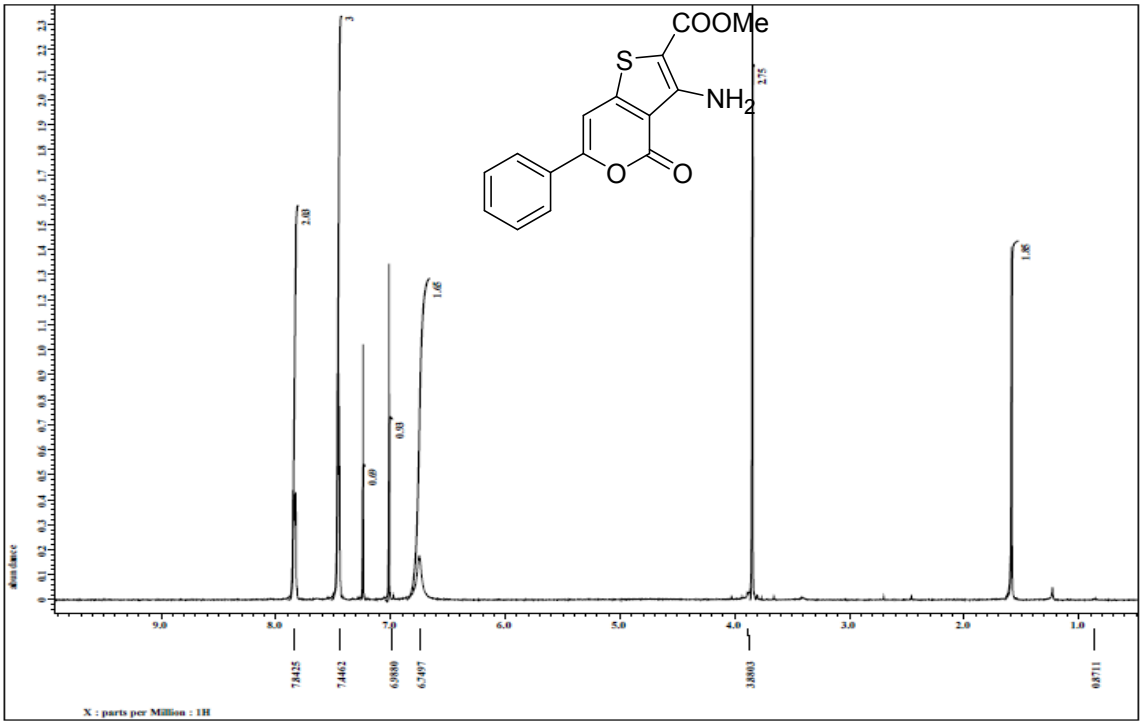
Electronic Supplementary Material (ESI) for RSC Advances.

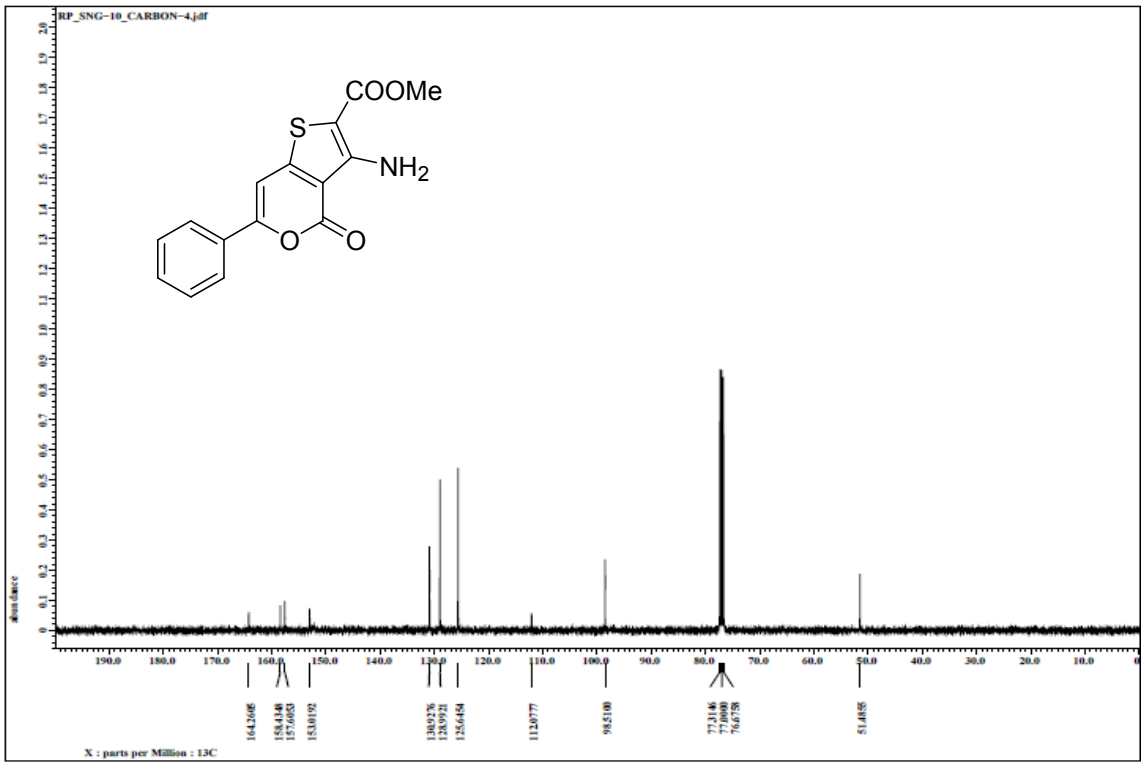
Substituent dependent tunable fluorescence in thieno[3,2-*c*]pyrans

Satya Narayan Sahu,[a] Maneesh Kumar Gupta,[a] Thaksen Jadhav,[b] Pratik Yadav,[a] Surjeet Singh,[a] Rajneesh Misra[b,*] and Ramendra Pratap[a,*]

