Electronic Supplementary Material (ESI) for RSC Advances.

Sulphur bridged [22]annulene[2.1.2.1]s based organic field-effect transistors: Interplay of the steric bulk and charge transport

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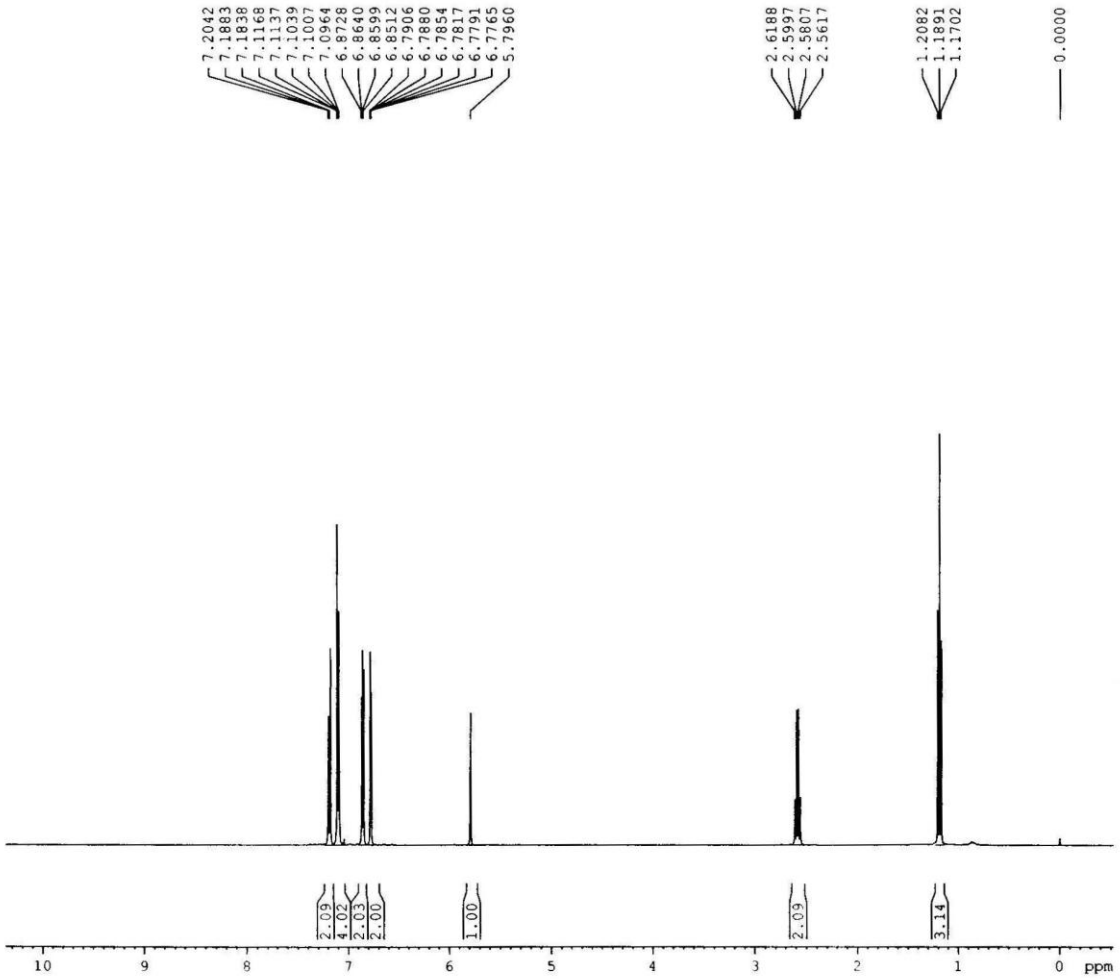


Figure S1: ^{1}H NMR spectrum of **3a**.

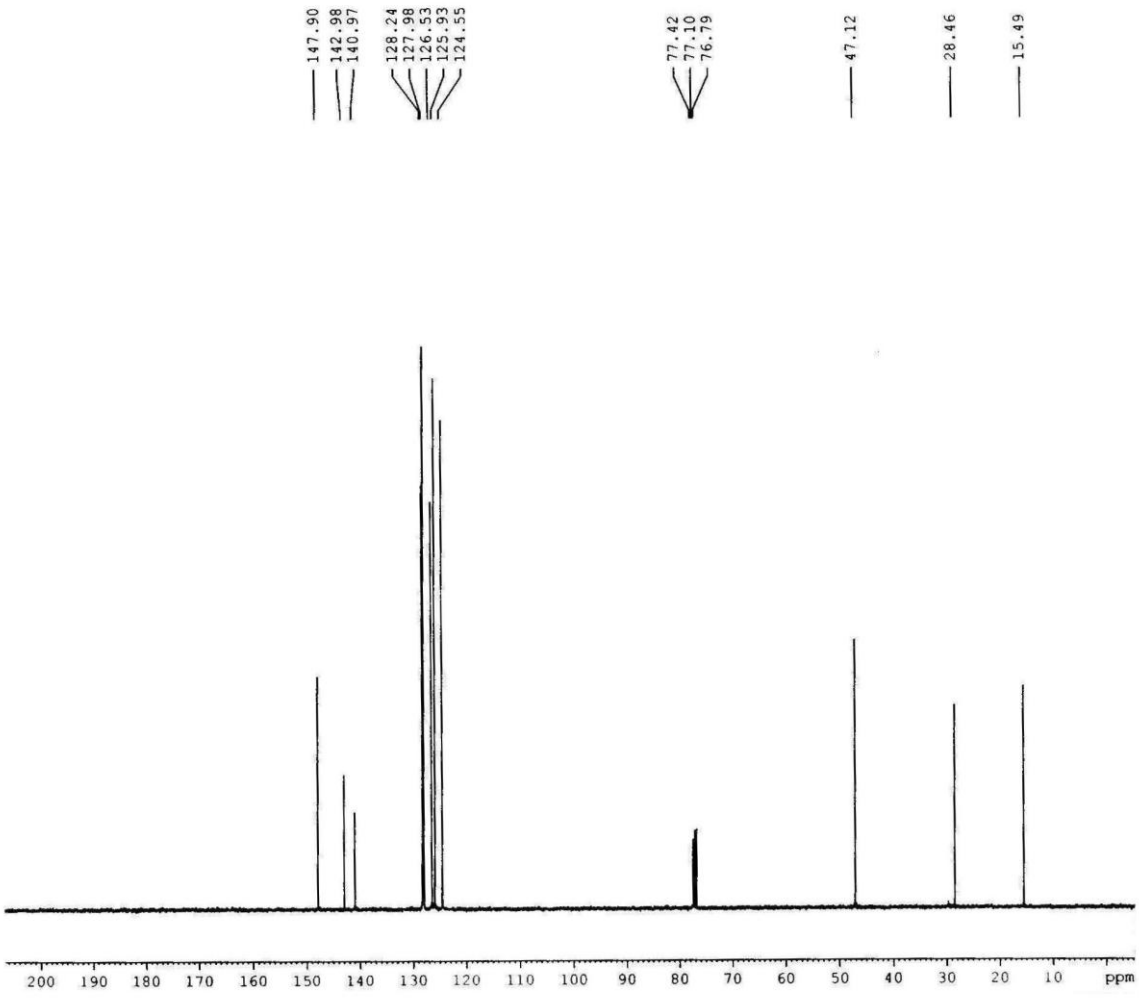


Figure S2: ^{13}C NMR spectrum of **3a**.

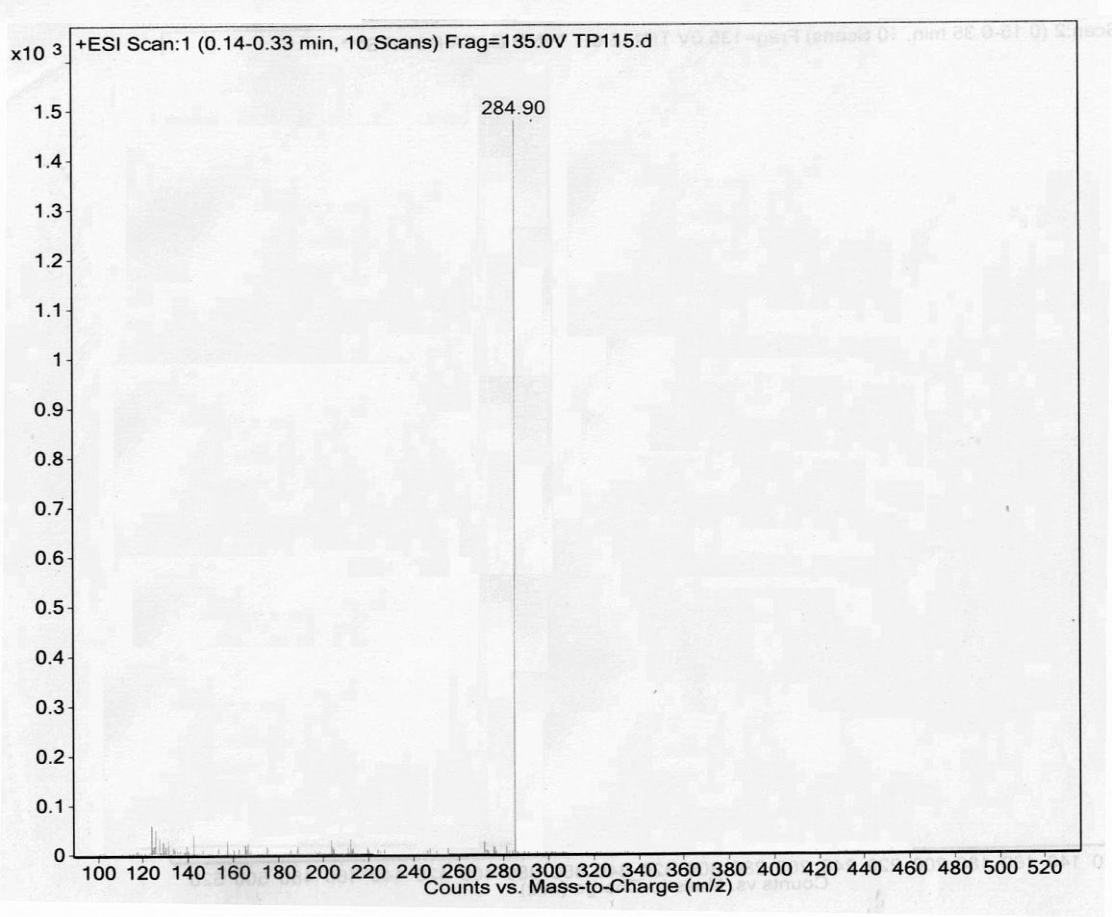


Figure **S3**: Mass spectrum of **3a**.

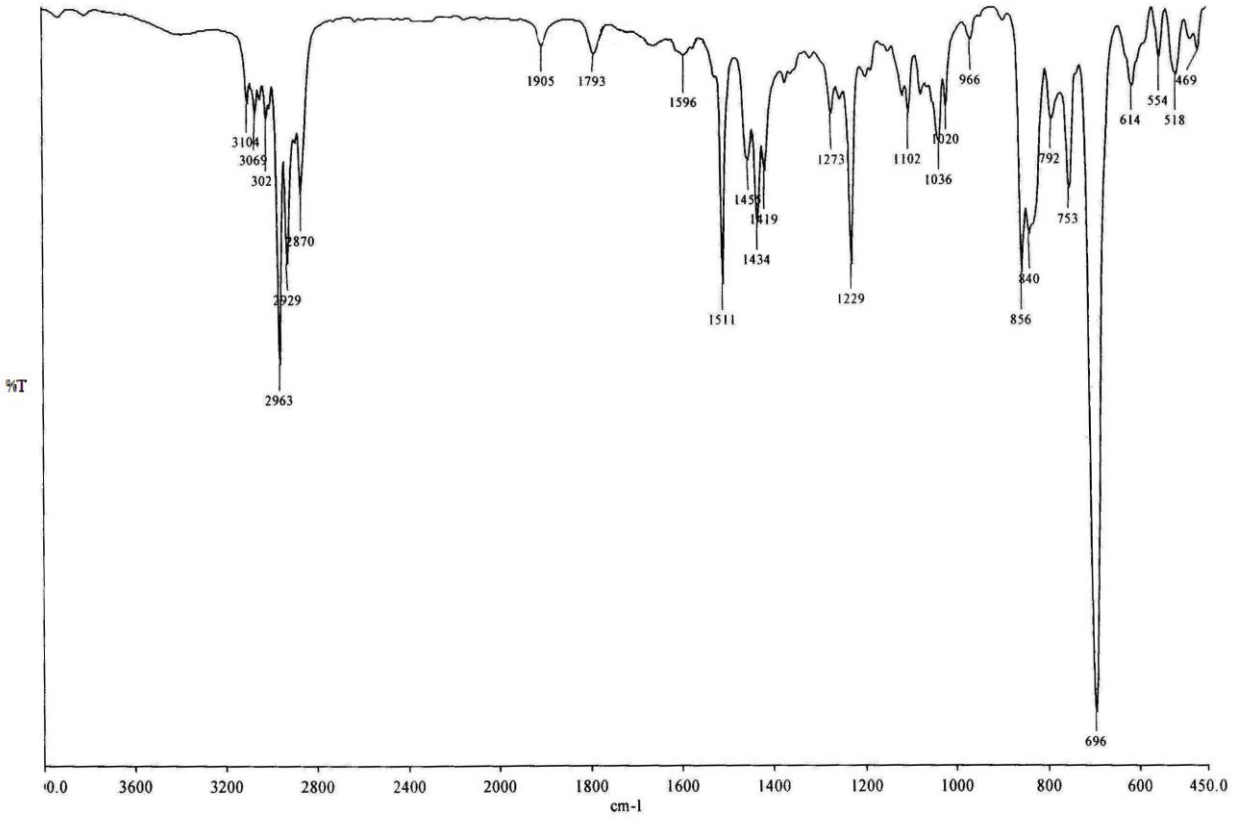
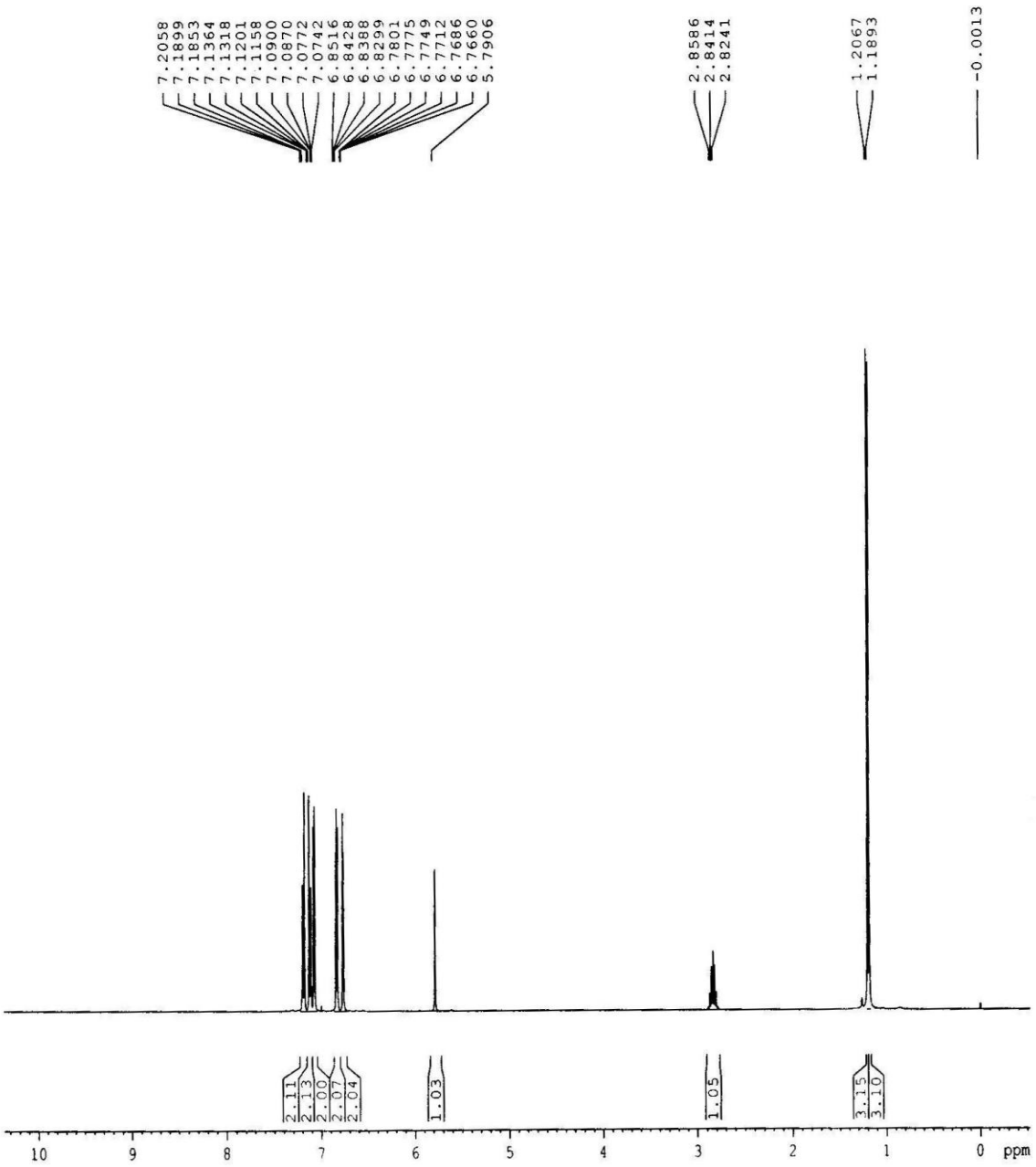


Figure **S4**: IR spectrum of **3a**.



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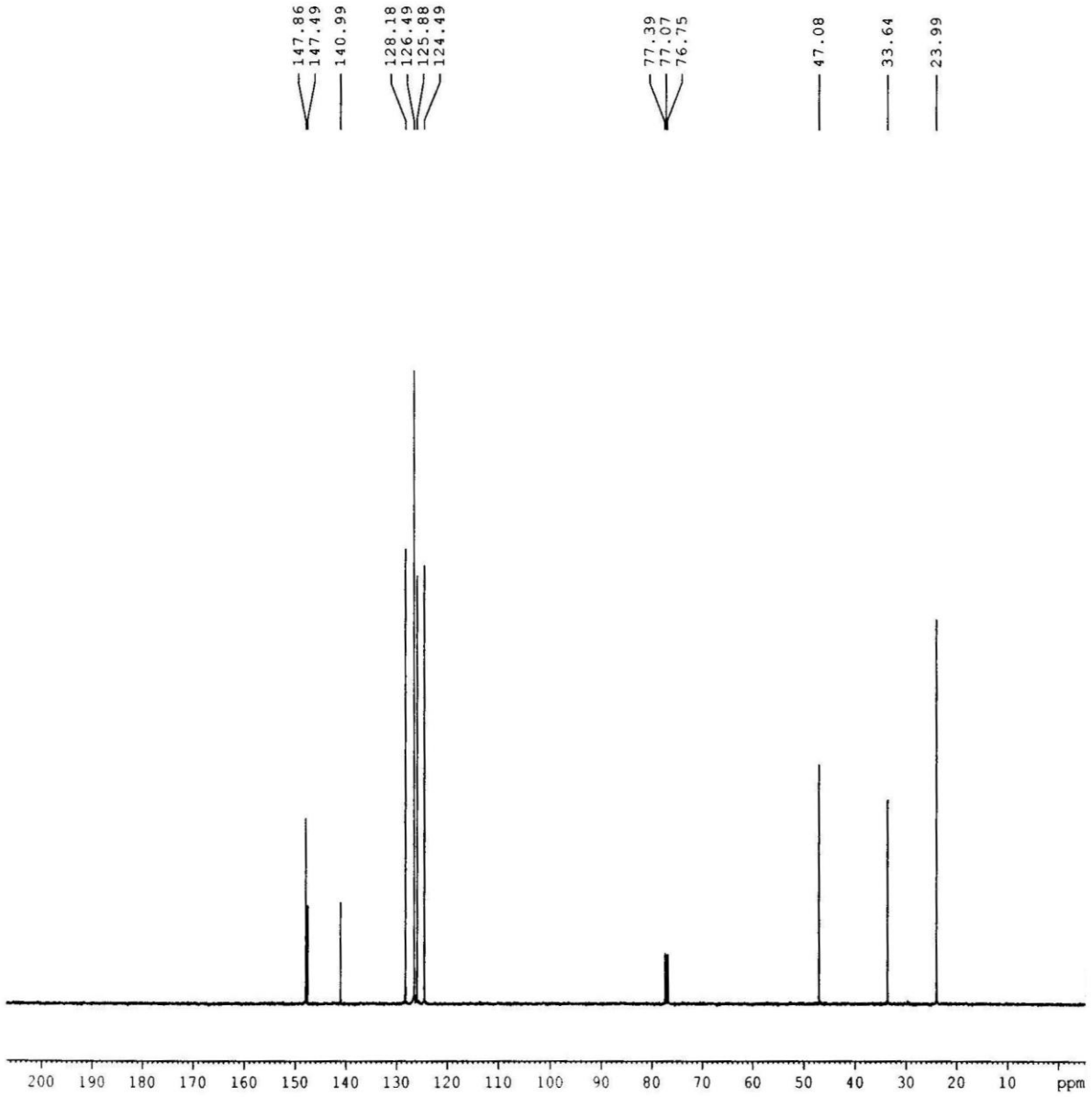


Figure **S6**: ^{13}C NMR spectrum of **3b**.

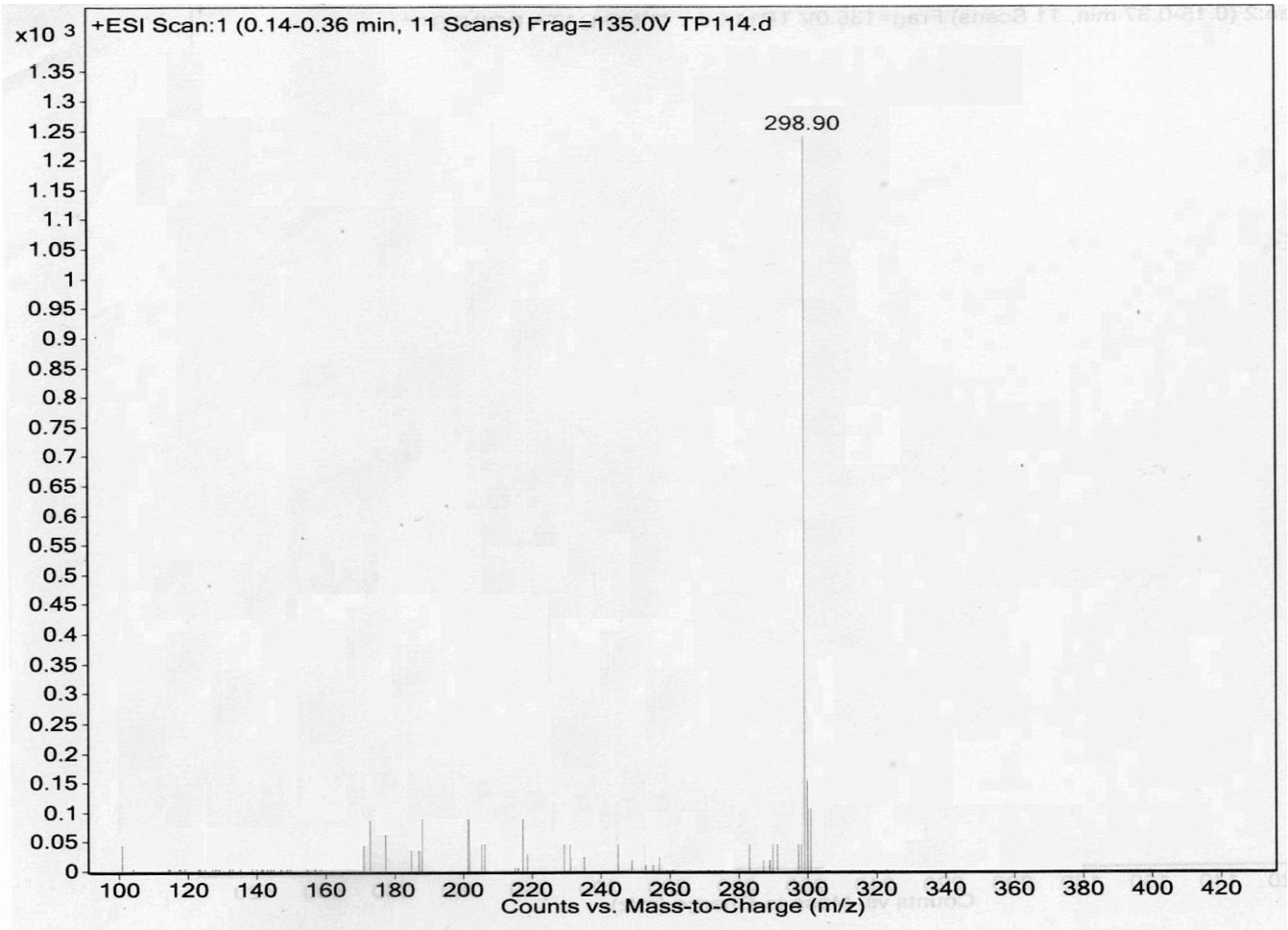
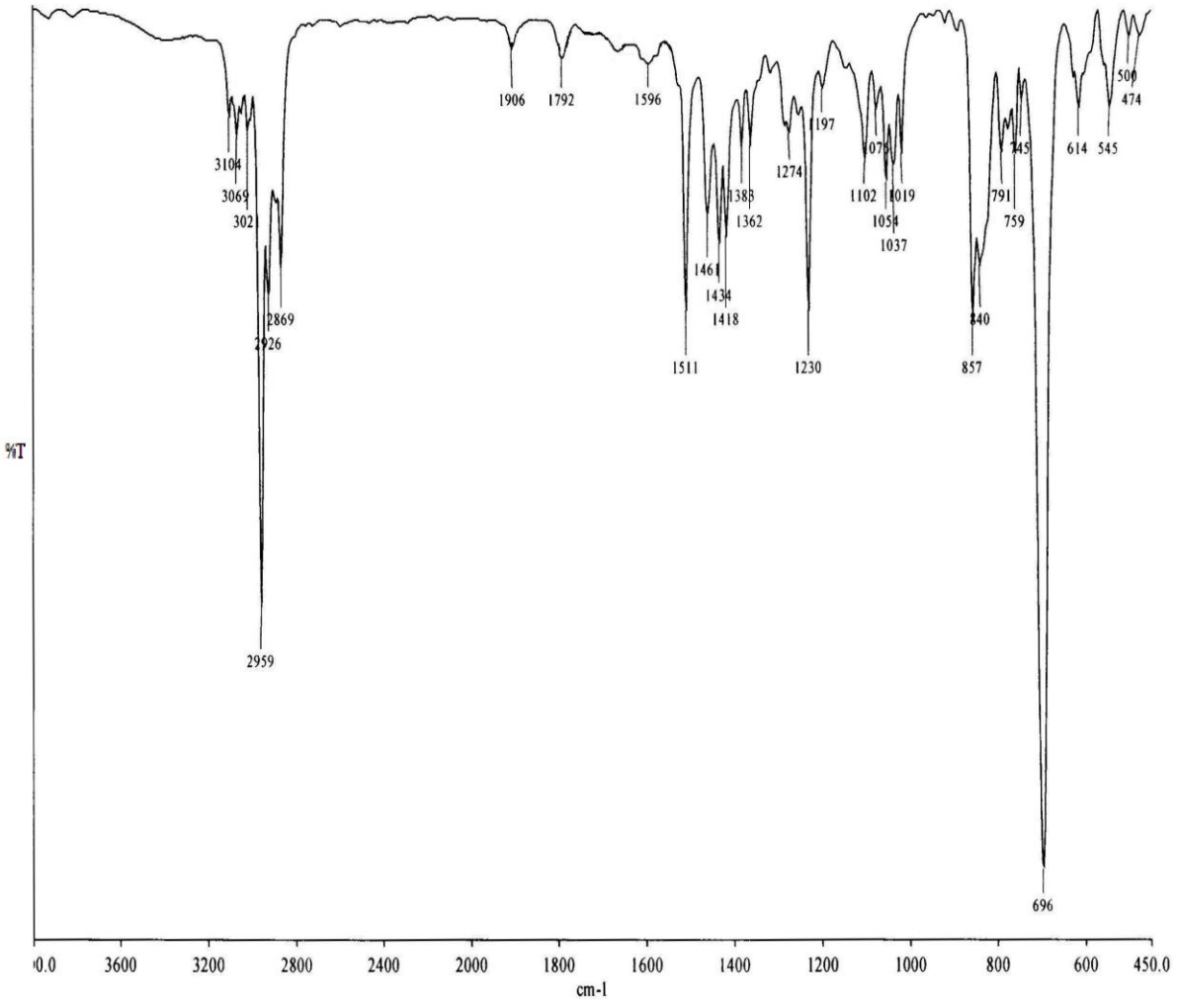


Figure **S7**: Mass spectrum of **3b**.



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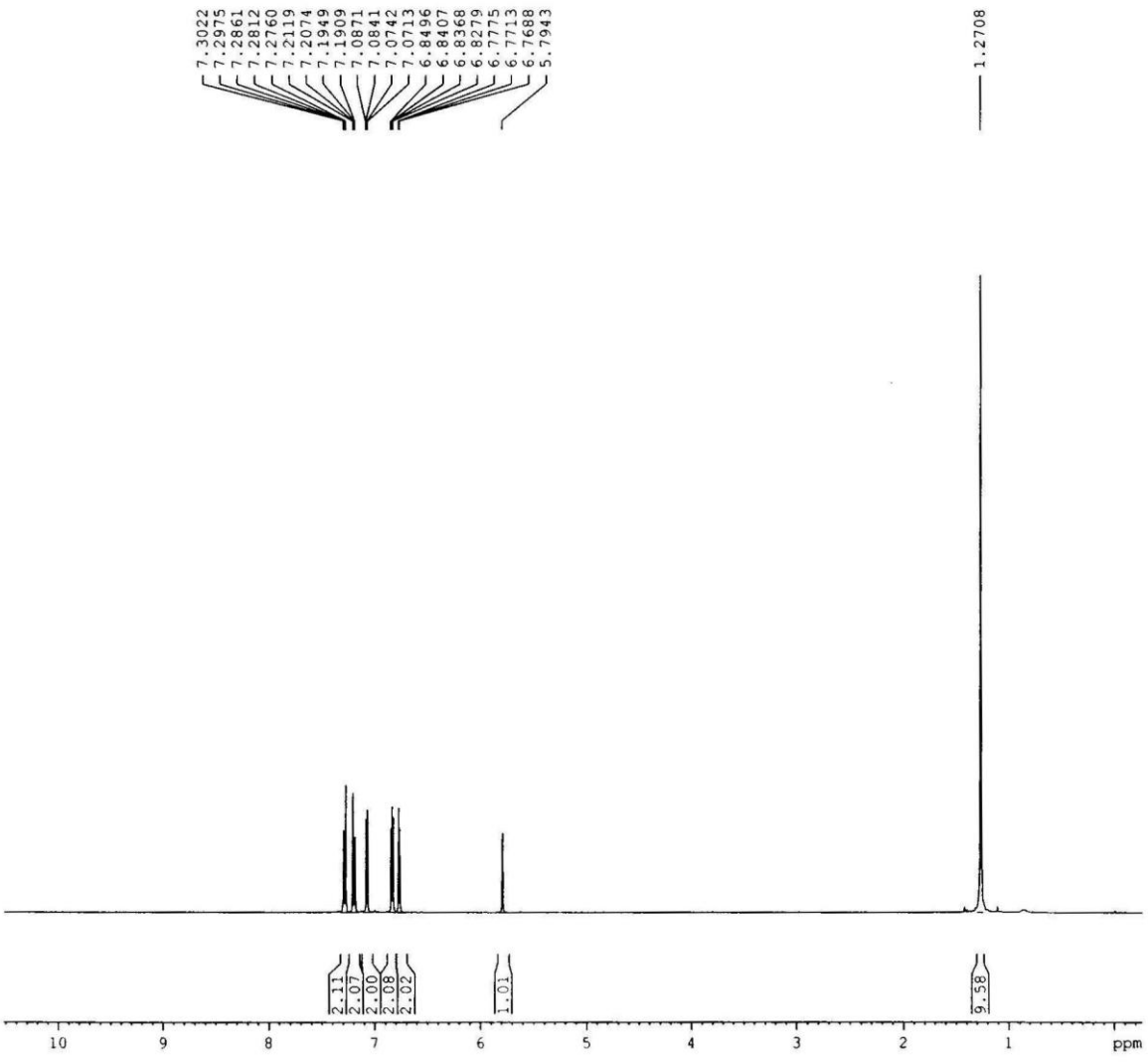

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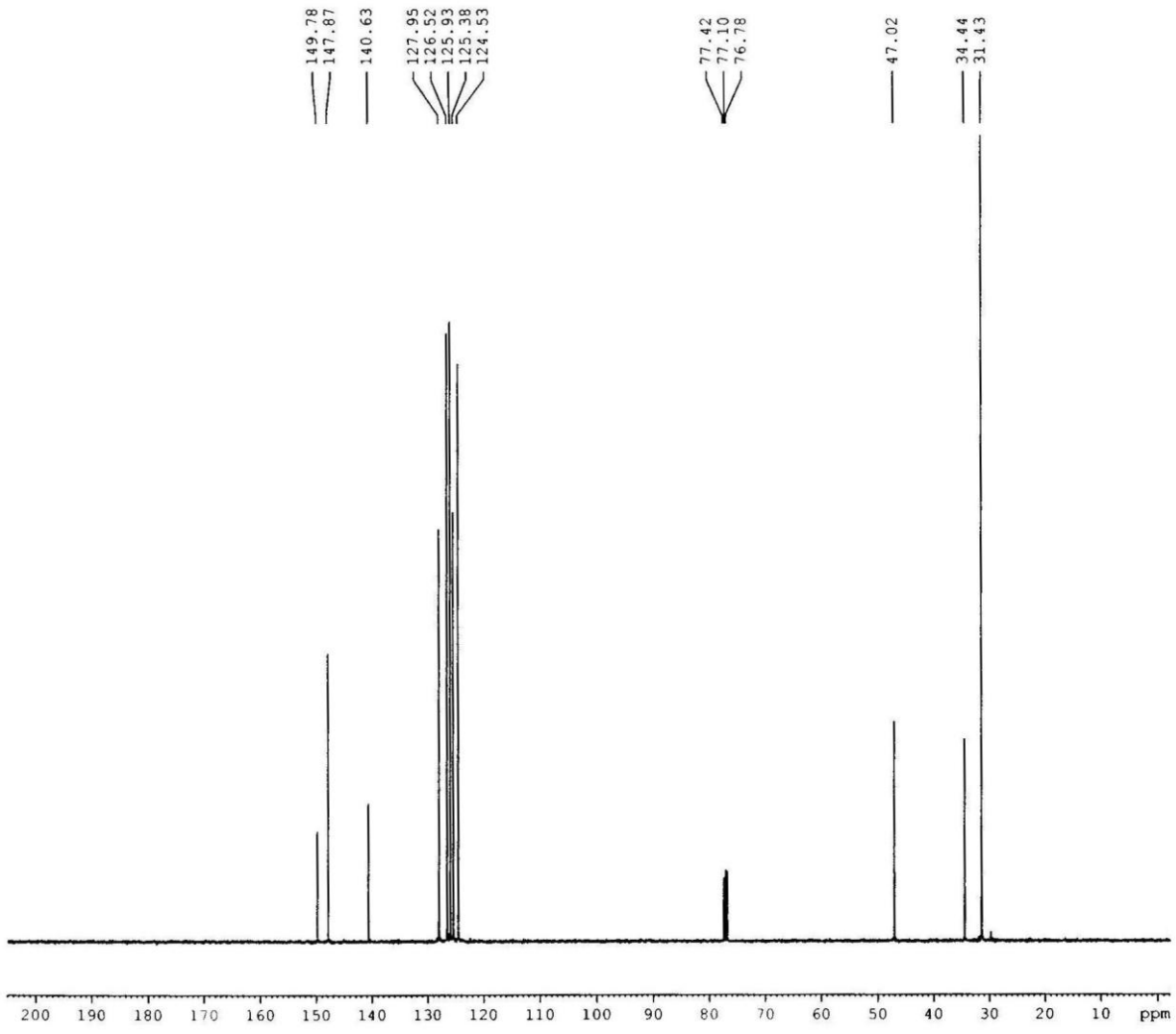
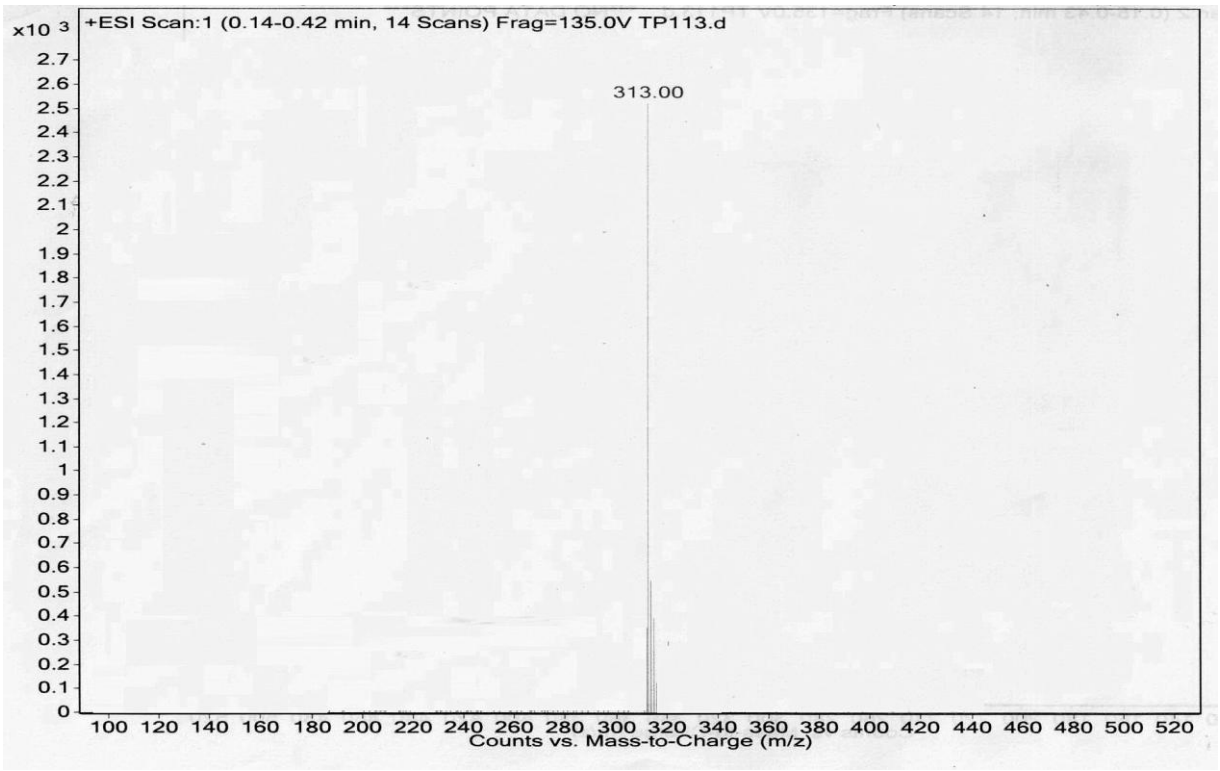


