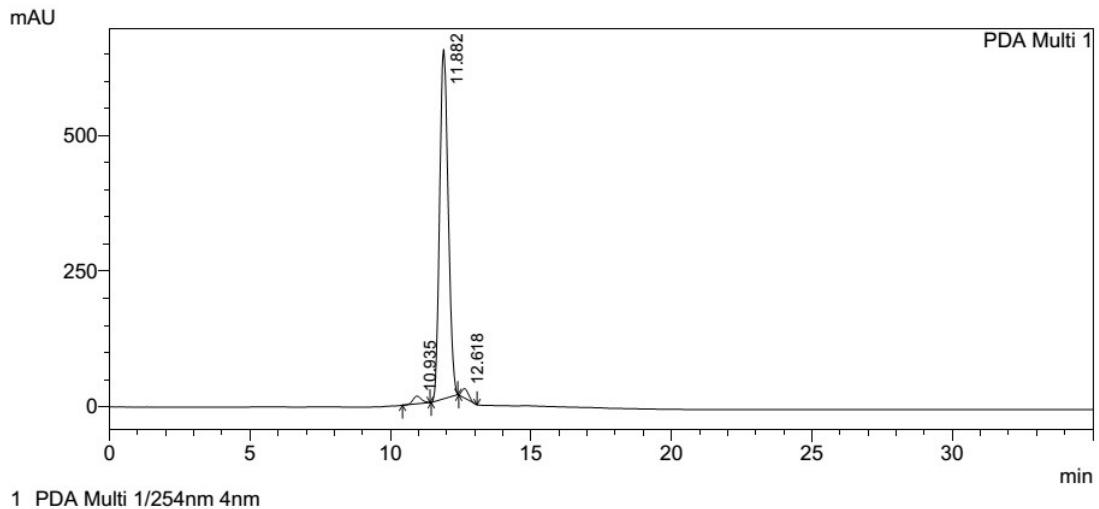




HRMS spectrum of **4a**



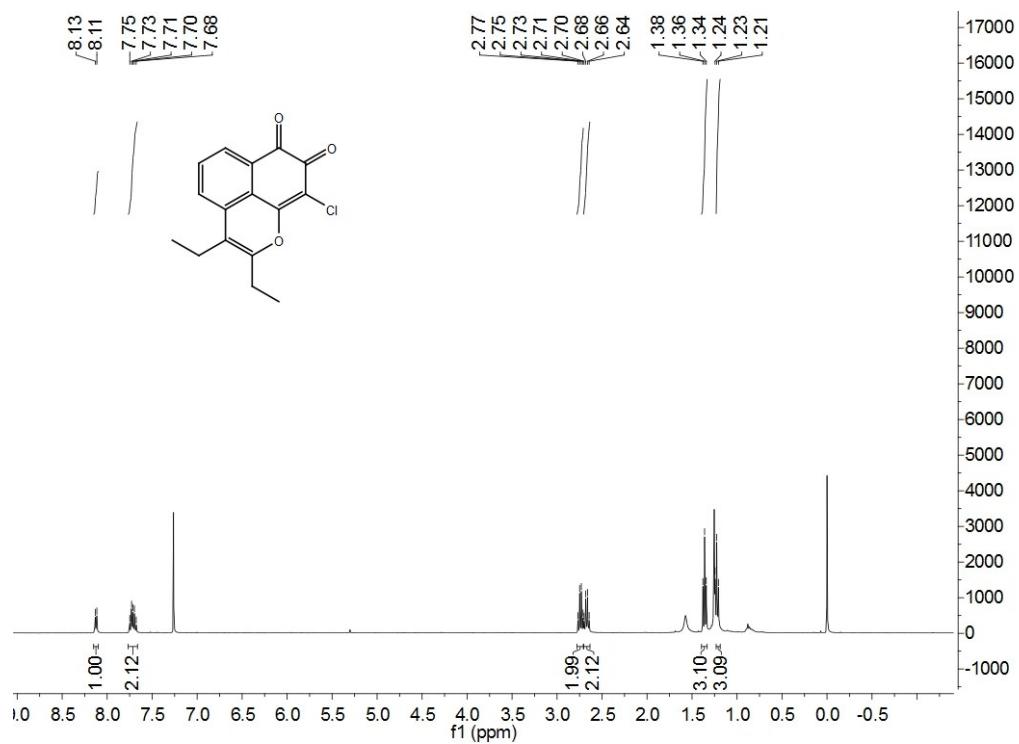
IR spectra of **4a**



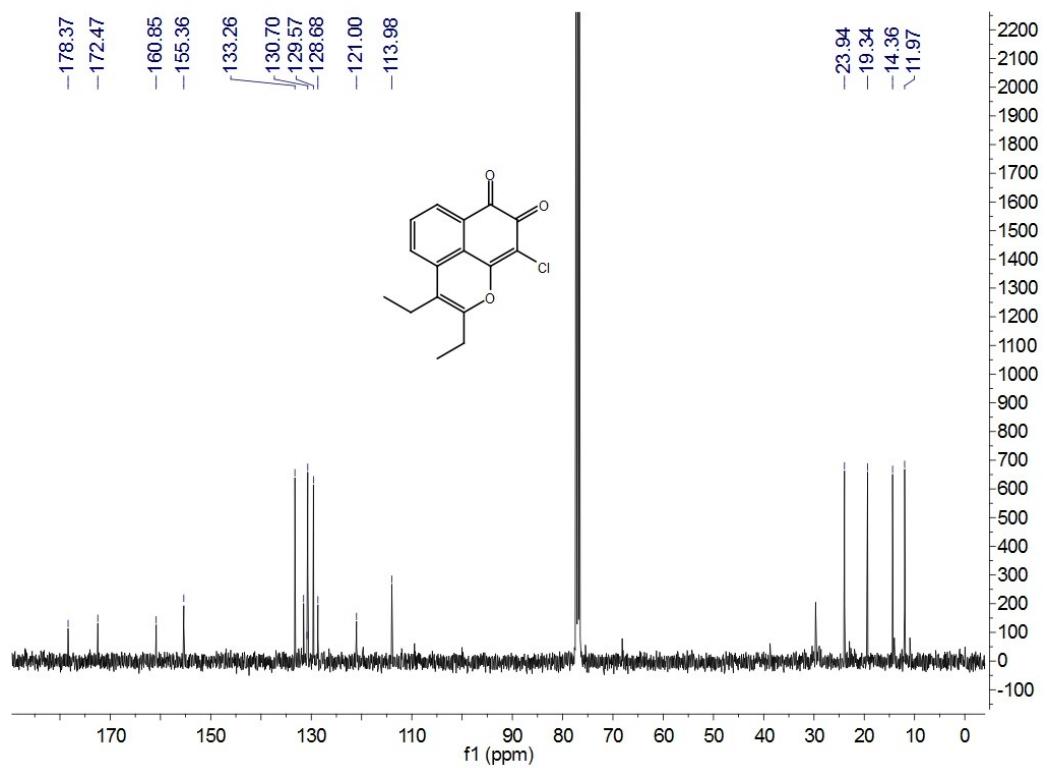
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.935	298752	14175	2.099	2.100
2	11.882	13652691	643802	95.943	95.393
3	12.618	278587	16917	1.958	2.507
Total		14230031	674893	100.000	100.000

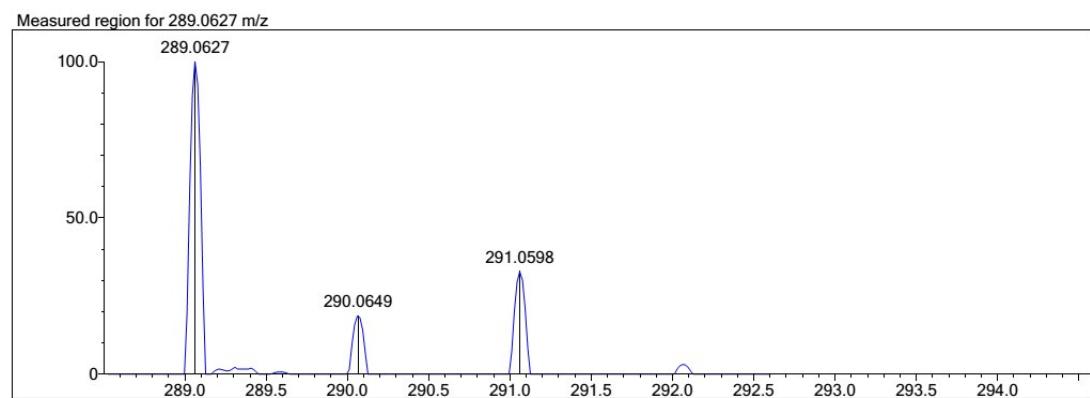
HPLC profile of 4a



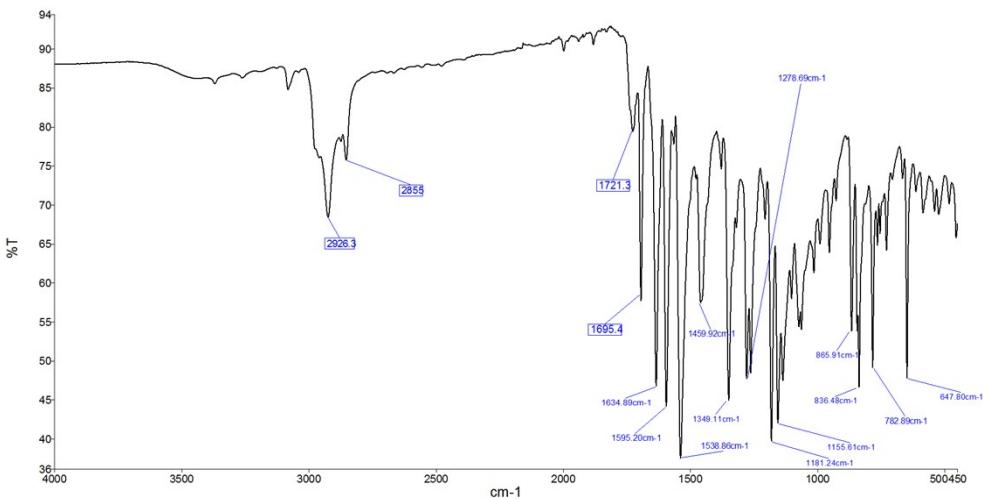
¹H NMR spectra of 5a



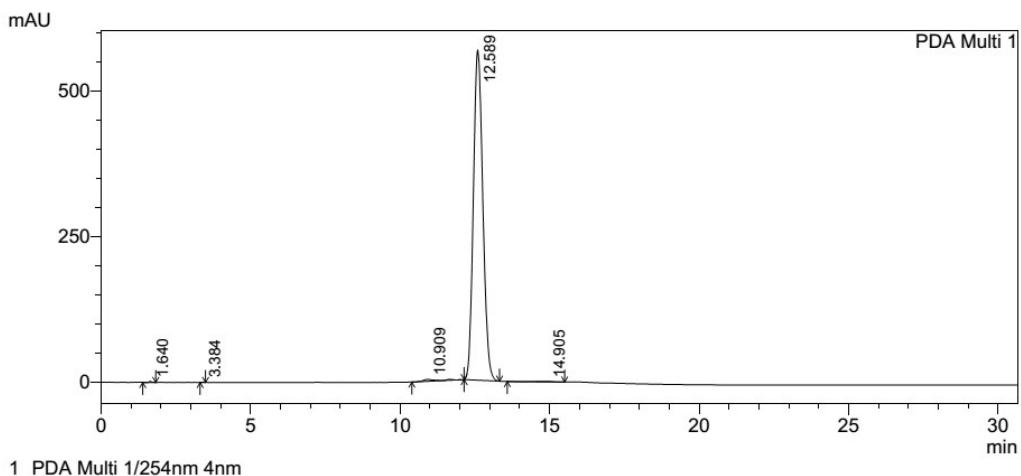
¹³C NMR spectra of **5a**



HRMS spectrum of **5a**

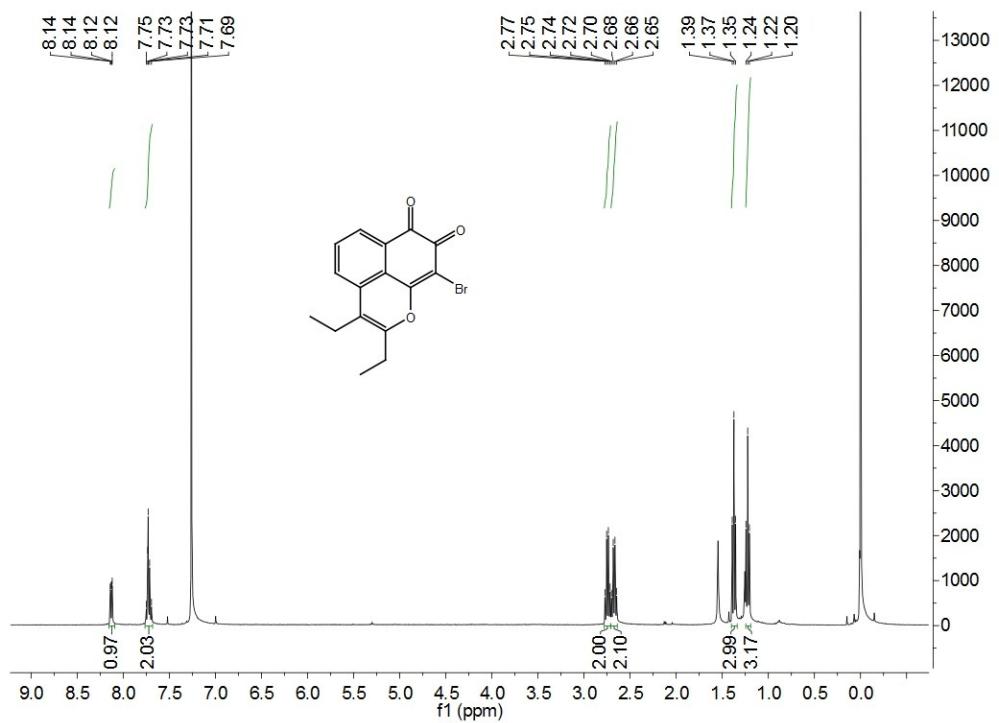


IR spectra of **5a**

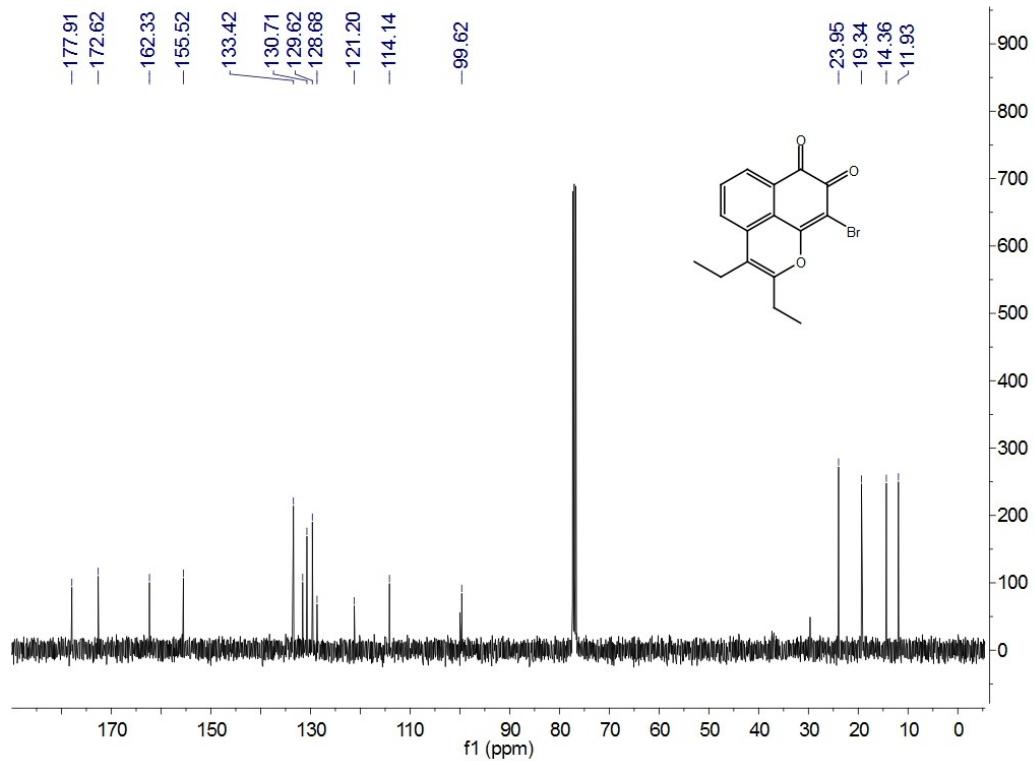


PeakTable					
PDA Ch1 254nm 4nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	1.640	9962	2190	0.079	0.381
2	3.384	2046	617	0.016	0.108
3	10.909	102999	3558	0.818	0.620
4	12.589	12438971	567153	98.829	98.757
5	14.905	32409	770	0.257	0.134
Total		12586387	574289	100.000	100.000

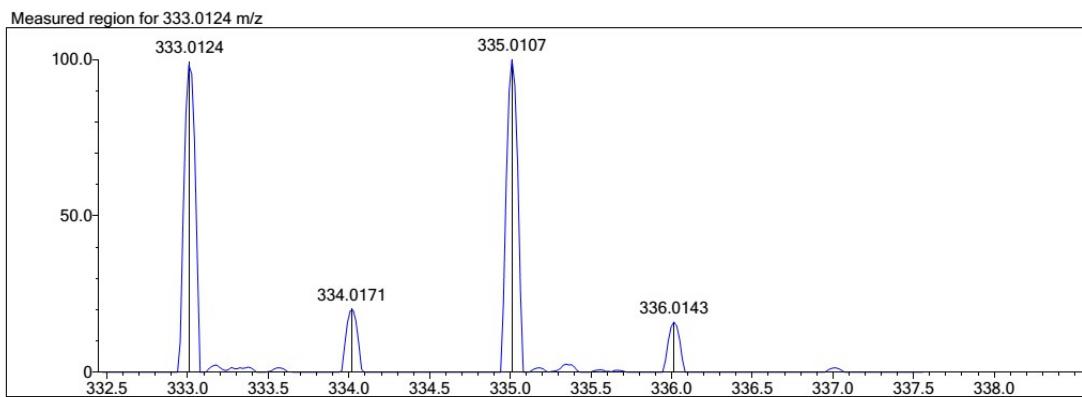
HPLC profile of **5a**



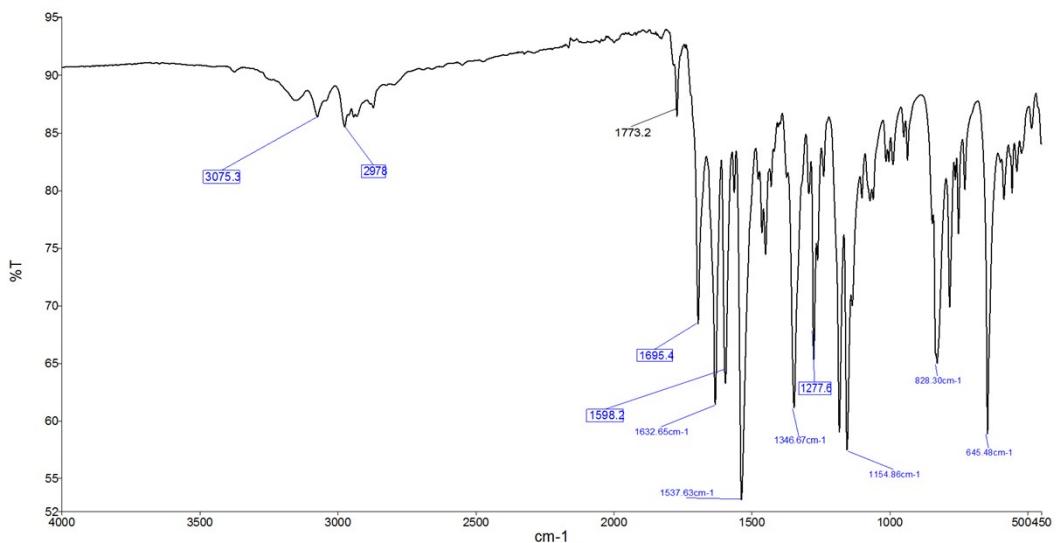
¹H NMR spectra of **6a**



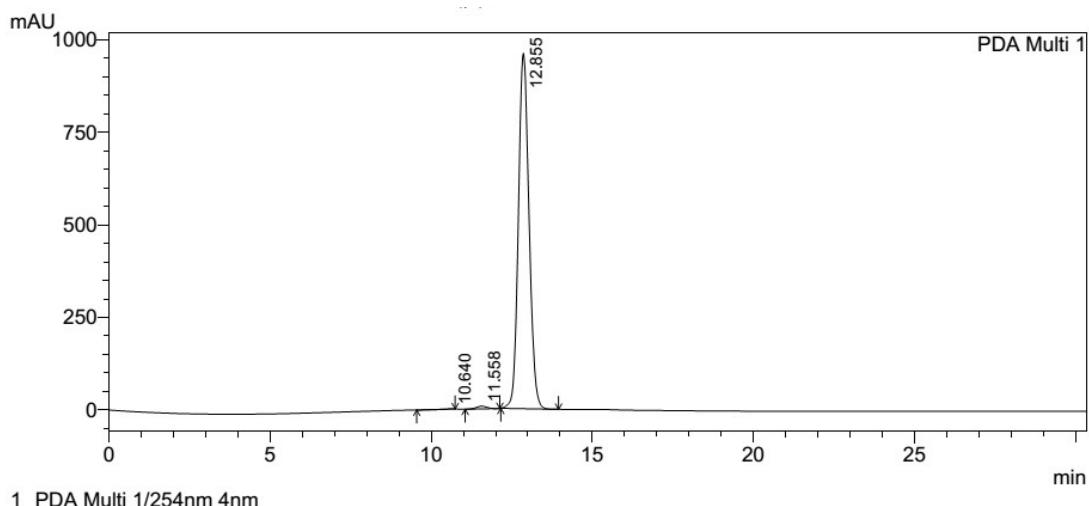
¹³C NMR spectra of **6a**



HRMS spectrum of **6a**



IR spectra of **6a**

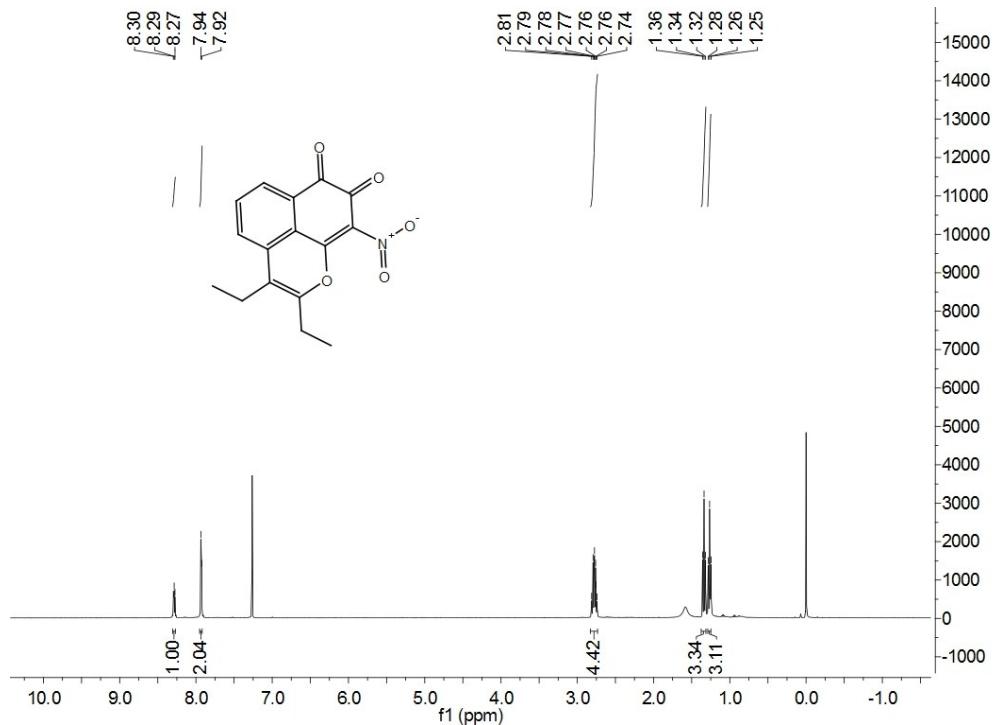


PeakTable

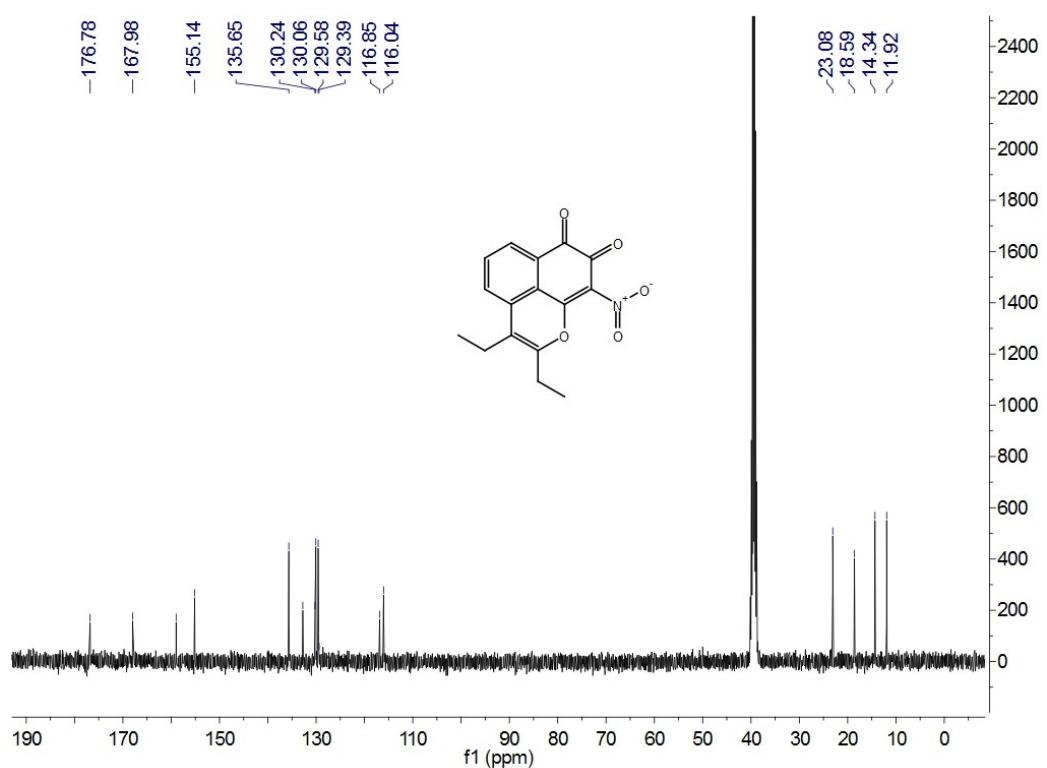
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.640	-12505	819	-0.056	0.085
2	11.558	159586	7279	0.720	0.751
3	12.855	22009092	960869	99.336	99.164
Total		22156173	968967	100.000	100.000

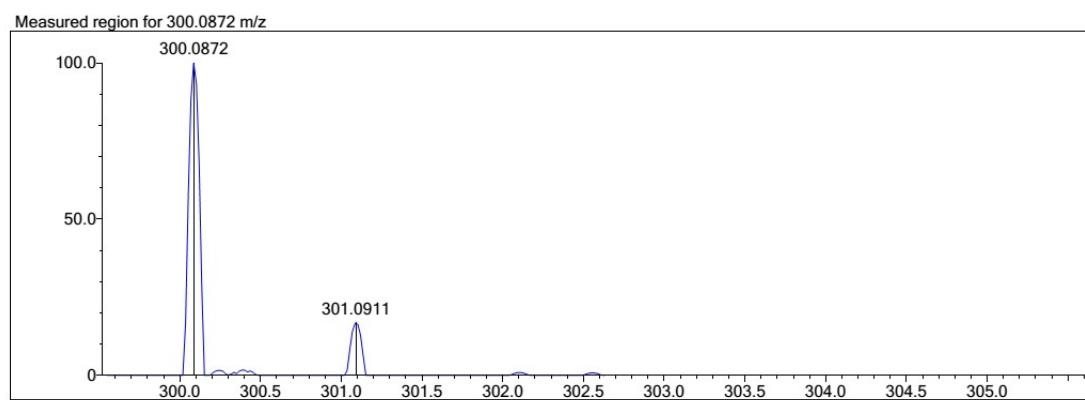
HPLC profile of **6a**



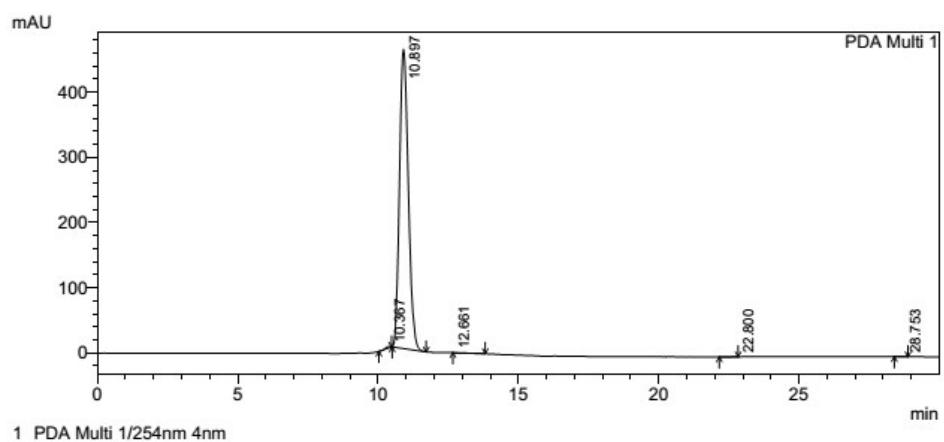
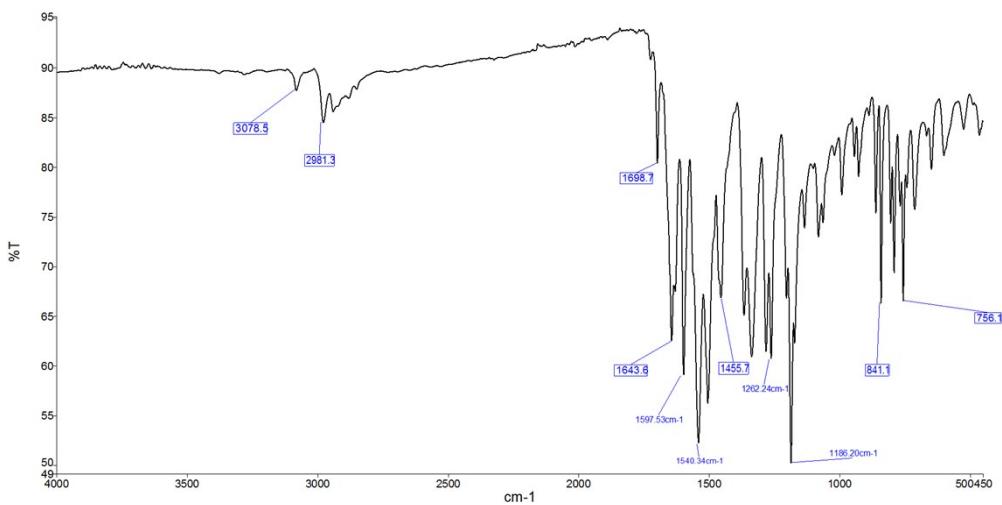
¹H NMR spectra of **7a**



^{13}C NMR spectra of **7a**

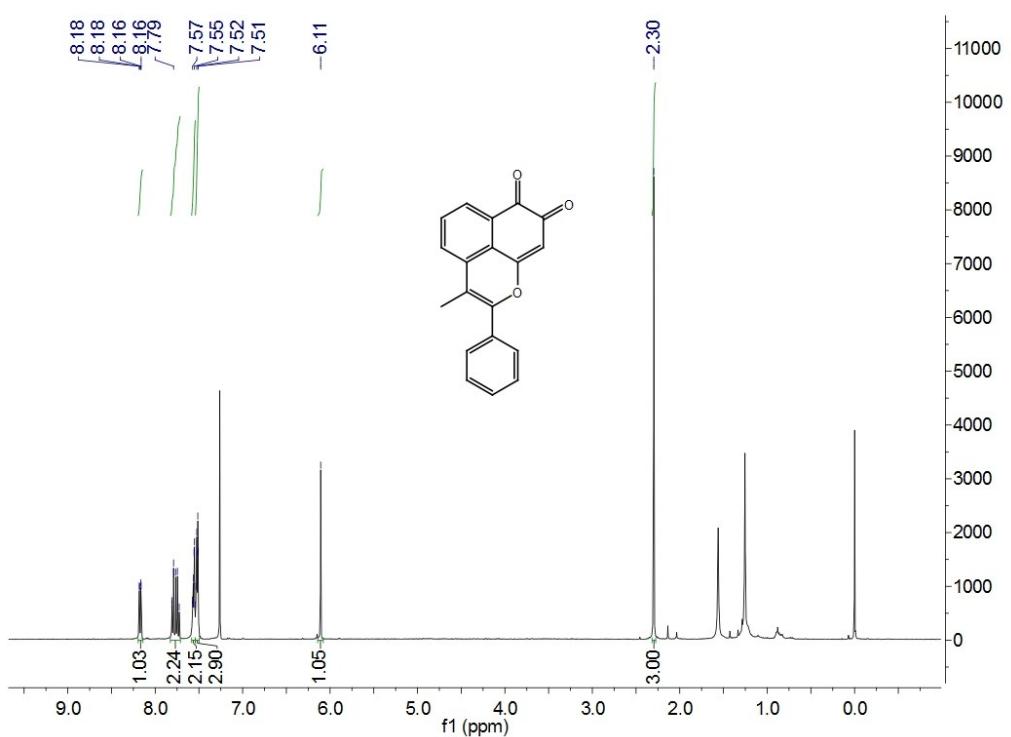


HRMS spectrum of **7a**

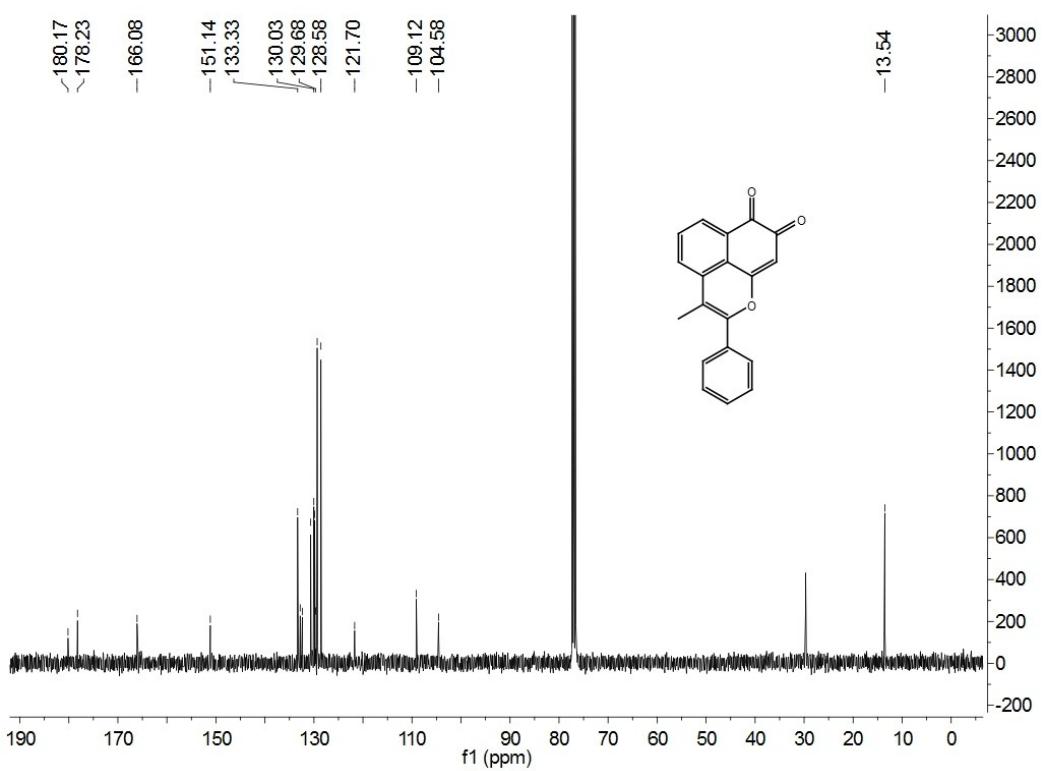


PeakTable					
PDA Ch1 254nm 4nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.367	30761	2476	0.308	0.536
2	10.897	9994577	459350	99.987	99.436
3	12.661	-22043	0	-0.221	0.000
4	22.800	-9820	1	-0.098	0.000
5	28.753	2363	127	0.024	0.028
Total		9995839	461955	100.000	100.000