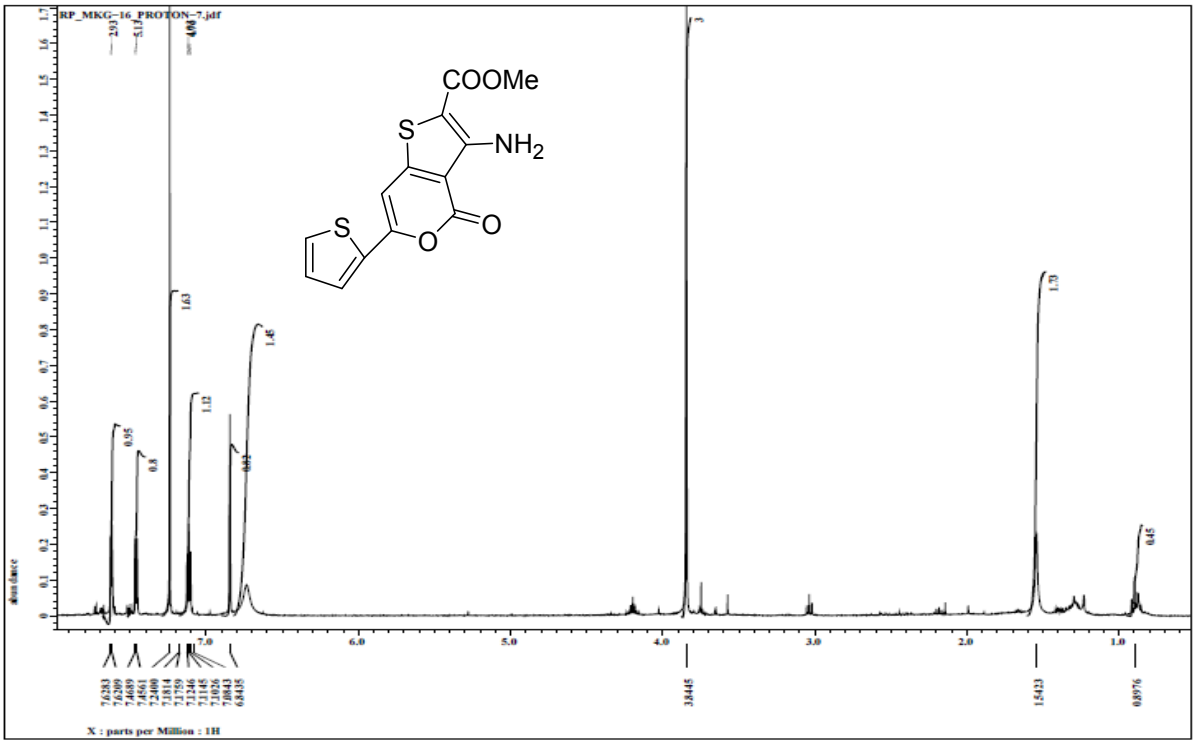
Supporting information

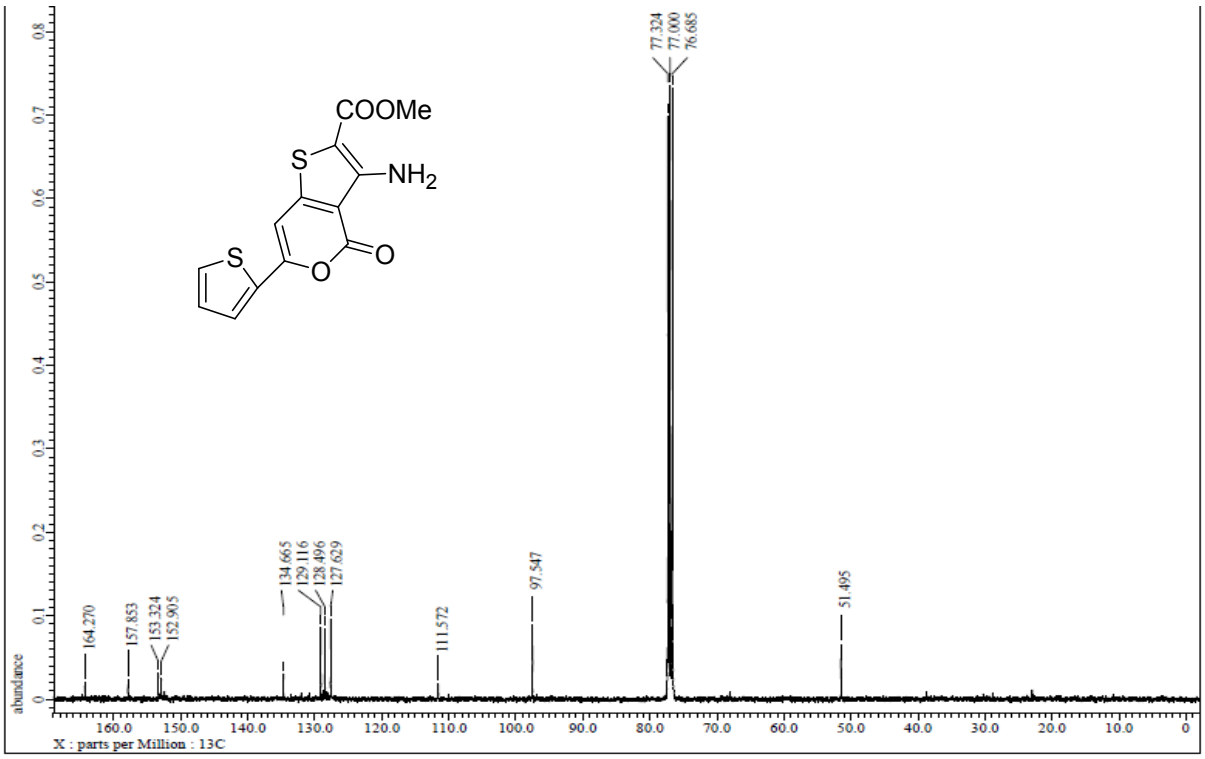
Contents



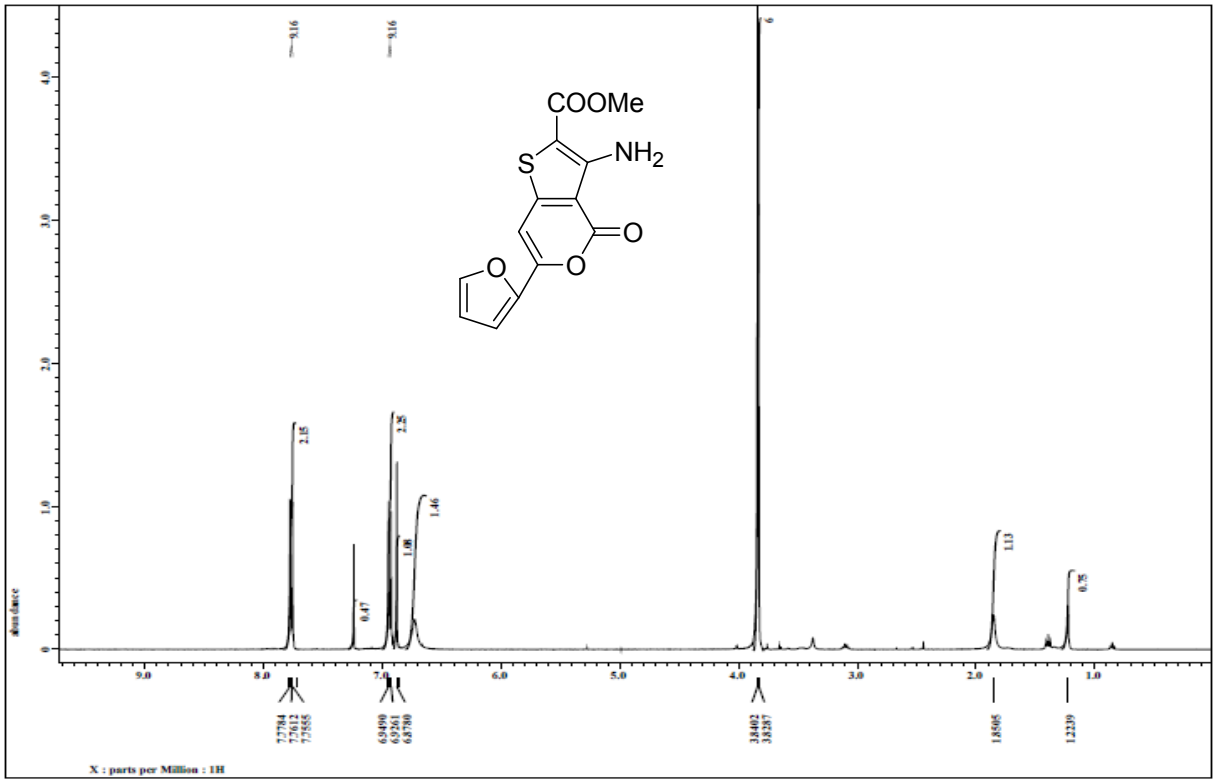


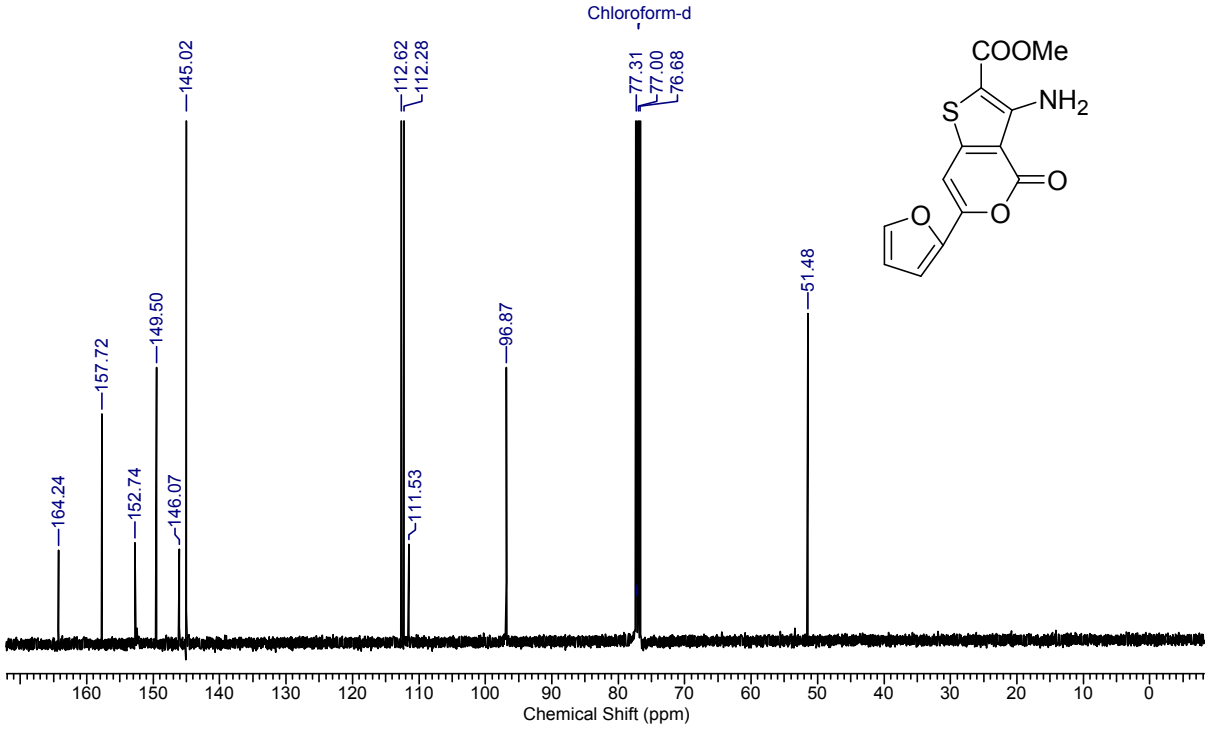
Spectra of 3-amino-4-oxo-6-phenyl-4*H*-thieno[3,2-*c*]pyran-2-carboxylic acid methyl ester (3a)



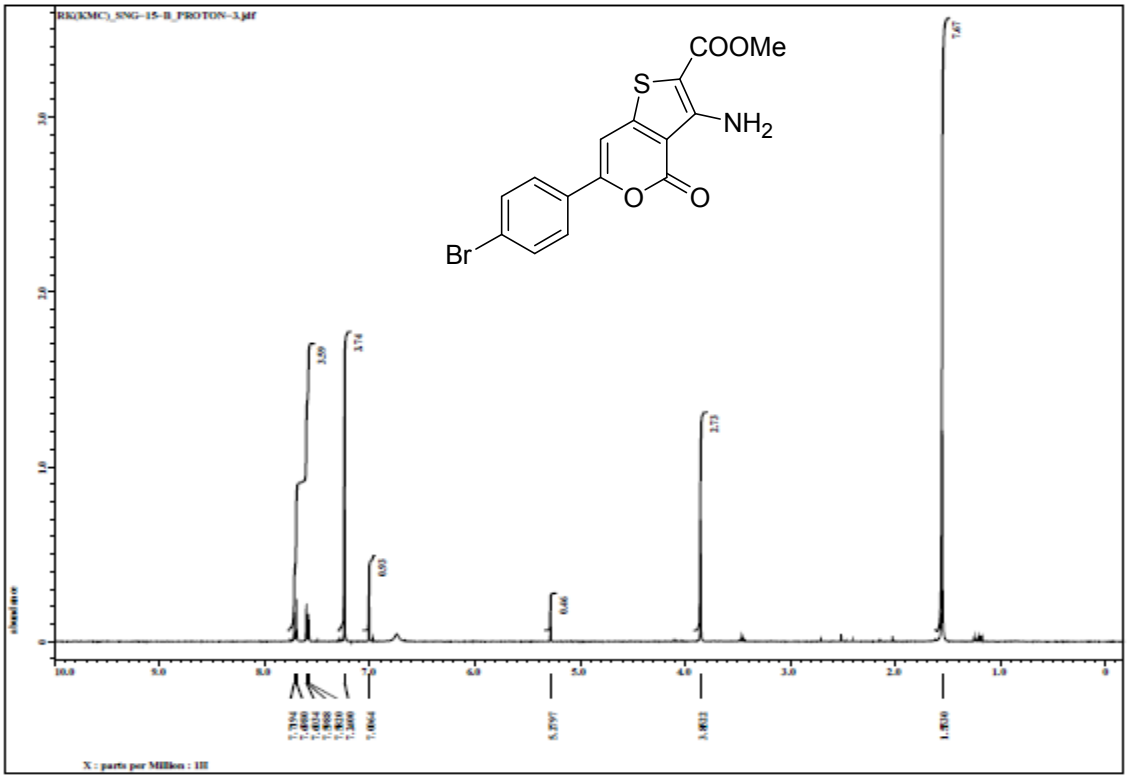


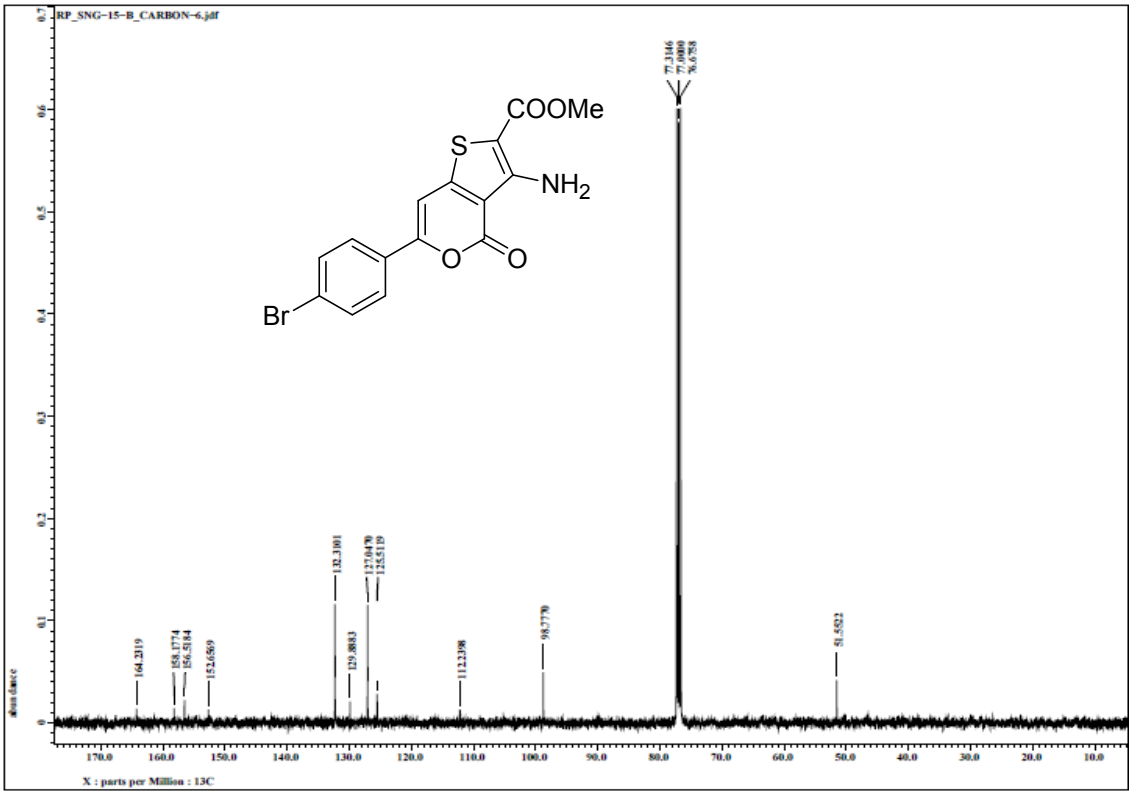
Spectra of 3-amino-4-oxo-6-thiophen-2-yl-4*H*-thieno[3,2-*c*]pyran-2-carboxylic acid methyl ester (3b)