Figure **S10**: ^{13}C NMR spectrum of **3c.**



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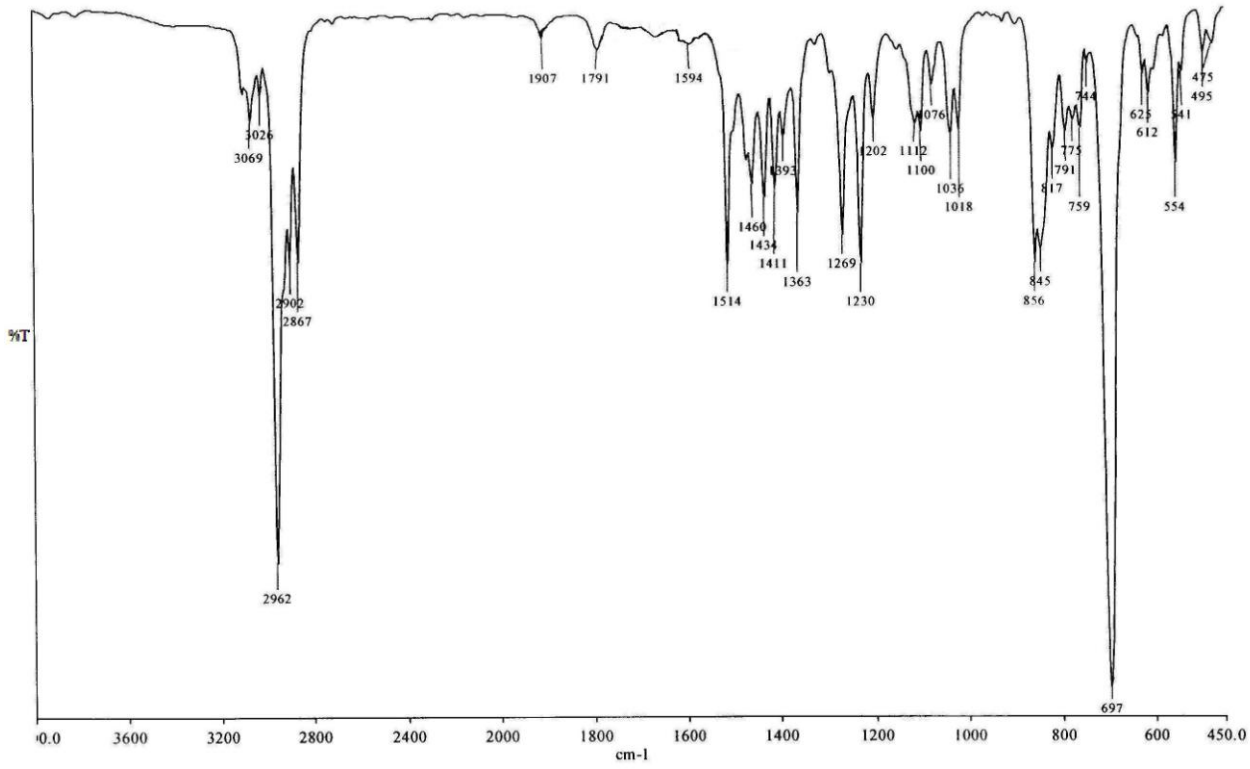

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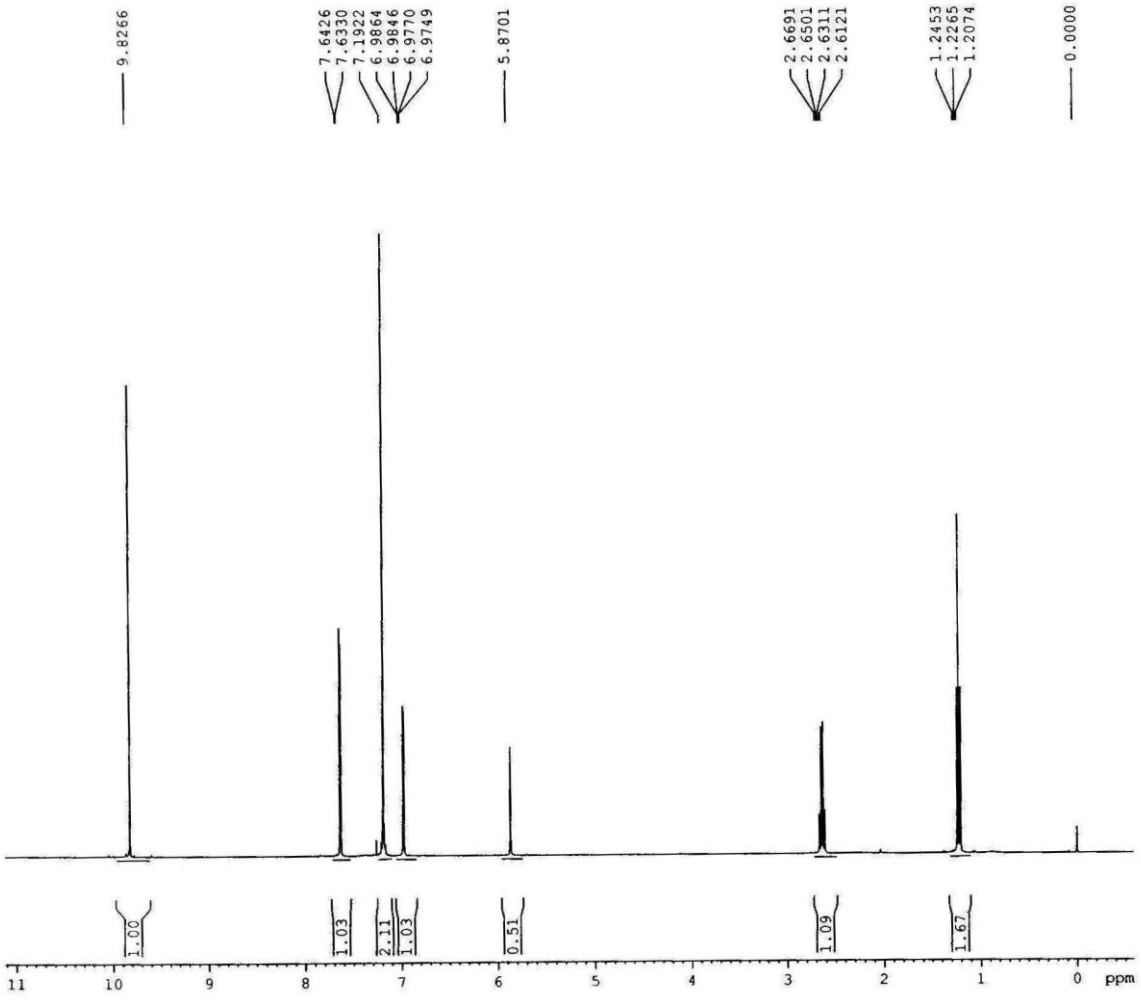

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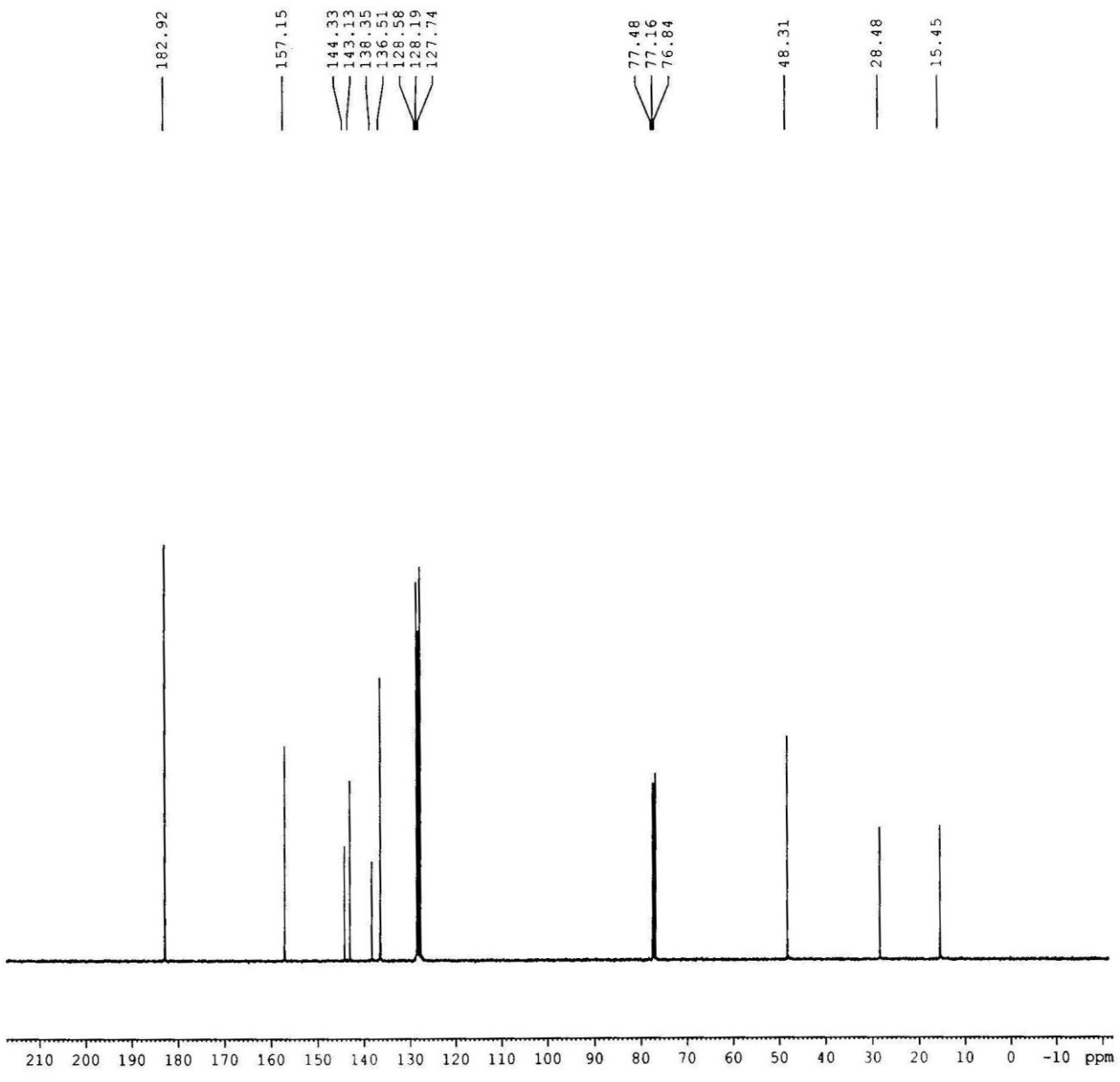


Figure **S14**: ^{13}C NMR spectrum of **4a**.

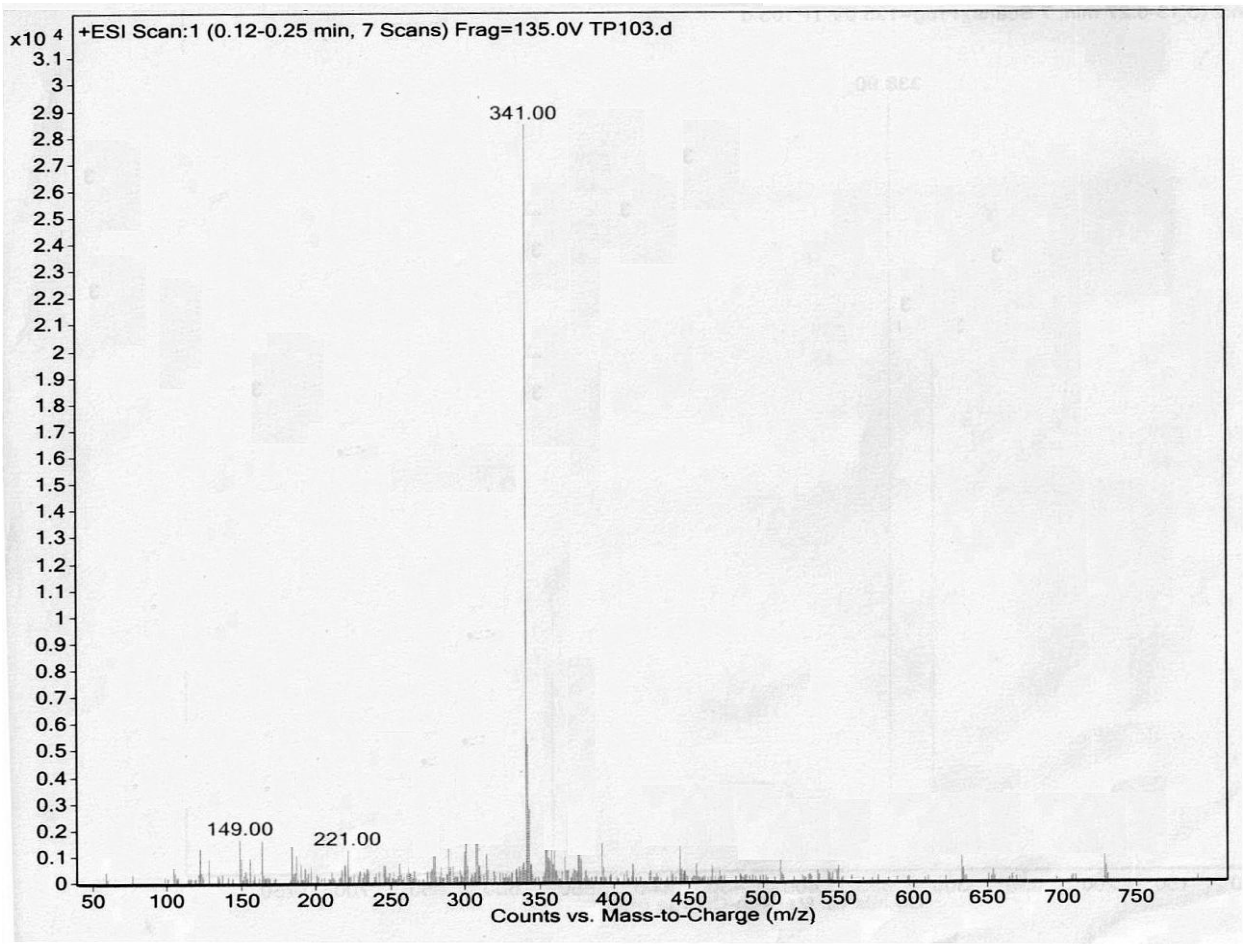


Figure **S15**: Mass spectrum of **4a.**

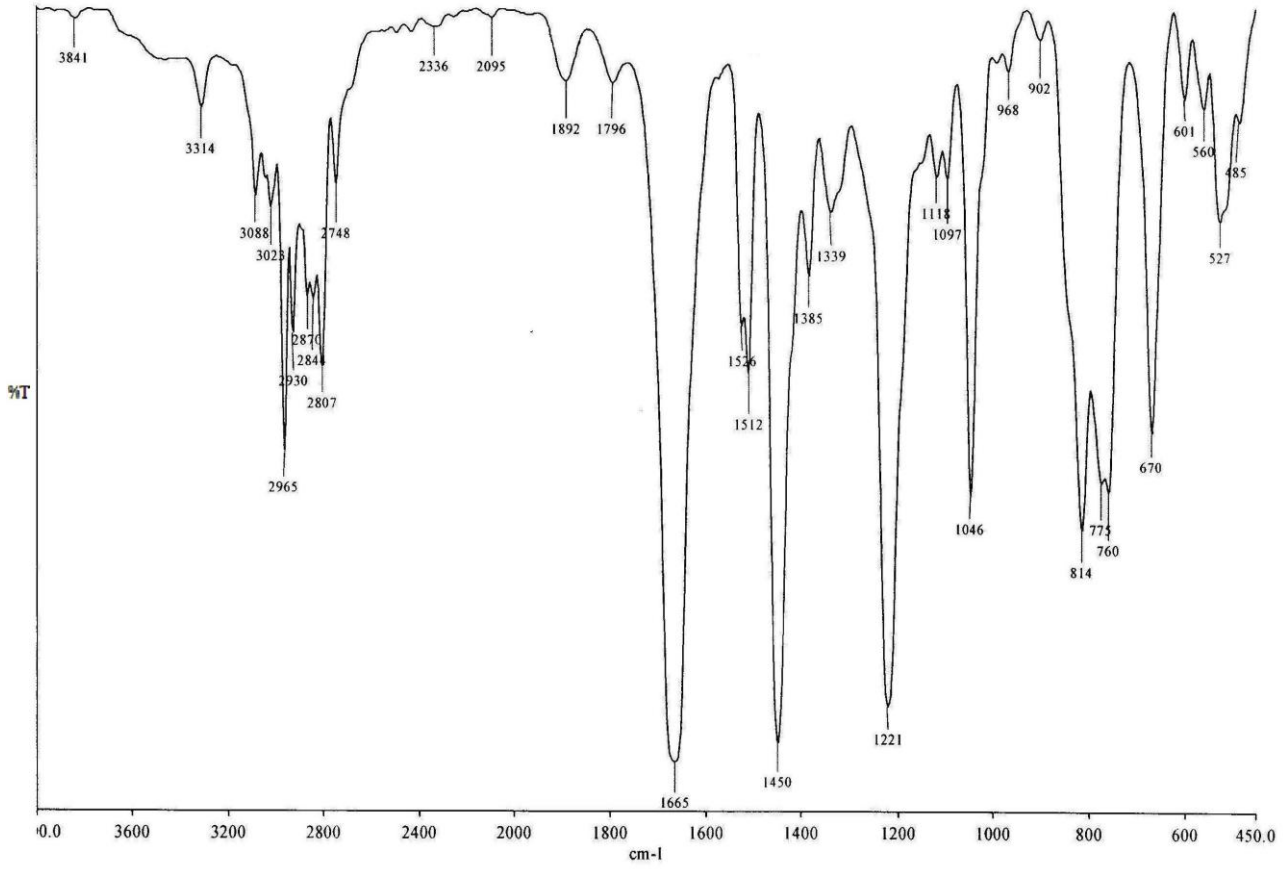
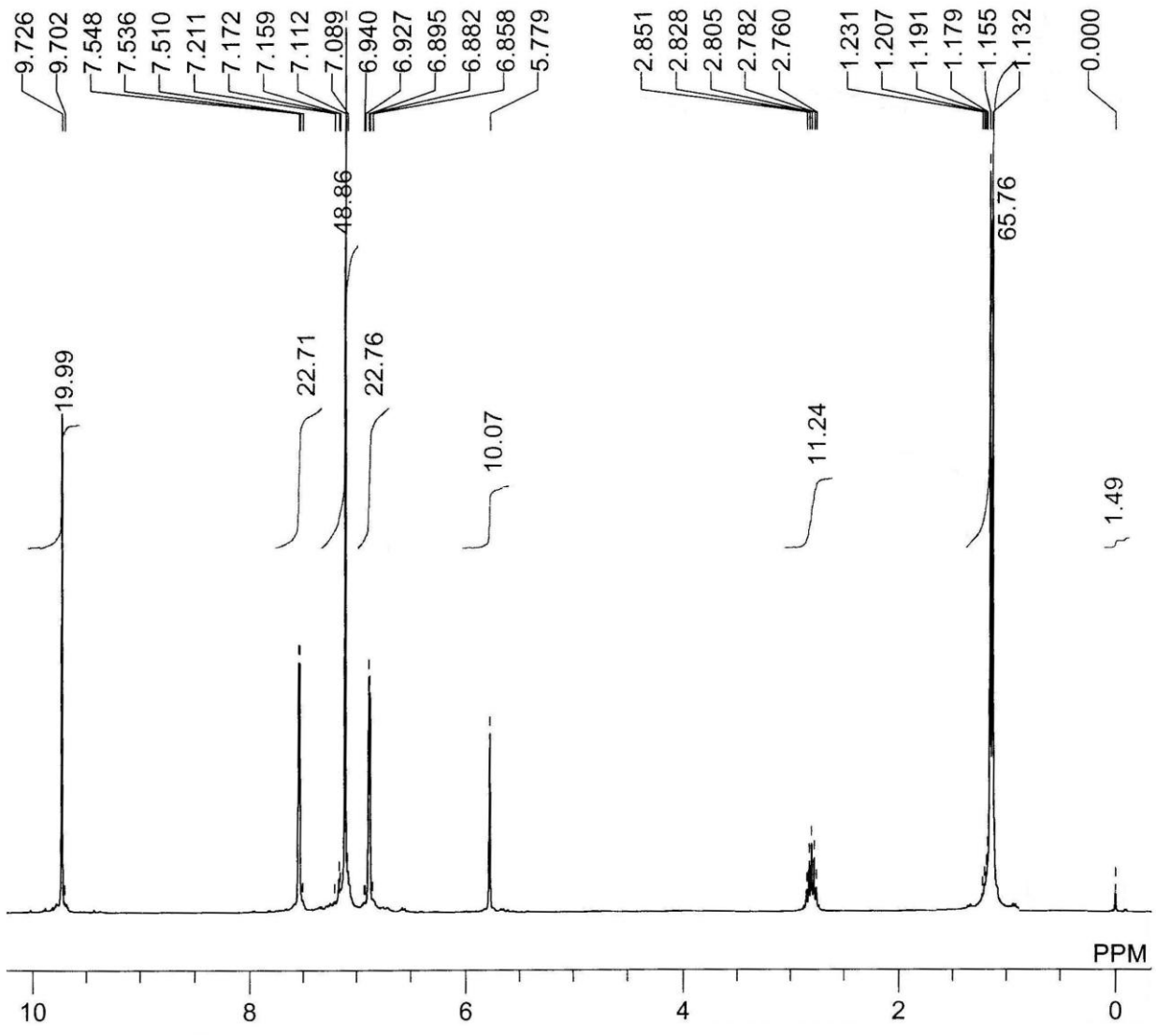


Figure **S16**: IR Spectrum of **4a**.



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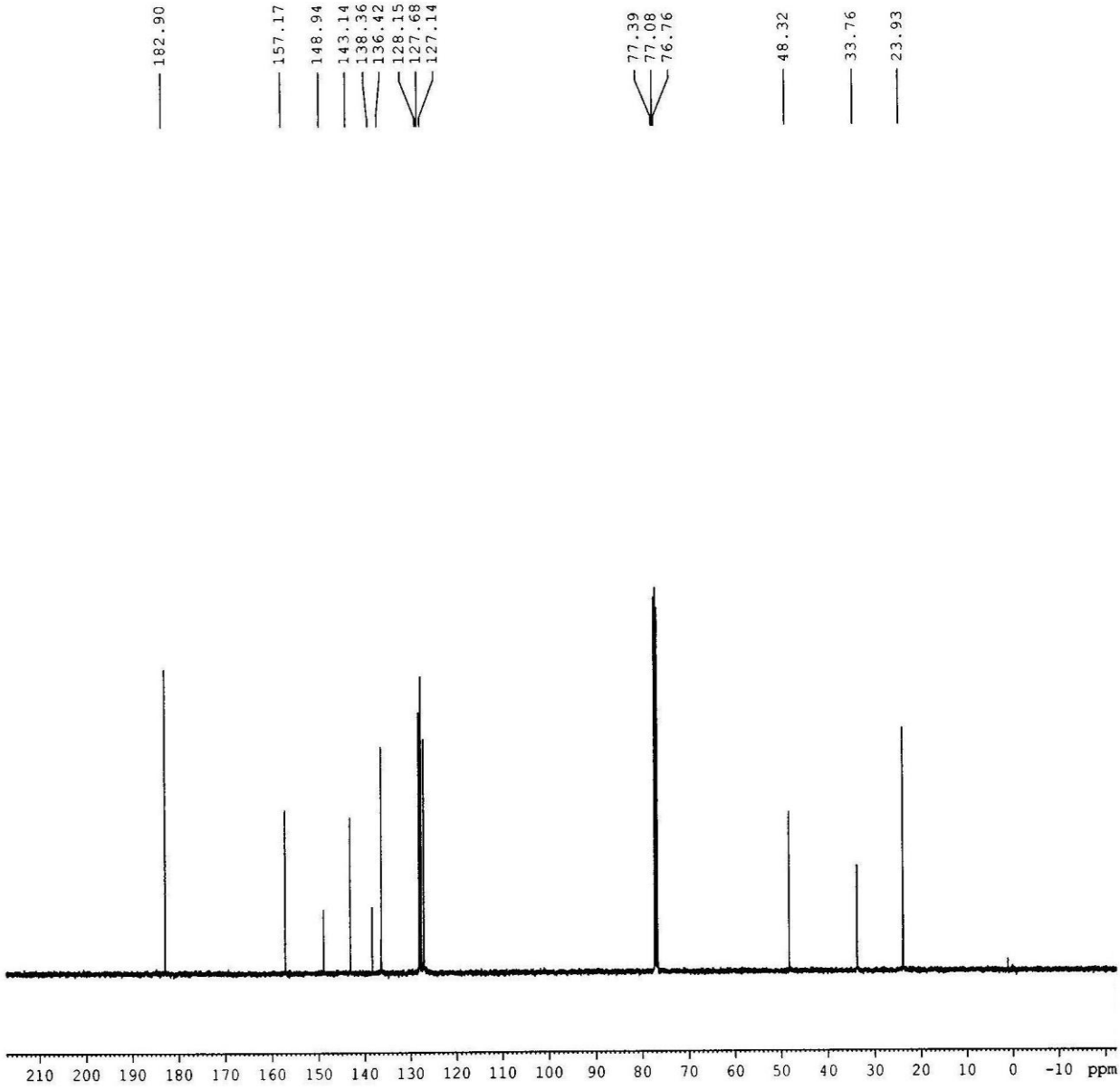

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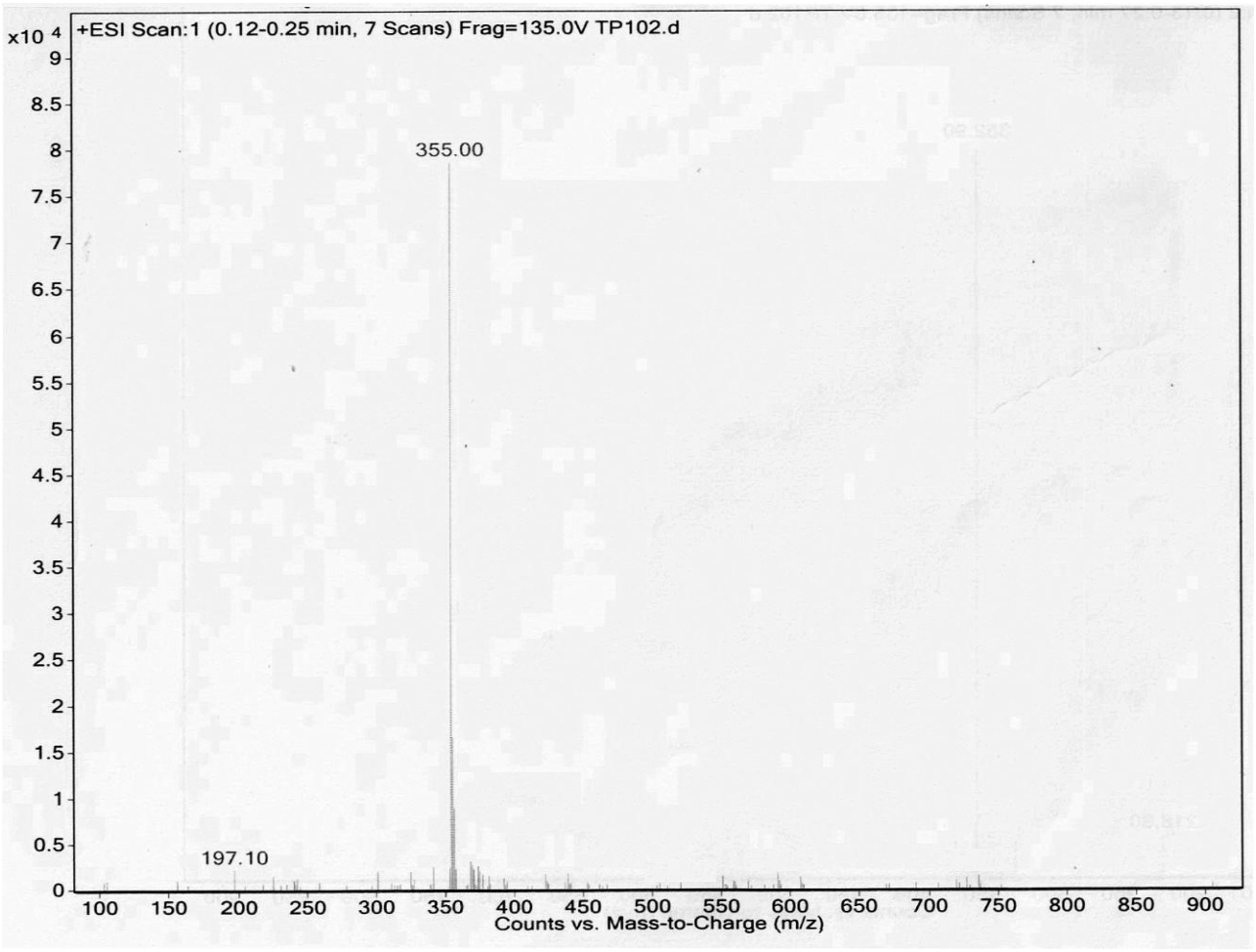

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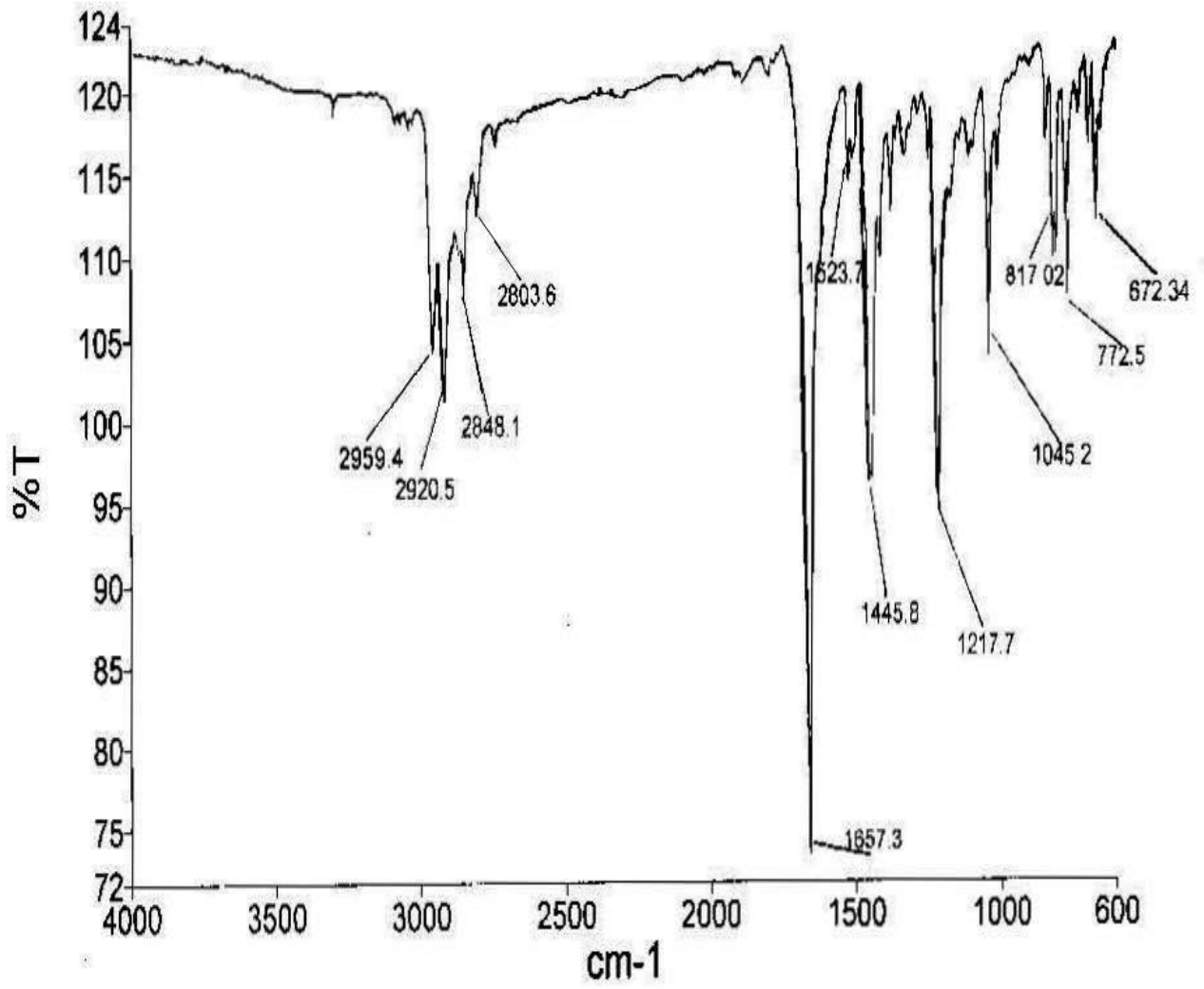

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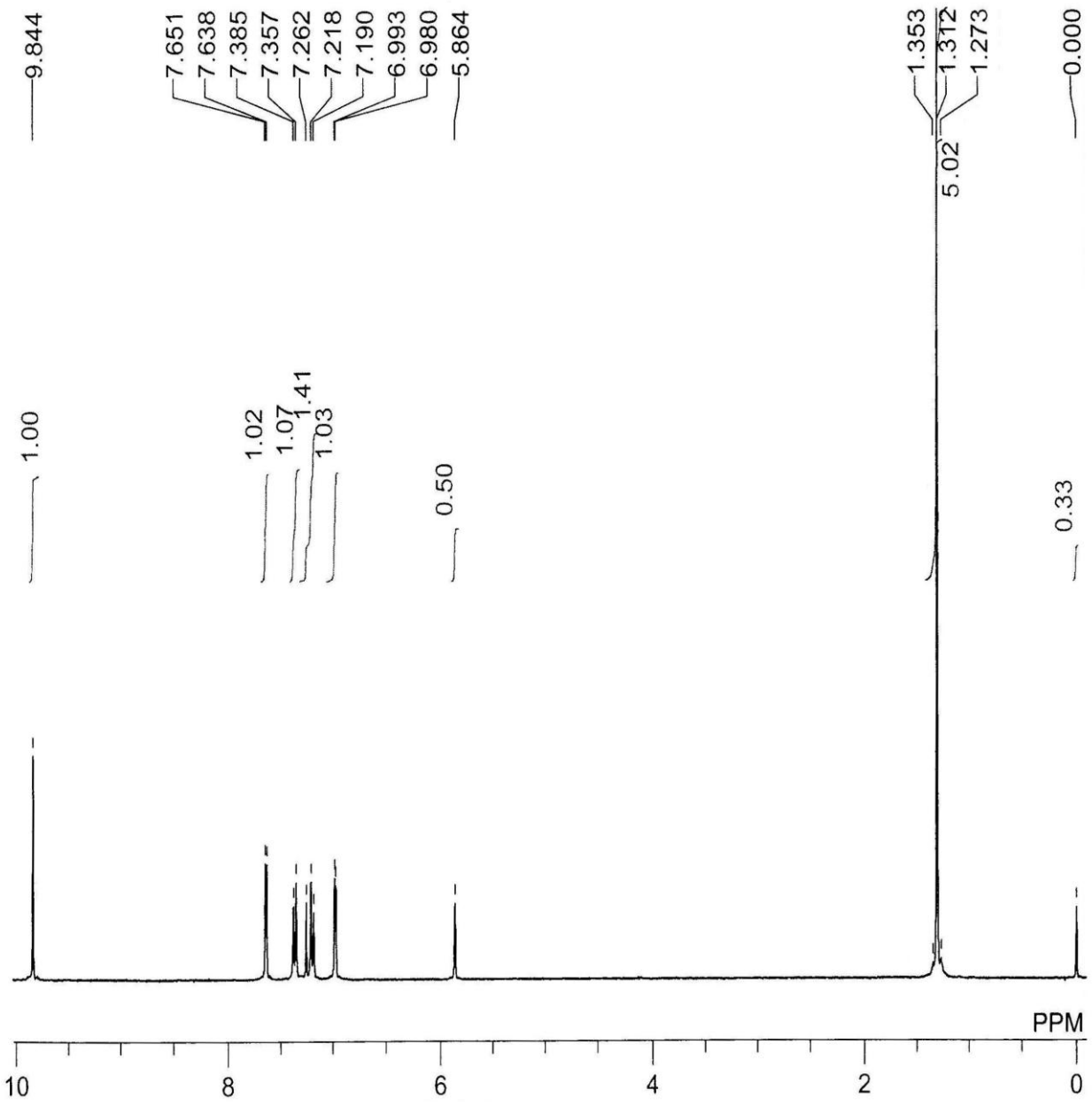


Figure **S21**: ^{1}H NMR Spectrum of **4c**.

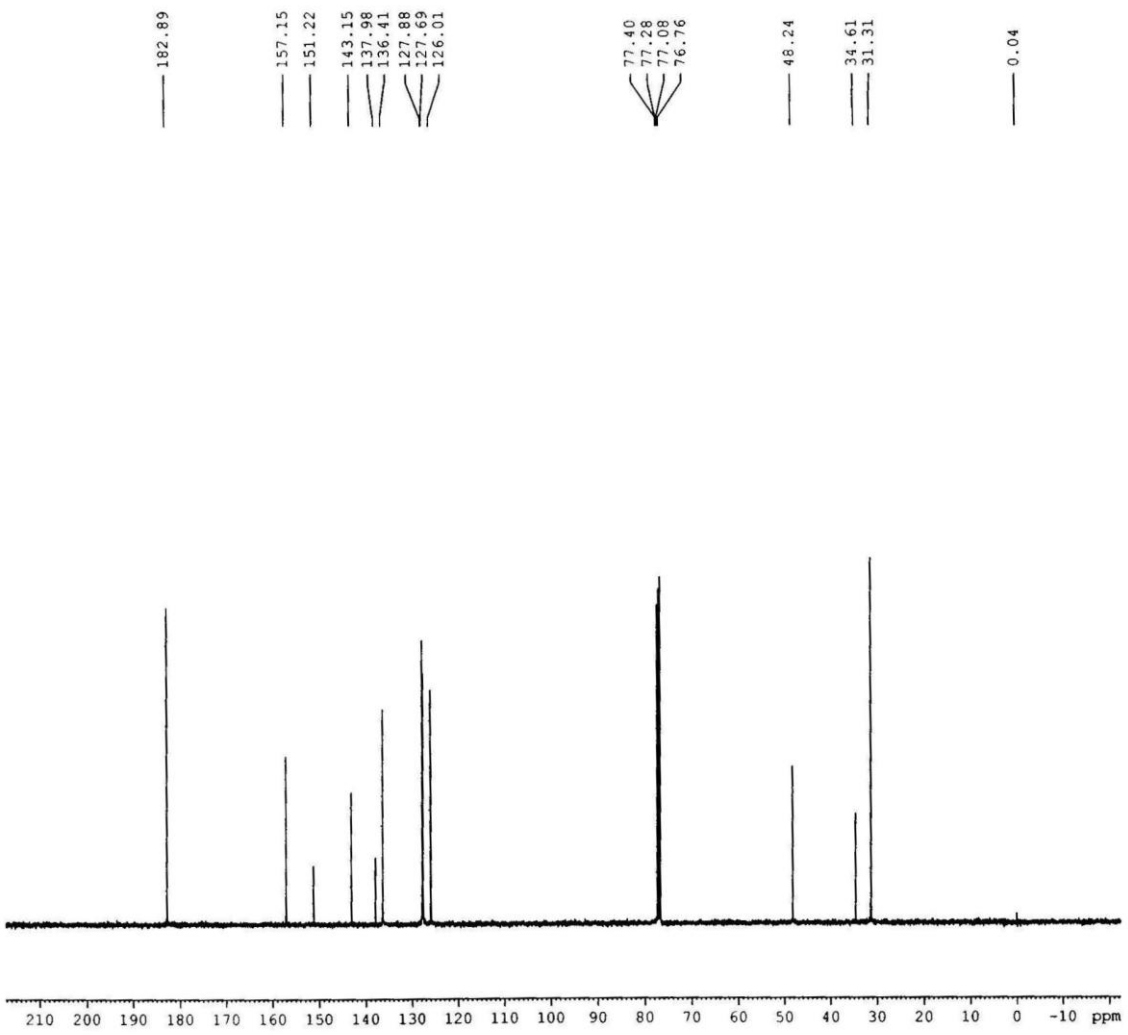


Figure **S22**: ^{13}C NMR Spectrum of **4c**.