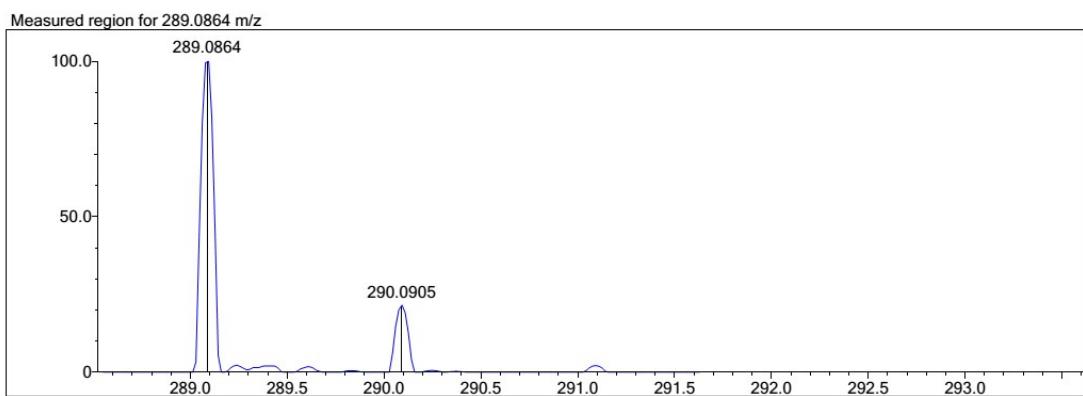
HPLC profile of **7a**



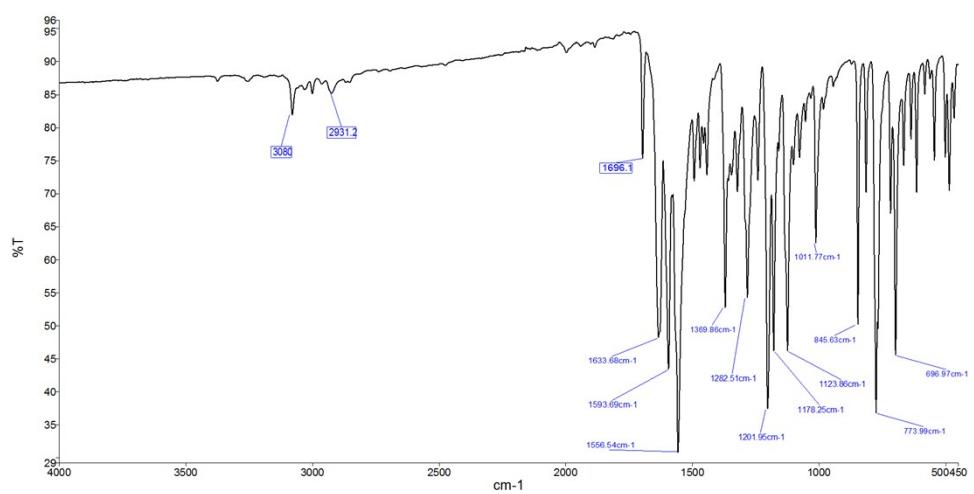
¹H NMR spectra of **3b**



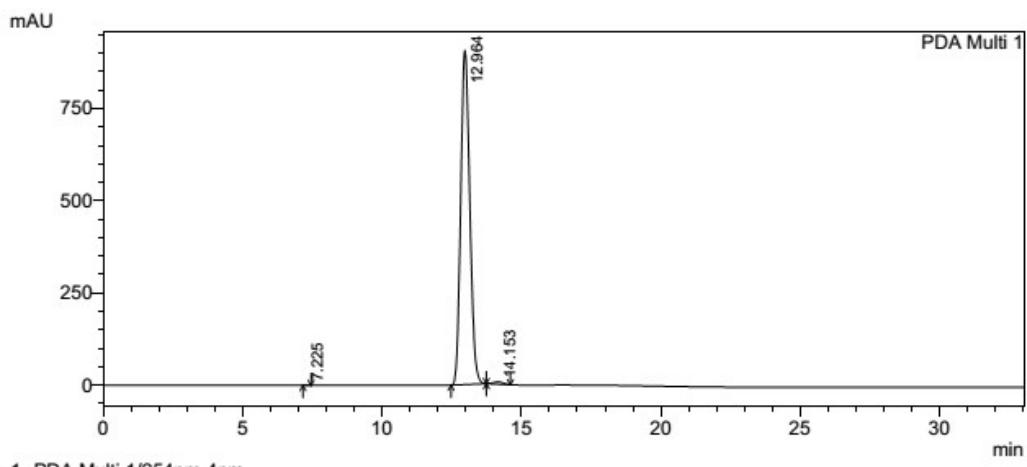
¹³C NMR spectra of **3b**



HRMS spectrum of **3b**



IR spectra of **3b**

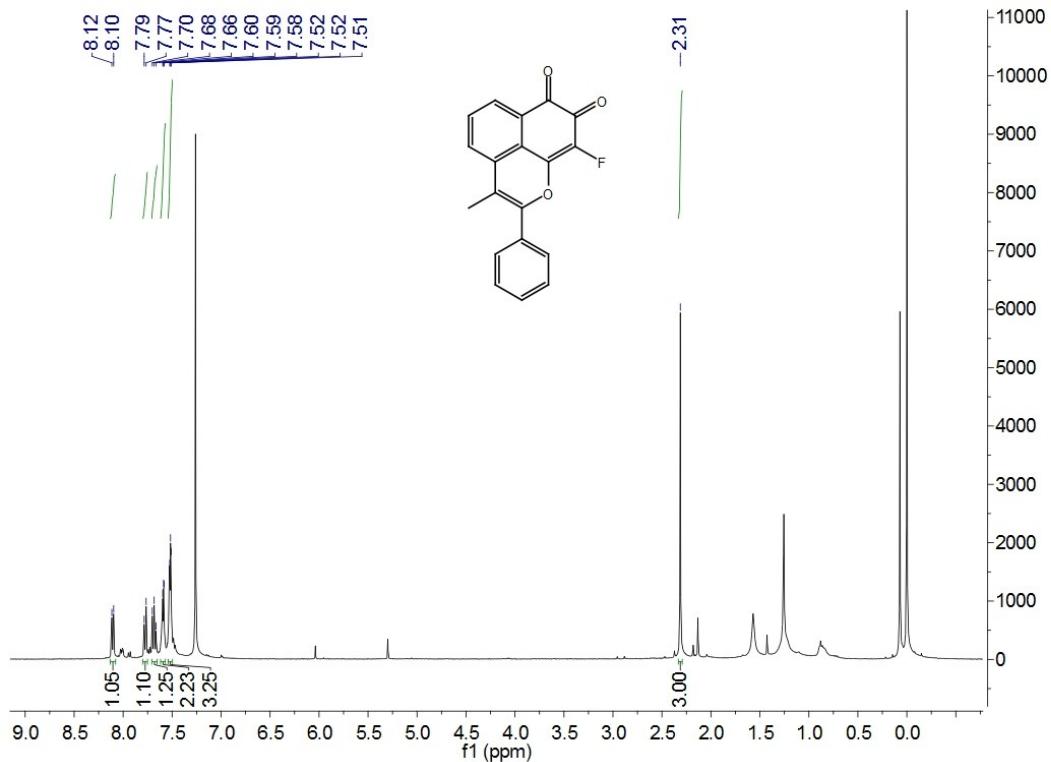


PeakTable

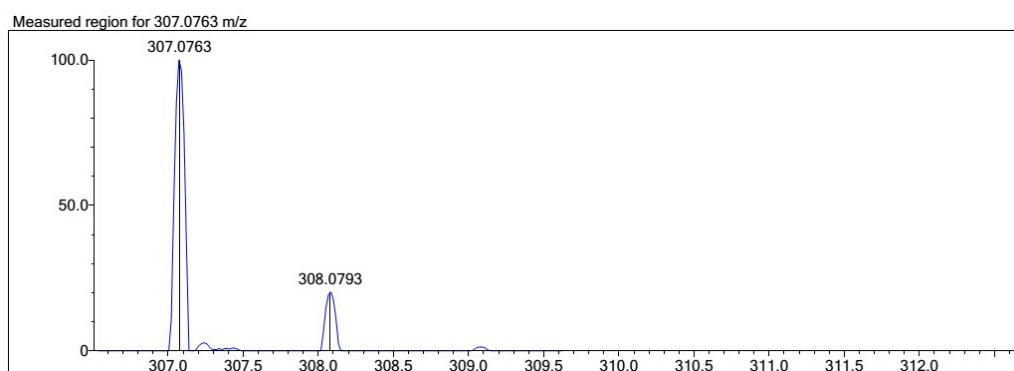
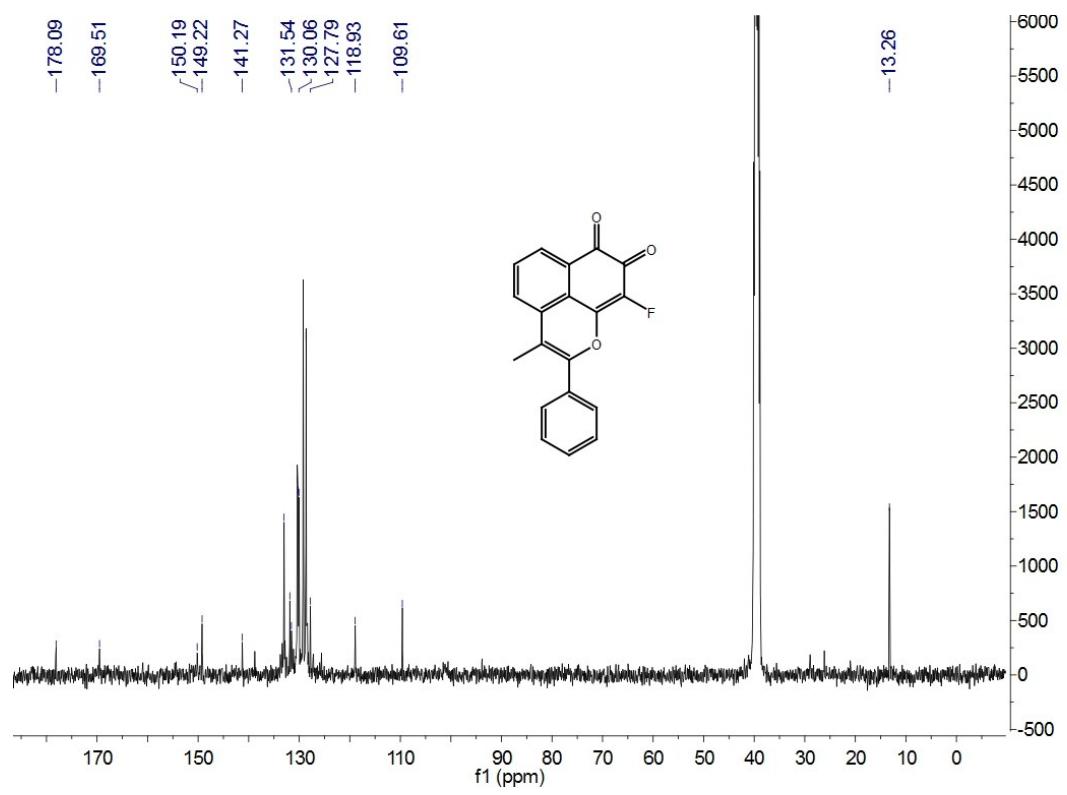
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.225	2270	183	0.011	0.020
2	12.964	20428055	906877	99.227	99.312
3	14.153	156956	6101	0.762	0.668
Total		20587282	913161	100.000	100.000

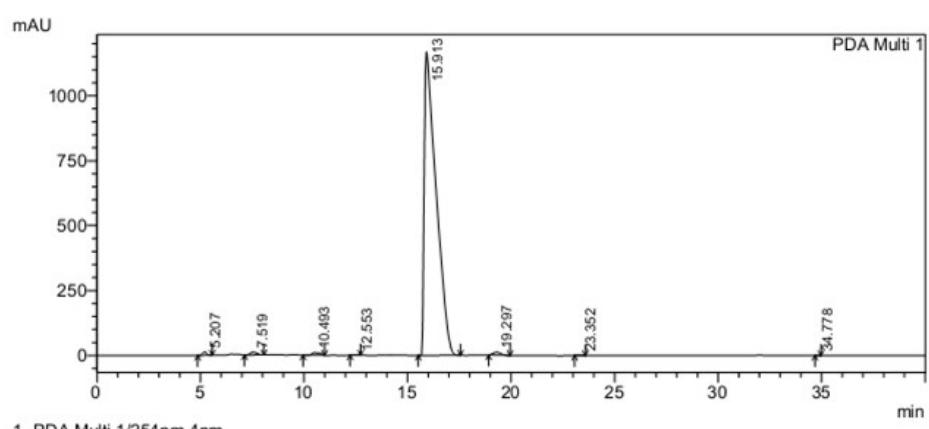
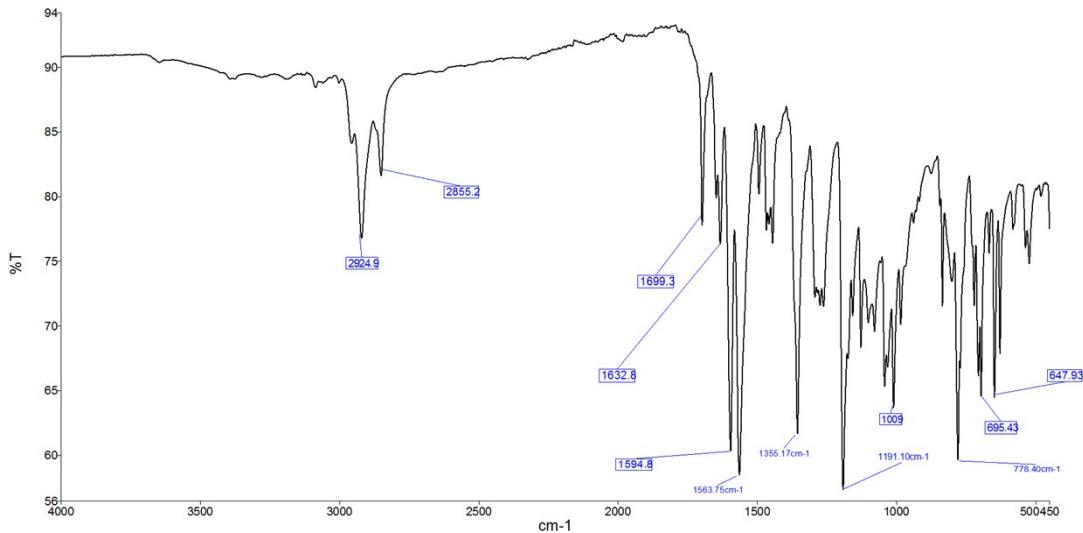
HPLC profile of 3b



¹H NMR spectra of 4b

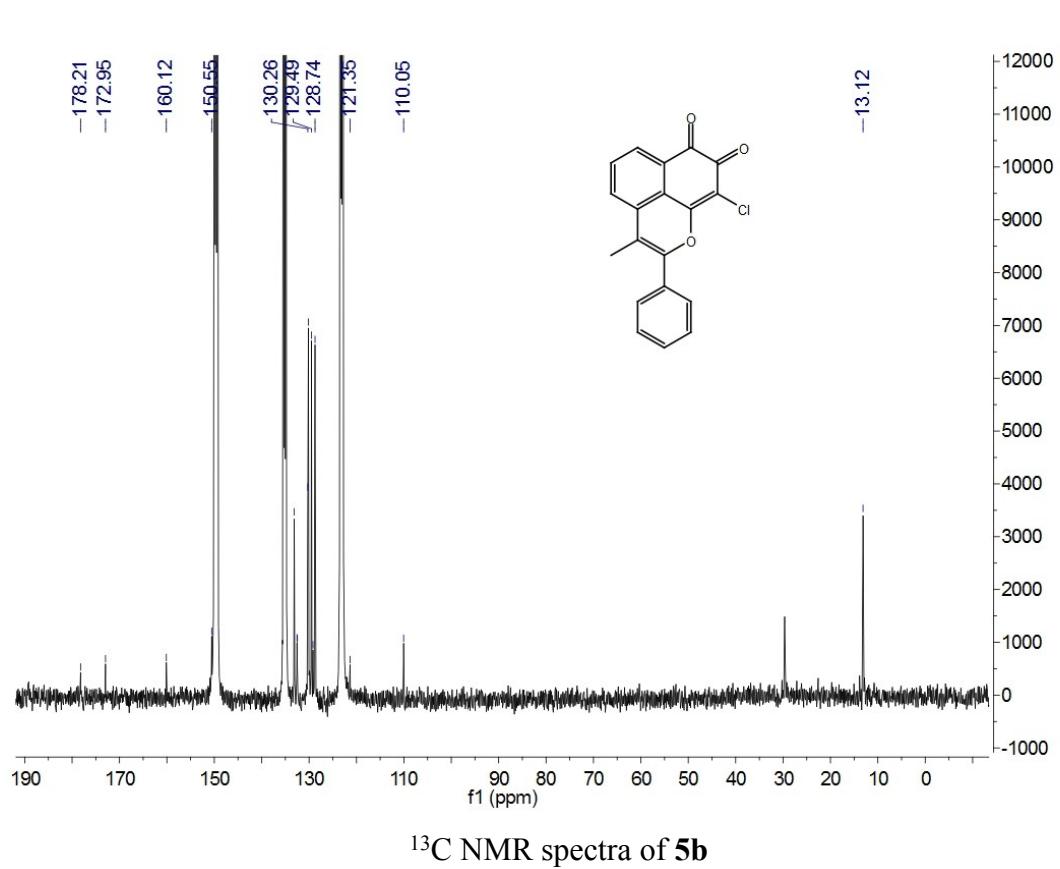
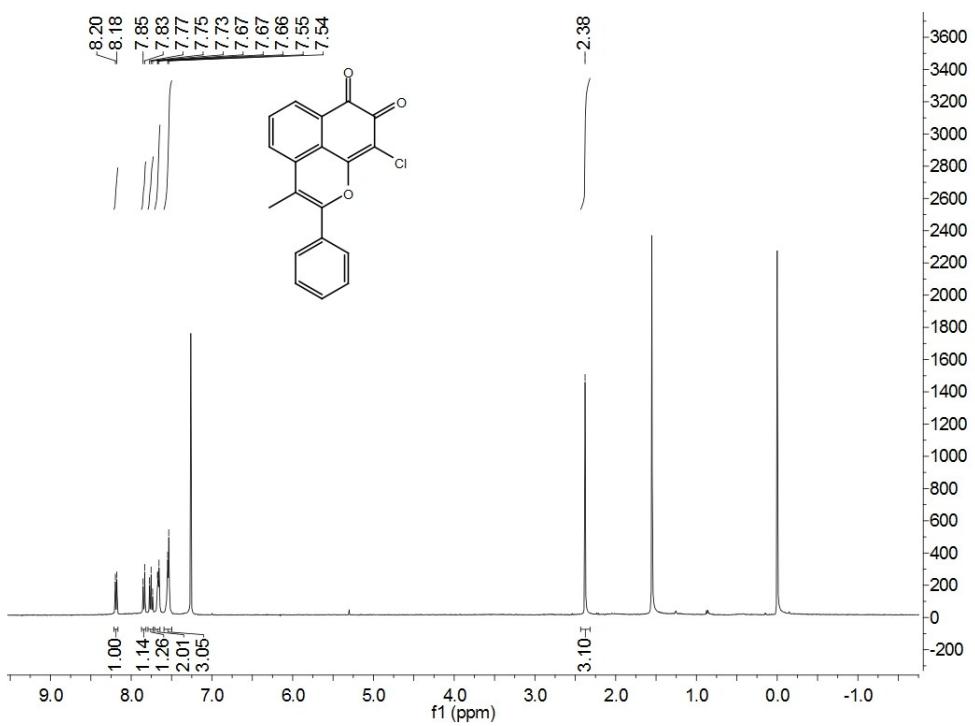


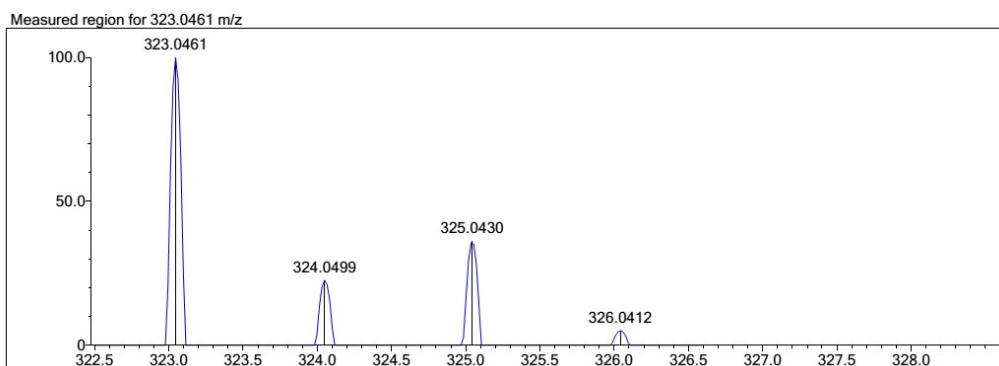
HRMS spectrum of **4b**



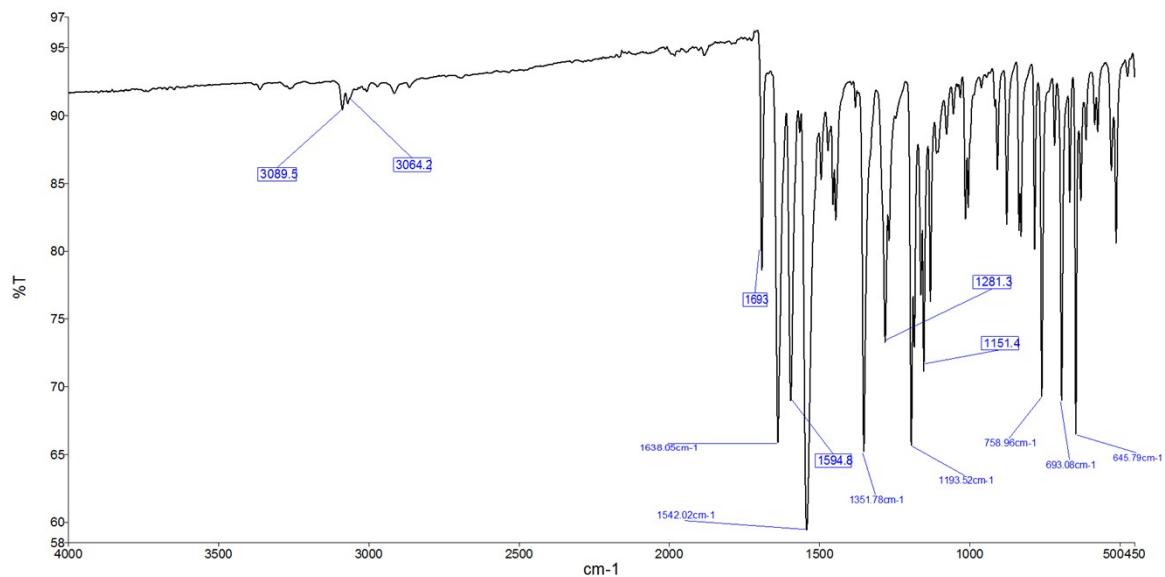
PeakTable						
Peak#	Ret. Time	Area	Height	Area %	Height %	
1	5.207	169692	13183	0.357	1.085	
2	7.519	256451	10424	0.540	0.858	
3	10.493	273322	9732	0.575	0.801	
4	12.553	10233	472	0.022	0.039	
5	15.913	46522556	1169482	97.899	96.250	
6	19.297	284292	11424	0.598	0.940	
7	23.352	3565	213	0.008	0.018	
8	34.778	1048	118	0.002	0.010	
Total		47521158	1215049	100.000	100.000	

HPLC profile of **4b**

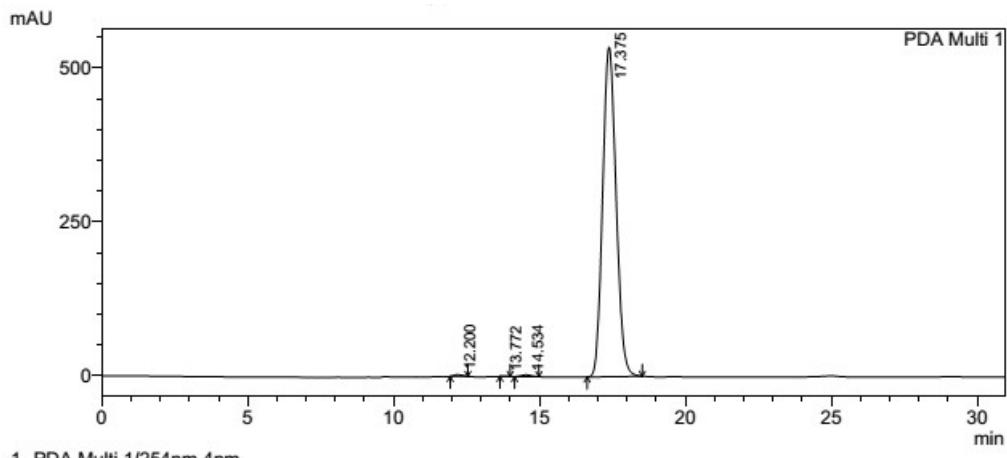




HRMS spectrum of **5b**



IR spectra of **5b**

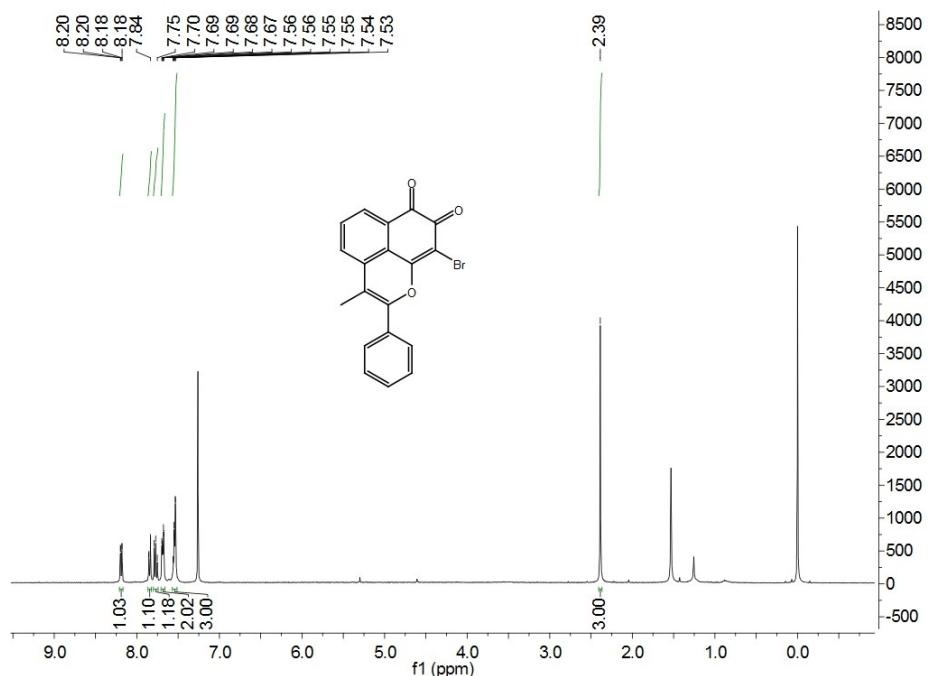


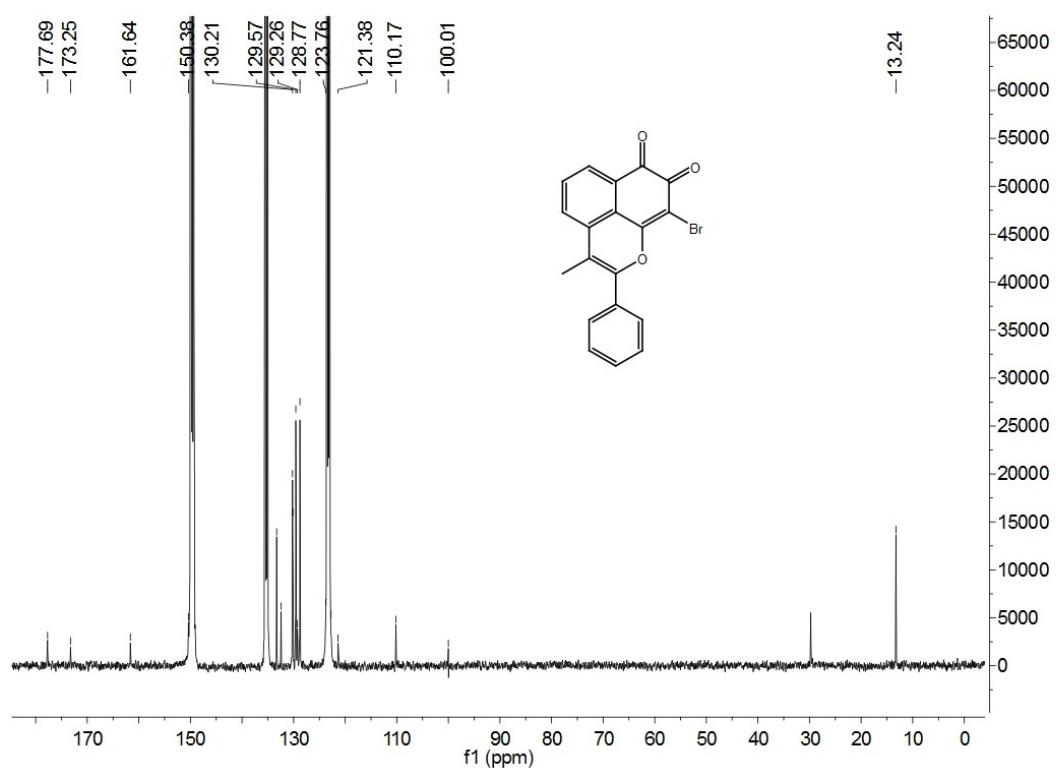
PeakTable

PDA Ch1 254nm 4nm

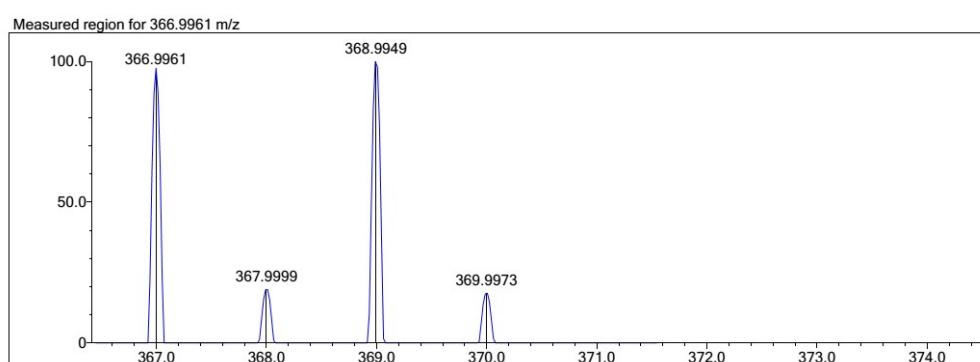
Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.200	57481	2780	0.332	0.513
2	13.772	3790	307	0.022	0.057
3	14.534	67730	2816	0.391	0.520
4	17.375	17203860	536187	99.256	98.911
Total		17332861	542089	100.000	100.000

HPLC profile of **5b**

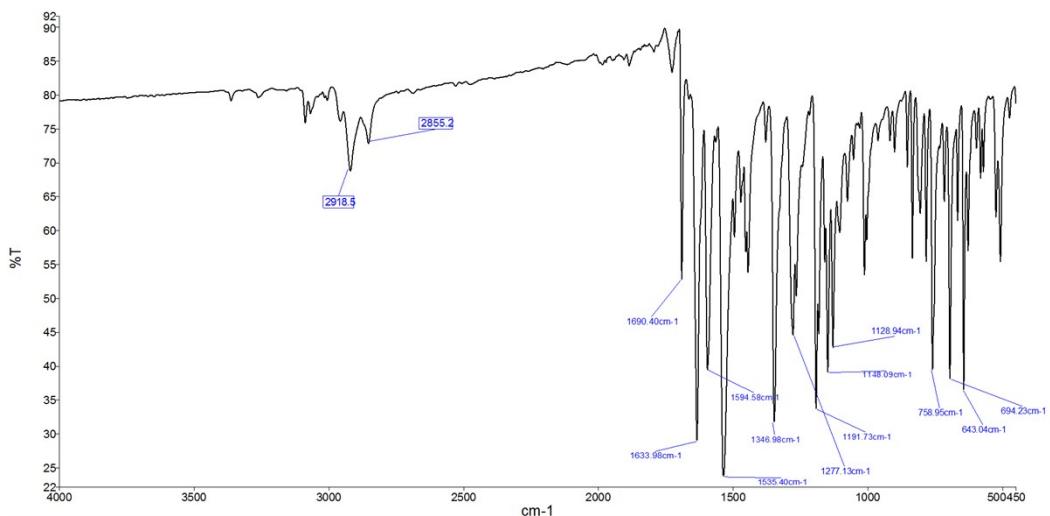




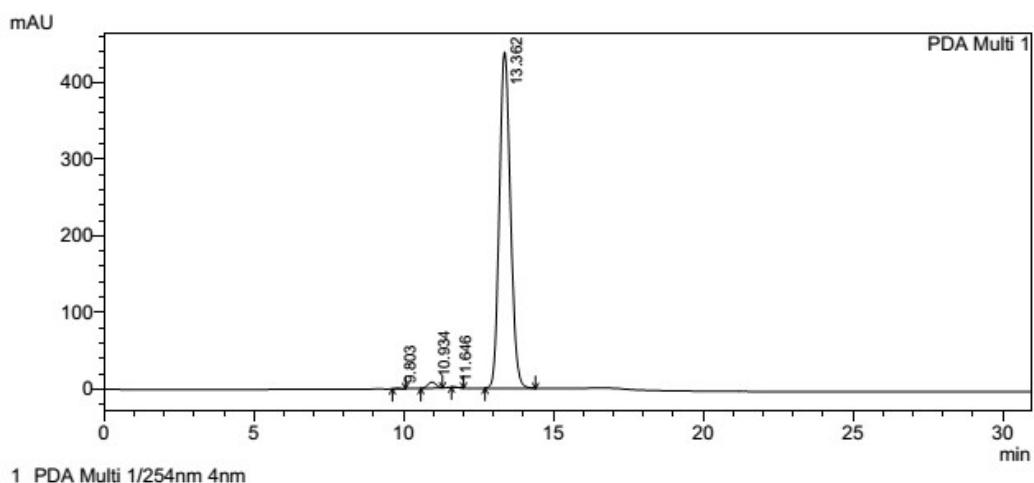
^{13}C NMR spectra of **6b**



HRMS spectrum of **6b**

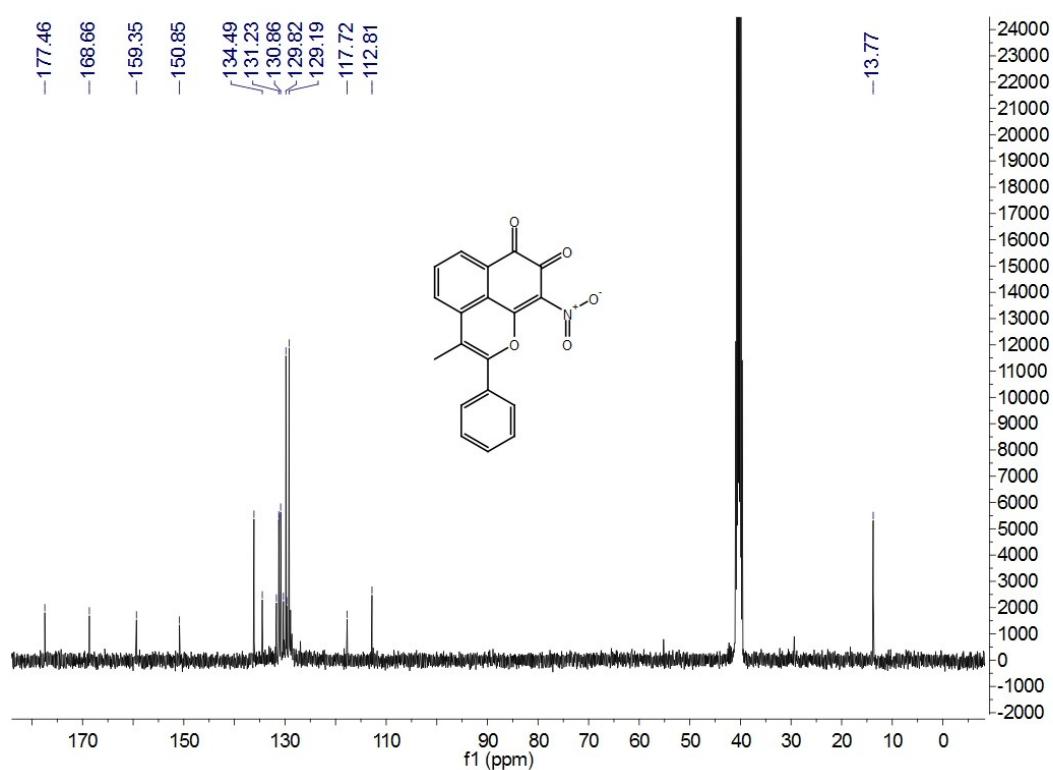
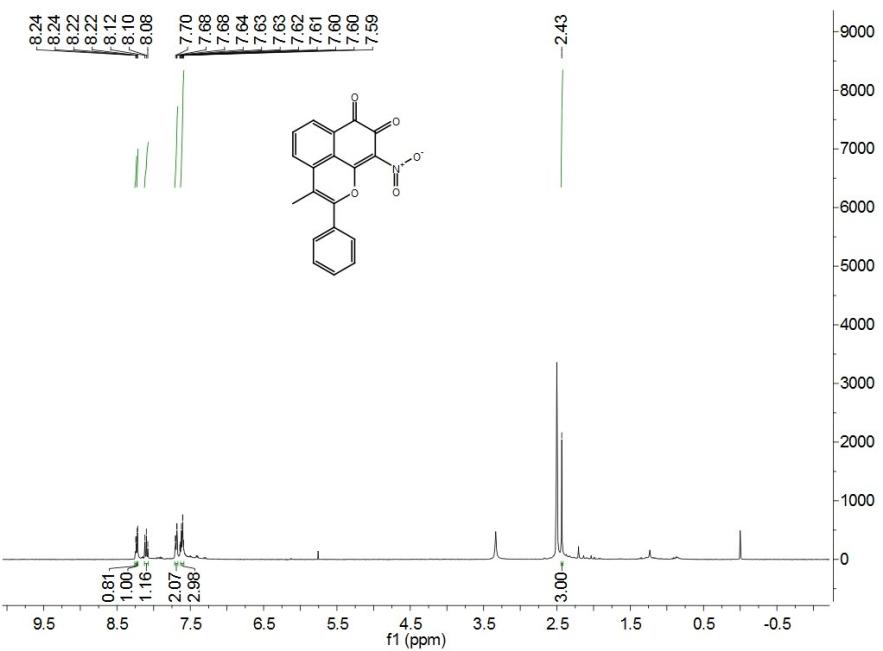