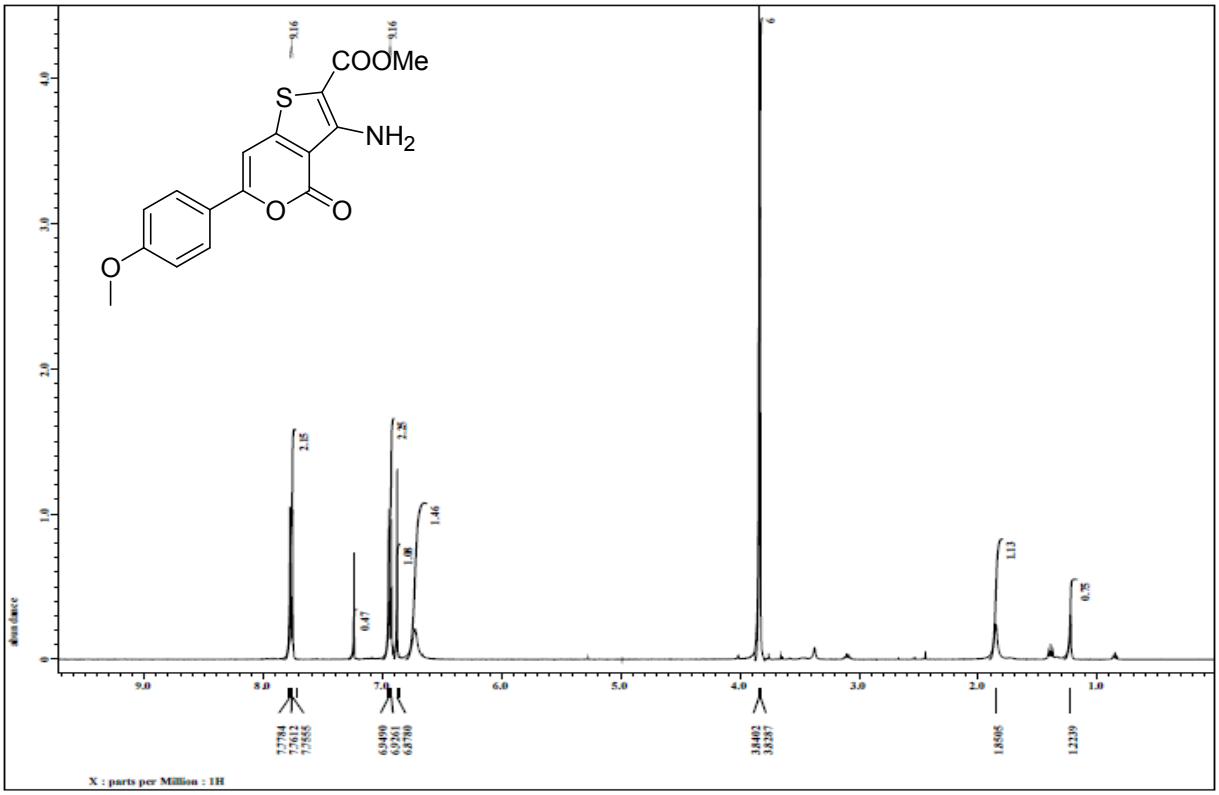


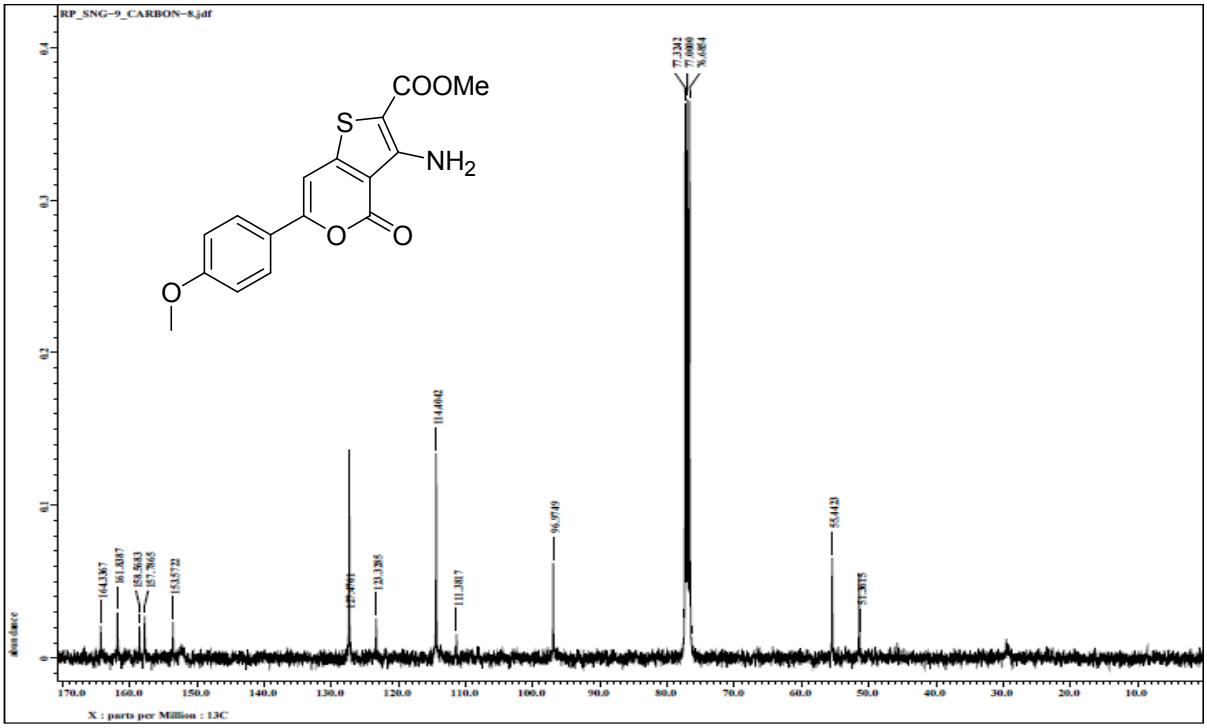
Spectra of 3-amino-4-oxo-6-furan-2-yl-4*H*-thieno[3,2-*c*]pyran-2-carboxylic acid methyl ester (3c)



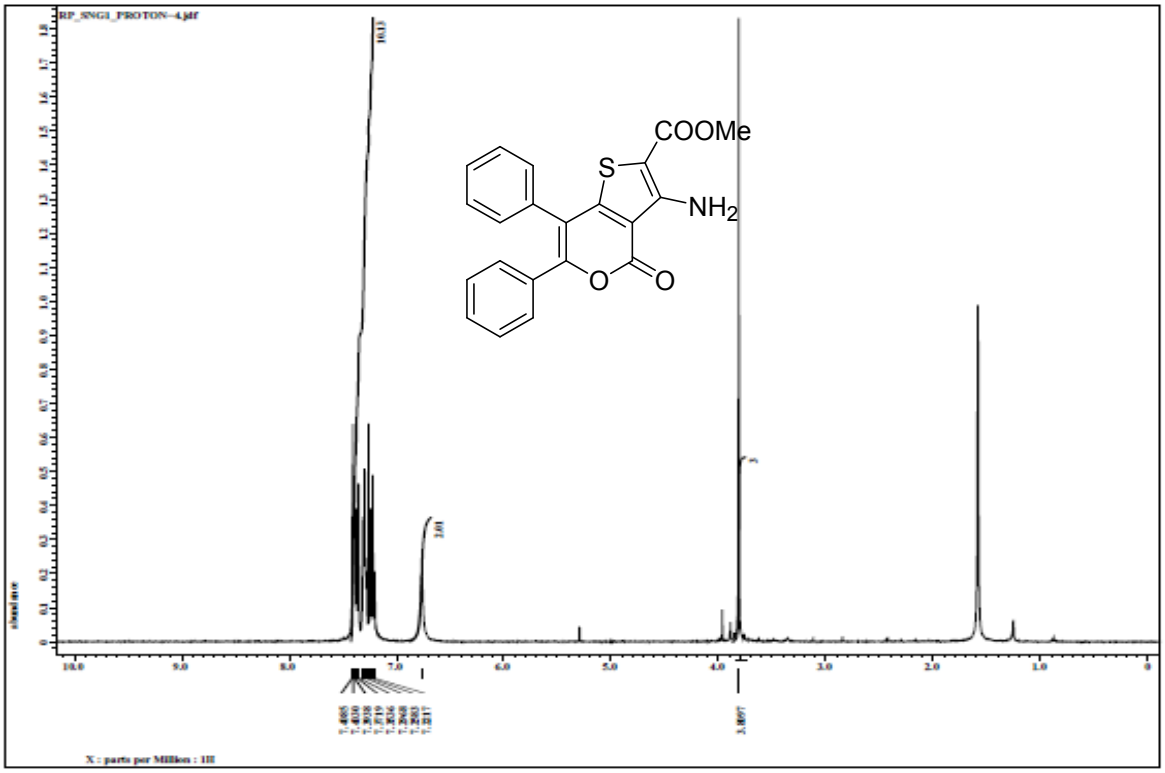


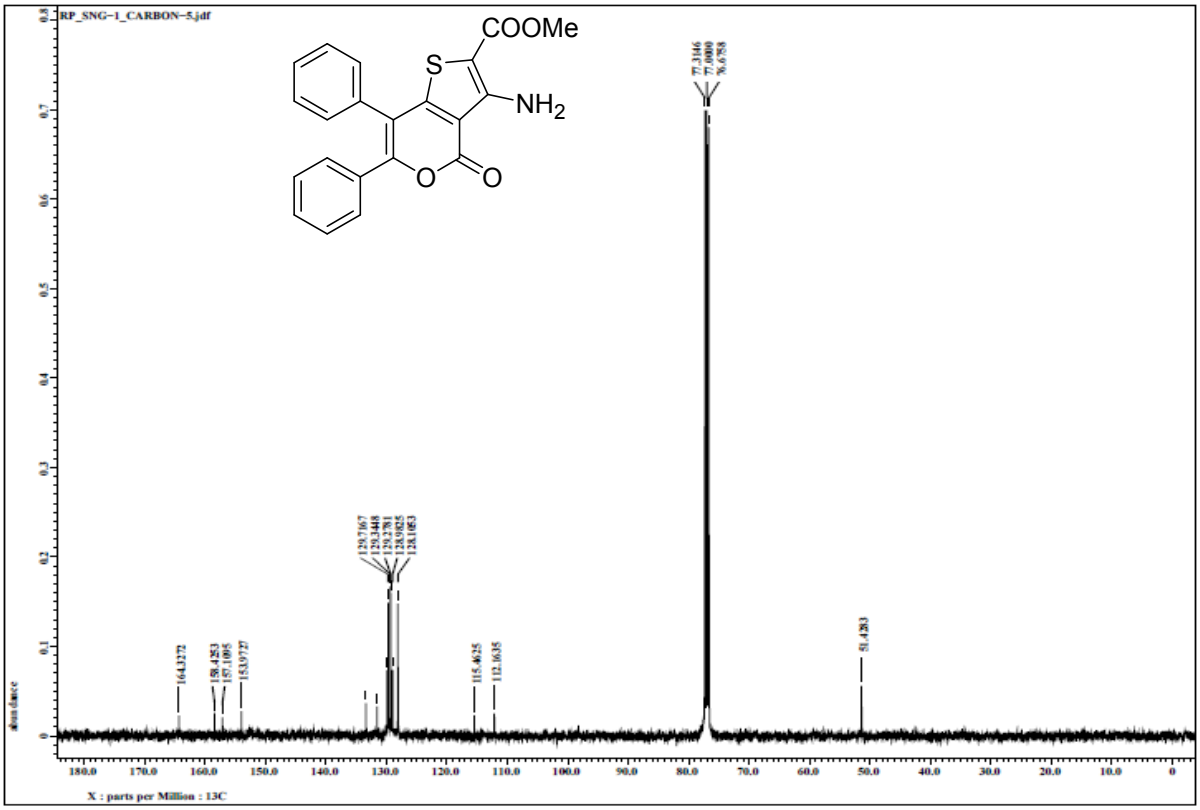
Spectra of 3-amino-6-(4-bromo-phenyl)-4-oxo-4*H*-thieno[3,2-*c*]pyran-2-carboxylic acid methyl ester (3d)