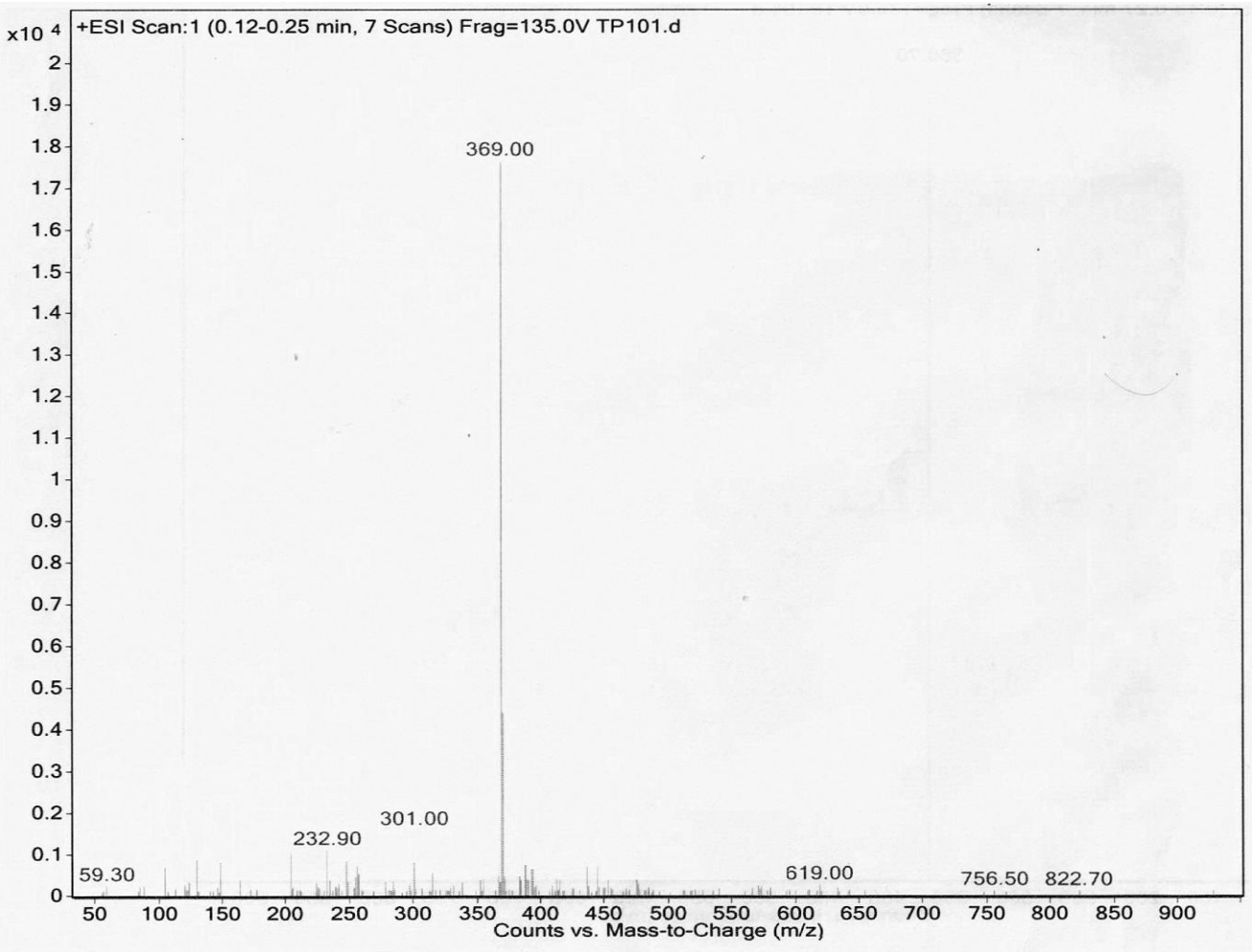
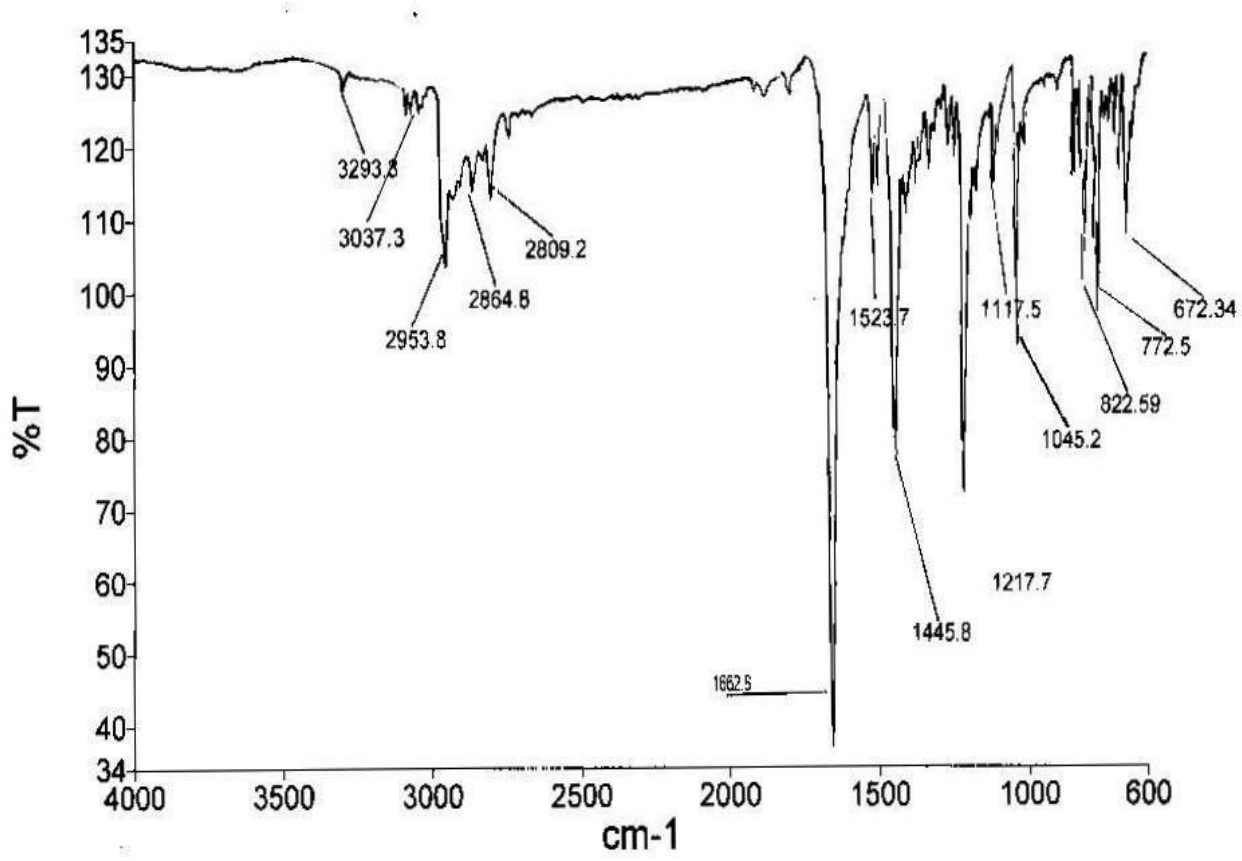


Figure **S23**: Mass spectrum of **4c**.



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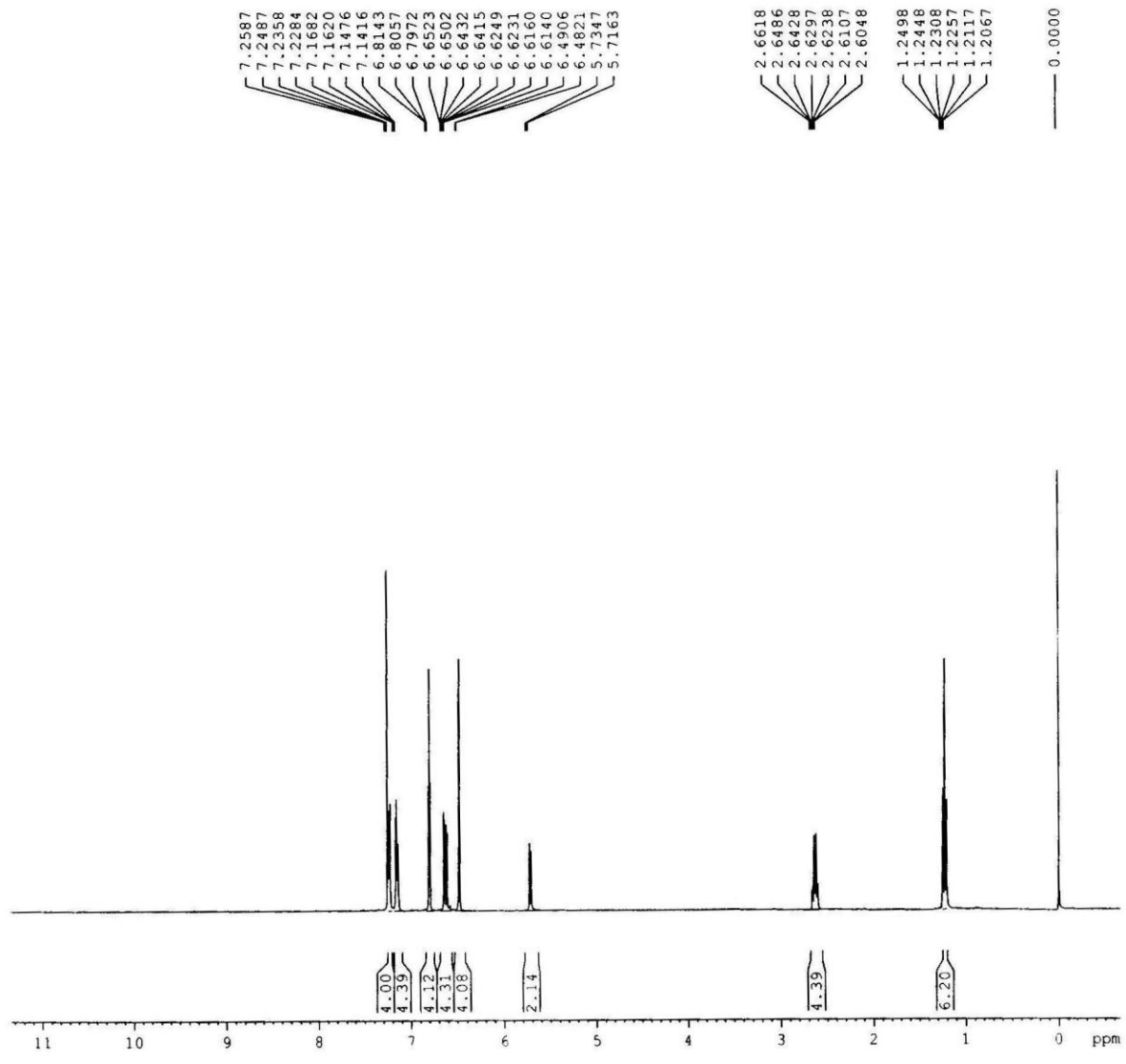


Figure **S25**: ^{1}H NMR Spectrum of **5a**.

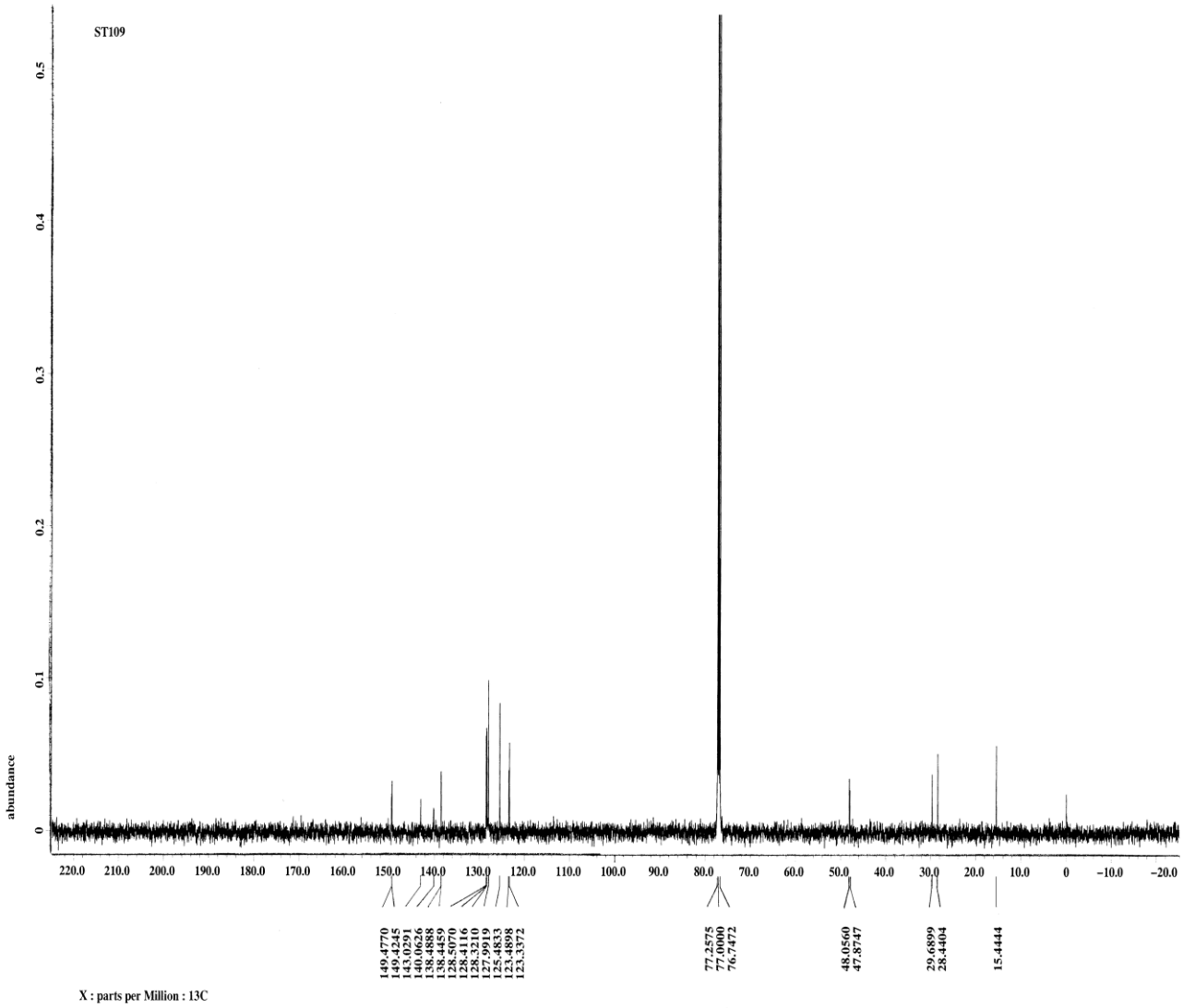
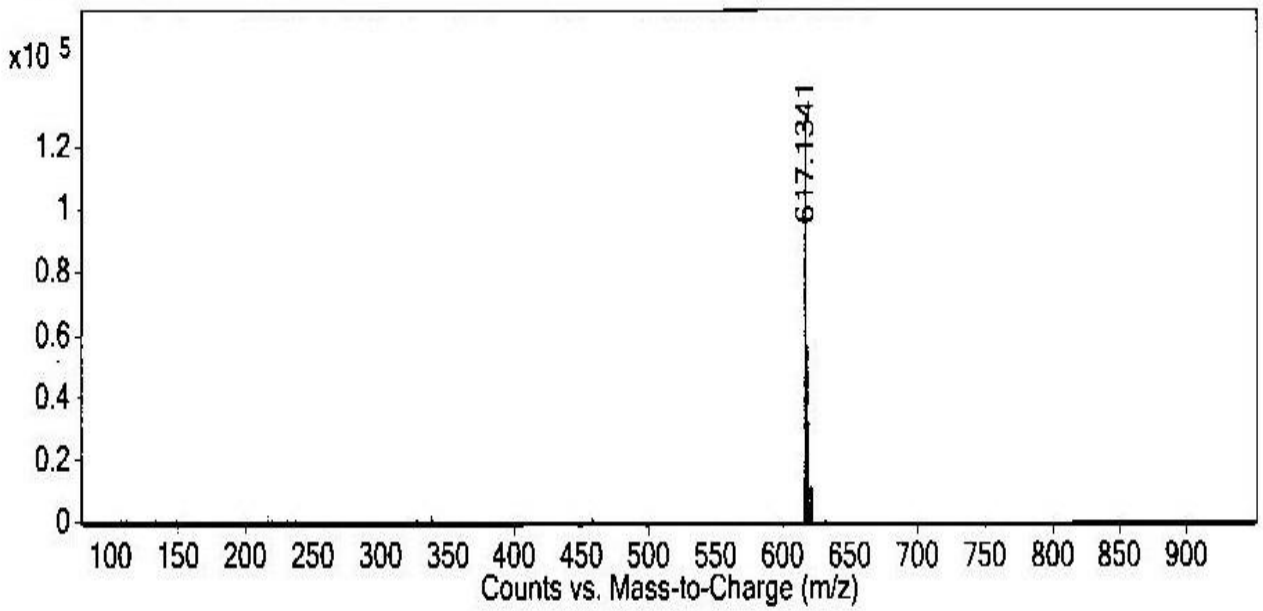


Figure **S26**: ^{13}C NMR Spectrum of **5a**.



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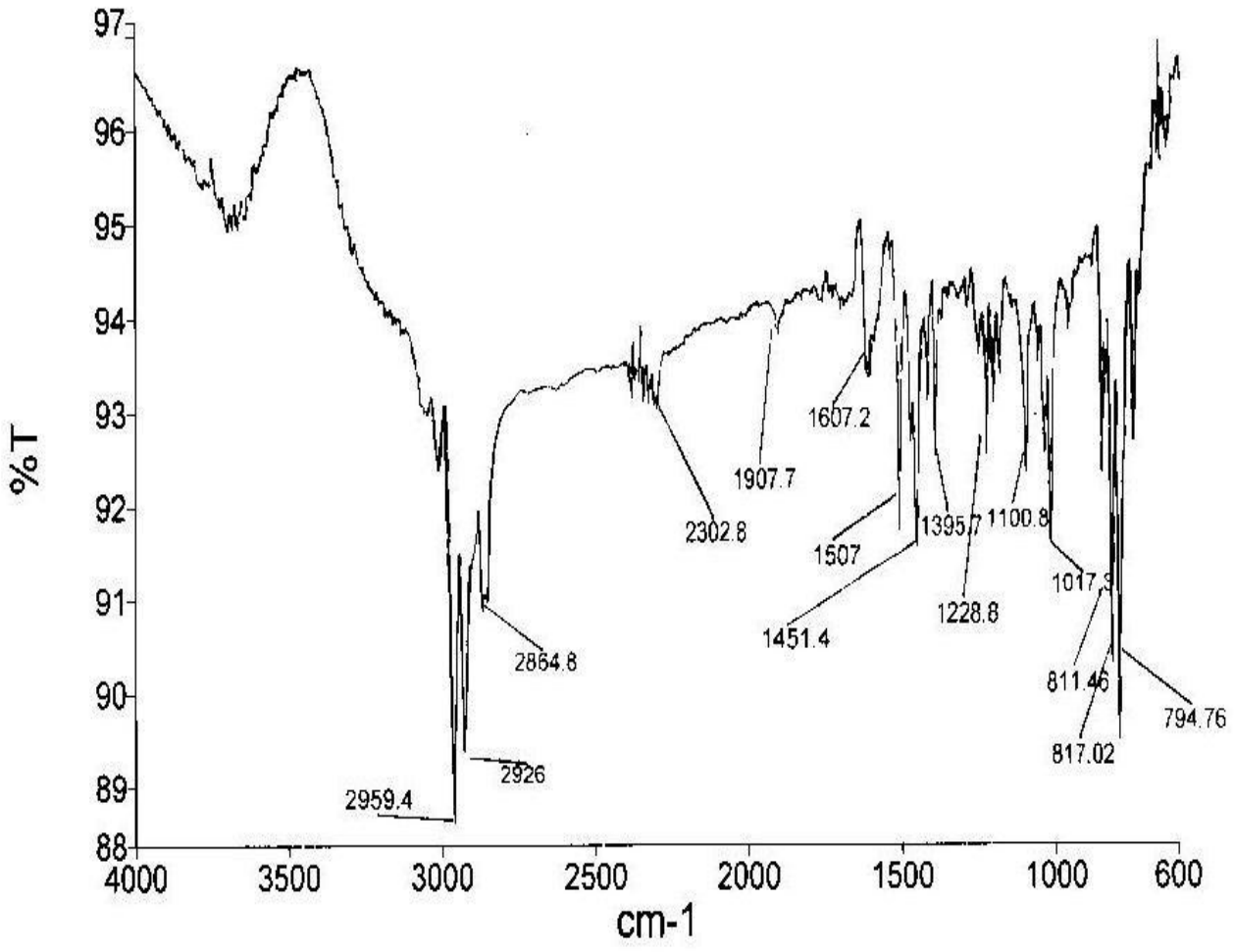
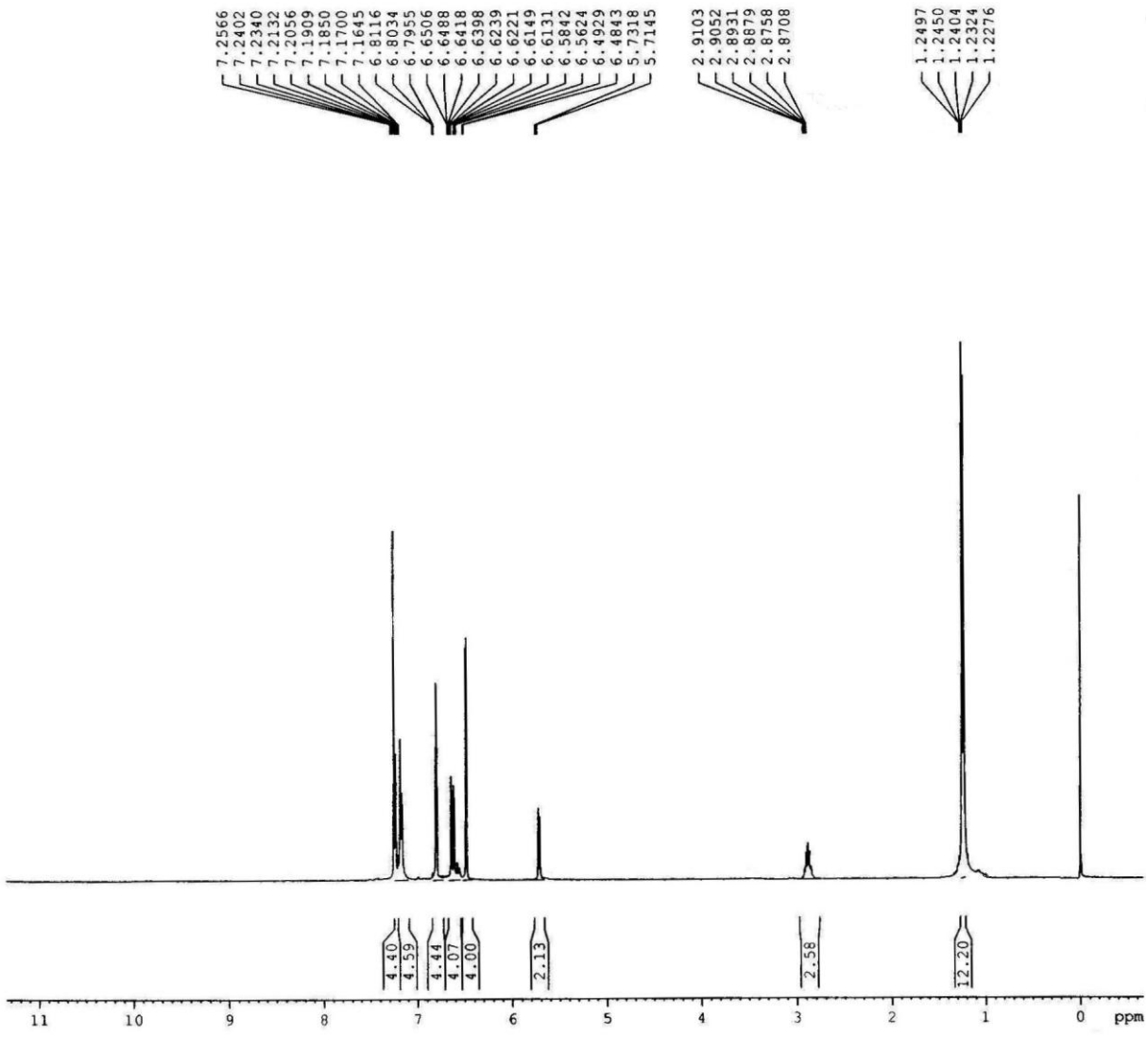


Figure **S28**: IR Spectrum of **5a**.



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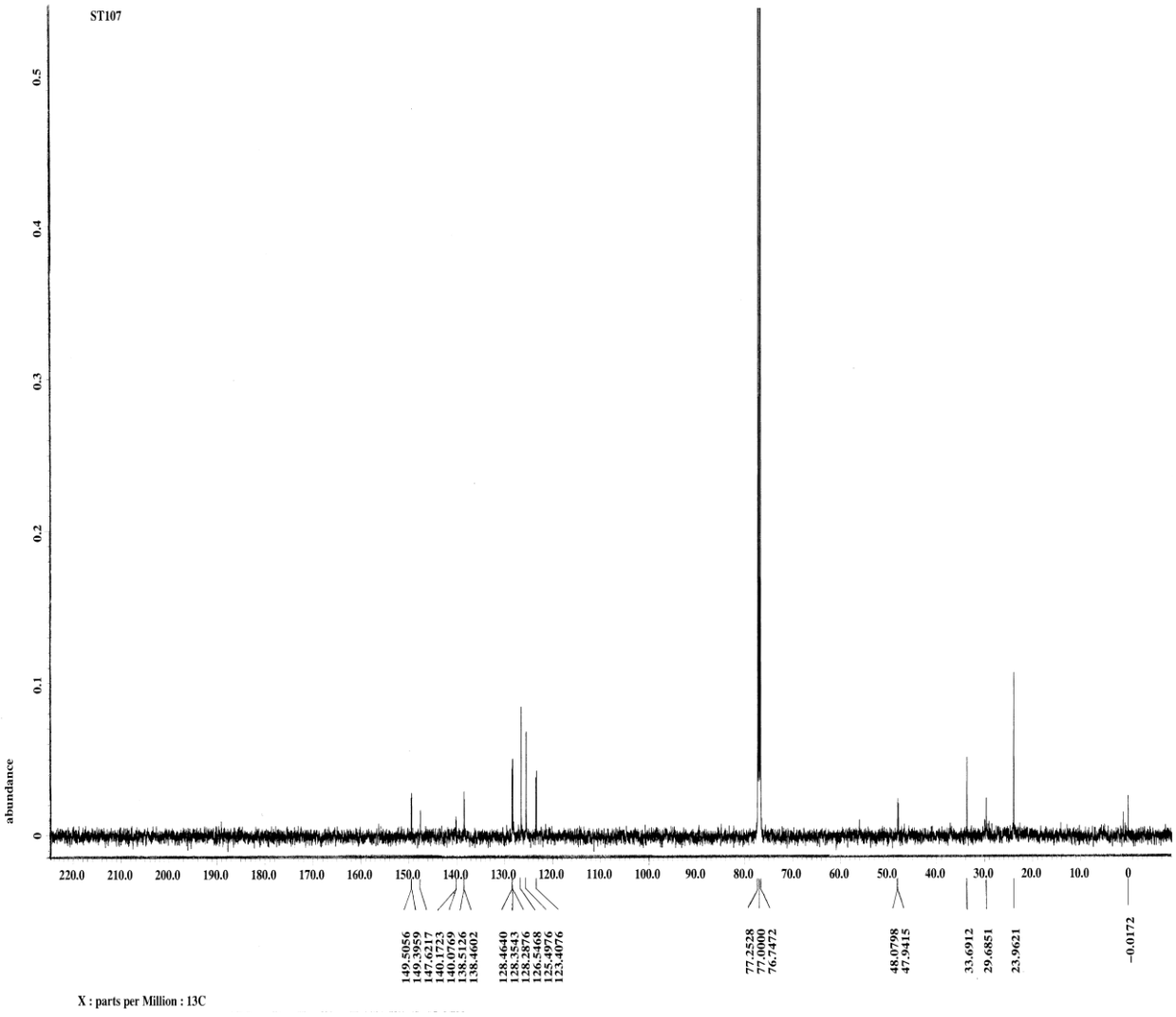


Figure **S30**: ^{13}C NMR Spectrum of **5b**.

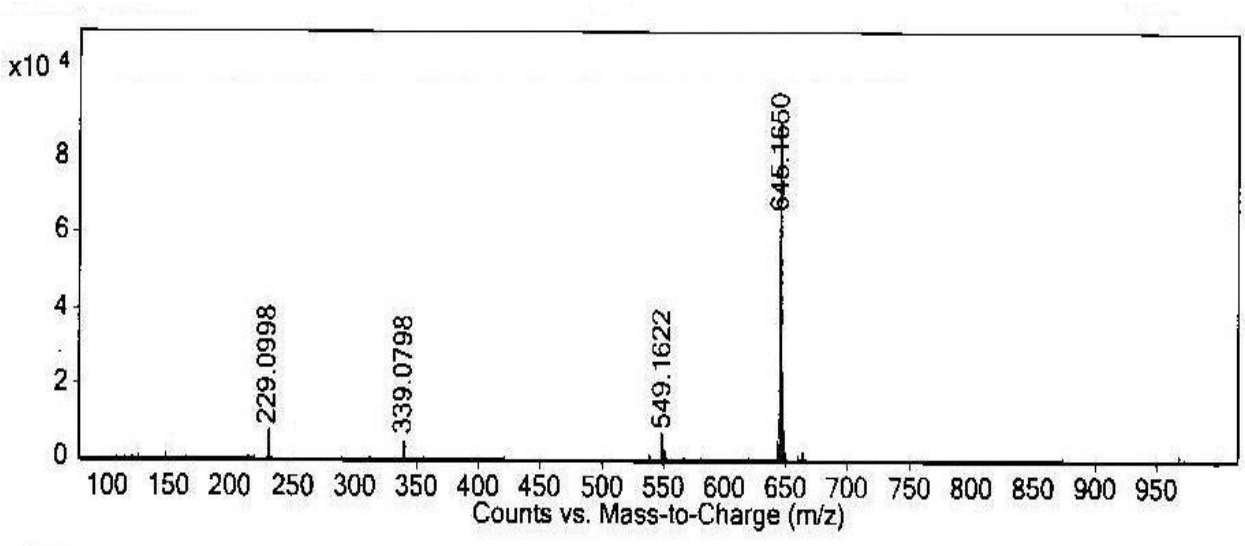


Figure **S31**: Mass spectrum of **5b**.

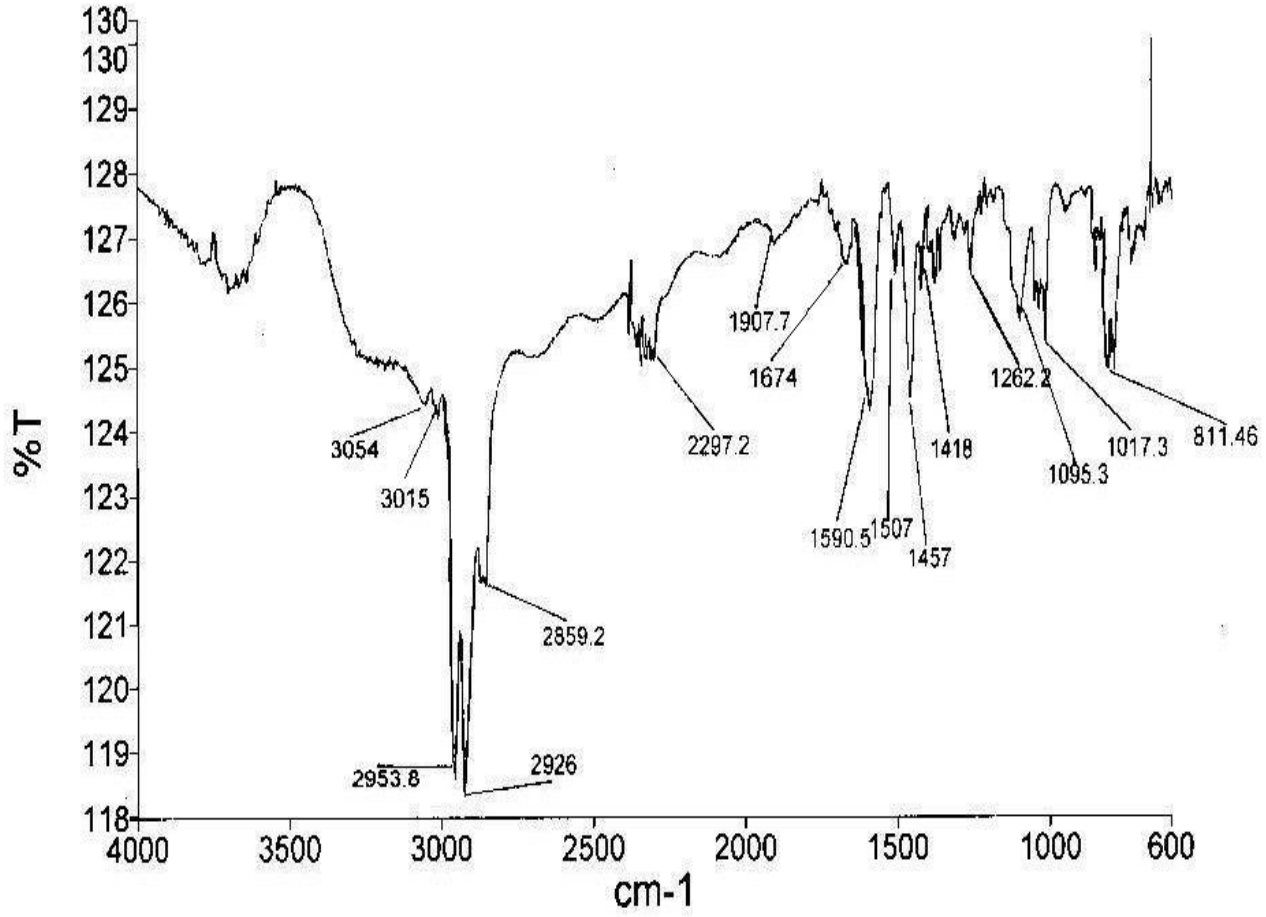


Figure **S32**: IR Spectrum of **5b**.

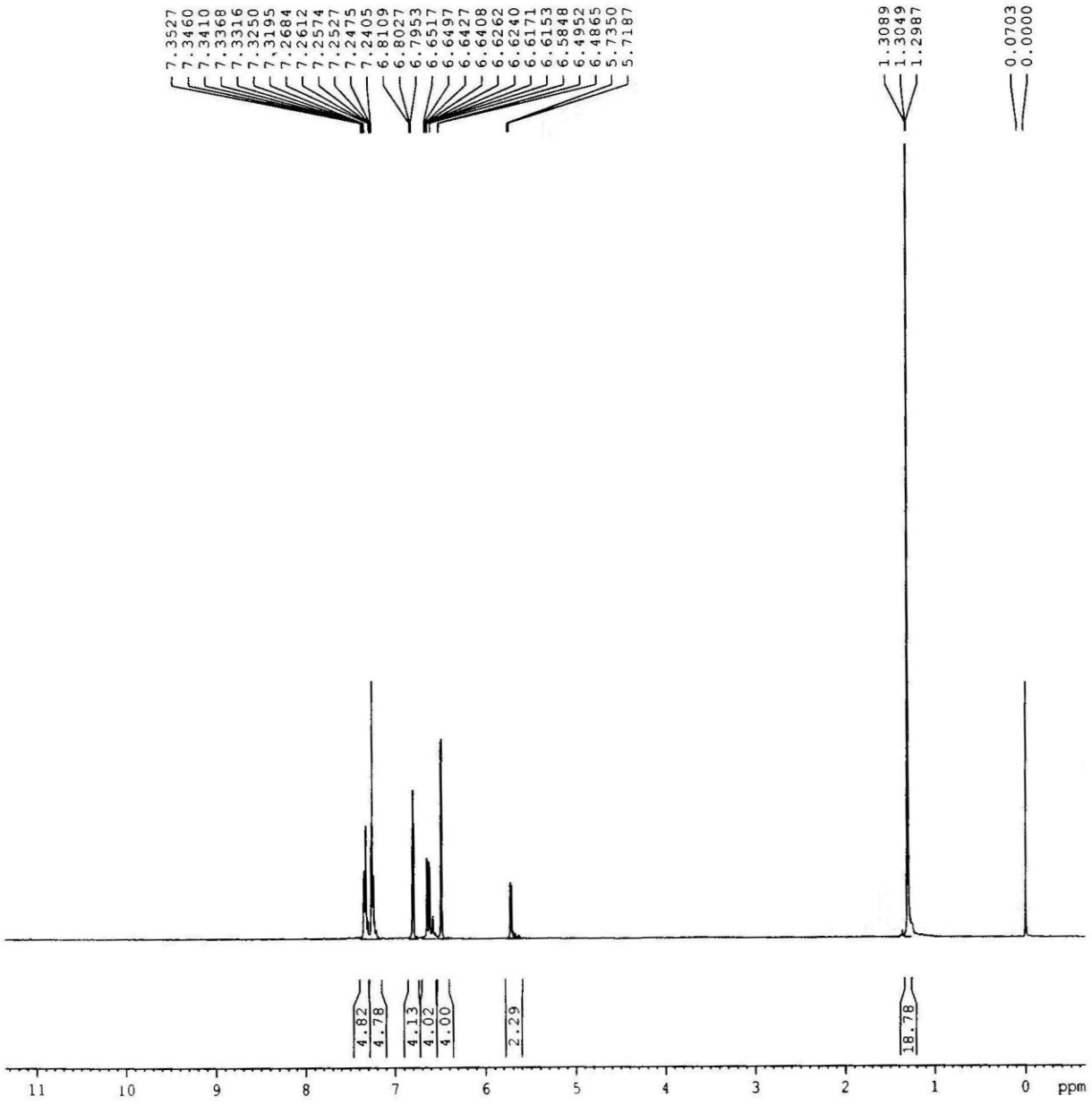


Figure **S33**: ^{1}H NMR Spectrum of **5c**.