IR spectra of **6b**

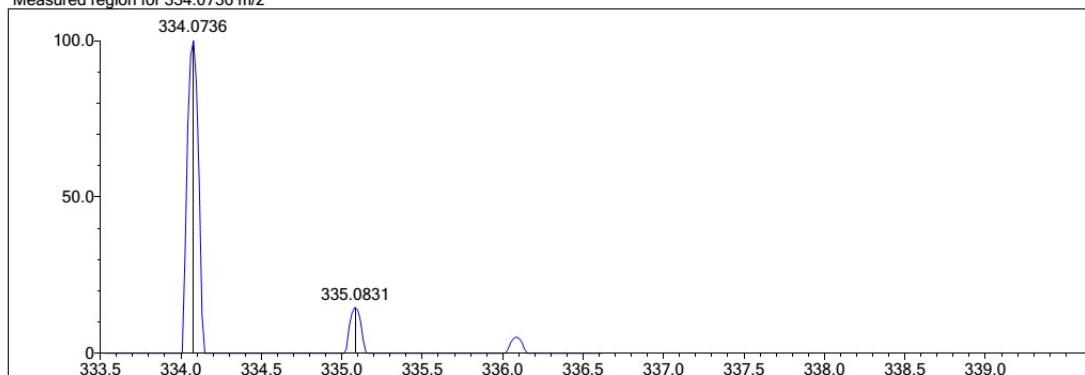


PDA Ch1 254nm 4nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.803	7316	802	0.064	0.179
2	10.934	154525	7937	1.355	1.773
3	11.646	3340	268	0.029	0.060
4	13.362	11240710	438711	98.552	97.988
Total		11405891	447718	100.000	100.000

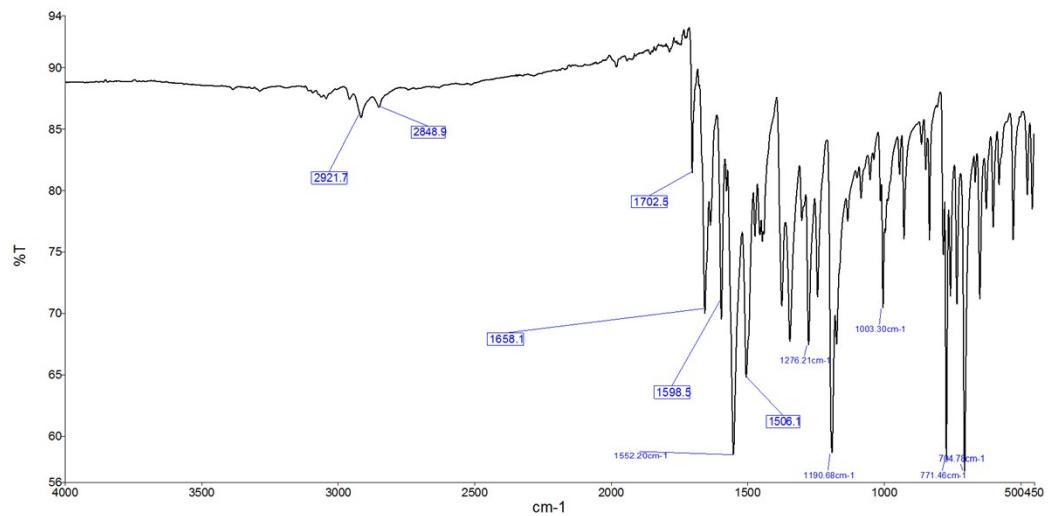
HPLC profile of **6b**



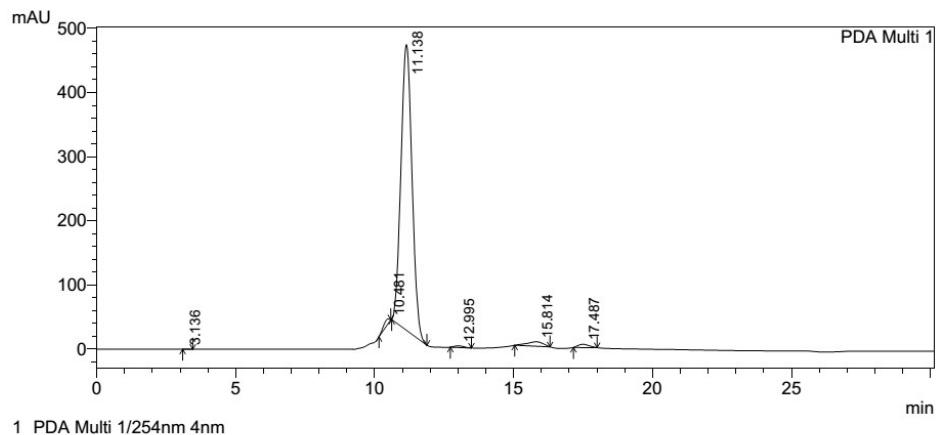
Measured region for 334.0736 m/z



HRMS spectrum of **7b**



IR spectra of **7b**

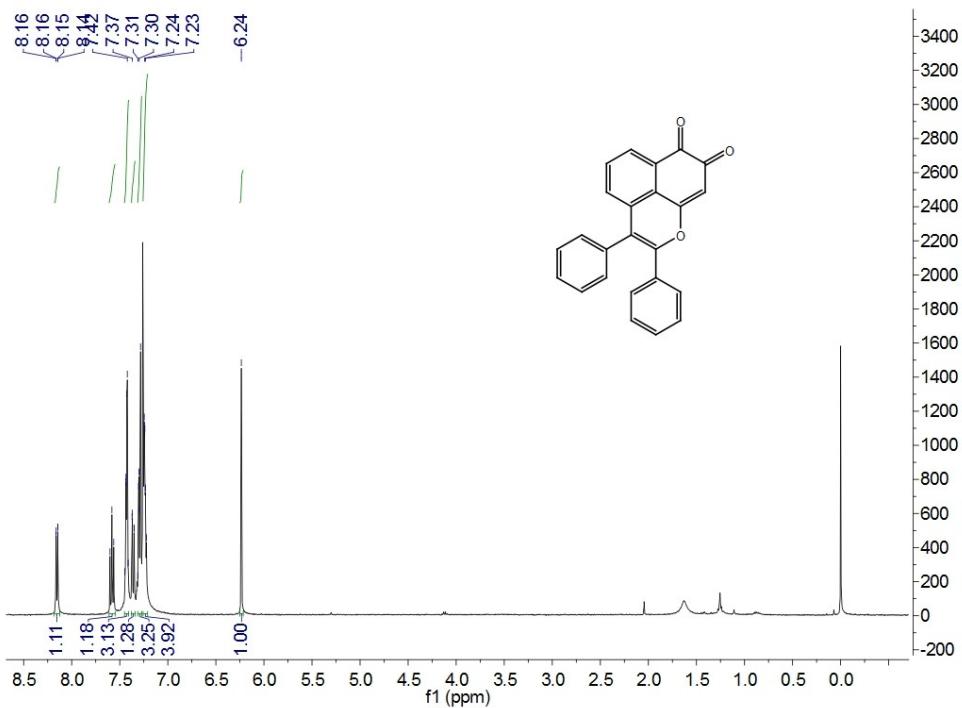


PeakTable

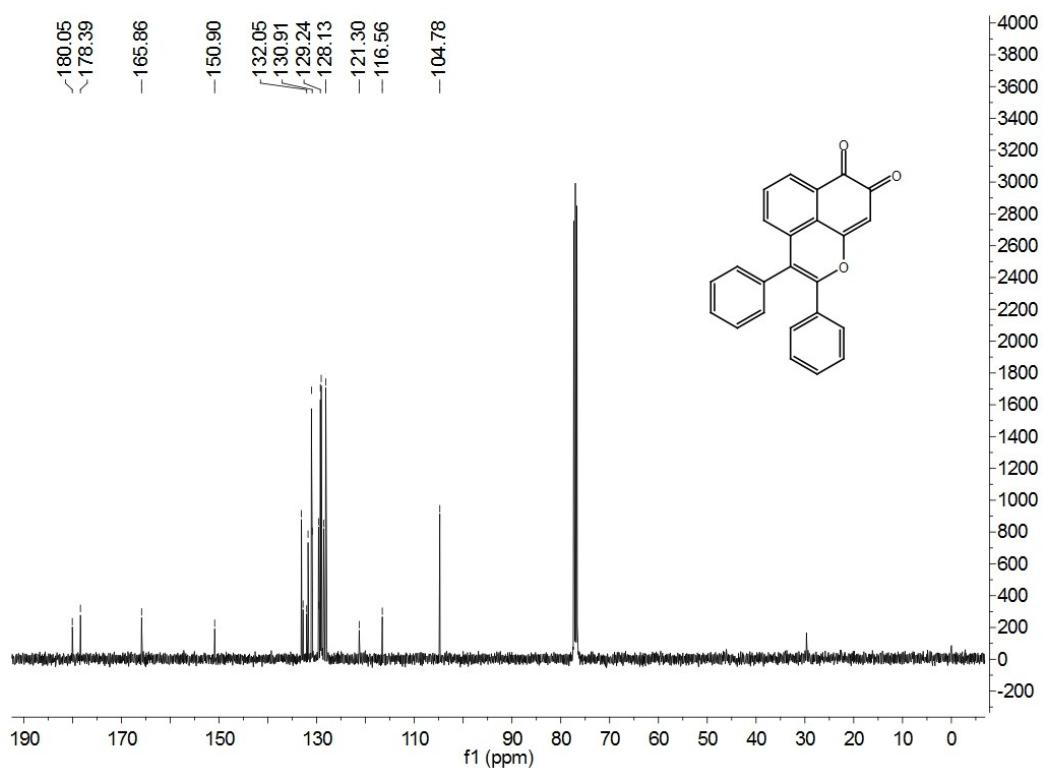
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.136	1028	48	0.008	0.010
2	10.481	144007	7422	1.110	1.587
3	11.138	12343111	445378	95.111	95.226
4	12.995	63129	2670	0.486	0.571
5	15.814	281606	6893	2.170	1.474
6	17.487	144654	5296	1.115	1.132
Total		12977536	467705	100.000	100.000

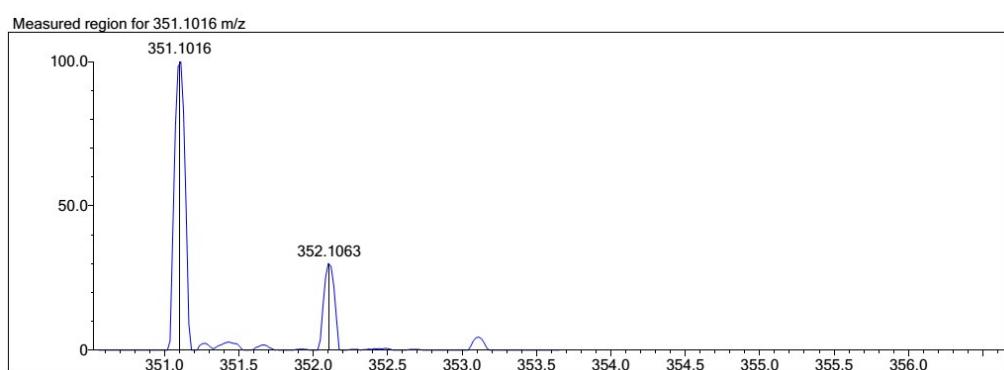
HPLC profile of 7b



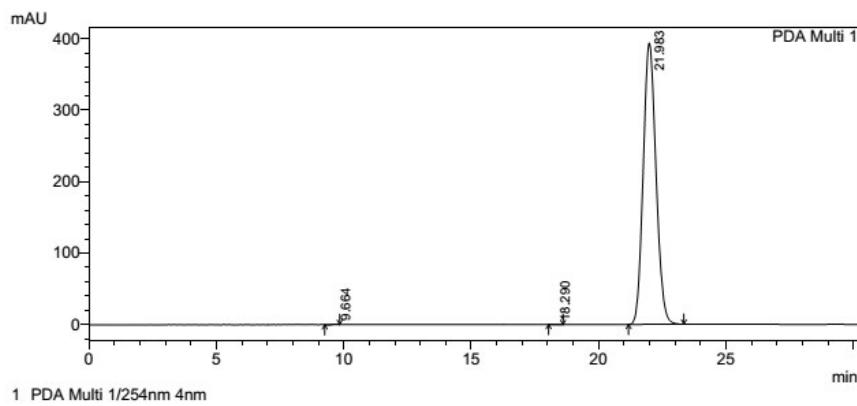
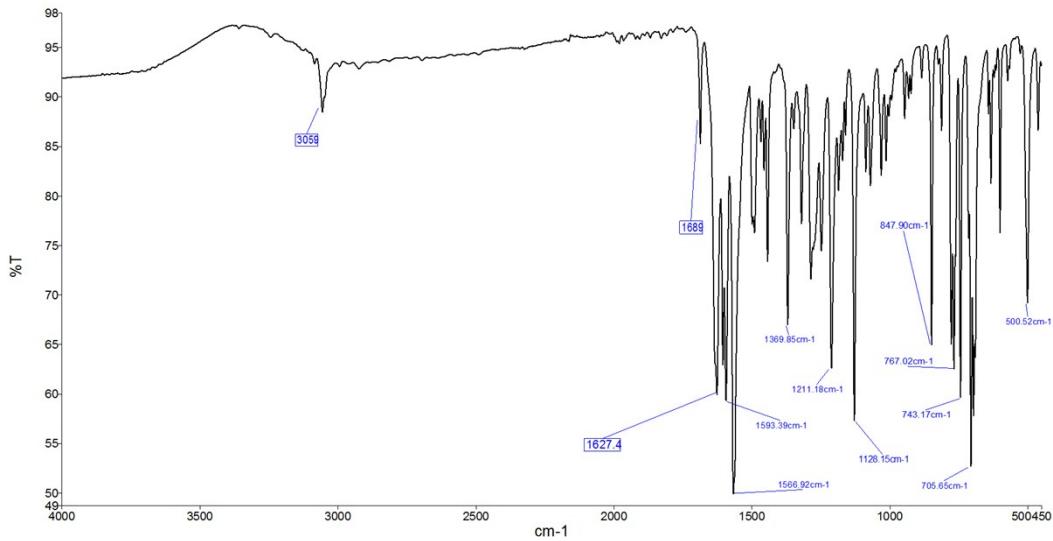
¹H NMR spectra of 3c



^{13}C NMR spectra of **3c**

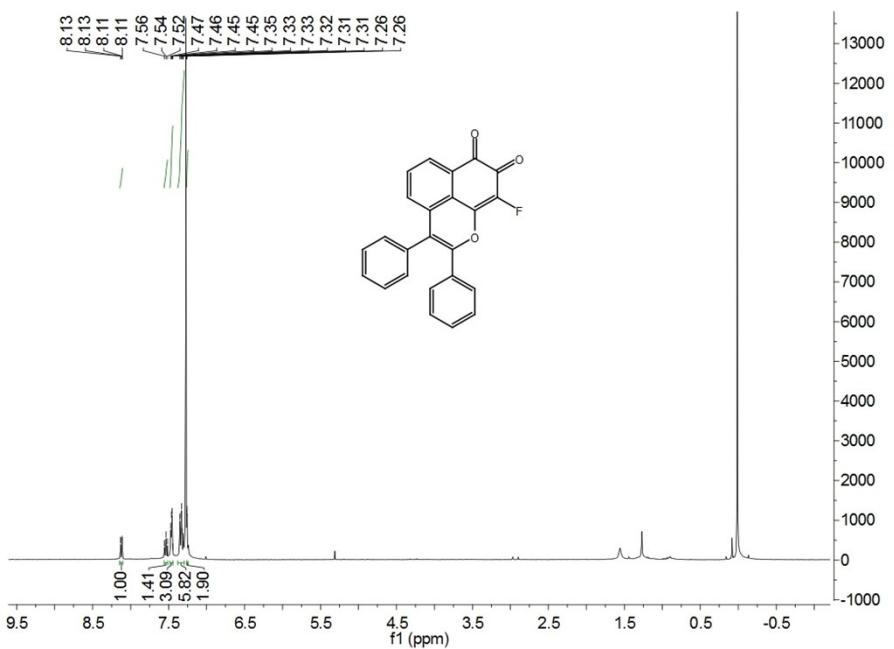


HRMS spectrum of **3c**

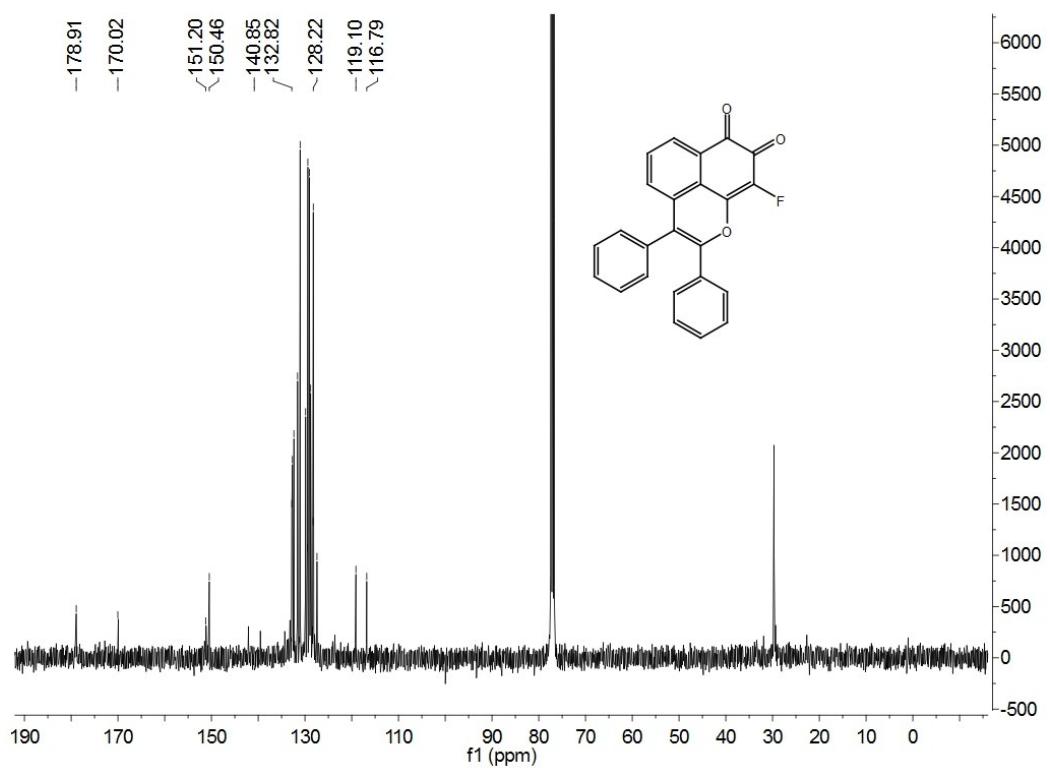


PeakTable					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.664	3762	752	0.027	0.190
2	18.290	6094	321	0.044	0.081
3	21.983	13735975	393811	99.928	99.728
Total		13745831	394884	100.000	100.000

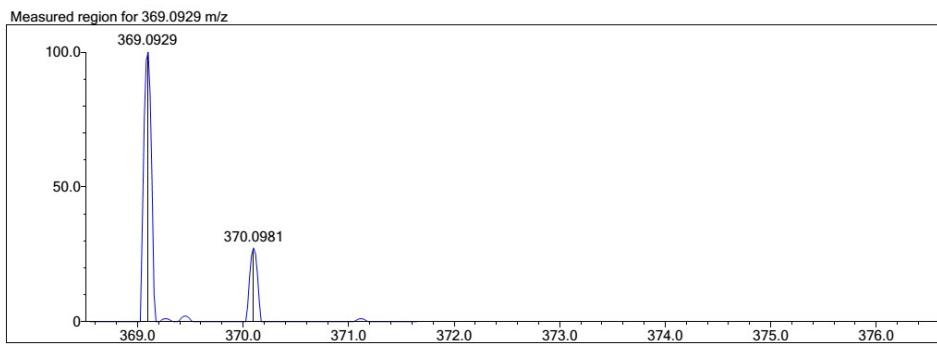
HPLC profile of **3c**



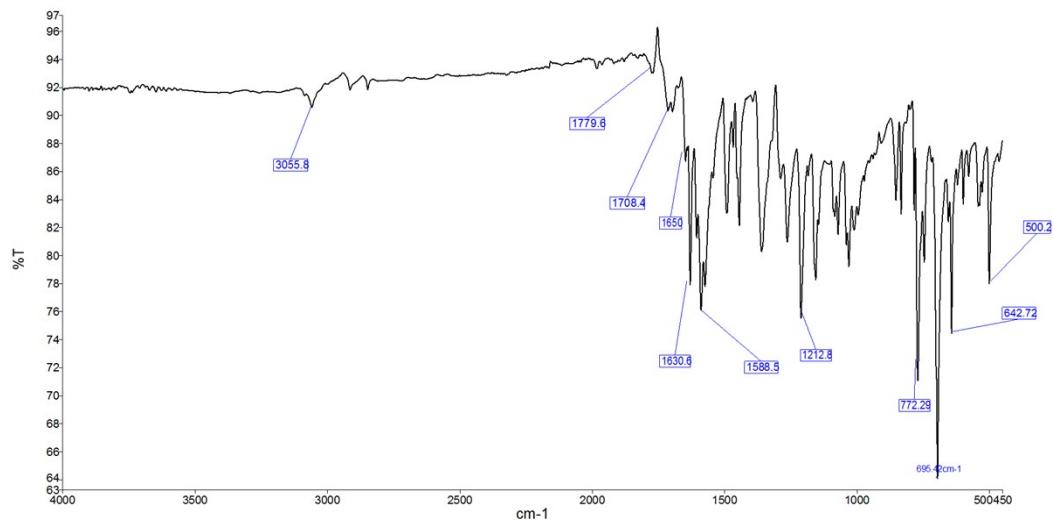
¹H NMR spectra of **4c**



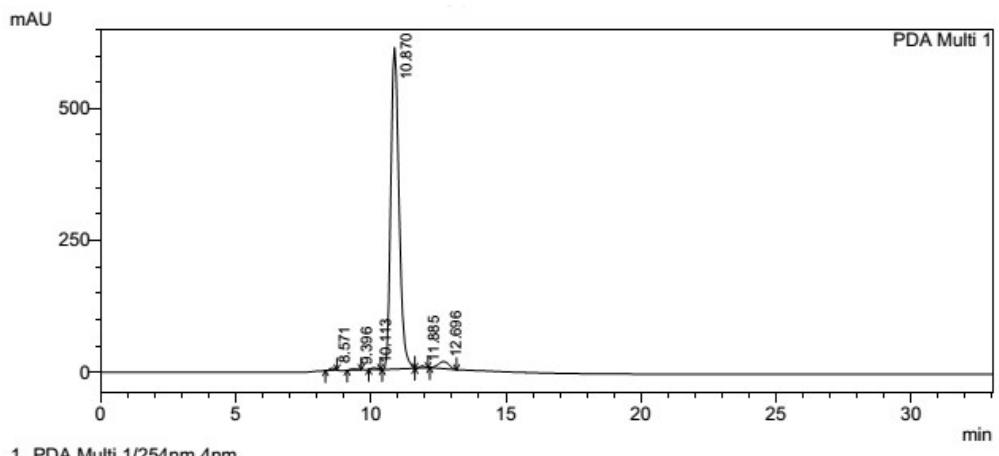
¹³C NMR spectra of **4c**



HRMS spectrum of **4c**



IR spectra of **4c**

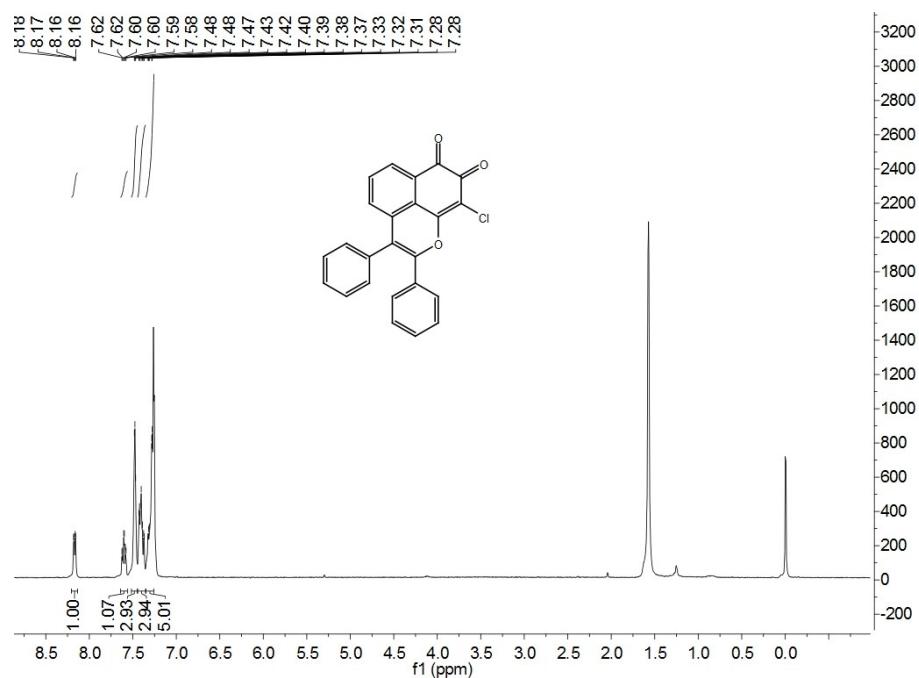


PeakTable

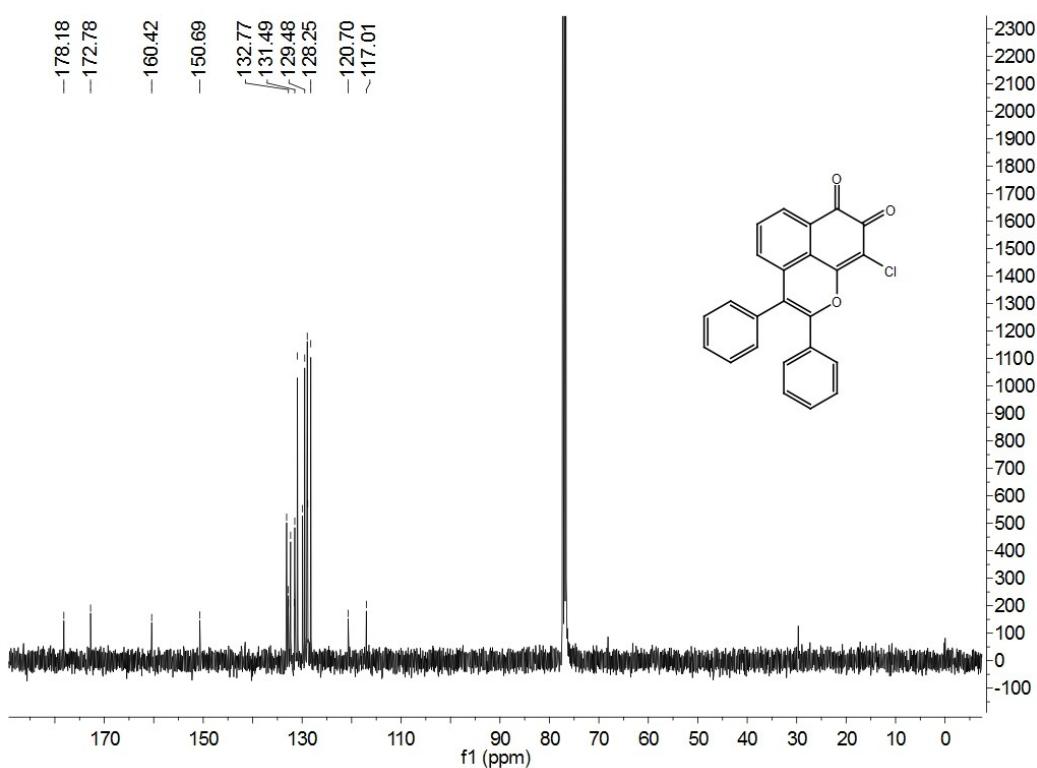
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.571	54346	4004	0.403	0.630
2	9.396	27055	1435	0.200	0.226
3	10.113	39657	2568	0.294	0.404
4	10.870	12942991	610003	95.909	95.955
5	11.885	49301	3693	0.365	0.581
6	12.696	381765	14015	2.829	2.205
Total		13495115	635717	100.000	100.000

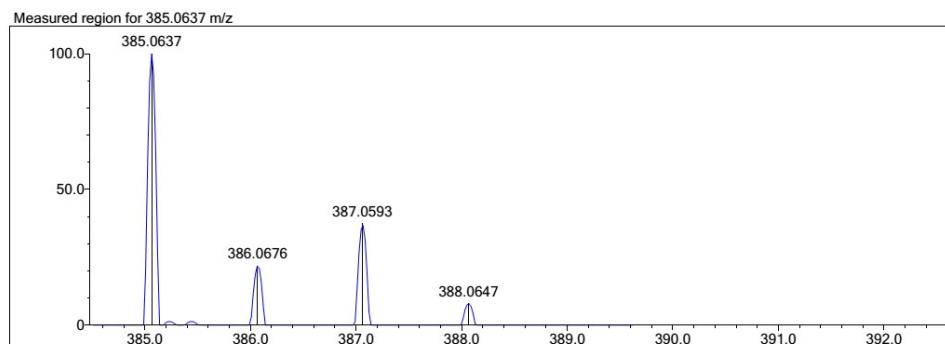
HPLC profile of 4c



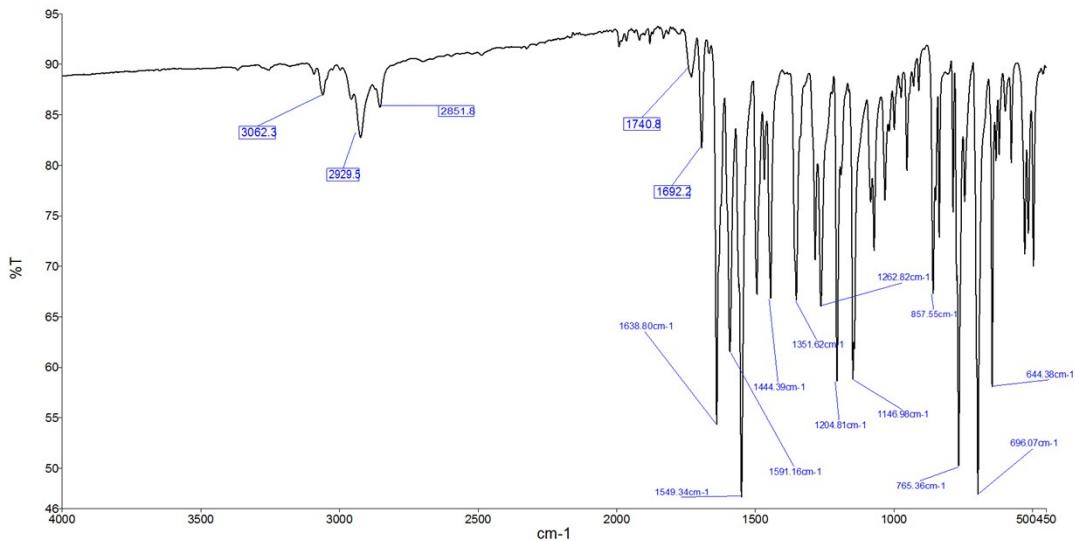
¹H NMR spectra of 5c



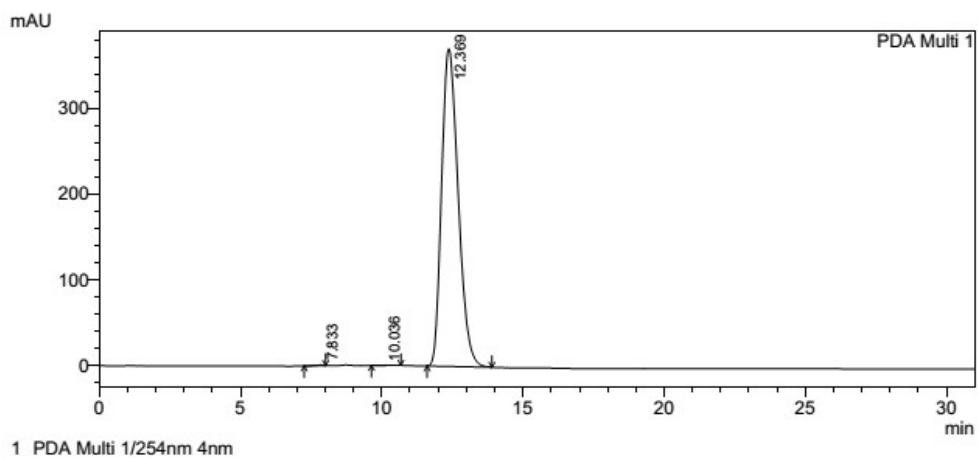
^{13}C NMR spectra of **5c**



HRMS spectrum of **5c**

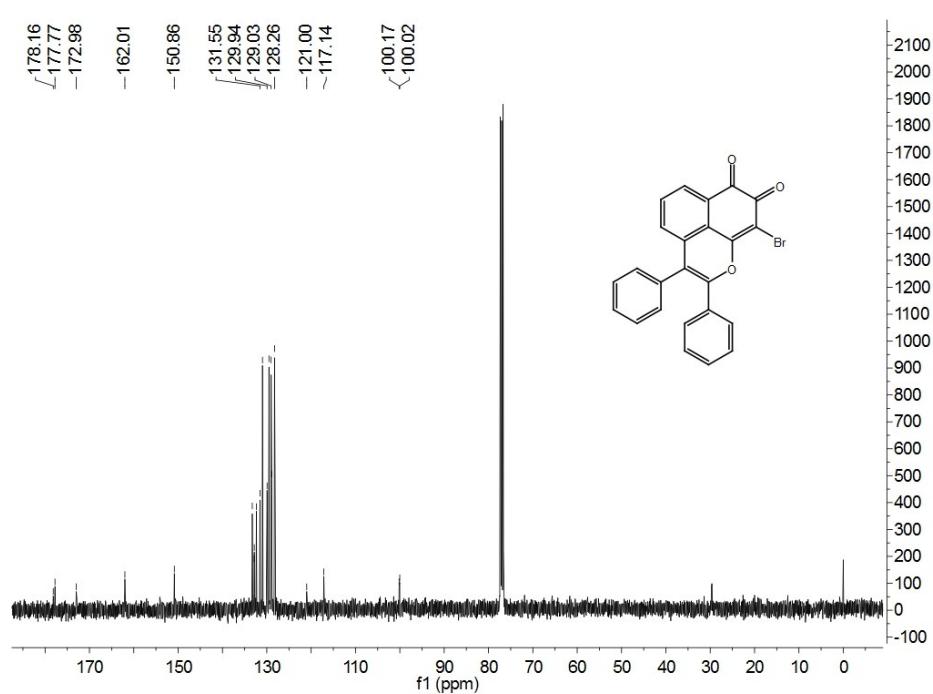
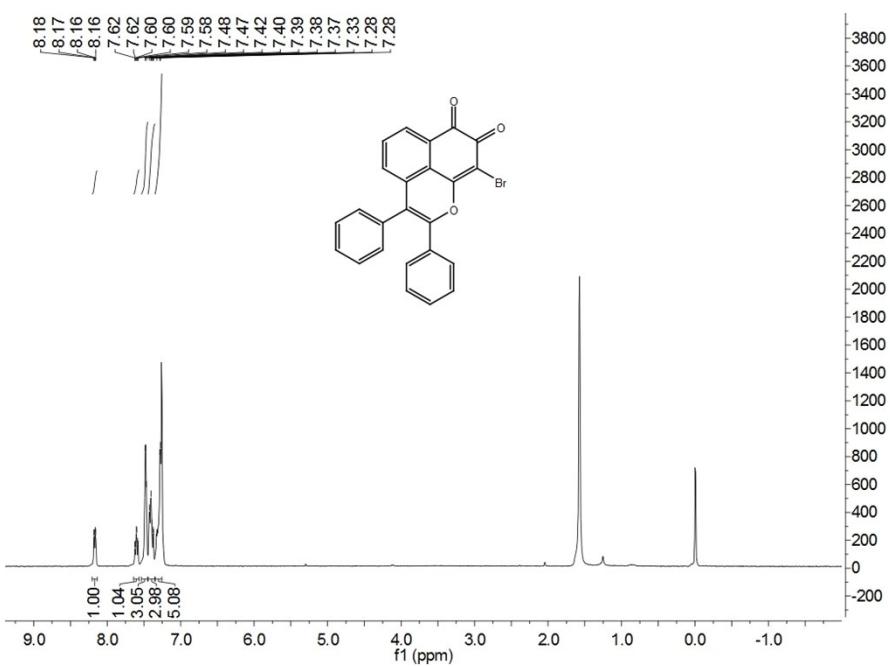