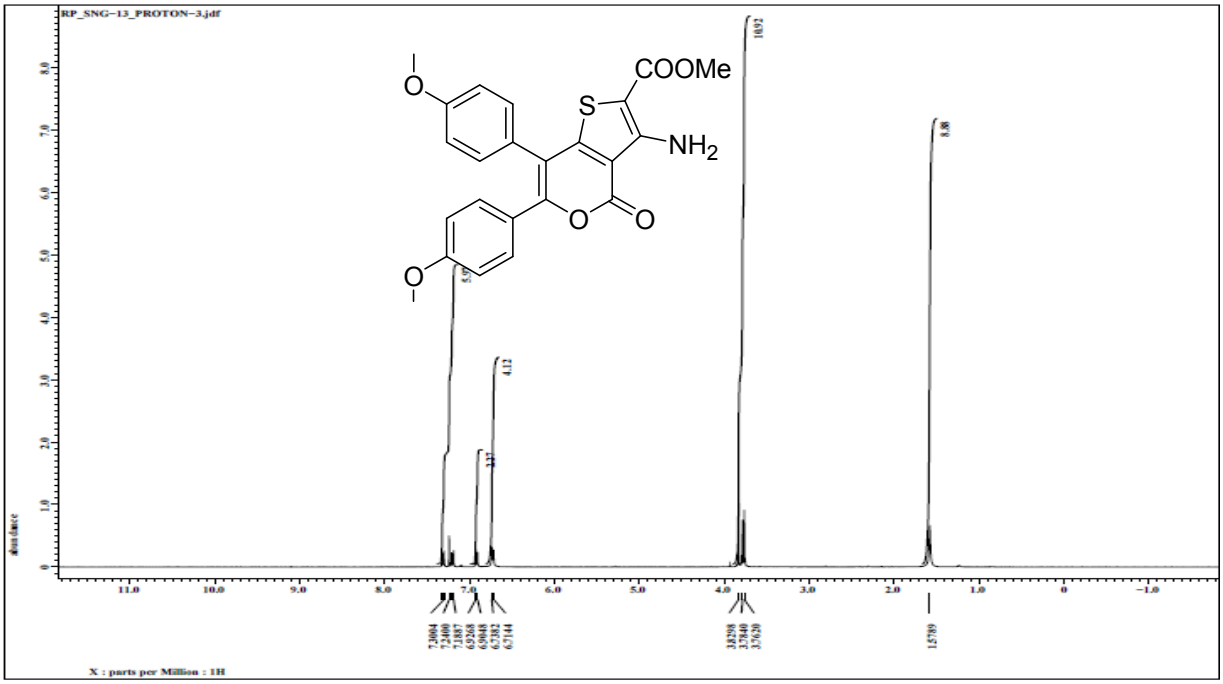


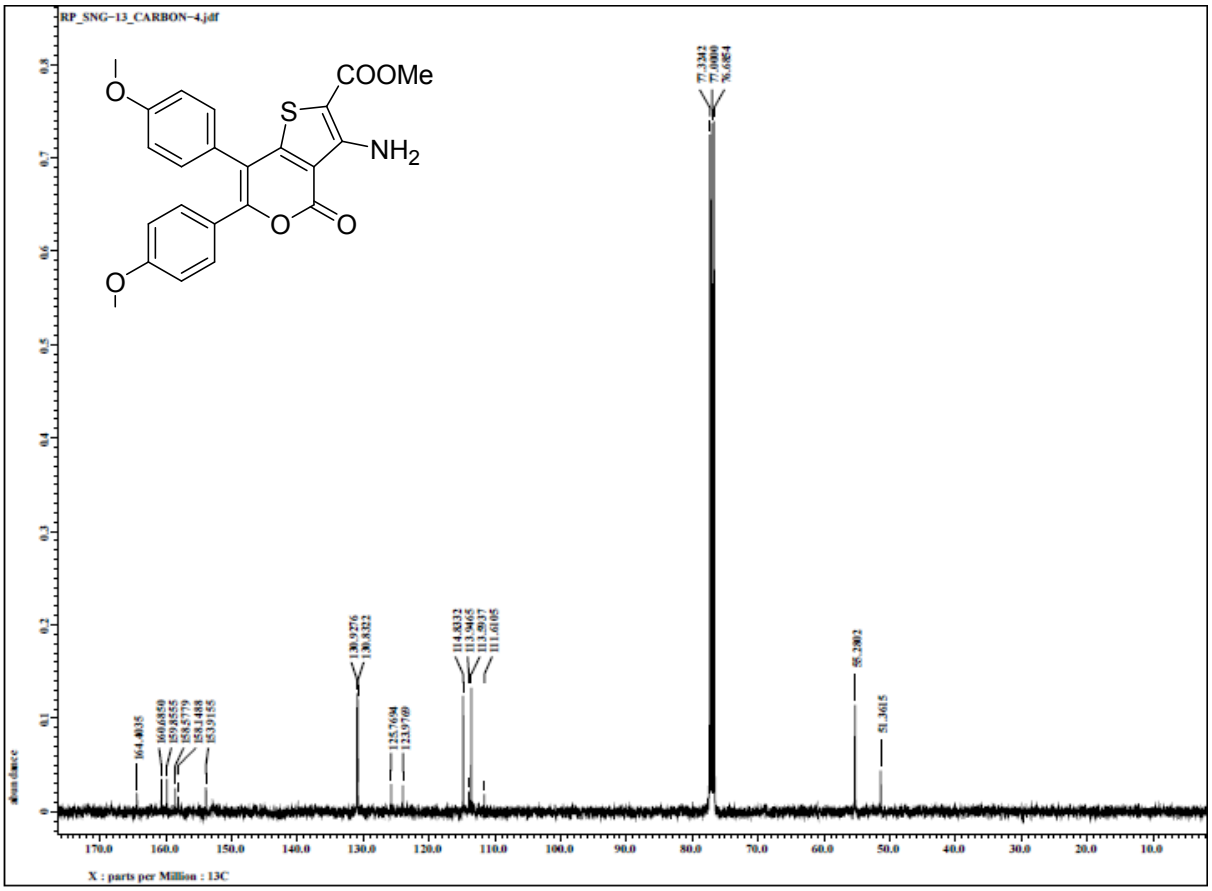
Spectra of 3-amino-6-(4-methoxy-phenyl)-4-oxo-4*H*-thieno[3,2-*c*]pyran-2-carboxylic acid methyl ester (3e)



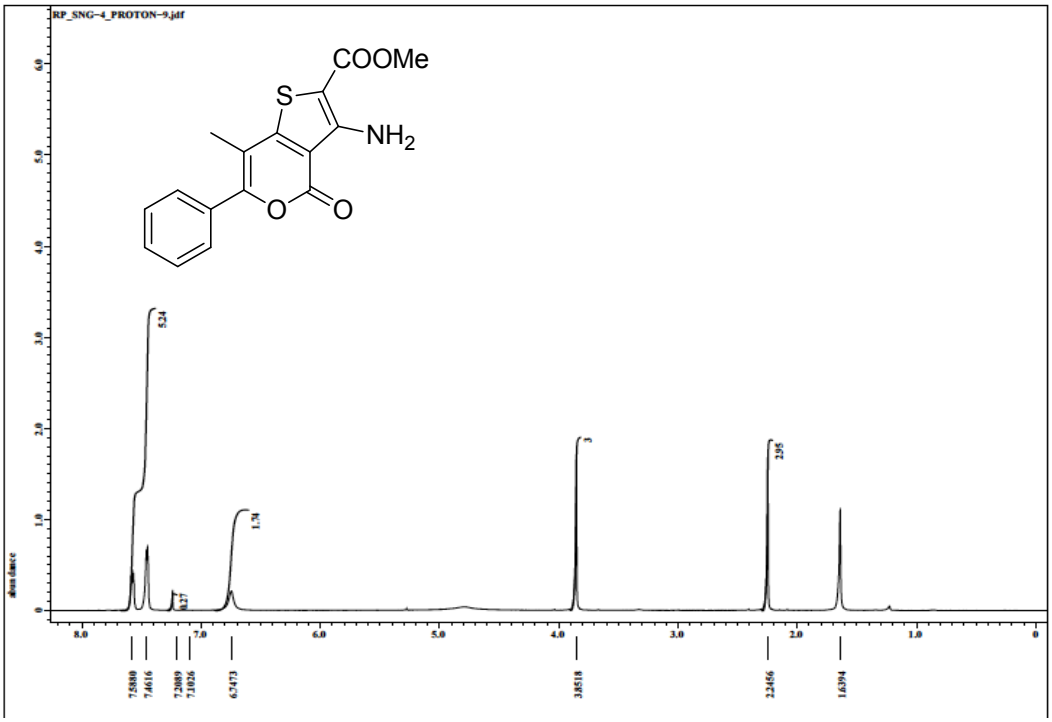


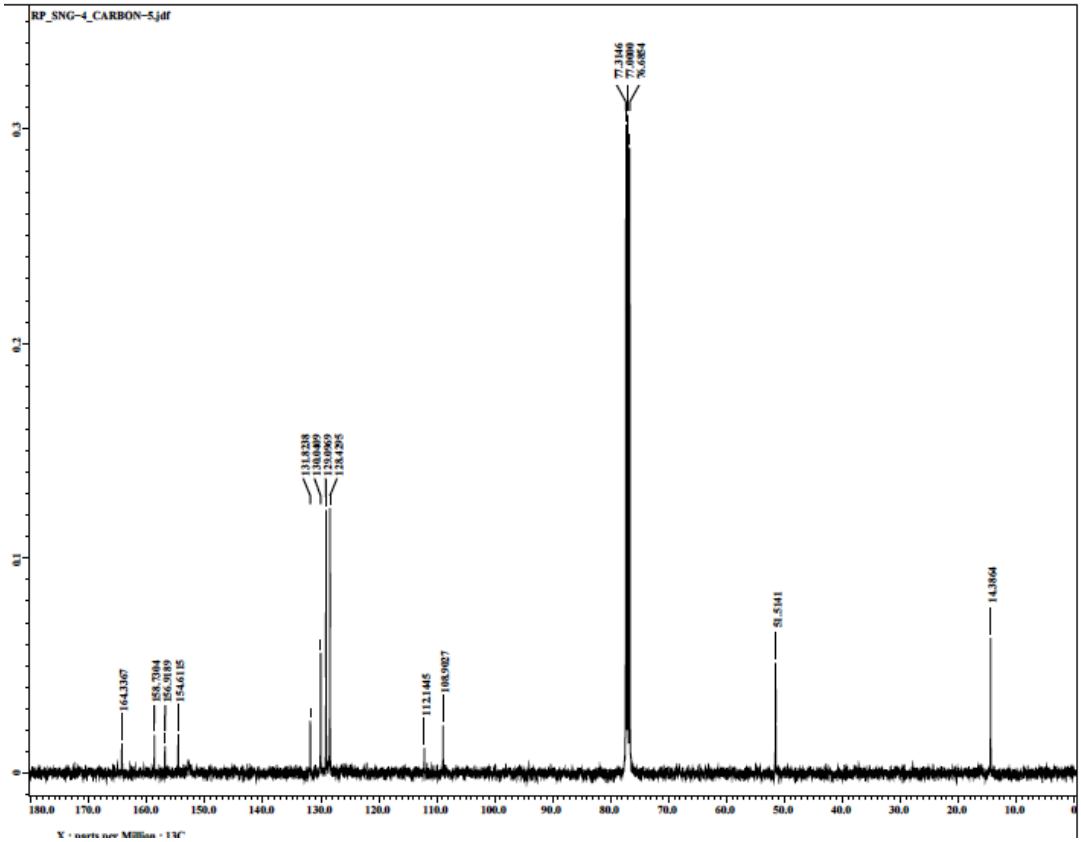
Spectra of 3-amino-4-oxo-6,7-diphenyl-4H-thieno[3,2-c]pyran-2-carboxylic acid methyl ester (3f)