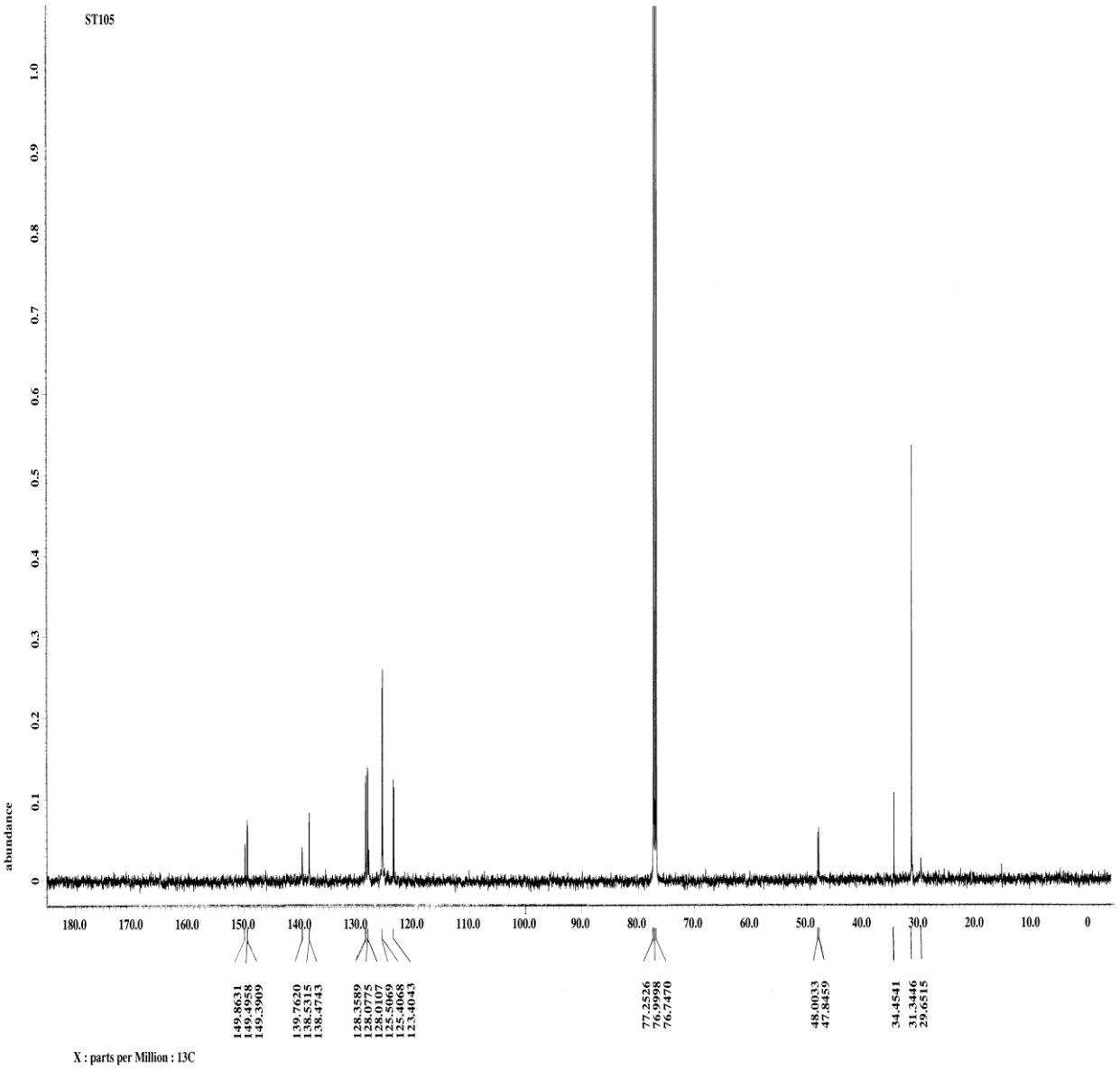
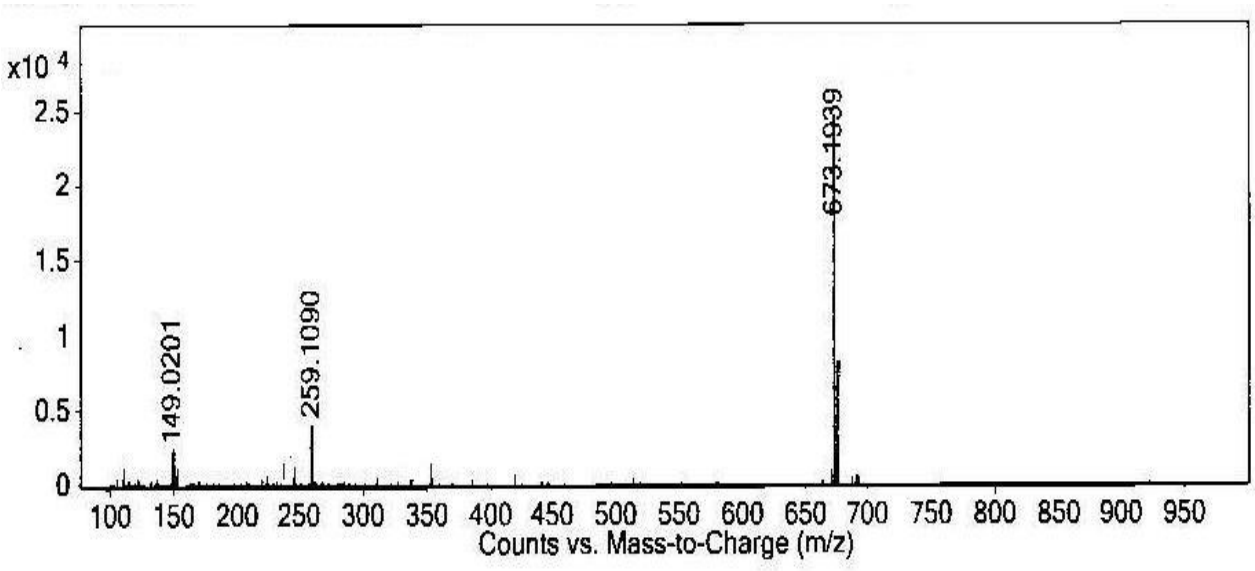


Figure **S34**: ^{13}C NMR Spectrum of **5c**.



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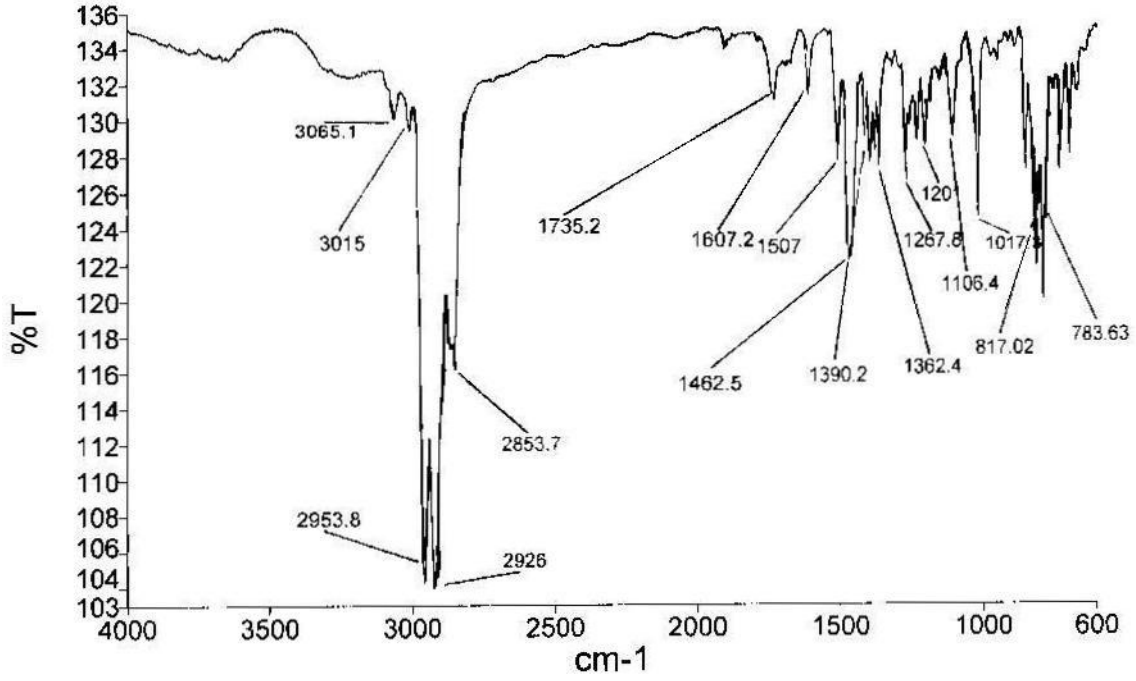


Figure **S36**: IR Spectrum of **5c**.

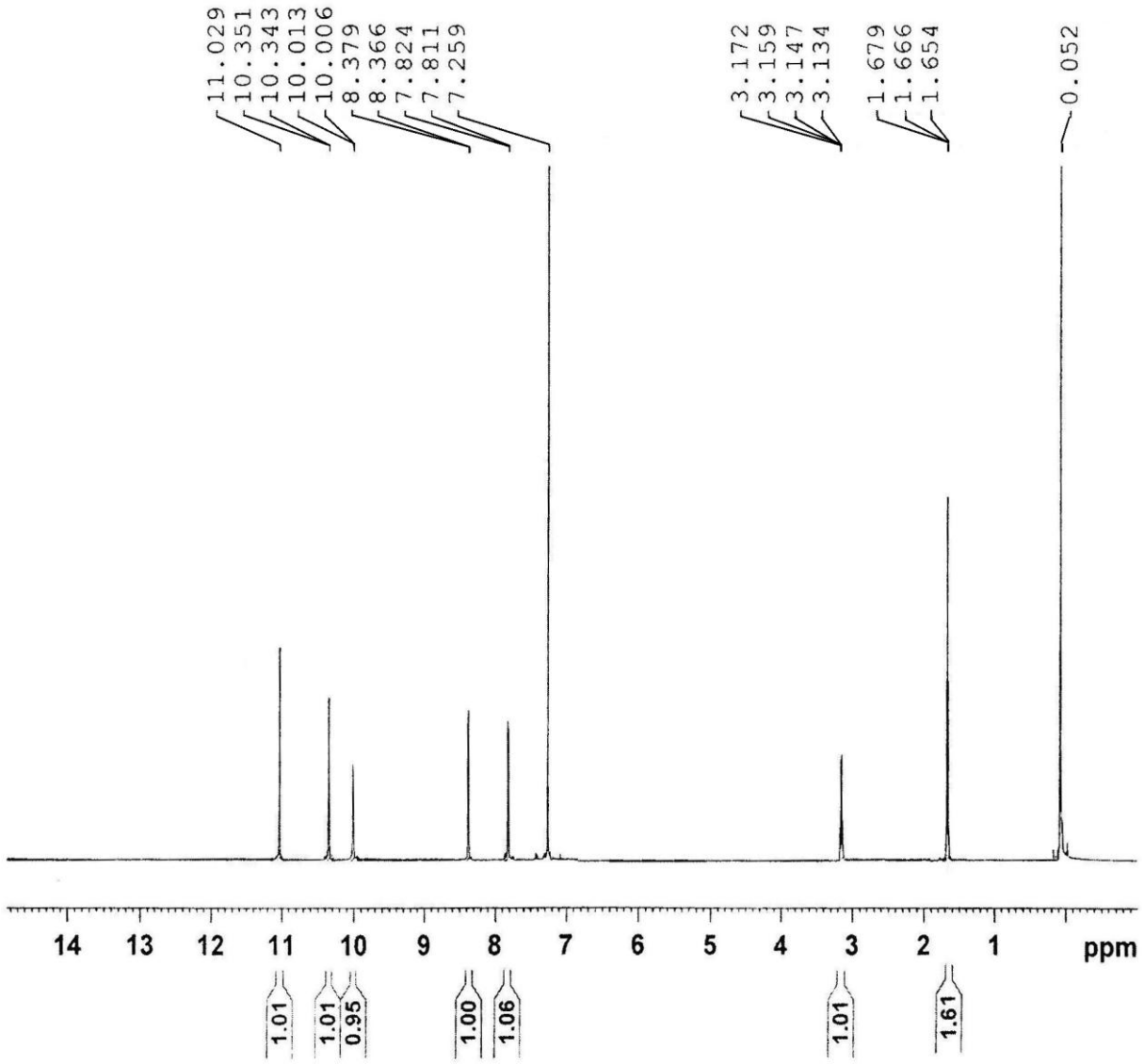


Figure **S37**: ^{1}H NMR Spectrum of **6a**.

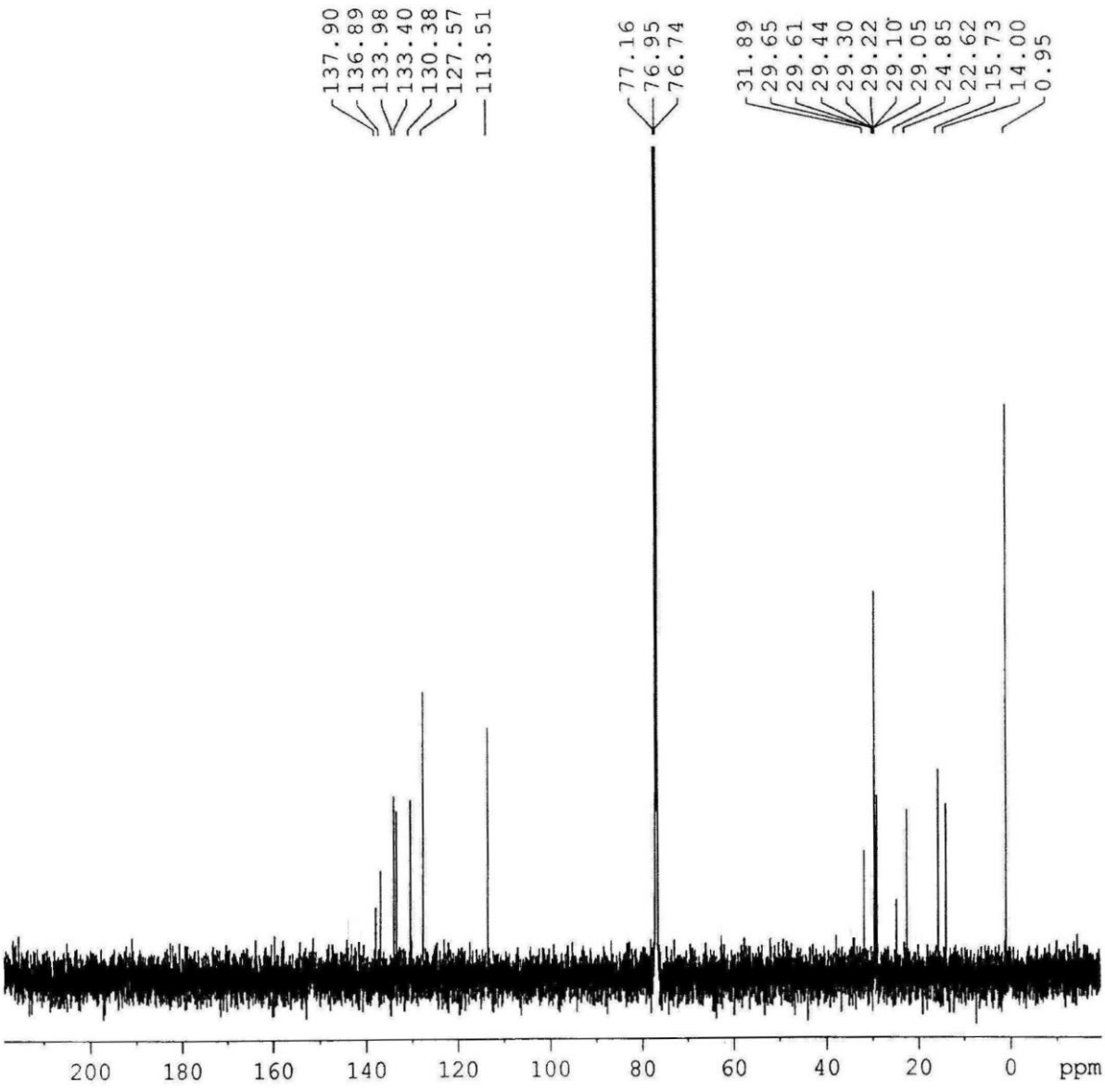


Figure **S38**: ^{13}C NMR Spectrum of **6a**.

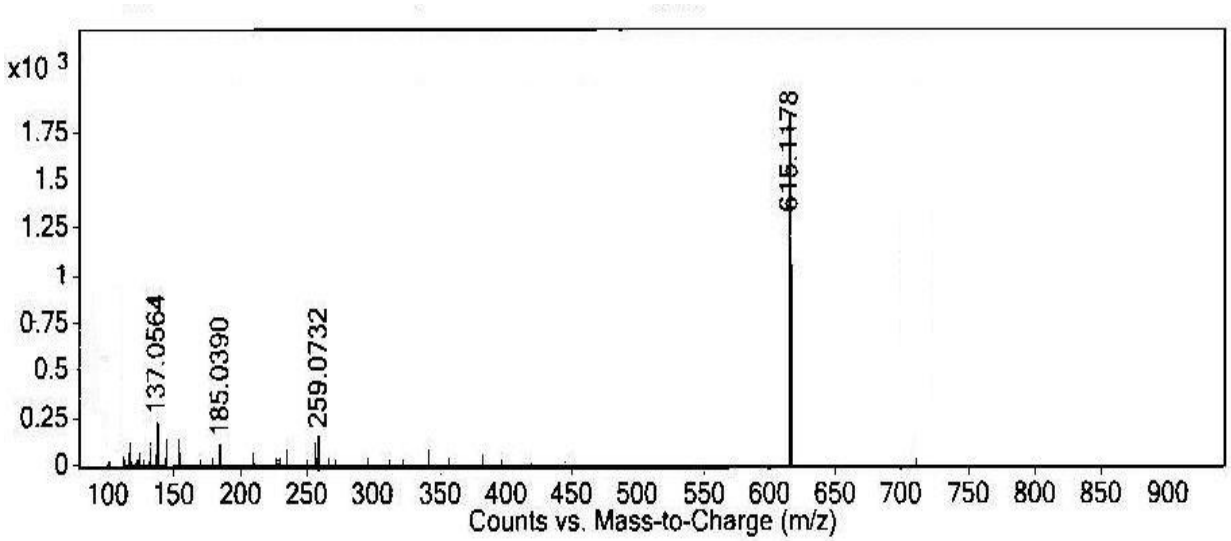


Figure **S39**: Mass Spectrum of **6a**.

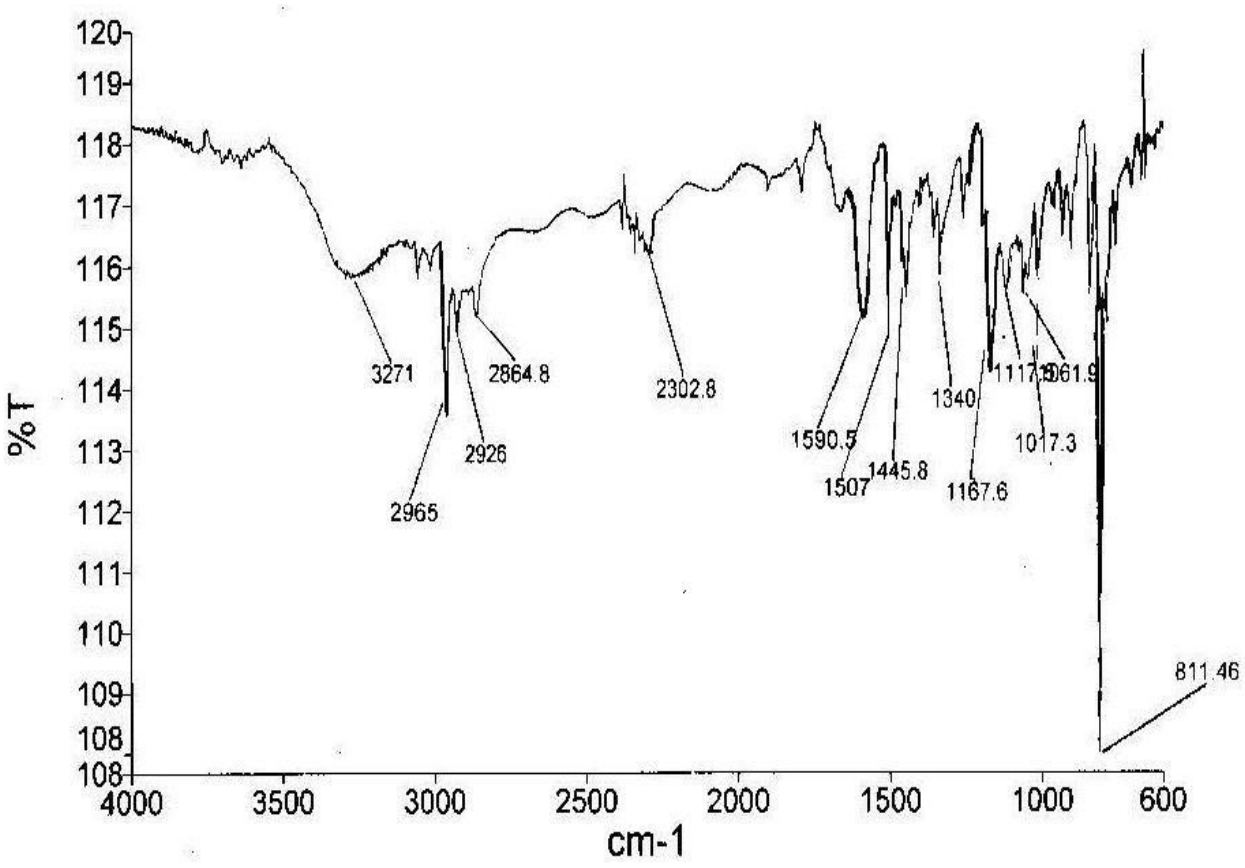


Figure **S40**: IR Spectrum of **6a**.

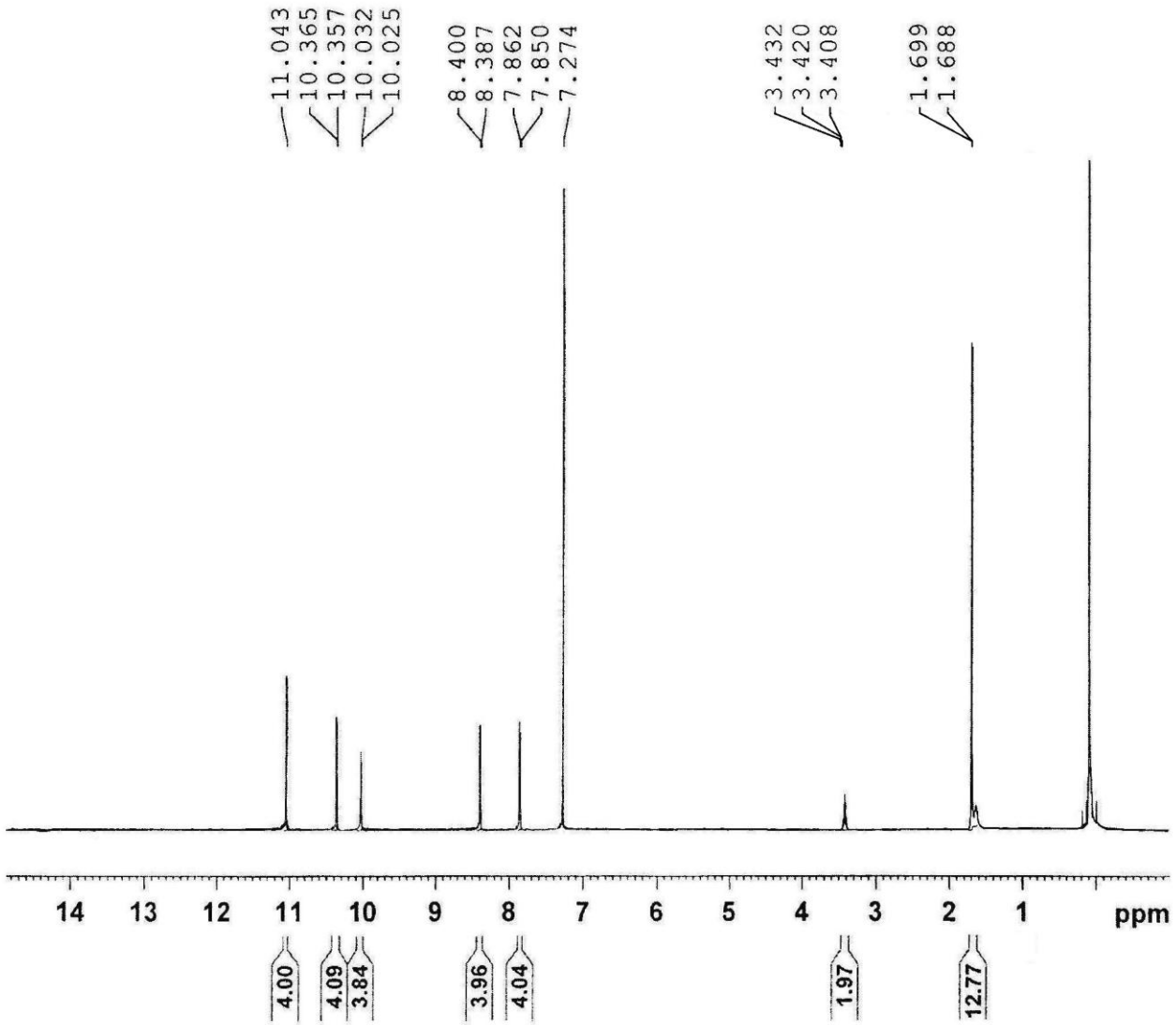


Figure **S41**: ^{1}H NMR Spectrum of **6b**.

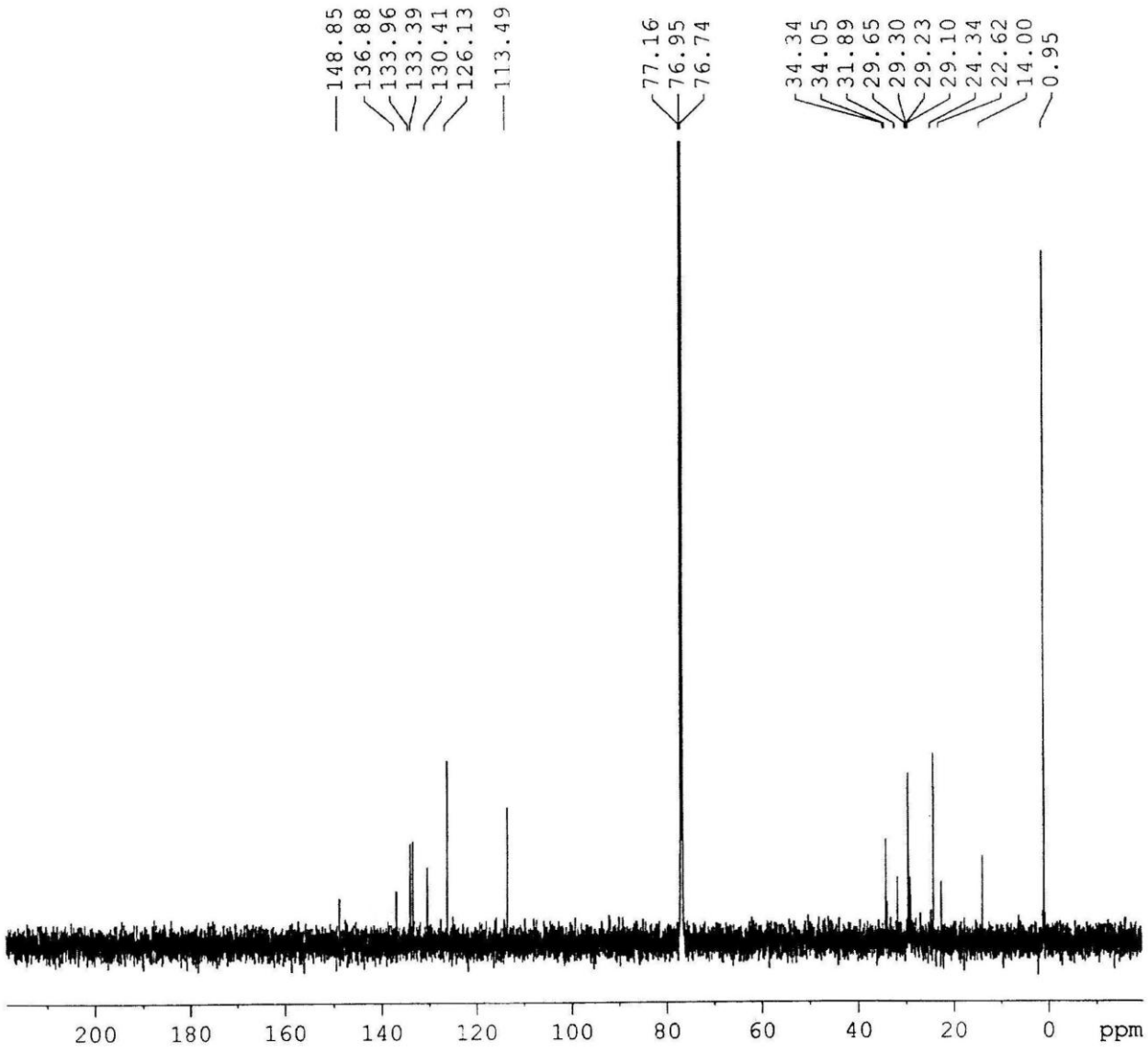


Figure **S42**: ^{13}C NMR Spectrum of **6b**.

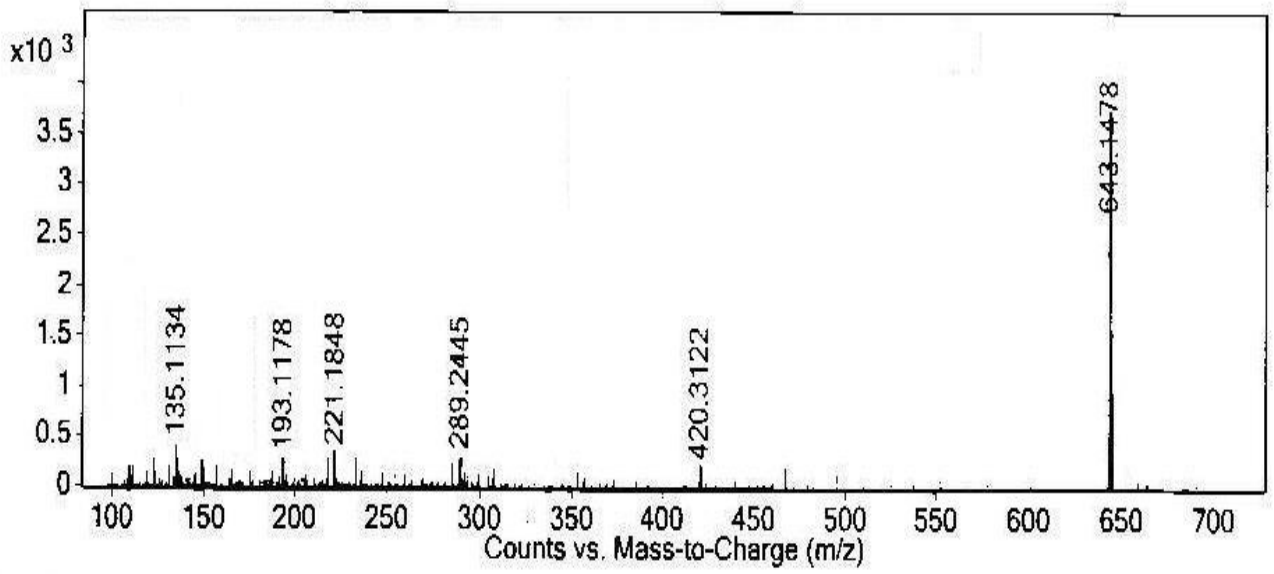


Figure **S43**: Mass Spectrum of **6b**.

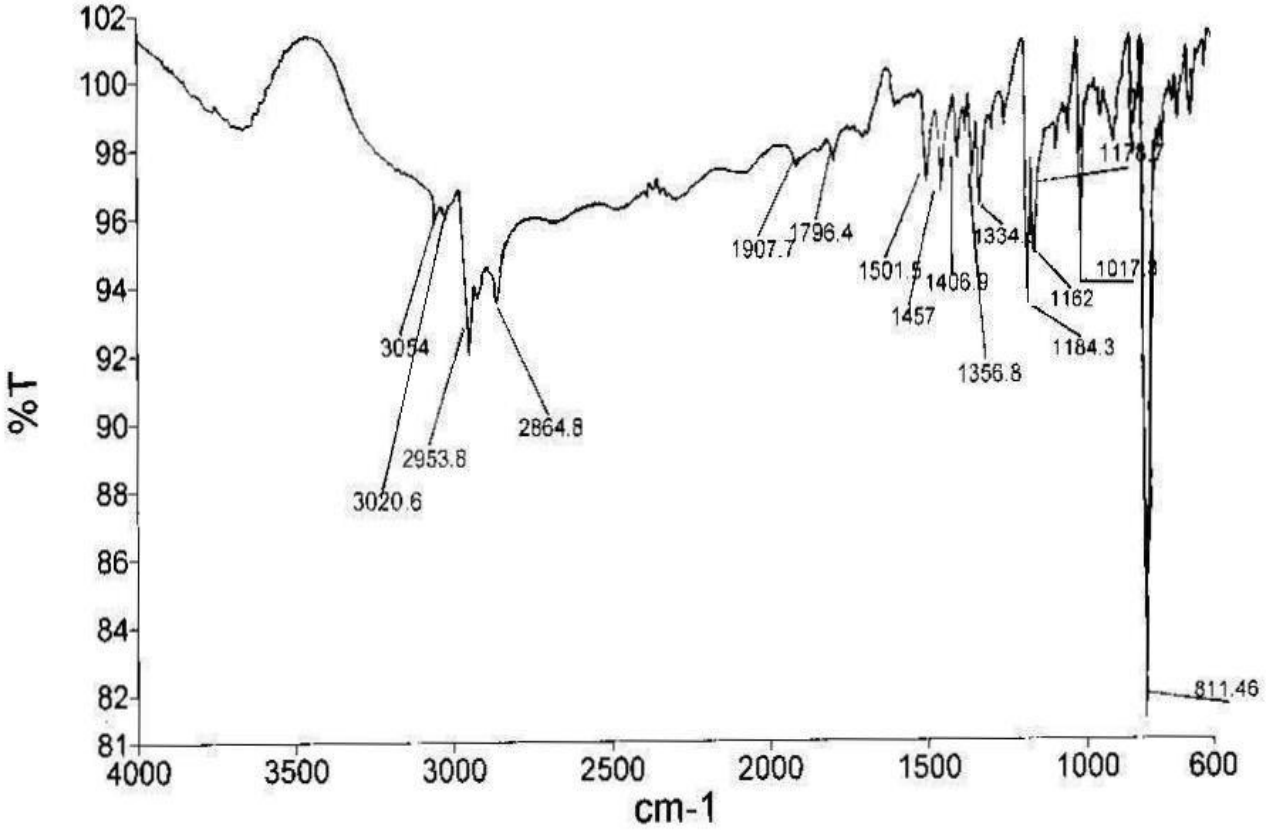


Figure **S44**: IR Spectrum of **6b**.

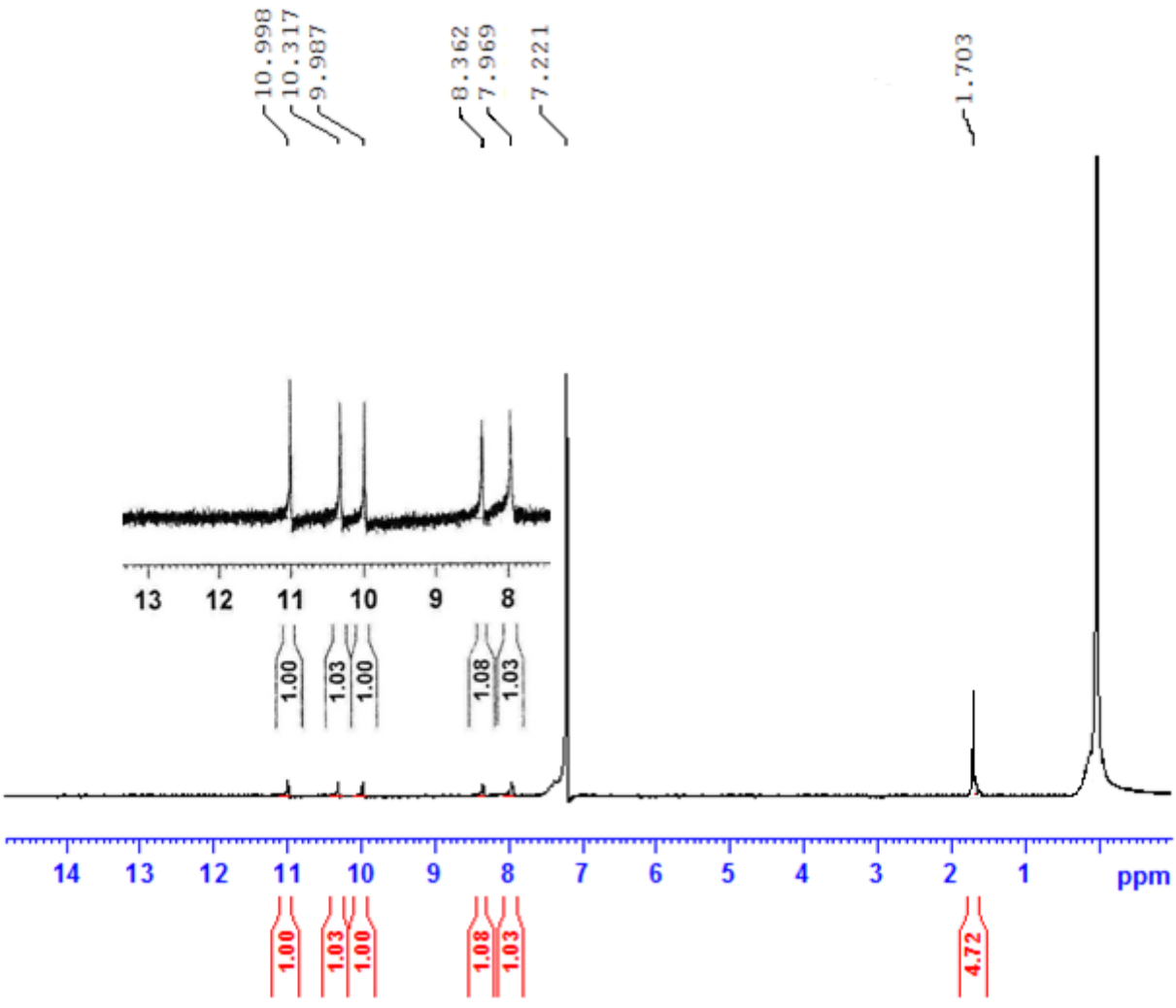


Figure **S45**: ^{1}H NMR Spectrum of **6c**.