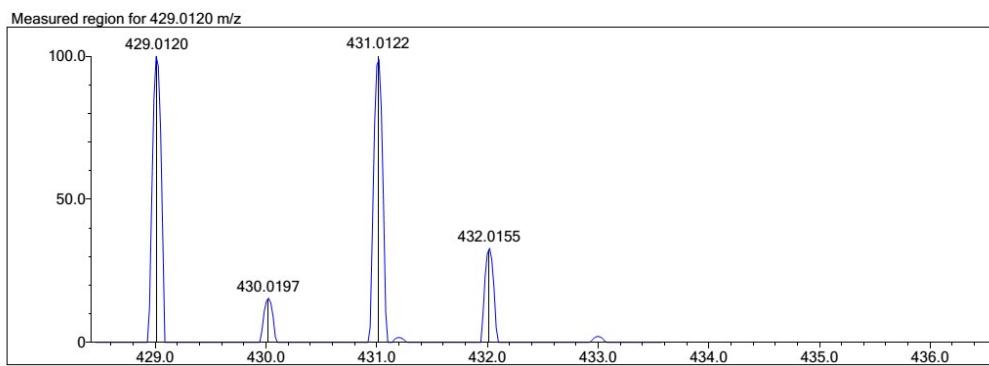
IR spectra of **5c**



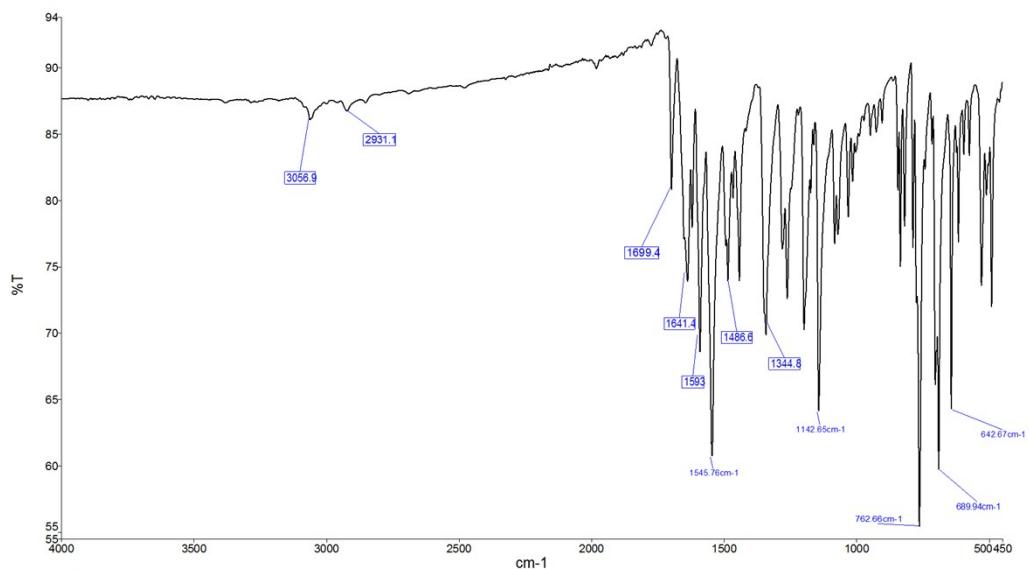
PeakTable					
PDA Ch1 254nm 4nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.833	5940	844	0.039	0.227
2	10.036	13562	393	0.090	0.106
3	12.369	15115860	370710	99.871	99.668
Total		15135363	371947	100.000	100.000

HPLC profile of **5c**

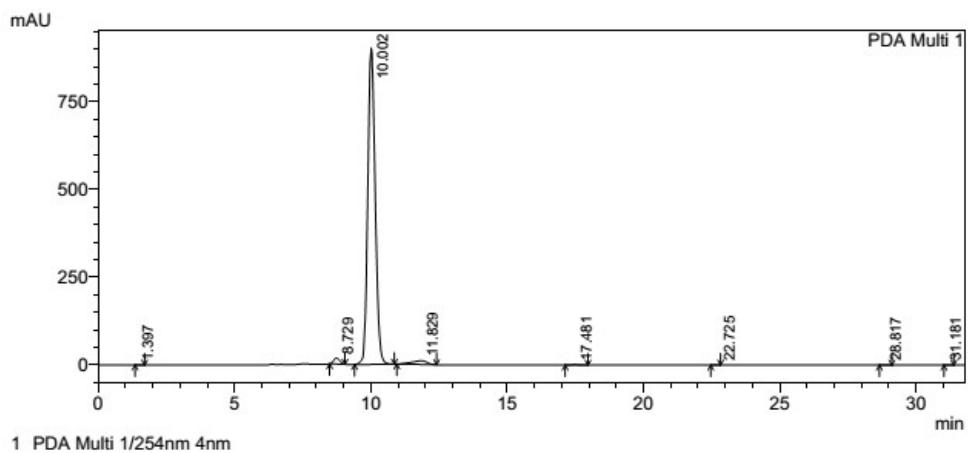




HRMS spectrum of **6c**



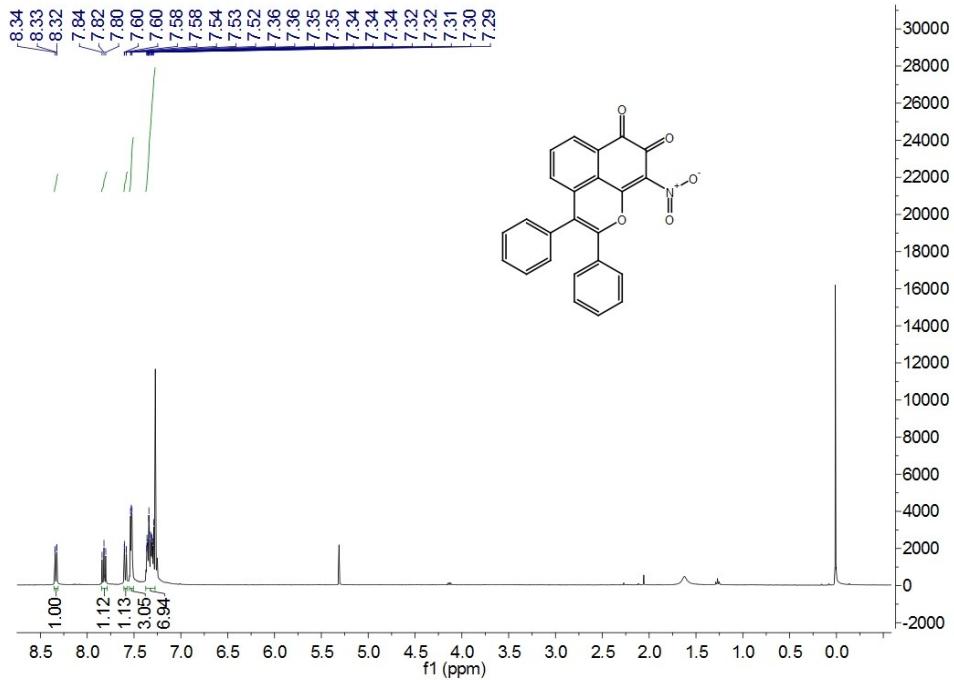
IR spectra of **6c**



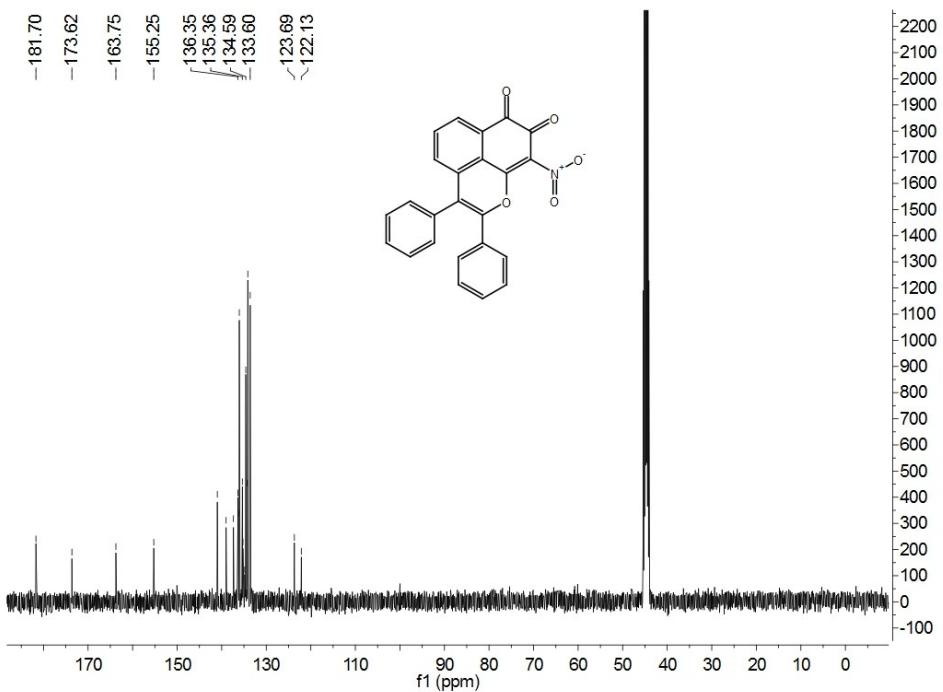
PeakTable

PDA Ch1 254nm 4nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	1.397	1070	58	0.006	0.006
2	8.729	266684	17174	1.511	1.842
3	10.002	16941325	902949	95.981	96.850
4	11.829	415852	10971	2.356	1.177
5	17.481	21169	887	0.120	0.095
6	22.725	1086	70	0.006	0.008
7	28.817	2309	123	0.013	0.013
8	31.181	1150	85	0.007	0.009
Total		17650644	932316	100.000	100.000

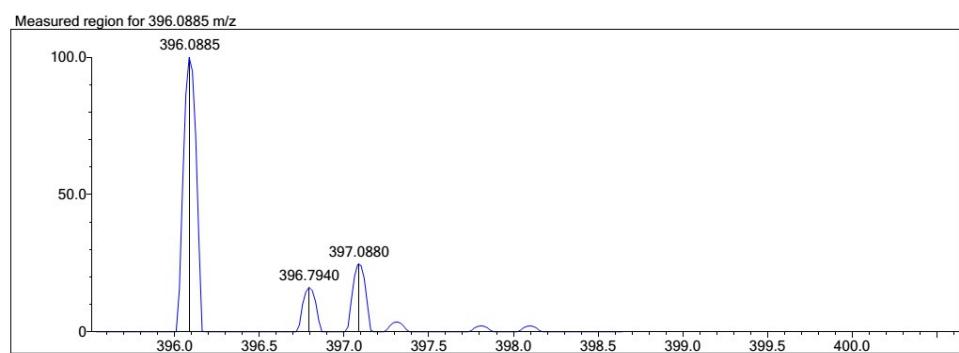
HPLC profile of 6c



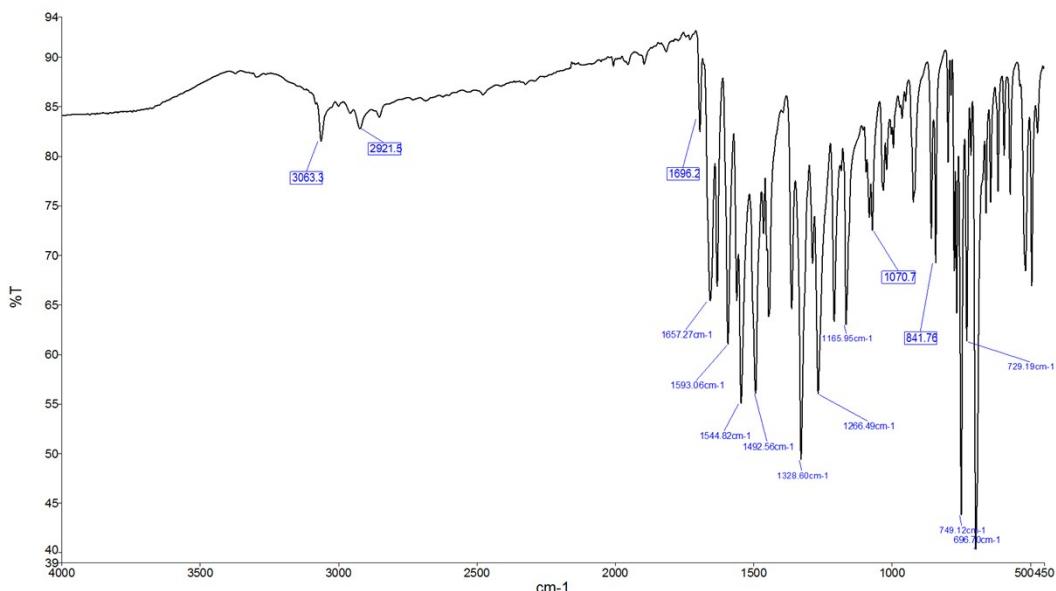
¹H NMR spectra of 7c



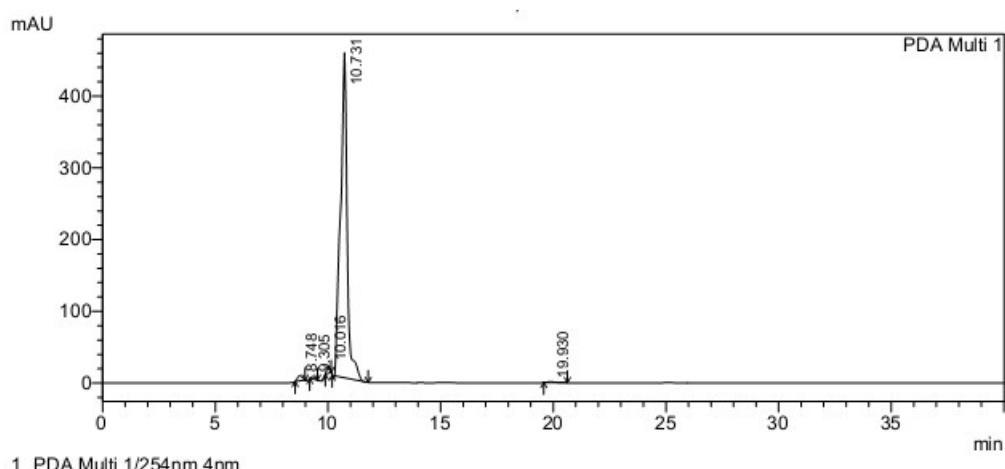
^{13}C NMR spectra of **7c**



HRMS spectrum of **7c**

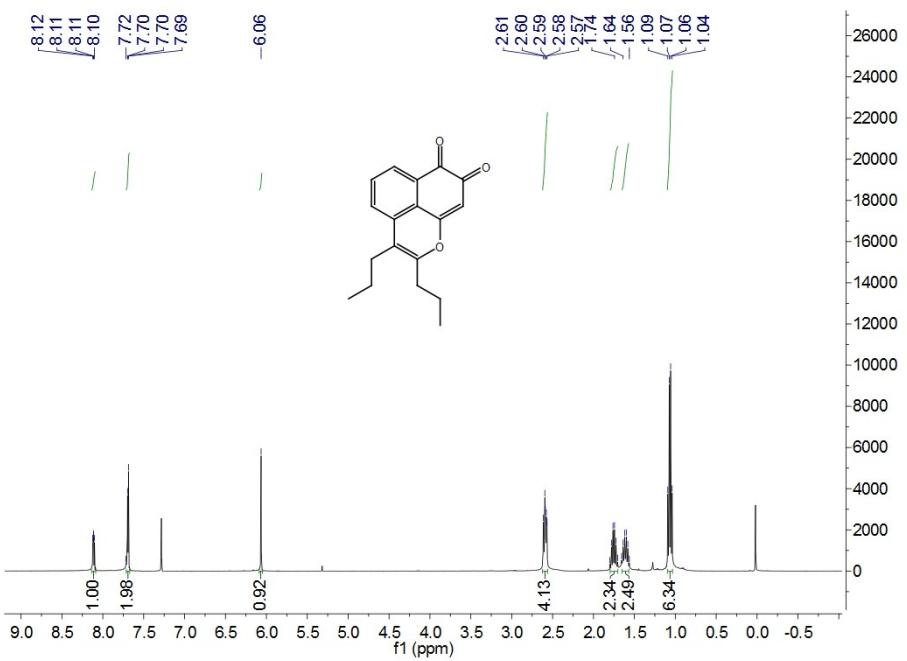


IR spectra of **7c**

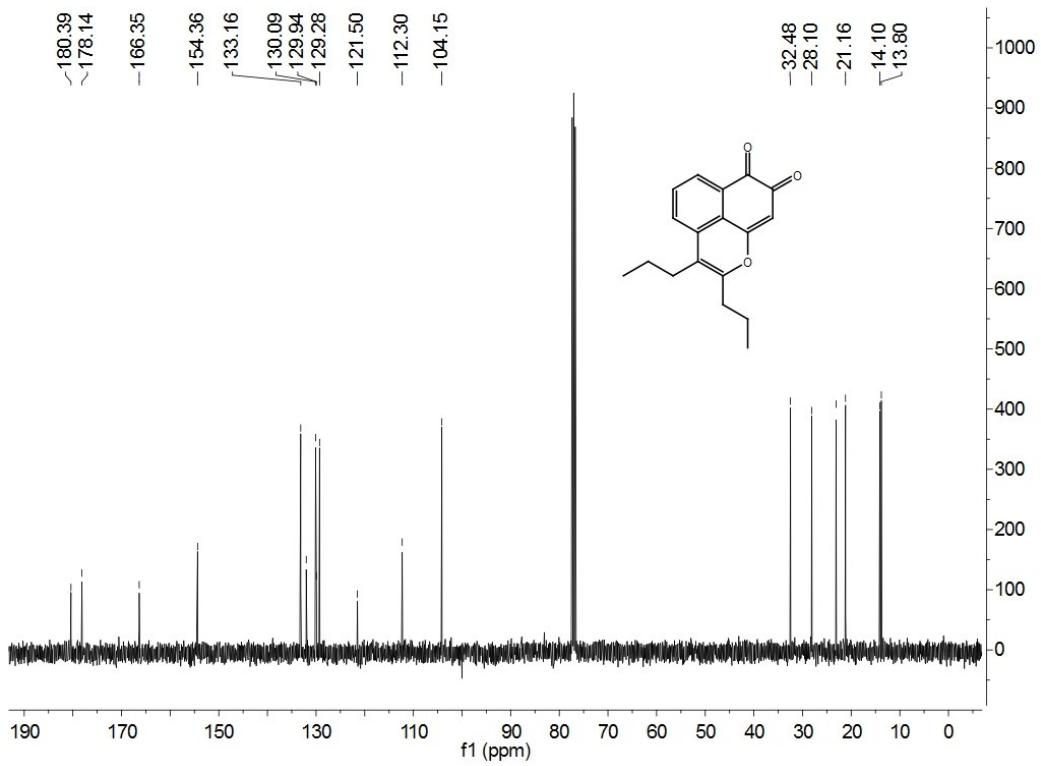


PeakTable					
PDA Ch1 254nm 4nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.748	106003	6988	1.110	1.471
2	9.305	37354	3068	0.391	0.646
3	10.016	101577	10610	1.063	2.234
4	10.731	9280649	453285	97.155	95.454
5	19.930	26820	921	0.281	0.194
Total		9552403	474871	100.000	100.000

HPLC profile of **7c**

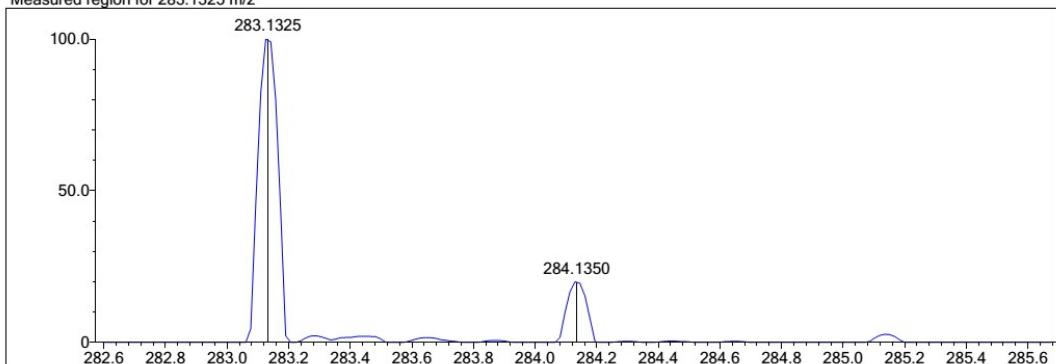


¹H NMR spectra of 3d

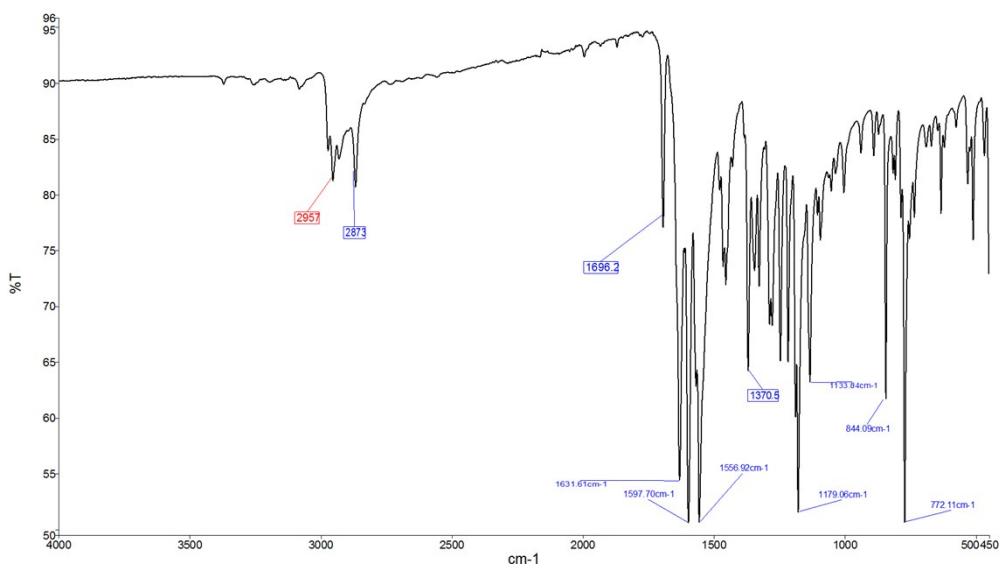


¹³C NMR spectra of **3d**

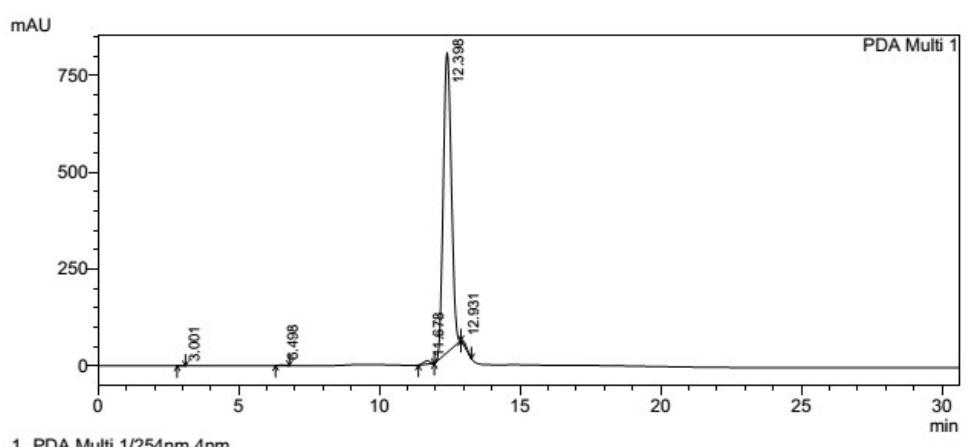
Measured region for 283.1325 m/z



HRMS spectrum of **3d**



IR spectra of **3d**

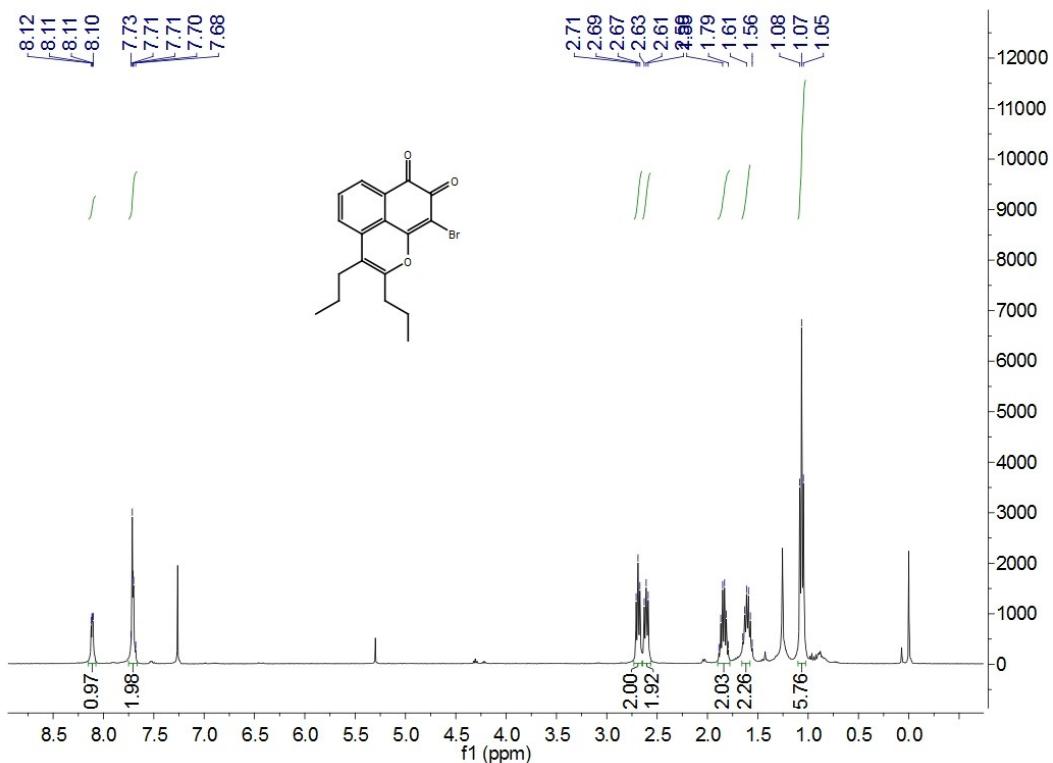


PeakTable

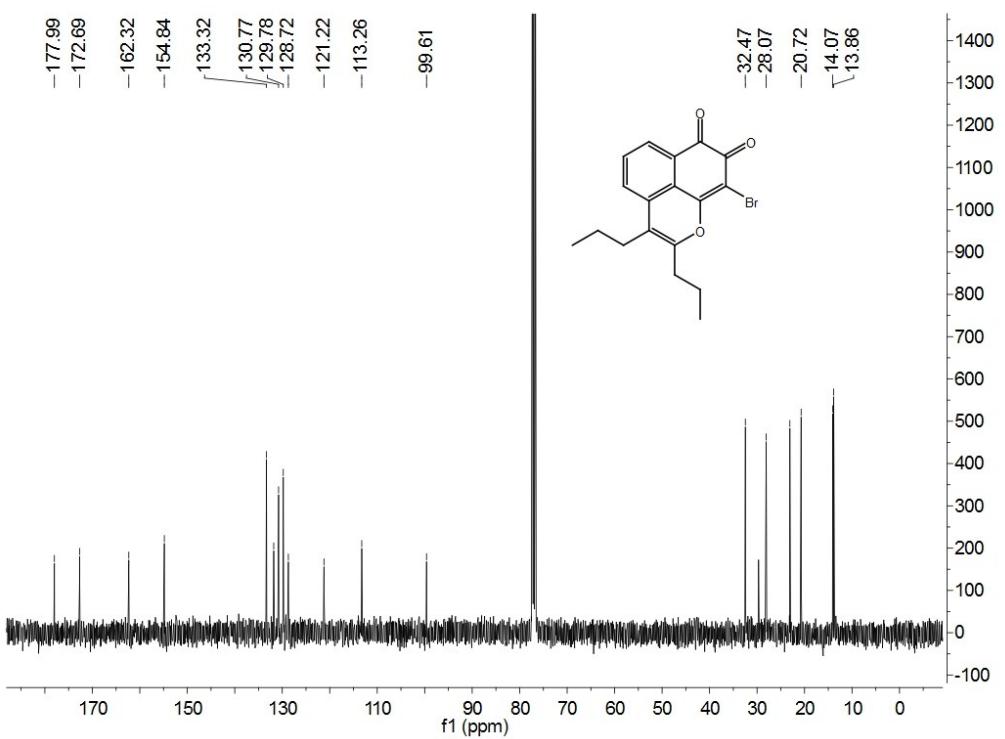
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	3.001	1068	99	0.007	0.012
2	6.498	37270	2528	0.238	0.319
3	11.678	151299	8751	0.967	1.105
4	12.398	15355914	775048	98.108	97.911
5	12.931	106439	5155	0.680	0.651
Total		15651990	791581	100.000	100.000

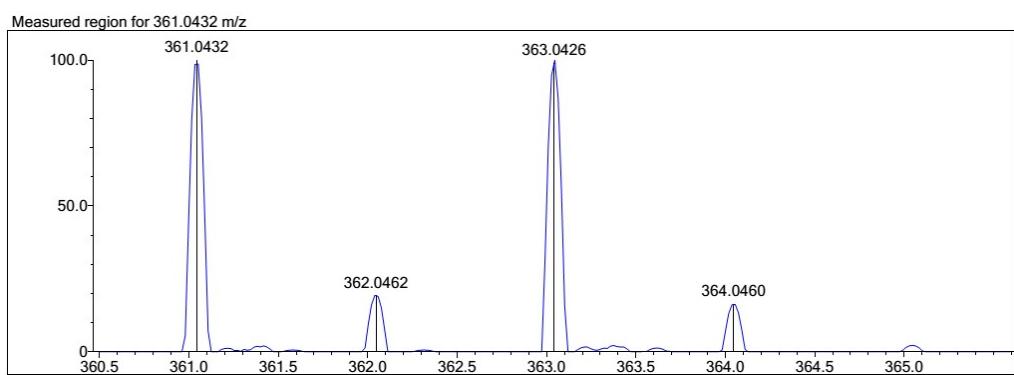
HPLC profile of 3d



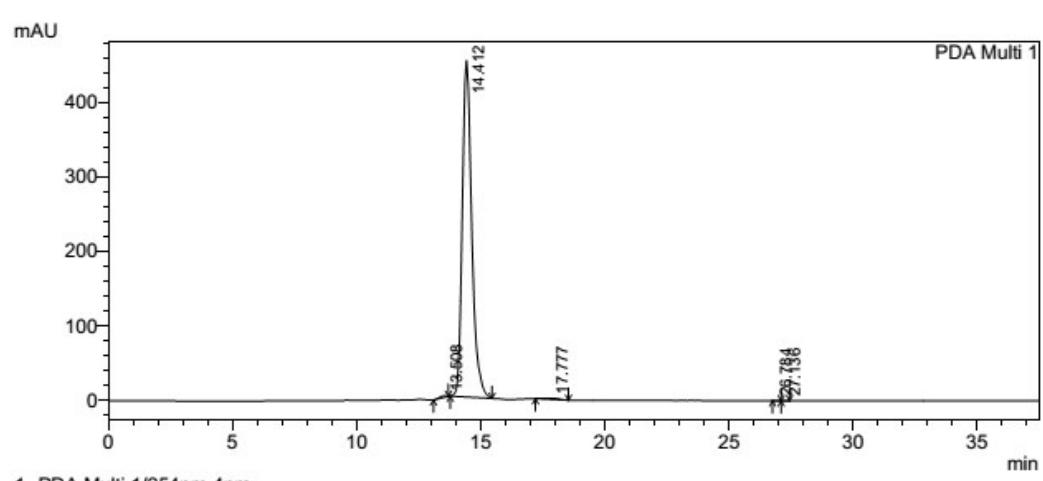
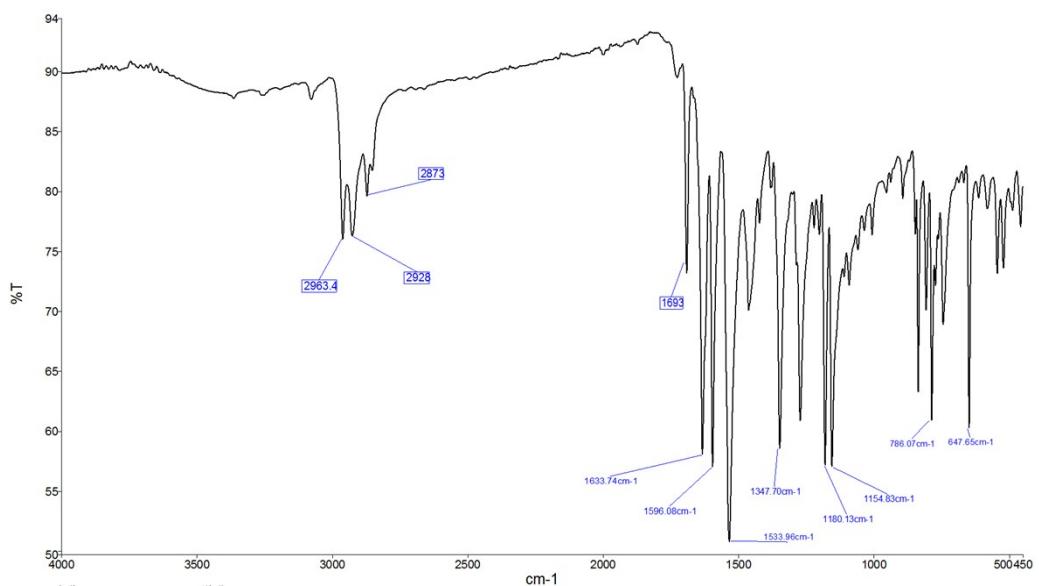
¹H NMR spectra of 6d