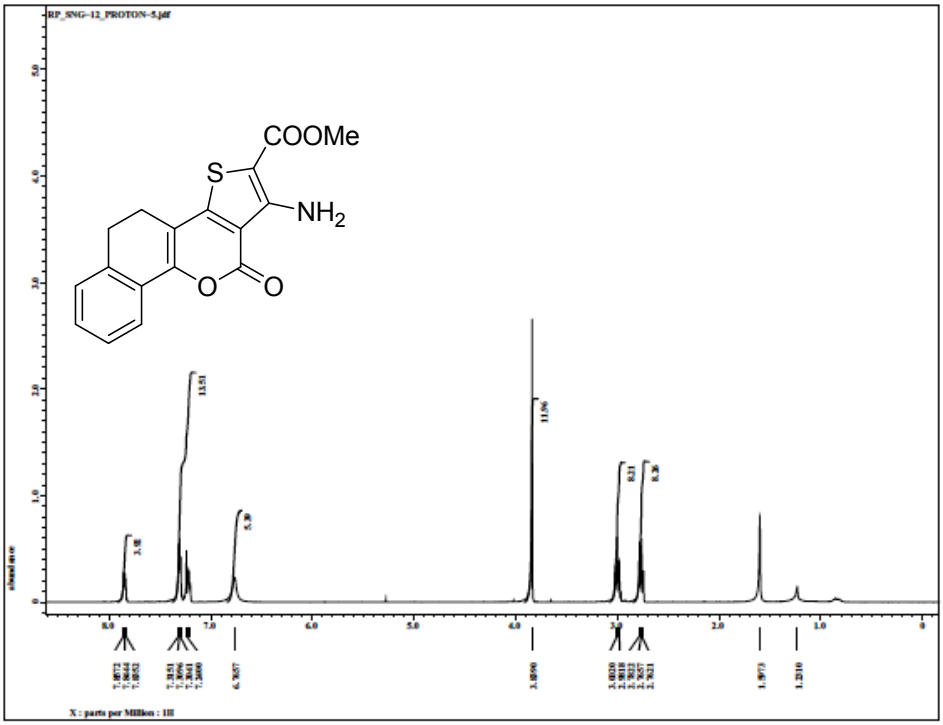


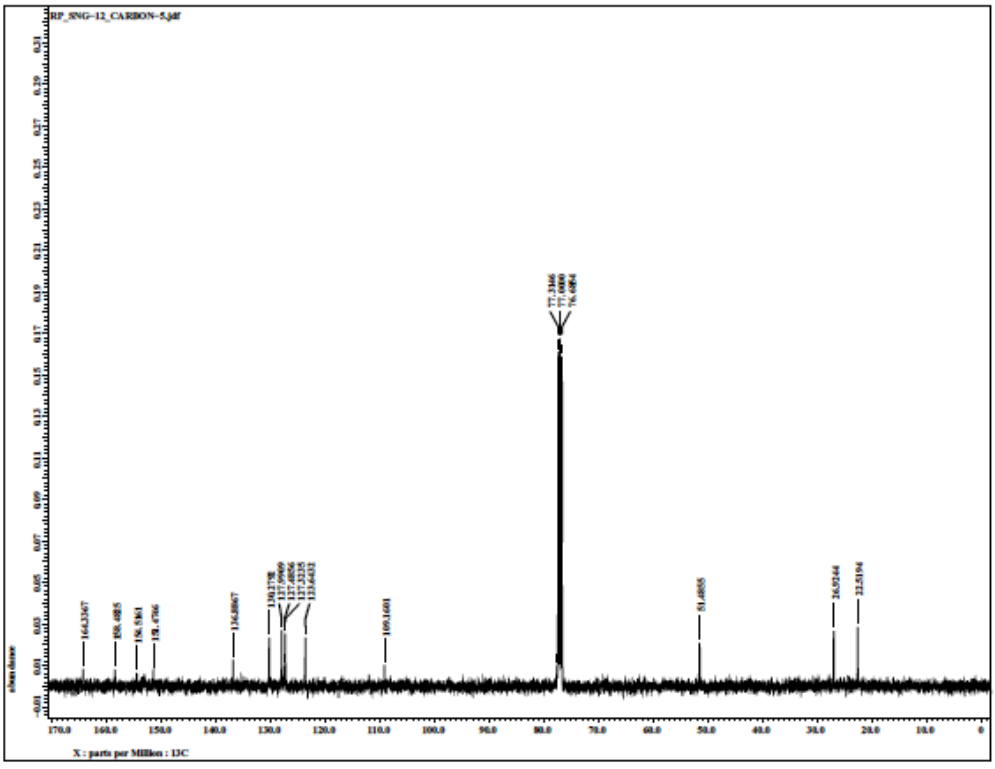
Spectra of 3-amino-6,7-bis-(4-methoxy-phenyl)-4-oxo-4H-thieno[3,2-c]pyran-2-carboxylic acid methyl ester (3g)





Spectra of 3-Amino-7-methyl-4-oxo-6-phenyl-4H-thieno[3,2-c]pyran-2-carboxylic acid methyl ester(3h)





Spectra of 17-Amino-12-oxo-6,12-dihydro-7H-11-oxa-15-thia-cyclopenta[a]phenanthrene-16-carboxylic acid methyl ester (5)

Thermogravimetric analysis :

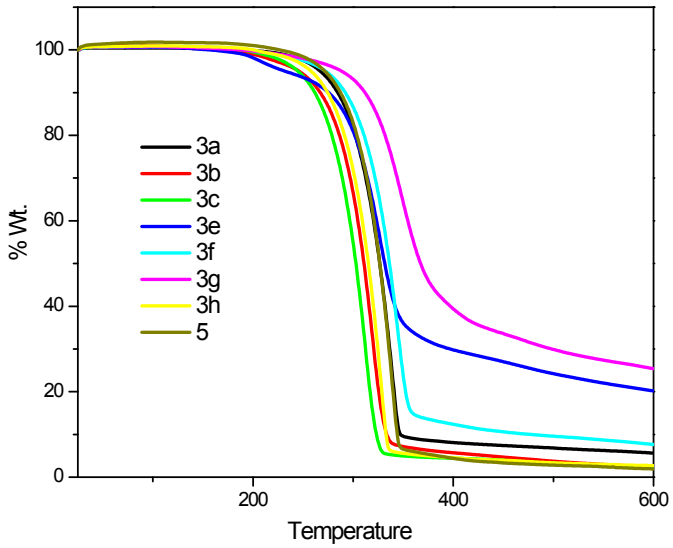


Figure S1 Thermogravimetric analysis of thieno[3,2-c]pyrans **3a-3g**, measured at a heating rate of 10° C/ min under nitrogen atmosphere.

Solvent effect:

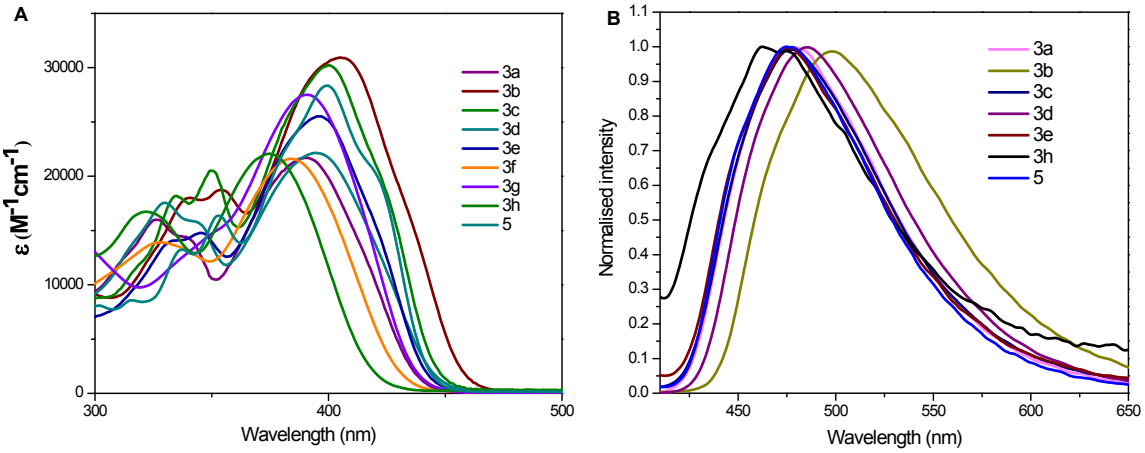


Figure S2: Electronic absorption (A) and fluorescence (B) spectra of thieno[3,2-*c*]pyrans recorded in dichloromethane

Solvatochromic effect of 3a:

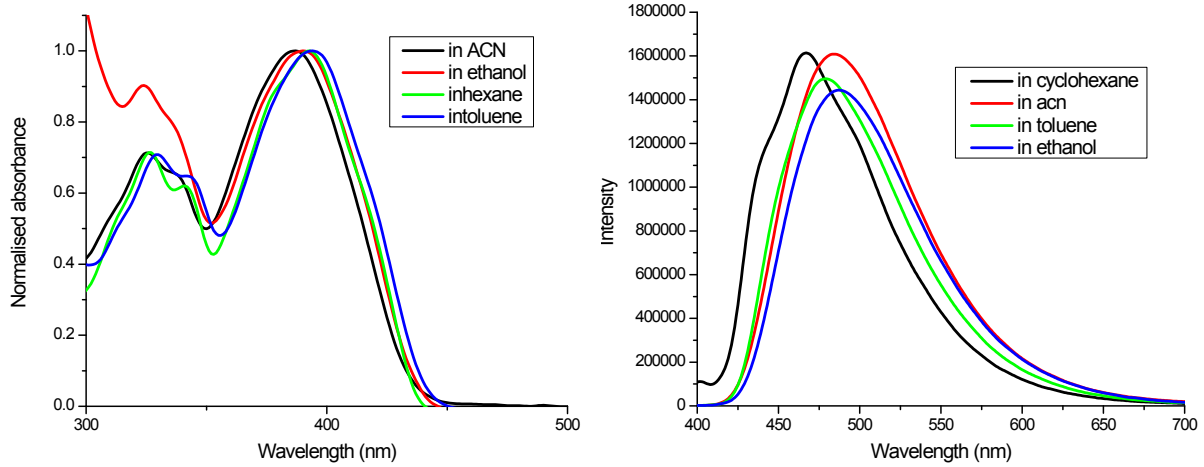


Figure S3- solvent effect on absorption and fluorescence spectra for **3a**.

Table S2: Solvatochromic Data of **3a**

Solvent	**λ_{max}(nm)**	**λ_{em}.(nm)**	**Stokes Shift(cm^{-1})**	**Φ_f^b**
Cyclohexane	393	467	4032	93
Toluene	394	479	4504	93
Dichloromethane	390	478	4721	89
Ethanol	390	487	5108	89
Acetonitrile	387	484	5178	81

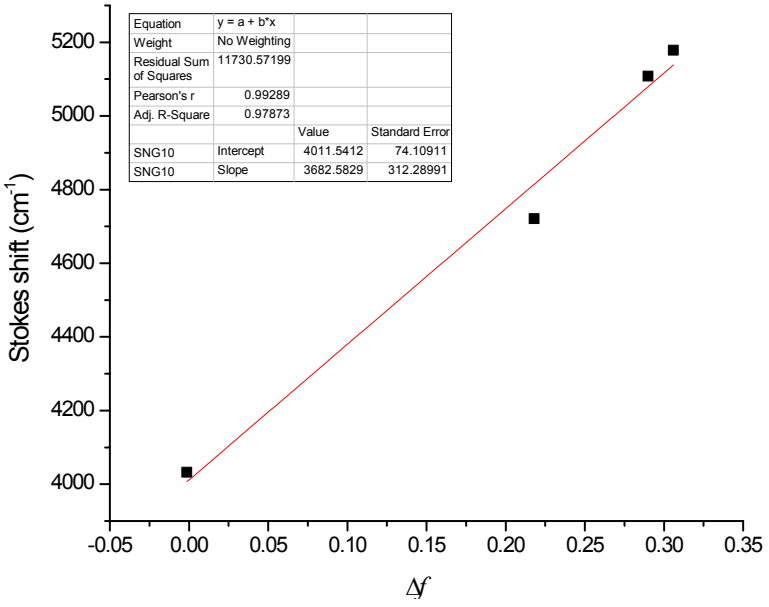


Figure S4 Lippert–Mataga plot of **3a** in solvents of increasing polarity.

Solvatochromic effect of 3b:

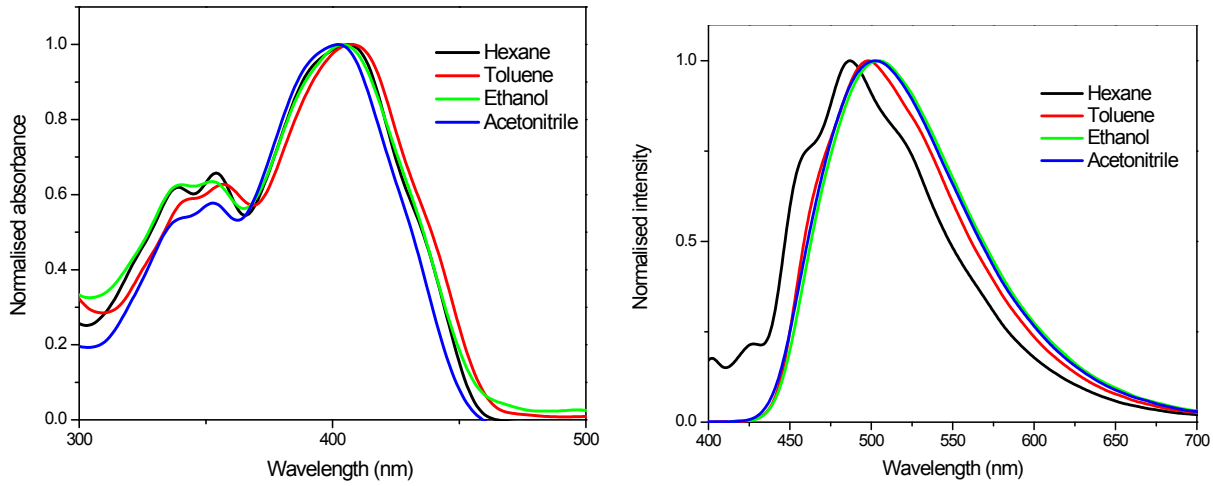


Figure S5- solvent effect on absorption and fluorescence spectra for **3b**.