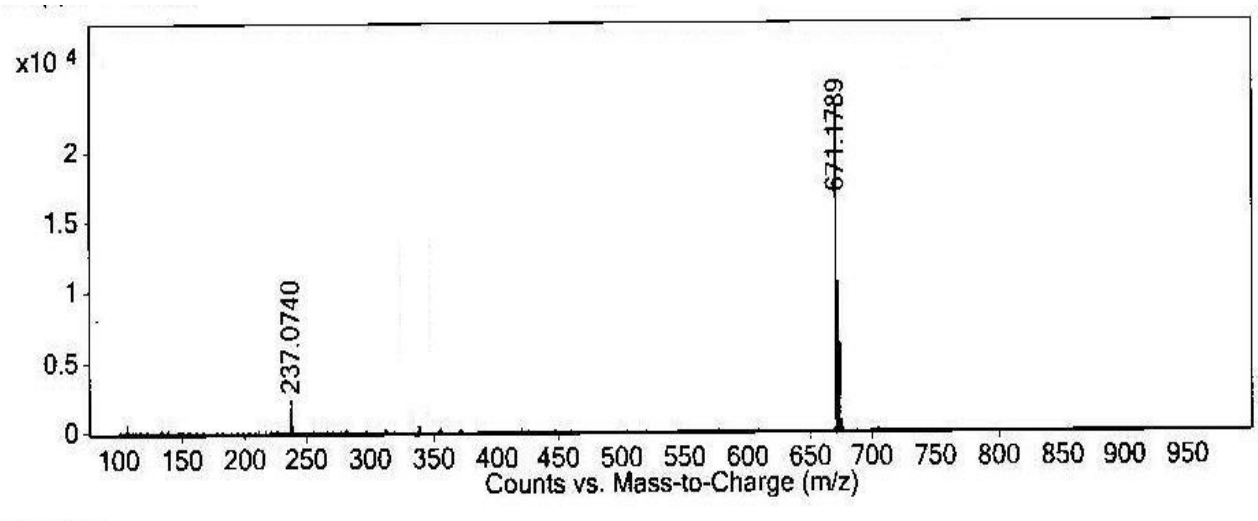


Figure **S46**: Mass Spectrum of **6c**.

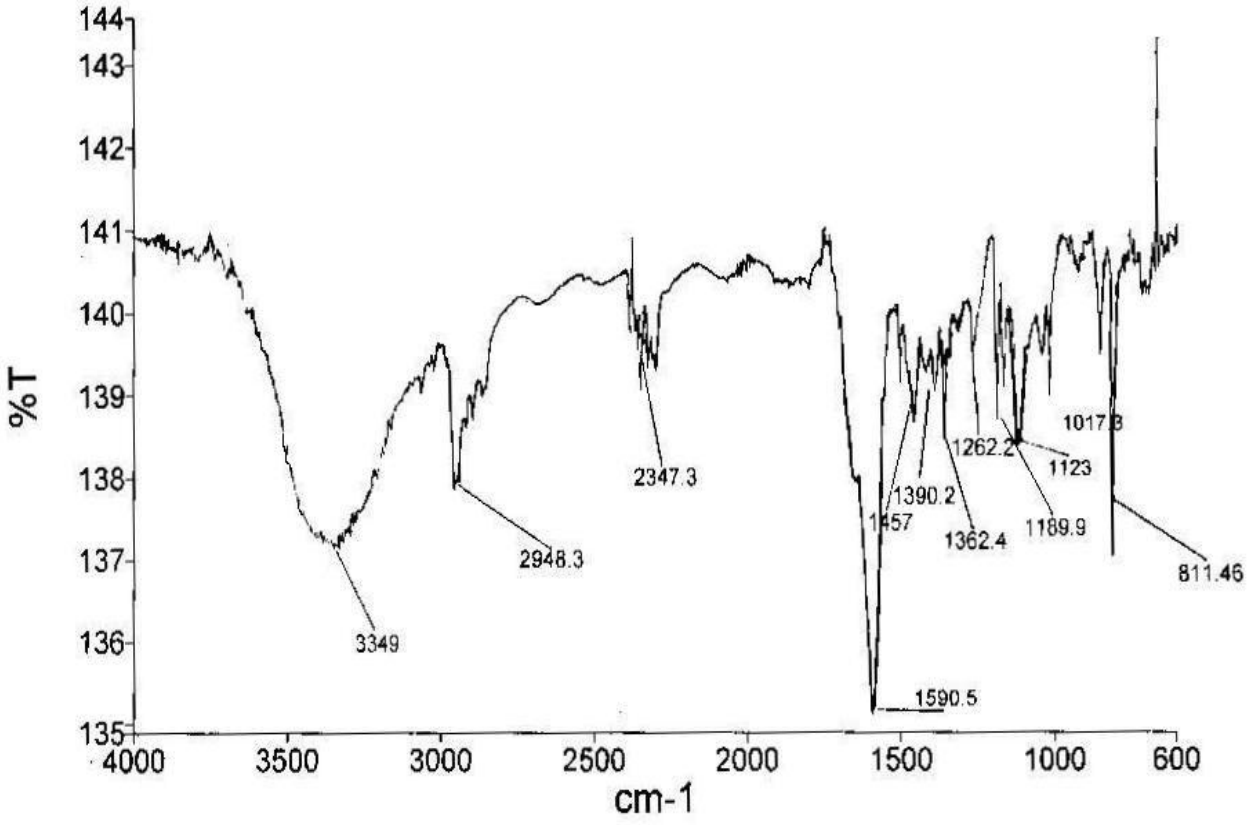


Figure **S47**: IR Spectrum of **6c**.

Theoretical Calculations

Computational methods

All the calculations were performed at the density functional theory (DFT) level with the B3LYP functional, the gradient correction of the exchange functional by Becke and the correlation functional by Lee, Yang and Parr. The 6-311G(d) split valence plus polarization basis set was used in Gaussian 09 program.[1],[2] The results were analyzed and visualized on Gauss View 5.0.9.

[1] Gaussian 09, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, W. H. G. E.; Robb, M. A.;Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.;Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M; Toyota, K.; Fukuda,R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta,Jr., J. E.; Ogliaro, F.;Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi,R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.;Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski,V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J.V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2010.

[2] Details including the references for the DFT method and basis set can be found online at the homepage of Gaussian, Inc.; http://www.gaussian.com/

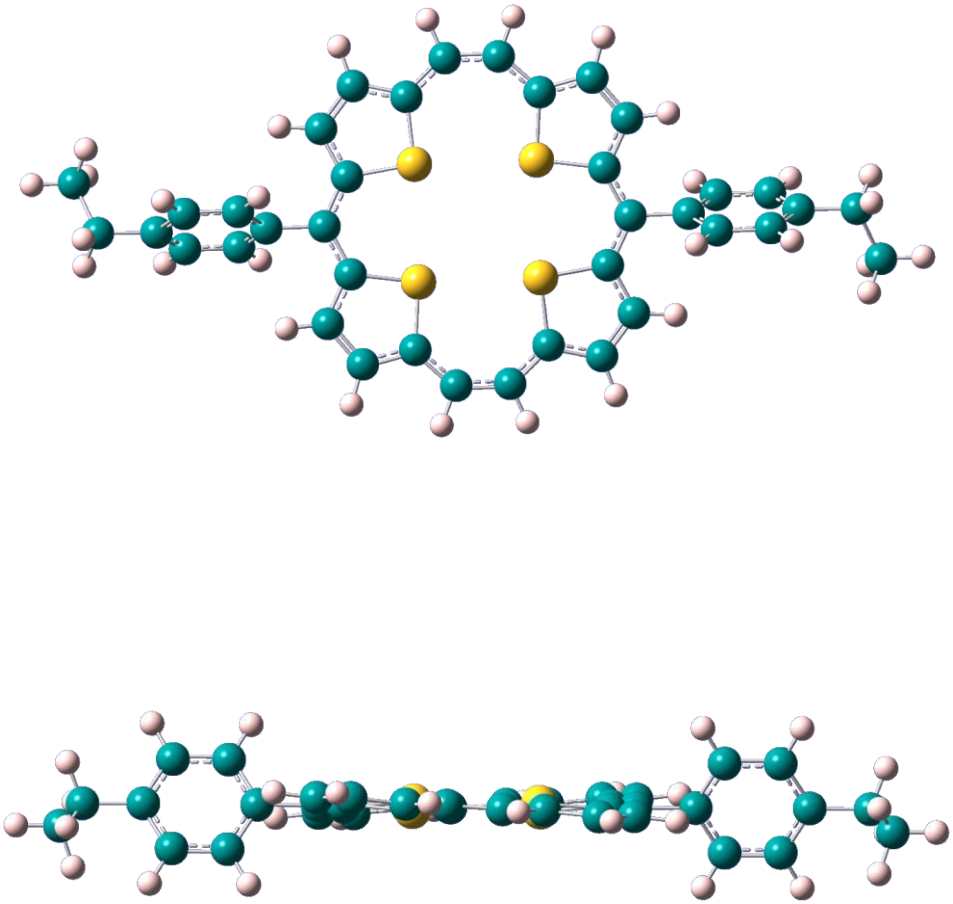


Figure S48: Energy minimized structure of **6a** by DFT method at B3LYP/6-311G(d) level using the Gaussion09 program (Top and side views shown above).

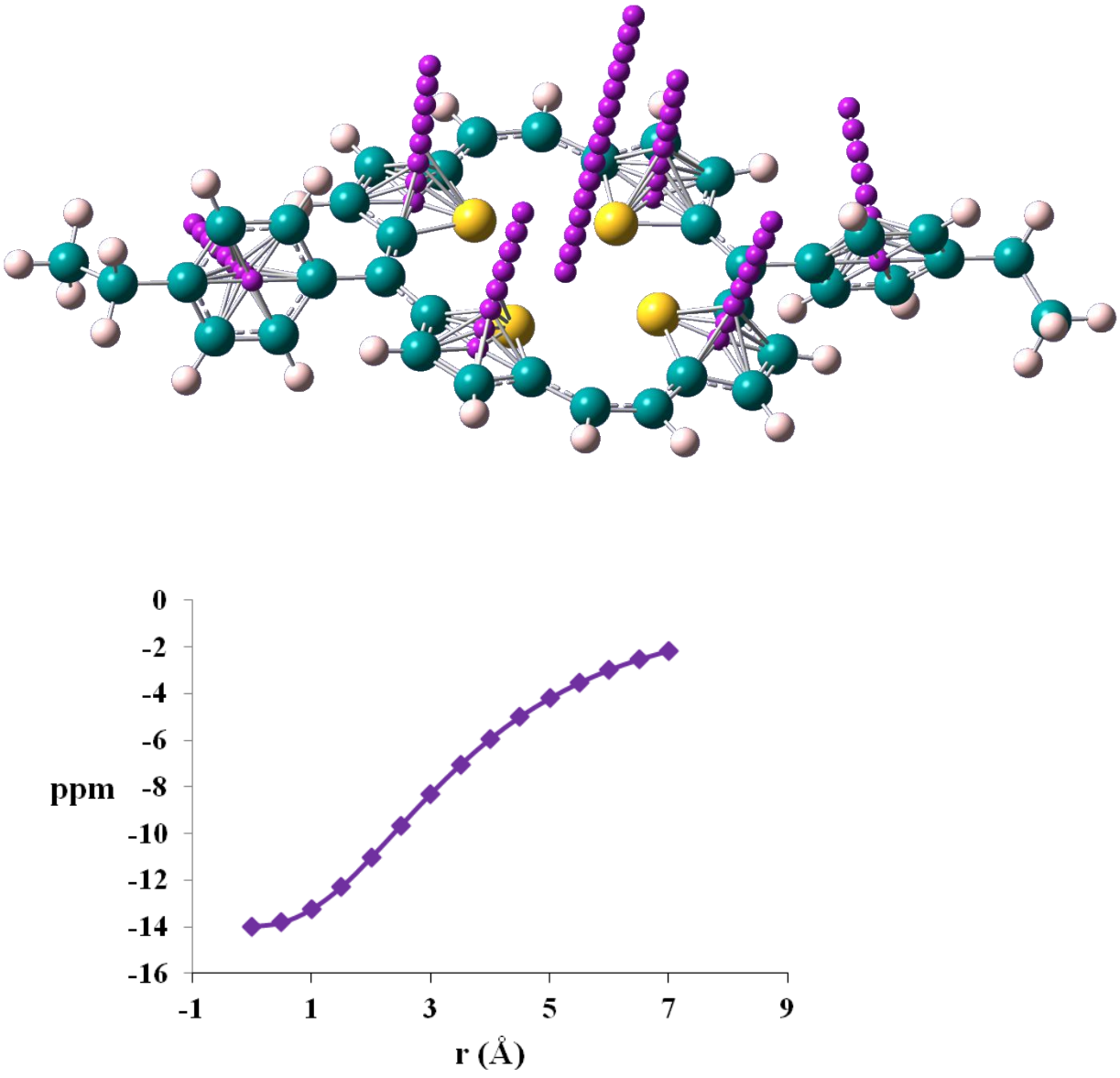
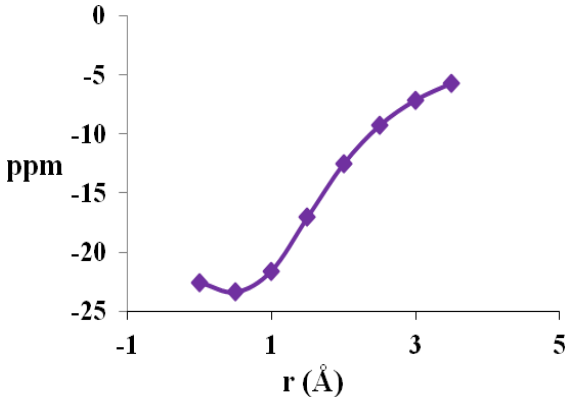
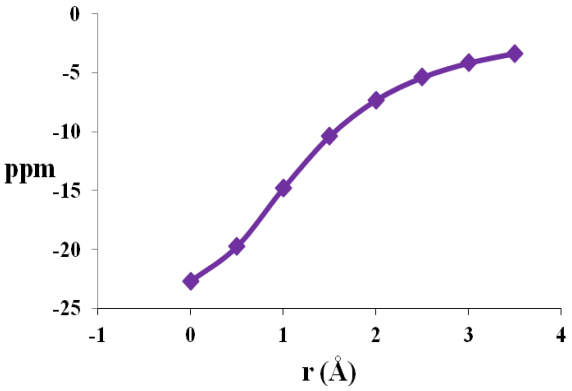


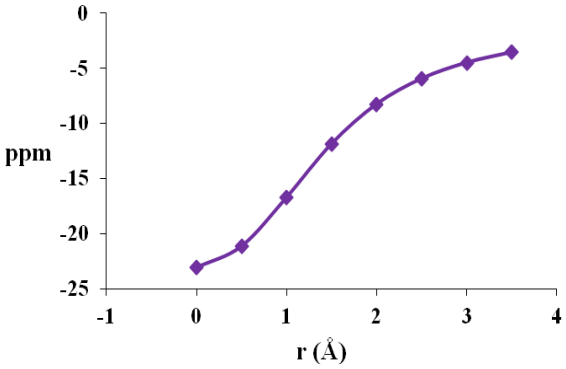
Figure S49: The ghost (Bq) atoms (in purple) were placed (0.5 Å interval) in the centre of **6a**. The -ve NICS values clearly indicate the aromaticity of **6a**. NICS is maximum at 0 Å and decreases as the distance of the ghost atom is increased in 0.5 Å intervals.



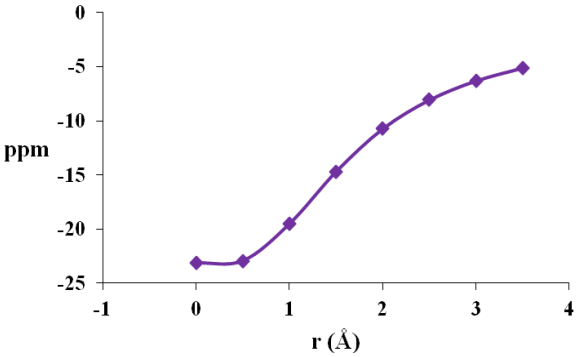
Thiophene ring 1



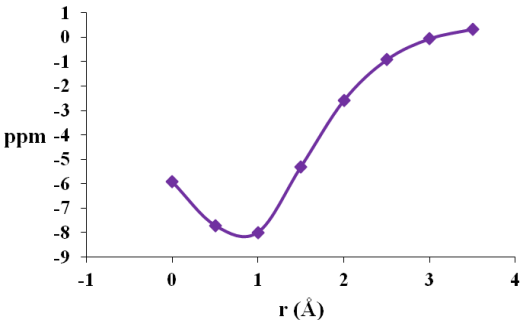
Thiophene ring 2



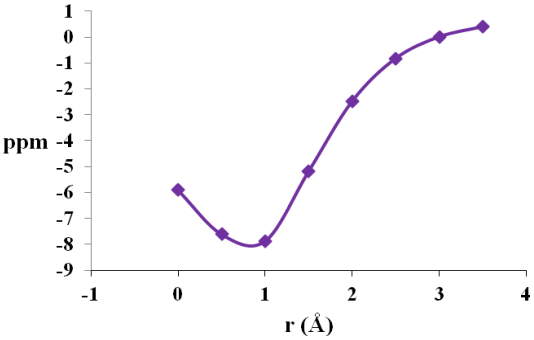
Thiophene ring 3



Thiophene ring 4



Phenyl ring 1



Phenyl ring 2

Figure S50: As shown above is the behaviour of the four thiophene rings of **6a**. The NICS are negative and maximum at their centres and decreases as we move farther. Further the NICS at the centre is far higher than the normal thiophene showing their increased aromatic character when they are part of the annulene ring. Phenyl rings are showing the normal behavior like benzene but with slightly decreased NICS values.

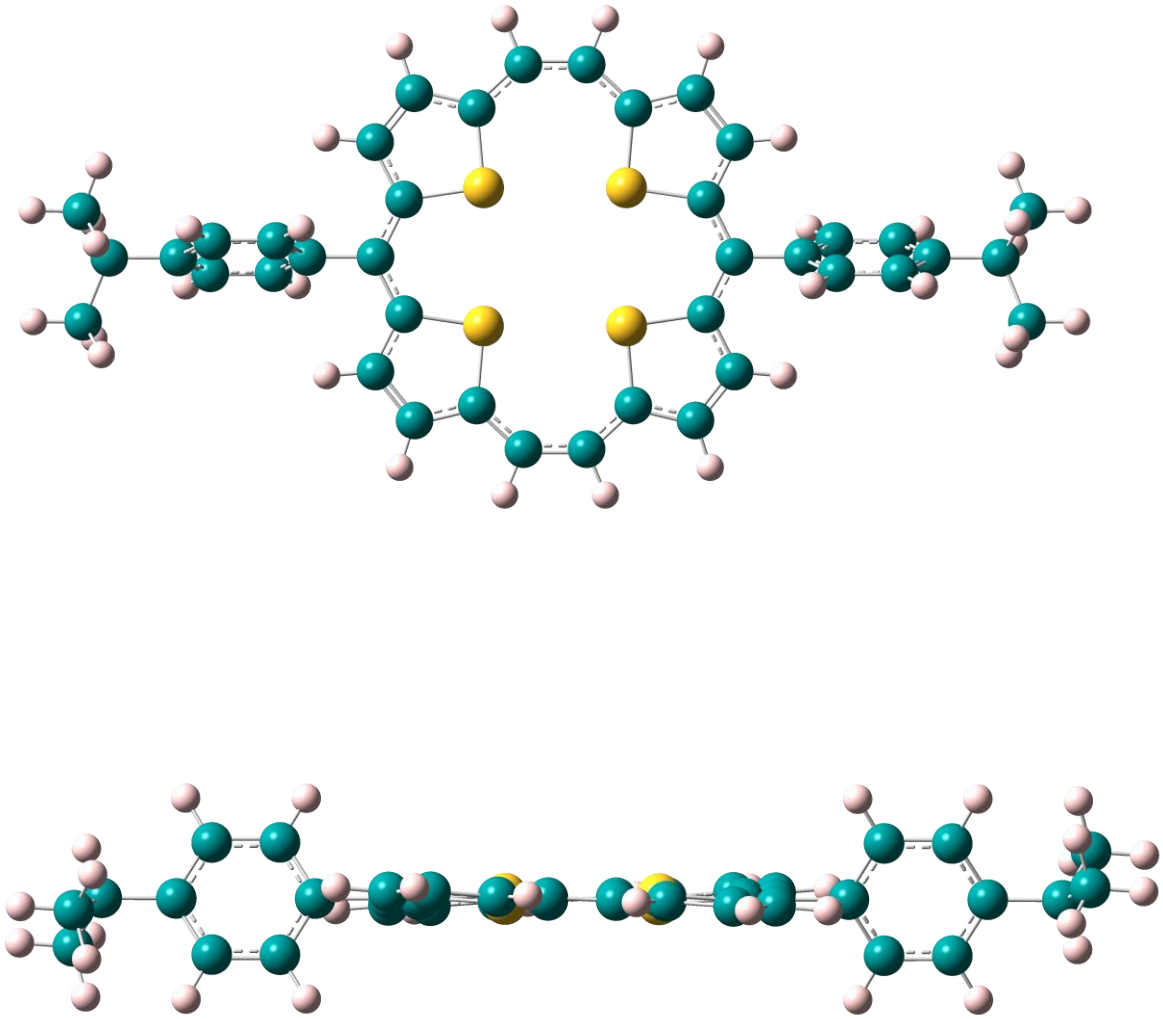


Figure S51: Energy minimized structure of **6b** by DFT method at B3LYP/6-311G(d) level using the Gaussion09 program (Top and side views shown above).

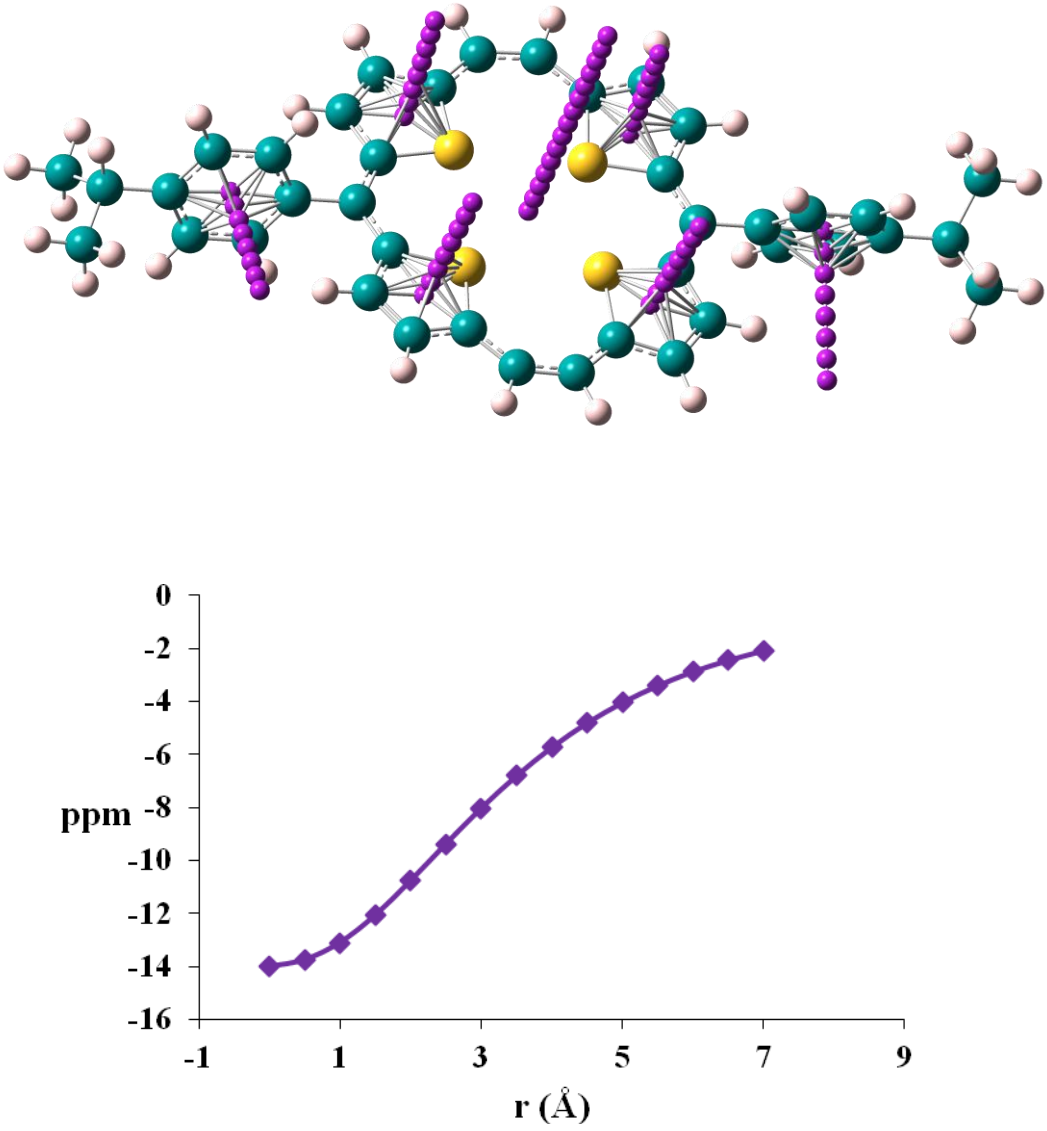
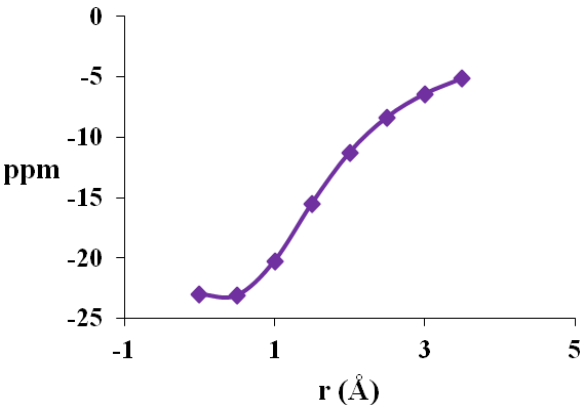
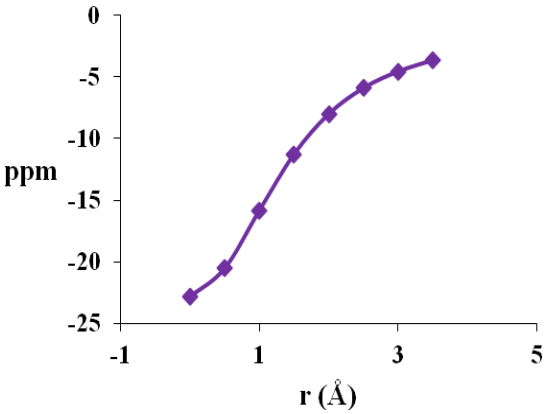


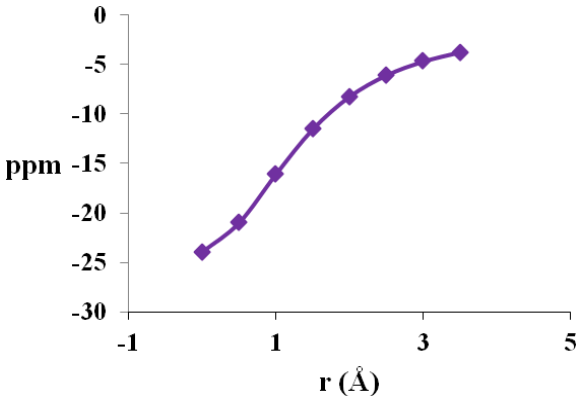
Figure S52: The ghost (Bq) atoms were placed (0.5 Å interval) in the centre of the molecule (in purple). The -ve NICS values clearly indicate the aromaticity of **6b**. NICS is maximum at 0 Å and decreases as the distance of the ghost atoms is increased in 0.5 Å intervals.



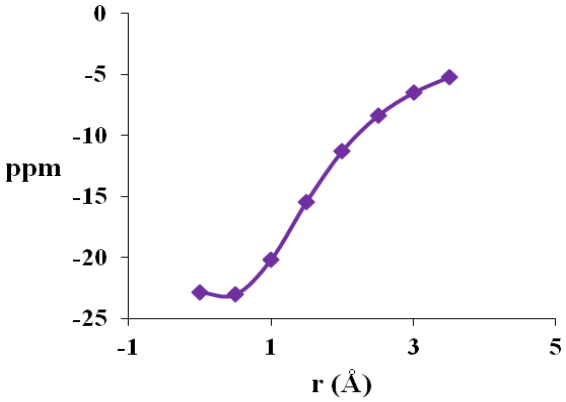
Thiophene ring 1



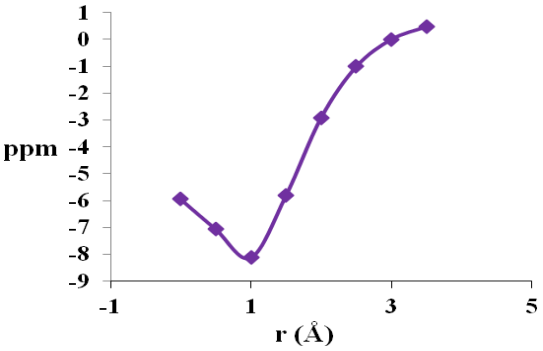
Thiophene ring 2



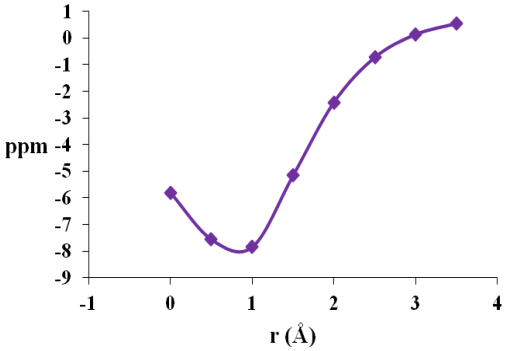
Thiophene ring 3



Thiophene ring 4



Phenyl ring 1



Phenyl ring 2

Figure S53: As shown above is the behaviour of the four thiophene rings of **6b**. The NICS are negative and maximum at their centres and decreases as we move farther. Further the NICS at the centre is far higher than the normal thiophene showing their increased aromatic character when they are part of the annulene ring. Phenyl rings are showing the normal behaviour like benzene but with slightly decreased NICS values.

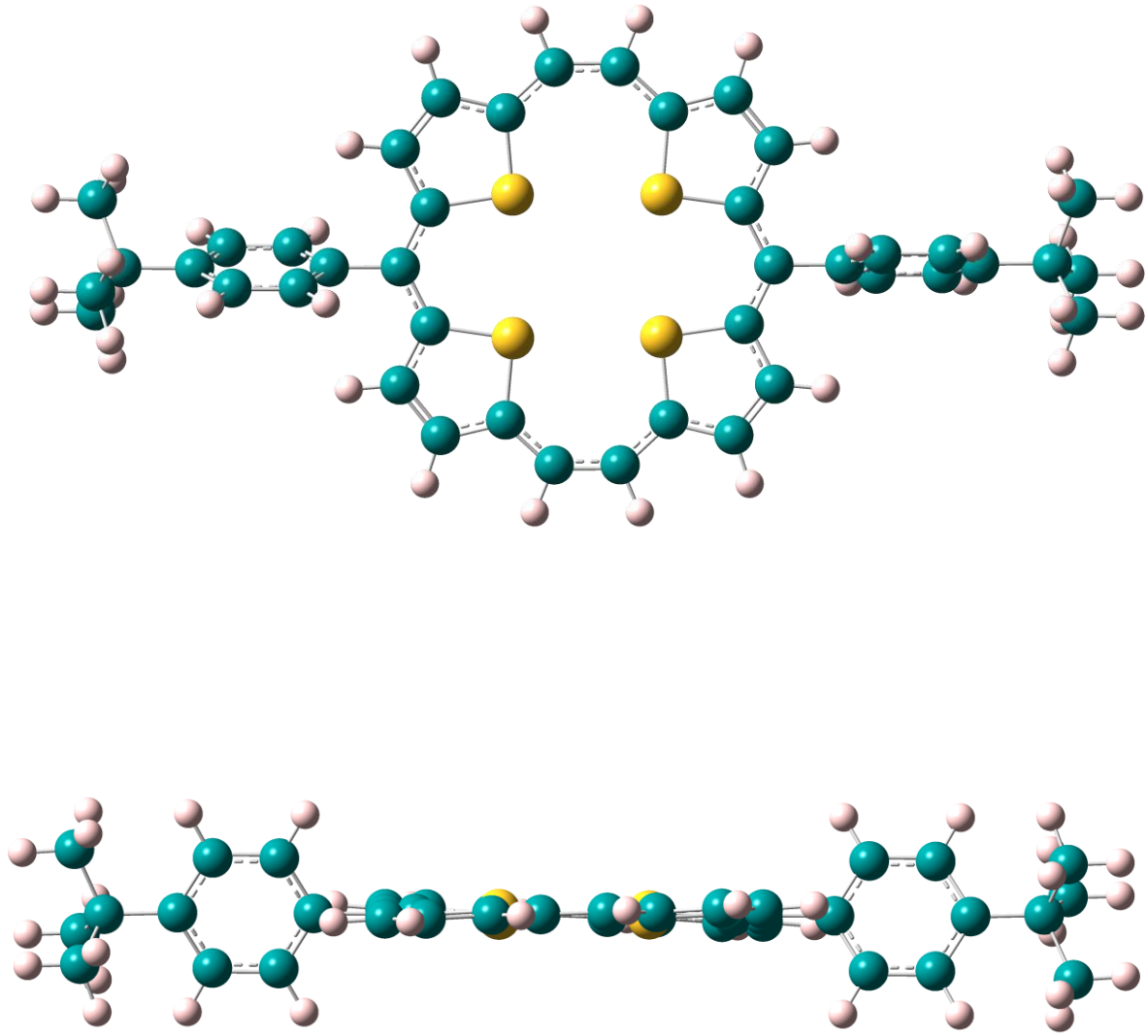


Figure S54: Energy minimized structure of **6c** by DFT method at B3LYP/6-311G(d) level using the Gaussion09 program (Top and side views shown above).

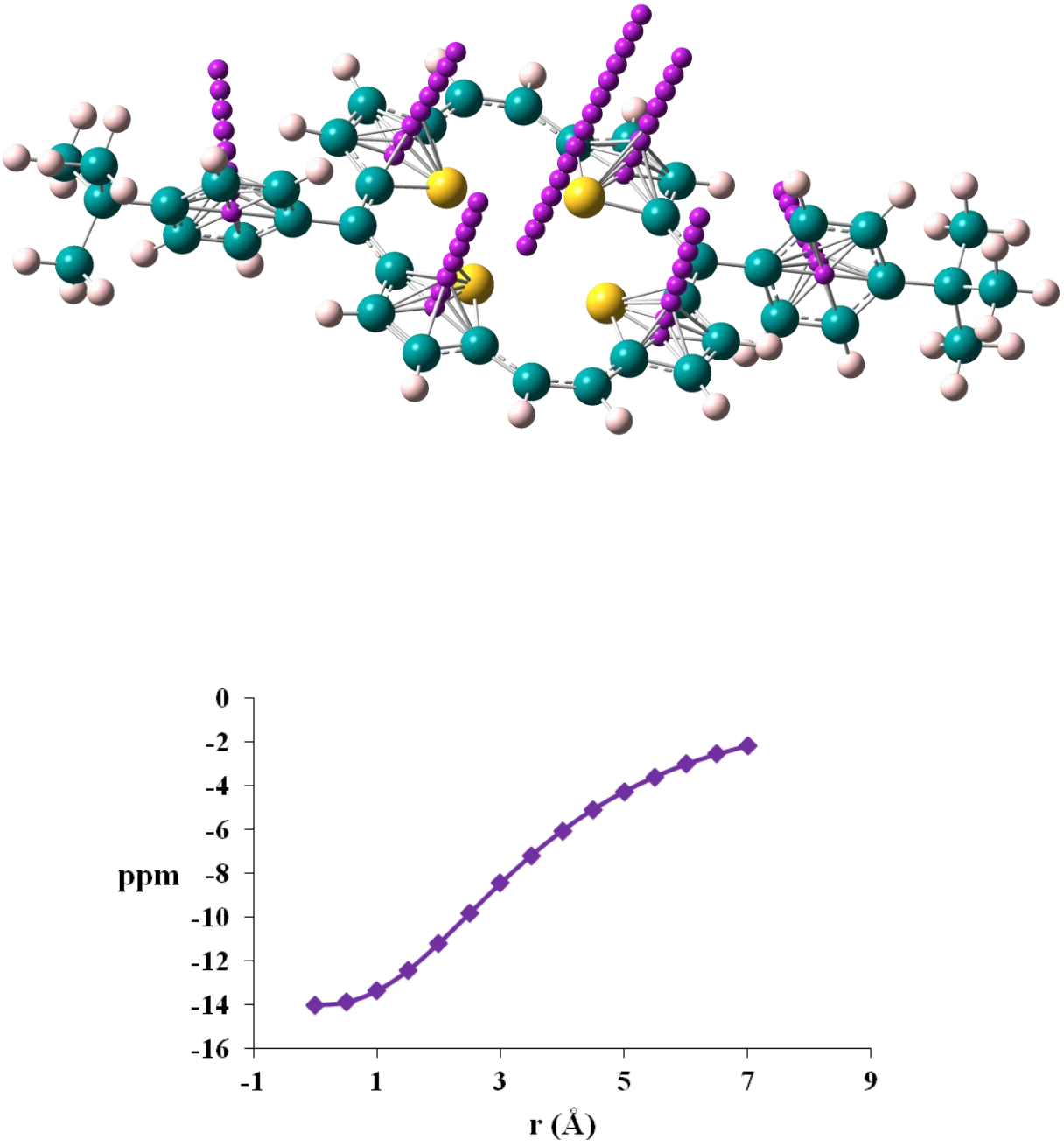
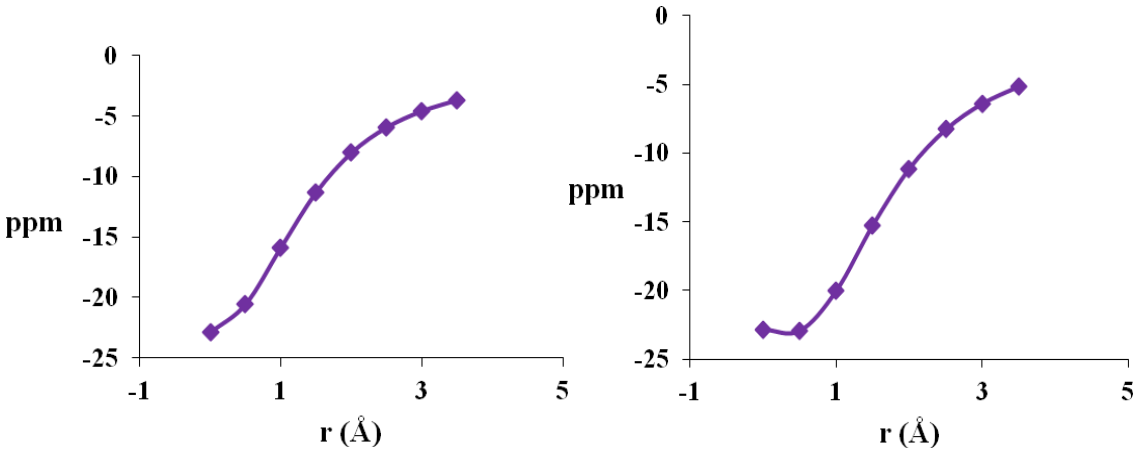
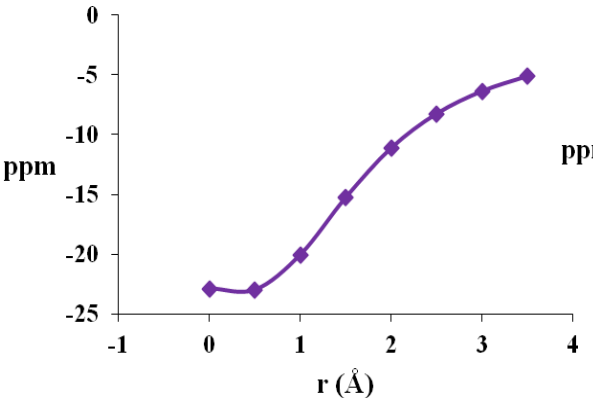


Figure S55: The ghost (Bq) atoms (in purple) were placed (0.5 Å interval) in the centre of **6c**. The -ve NICS values clearly indicate the aromaticity of **6c**. NICS is maximum at 0 Å and decreases as the distance of the ghost atom is increased in 0.5 Å intervals.