^{13}C NMR spectra of **6d**

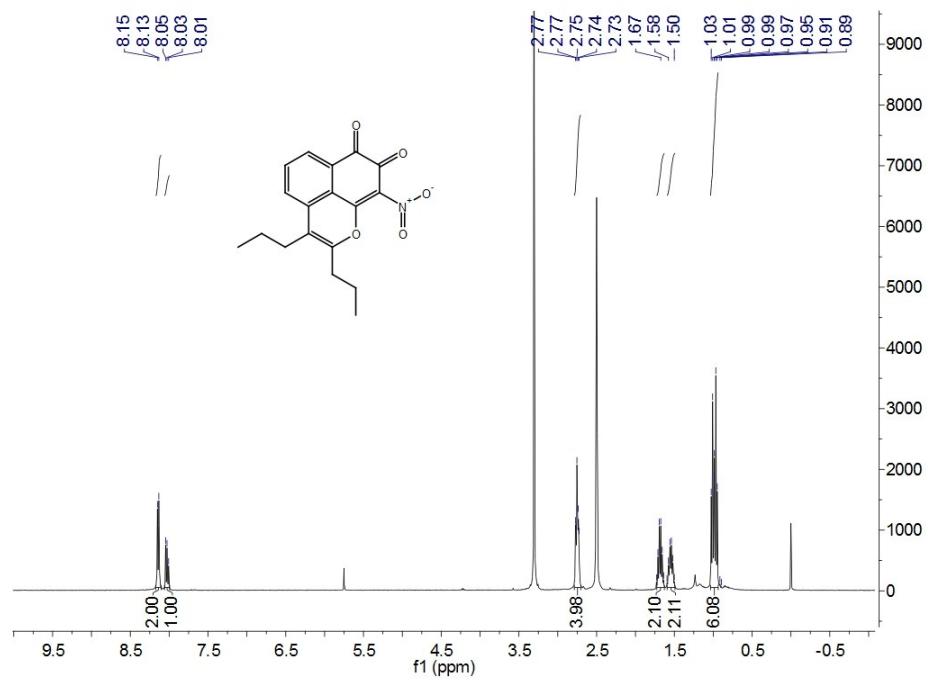


HRMS spectrum of **6d**

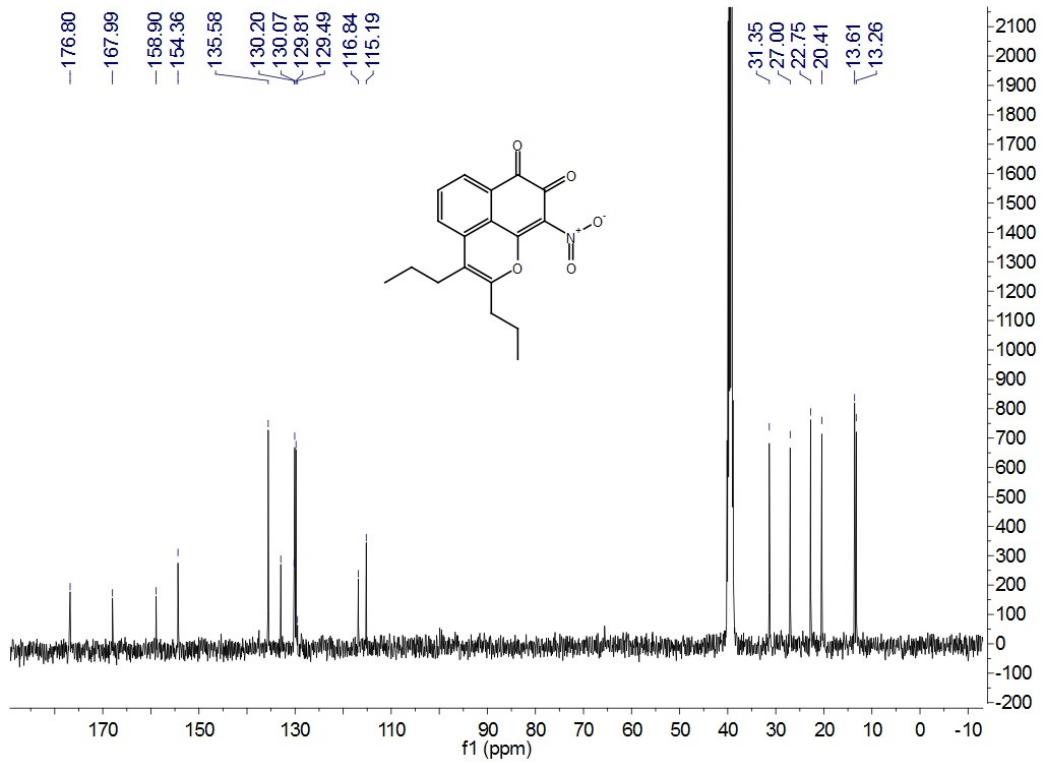


PDA Ch1 254nm 4nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.508	39796	2067	0.331	0.454
2	14.412	11909002	451282	99.116	99.199
3	17.777	63944	1368	0.532	0.301
4	26.784	1160	103	0.010	0.023
5	27.136	1327	107	0.011	0.023
Total		12015229	454926	100.000	100.000

HPLC profile of **6d**

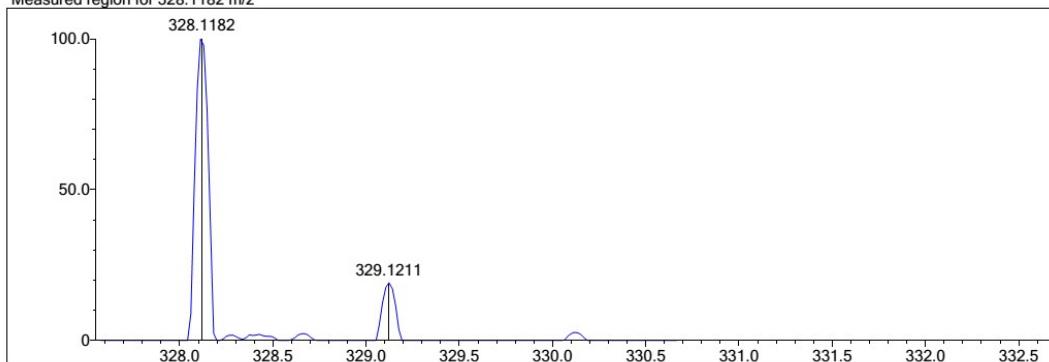


¹H NMR spectra of **7d**

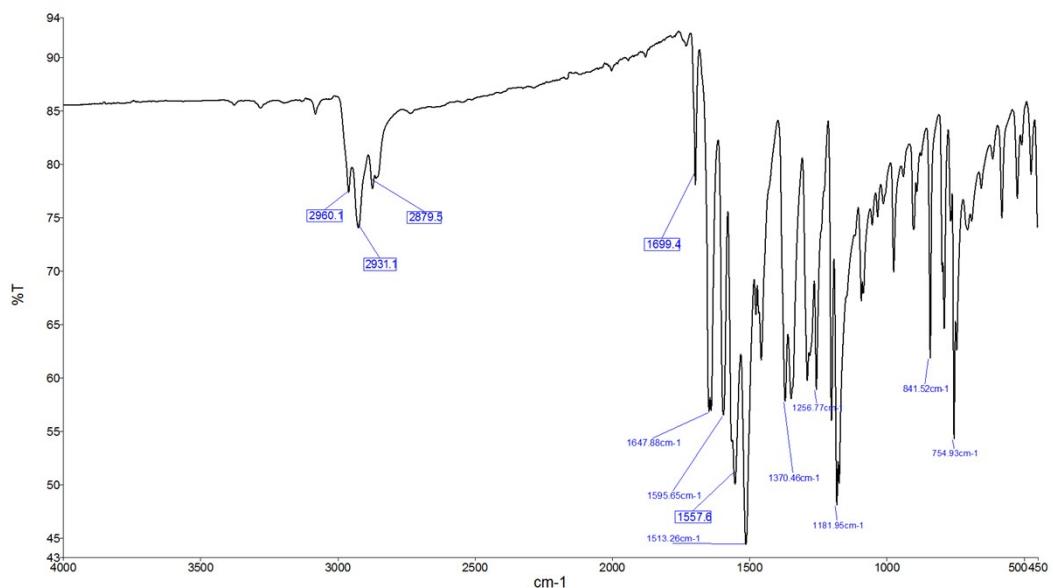


¹³C NMR spectra of **7d**

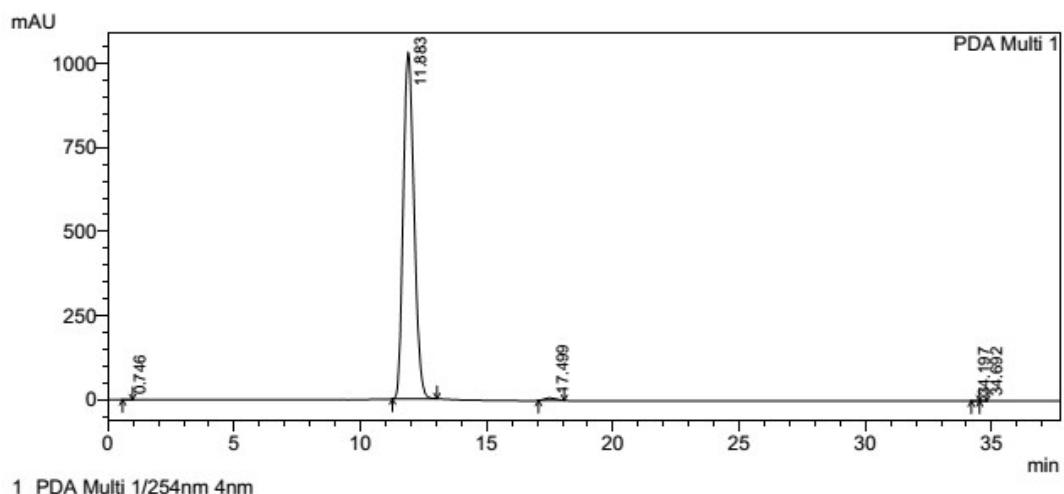
Measured region for 328.1182 m/z



HRMS spectrum of **7d**



IR spectra of **7d**

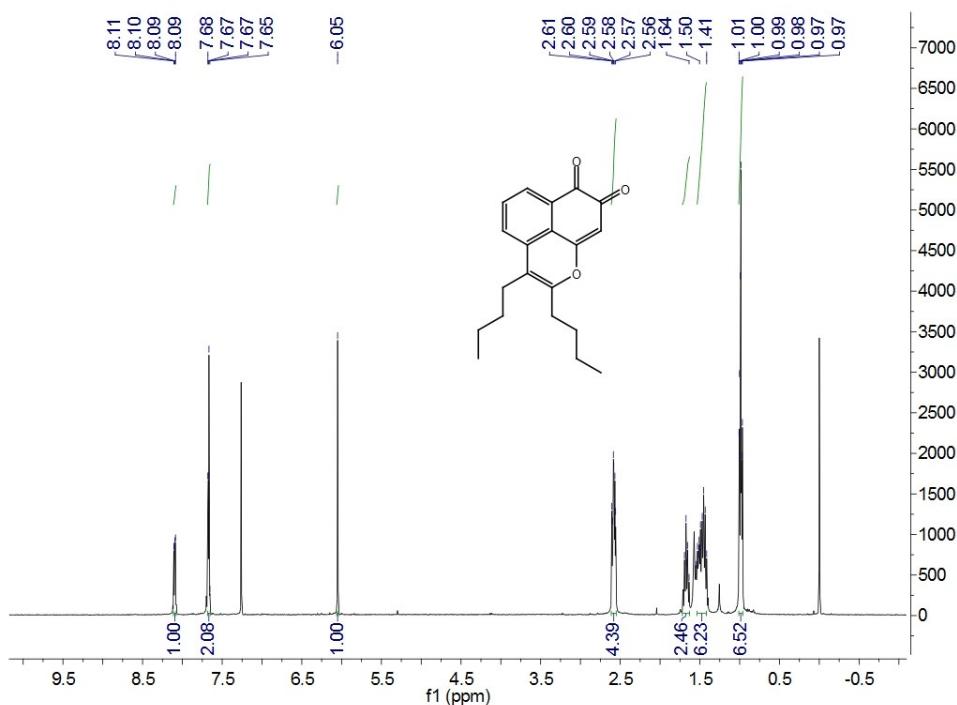


PeakTable

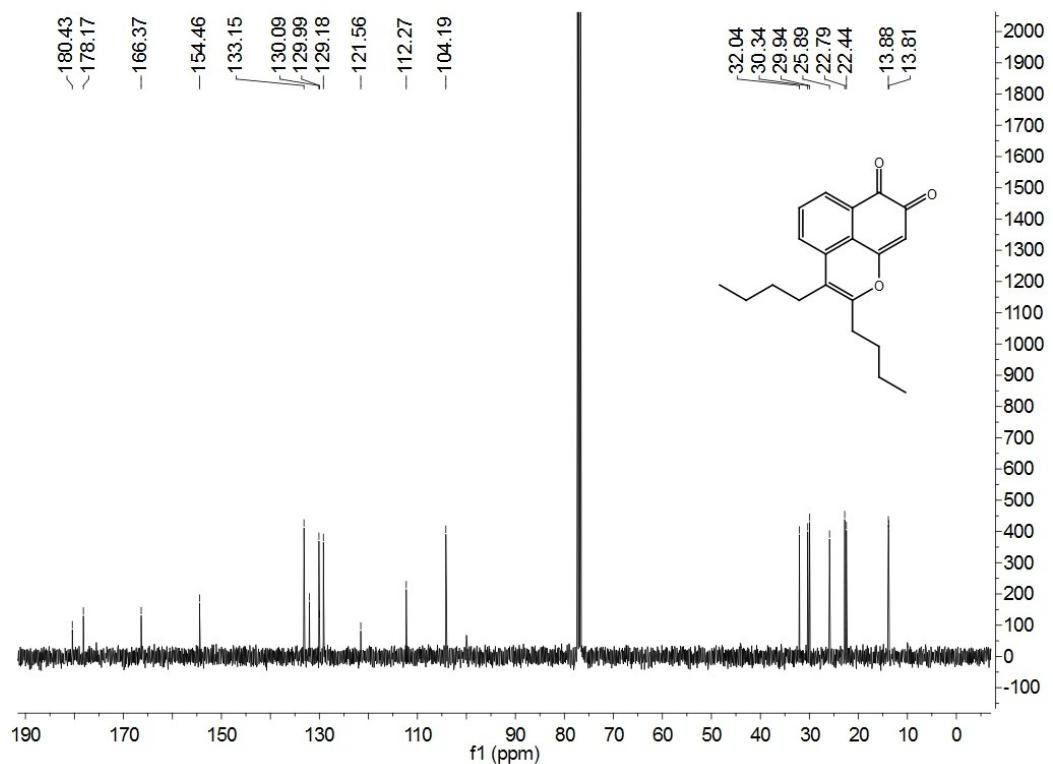
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	0.746	1326	103	0.004	0.010
2	11.883	30590019	1032607	99.241	99.313
3	17.499	230685	6907	0.748	0.664
4	34.197	1032	46	0.003	0.004
5	34.692	1045	86	0.003	0.008
Total		30824108	1039748	100.000	100.000

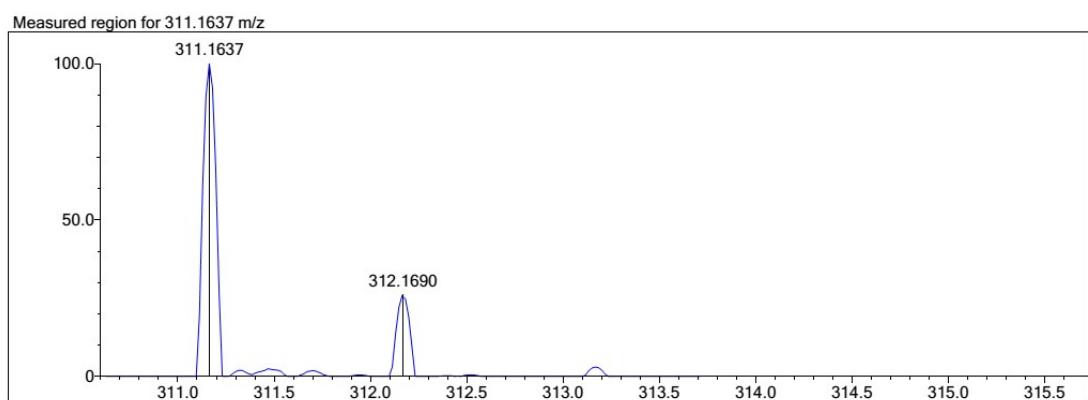
HPLC profile of 7d



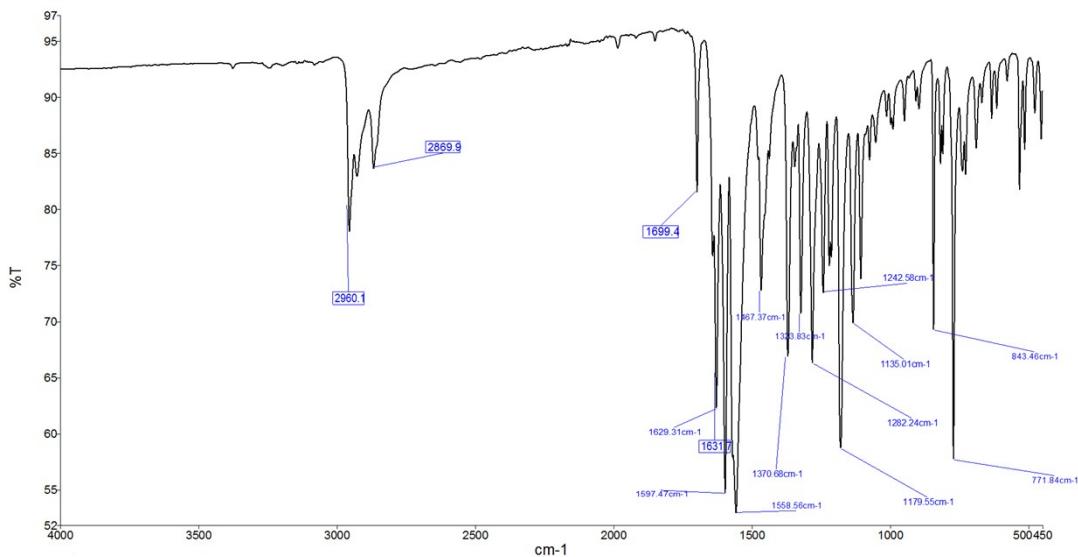
¹H NMR spectra of 3e



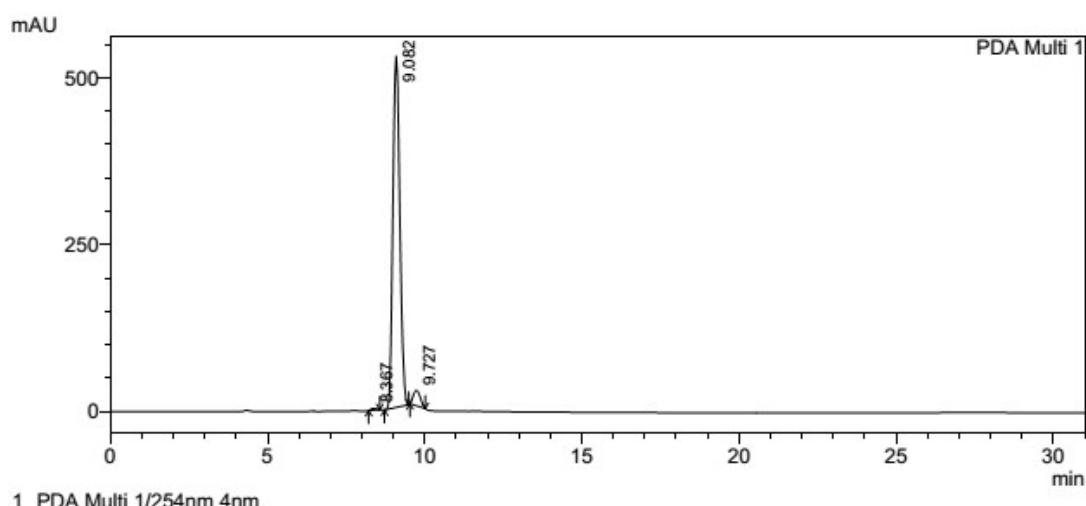
¹³C NMR spectra of **3e**



HRMS spectrum of **3e**



IR spectra of **3e**

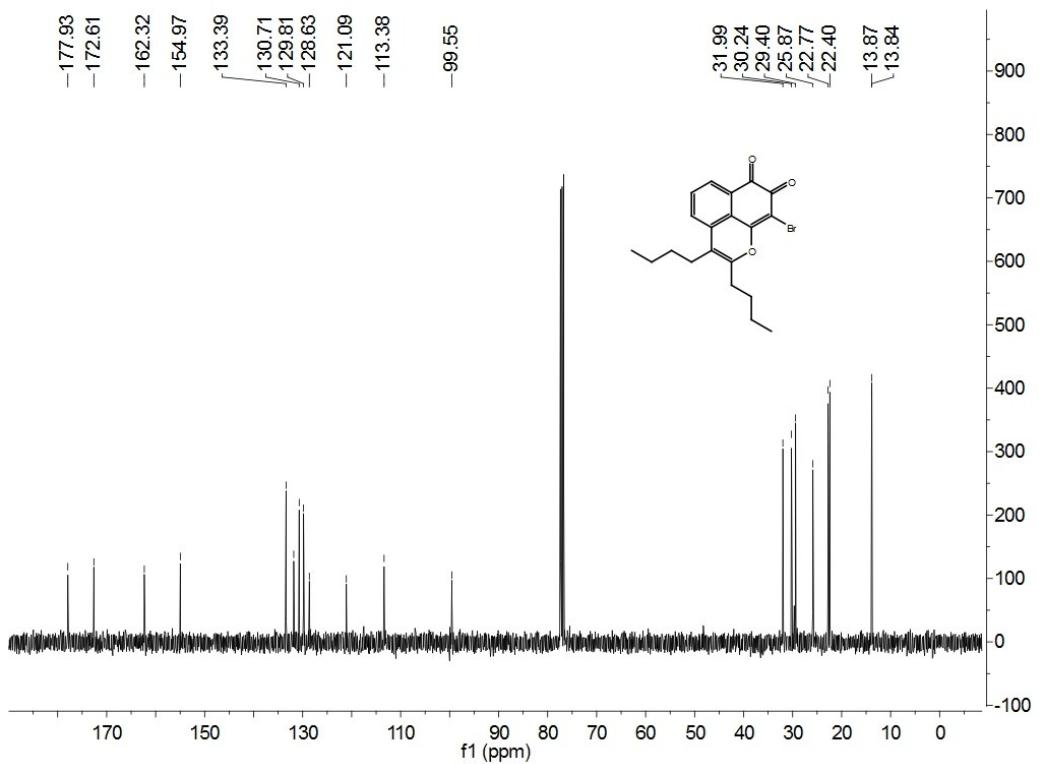
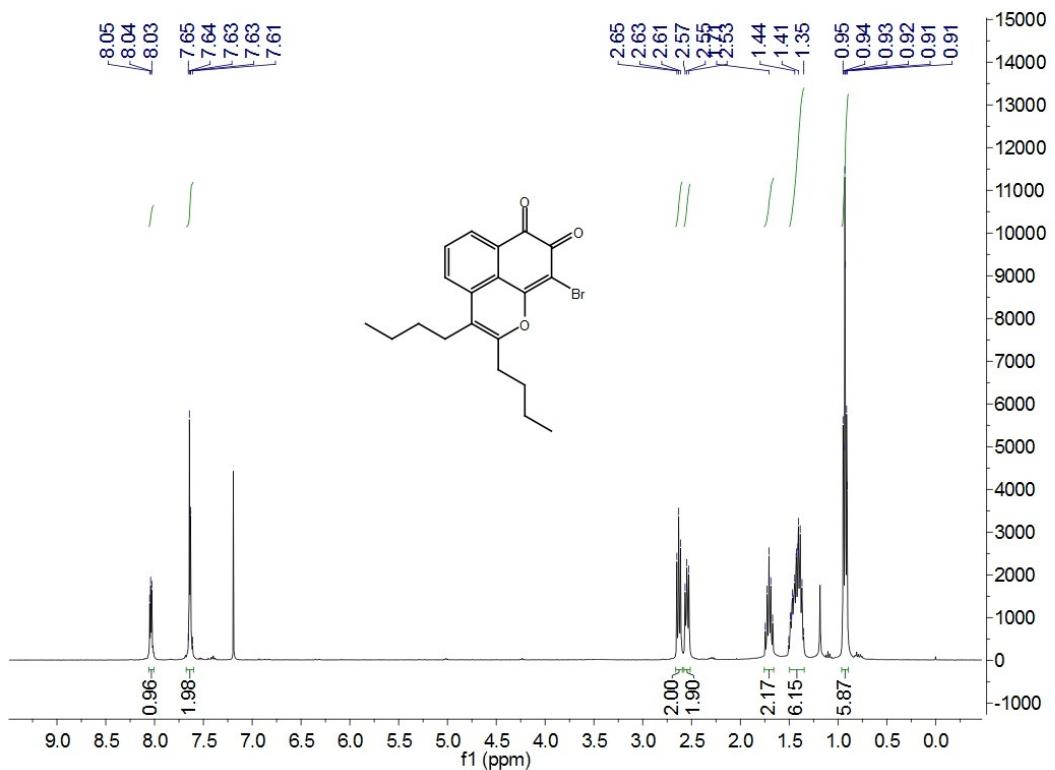


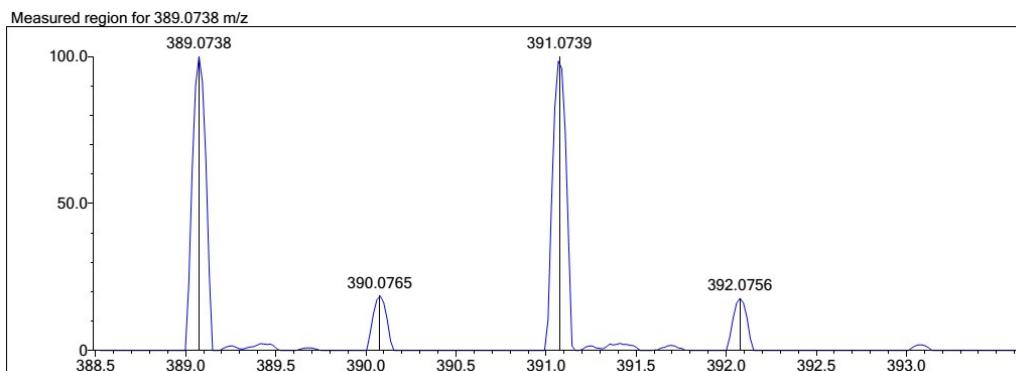
PDA Ch1 254nm 4nm

PeakTable

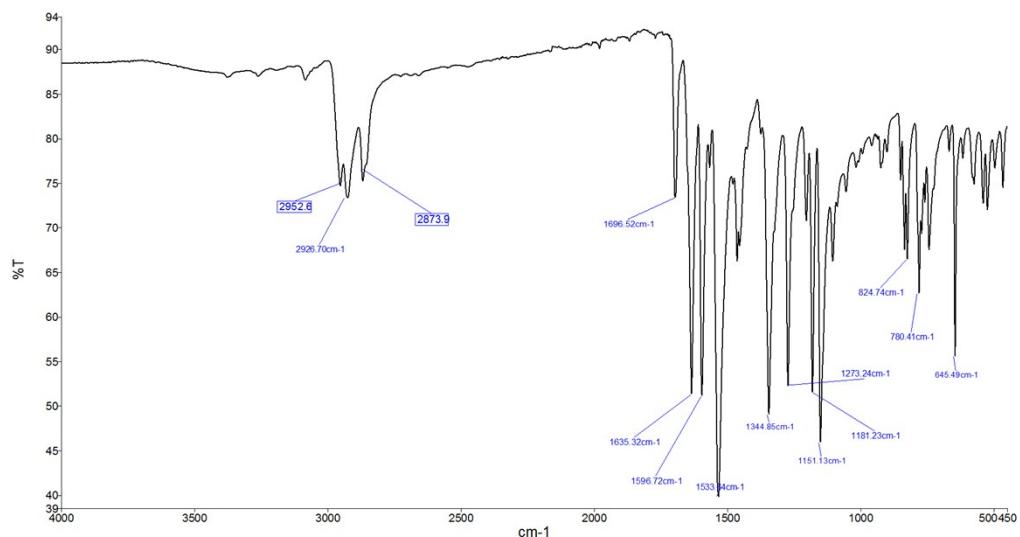
Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.367	34500	2969	0.411	0.537
2	9.082	7998966	527146	95.307	95.285
3	9.727	359347	23115	4.282	4.178
Total		8392813	553230	100.000	100.000

HPLC profile of **3e**

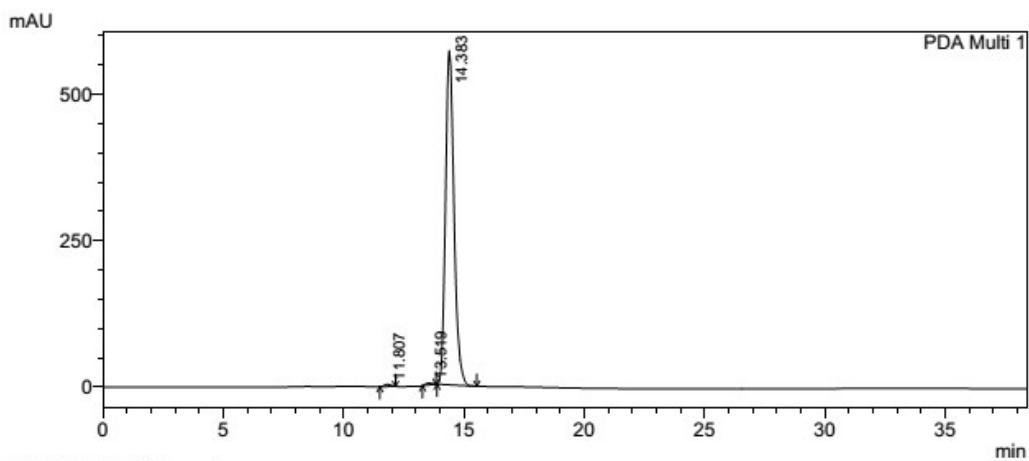




HRMS spectrum of **6e**



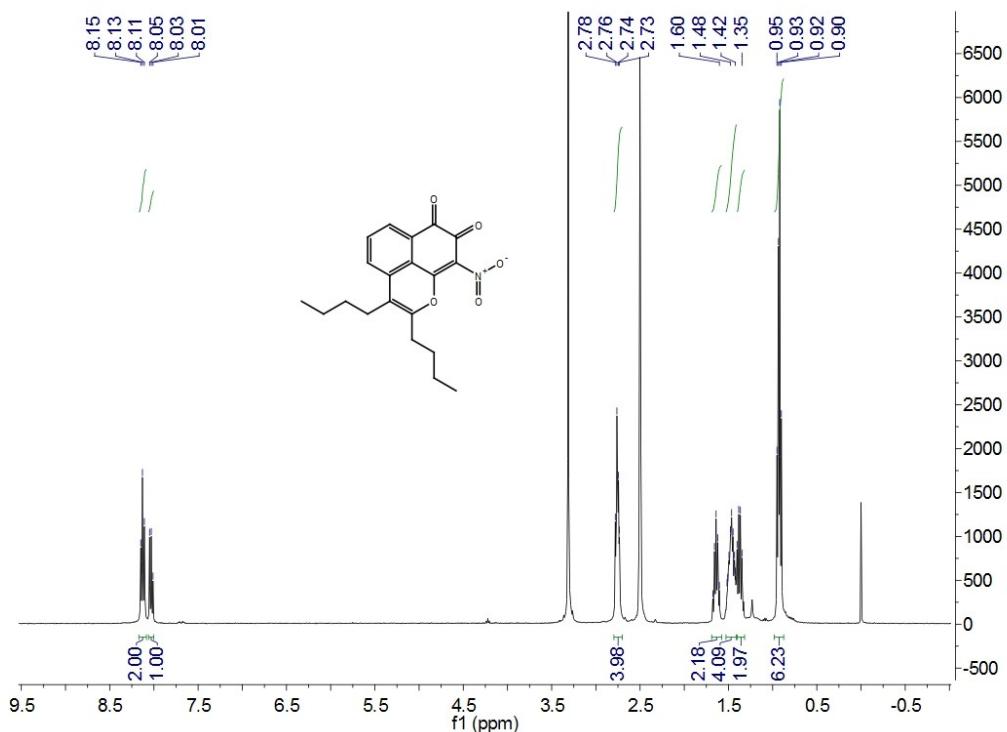
IR spectra of **6e**



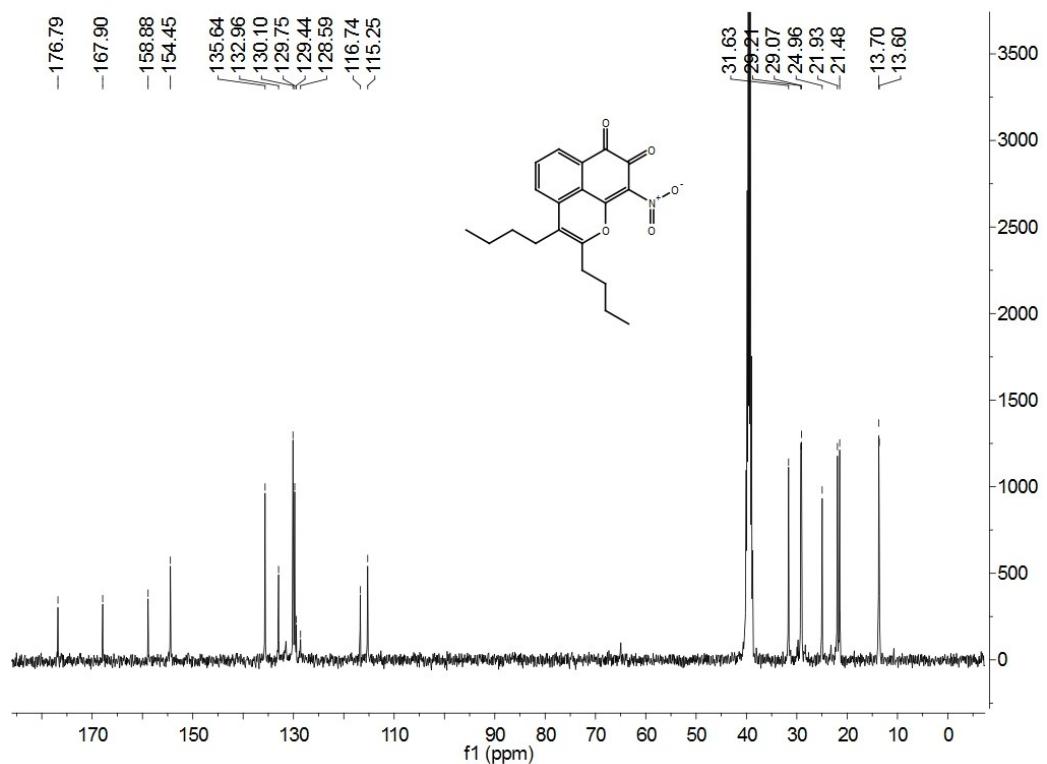
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.807	73587	3692	0.523	0.638
2	13.519	67171	3471	0.477	0.600
3	14.383	13934321	571238	99.000	98.762
Total		14075079	578401	100.000	100.000