Table S3: Solvatochromic Data of **3b**

Solvent	**λ_{max}(nm)**	**λ_{em} .(nm)**	**Stokes Shift(cm^{-1})**	**Φ_f^b**
Cyclohexane	406	487	4032	93
Toluene	408	498	4504	93
Dichloromethane	405	498	4611	73
Ethanol	404	504	5108	38
Acetonitrile	402	502	5178	64

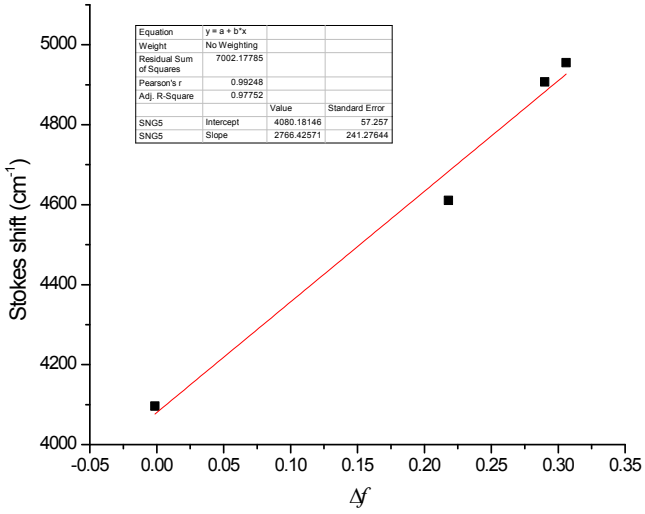


Figure S6 Lippert–Mataga plot of **3b** in solvents of increasing polarity.

AIE study of 3g:

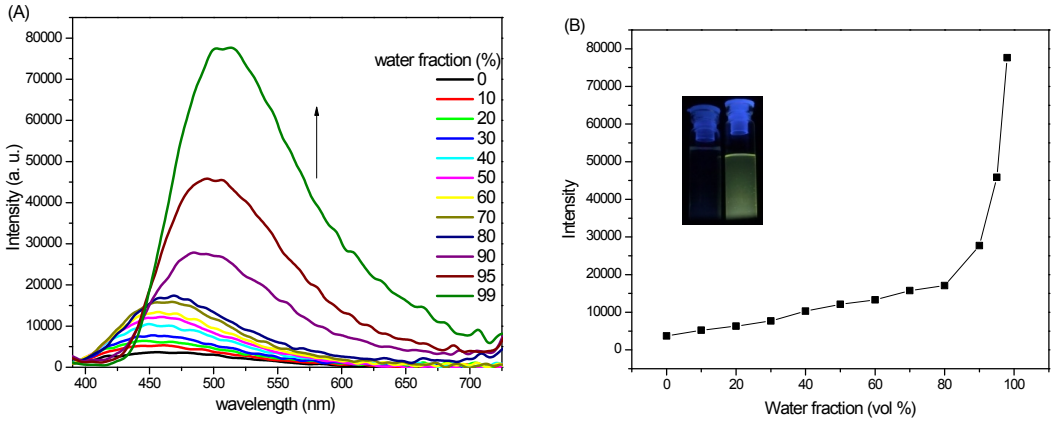


Figure S7 (A) Fluorescence spectra of **3g** in THF–water mixtures with different water fractions. (B) Plot of PL peak intensity vs. water fraction (fw) of the aqueous mixture. concentration: 20 μm; excitation wavelength: 370 nm. Inset: solution of **3g** in THF (fw = 0%) and its suspension in a THF–water mixture with fw = 98%; photographs taken under UV illumination.

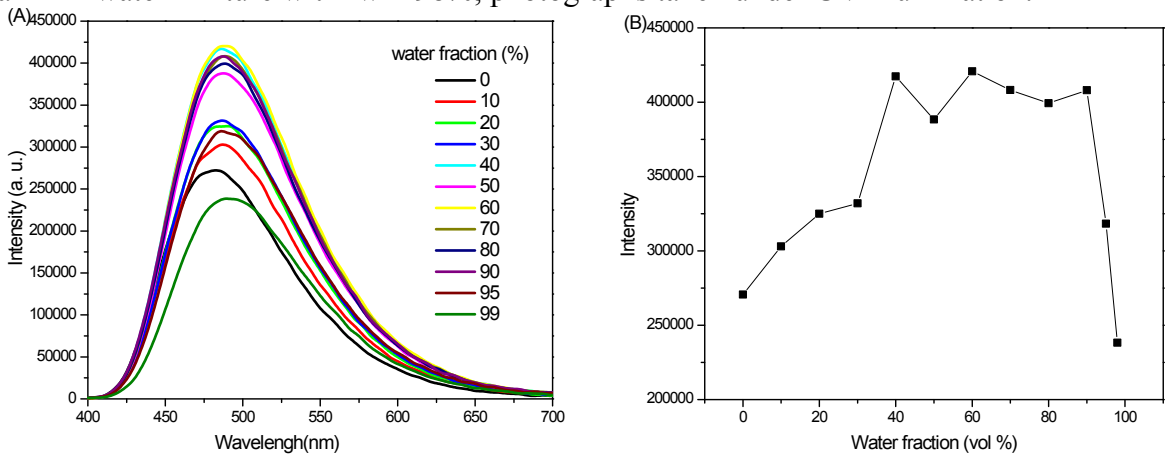
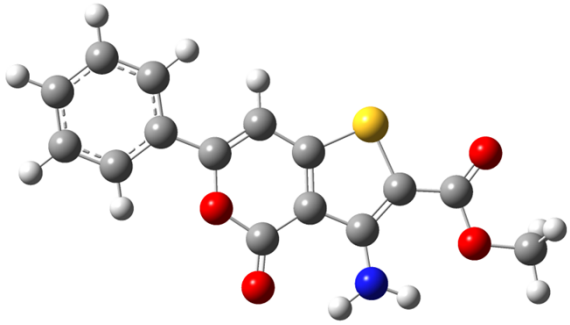


Figure- S8 (A) Fluorescence spectra of **3h** in THF–water mixtures with different water fractions. (B) Plot of PL peak intensity at 488 nm vs. water fraction of the aqueous mixture. Luminogen concentration: 20 μm; excitation wavelength: 370 nm. Inset: solution of **3h** in THF (fw = 0%) and its suspension in a THF–water mixture with fw = 98%; photographs taken under UV illumination.

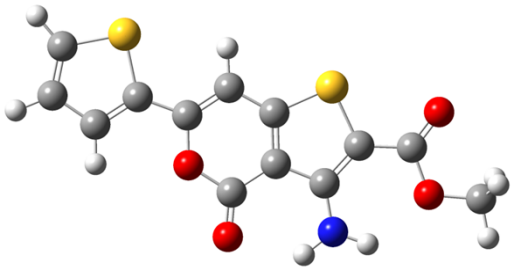
Theoretical study:

Energy optimized structures:

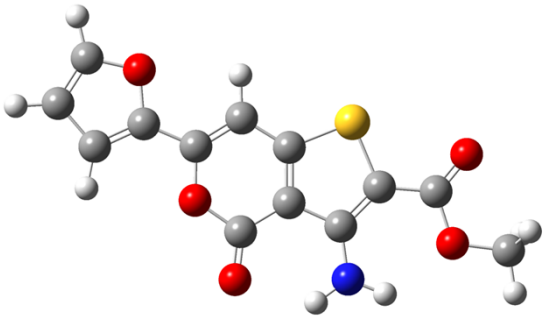
3a-



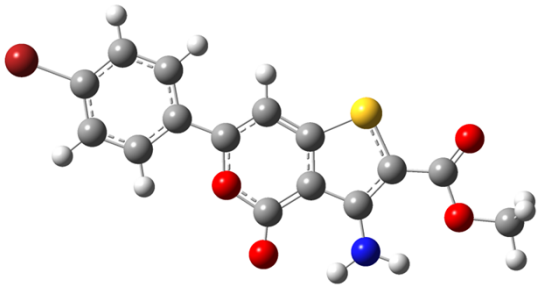
3b-



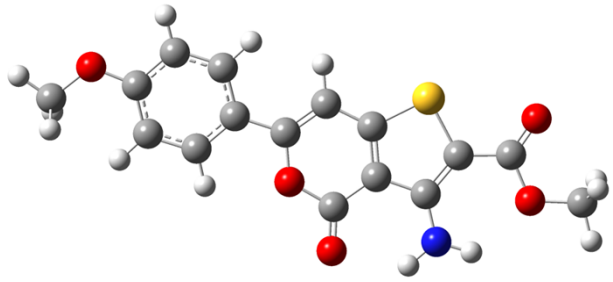
3c-



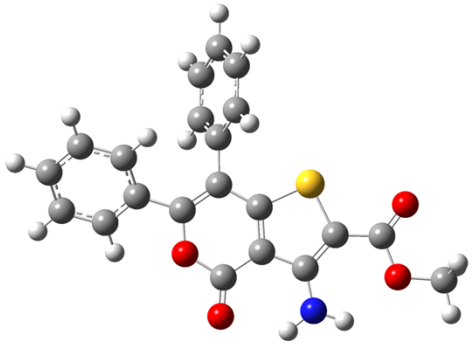
3d-



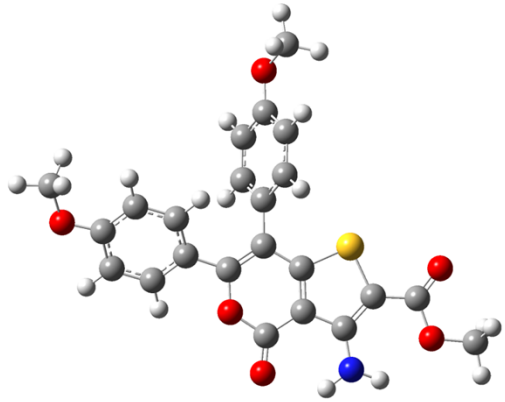
3e-



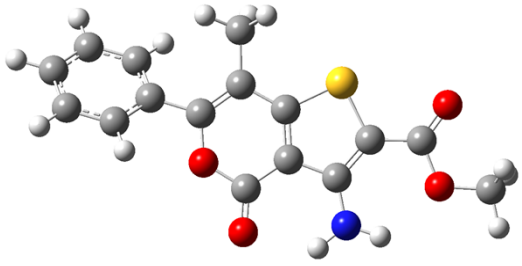
3f-



3g-



3h



5

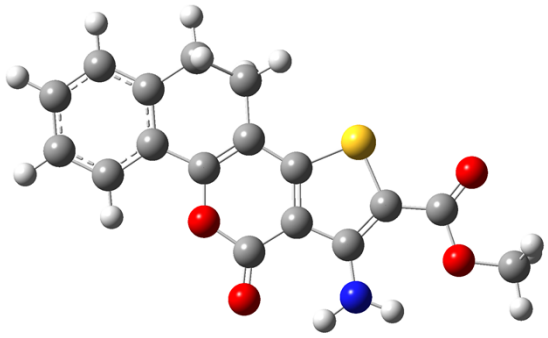
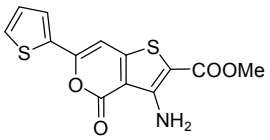
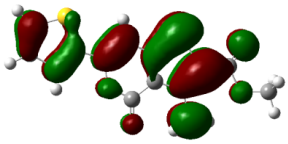
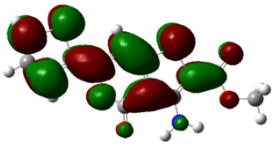
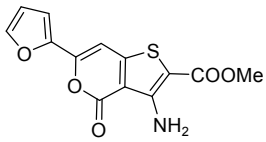
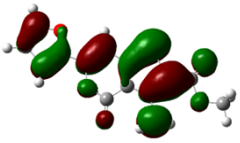
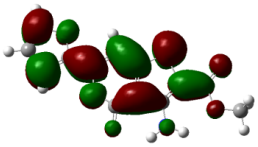
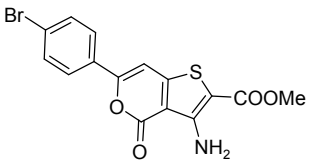
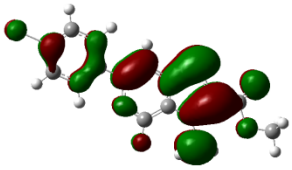
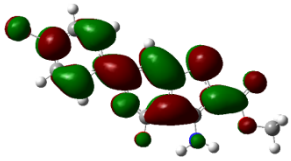
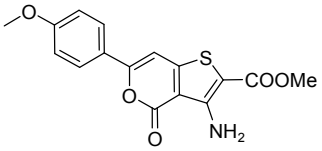
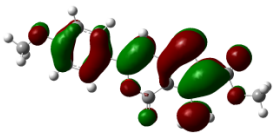
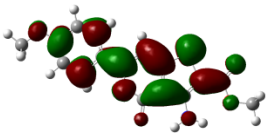


Figure S9 - Energy optimized structures of thieno[3,2-c]pyrans **3a-3g and 5** at the B3LYP/6-31G (d) level.