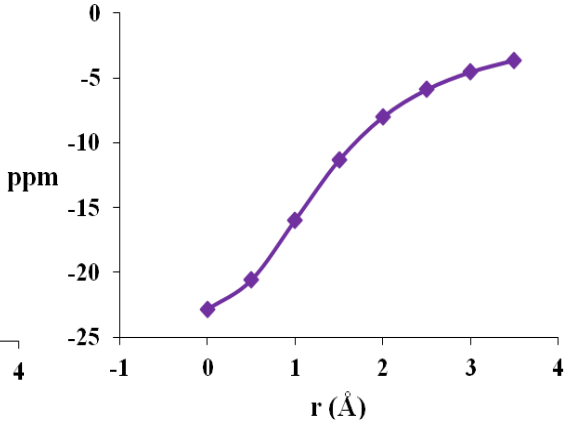


Thiophene ring 1

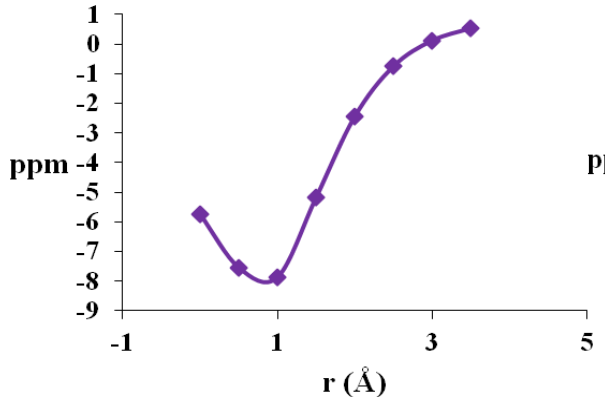
Thiophene ring 2



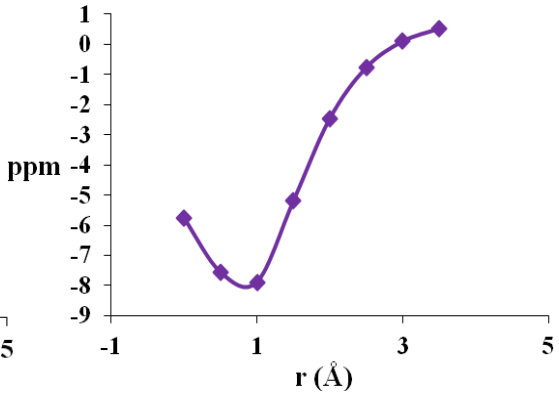
Thiophene ring 3



Thiophene ring 4



Phenyl ring 1



Phenyl ring 2

Figure S56: As shown above is the behaviour of the four thiophene rings of **6c**. The NICS are negative and maximum at their centres and decreases as we move farther. Further the NICS at the centre is far higher than the normal thiophene showing their increased aromatic character when they are part of the annulene ring. Phenyl rings are showing the normal behaviour like benzene but with slightly decreased NICS values.

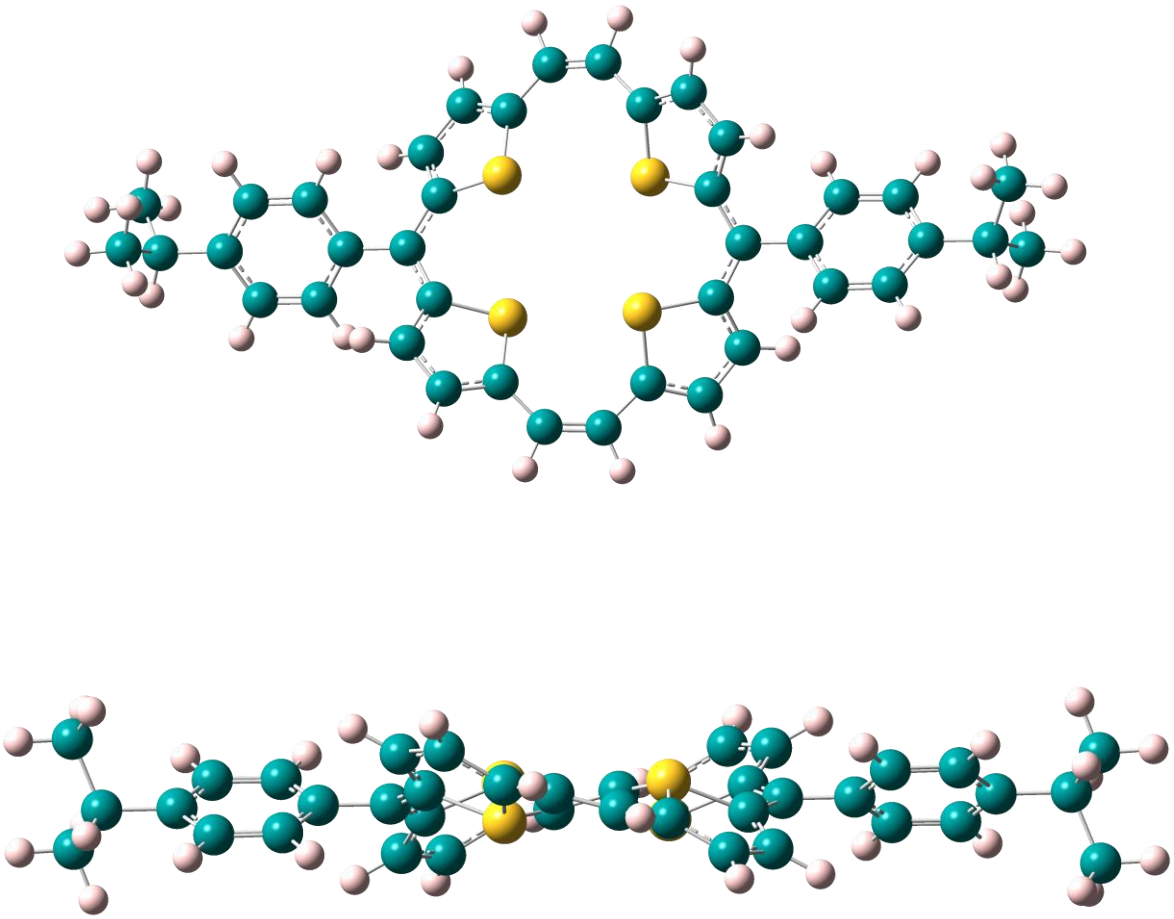


Figure S57: Energy minimized structure of antiaromatic dication **7b**. Upper (top view), lower (side view). The antiaromatic dication is no longer planar and is highly puckered. The aromaticity is thus lost.

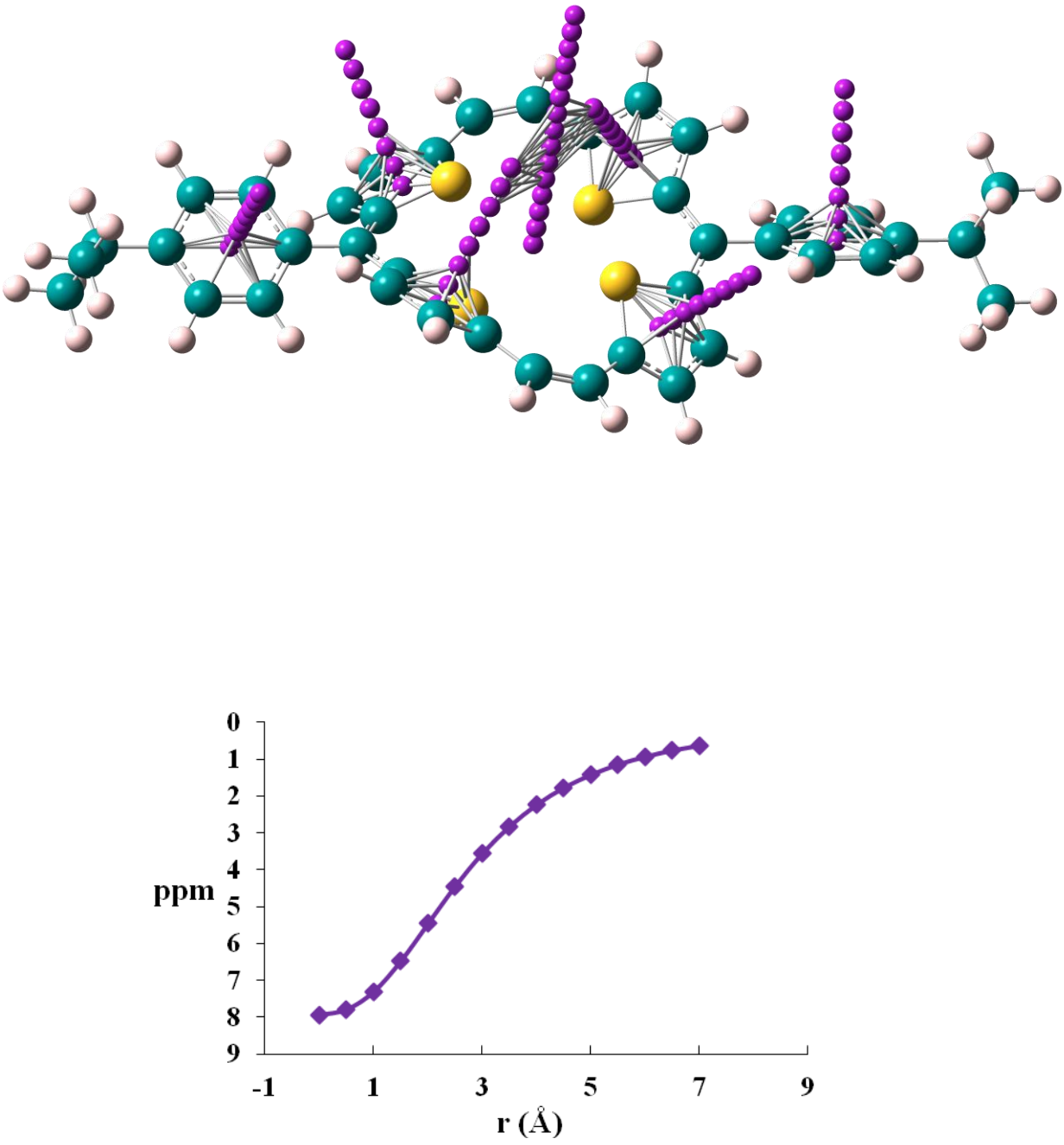
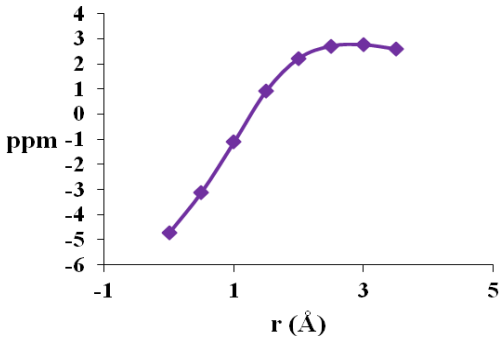
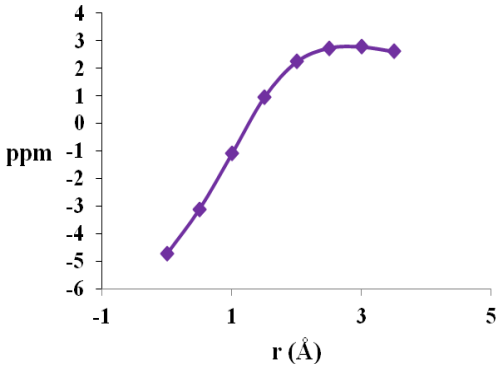


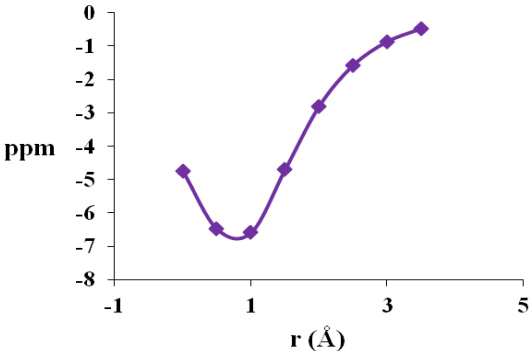
Figure S58: Placement of the ghost atoms (at 0.5 Å intervals) at the centre of all the individual rings as well as the main ring of **7b** (anti aromatic). The +ve NICS values (NICS 1 = 7.3) indicates the antiaromatic behaviour of the dication **7b**. The resulting NICS vs. r (distance from centre in Å) graph is also shown for the main centre of the **7b**. The graphs for the four thiophene rings are also shown below (Figure **S59**).



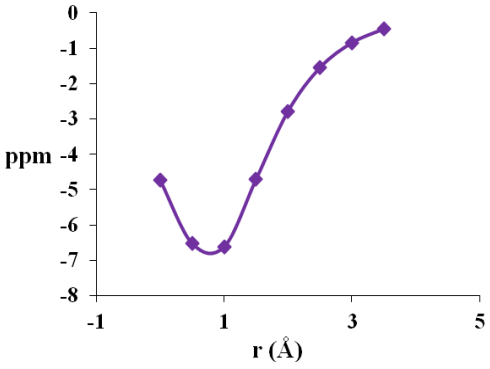
Thiophene ring 1



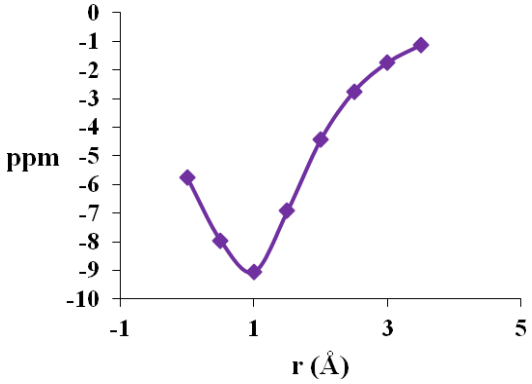
Thiophene ring 2



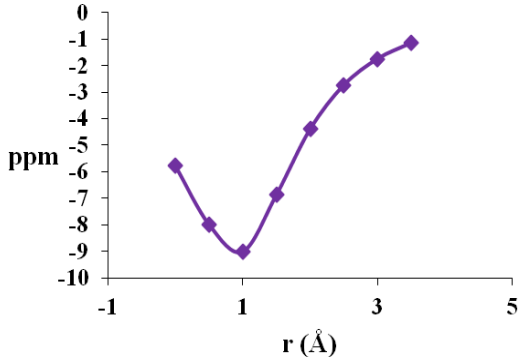
Thiophene ring 3



Thiophene ring 4



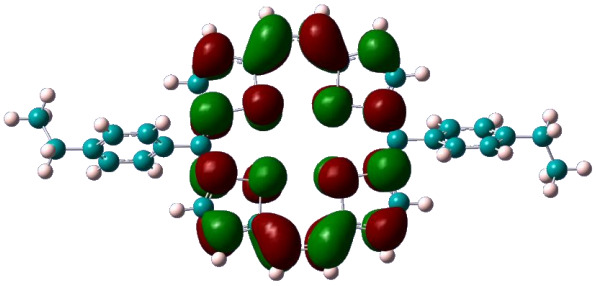
Phenyl ring 1



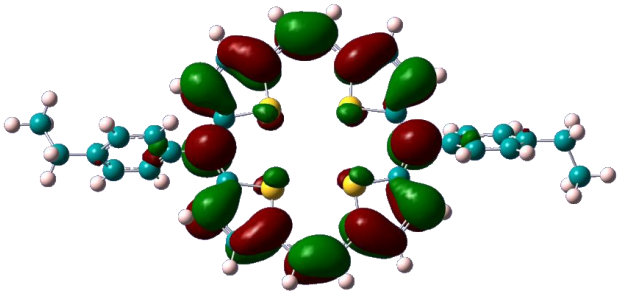
Phenyl ring 2

Figure S59: For **7b,** as shown at the top, at the centre of a set of two thiophene rings aromaticity (-ve NICS) is lost after 1Å distance and antiaromatic ring current is then observed due to the impact of the main annulene ring. The other set of thiophenes maintain their aromaticity as they points outwards to the annulene core as shown in Fig. **S58**. They also show a dip at 1 Å which is not shown by a free thiophene ring. The *p-iso*propylphenyl rings shows the normal aromaticity.

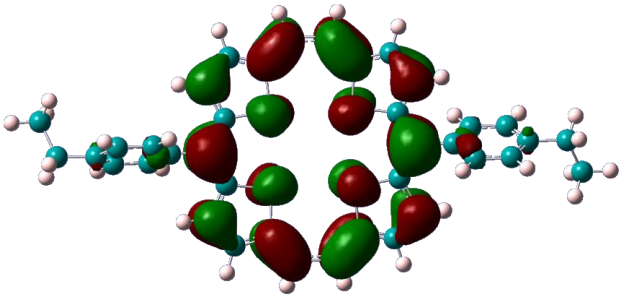
LUMO+1 (163), -0.07502 a.u.



LUMO (162), -0.09383 a.u.



HOMO (161), -0.17117 a.u.



HOMO-1 (160), -0.18602 a.u.

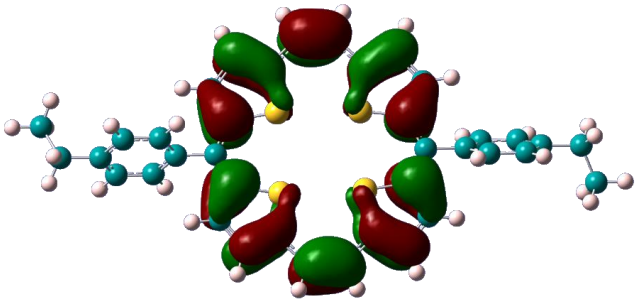
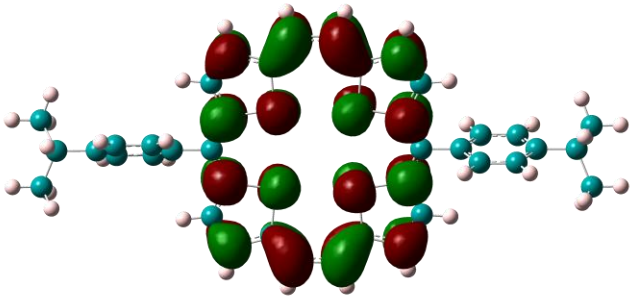
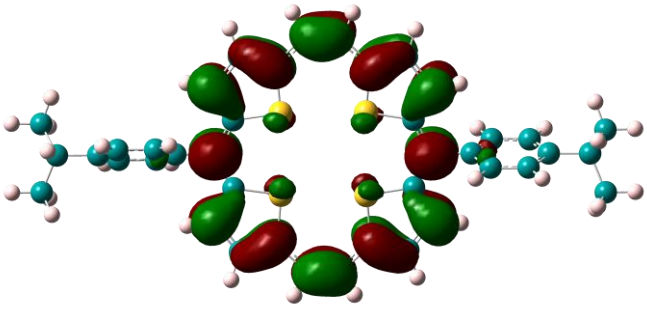


Figure S60: HOMO-LUMO and their neighbouring energy levels for **6a** are shown along with their energies (left) in a.u.. HOMO-LUMO levels are showing high degree of delocalisation on the 22Π porphyrin ring periphery.

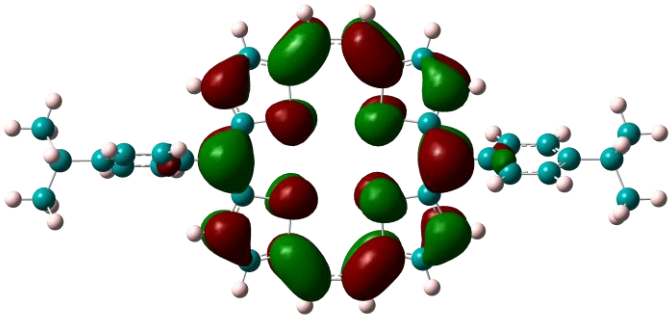
LUMO+1 (171), -0.07457 a.u.



LUMO (170), -0.09384 a.u.



HOMO (169), -0.17163 a.u.



HOMO-1 (168), -0.18595 a.u.

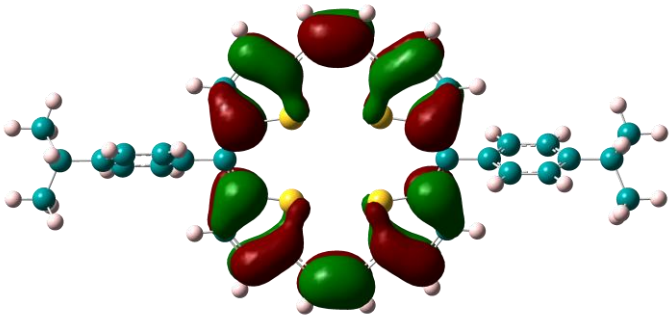
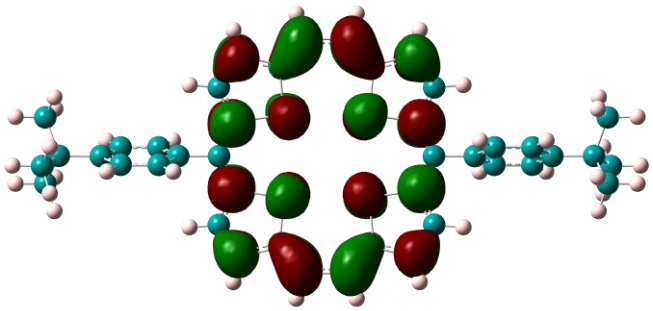
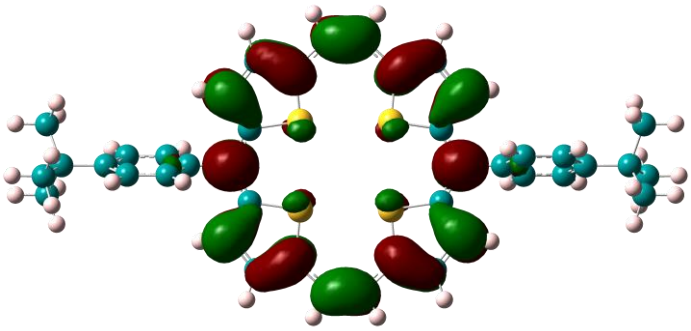


Figure S61: HOMO-LUMO and their neighbouring energy levels for **6b** are shown along with their energies (left) in a.u.. HOMO-LUMO levels are showing high degree of delocalisation on the 22Π porphyrin ring periphery.

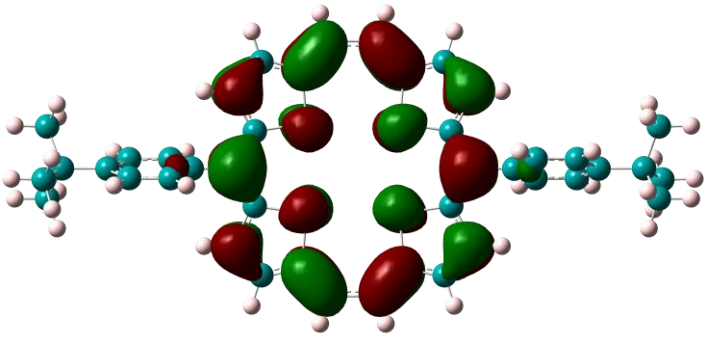
LUMO+1 (179), -0.07429a.u.



LUMO (178), -0.09367 a.u.



HOMO (177), -0.17158 a.u.



HOMO-1 (176), -0.18577 a.u.

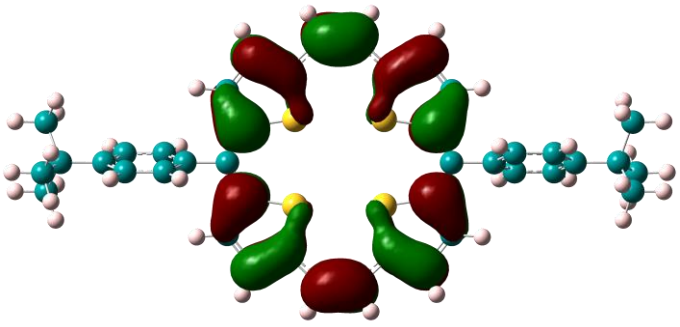


Figure S62: HOMO-LUMO and their neighbouring energy levels for **6c** are shown along with their energies (left) in a.u.. HOMO-LUMO levels are showing high degree of delocalisation on the 22Π porphyrin ring periphery.

Cartesian coordinates

Table S1: Cartesian coordinates of **6a**

SCF Done: E (RB3LYP) = -3059.21133209 a.u.. after 17 cycles.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-1.521043	-1.575011	-0.078609
2	6	0	-0.545640	-4.248436	0.068016
3	6	0	-1.604901	-3.324570	0.090890
4	6	0	-2.959524	-3.699417	0.233653
5	1	0	-3.246780	-4.738308	0.350324
6	6	0	-3.857933	-2.655015	0.228105
7	1	0	-4.924863	-2.782124	0.350296
8	6	0	-3.272555	-1.375805	0.068422
9	6	0	-3.946420	-0.138715	0.030080
10	6	0	-5.445588	-0.190573	0.034451
11	6	0	-6.152001	-0.673857	-1.073116
12	1	0	-5.603766	-1.011504	-1.946737
13	6	0	-7.543047	-0.723072	-1.064859
14	1	0	-8.066717	-1.102644	-1.938339
15	6	0	-8.277181	-0.295764	0.046683
16	1	0	-0.921890	-5.268542	0.120147
17	16	0	-1.626845	1.464538	0.130952
18	6	0	-0.842786	4.199674	-0.017595
19	6	0	-1.834493	3.203582	-0.038545
20	6	0	-3.212399	3.482130	-0.178267
21	1	0	-3.572392	4.498145	-0.294703
22	6	0	-4.035082	2.377110	-0.169539
23	1	0	-5.108635	2.428370	-0.289137
24	6	0	-3.360662	1.142465	-0.010742
25	6	0	-6.176252	0.238180	1.148492
26	1	0	-5.646646	0.606509	2.021196
27	6	0	-7.567265	0.183449	1.152484
28	1	0	-8.109679	0.511801	2.035169
29	1	0	-1.289779	5.190779	-0.070442
30	16	0	1.521045	1.575012	-0.078605
31	6	0	0.545639	4.248438	0.068002
32	6	0	1.604898	3.324571	0.090891
33	6	0	2.959519	3.699419	0.233670
34	1	0	3.246773	4.738311	0.350343
35	6	0	3.857930	2.655019	0.228134
36	1	0	4.924857	2.782131	0.350338
37	6	0	3.272556	1.375808	0.068444
38	6	0	3.946424	0.138719	0.030101
39	6	0	5.445591	0.190574	0.034483
40	6	0	6.176249	-0.238210	1.148516
41	1	0	5.646639	-0.606560	2.021207

42	6	0	7.567263	-0.183494	1.152511
43	1	0	8.109674	-0.511878	2.035187
44	6	0	8.277186	0.295740	0.046724
45	1	0	0.921890	5.268544	0.120128
46	16	0	1.626845	-1.464531	0.130956
47	6	0	0.842785	-4.199670	-0.017574
48	6	0	1.834491	-3.203577	-0.038530
49	6	0	3.212397	-3.482127	-0.178248
50	1	0	3.572389	-4.498143	-0.294679
51	6	0	4.035081	-2.377108	-0.169524
52	1	0	5.108634	-2.428373	-0.289120
53	6	0	3.360664	-1.142462	-0.010731
54	6	0	6.152012	0.673880	-1.073071
55	1	0	5.603780	1.011555	-1.946683
56	6	0	7.543056	0.723084	-1.064809
57	1	0	8.066731	1.102675	-1.938277
58	1	0	1.289779	-5.190775	-0.070410
59	6	0	-9.789716	-0.315795	0.037808
60	6	0	-10.403356	0.975160	-0.529374
61	1	0	-10.158951	-0.473361	1.056601
62	1	0	-10.140797	-1.170187	-0.550521
63	1	0	-11.496055	0.926718	-0.521720
64	1	0	-10.101169	1.846594	0.057776
65	1	0	-10.081518	1.145078	-1.560355
66	6	0	9.789721	0.315755	0.037850
67	6	0	10.403342	-0.975112	-0.529556
68	1	0	10.158958	0.473141	1.056670
69	1	0	10.140815	1.170241	-0.550333
70	1	0	11.496042	-0.926684	-0.521902
71	1	0	10.101148	-1.846640	0.057450
72	1	0	10.081494	-1.144853	-1.560563

Table S2: Cartesian coordinates of **6b**

SCF Done: E (RB3LYP) = -3137.85301104 a.u. after 6 cycles.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.573998	-1.493556	0.046314
2	6	0	0.694730	-4.202217	-0.044847
3	6	0	1.720981	-3.242439	-0.080798
4	6	0	3.088970	-3.571367	-0.211942

5	1	0	3.413839	-4.601688	-0.303274
6	6	0	3.949377	-2.495618	-0.226183
7	1	0	5.021221	-2.586651	-0.337621
8	6	0	3.317502	-1.234863	-0.098160
9	6	0	3.946474	0.025550	-0.087888
10	6	0	5.447355	0.024007	-0.120159
11	6	0	6.189519	-0.333273	1.011925
12	1	0	5.667953	-0.605611	1.923973
13	6	0	7.580354	-0.336938	0.981599
14	1	0	8.122463	-0.614564	1.880615
15	6	0	8.282681	0.010739	-0.179340
16	1	0	1.106286	-5.208849	-0.091435
17	16	0	1.570753	1.544563	-0.116983
18	6	0	0.696115	4.252969	0.013680
19	6	0	1.723062	3.293405	0.004106
20	6	0	3.095630	3.622397	0.074566
21	1	0	3.424190	4.652716	0.151710
22	6	0	3.955897	2.546756	0.050155
23	1	0	5.031698	2.637519	0.113741
24	6	0	3.318994	1.285963	-0.050124
25	6	0	6.142555	0.375827	-1.280477
26	1	0	5.586836	0.652542	-2.170754
27	6	0	7.535839	0.366039	-1.306202
28	1	0	8.051079	0.637678	-2.223615
29	1	0	1.109163	5.259663	0.042122
30	16	0	-1.570730	1.544562	0.116566
31	6	0	-0.696101	4.252970	-0.014051
32	6	0	-1.723048	3.293408	-0.004445
33	6	0	-3.095623	3.622405	-0.074769
34	1	0	-3.424187	4.652727	-0.151847
35	6	0	-3.955889	2.546765	-0.050289
36	1	0	-5.031698	2.637529	-0.113747
37	6	0	-3.318977	1.285970	0.049888
38	6	0	-3.946460	0.025562	0.087698

39	6	0	-5.447339	0.024031	0.120189
40	6	0	-6.189697	-0.333014	-1.011839
41	1	0	-5.668291	-0.605167	-1.924034
42	6	0	-7.580529	-0.336694	-0.981268
43	1	0	-8.122791	-0.614147	-1.880246
44	6	0	-8.282654	0.010739	0.179866
45	1	0	-1.109148	5.259665	-0.042477
46	16	0	-1.574004	-1.493556	-0.046671
47	6	0	-0.694746	-4.202219	0.044399
48	6	0	-1.720994	-3.242441	0.080397
49	6	0	-3.088981	-3.571366	0.211573
50	1	0	-3.413853	-4.601688	0.302882
51	6	0	-3.949380	-2.495612	0.225884
52	1	0	-5.021221	-2.586642	0.337354
53	6	0	-3.317501	-1.234856	0.097884
54	6	0	-6.142337	0.375613	1.280700
55	1	0	-5.586462	0.652151	2.170935
56	6	0	-7.535615	0.365813	1.306668
57	1	0	-8.050696	0.637264	2.224226
58	1	0	-1.106301	-5.208853	0.090955
59	6	0	9.803846	0.004396	-0.221888
60	6	0	10.379004	-1.402395	0.018400
61	6	0	10.410665	1.024840	0.756952
62	1	0	10.096568	0.308858	-1.233849
63	1	0	9.980144	-2.122862	-0.700212
64	1	0	11.468847	-1.397187	-0.078088
65	1	0	10.138695	-1.767076	1.021409
66	1	0	10.034289	2.032730	0.564469
67	1	0	10.173132	0.775238	1.795281
68	1	0	11.500697	1.048410	0.665221
69	6	0	-9.803813	0.004362	0.222703
70	6	0	-10.378989	-1.402423	-0.017587
71	6	0	-10.410854	1.024880	-0.755919
72	1	0	-10.096335	0.308728	1.234750

73	1	0	-9.979973	-2.122939	0.700888
74	1	0	-11.468814	-1.397244	0.079115
75	1	0	-10.138869	-1.767018	-1.020673
76	1	0	-10.034444	2.032757	-0.563436
77	1	0	-10.173554	0.775370	-1.794324
78	1	0	-11.500866	1.048434	-0.663942

Table S3: Cartesian coordinates of **6c**

SCF Done: E (RB3LYP) = -3216.48950982 a.u. after 7 cycles.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.572439	1.515694	0.070320
2	6	0	0.695720	4.224839	-0.027351
3	6	0	1.722775	3.265357	-0.040788
4	6	0	3.093920	3.594726	-0.133676
5	1	0	3.421233	4.625554	-0.209314
6	6	0	3.954313	2.518848	-0.131893
7	1	0	5.028928	2.609937	-0.212883
8	6	0	3.318989	1.257483	-0.029263
9	6	0	3.947080	-0.003039	-0.011921
10	6	0	5.448371	-0.002787	-0.017157
11	6	0	6.165407	-0.323244	-1.170770
12	1	0	5.627147	-0.573002	-2.079679
13	6	0	7.560446	-0.320834	-1.174599
14	1	0	8.068432	-0.571266	-2.097827
15	6	0	8.295127	-0.003135	-0.027341
16	1	0	1.108154	5.231606	-0.061550
17	16	0	1.571983	-1.521501	-0.077110
18	6	0	0.695920	-4.230712	0.023340

19	6	0	1.722934	-3.271333	0.031159
20	6	0	3.094752	-3.600831	0.114605
21	1	0	3.422498	-4.631747	0.187141
22	6	0	3.955156	-2.525116	0.107385
23	1	0	5.030328	-2.616285	0.180218
24	6	0	3.319264	-1.263506	0.009847
25	6	0	6.173737	0.319089	1.135813
26	1	0	5.640453	0.568818	2.047620
27	6	0	7.563765	0.315540	1.127379
28	1	0	8.084209	0.566040	2.045912
29	1	0	1.108497	-5.237508	0.054833
30	16	0	-1.571985	-1.521489	0.077271
31	6	0	-0.695929	-4.230713	-0.022874
32	6	0	-1.722940	-3.271332	-0.030800
33	6	0	-3.094759	-3.600837	-0.114207
34	1	0	-3.422508	-4.631760	-0.186627
35	6	0	-3.955161	-2.525119	-0.107107
36	1	0	-5.030333	-2.616294	-0.179927
37	6	0	-3.319266	-1.263499	-0.009710
38	6	0	-3.947080	-0.003028	0.011923
39	6	0	-5.448371	-0.002775	0.017158
40	6	0	-6.165408	-0.323107	1.170804
41	1	0	-5.627150	-0.572765	2.079742
42	6	0	-7.560447	-0.320702	1.174631
43	1	0	-8.068434	-0.571039	2.097885
44	6	0	-8.295128	-0.003131	0.027337
45	1	0	-1.108508	-5.237511	-0.054252
46	16	0	-1.572436	1.515691	-0.070476
47	6	0	-0.695711	4.224844	0.026897
48	6	0	-1.722768	3.265366	0.040440
49	6	0	-3.093913	3.594748	0.133289
50	1	0	-3.421223	4.625585	0.208814
51	6	0	-3.954307	2.518871	0.131622
52	1	0	-5.028922	2.609972	0.212600

53	6	0	-3.318986	1.257494	0.029131
54	6	0	-6.173736	0.318975	-1.135848
55	1	0	-5.640452	0.568607	-2.047682
56	6	0	-7.563765	0.315425	-1.127415
57	1	0	-8.084209	0.565827	-2.045975
58	1	0	-1.108142	5.231616	0.060985
59	6	0	9.833188	0.006602	0.007059
60	6	0	10.332365	1.419124	0.386751
61	6	0	10.332145	-1.010687	1.058337
62	6	0	10.451107	-0.368443	-1.351352
63	1	0	10.001772	2.162560	-0.343767
64	1	0	9.967266	1.733204	1.367348
65	1	0	11.426021	1.442014	0.419100
66	1	0	9.997391	-2.022965	0.815558
67	1	0	11.425983	-1.017103	1.094909
68	1	0	9.970451	-0.774239	2.061639
69	1	0	11.541890	-0.348202	-1.279963
70	1	0	10.164767	-1.374669	-1.669389
71	1	0	10.163662	0.332161	-2.140025
72	6	0	-9.833188	0.006597	-0.007068
73	6	0	-10.332369	1.419084	-0.386885
74	6	0	-10.332140	-1.010785	-1.058258
75	6	0	-10.451109	-0.368334	1.351374
76	1	0	-10.001782	2.162585	0.343571
77	1	0	-9.967262	1.733079	-1.367507
78	1	0	-11.426024	1.441968	-0.419243
79	1	0	-9.997378	-2.023040	-0.815394
80	1	0	-11.425977	-1.017211	-1.094829
81	1	0	-9.970449	-0.774419	-2.061581
82	1	0	-11.541892	-0.348109	1.279980
83	1	0	-10.164760	-1.374529	1.669500
84	1	0	-10.163674	0.332342	2.139987

Table S4: Cartesian coordinates of **7b**

SCF Done: E (RB3LYP) = -3137.33883693 a.u. after 17 cycles.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.657807	-1.548426	0.371858
2	6	0	0.653938	-4.149680	-0.179051
3	6	0	1.654565	-3.119886	-0.367877
4	6	0	2.836532	-3.332127	-1.077472
5	1	0	3.032429	-4.252641	-1.613095
6	6	0	3.720016	-2.254818	-1.035778
7	1	0	4.663024	-2.228998	-1.564834
8	6	0	3.249932	-1.172754	-0.286166
9	6	0	3.937110	0.055534	-0.035558
10	6	0	5.387792	0.059443	-0.054371
11	6	0	6.131345	-1.030729	0.466383
12	1	0	5.610242	-1.856607	0.935884
13	6	0	7.511396	-1.012406	0.455695
14	1	0	8.050738	-1.842838	0.896840
15	6	0	8.226057	0.065988	-0.102650
16	1	0	1.069512	-5.141156	-0.340882
17	16	0	1.649253	1.658092	-0.398359
18	6	0	0.656662	4.260040	0.168452
19	6	0	1.659769	3.229808	0.340934
20	6	0	2.853858	3.441521	1.029891
21	1	0	3.059508	4.361956	1.561989
22	6	0	3.736338	2.363958	0.972234
23	1	0	4.688691	2.337695	1.484269
24	6	0	3.252692	1.282227	0.230905
25	6	0	6.106454	1.152903	-0.597447
26	1	0	5.567181	1.976481	-1.050036
27	6	0	7.488140	1.139269	-0.632374
28	1	0	8.015350	1.969656	-1.090022

29	1	0	1.075033	5.251406	0.323557
30	16	0	-1.649233	1.658102	0.398107
31	6	0	-0.656679	4.260021	-0.168921
32	6	0	-1.659789	3.229773	-0.341284
33	6	0	-2.853913	3.441440	-1.030194
34	1	0	-3.059591	4.361841	-1.562340
35	6	0	-3.736390	2.363881	-0.972422
36	1	0	-4.688770	2.337585	-1.484405
37	6	0	-3.252705	1.282198	-0.231050
38	6	0	-3.937109	0.055520	0.035523
39	6	0	-5.387790	0.059432	0.054417
40	6	0	-6.131375	-1.030768	-0.466232
41	1	0	-5.610302	-1.856674	-0.935717
42	6	0	-7.511426	-1.012442	-0.455464
43	1	0	-8.050795	-1.842898	-0.896529
44	6	0	-8.226051	0.065986	0.102860
45	1	0	-1.075052	5.251370	-0.324130
46	16	0	-1.657825	-1.548460	-0.371919
47	6	0	-0.653921	-4.149678	0.179080
48	6	0	-1.654544	-3.119879	0.367902
49	6	0	-2.836477	-3.332085	1.077564
50	1	0	-3.032348	-4.252570	1.613246
51	6	0	-3.719963	-2.254777	1.035858
52	1	0	-4.662945	-2.228929	1.564960
53	6	0	-3.249917	-1.172753	0.286165
54	6	0	-6.106418	1.152925	0.597472
55	1	0	-5.567117	1.976528	1.049982
56	6	0	-7.488102	1.139295	0.632480
57	1	0	-8.015284	1.969710	1.090111
58	1	0	-1.069495	-5.141152	0.340927
59	6	0	9.738689	0.079071	-0.128674
60	6	0	10.306464	-1.119835	-0.912892
61	6	0	10.319633	0.141754	1.299033
62	1	0	10.045359	0.991861	-0.649885

63	1	0	9.913508	-1.159200	-1.931485
64	1	0	11.393465	-1.037876	-0.978083
65	1	0	10.079814	-2.071205	-0.424170
66	1	0	9.943171	1.005758	1.851457
67	1	0	10.082554	-0.757538	1.873854
68	1	0	11.407588	0.223754	1.251782
69	6	0	-9.738682	0.079076	0.128968
70	6	0	-10.306424	-1.119803	0.913248
71	6	0	-10.319700	0.141722	-1.298712
72	1	0	-10.045320	0.991883	0.650168
73	1	0	-9.913416	-1.159141	1.931822
74	1	0	-11.393422	-1.037836	0.978492
75	1	0	-10.079806	-2.071189	0.424542
76	1	0	-9.943263	1.005710	-1.851179
77	1	0	-10.082652	-0.757587	-1.873520
78	1	0	-11.407652	0.223727	-1.251407

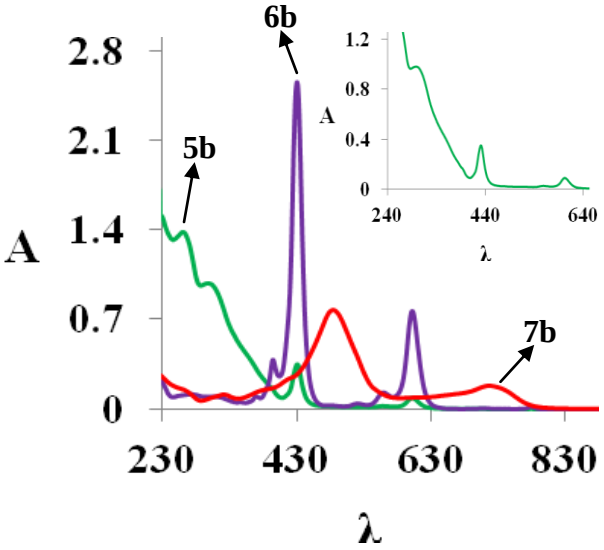


Figure S63: UV-Vis. spectra of **5b** (DCM), **6b** (DCM) and **7b** (H_2SO_4). (Inset shows the partial auto-oxidation of **5b** into **6b**).