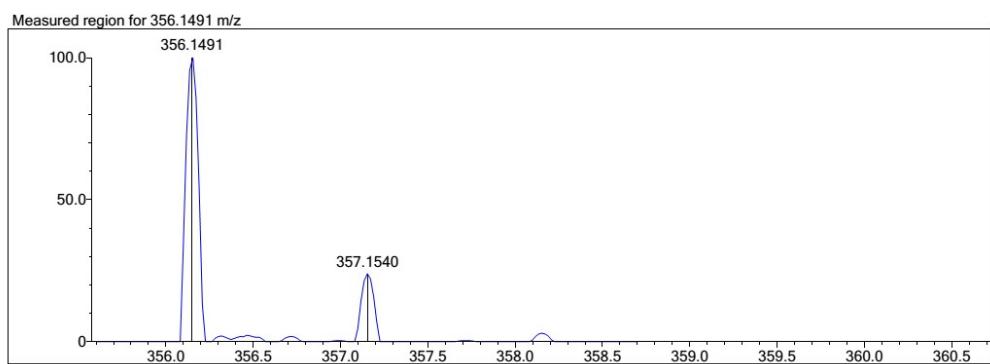
HPLC profile of 6e



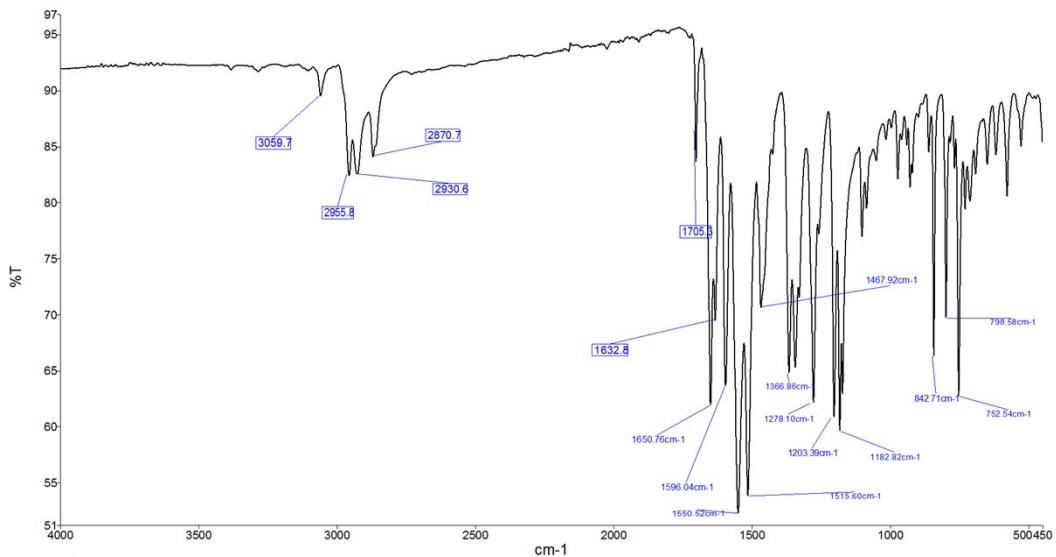
¹H NMR spectra of 7e



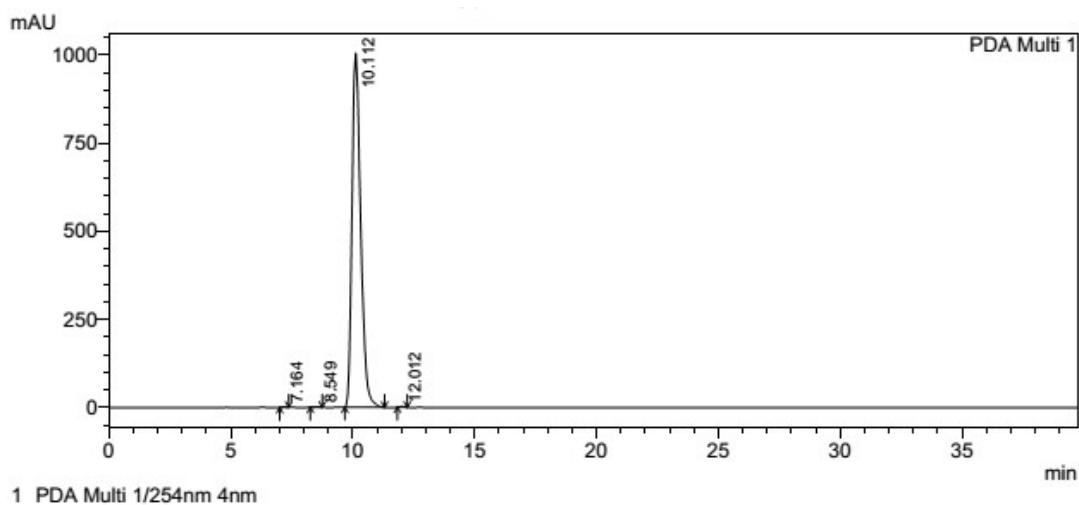
^{13}C NMR spectra of **7e**



HRMS spectrum of **7e**

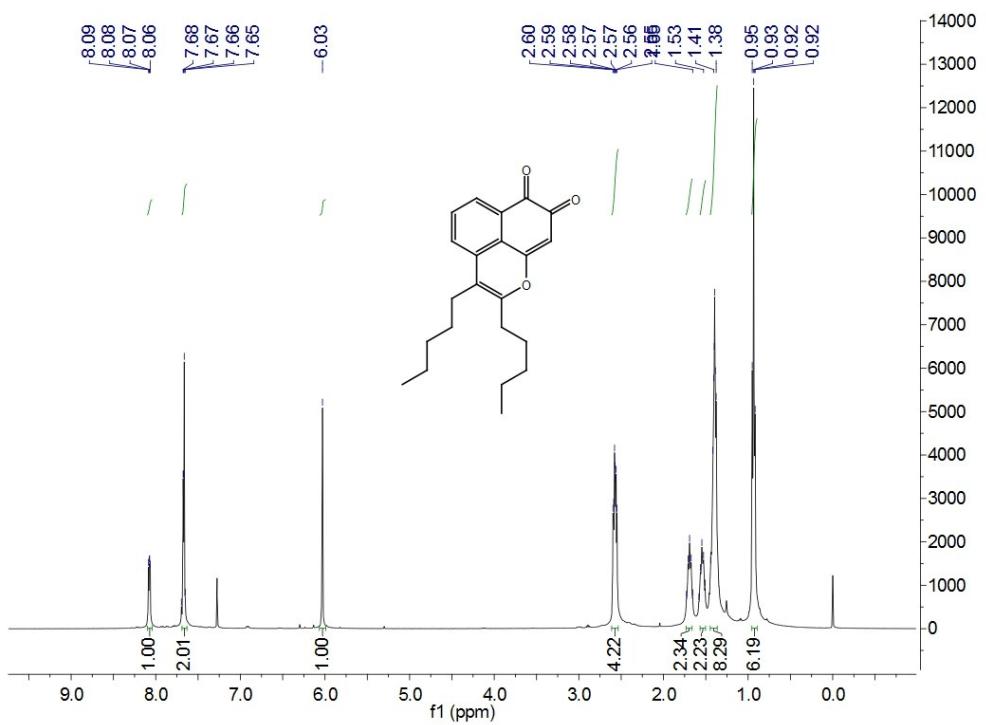


IR spectra of **7e**

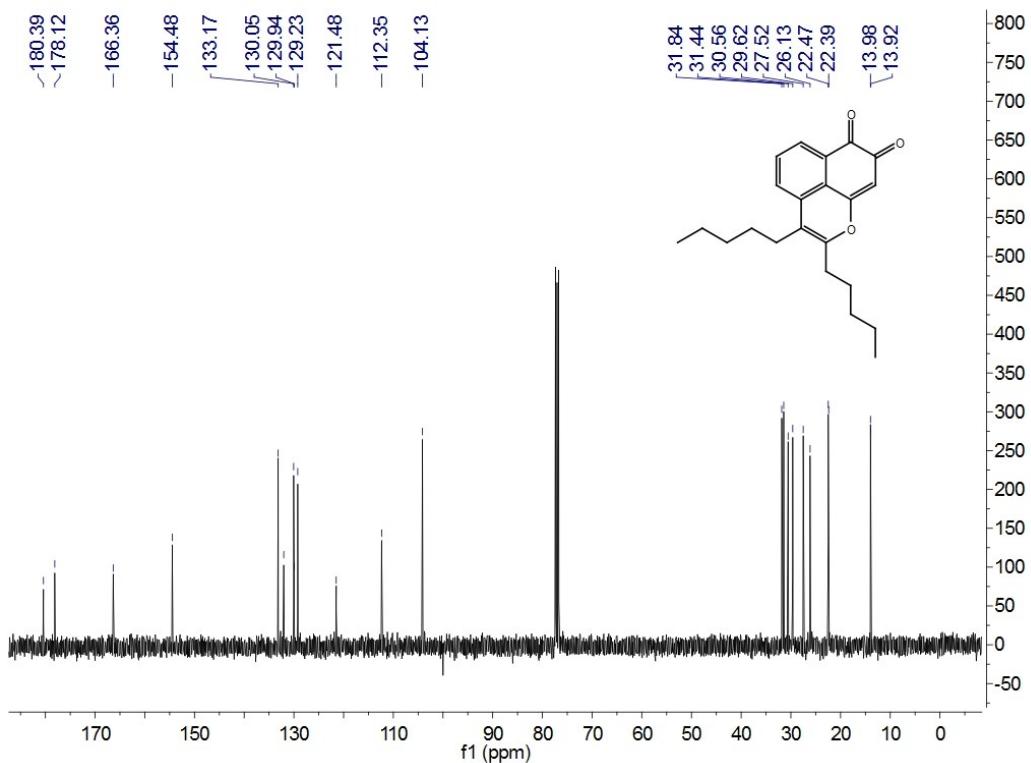


PeakTable					
PDA Ch1 254nm 4nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.164	14783	1196	0.059	0.119
2	8.549	17195	1074	0.069	0.106
3	10.112	24898057	1004497	99.754	99.566
4	12.012	29307	2111	0.117	0.209
Total		24959342	1008880	100.000	100.000

HPLC profile of **7e**

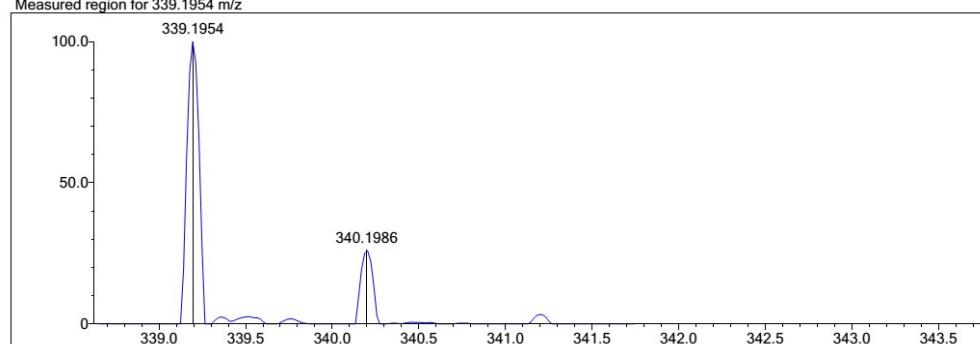


¹H NMR spectra of **3f**

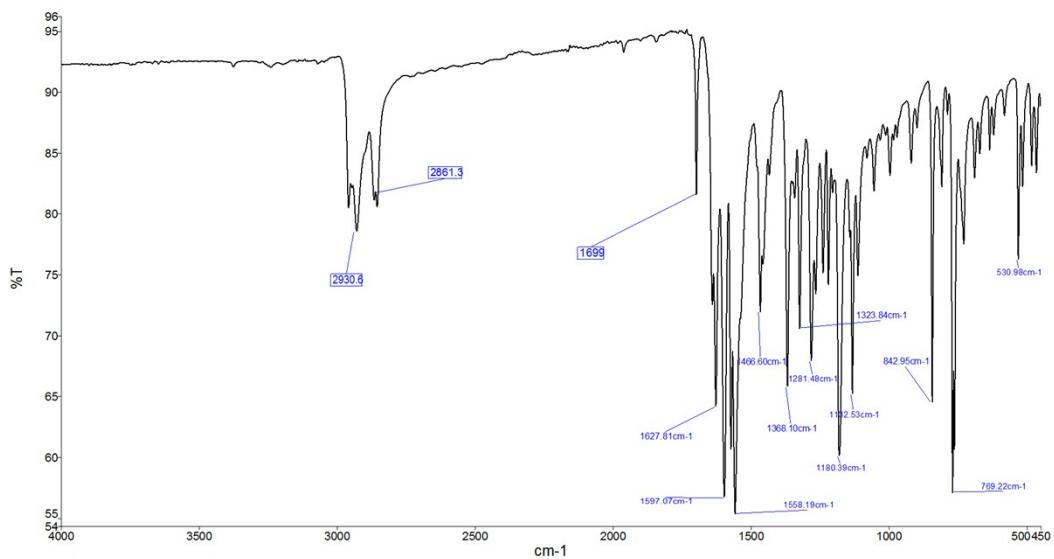


¹³C NMR spectra of **3f**

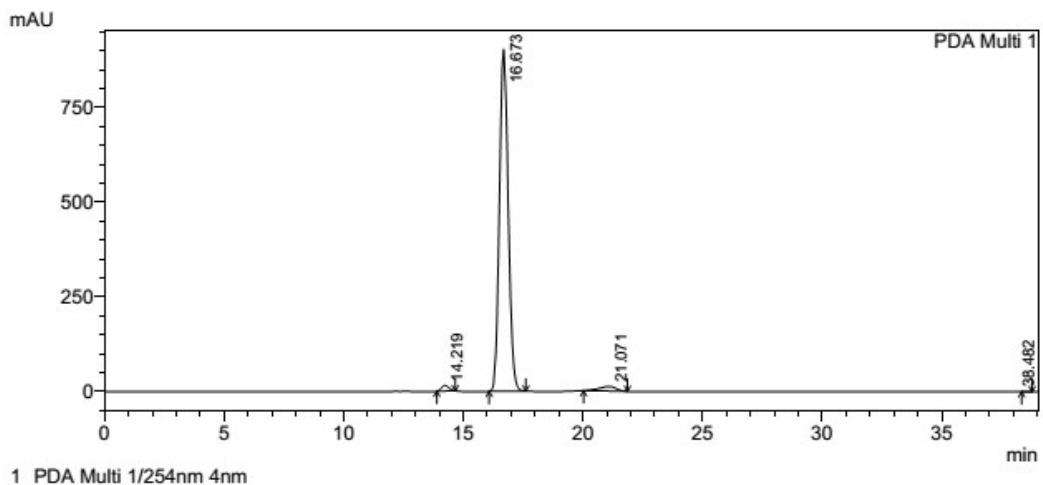
Measured region for 339.1954 m/z



HRMS spectrum of **3f**



IR spectra of **3f**

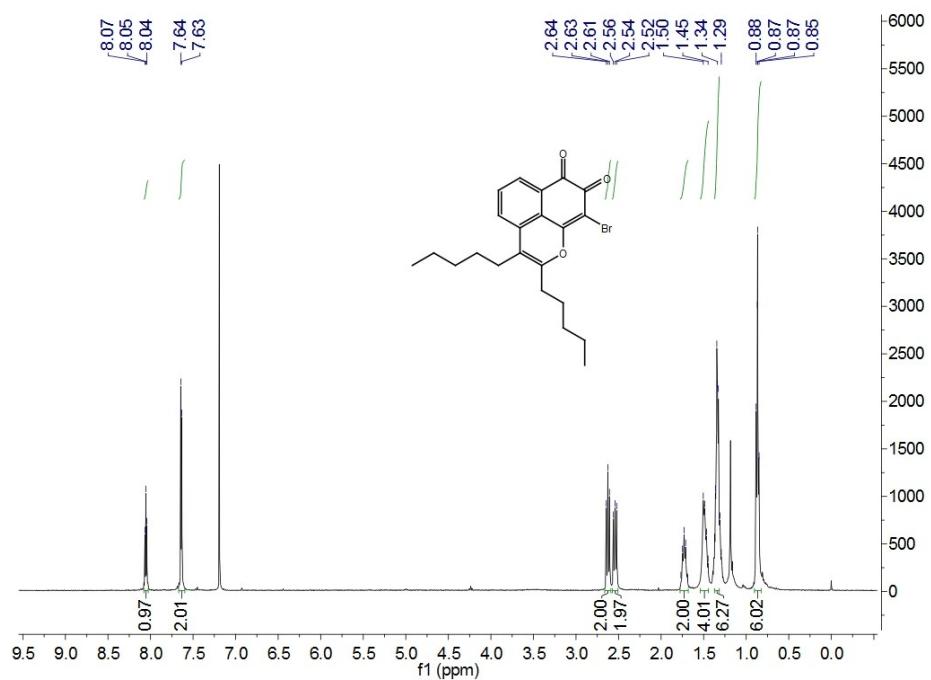


PeakTable

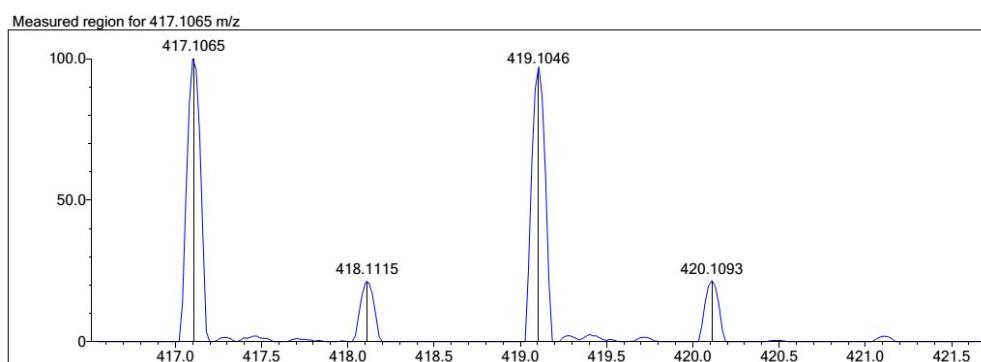
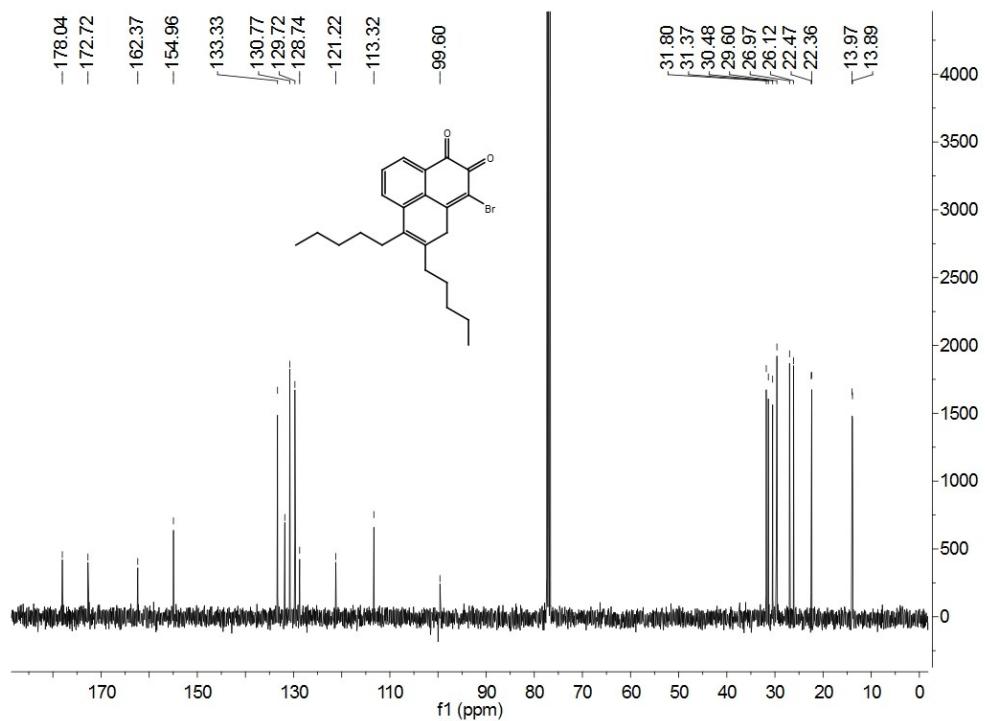
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.219	323563	14677	1.348	1.578
2	16.673	23076282	903181	96.149	97.090
3	21.071	599119	12307	2.496	1.323
4	38.482	1487	85	0.006	0.009
Total		24000451	930250	100.000	100.000

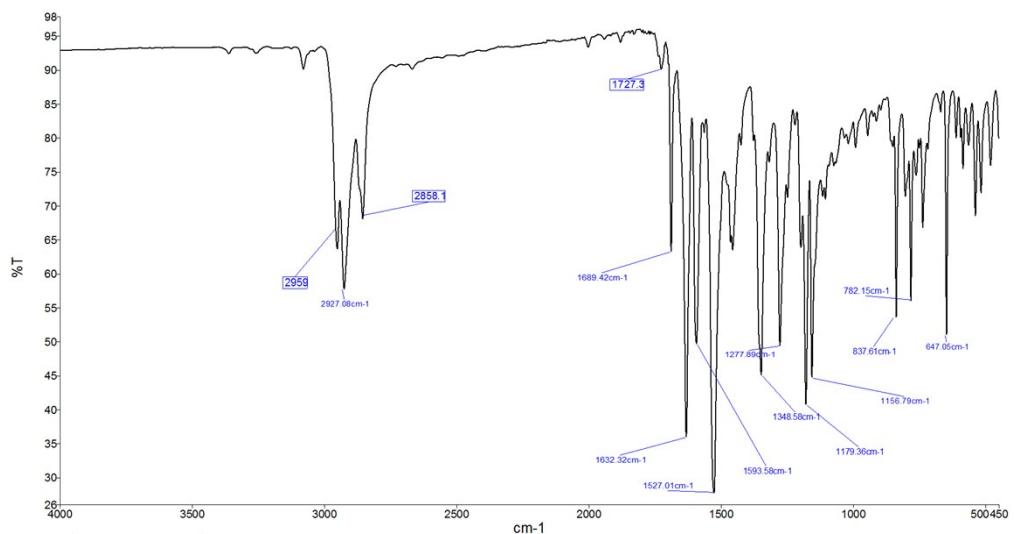
HPLC profile of **3f**



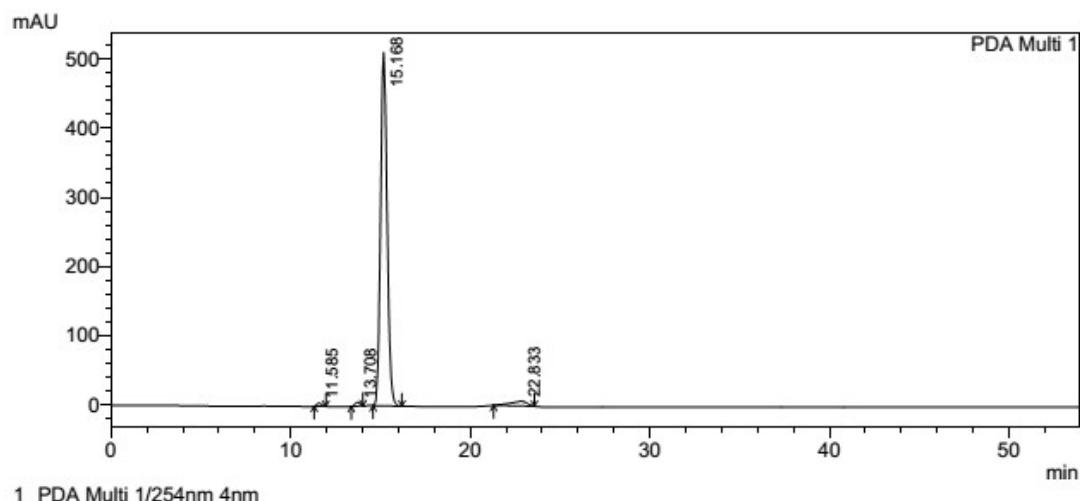
¹H NMR spectra of **6f**



HRMS spectrum of **6f**

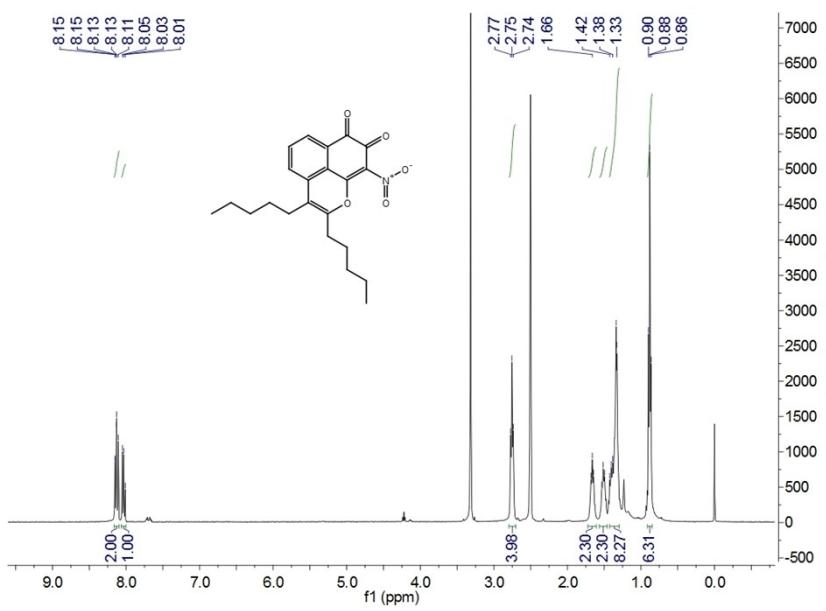


IR spectra of **6f**

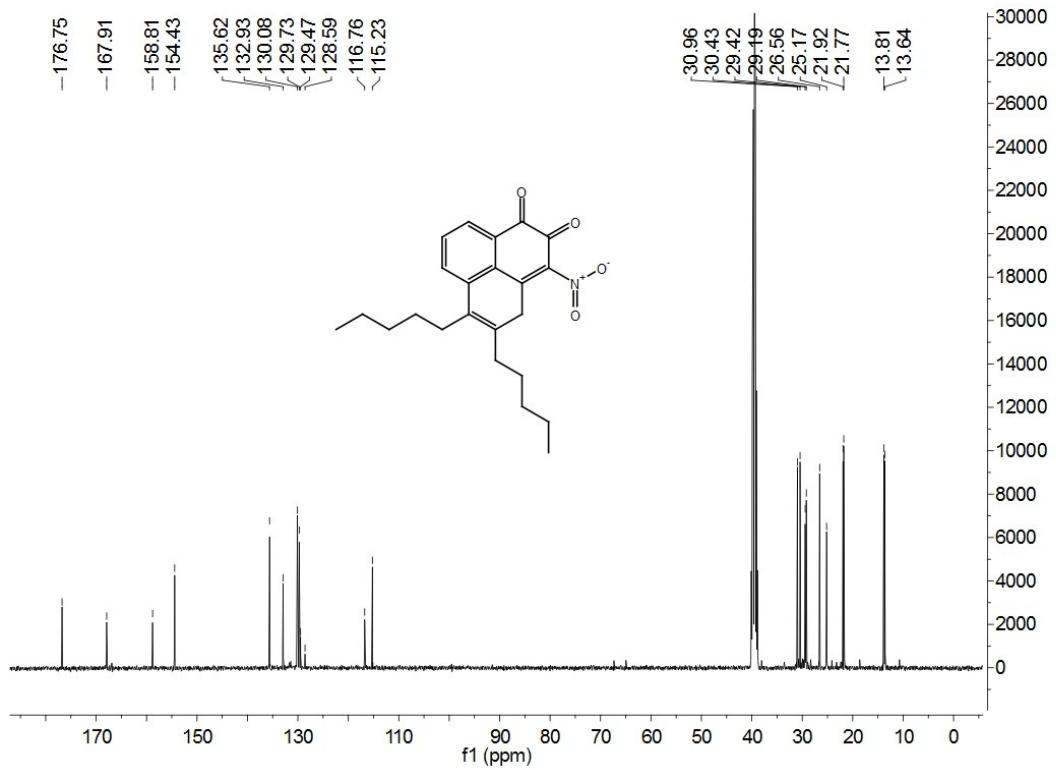


PeakTable					
PDA Ch1 254nm 4nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.585	88919	4421	0.655	0.839
2	13.708	104952	5251	0.774	0.997
3	15.168	12922513	510321	95.250	96.877
4	22.833	450496	6777	3.321	1.287
Total		13566881	526771	100.000	100.000

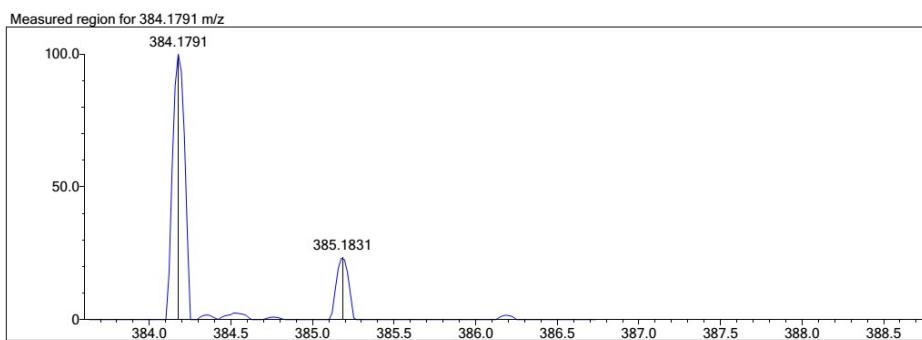
HPLC profile of **6f**



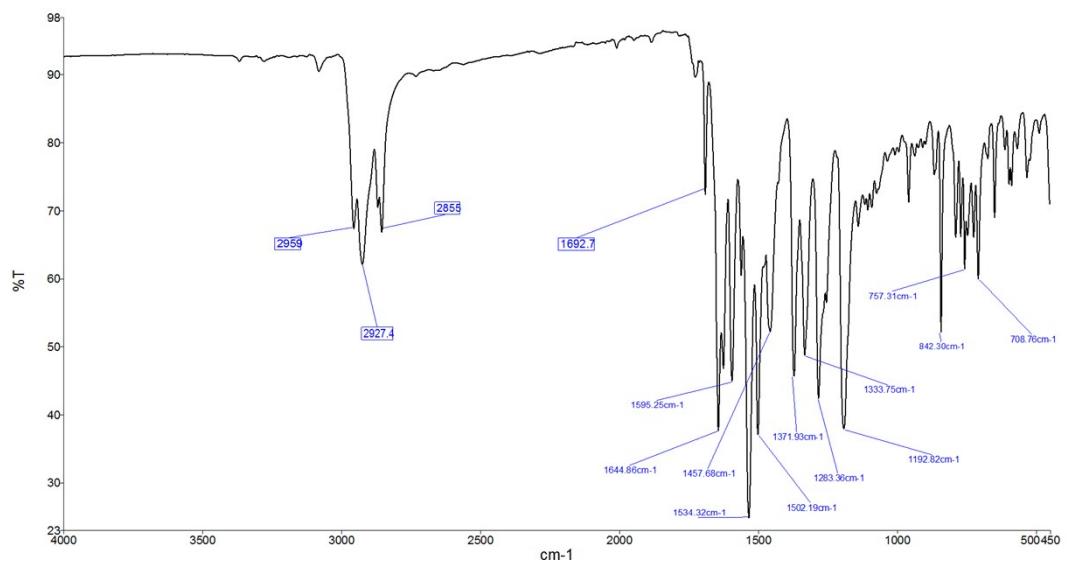
¹H NMR spectra of 7f



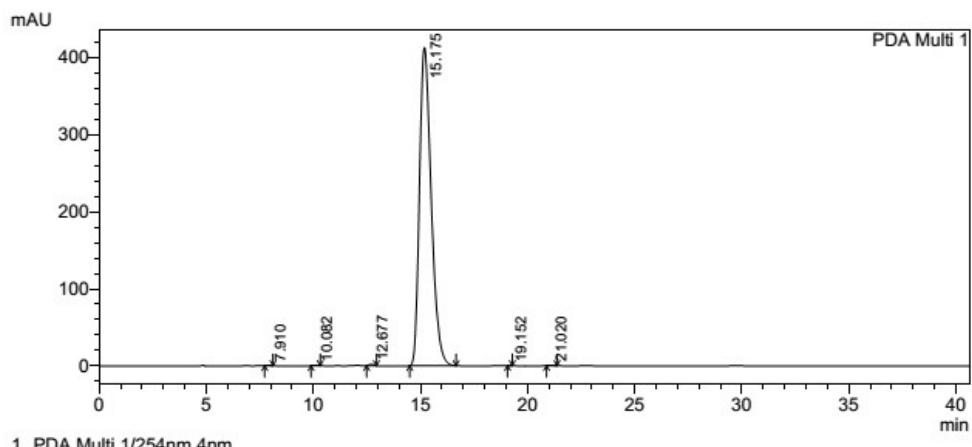
¹³C NMR spectra of 7f



HRMS spectrum of **7f**



IR spectra of **7f**

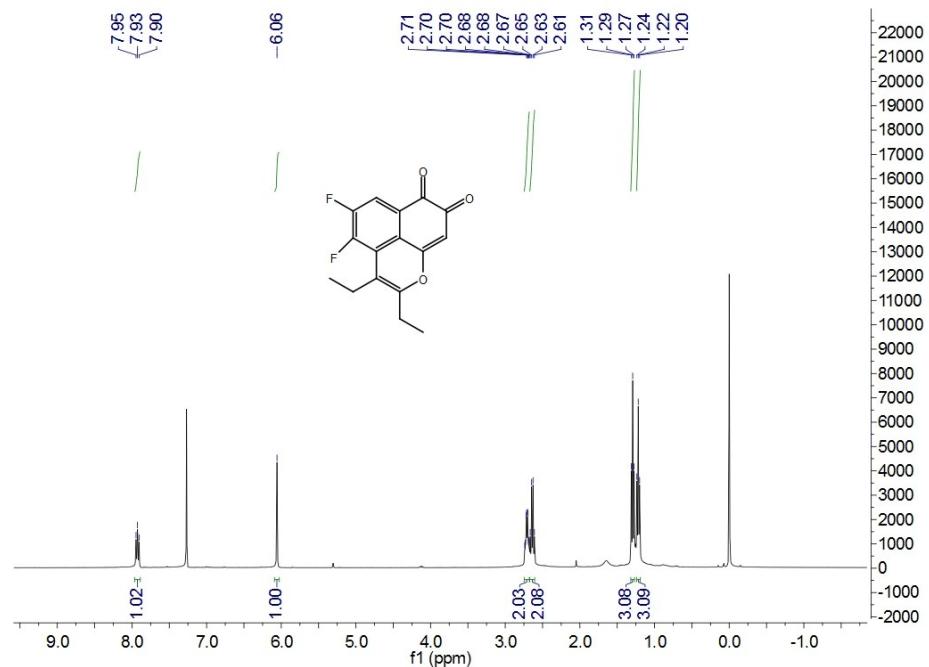


PeakTable

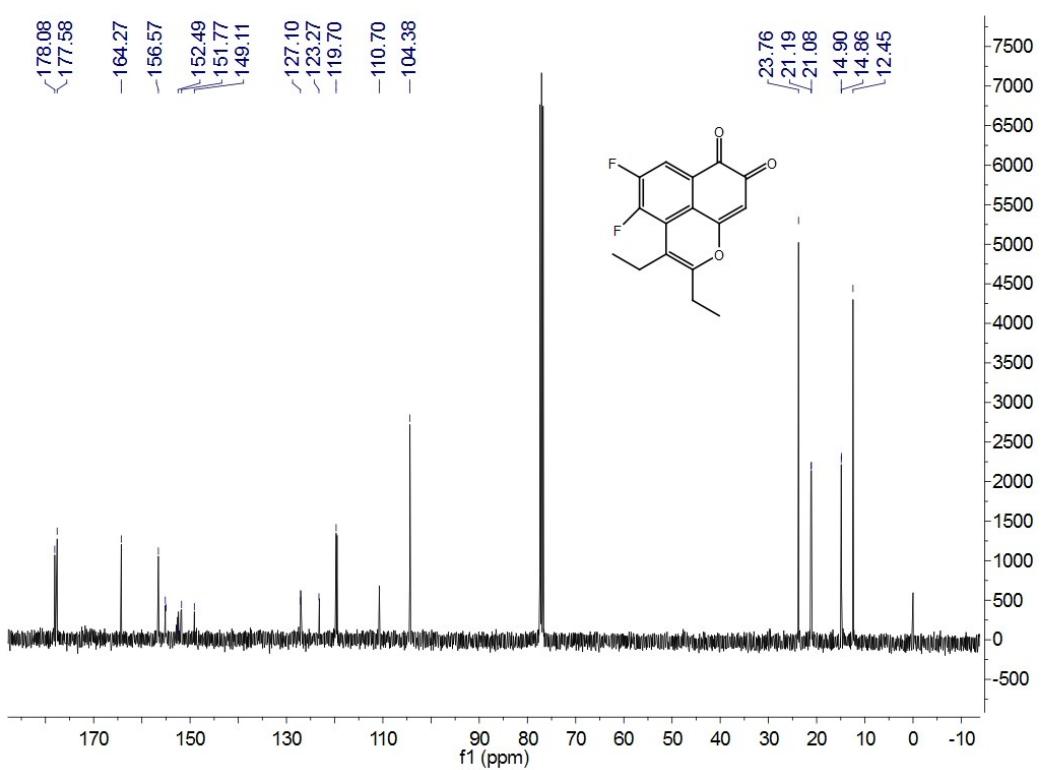
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.910	6217	517	0.040	0.124
2	10.082	10623	699	0.068	0.168
3	12.677	25825	1694	0.165	0.407
4	15.175	15621447	413022	99.685	99.195
5	19.152	785	116	0.005	0.028
6	21.020	5910	325	0.038	0.078
Total		15670806	416373	100.000	100.000