Distribution of molecular orbital:

Compounds	HOMO	LUMO	Homo-Lumo Gap
			**3.24**
3b	**-5.50 eV**	**-2.26 eV**	
			**3.32**
3c	**-5.46 eV**	**-2.14 eV**	
			**3.29**
3d	**-5.63 eV**	**-2.34 eV**	
			**3.40**
3e	**-5.38 eV**	**-1.98 eV**	

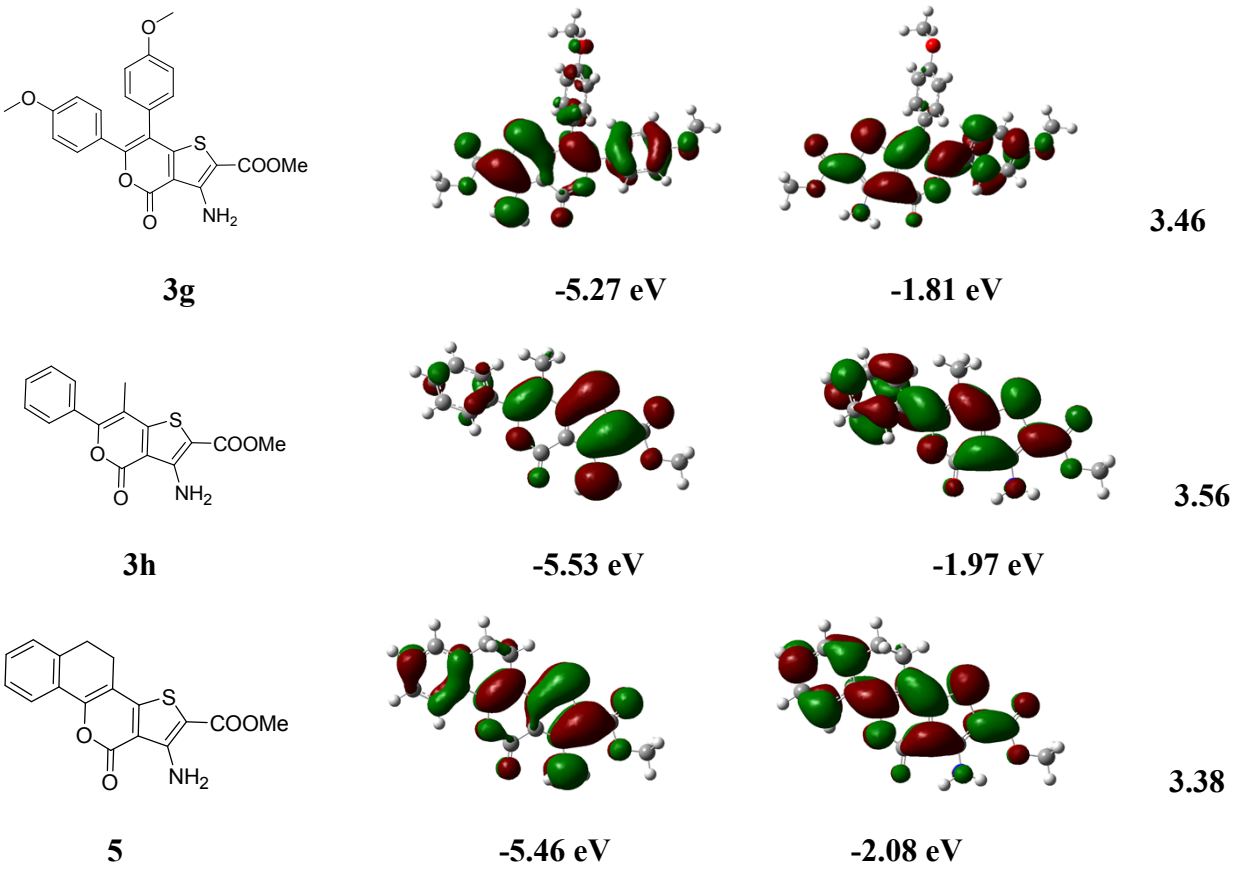


Figure S10 HOMO and LUMO frontier orbitals of thieno[3,2-c]pyrans **3b-3g** at the B3LYP/6-31G (d) level.

TD-DFT data:

Table S4. Computed Vertical Transitions and Their Oscillator Strengths and Configurations at CAMB3LYP/6-31G(d) / CAMB3LYP/6-31G(d) level.[1]

compound	DCM			Gas		
	λ_{max}[nm]	*f*	configuration	λ_{max}[nm]	*f*	Configuration
3a	434.3	0.9979	HOMO→LUMO(-0.68830)	400.8	0.6580	HOMO→LUMO(0.69273)
	319.6	0.2085	HOMO-1 → LUMO(-0.68414)	312.7	0.1939	HOMO-1→LUMO(0.68446)
	270.8	0.1508	HOMO→LUMO+1(0.62467)	263.8	0.0525	HOMO→LUMO+1(0.56377) HOMO→LUMO+2(0.26901)
3b	455.7	1.019	HOMO→LUMO(0.68462) HOMO-1 → LUMO(0.12612)	414.8	0.6821	HOMO→LUMO(0.69103)
				322.1	0.1499	HOMO-1→LUMO(0.6842)
	327.9	0.154	HOMO-1 → LUMO(0.67888)			
				266.6	0.0299	HOMO-1→LUMO(0.20774)
	272.5	0.141	HOMO→LUMO+1(0.47806) HOMO→LUMO+2(0.42929)			HOMO→LUMO+1(0.5219) HOMO→LUMO+2(0.38956)

3f	465.42	0.8810	HOMO→LUMO(-0.6869)	429.9	0.5701	HOMO→LUMO(-0.68878)
	343.23	0.0153	HOMO-1 → LUMO(-0.6790)	340.8	0.0143	HOMO-1 → LUMO(0.68198)
	283.05	0.1777	HOMO-2 →LUMO (0.49846) HOMO→LUMO+1 (-0.35889)	283.9	0.0793	HOMO→LUMO+1(0.67042)
	281.83	0.1210	HOMO→LUMO+1 (0.55681) HOMO-2 →LUMO(0.29058)	276.8	0.0572	HOMO-2 → LUMO(0.62131)

Optimized Parameters :

3a-

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.632976	0.642046	-0.035857
2	6	0	0.230679	-0.690363	0.020507
3	6	0	-1.147098	-1.035879	0.038752
4	6	0	-2.065454	-0.026253	-0.014848
5	6	0	-0.336695	1.701605	-0.070513
6	6	0	2.062972	0.817154	-0.040867
7	6	0	2.713680	-0.417978	0.015985
8	1	0	-1.464992	-2.067260	0.112498
9	8	0	-1.671381	1.280371	-0.066861
10	8	0	-0.125810	2.899247	-0.104155
11	16	0	1.577273	-1.772533	0.072316
12	7	0	2.630400	2.040681	-0.099998
13	1	0	2.022076	2.849066	-0.107487
14	1	0	3.634736	2.123769	-0.075227
15	6	0	4.124384	-0.734213	0.036580
16	8	0	4.592646	-1.859229	0.087678
17	8	0	4.907380	0.390861	-0.007582
18	6	0	6.321750	0.140842	0.010224
19	1	0	6.616811	-0.462058	-0.852445
20	1	0	6.793142	1.123704	-0.030396
21	1	0	6.608321	-0.384609	0.924858
22	6	0	-3.528486	-0.178500	-0.006604
23	6	0	-4.352861	0.934188	0.238922
24	6	0	-4.131193	-1.427995	-0.241189
25	6	0	-5.738441	0.793907	0.263488
26	1	0	-3.898966	1.902973	0.411969
27	6	0	-5.515654	-1.561956	-0.214754
28	1	0	-3.520189	-2.296312	-0.466542
29	6	0	-6.325819	-0.452275	0.040004
30	1	0	-6.360529	1.662927	0.458532
31	1	0	-5.963873	-2.533583	-0.402392
32	1	0	-7.406824	-0.558852	0.057940

Total Energy (HF) = -1332.0871291 Hartree

3b-

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.645724	0.702373	-0.004000
2	6	0	-0.206689	-0.621133	-0.002685
3	6	0	1.178467	-0.928436	-0.001319
4	6	0	2.064470	0.113358	-0.000406
5	6	0	0.291598	1.791194	0.000311
6	6	0	-2.079856	0.837142	-0.005459
7	6	0	-2.696299	-0.416949	-0.002677
8	1	0	1.533251	-1.951934	-0.000885
9	8	0	1.641019	1.411847	0.000440
10	8	0	0.045873	2.982230	0.004844
11	16	0	-1.523058	-1.740923	-0.001724
12	7	0	-2.682567	2.045079	-0.013983
13	1	0	-2.098522	2.870815	0.007502
14	1	0	-3.689024	2.097489	0.008976
15	6	0	-4.097427	-0.773026	0.000810
16	8	0	-4.534017	-1.911847	0.002159
17	8	0	-4.911889	0.330620	0.003465
18	6	0	-6.318607	0.040433	0.006910
19	1	0	-6.591732	-0.530831	0.897916
20	1	0	-6.817486	1.010506	0.006388
21	1	0	-6.595377	-0.533662	-0.881099
22	6	0	3.510529	0.017005	0.000609
23	6	0	4.410898	1.062183	0.002299
24	16	0	4.348621	-1.522747	-0.000167
25	6	0	5.765404	0.632705	0.002889
26	1	0	4.095139	2.098064	0.003084
27	6	0	5.889466	-0.731150	0.001579
28	1	0	6.612701	1.309182	0.004180
29	1	0	6.794740	-1.323456	0.001643

Total Energy (HF) = -1652.8423277Hartree

3c-

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.358442	0.658211	-0.003658
2	6	0	0.050611	-0.675878	-0.002353
3	6	0	1.428611	-1.013662	-0.001044
4	6	0	2.326896	0.015708	-0.000132
5	6	0	0.600458	1.729092	0.000045
6	6	0	-1.789500	0.824532	-0.005022

7	6	0	-2.433862	-0.415555	-0.002511
8	1	0	1.779943	-2.037212	-0.000693
9	8	0	1.943060	1.324473	0.000376
10	8	0	0.377496	2.924606	0.003931
11	16	0	-1.290544	-1.765369	-0.001680
12	7	0	-2.365763	2.045336	-0.012596
13	1	0	-1.763731	2.858104	0.006227
14	1	0	-3.370897	2.119502	0.007521
15	6	0	-3.842527	-0.739900	0.000571
16	8	0	-4.305047	-1.868497	0.002061
17	8	0	-4.632230	0.381891	0.003174
18	6	0	-6.044945	0.123059	0.006548
19	1	0	-6.330758	-0.442429	0.897268
20	1	0	-6.522210	1.103962	0.006482
21	1	0	-6.334531	-0.444374	-0.881675
22	6	0	3.761722	-0.122623	0.000784
23	6	0	4.781915	0.795179	0.002045
24	6	0	5.994931	0.044282	0.002381
25	1	0	4.665336	1.868832	0.002635
26	6	0	5.629860	-1.270139	0.001322
27	1	0	7.004115	0.431135	0.003283
28	1	0	6.181789	-2.197637	0.001120
29	8	0	4.274923	-1.393121	0.000336

Total Energy (HF) = -1329.8649158 Hartree

3d-

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.143732	0.646187	-0.000003
2	6	0	1.668537	-0.663518	-0.000059
3	6	0	0.282826	-0.961851	-0.000075
4	6	0	-0.610437	0.077522	0.000054
5	6	0	1.233612	1.753529	0.000061
6	6	0	3.586349	0.764841	0.000089
7	6	0	4.210237	-0.483950	0.000073
8	1	0	-0.059561	-1.986246	-0.000275
9	8	0	-0.147768	1.387905	0.000152
10	8	0	1.500161	2.961996	0.000035
11	16	0	2.999415	-1.859641	-0.000024
12	7	0	4.204474	1.969615	0.000189
13	1	0	3.639296	2.807857	0.000132
14	1	0	5.213015	1.994894	0.000212
15	6	0	5.602020	-0.821715	-0.000058
16	8	0	6.085311	-1.967623	-0.000136
17	8	0	6.418489	0.317536	-0.000042
18	6	0	7.865619	0.063876	-0.000114
19	1	0	8.148616	-0.502412	-0.889614
20	1	0	8.322411	1.052128	-0.001803
21	1	0	8.149181	-0.499547	0.891040