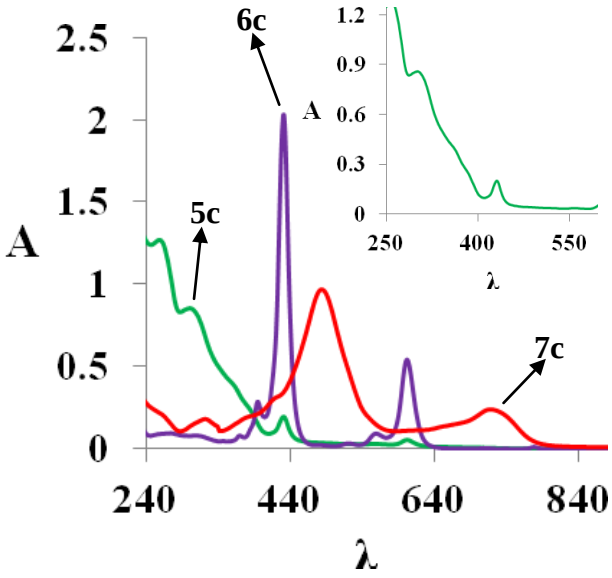


Figure S64: UV-Vis. spectra of **5c** (DCM), **6c** (DCM) and **7c** (H_2SO_4). (Inset shows the partial auto-oxidation of **5c** into **6c**).

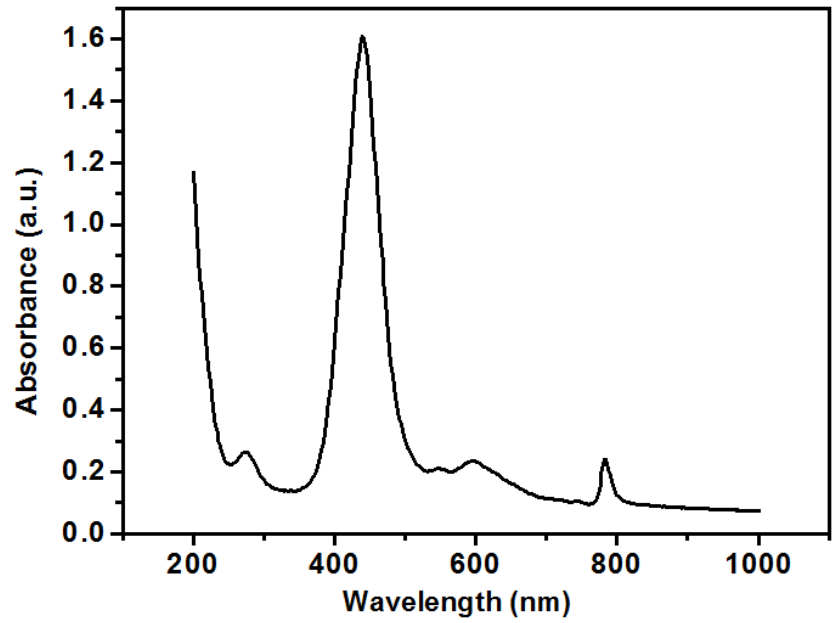


Figure S65: Normalised UV-Vis. absorption spectra of thin film of **6a** at room temperature.

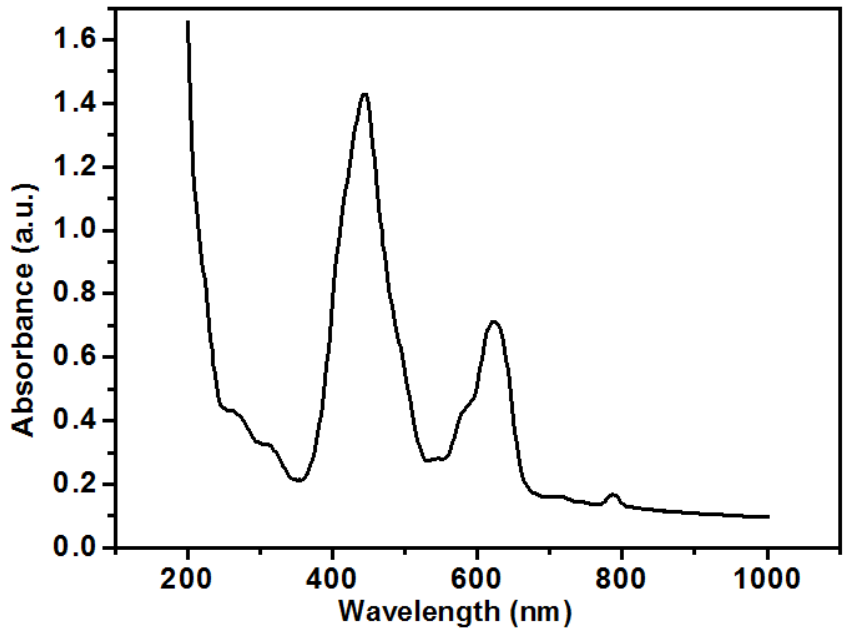


Figure S66: Normalised UV-Vis. absorption spectra of thin film of **6b** at room temperature.

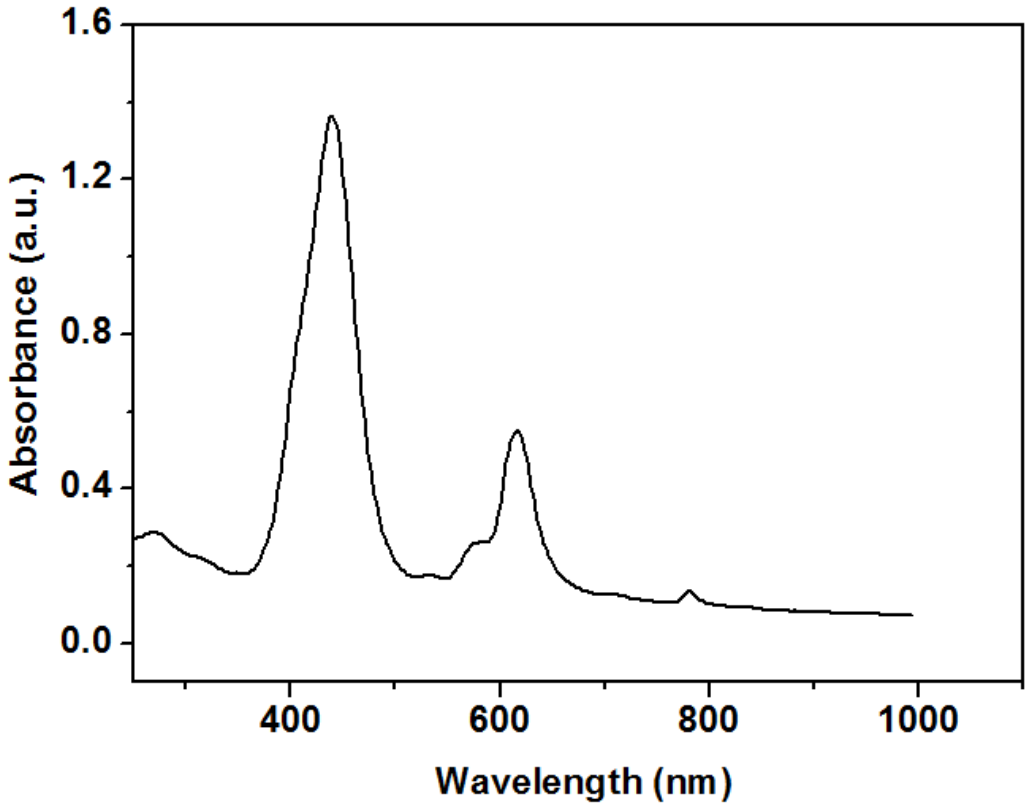


Figure S67: Normalised UV-Vis. absorption spectra of thin film of **6c** at room temperature.

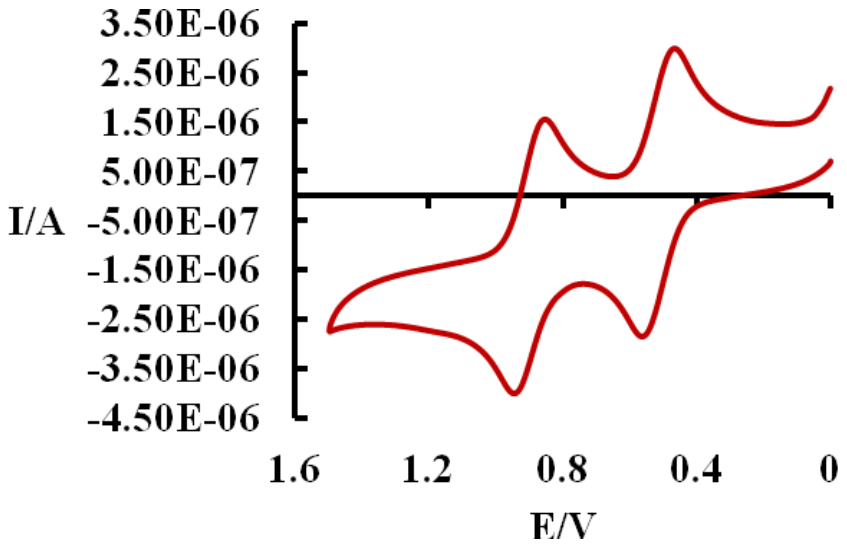


Figure S68: Cyclic voltammogram (CV) for **6b** (DCM, electrolyte $TBAPF_6$; working electrode: Pt; ref. electrode: Ag/AgCl; Scan rate 100 mV s^{-1}).

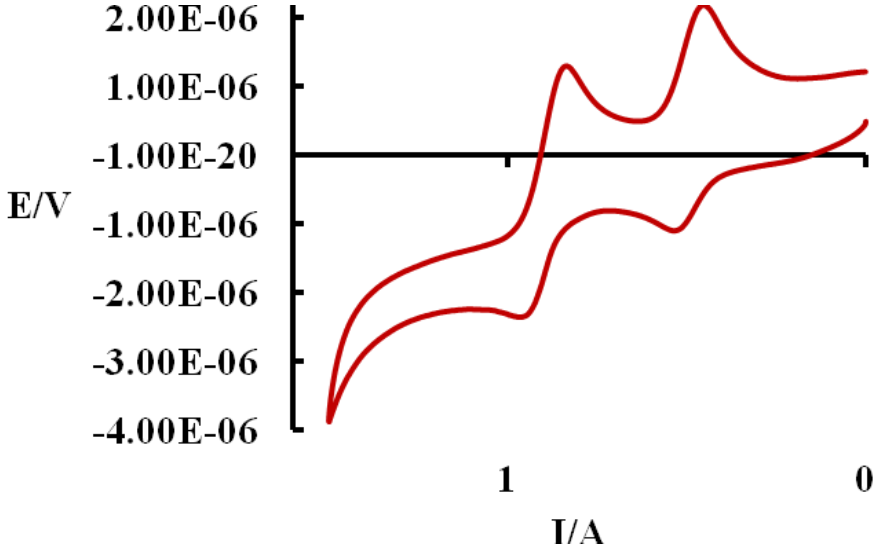


Figure S69: Cyclic voltammogram (CV) for **6c** (DCM, electrolyte $TBAPF_6$; working electrode: Pt; ref. electrode: Ag/AgCl; Scan rate 100 mV s^{-1}).

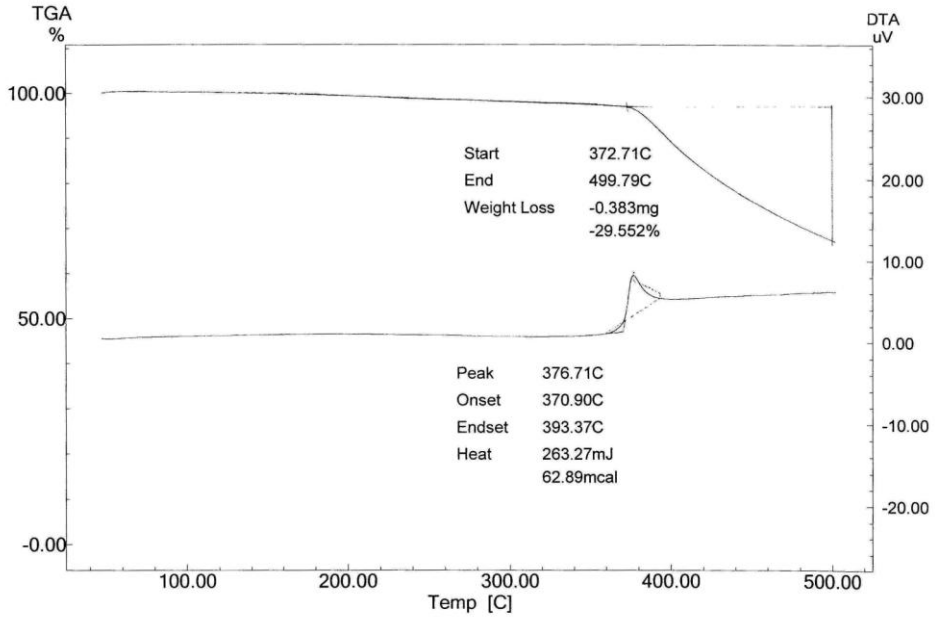


Figure S70: TGA Analysis of **6a** under N_2 with temperature rise of 10°C per minute. **6a** is highly stable as it is having a high thermal decomposition temp. of about >371°C.

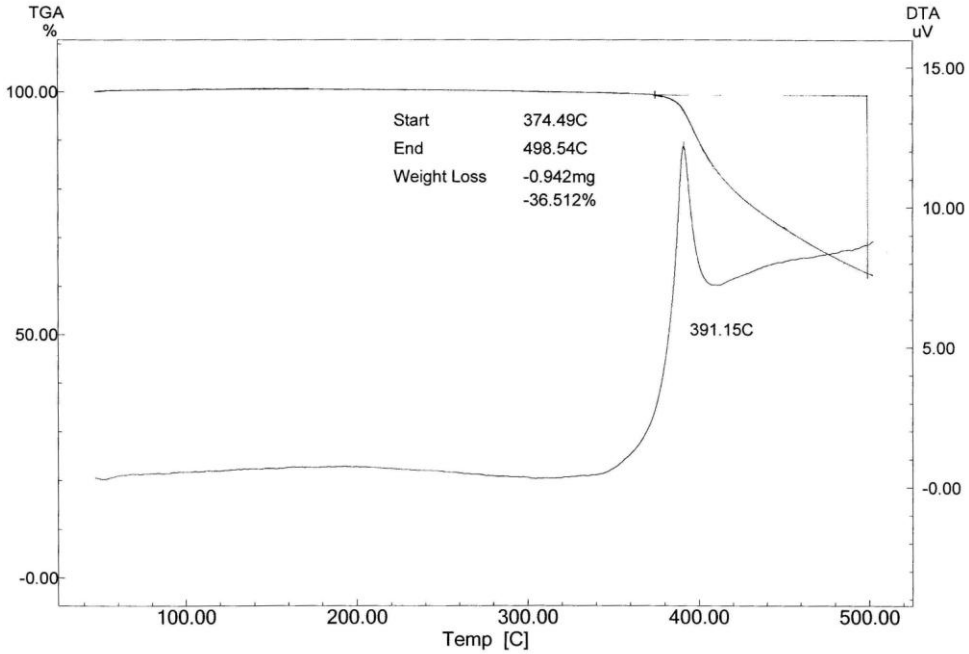


Figure S71: TGA Analysis of **6b** under N_2 with temperature rise of 10°C per minute. **6b** is highly stable as it is having a high thermal decomposition temp. of about >391°C.

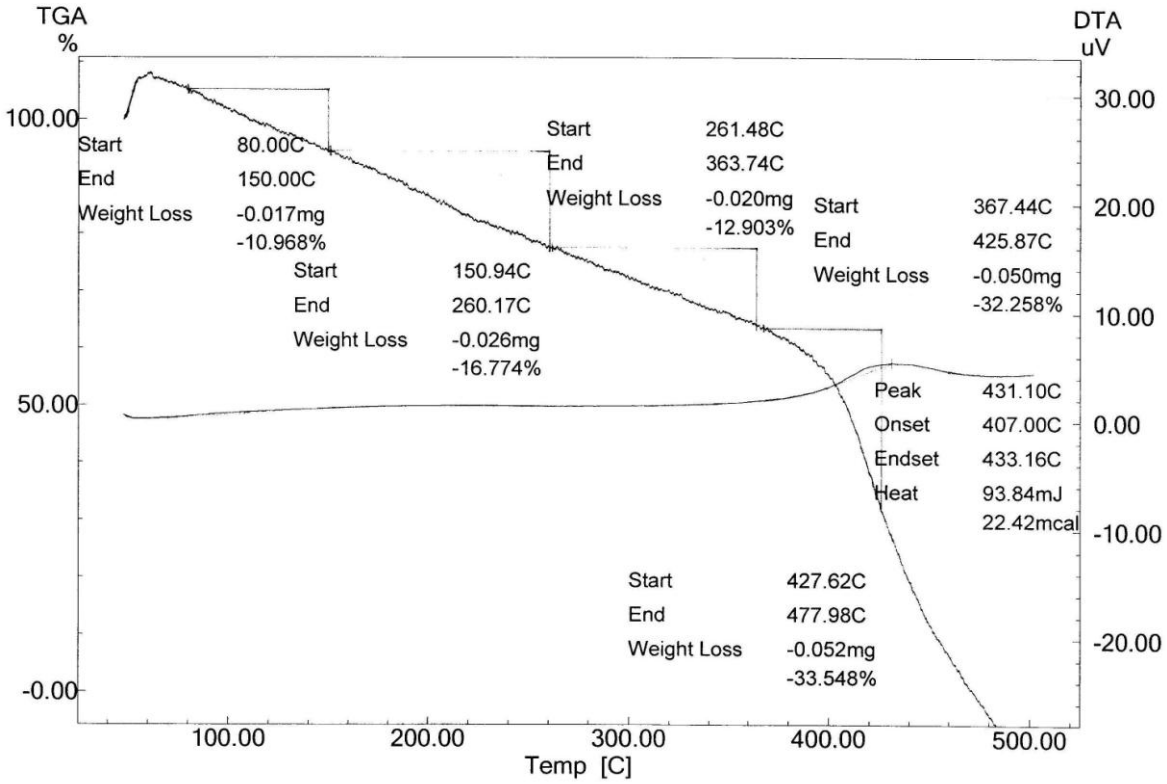


Figure S72: TGA Analysis of **6c** under N_2 with temperature rise of 10°C per minute. **6c** is highly stable as it is having a high thermal decomposition temp. of about >407°C.

X-Ray Diffraction Analysis of 6a:
Single crystals of **6a** suitable for an X-Ray crystal structure determination were grown in a dark, quiet and undisturbed place from dry Toluene (3 weeks).

Table S5: The crystallographic data and structure refinement for **6a:**

Empirical formula	C38 H30 S4
Formula weight	614.86
Temperature	150(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/n
Unit cell dimensions	a = 8.3972(2) A alpha = 90 deg. b = 15.4871(4) A beta = 92.993(3) deg. c = 11.8460(5) A gamma = 90 deg.
Volume	1538.45(8) A^3
Z, Calculated density	2, 1.327 Mg/m^3
Absorption coefficient	0.336 mm^-1
F(000)	644
Crystal size	0.33 x 0.26 x 0.21 mm
Theta range for data collection	2.90 to 25.00 deg.
Limiting indices	-9<=h<=9, -18<=k<=15, -13<=l<=14
Reflections collected / unique	10334 / 2692 [R(int) = 0.0444]
Completeness to theta = 25.00	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9328 and 0.8972
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2692 / 0 / 192
Goodness-of-fit on F^2	1.049
Final R indices [I>2sigma(I)]	R1 = 0.0381, wR2 = 0.0957

R indices (all data)	R1 = 0.0525, wR2 = 0.1089
Extinction coefficient	0.0107(13)
Largest diff. peak and hole	0.195 and -0.197 e.A^-3

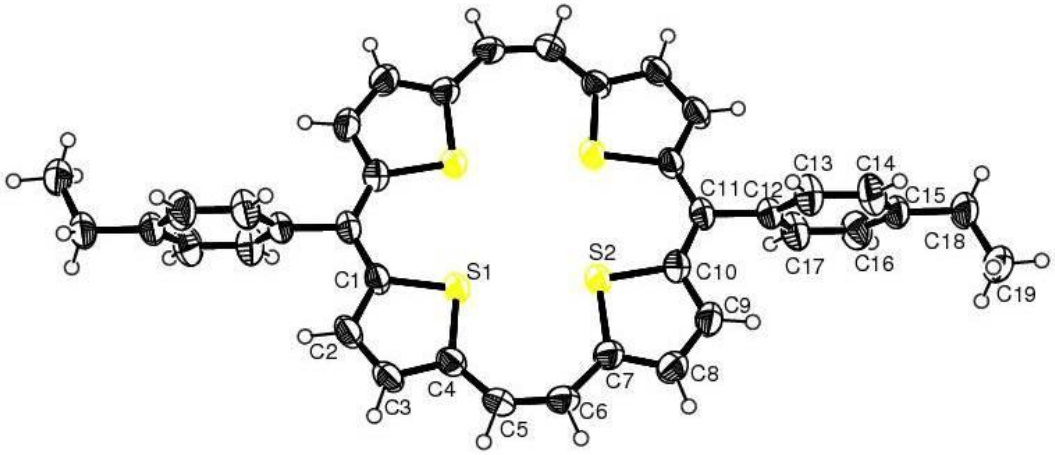


Table S6: Torsion angles [deg] for **6a**:

C(4)-S(1)-C(1)-C(11)#1	179.8(2)
C(4)-S(1)-C(1)-C(2)	0.00(18)
C(11)#1-C(1)-C(2)-C(3)	180.0(2)
S(1)-C(1)-C(2)-C(3)	-0.2(3)
C(1)-C(2)-C(3)-C(4)	0.3(3)
C(2)-C(3)-C(4)-C(5)	179.1(2)
C(2)-C(3)-C(4)-S(1)	-0.3(3)
C(1)-S(1)-C(4)-C(5)	-179.2(2)
C(1)-S(1)-C(4)-C(3)	0.18(18)
C(3)-C(4)-C(5)-C(6)	-175.0(3)
S(1)-C(4)-C(5)-C(6)	4.3(4)
C(4)-C(5)-C(6)-C(7)	1.0(5)
C(5)-C(6)-C(7)-C(8)	-178.6(3)
C(5)-C(6)-C(7)-S(2)	1.3(4)
C(10)-S(2)-C(7)-C(8)	1.76(19)
C(10)-S(2)-C(7)-C(6)	-178.1(2)
C(6)-C(7)-C(8)-C(9)	178.5(2)
S(2)-C(7)-C(8)-C(9)	-1.4(3)
C(7)-C(8)-C(9)-C(10)	0.1(3)
C(8)-C(9)-C(10)-C(11)	-175.6(2)
C(8)-C(9)-C(10)-S(2)	1.2(3)
C(7)-S(2)-C(10)-C(9)	-1.69(18)
C(7)-S(2)-C(10)-C(11)	175.2(2)
C(9)-C(10)-C(11)-C(1)#1	177.4(2)
S(2)-C(10)-C(11)-C(1)#1	1.1(3)
C(9)-C(10)-C(11)-C(12)	-0.8(3)
S(2)-C(10)-C(11)-C(12)	-177.07(16)
C(1)#1-C(11)-C(12)-C(17)	-84.2(3)
C(10)-C(11)-C(12)-C(17)	94.2(3)
C(1)#1-C(11)-C(12)-C(13)	96.4(3)
C(10)-C(11)-C(12)-C(13)	-85.2(3)
C(17)-C(12)-C(13)-C(14)	0.8(4)
C(11)-C(12)-C(13)-C(14)	-179.8(2)
C(12)-C(13)-C(14)-C(15)	-0.2(4)
C(13)-C(14)-C(15)-C(16)	-0.3(4)
C(13)-C(14)-C(15)-C(18)	179.4(2)
C(14)-C(15)-C(16)-C(17)	0.1(4)
C(18)-C(15)-C(16)-C(17)	-179.5(2)
C(13)-C(12)-C(17)-C(16)	-0.9(4)
C(11)-C(12)-C(17)-C(16)	179.7(2)
C(15)-C(16)-C(17)-C(12)	0.5(4)
C(14)-C(15)-C(18)-C(19)	81.4(3)
C(16)-C(15)-C(18)-C(19)	-99.0(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y,-z

The crystal structure has been deposited at the Cambridge Crystallographic Data Centre (CCDC 986822). The data can be obtained free of charge via the Internet at www.ccdc.cam.ac.uk/data_request/cif.

X-Ray Diffraction Analysis of 6b:
Single crystals of **6b** suitable for an X-Ray crystal structure determination were grown in a dark, quiet and undisturbed place from dry DCM with a toluene layer upon it (2 weeks).

Table S7: The crystallographic data and structure refinement for **6b:**

Empirical formula	C80 H68 S8
Formula weight	1285.82
Temperature	150(2) K
Wavelength	1.5418 A
Crystal system, space group	Orthorhombic, P n a 21
Unit cell dimensions	a = 19.7591(3) A alpha = 90 deg. b = 34.5783(4) A beta = 90 deg. c = 9.5257(2) A gamma = 90 deg.
Volume	6508.30(18) A^3
Z, Calculated density	4, 1.312 Mg/m^3
Absorption coefficient	2.888 mm^-1
F(000)	2704
Crystal size	0.33 x 0.26 x 0.21 mm
Theta range for data collection	3.40 to 49.99 deg.
Limiting indices	-19<=h<=19, -34<=k<=34, -7<=l<=9
Reflections collected / unique	27082 / 5655 [R(int) = 0.0229]
Completeness to theta = 25.00	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.5822 and 0.4491
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5655 / 1 / 802
Goodness-of-fit on F^2	1.014
Final R indices [I>2sigma(I)]	R1 = 0.0387, wR2 = 0.1022

R indices (all data)	R1 = 0.0407, wR2 = 0.1048
Absolute structure parameter	-0.01(2)
Extinction coefficient	0.00021(3)
Largest diff. peak and hole	0.299 and -0.211 e.A^-3

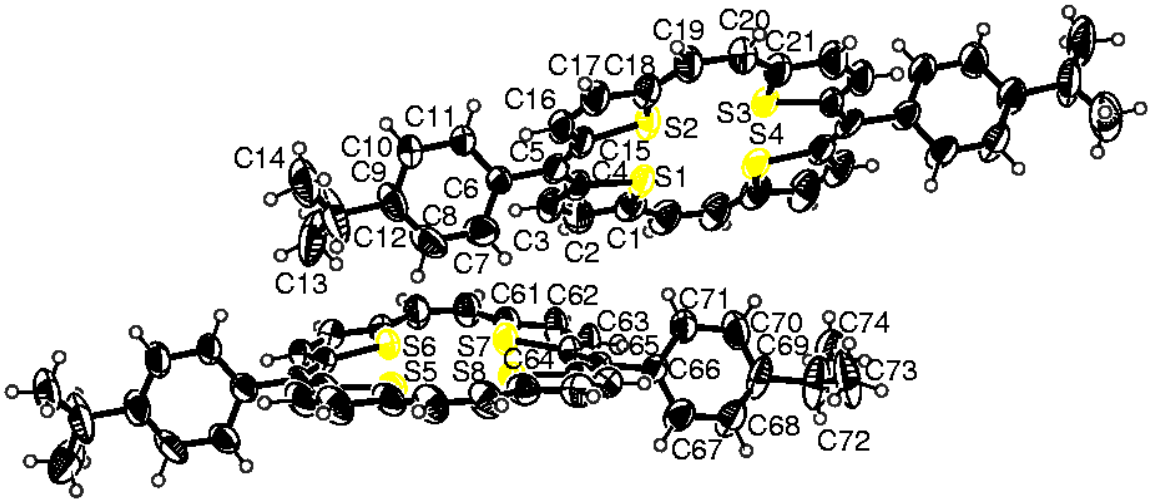


Table S8: Torsion angles [deg] for **6b**:

C(40)-C(1)-C(2)-C(3)	177.2(5)
S(1)-C(1)-C(2)-C(3)	-0.2(6)
C(1)-C(2)-C(3)-C(4)	0.1(7)
C(2)-C(3)-C(4)-C(5)	178.0(5)
C(2)-C(3)-C(4)-S(1)	0.1(6)
C(3)-C(4)-C(5)-C(15)	-172.3(5)
S(1)-C(4)-C(5)-C(15)	5.2(8)
C(3)-C(4)-C(5)-C(6)	7.5(7)
S(1)-C(4)-C(5)-C(6)	-174.9(3)
C(15)-C(5)-C(6)-C(7)	-115.2(6)
C(4)-C(5)-C(6)-C(7)	64.9(7)
C(15)-C(5)-C(6)-C(11)	65.4(7)
C(4)-C(5)-C(6)-C(11)	-114.5(6)
C(11)-C(6)-C(7)-C(8)	-0.8(9)
C(5)-C(6)-C(7)-C(8)	179.8(6)
C(6)-C(7)-C(8)-C(9)	-1.1(11)
C(7)-C(8)-C(9)-C(10)	3.4(11)
C(7)-C(8)-C(9)-C(12)	176.8(7)
C(8)-C(9)-C(10)-C(11)	-3.9(11)
C(12)-C(9)-C(10)-C(11)	-177.1(7)
C(7)-C(6)-C(11)-C(10)	0.4(9)
C(5)-C(6)-C(11)-C(10)	179.8(6)
C(9)-C(10)-C(11)-C(6)	2.0(10)
C(8)-C(9)-C(12)-C(13)	-62.0(14)
C(10)-C(9)-C(12)-C(13)	111.1(11)
C(8)-C(9)-C(12)-C(14)	139.3(9)
C(10)-C(9)-C(12)-C(14)	-47.7(12)
C(4)-C(5)-C(15)-C(16)	-177.6(5)
C(6)-C(5)-C(15)-C(16)	2.6(7)
C(4)-C(5)-C(15)-S(2)	3.9(8)
C(6)-C(5)-C(15)-S(2)	-176.0(3)
C(5)-C(15)-C(16)-C(17)	-176.9(5)
S(2)-C(15)-C(16)-C(17)	1.9(6)
C(15)-C(16)-C(17)-C(18)	-2.5(7)
C(16)-C(17)-C(18)-C(19)	-178.7(5)
C(16)-C(17)-C(18)-S(2)	1.8(6)
C(17)-C(18)-C(19)-C(20)	173.9(6)
S(2)-C(18)-C(19)-C(20)	-6.7(10)
C(18)-C(19)-C(20)-C(21)	-0.1(12)
C(19)-C(20)-C(21)-C(22)	-171.8(6)
C(19)-C(20)-C(21)-S(3)	7.2(10)
C(20)-C(21)-C(22)-C(23)	178.7(5)
S(3)-C(21)-C(22)-C(23)	-0.4(6)
C(21)-C(22)-C(23)-C(24)	-0.3(7)
C(22)-C(23)-C(24)-C(25)	-179.7(5)
C(22)-C(23)-C(24)-S(3)	0.8(6)
C(23)-C(24)-C(25)-C(35)	176.0(5)
S(3)-C(24)-C(25)-C(35)	-4.6(8)
C(23)-C(24)-C(25)-C(26)	-3.8(8)
S(3)-C(24)-C(25)-C(26)	175.6(3)
C(35)-C(25)-C(26)-C(27)	96.8(7)
C(24)-C(25)-C(26)-C(27)	-83.4(7)
C(35)-C(25)-C(26)-C(31)	-81.5(8)
C(24)-C(25)-C(26)-C(31)	98.3(7)
C(31)-C(26)-C(27)-C(28)	-4.7(11)

C(25)-C(26)-C(27)-C(28)	176.9(7)
C(26)-C(27)-C(28)-C(29)	0.6(12)
C(27)-C(28)-C(29)-C(30)	2.8(12)
C(27)-C(28)-C(29)-C(32)	-177.8(8)
C(28)-C(29)-C(30)-C(31)	-2.1(12)
C(32)-C(29)-C(30)-C(31)	178.5(8)
C(27)-C(26)-C(31)-C(30)	5.4(11)
C(25)-C(26)-C(31)-C(30)	-176.3(6)
C(29)-C(30)-C(31)-C(26)	-2.0(11)
C(30)-C(29)-C(32)-C(34)	171.0(11)
C(28)-C(29)-C(32)-C(34)	-8.4(17)
C(30)-C(29)-C(32)-C(33)	-15.4(14)
C(28)-C(29)-C(32)-C(33)	165.2(9)
C(24)-C(25)-C(35)-C(36)	178.4(5)
C(26)-C(25)-C(35)-C(36)	-1.8(9)
C(24)-C(25)-C(35)-S(4)	-1.2(8)
C(26)-C(25)-C(35)-S(4)	178.6(4)
C(25)-C(35)-C(36)-C(37)	-178.8(5)
S(4)-C(35)-C(36)-C(37)	0.9(7)
C(35)-C(36)-C(37)-C(38)	-0.3(8)
C(36)-C(37)-C(38)-C(39)	177.5(6)
C(36)-C(37)-C(38)-S(4)	-0.4(7)
C(37)-C(38)-C(39)-C(40)	-177.8(6)
S(4)-C(38)-C(39)-C(40)	-0.2(11)
C(38)-C(39)-C(40)-C(1)	-1.6(12)
C(2)-C(1)-C(40)-C(39)	179.5(6)
S(1)-C(1)-C(40)-C(39)	-3.7(10)
C(80)-C(41)-C(42)-C(43)	179.5(6)
S(5)-C(41)-C(42)-C(43)	-0.8(7)
C(41)-C(42)-C(43)-C(44)	-0.5(8)
C(42)-C(43)-C(44)-C(45)	-178.1(5)
C(42)-C(43)-C(44)-S(5)	1.6(7)
C(43)-C(44)-C(45)-C(55)	170.2(5)
S(5)-C(44)-C(45)-C(55)	-9.4(8)
C(43)-C(44)-C(45)-C(46)	-8.1(8)
S(5)-C(44)-C(45)-C(46)	172.3(4)
C(44)-C(45)-C(46)-C(51)	113.4(7)
C(55)-C(45)-C(46)-C(51)	-65.1(8)
C(44)-C(45)-C(46)-C(47)	-66.9(7)
C(55)-C(45)-C(46)-C(47)	114.6(6)
C(51)-C(46)-C(47)-C(48)	2.4(9)
C(45)-C(46)-C(47)-C(48)	-177.4(6)
C(46)-C(47)-C(48)-C(49)	-1.0(10)
C(47)-C(48)-C(49)-C(50)	-0.5(11)
C(47)-C(48)-C(49)-C(52)	177.8(7)
C(48)-C(49)-C(50)-C(51)	0.7(12)
C(52)-C(49)-C(50)-C(51)	-177.6(8)
C(47)-C(46)-C(51)-C(50)	-2.2(10)
C(45)-C(46)-C(51)-C(50)	177.5(7)
C(49)-C(50)-C(51)-C(46)	0.7(12)
C(48)-C(49)-C(52)-C(53)	-33.4(15)
C(50)-C(49)-C(52)-C(53)	144.8(10)
C(48)-C(49)-C(52)-C(54)	120.1(9)
C(50)-C(49)-C(52)-C(54)	-61.7(12)
C(44)-C(45)-C(55)-C(56)	178.3(5)
C(46)-C(45)-C(55)-C(56)	-3.4(7)
C(44)-C(45)-C(55)-S(6)	-1.5(8)
C(46)-C(45)-C(55)-S(6)	176.9(4)

C(45)-C(55)-C(56)-C(57)	178.7(5)
S(6)-C(55)-C(56)-C(57)	-1.5(6)
C(55)-C(56)-C(57)-C(58)	2.8(7)
C(58)-C(59)-C(60)-C(61)	0.9(12)
C(59)-C(60)-C(61)-C(62)	165.2(7)
C(59)-C(60)-C(61)-S(7)	-14.7(10)
C(60)-C(61)-C(62)-C(63)	-178.6(5)
S(7)-C(61)-C(62)-C(63)	1.2(6)
C(61)-C(62)-C(63)-C(64)	-1.1(8)
C(62)-C(63)-C(64)-C(65)	-176.9(5)
C(62)-C(63)-C(64)-S(7)	0.5(7)
C(63)-C(64)-C(65)-C(75)	179.4(5)
S(7)-C(64)-C(65)-C(75)	2.4(8)
C(63)-C(64)-C(65)-C(66)	1.7(8)
S(7)-C(64)-C(65)-C(66)	-175.4(4)
C(75)-C(65)-C(66)-C(71)	-108.8(6)
C(64)-C(65)-C(66)-C(71)	69.2(7)
C(75)-C(65)-C(66)-C(67)	69.8(7)
C(64)-C(65)-C(66)-C(67)	-112.3(6)
C(71)-C(66)-C(67)-C(68)	-1.7(9)
C(65)-C(66)-C(67)-C(68)	179.7(6)
C(66)-C(67)-C(68)-C(69)	-0.5(11)
C(67)-C(68)-C(69)-C(70)	2.5(11)
C(67)-C(68)-C(69)-C(72)	-177.7(6)
C(68)-C(69)-C(70)-C(71)	-2.3(11)
C(72)-C(69)-C(70)-C(71)	177.9(7)
C(67)-C(66)-C(71)-C(70)	1.9(10)
C(65)-C(66)-C(71)-C(70)	-179.5(7)
C(69)-C(70)-C(71)-C(66)	0.1(12)
C(68)-C(69)-C(72)-C(73)	-90.7(10)
C(70)-C(69)-C(72)-C(73)	89.0(9)
C(68)-C(69)-C(72)-C(74)	134.2(7)
C(70)-C(69)-C(72)-C(74)	-46.0(10)
C(64)-C(65)-C(75)-C(76)	-172.3(5)
C(66)-C(65)-C(75)-C(76)	5.4(7)
C(64)-C(65)-C(75)-S(8)	7.7(7)
C(66)-C(65)-C(75)-S(8)	-174.5(3)
C(65)-C(75)-C(76)-C(77)	179.6(5)
S(8)-C(75)-C(76)-C(77)	-0.5(6)
C(75)-C(76)-C(77)-C(78)	1.6(7)
C(76)-C(77)-C(78)-C(79)	176.5(5)
C(76)-C(77)-C(78)-S(8)	-1.9(6)
C(77)-C(78)-C(79)-C(80)	-176.8(7)
S(8)-C(78)-C(79)-C(80)	1.3(11)
C(78)-C(79)-C(80)-C(41)	-0.2(13)
C(42)-C(41)-C(80)-C(79)	-179.3(6)
S(5)-C(41)-C(80)-C(79)	1.0(11)
C(56)-C(57)-C(58)-C(59)	178.3(5)
C(56)-C(57)-C(58)-S(6)	-2.7(6)
C(60)-C(59)-C(58)-C(57)	-167.6(6)
C(60)-C(59)-C(58)-S(6)	13.5(10)
C(3)-C(4)-S(1)-C(1)	-0.2(4)
C(5)-C(4)-S(1)-C(1)	-178.1(4)
C(40)-C(1)-S(1)-C(4)	-176.9(5)
C(2)-C(1)-S(1)-C(4)	0.2(4)
C(19)-C(18)-S(2)-C(15)	180.0(5)
C(17)-C(18)-S(2)-C(15)	-0.6(4)
C(16)-C(15)-S(2)-C(18)	-0.7(4)

C(5)-C(15)-S(2)-C(18)	178.1(4)
C(20)-C(21)-S(3)-C(24)	-178.3(5)
C(22)-C(21)-S(3)-C(24)	0.8(4)
C(23)-C(24)-S(3)-C(21)	-0.9(4)
C(25)-C(24)-S(3)-C(21)	179.6(4)
C(25)-C(35)-S(4)-C(38)	178.7(5)
C(36)-C(35)-S(4)-C(38)	-1.0(4)
C(39)-C(38)-S(4)-C(35)	-177.1(6)
C(37)-C(38)-S(4)-C(35)	0.8(4)
C(43)-C(44)-S(5)-C(41)	-1.7(4)
C(45)-C(44)-S(5)-C(41)	177.9(5)
C(80)-C(41)-S(5)-C(44)	-178.9(6)
C(42)-C(41)-S(5)-C(44)	1.4(4)
C(57)-C(58)-S(6)-C(55)	1.5(4)
C(59)-C(58)-S(6)-C(55)	-179.5(5)
C(56)-C(55)-S(6)-C(58)	-0.1(4)
C(45)-C(55)-S(6)-C(58)	179.7(4)
C(62)-C(61)-S(7)-C(64)	-0.8(4)
C(60)-C(61)-S(7)-C(64)	179.1(5)
C(63)-C(64)-S(7)-C(61)	0.2(4)
C(65)-C(64)-S(7)-C(61)	177.7(5)
C(79)-C(78)-S(8)-C(75)	-177.0(5)
C(77)-C(78)-S(8)-C(75)	1.4(4)
C(65)-C(75)-S(8)-C(78)	179.4(4)
C(76)-C(75)-S(8)-C(78)	-0.6(4)

The crystal structure has been deposited at the Cambridge Crystallographic Data Centre (CCDC 948111). The data can be obtained free of charge via the Internet at www.ccdc.cam.ac.uk/data_request/cif.