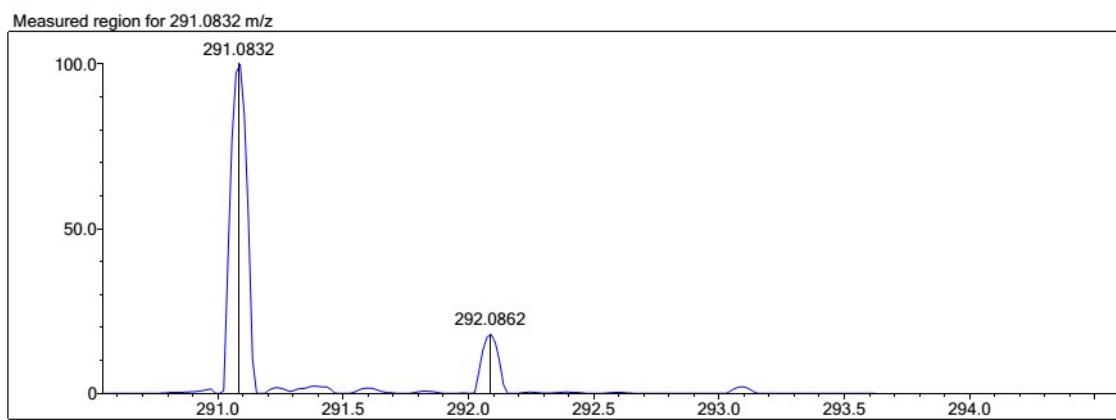
HPLC profile of **7f**



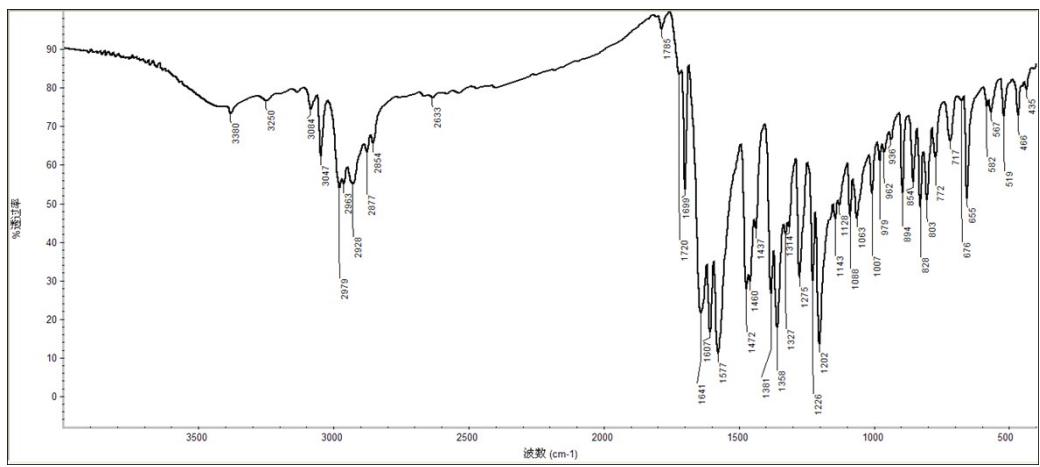
¹H NMR spectra of **13**



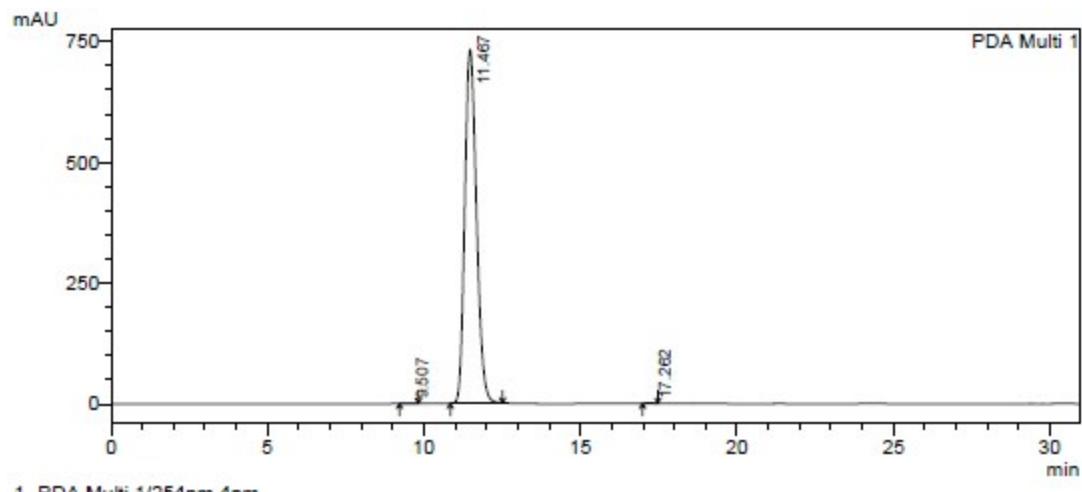
^{13}C NMR spectra of **13**



HRMS spectrum of **13**

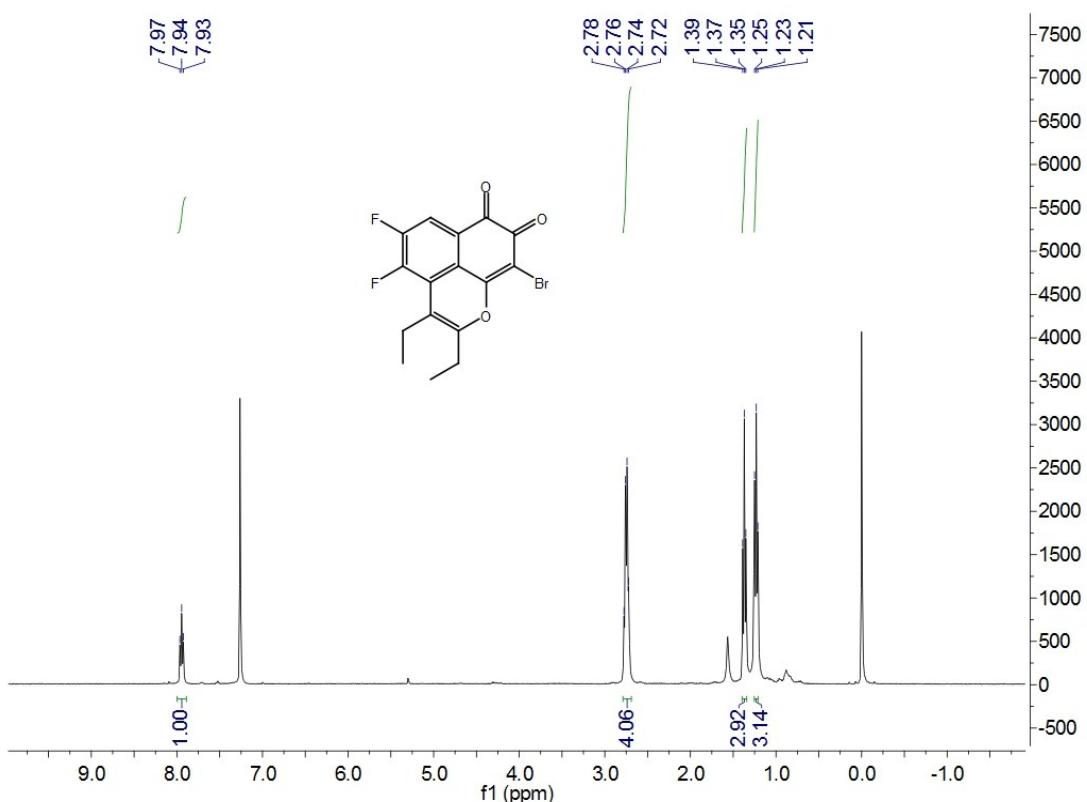


IR spectra of **13**

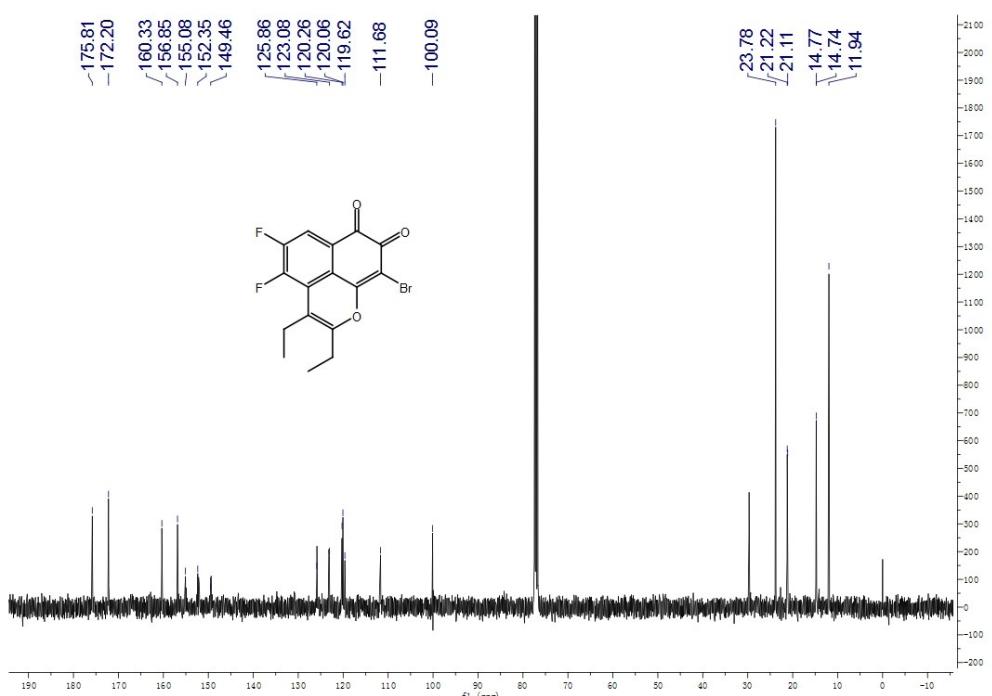


PeakTable					
PDA Ch1 254nm 4nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.507	11076	515	0.058	0.070
2	11.467	18996498	731921	99.900	99.870
3	17.262	7926	439	0.042	0.060
Total		19015500	732875	100.000	100.000

HPLC profile of **13**

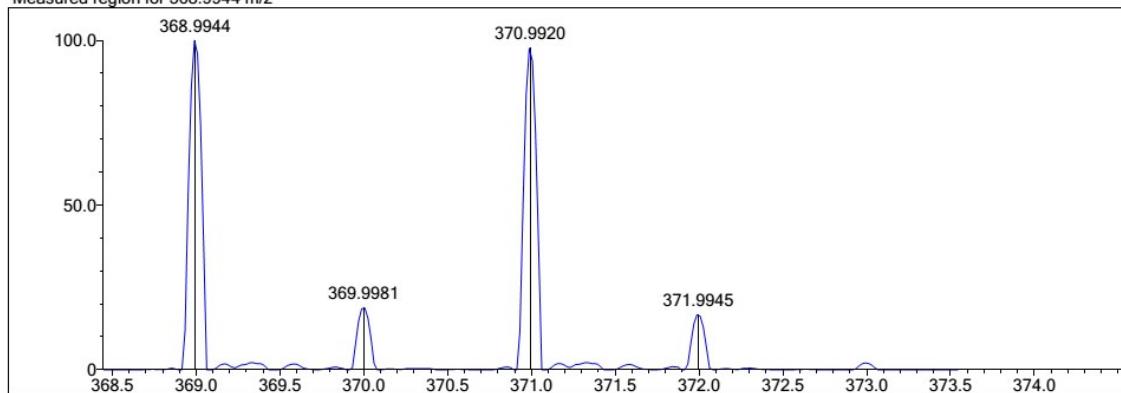


¹H NMR spectra of **14**

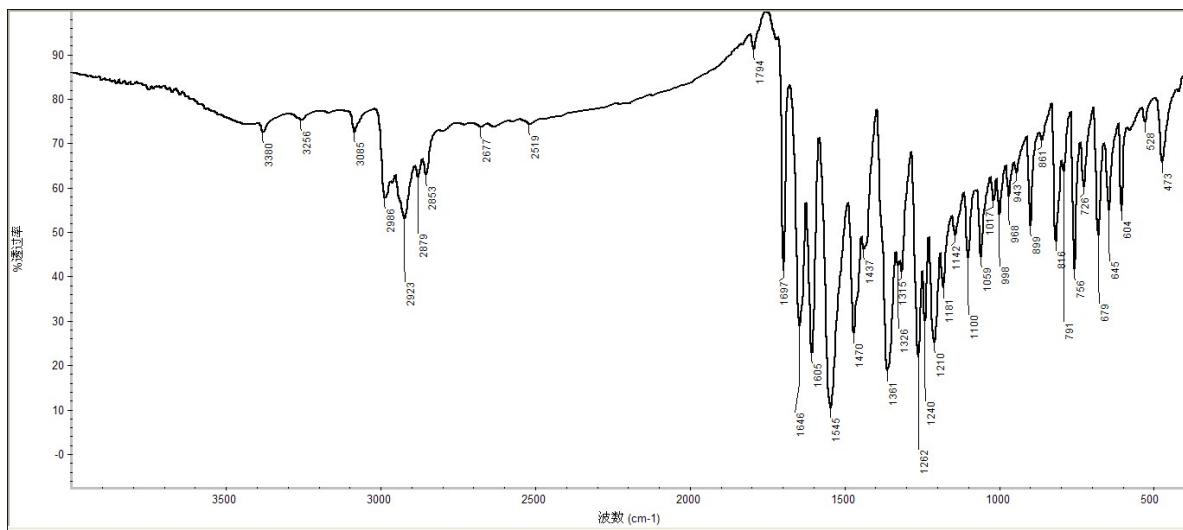


¹³C NMR spectra of **14**

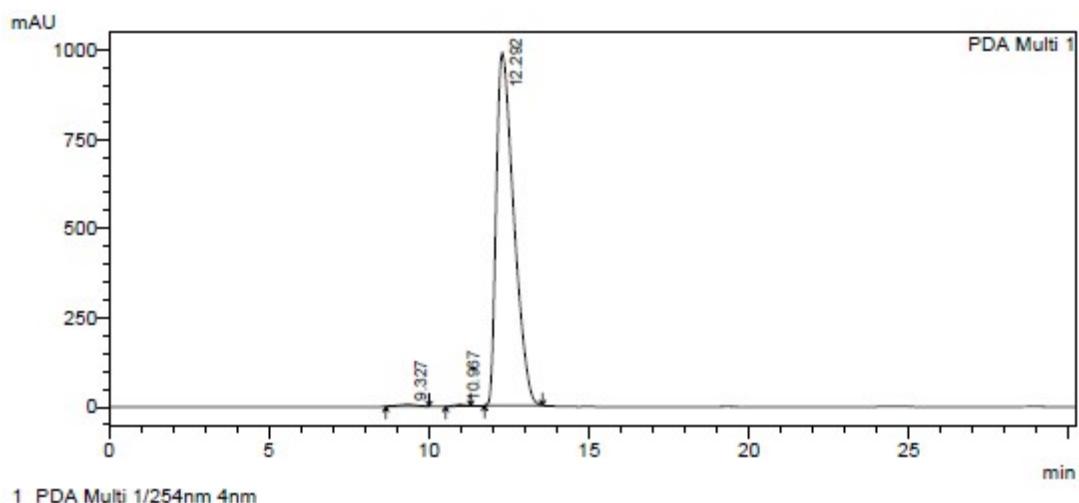
Measured region for 368.9944 m/z



HRMS spectrum of **14**



IR spectra of **14**

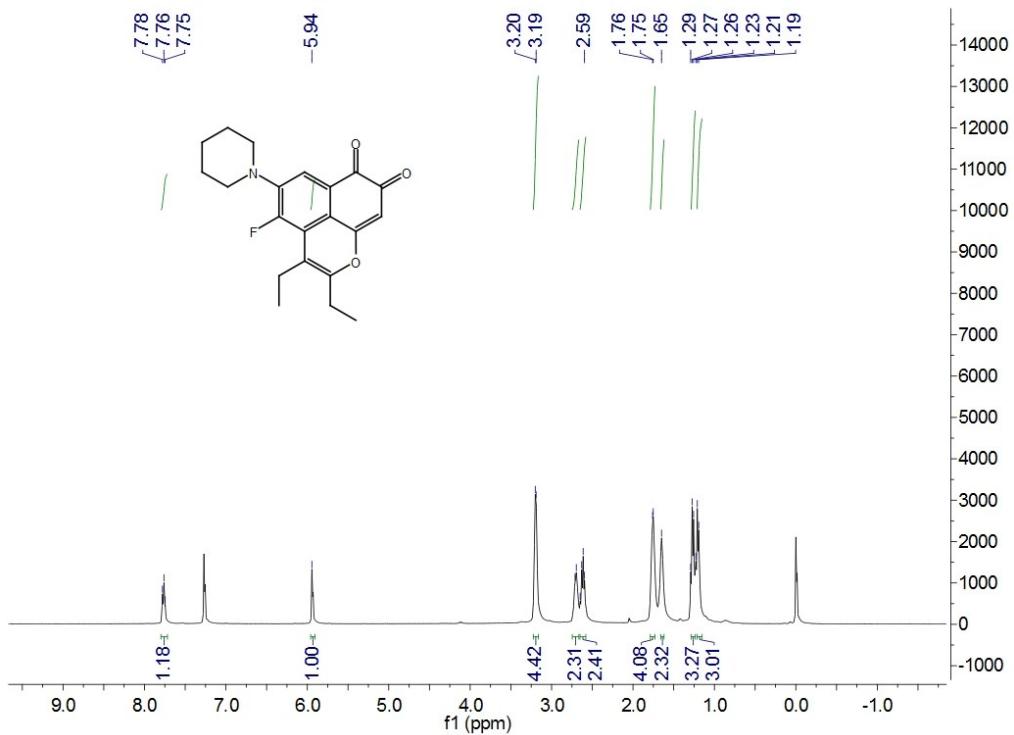


PeakTable

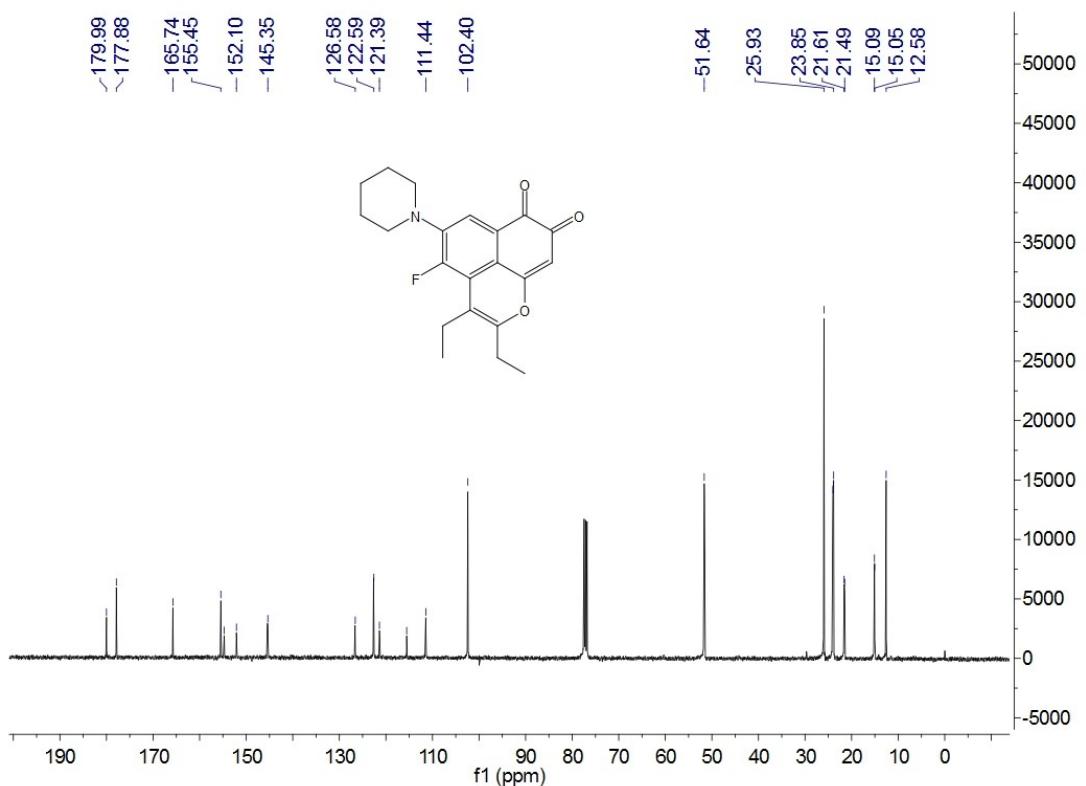
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.327	199891	5235	0.526	0.524
2	10.967	89355	3921	0.235	0.393
3	12.292	37692841	989318	99.238	99.083
Total		37982088	998474	100.000	100.000

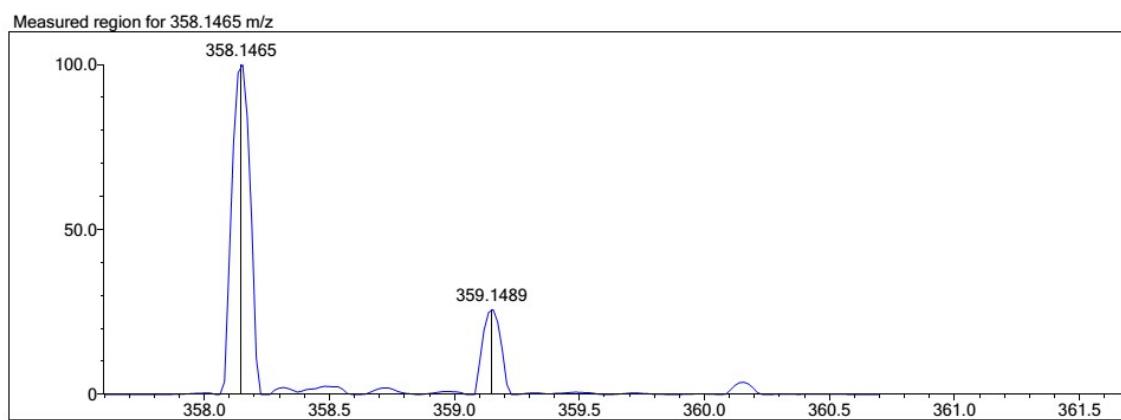
HPLC profile of **14**



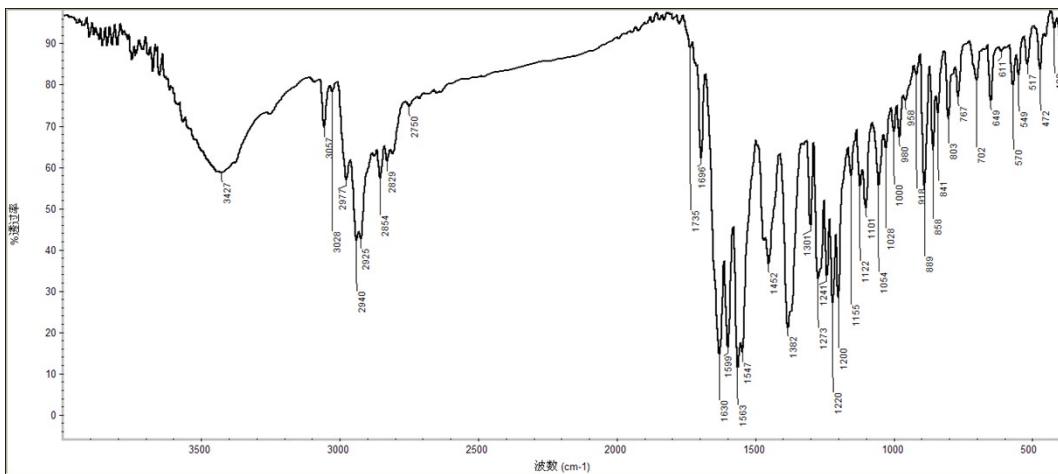
¹H NMR spectra of **16a**



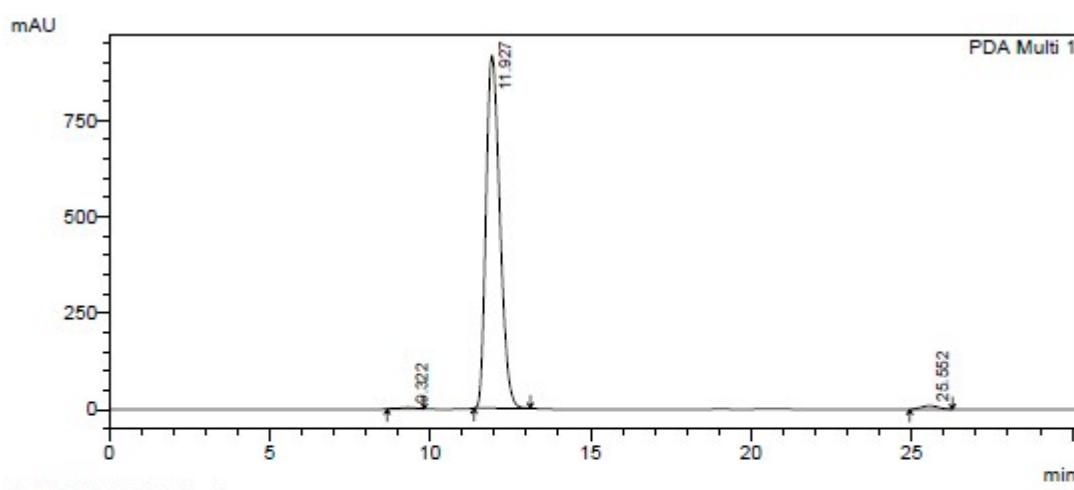
^{13}C NMR spectra of **16a**



HRMS spectrum of **16a**



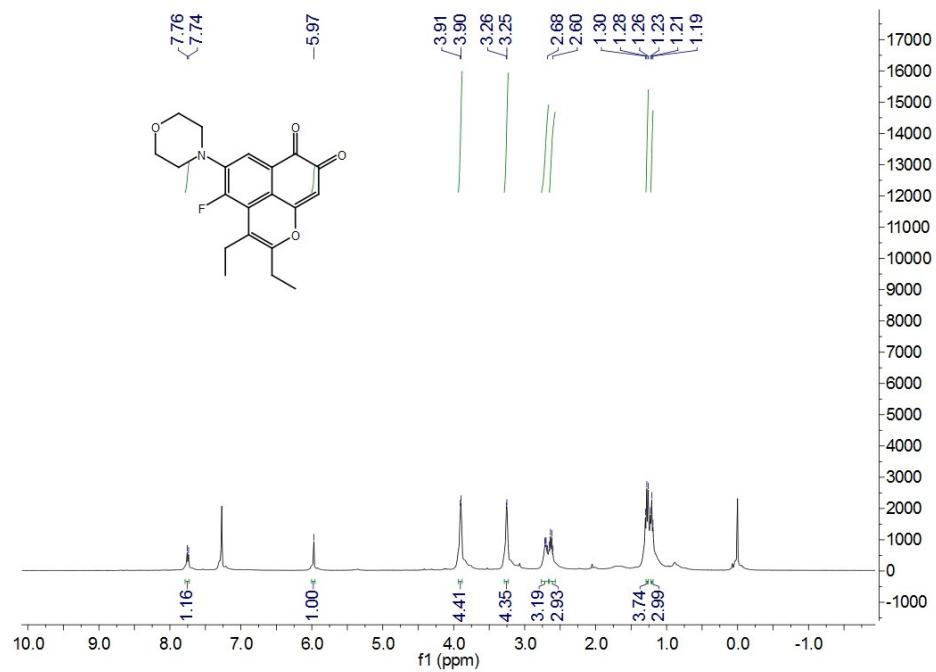
IR spectra of **16a**



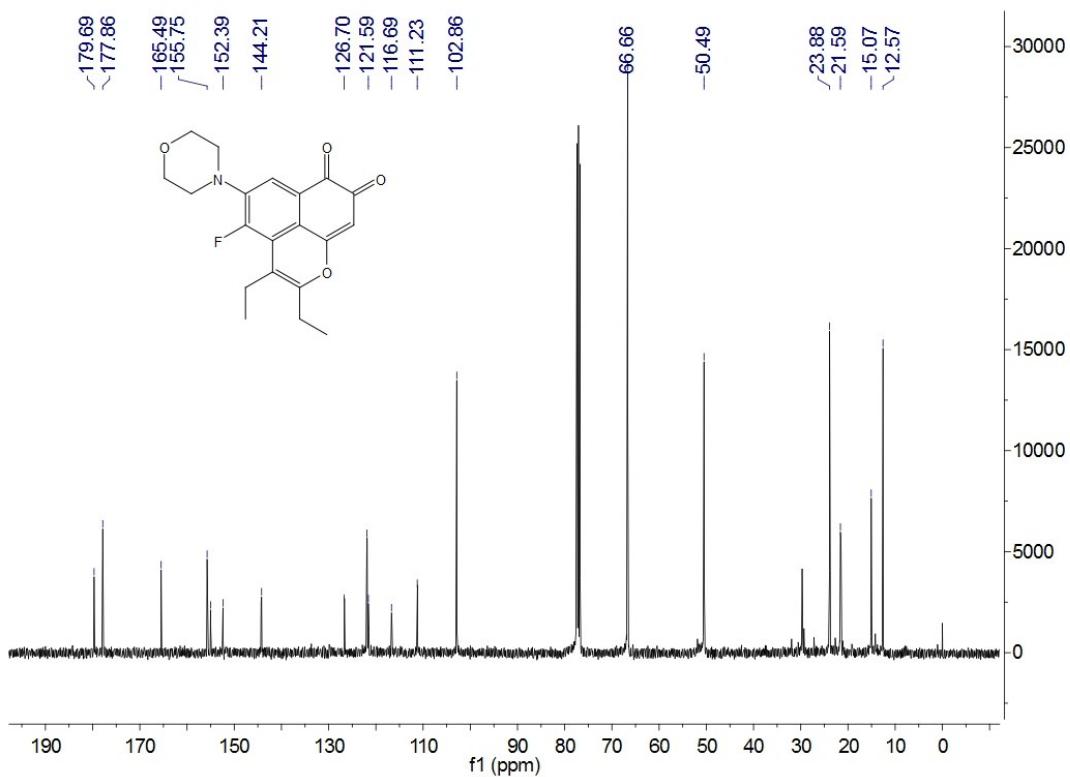
1 PDA Multi 1/254nm 4nm

PeakTable					
PDA Ch1 254nm 4nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.322	107459	2977	0.385	0.321
2	11.927	27417733	914395	98.340	98.631
3	25.552	355363	9716	1.275	1.048
Total		27880555	927088	100.000	100.000

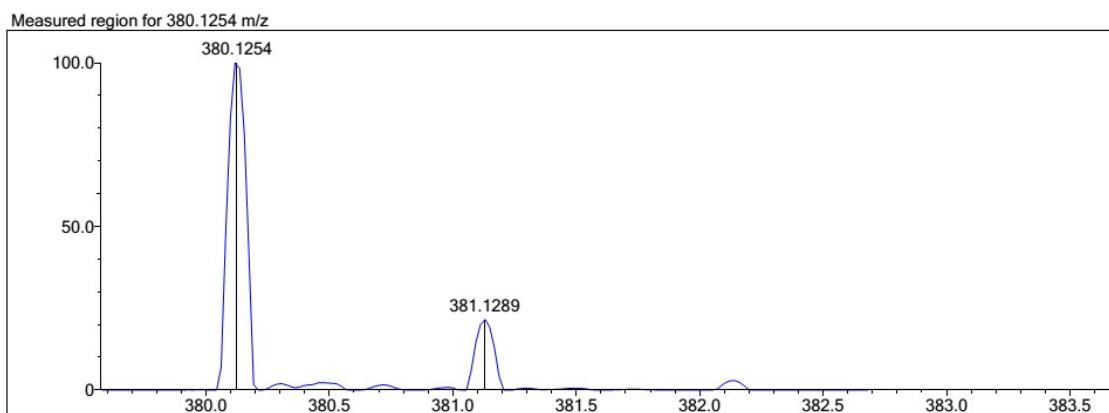
HPLC profile of **16a**



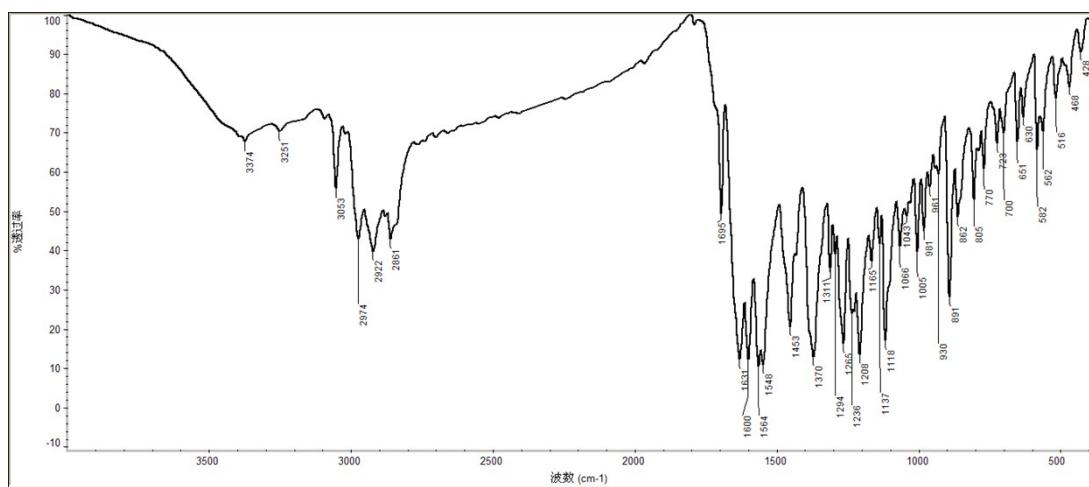
¹H NMR spectra of 16b



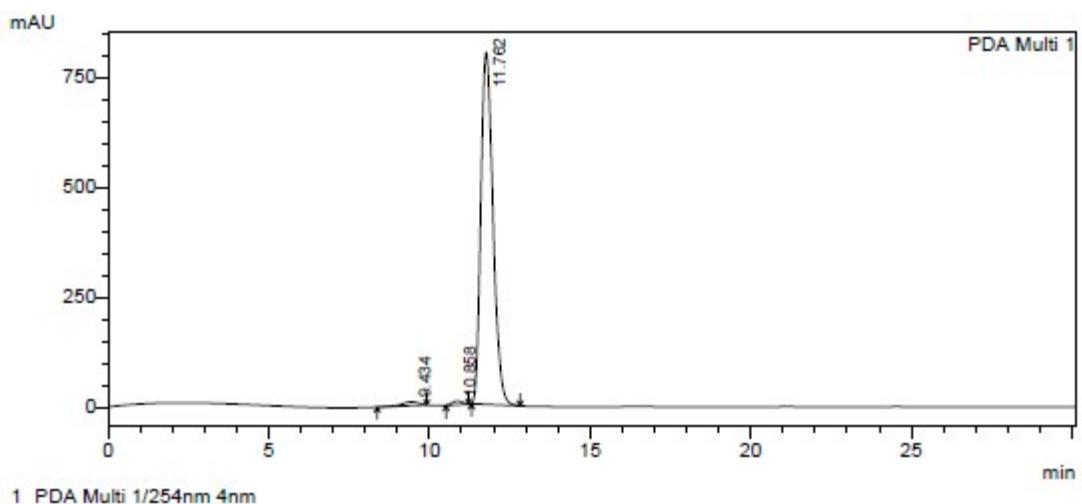
¹³C NMR spectra of **16b**



HRMS spectrum of **16b**



IR spectra of **16b**

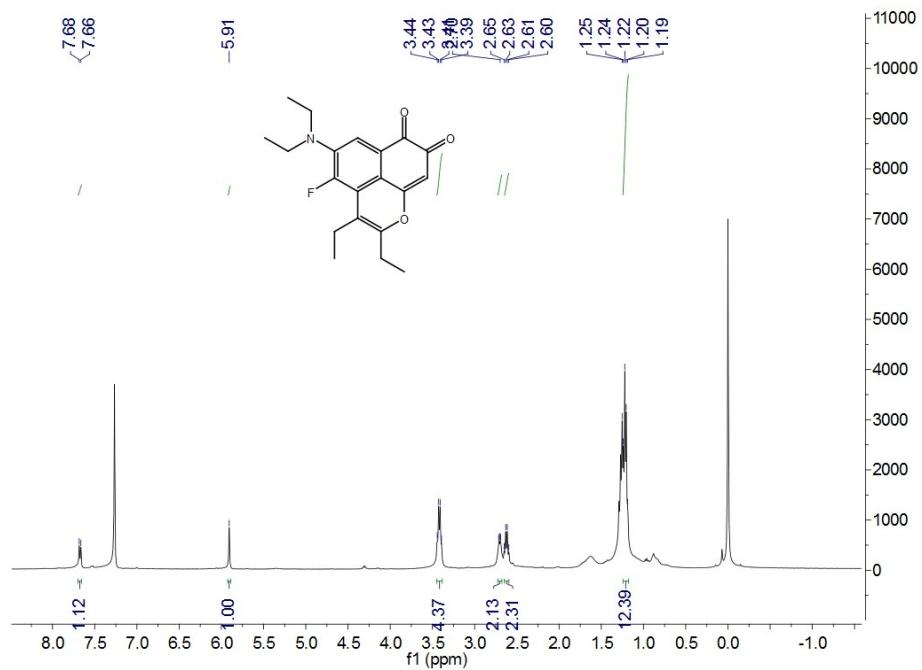


PeakTable

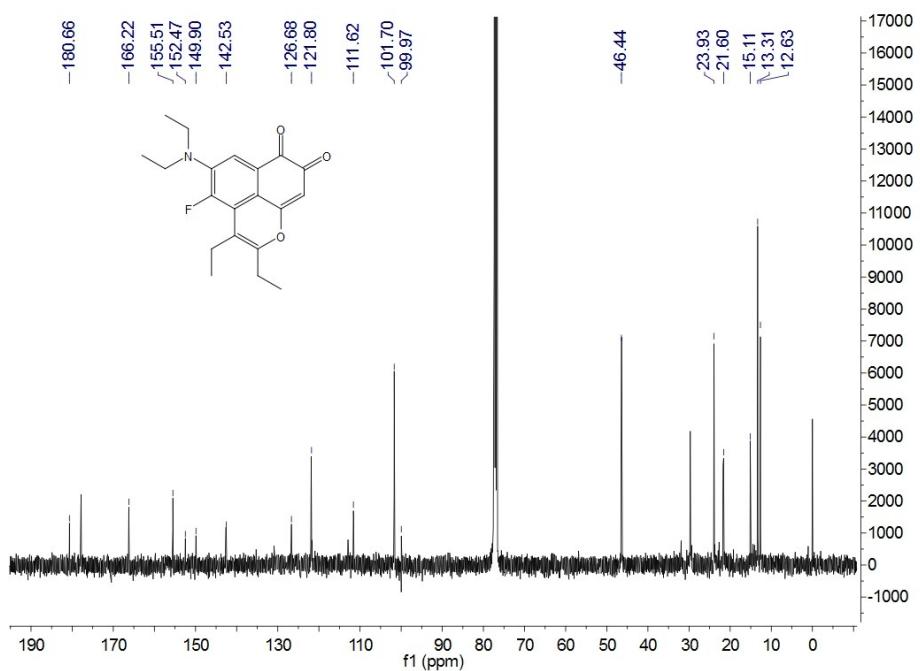
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.434	304640	8599	1.417	1.052
2	10.858	191746	8808	0.892	1.078
3	11.762	21009086	799802	97.692	97.870
Total		21505472	817208	100.000	100.000