22	6	0	-2.074345	-0.006451	0.000053
23	6	0	-2.847478	1.172963	-0.000199
24	6	0	-2.738476	-1.251243	0.000302
25	6	0	-4.241288	1.111043	-0.000232
26	1	0	-2.347428	2.132545	-0.000370
27	6	0	-4.130409	-1.317109	0.000268
28	1	0	-2.176312	-2.177928	0.000571
29	6	0	-4.867555	-0.133082	-0.000005
30	1	0	-4.830794	2.019532	-0.000432
31	1	0	-4.635888	-2.274845	0.000471
32	35	0	-6.805477	-0.225823	-0.000053

Total Energy (HF) = -3902.759665 Hartree

3e-

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.399234	0.642067	-0.031813
2	6	0	0.998162	-0.692171	0.004771
3	6	0	-0.376996	-1.041908	0.012562
4	6	0	-1.300587	-0.033566	-0.026641
5	6	0	0.427785	1.698701	-0.055525
6	6	0	2.828665	0.819784	-0.029684
7	6	0	3.482801	-0.413919	0.013147
8	1	0	-0.689562	-2.076273	0.061523
9	8	0	-0.905657	1.274377	-0.059393
10	8	0	0.634381	2.898080	-0.073333
11	16	0	2.348121	-1.772414	0.045654
12	7	0	3.393046	2.045744	-0.072250
13	1	0	2.781918	2.852022	-0.064341
14	1	0	4.396756	2.131171	-0.034356
15	6	0	4.893279	-0.726121	0.036822
16	8	0	5.366451	-1.849855	0.074328
17	8	0	5.673838	0.402650	0.013546
18	6	0	7.088188	0.156031	0.035741
19	1	0	7.389872	-0.435681	-0.832430
20	1	0	7.557556	1.140456	0.009522
21	1	0	7.371894	-0.379728	0.945386
22	6	0	-2.758803	-0.183483	-0.028317
23	6	0	-3.590679	0.938832	0.112509
24	6	0	-3.372566	-1.446215	-0.169549
25	6	0	-4.978371	0.818251	0.123670
26	1	0	-3.142732	1.920042	0.217175
27	6	0	-4.749352	-1.577275	-0.159395
28	1	0	-2.768876	-2.338116	-0.303030
29	6	0	-5.568792	-0.444696	-0.010298
30	1	0	-5.584555	1.709475	0.236866
31	1	0	-5.221923	-2.547647	-0.271967

32	8	0	-6.906340	-0.680939	-0.013159
33	6	0	-7.790051	0.423334	0.133070
34	1	0	-8.796811	0.003781	0.105056
35	1	0	-7.635431	0.935986	1.090895
36	1	0	-7.672247	1.142561	-0.687357

Total Energy (HF) = -1446.611731Hartree

3f-

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.211717	-1.256426	-0.053213
2	6	0	-0.620368	0.003682	-0.052404
3	6	0	0.804911	0.176899	-0.040382
4	6	0	1.555958	-0.974136	-0.061603
5	6	0	-0.406355	-2.443445	-0.021329
6	6	0	-2.651939	-1.228512	-0.036980
7	6	0	-3.118953	0.086965	-0.014493
8	8	0	0.967537	-2.211318	-0.044184
9	8	0	-0.785248	-3.599552	0.021696
10	16	0	-1.804087	1.267434	-0.018463
11	7	0	-3.386909	-2.362414	-0.057512
12	1	0	-2.897197	-3.245459	0.010951
13	1	0	-4.389262	-2.300805	0.032264
14	6	0	-4.470885	0.600328	0.012380
15	8	0	-4.775948	1.781102	0.024955
16	8	0	-5.405870	-0.403330	0.025250
17	6	0	-6.769784	0.045493	0.052245
18	1	0	-6.992198	0.653945	-0.828124
19	1	0	-7.376430	-0.861112	0.054147
20	1	0	-6.962654	0.638105	0.950332
21	6	0	3.027366	-1.103769	-0.098483
22	6	0	3.838396	-0.191609	-0.795931
23	6	0	3.635854	-2.199470	0.541206
24	6	0	5.220211	-0.362604	-0.833435
25	1	0	3.387429	0.641351	-1.322161
26	6	0	5.018470	-2.360172	0.506951
27	6	0	5.816494	-1.441869	-0.178200
28	1	0	5.472494	-3.207281	1.013597
29	1	0	5.831508	0.346860	-1.384207
30	1	0	3.016971	-2.921817	1.061918
31	6	0	1.382349	1.548977	0.063894
32	6	0	1.169537	2.491566	-0.954415
33	6	0	2.107754	1.934056	1.201750
34	6	0	1.681002	3.785318	-0.841216
35	1	0	0.609924	2.206477	-1.840956
36	6	0	2.619091	3.226066	1.312233
37	1	0	2.268546	1.214462	1.999233

38	6	0	2.407983	4.155092	0.291010
39	1	0	1.510540	4.502341	-1.639559
40	1	0	3.178238	3.509013	2.199917
41	1	0	2.804804	5.162700	0.379531
42	1	0	6.895016	-1.570605	-0.208139

Total Energy (HF) = -1563.1362368 Hartree

3g-

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.008775	-1.522539	-0.038525
2	6	0	-1.368697	-0.285996	-0.031484
3	6	0	0.059963	-0.164193	0.013394
4	6	0	0.769299	-1.344354	0.013592
5	6	0	-1.250133	-2.737834	0.026022
6	6	0	-3.446528	-1.439810	-0.058262
7	6	0	-3.864821	-0.107901	-0.055978
8	8	0	0.130680	-2.558000	0.031375
9	8	0	-1.673474	-3.878994	0.074281
10	16	0	-2.505104	1.022561	-0.034906
11	7	0	-4.222372	-2.546424	-0.091571
12	1	0	-3.765970	-3.444416	0.007966
13	1	0	-5.222711	-2.446776	-0.014131
14	6	0	-5.196210	0.454429	-0.065447
15	8	0	-5.459979	1.645558	-0.070313
16	8	0	-6.168412	-0.514811	-0.066016
17	6	0	-7.514436	-0.015964	-0.076198
18	1	0	-7.694210	0.589900	-0.968147
19	1	0	-8.154420	-0.899453	-0.078807
20	1	0	-7.706666	0.594107	0.810345
21	6	0	2.229883	-1.533647	0.001023
22	6	0	3.099588	-0.643689	-0.647697
23	6	0	2.788980	-2.676102	0.612854
24	6	0	4.475224	-0.862844	-0.673836
25	1	0	2.702432	0.226864	-1.155721
26	6	0	4.155438	-2.898238	0.599907
27	6	0	5.013910	-1.991526	-0.042199
28	1	0	4.586655	-3.771735	1.078399
29	1	0	5.111397	-0.155885	-1.193536
30	8	0	6.337899	-2.299035	-0.000960
31	6	0	7.256740	-1.423356	-0.639147
32	1	0	7.226791	-0.418669	-0.198210
33	1	0	8.244070	-1.859469	-0.478734
34	1	0	7.061698	-1.352127	-1.716937
35	1	0	2.135690	-3.391239	1.100035
36	6	0	0.684619	1.184804	0.126441
37	6	0	0.525369	2.140680	-0.883936
38	6	0	1.411928	1.551350	1.273830

39	6	0	1.074832	3.420952	-0.771936
40	1	0	-0.030303	1.885013	-1.781912
41	6	0	1.965085	2.816892	1.397445
42	1	0	1.540917	0.830308	2.075708
43	6	0	1.799788	3.764349	0.374421
44	1	0	0.929255	4.131648	-1.577179
45	1	0	2.523108	3.102852	2.283482
46	8	0	2.378416	4.978426	0.593955
47	6	0	2.212966	5.990650	-0.387849
48	1	0	2.733771	6.868674	-0.002001
49	1	0	2.658120	5.698455	-1.348136
50	1	0	1.153514	6.234097	-0.540174

Total Energy (HF) = -1792.1838083 Hartree

3h

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.713202	0.736615	0.058376
2	6	0	0.302373	-0.587544	-0.054546
3	6	0	-1.080890	-0.959601	-0.105500
4	6	0	-1.980589	0.069953	0.003019
5	6	0	-0.249910	1.799878	0.109075
6	6	0	2.143641	0.906548	0.084712
7	6	0	2.790699	-0.326987	-0.014371
8	8	0	-1.577054	1.378198	0.093345
9	8	0	-0.032749	2.996776	0.167215
10	16	0	1.650461	-1.672169	-0.133343
11	7	0	2.712271	2.125877	0.201745
12	1	0	2.103970	2.934751	0.203008
13	1	0	3.716176	2.209458	0.163026
14	6	0	4.200599	-0.647079	-0.035773
15	8	0	4.666900	-1.770526	-0.125125
16	8	0	4.986429	0.473448	0.055952
17	6	0	6.399998	0.219904	0.041773
18	1	0	6.693677	-0.273408	-0.888414
19	1	0	6.873809	1.199193	0.121923
20	1	0	6.685681	-0.414449	0.884858
21	6	0	-3.454473	-0.019535	0.013291
22	6	0	-4.212598	0.962652	-0.649647
23	6	0	-4.127558	-1.039512	0.706900
24	6	0	-5.603271	0.902640	-0.646504
25	1	0	-3.701968	1.768929	-1.165229
26	6	0	-5.520713	-1.092480	0.711424
27	1	0	-3.562317	-1.772530	1.272554
28	6	0	-6.262565	-0.126925	0.029822
29	1	0	-6.174496	1.663386	-1.171202
30	1	0	-6.025660	-1.882931	1.259697
31	1	0	-7.348213	-0.169792	0.033786
32	6	0	-1.454762	-2.406106	-0.317147

33	1	0	-1.365995	-2.991745	0.607103
34	1	0	-2.475046	-2.513293	-0.688850
35	1	0	-0.780205	-2.861696	-1.051518

Total Energy (HF) = -1371.4006042 Hartree

5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.859112	0.851035	0.055950
2	6	0	-0.374694	-0.454451	-0.018699
3	6	0	1.022989	-0.724646	-0.025763
4	6	0	1.856291	0.360600	0.033285
5	6	0	0.037153	1.973170	0.115465
6	6	0	-2.297252	0.937261	0.053593
7	6	0	-2.871753	-0.333763	-0.030035
8	8	0	1.394696	1.641482	0.106191
9	8	0	-0.255946	3.153428	0.171899
10	16	0	-1.655750	-1.615650	-0.101166
11	7	0	-2.939835	2.122090	0.129825
12	1	0	-2.382064	2.965971	0.157807
13	1	0	-3.947234	2.142974	0.099213
14	6	0	-4.259676	-0.735402	-0.067916
15	8	0	-4.658132	-1.885845	-0.144034
16	8	0	-5.111462	0.338368	-0.008037
17	6	0	-6.507173	0.001691	-0.041375
18	1	0	-6.768573	-0.640714	0.803440
19	1	0	-7.039075	0.952018	0.021270
20	1	0	-6.756405	-0.516497	-0.971067
21	6	0	3.313508	0.243362	-0.017639
22	6	0	4.135001	1.354808	-0.261209
23	6	0	3.886171	-1.034880	0.172028
24	6	0	5.517185	1.200218	-0.329880
25	1	0	3.680385	2.329583	-0.400061
26	6	0	5.271753	-1.168750	0.096819
27	6	0	6.087056	-0.062320	-0.155011
28	1	0	6.147887	2.063158	-0.523435
29	1	0	5.718991	-2.149404	0.241680
30	1	0	7.164796	-0.187626	-0.213202
31	6	0	1.617038	-2.107294	-0.171297
32	1	0	1.720068	-2.347539	-1.240302
33	1	0	0.937990	-2.856464	0.251228
34	6	0	2.983113	-2.198753	0.522953
35	1	0	3.470536	-3.147764	0.275252
36	1	0	2.824706	-2.202689	1.612293

Total Energy (HF) = -1409.5222576 Hartree

References:

T. Yanai, D. P. Tew, and N. C. Handy, *Chem. Phys. Lett*., 2004, **393**, 51.