Transfer and output curves:

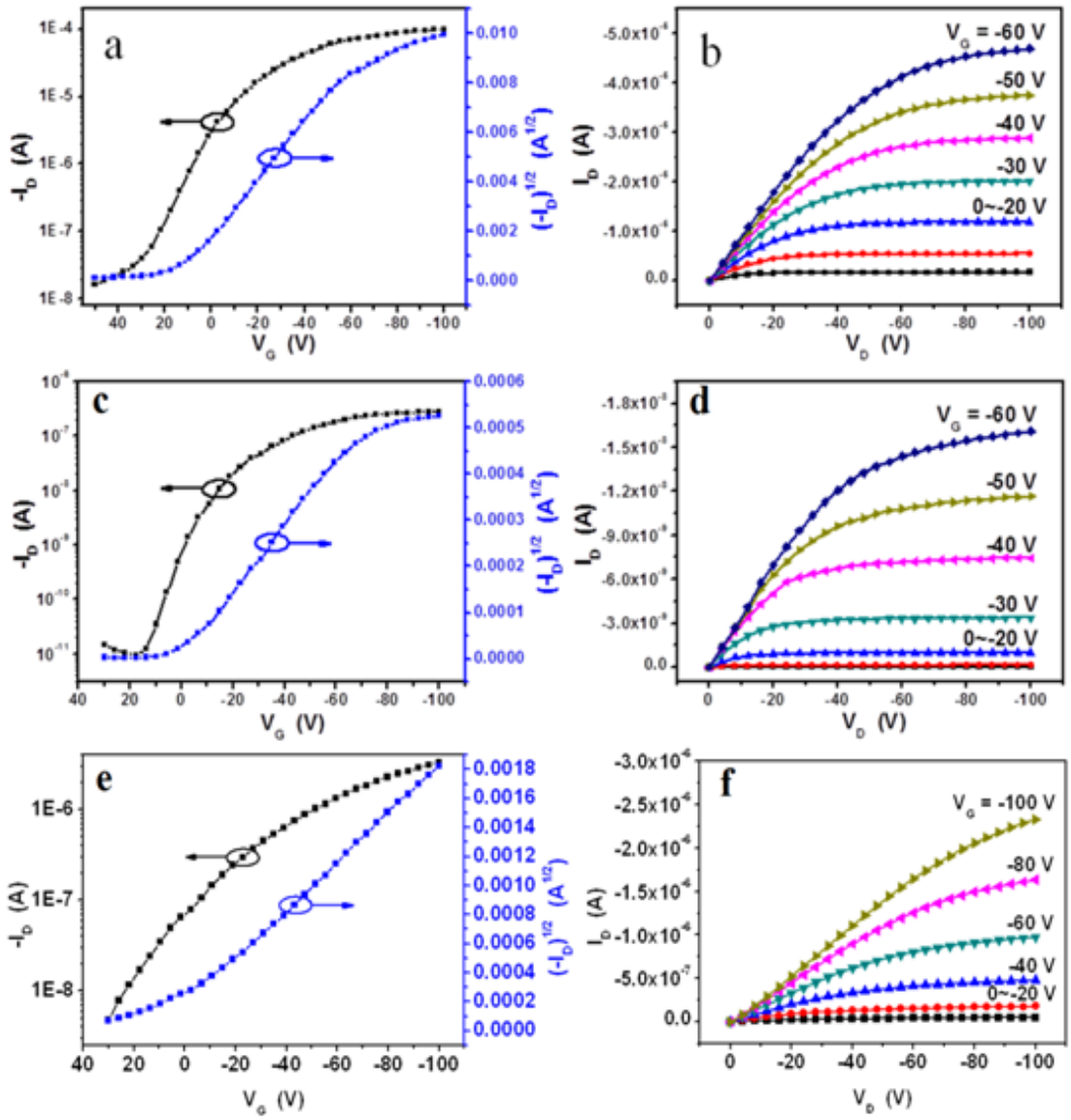


Figure S73: Typical transfer (a) and output (b) characteristics of FET devices based on **6a,** with OTS-treated SiO_2/Si substrate (T_s = 100 ^oC). Typical transfer (c) and output (d) characteristics of FET devices based on **6b,** with OTS-treated SiO_2/Si substrate (T_s = 25 ^oC). Typical transfer (e) and output (f) characteristics of FET devices based on **6c,** with OTS-treated SiO_2/Si substrate (T_s = 25 ^oC).

CIF Files for **6a**:

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_cell_angle_gamma                 90.00
_cell_volume                      1538.45(8)
_cell_formula_units_Z             2
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CrysAlis RED, Oxford Diffraction Ltd.,
Version 1.171.31.7 (release 18-10-2006 CrysAlis171 .NET)
(compiled Oct 18 2006,16:28:17)
Empirical absorption correction using spherical harmonics,
 implemented in SCALE3 ABSPACK scaling algorithm.
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of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
 not relevant to the choice of reflections for refinement.  R-factors
based
 on F^2^ are statistically about twice as large as those based on F,
and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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C6 C 0.6095(2) 0.10648(15) 0.1720(2) 0.0504(6) Uani 1 1 d . . .
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C7 C 0.7432(2) 0.15456(15) 0.1402(2) 0.0467(6) Uani 1 1 d . . .
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C9 C 0.9031(3) 0.27749(14) 0.1323(2) 0.0517(6) Uani 1 1 d . . .
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C10 C 0.9995(2) 0.22021(13) 0.07435(19) 0.0443(5) Uani 1 1 d . . .
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C13 C 1.1763(3) 0.39434(15) -0.0158(2) 0.0593(7) Uani 1 1 d . . .
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C14 C 1.2356(3) 0.47688(15) 0.0047(3) 0.0640(7) Uani 1 1 d . . .
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C4 0.0391(11) 0.0492(13) 0.0476(14) 0.0001(11) 0.0063(10) -0.0072(10)
C5 0.0402(11) 0.0547(15) 0.0547(15) -0.0005(12) 0.0145(10) -0.0054(10)
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C9 0.0558(13) 0.0391(13) 0.0603(16) -0.0092(12) 0.0031(12) -0.0060(10)
C10 0.0453(12) 0.0387(12) 0.0485(14) -0.0032(10) -0.0015(10) -0.0056(9)
C11 0.0463(12) 0.0361(12) 0.0495(15) 0.0004(10) -0.0009(11) -0.0114(9)
C12 0.0459(12) 0.0362(12) 0.0531(15) -0.0009(11) 0.0050(11) -0.0083(10)
C13 0.0643(15) 0.0447(14) 0.0674(18) 0.0020(13) -0.0117(14) -0.0112(12)
C14 0.0679(15) 0.0395(14) 0.084(2) 0.0132(13) -0.0014(15) -0.0052(12)
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0.0213(13)
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taken
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angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
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C12 C17 C16 121.2(2) . . ?
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C5 C6 C7 C8 -178.6(3) . . . . ?
C5 C6 C7 S2 1.3(4) . . . . ?
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C6 C7 C8 C9 178.5(2) . . . . ?
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C9 C10 C11 C12 -0.8(3) . . . . ?
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C10 C11 C12 C17 94.2(3) . . . . ?
C1 C11 C12 C13 96.4(3) 3_755 . . . ?
C10 C11 C12 C13 -85.2(3) . . . . ?
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C11 C12 C13 C14 -179.8(2) . . . . ?
C12 C13 C14 C15 -0.2(4) . . . . ?
C13 C14 C15 C16 -0.3(4) . . . . ?
C13 C14 C15 C18 179.4(2) . . . . ?
C14 C15 C16 C17 0.1(4) . . . . ?
C18 C15 C16 C17 -179.5(2) . . . . ?
C13 C12 C17 C16 -0.9(4) . . . . ?
C11 C12 C17 C16 179.7(2) . . . . ?
C15 C16 C17 C12 0.5(4) . . . . ?
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CIF Files for **6b**:

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 'S'  'S'   0.3331   0.5567
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_symmetry_space_group_name_H-M   'P n a 21'

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_cell_formula_units_Z             4
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_exptl_absorpt_process_details
;
CrysAlis RED, Oxford Diffraction Ltd.,
Version 1.171.31.7 (release 18-10-2006 CrysAlis171 .NET)
(compiled Oct 18 2006,16:28:17)
Empirical absorption correction using spherical harmonics,
 implemented in SCALE3 ABSPACK scaling algorithm.
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_diffrn_radiation_monochromator   graphite
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_diffrn_measurement_method        '\w/q-scan'
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_diffrn_standards_interval_count  ?
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_diffrn_reflns_number             27082
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_diffrn_reflns_av_sigmaI/netI     0.0182
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_diffrn_reflns_limit_h_max        19
_diffrn_reflns_limit_k_min        -34
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_diffrn_reflns_limit_l_min        -7
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Ltd.,'
_computing_cell_refinement        'CrysAlis RED, Oxford Diffraction
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Ltd.,'
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_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR
and
 goodness of fit S are based on F^2^, conventional R-factors R are
based
 on F, with F set to zero for negative F^2^. The threshold expression
of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
 not relevant to the choice of reflections for refinement.  R-factors
based
 on F^2^ are statistically about twice as large as those based on F,
and R-
 factors based on ALL data will be even larger.
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P=(Fo^2^+2Fc^2^)/3'
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_refine_ls_extinction_method      SHELXL
_refine_ls_extinction_coef        0.00021(3)
_refine_ls_extinction_expression
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_refine_ls_abs_structure_Flack    -0.01(2)
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C2 C 0.4107(3) 1.34069(16) 0.0145(7) 0.0755(16) Uani 1 1 d . . .
H2 H 0.4005 1.3507 -0.0759 0.091 Uiso 1 1 calc R . .
C3 C 0.4254(3) 1.36379(15) 0.1248(7) 0.0679(16) Uani 1 1 d . . .
H3 H 0.4262 1.3912 0.1175 0.082 Uiso 1 1 calc R . .
C4 C 0.4393(2) 1.34445(14) 0.2500(6) 0.0558(14) Uani 1 1 d . . .
C5 C 0.4579(3) 1.36157(13) 0.3783(7) 0.0583(14) Uani 1 1 d . . .
C6 C 0.4542(2) 1.40487(12) 0.3828(6) 0.0531(13) Uani 1 1 d . . .
C7 C 0.3934(3) 1.42379(16) 0.3699(7) 0.0749(17) Uani 1 1 d . . .
H7 H 0.3530 1.4092 0.3576 0.090 Uiso 1 1 calc R . .
C8 C 0.3901(3) 1.46364(17) 0.3745(8) 0.089(2) Uani 1 1 d . . .
H8 H 0.3475 1.4760 0.3636 0.106 Uiso 1 1 calc R . .
C9 C 0.4463(3) 1.48569(15) 0.3941(7) 0.0820(19) Uani 1 1 d . . .
C10 C 0.5075(3) 1.46714(14) 0.4020(7) 0.0792(19) Uani 1 1 d . . .
H10 H 0.5479 1.4819 0.4098 0.095 Uiso 1 1 calc R . .
C11 C 0.5114(3) 1.42708(13) 0.3985(7) 0.0665(16) Uani 1 1 d . . .
H11 H 0.5543 1.4148 0.4071 0.080 Uiso 1 1 calc R . .
C12 C 0.4416(5) 1.53021(17) 0.3910(10) 0.146(4) Uani 1 1 d . . .
H12 H 0.3975 1.5322 0.4420 0.175 Uiso 1 1 calc R . .
C13 C 0.4221(5) 1.54745(19) 0.2778(11) 0.153(4) Uani 1 1 d . . .
H13A H 0.4603 1.5496 0.2127 0.229 Uiso 1 1 calc R . .
H13B H 0.4054 1.5734 0.3011 0.229 Uiso 1 1 calc R . .
H13C H 0.3857 1.5325 0.2337 0.229 Uiso 1 1 calc R . .
C14 C 0.4823(4) 1.54837(16) 0.4975(9) 0.129(3) Uani 1 1 d . . .
H14A H 0.4676 1.5752 0.5103 0.193 Uiso 1 1 calc R . .
H14B H 0.5299 1.5480 0.4687 0.193 Uiso 1 1 calc R . .
H14C H 0.4773 1.5343 0.5862 0.193 Uiso 1 1 calc R . .
C15 C 0.4793(2) 1.34276(13) 0.5008(7) 0.0566(14) Uani 1 1 d . . .
C16 C 0.4953(2) 1.35963(15) 0.6286(6) 0.0626(16) Uani 1 1 d . . .
H16 H 0.4908 1.3866 0.6453 0.075 Uiso 1 1 calc R . .
C17 C 0.5180(3) 1.33457(15) 0.7281(7) 0.0678(16) Uani 1 1 d . . .
H17 H 0.5322 1.3430 0.8184 0.081 Uiso 1 1 calc R . .
C18 C 0.5192(3) 1.29537(14) 0.6883(6) 0.0616(14) Uani 1 1 d . . .
C19 C 0.5394(3) 1.26561(15) 0.7765(7) 0.0711(16) Uani 1 1 d . . .
H19 H 0.5568 1.2748 0.8631 0.085 Uiso 1 1 calc R . .
C20 C 0.5403(3) 1.22537(15) 0.7679(7) 0.0763(17) Uani 1 1 d . . .
H20 H 0.5583 1.2141 0.8509 0.092 Uiso 1 1 calc R . .
C21 C 0.5220(3) 1.19742(15) 0.6716(7) 0.0709(17) Uani 1 1 d . . .
C22 C 0.5218(3) 1.15763(15) 0.7033(8) 0.0779(17) Uani 1 1 d . . .
H22 H 0.5351 1.1476 0.7920 0.094 Uiso 1 1 calc R . .
C23 C 0.5005(3) 1.13436(16) 0.5929(9) 0.083(2) Uani 1 1 d . . .
H23 H 0.4983 1.1070 0.6007 0.100 Uiso 1 1 calc R . .
C24 C 0.4829(2) 1.15319(14) 0.4729(8) 0.0704(19) Uani 1 1 d . . .
C25 C 0.4591(3) 1.13638(14) 0.3448(8) 0.0674(18) Uani 1 1 d . . .
C26 C 0.4586(2) 1.09280(13) 0.3480(7) 0.0691(17) Uani 1 1 d . . .
C27 C 0.5162(3) 1.07268(14) 0.3192(8) 0.087(2) Uani 1 1 d . . .
H27 H 0.5559 1.0863 0.2926 0.104 Uiso 1 1 calc R . .
C28 C 0.5179(3) 1.03307(16) 0.3279(9) 0.101(3) Uani 1 1 d . . .
H28 H 0.5590 1.0200 0.3080 0.121 Uiso 1 1 calc R . .
C29 C 0.4613(3) 1.01146(14) 0.3649(8) 0.0826(19) Uani 1 1 d . . .
C30 C 0.4030(3) 1.03189(15) 0.3862(8) 0.088(2) Uani 1 1 d . . .
H30 H 0.3626 1.0183 0.4086 0.106 Uiso 1 1 calc R . .
C31 C 0.4010(3) 1.07228(15) 0.3758(7) 0.083(2) Uani 1 1 d . . .
H31 H 0.3593 1.0855 0.3883 0.099 Uiso 1 1 calc R . .
C32 C 0.4662(4) 0.96735(16) 0.3785(13) 0.149(4) Uani 1 1 d . . .
H32 H 0.4444 0.9634 0.2848 0.179 Uiso 1 1 calc R . .
C33 C 0.4107(4) 0.94872(19) 0.4499(10) 0.142(4) Uani 1 1 d . . .
H33A H 0.4114 0.9559 0.5494 0.213 Uiso 1 1 calc R . .
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H33B H 0.4153 0.9206 0.4411 0.213 Uiso 1 1 calc R . .
H33C H 0.3679 0.9570 0.4078 0.213 Uiso 1 1 calc R . .
C34 C 0.5202(4) 0.94961(17) 0.3394(15) 0.199(7) Uani 1 1 d . . .
H34A H 0.5138 0.9217 0.3499 0.299 Uiso 1 1 calc R . .
H34B H 0.5583 0.9580 0.3978 0.299 Uiso 1 1 calc R . .
H34C H 0.5297 0.9557 0.2409 0.299 Uiso 1 1 calc R . .
C35 C 0.4376(3) 1.15493(15) 0.2257(8) 0.0693(17) Uani 1 1 d . . .
C36 C 0.4156(3) 1.13797(18) 0.0988(8) 0.0818(19) Uani 1 1 d . . .
H36 H 0.4132 1.1108 0.0860 0.098 Uiso 1 1 calc R . .
C37 C 0.3984(3) 1.16330(18) -0.0032(9) 0.094(2) Uani 1 1 d . . .
H37 H 0.3832 1.1551 -0.0930 0.113 Uiso 1 1 calc R . .
C38 C 0.4044(3) 1.20230(16) 0.0316(7) 0.0756(18) Uani 1 1 d . . .
C39 C 0.3915(3) 1.23247(18) -0.0602(7) 0.0842(19) Uani 1 1 d . . .
H39 H 0.3765 1.2233 -0.1488 0.101 Uiso 1 1 calc R . .
C40 C 0.3947(3) 1.27228(16) -0.0576(7) 0.0788(18) Uani 1 1 d . . .
H40 H 0.3825 1.2834 -0.1451 0.095 Uiso 1 1 calc R . .
C41 C 0.1942(3) 1.51187(16) 0.4628(7) 0.0731(18) Uani 1 1 d . . .
C42 C 0.1967(3) 1.55164(18) 0.4929(8) 0.087(2) Uani 1 1 d . . .
H42 H 0.1865 1.5616 0.5834 0.104 Uiso 1 1 calc R . .
C43 C 0.2146(3) 1.57499(18) 0.3832(8) 0.082(2) Uani 1 1 d . . .
H43 H 0.2176 1.6023 0.3912 0.098 Uiso 1 1 calc R . .
C44 C 0.2282(3) 1.55542(15) 0.2591(8) 0.0669(16) Uani 1 1 d . . .
C45 C 0.2493(2) 1.57154(14) 0.1319(8) 0.0655(17) Uani 1 1 d . . .
C46 C 0.2499(3) 1.61500(14) 0.1191(7) 0.0690(17) Uani 1 1 d . . .
C47 C 0.1886(3) 1.63523(15) 0.1210(7) 0.0795(19) Uani 1 1 d . . .
H47 H 0.1470 1.6219 0.1342 0.095 Uiso 1 1 calc R . .
C48 C 0.1895(3) 1.67572(16) 0.1030(8) 0.094(2) Uani 1 1 d . . .
H48 H 0.1475 1.6891 0.1029 0.112 Uiso 1 1 calc R . .
C49 C 0.2473(3) 1.69651(16) 0.0857(8) 0.095(2) Uani 1 1 d . . .
C50 C 0.3056(3) 1.67570(15) 0.0881(9) 0.099(2) Uani 1 1 d . . .
H50 H 0.3472 1.6892 0.0775 0.119 Uiso 1 1 calc R . .
C51 C 0.3078(3) 1.63626(14) 0.1048(8) 0.089(2) Uani 1 1 d . . .
H51 H 0.3504 1.6235 0.1065 0.106 Uiso 1 1 calc R . .
C52 C 0.2466(5) 1.74004(17) 0.0614(11) 0.147(4) Uani 1 1 d . . .
H52 H 0.2820 1.7412 -0.0135 0.176 Uiso 1 1 calc R . .
C53 C 0.1958(4) 1.7558(2) -0.0107(11) 0.148(4) Uani 1 1 d . . .
H53A H 0.2035 1.7837 -0.0203 0.222 Uiso 1 1 calc R . .
H53B H 0.1531 1.7514 0.0392 0.222 Uiso 1 1 calc R . .
H53C H 0.1934 1.7440 -0.1041 0.222 Uiso 1 1 calc R . .
C54 C 0.2829(4) 1.76015(17) 0.1692(8) 0.109(3) Uani 1 1 d . . .
H54A H 0.2558 1.7605 0.2554 0.163 Uiso 1 1 calc R . .
H54B H 0.2917 1.7867 0.1389 0.163 Uiso 1 1 calc R . .
H54C H 0.3259 1.7470 0.1872 0.163 Uiso 1 1 calc R . .
C55 C 0.2725(2) 1.55138(13) 0.0116(8) 0.0630(15) Uani 1 1 d . . .
C56 C 0.2922(3) 1.56755(15) -0.1171(8) 0.0687(17) Uani 1 1 d . . .
H56 H 0.2904 1.5946 -0.1343 0.082 Uiso 1 1 calc R . .
C57 C 0.3143(2) 1.54149(14) -0.2175(8) 0.0745(17) Uani 1 1 d . . .
H57 H 0.3307 1.5491 -0.3071 0.089 Uiso 1 1 calc R . .
C59 C 0.3286(3) 1.47185(14) -0.2633(7) 0.0712(16) Uani 1 1 d . . .
H59 H 0.3522 1.4805 -0.3443 0.085 Uiso 1 1 calc R . .
C60 C 0.3207(3) 1.43220(14) -0.2615(7) 0.0703(16) Uani 1 1 d . . .
H60 H 0.3409 1.4204 -0.3411 0.084 Uiso 1 1 calc R . .
C61 C 0.2904(3) 1.40482(14) -0.1724(6) 0.0641(15) Uani 1 1 d . . .
C62 C 0.2769(3) 1.36657(14) -0.2123(7) 0.0740(16) Uani 1 1 d . . .
H62 H 0.2883 1.3565 -0.3020 0.089 Uiso 1 1 calc R . .
C63 C 0.2458(3) 1.34497(14) -0.1098(7) 0.0685(16) Uani 1 1 d . . .
H63 H 0.2333 1.3188 -0.1244 0.082 Uiso 1 1 calc R . .
C64 C 0.2339(2) 1.36377(13) 0.0158(7) 0.0573(14) Uani 1 1 d . . .
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C65 C 0.2056(2) 1.34783(14) 0.1393(6) 0.0547(14) Uani 1 1 d . . .
C66 C 0.1885(2) 1.30548(14) 0.1329(6) 0.0549(13) Uani 1 1 d . . .
C67 C 0.1227(3) 1.29297(15) 0.1363(7) 0.0767(18) Uani 1 1 d . . .
H67 H 0.0871 1.3113 0.1432 0.092 Uiso 1 1 calc R . .
C68 C 0.1075(3) 1.25418(16) 0.1297(7) 0.087(2) Uani 1 1 d . . .
H68 H 0.0614 1.2464 0.1331 0.104 Uiso 1 1 calc R . .
C69 C 0.1556(4) 1.22688(16) 0.1186(7) 0.0797(19) Uani 1 1 d . . .
C70 C 0.2224(4) 1.23880(17) 0.1195(9) 0.101(2) Uani 1 1 d . . .
H70 H 0.2577 1.2202 0.1154 0.121 Uiso 1 1 calc R . .
C71 C 0.2383(3) 1.27803(15) 0.1265(9) 0.089(2) Uani 1 1 d . . .
H71 H 0.2844 1.2858 0.1269 0.107 Uiso 1 1 calc R . .
C72 C 0.1366(4) 1.18362(17) 0.1060(8) 0.111(3) Uani 1 1 d . . .
H72 H 0.0891 1.1839 0.0701 0.133 Uiso 1 1 calc R . .
C73 C 0.1323(5) 1.16501(17) 0.2328(10) 0.149(4) Uani 1 1 d . . .
H73A H 0.1778 1.1611 0.2710 0.224 Uiso 1 1 calc R . .
H73B H 0.1102 1.1399 0.2199 0.224 Uiso 1 1 calc R . .
H73C H 0.1057 1.1807 0.2982 0.224 Uiso 1 1 calc R . .
C74 C 0.1765(3) 1.16332(17) -0.0086(8) 0.103(2) Uani 1 1 d . . .
H74A H 0.1584 1.1372 -0.0225 0.155 Uiso 1 1 calc R . .
H74B H 0.2242 1.1617 0.0190 0.155 Uiso 1 1 calc R . .
H74C H 0.1727 1.1780 -0.0963 0.155 Uiso 1 1 calc R . .
C75 C 0.1943(2) 1.36676(13) 0.2654(6) 0.0545(14) Uani 1 1 d . . .
C76 C 0.1731(3) 1.34966(15) 0.3929(6) 0.0613(14) Uani 1 1 d . . .
H76 H 0.1645 1.3228 0.4020 0.074 Uiso 1 1 calc R . .
C77 C 0.1662(3) 1.37503(16) 0.5017(7) 0.0736(15) Uani 1 1 d . . .
H77 H 0.1534 1.3671 0.5934 0.088 Uiso 1 1 calc R . .
C78 C 0.1796(2) 1.41384(15) 0.4675(6) 0.0641(15) Uani 1 1 d . . .
C79 C 0.1719(3) 1.44394(17) 0.5609(7) 0.0810(18) Uani 1 1 d . . .
H79 H 0.1591 1.4347 0.6510 0.097 Uiso 1 1 calc R . .
C80 C 0.1776(3) 1.48377(18) 0.5604(7) 0.0793(17) Uani 1 1 d . . .
H80 H 0.1676 1.4946 0.6497 0.095 Uiso 1 1 calc R . .
C58 C 0.3101(2) 1.50276(13) -0.1744(7) 0.0653(17) Uani 1 1 d . . .
S1 S 0.43283(6) 1.29472(3) 0.22015(16) 0.0638(4) Uani 1 1 d . . .
S2 S 0.49193(7) 1.29266(3) 0.51427(17) 0.0644(4) Uani 1 1 d . . .
S3 S 0.49488(6) 1.20317(3) 0.49855(18) 0.0677(4) Uani 1 1 d . . .
S4 S 0.43321(6) 1.20521(4) 0.20558(19) 0.0716(5) Uani 1 1 d . . .
S5 S 0.21512(6) 1.50604(3) 0.28506(17) 0.0633(4) Uani 1 1 d . . .
S6 S 0.28122(6) 1.50119(3) -0.00137(18) 0.0609(4) Uani 1 1 d . . .
S7 S 0.26344(6) 1.41140(3) 0.00073(16) 0.0607(4) Uani 1 1 d . . .
S8 S 0.20407(6) 1.41661(3) 0.29154(16) 0.0570(4) Uani 1 1 d . . .

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C2 0.079(4) 0.063(4) 0.084(5) 0.003(4) 0.005(4) -0.004(3)
C3 0.075(4) 0.050(3) 0.078(5) -0.016(4) 0.020(3) -0.012(3)
C4 0.054(3) 0.046(3) 0.067(4) -0.002(3) 0.015(3) -0.010(2)
C5 0.049(3) 0.044(3) 0.082(4) -0.011(3) 0.015(3) -0.009(3)
C6 0.048(3) 0.039(3) 0.073(4) -0.011(3) 0.008(3) 0.001(2)
C7 0.060(4) 0.075(4) 0.089(5) -0.027(3) -0.006(3) 0.009(3)
C8 0.086(4) 0.074(4) 0.107(5) -0.038(4) -0.030(4) 0.038(4)
C9 0.113(5) 0.047(3) 0.086(5) -0.023(3) -0.036(4) 0.022(4)
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C10 0.074(4) 0.039(3) 0.125(6) 0.001(3) -0.007(4) -0.002(3)
C11 0.055(3) 0.040(3) 0.104(5) -0.003(3) 0.008(3) 0.000(2)
C12 0.256(11) 0.044(4) 0.137(7) -0.017(4) -0.111(8) 0.040(5)
C13 0.210(9) 0.067(4) 0.181(10) 0.054(6) -0.102(8) -0.059(5)
C14 0.174(7) 0.052(4) 0.160(8) -0.026(5) -0.073(7) 0.014(4)
C15 0.055(3) 0.039(3) 0.076(4) -0.010(3) 0.015(3) -0.010(2)
C16 0.064(3) 0.039(3) 0.085(5) -0.019(3) 0.009(3) -0.005(2)
C17 0.071(3) 0.050(3) 0.082(4) -0.016(3) 0.007(3) -0.008(3)
C18 0.066(3) 0.049(3) 0.069(4) -0.010(3) 0.007(3) -0.012(2)
C19 0.083(4) 0.049(3) 0.081(4) -0.006(3) -0.003(3) -0.005(3)
C20 0.080(4) 0.050(3) 0.098(5) -0.001(3) -0.002(4) -0.003(3)
C21 0.064(3) 0.044(3) 0.105(5) -0.013(3) 0.009(3) -0.004(3)
C22 0.086(4) 0.047(3) 0.100(5) -0.010(4) 0.009(4) -0.003(3)
C23 0.073(4) 0.037(3) 0.141(7) -0.013(4) 0.026(4) -0.004(3)
C24 0.046(3) 0.033(3) 0.131(6) -0.006(4) 0.021(4) 0.000(2)
C25 0.041(3) 0.047(3) 0.114(6) -0.036(4) 0.020(3) -0.016(3)
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C29 0.075(4) 0.049(3) 0.124(6) -0.016(4) 0.040(4) -0.004(3)
C30 0.074(4) 0.057(4) 0.134(6) -0.037(4) 0.051(4) -0.027(3)
C31 0.053(3) 0.058(3) 0.137(6) -0.042(4) 0.037(4) -0.014(3)
C32 0.124(6) 0.038(3) 0.286(12) 0.011(5) 0.096(7) -0.007(4)
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C34 0.134(7) 0.037(3) 0.43(2) -0.002(7) 0.116(10) 0.004(4)
C35 0.050(3) 0.048(3) 0.110(5) -0.025(4) 0.022(3) -0.011(3)
C36 0.083(4) 0.061(4) 0.102(5) -0.039(4) 0.017(4) -0.029(3)
C37 0.115(5) 0.072(4) 0.094(6) -0.039(5) 0.018(5) -0.031(4)
C38 0.072(4) 0.063(4) 0.091(5) -0.038(4) 0.012(3) -0.020(3)
C39 0.094(4) 0.072(4) 0.087(5) -0.027(4) 0.004(4) -0.024(3)
C40 0.079(4) 0.073(4) 0.084(5) -0.027(3) 0.011(3) -0.016(3)
C41 0.075(4) 0.061(4) 0.084(5) -0.034(4) -0.018(3) 0.023(3)
C42 0.107(5) 0.073(4) 0.080(5) -0.031(4) -0.028(4) 0.028(3)
C43 0.087(4) 0.056(4) 0.102(6) -0.045(4) -0.026(4) 0.028(3)
C44 0.059(3) 0.046(3) 0.095(5) -0.021(4) -0.015(3) 0.013(3)
C45 0.048(3) 0.036(3) 0.112(5) -0.029(4) -0.029(3) 0.015(2)
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C48 0.097(5) 0.061(4) 0.123(6) -0.041(4) -0.063(4) 0.044(4)
C49 0.101(5) 0.045(3) 0.139(7) -0.022(4) -0.073(5) 0.007(4)
C50 0.098(5) 0.041(3) 0.159(7) -0.011(4) -0.065(5) 0.002(3)
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C55 0.047(3) 0.038(3) 0.104(5) -0.003(4) -0.017(3) -0.002(2)
C56 0.053(3) 0.039(3) 0.114(6) -0.017(4) -0.011(3) -0.001(3)
C57 0.066(3) 0.050(3) 0.107(5) 0.001(4) -0.004(4) -0.008(3)
C59 0.081(4) 0.048(3) 0.084(5) 0.000(3) 0.015(3) -0.001(3)
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C61 0.077(3) 0.048(3) 0.067(4) -0.006(3) 0.011(3) 0.001(3)
C62 0.106(4) 0.040(3) 0.077(4) -0.014(3) 0.006(4) -0.005(3)
C63 0.093(4) 0.033(3) 0.079(4) -0.006(3) 0.006(3) -0.008(3)
C64 0.058(3) 0.036(3) 0.078(4) -0.010(3) -0.001(3) -0.001(2)
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C66 0.051(3) 0.047(3) 0.067(4) -0.008(3) 0.004(3) -0.008(2)
C67 0.063(3) 0.064(4) 0.104(5) -0.032(3) 0.015(3) -0.013(3)
C68 0.078(4) 0.066(4) 0.116(6) -0.035(4) 0.042(4) -0.025(3)

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C69 0.112(5) 0.052(3) 0.075(4) -0.009(3) 0.043(4) -0.038(4)
C70 0.101(5) 0.045(4) 0.156(7) -0.005(4) 0.029(5) 0.009(3)
C71 0.070(4) 0.048(4) 0.149(7) -0.003(4) 0.026(4) -0.002(3)
C72 0.185(8) 0.056(4) 0.091(5) -0.020(4) 0.058(5) -0.034(4)
C73 0.236(10) 0.051(4) 0.161(8) 0.040(5) 0.099(8) 0.023(5)
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C75 0.036(3) 0.045(3) 0.083(4) -0.007(3) -0.007(3) 0.002(2)
C76 0.055(3) 0.056(3) 0.072(4) 0.000(3) 0.002(3) -0.002(3)
C77 0.070(4) 0.077(4) 0.074(4) -0.004(4) -0.001(3) 0.002(3)
C78 0.062(3) 0.067(4) 0.063(4) -0.011(3) 0.002(3) 0.007(3)
C79 0.094(4) 0.068(4) 0.080(5) -0.020(4) 0.005(3) 0.015(3)
C80 0.100(5) 0.075(4) 0.063(4) -0.014(4) -0.001(3) 0.018(3)
C58 0.052(3) 0.042(3) 0.102(5) -0.007(3) 0.008(3) -0.003(2)
S1 0.0641(8) 0.0462(7) 0.0811(10) -0.0149(7) 0.0152(8) -0.0142(6)
S2 0.0767(9) 0.0387(7) 0.0777(10) -0.0104(7) 0.0127(8) -0.0093(6)
S3 0.0524(7) 0.0411(7) 0.1096(13) -0.0206(8) 0.0024(8) -0.0059(5)
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S6 0.0588(8) 0.0368(6) 0.0873(10) -0.0140(7) -0.0011(8) 0.0014(5)
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_geom_special_details
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 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
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C20 C21 1.381(8) . ?
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C26 C31 1.367(7) . ?
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C28 H28 0.9500 . ?
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C29 C32 1.534(7) . ?
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C43 H43 0.9500 . ?
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C45 C46 1.508(7) . ?
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C46 C47 1.400(7) . ?
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H14B C14 H14C 109.5 . . ?
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