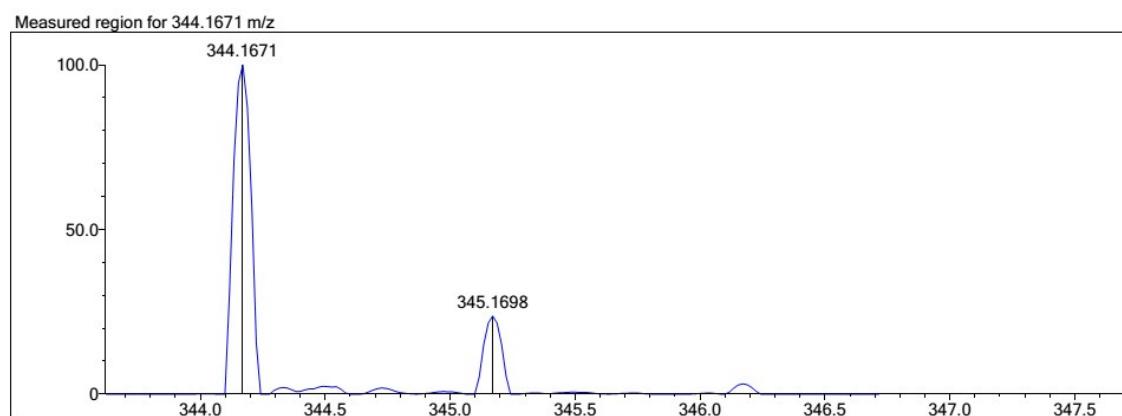
HPLC profile of **16b**



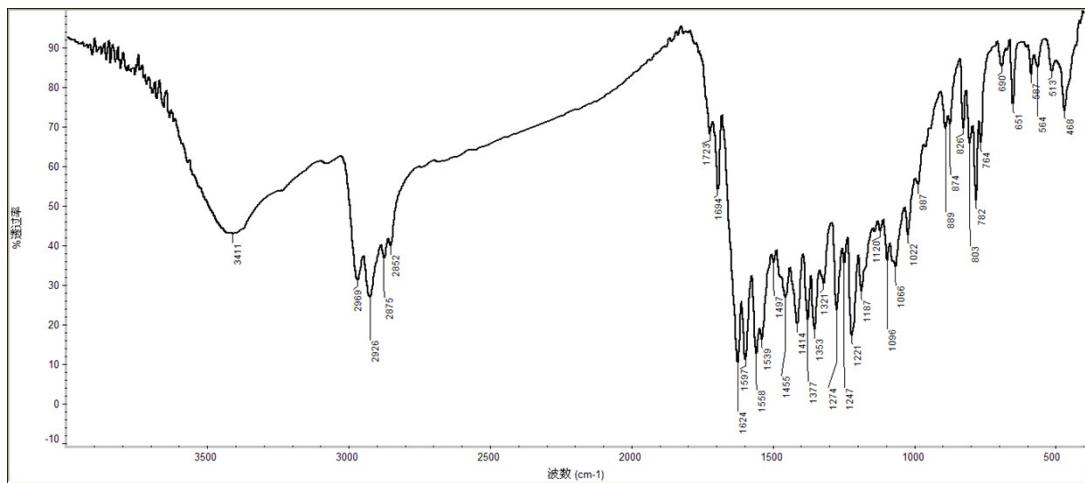
¹H NMR spectra of **16c**



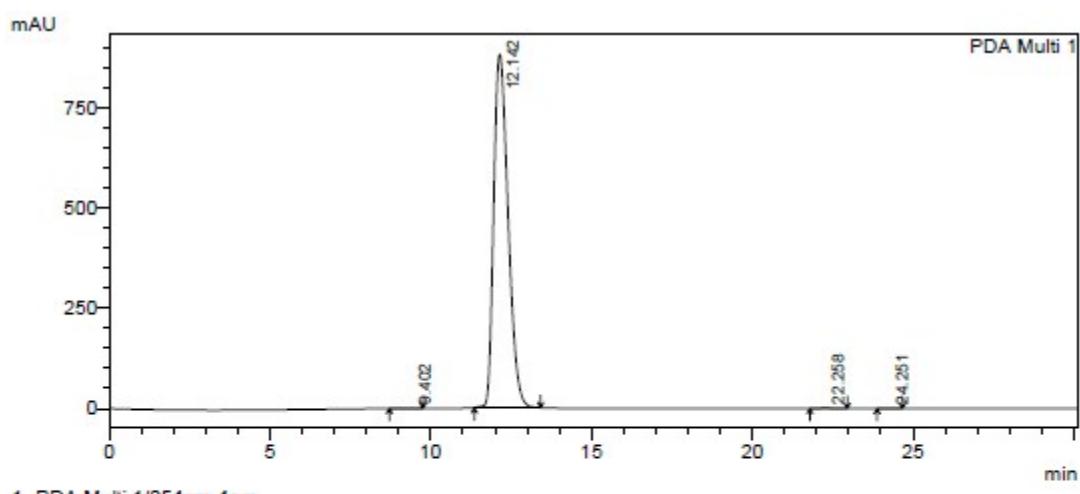
^{13}C NMR spectra of **16c**



HRMS spectrum of **16c**

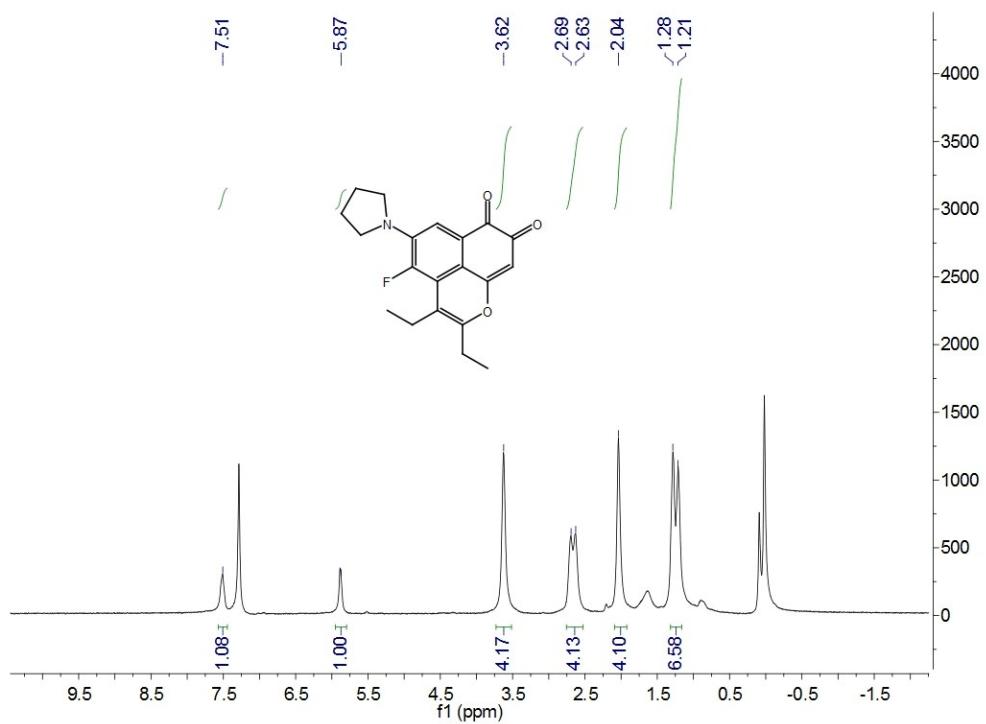


IR spectra of **16c**

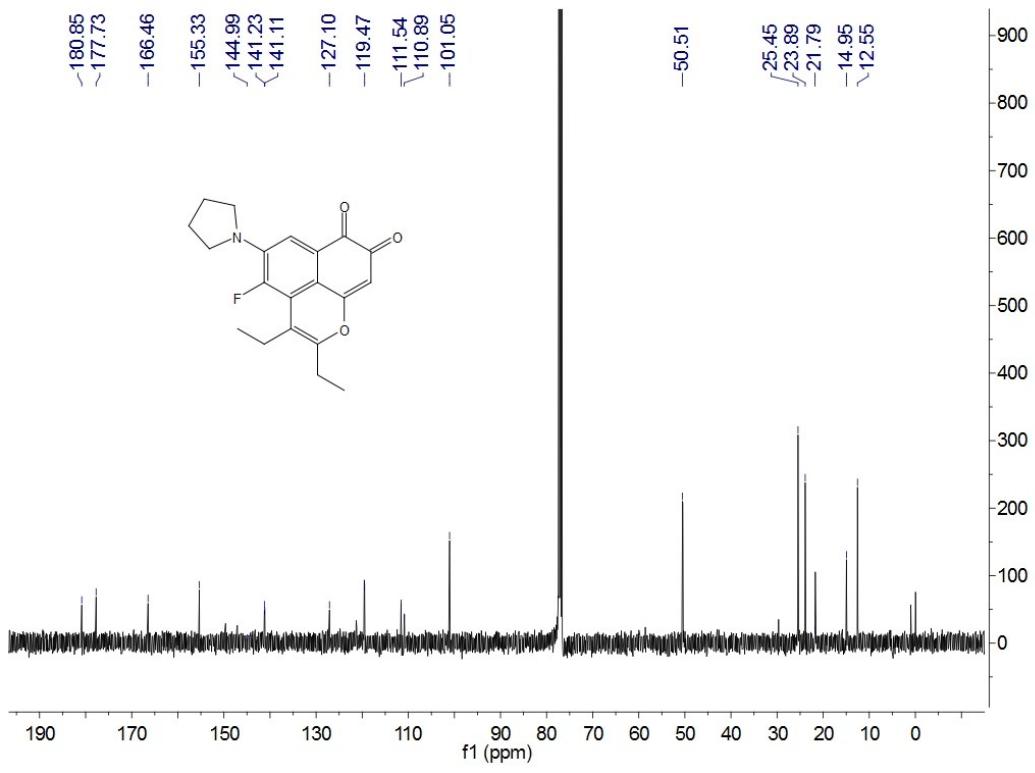


PeakTable					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.402	8945	298	0.033	0.034
2	12.142	27365626	881291	99.837	99.827
3	22.258	26358	868	0.096	0.098
4	24.251	9486	366	0.035	0.041
Total		27410415	882823	100.000	100.000

HPLC profile of **16c**

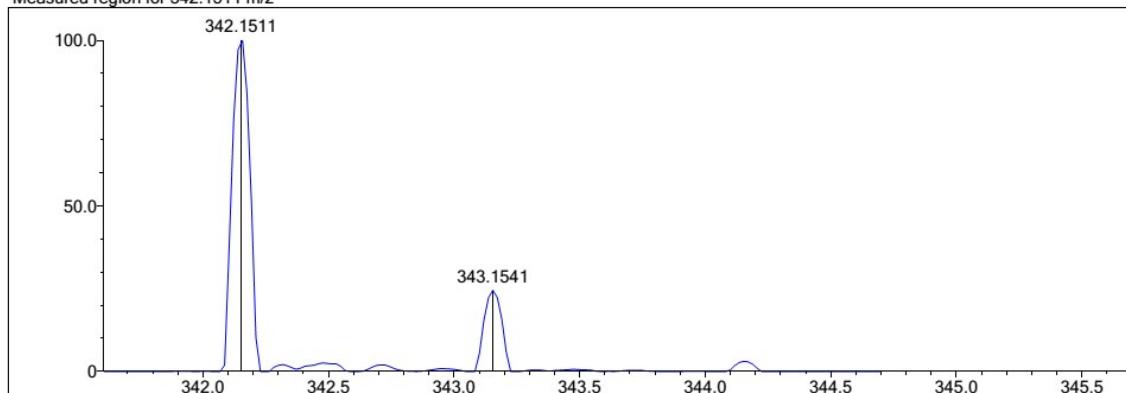


¹H NMR spectra of **16d**

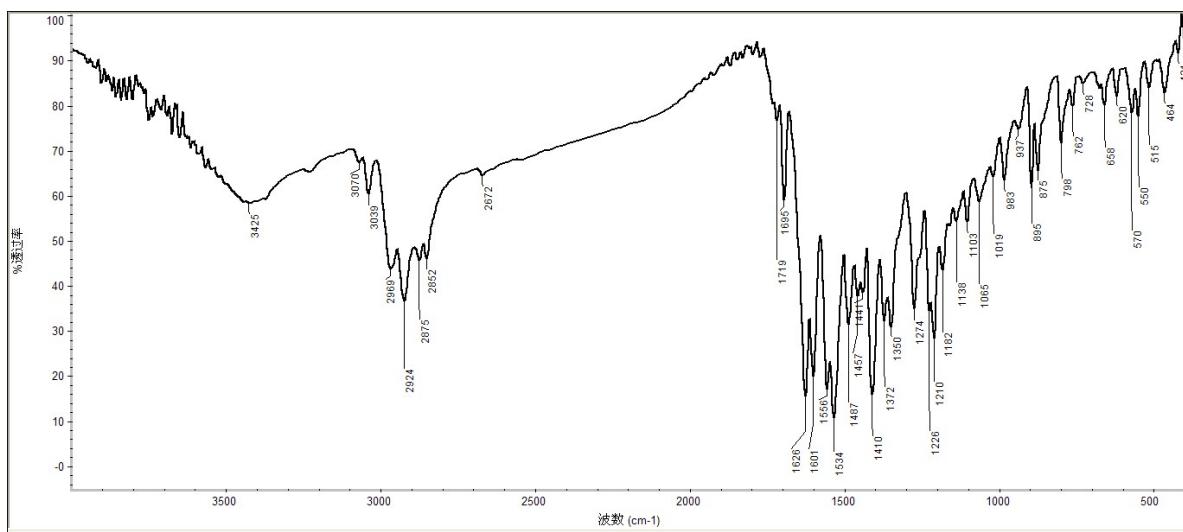


¹³C NMR spectra of **16d**

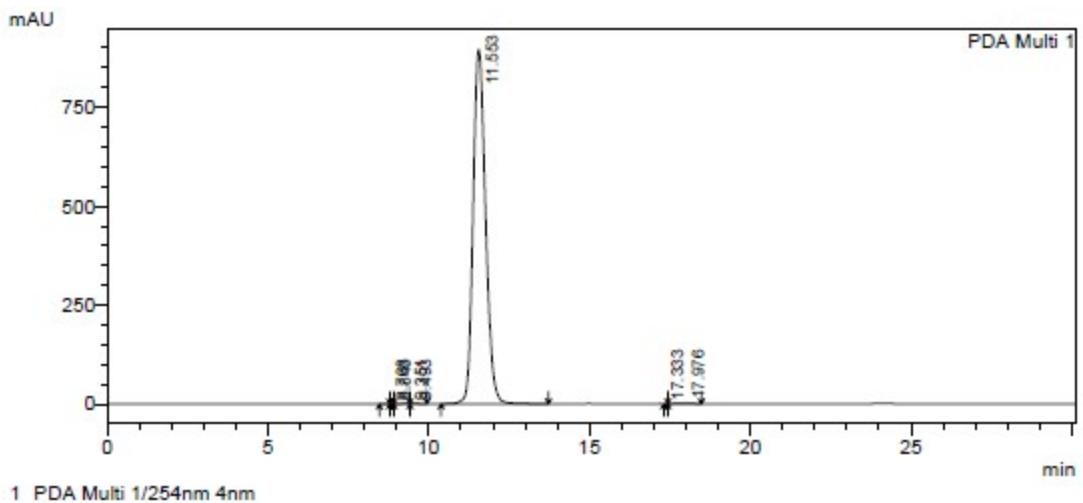
Measured region for 342.1511 m/z



HRMS spectrum of **16d**



IR spectra of **16d**

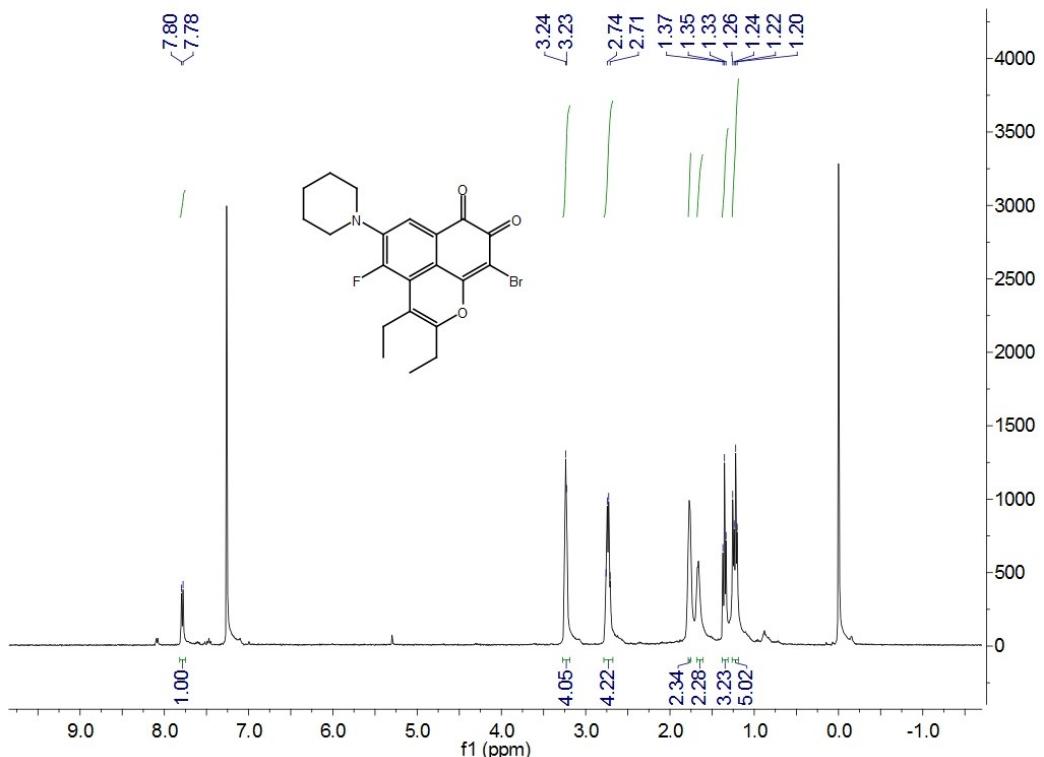


PDA Chl 254nm 4nm

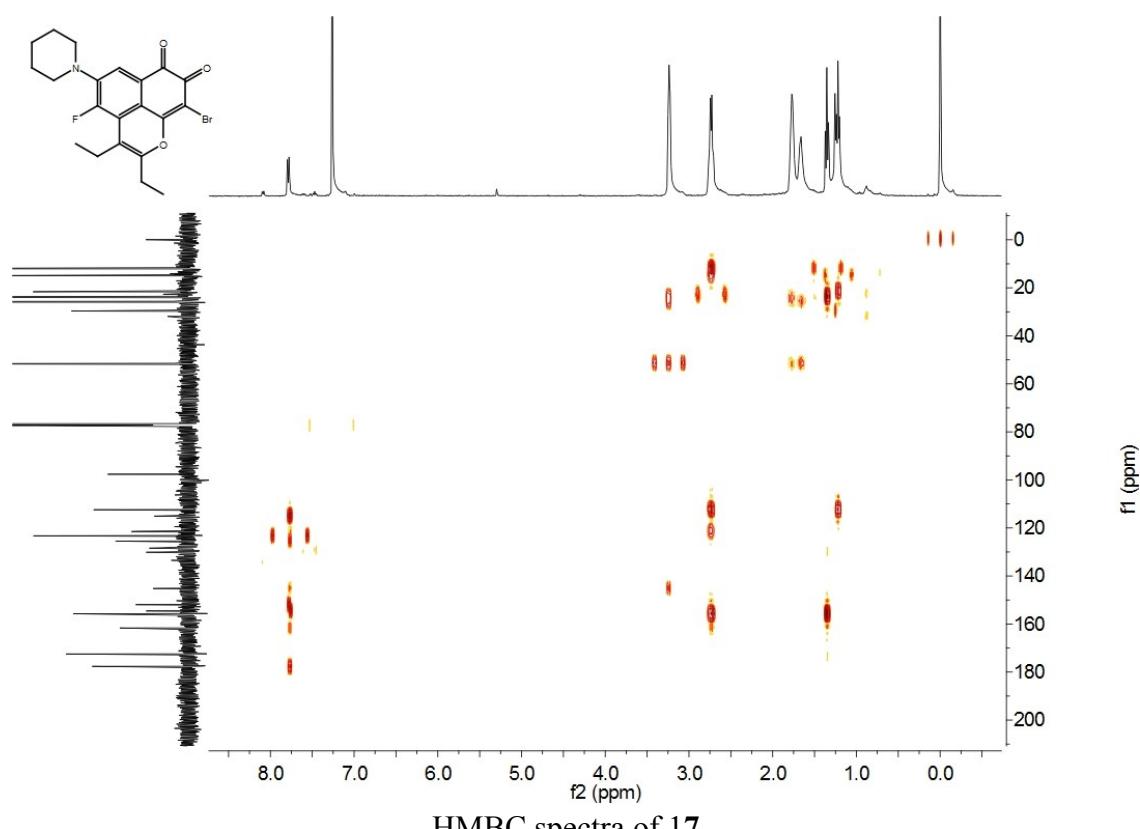
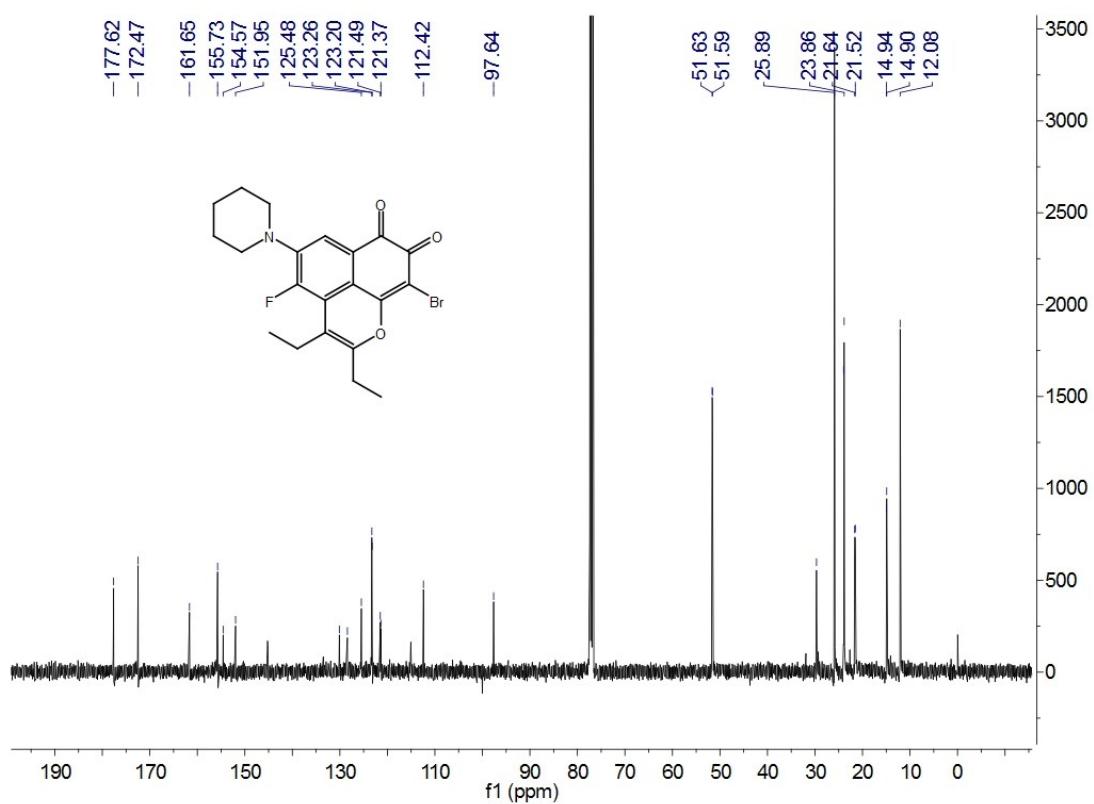
PeakTable

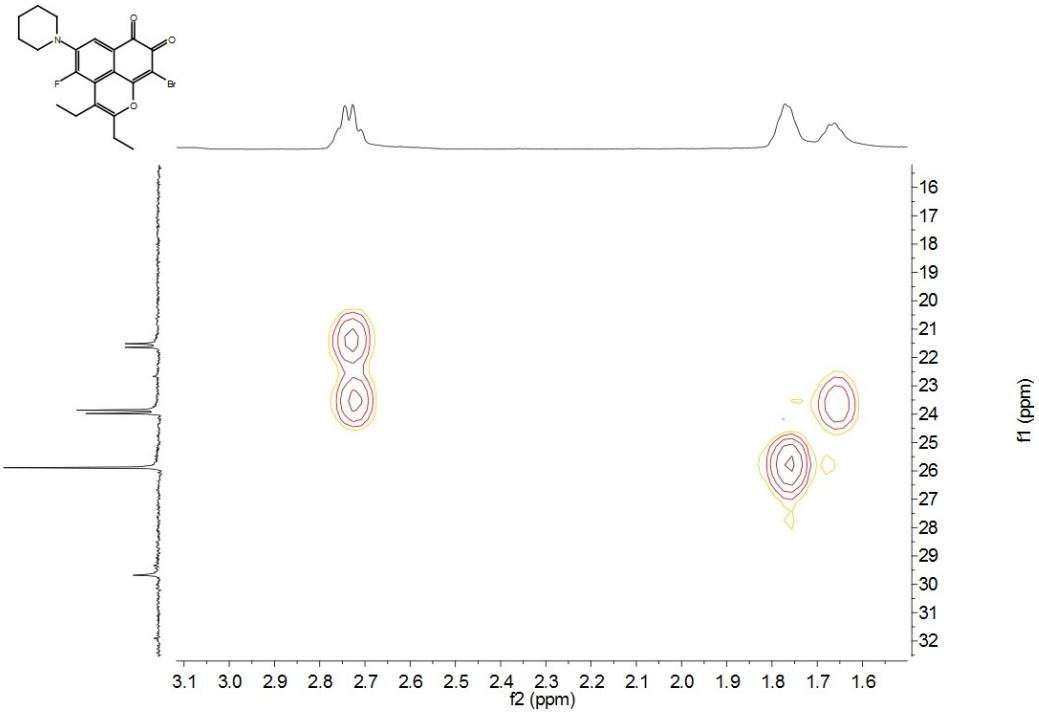
Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.768	3597	298	0.015	0.033
2	8.843	2344	322	0.010	0.036
3	9.351	16064	695	0.066	0.077
4	9.493	10608	615	0.044	0.068
5	11.553	24094937	895814	99.733	99.656
6	17.333	156	48	0.001	0.005
7	17.976	31832	1112	0.132	0.124
Total		24159536	898904	100.000	100.000

HPLC profile of 16d

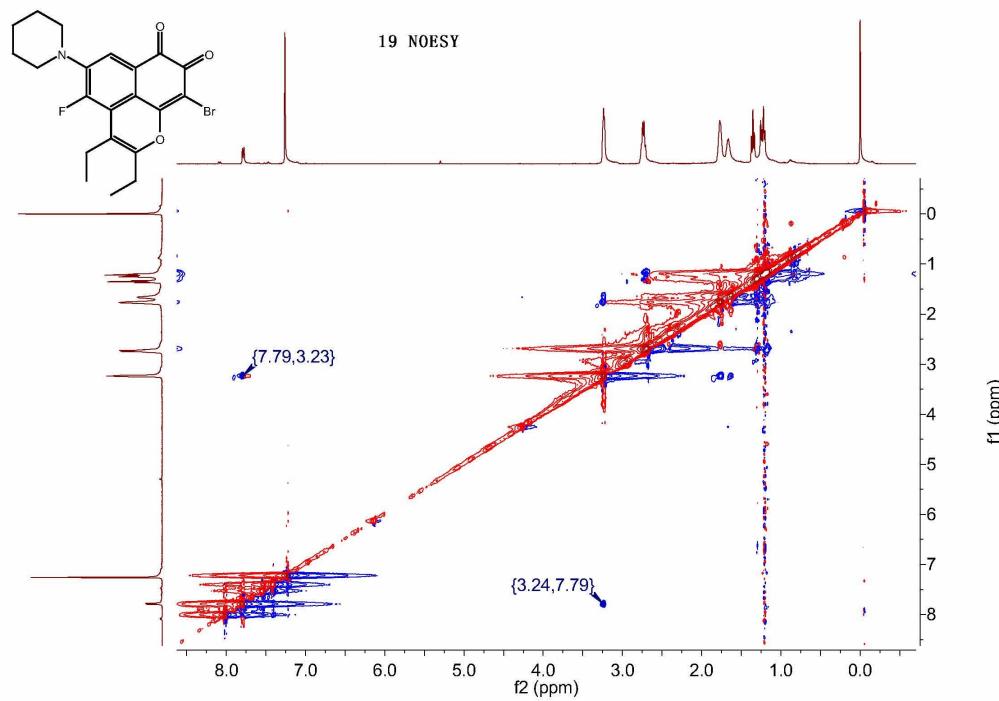


¹H NMR spectra of 17

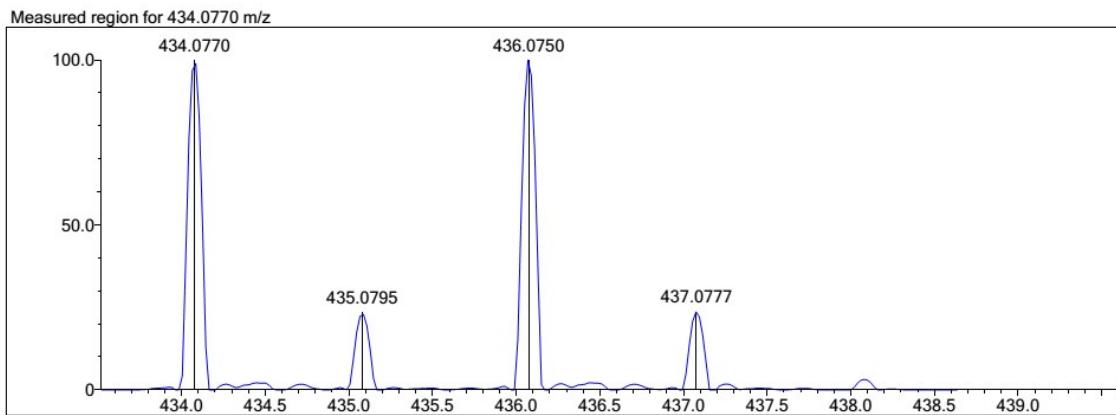




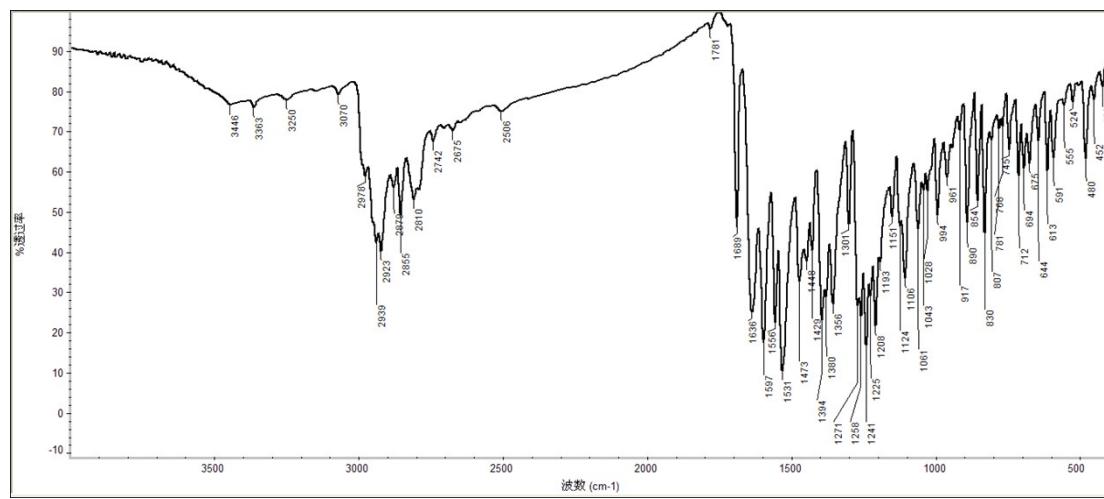
HSQC spectra of **17**



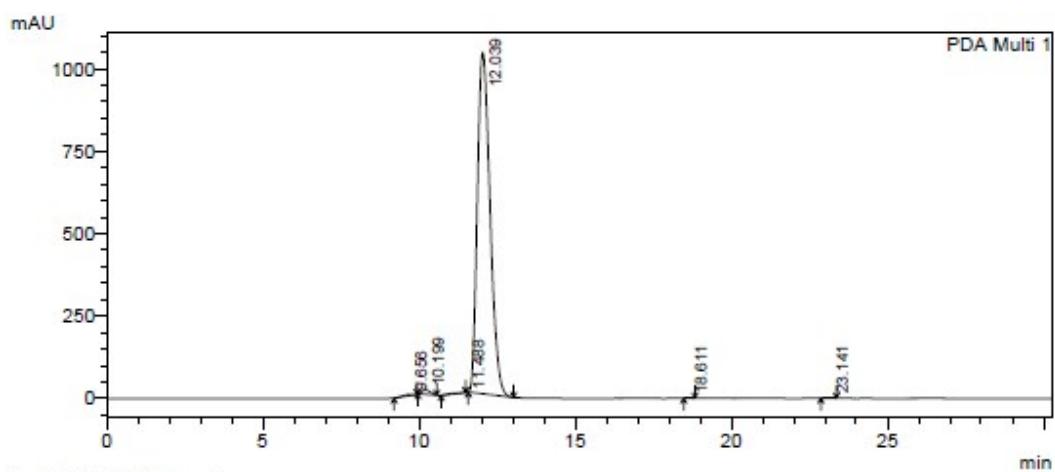
NOESY spectra of **17**



HRMS spectrum of **17**



IR spectra of **17**



1 PDA Multi 1/254nm 4nm

PeakTable					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.656	66135	4116	0.224	0.391
2	10.199	260648	13108	0.881	1.245
3	11.488	47886	26	0.162	0.002
4	12.039	29180409	1034585	98.678	98.264
5	18.611	5923	428	0.020	0.041
6	23.141	10421	604	0.035	0.057
Total		29571421	1052868	100.000	100.000

HPLC profile of 17