Supporting Information

Thienopyrrole and Selenophenopyrrole Donor Fused with Benzotriazole Acceptor: Microwave Assisted Synthesis and Electrochemical Polymerization

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Table 1. Crystallographic data and structure refinement parameters.

Formula	$C_{20}H_{19}N_5S_2.C_4H_8O_2$	$C_{20}H_{19}N_5Se_2.C_4H_8O_2$	$C_{22}H_{23}N_5S_2$	$C_{22}H_{23}N_5Se_2$
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
space group	P 1 21/c 1	P21/c	P 21/n	P 1 21/n 1
a [Å]	7.3225(2)	7.2332(3)	9.5446(4)	9.5962(4)
b [Å]	15.3272(5)	15.9927(6)	14.8256(5)	14.5492(5)
c [Å]	21.4586(6)	21.3756(8)	15.3905(6)	15.4086(6)
α [deg]	90	90.00	90.00	90
β [deg]	94.056(3)	95.932(3)	102.452(4)	102.721(4)
γ [deg]	90	90.00	90.00	90
V [Å3]	2402.34(12)	2459.45(17)	2126.61(14)	2098.50(14)
Z	4	4	4	4
λ [Å]	0.71073	1.54184	0.71073	0.71073
ρcalcd	1.3316	1.554	1.317	1.6312
F[000]	1017.3545	1160	888	1031.6812
μ [mm−1]	0.253	4.009	0.269	3.543
θ [deg]	3.09-27.97	3.4550-66.3150	1.93-28.22	2.2950- 28.0090
index ranges	$-5 \le h \le 8$ $-20 \le k \le 19$ $-25 \le l \le 28$	$-8 \le h \le 6$ $-18 \le k \le 18$ $-25 \le l \le 24$	$-11 \le h \le 12$ $-18 \le k \le 7$ $-20 \le l \le 9$	$-12 \le h \le 7$ $-19 \le k \le 12$ $-20 \le l \le 20$
T [K]	293.15	100.03(10)	293(2)	99.98(10)
R1	0.066472	0.0418	0.0591	0.045370
wR2	0.0944	0.1060	0.1384	0.1143
Rmerge	0.086986	0.0439	0.0895	0.059614
parameters	143	301	265	264
GOF	1.164225	1.104	1.068	1.142507
reflns total	9430	9009	7193	8088
unique reflns	4852	4273	4595	4595
obsd reflns	3697	4015	3049	3710
CCDC No.	1021387	1021388	999722	1021386

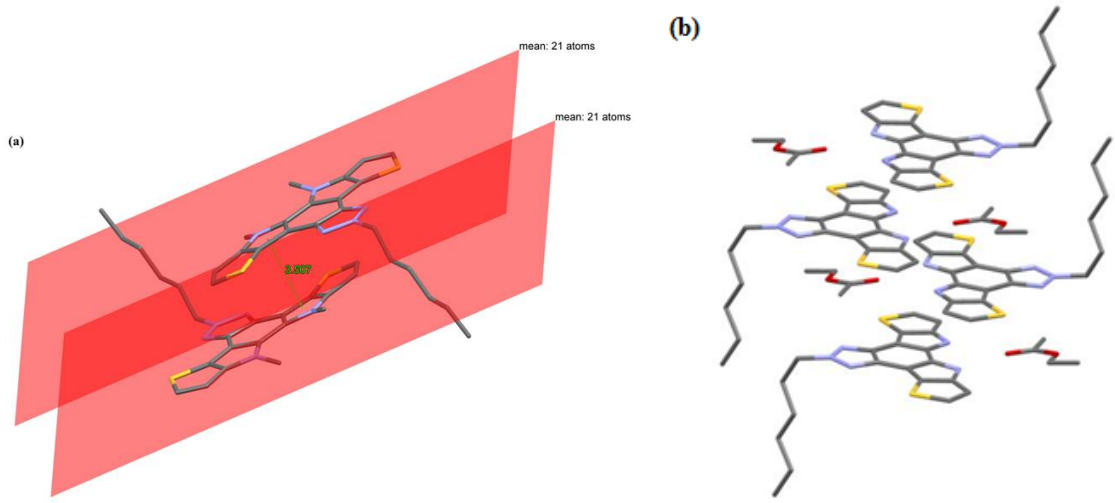


Figure S1. (a) Interplanar distance (by picking only the atoms of the rings) between two molecules of **6.** (b) Arrangement of neighboring molecules in the crystal packing of **4**.

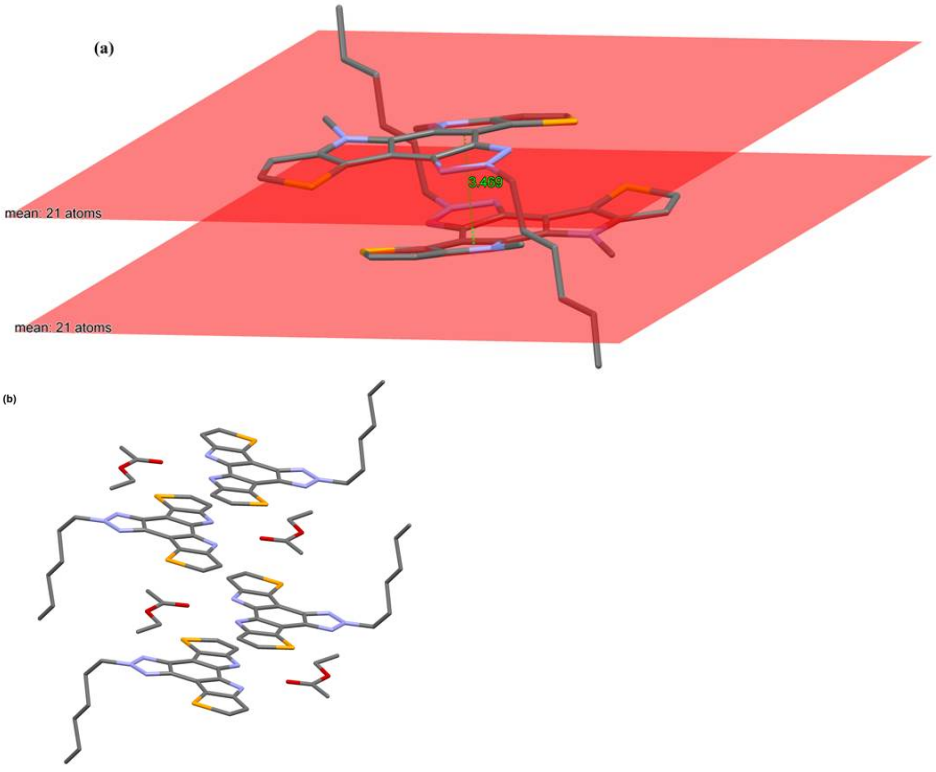


Figure S2. (a) Interplanar distance (by picking only the atoms of the rings) between two molecules of **7.** (b) Arrangement of neighboring molecules in the crystal packing of **5**.

UV-vis and fluorescence spectra

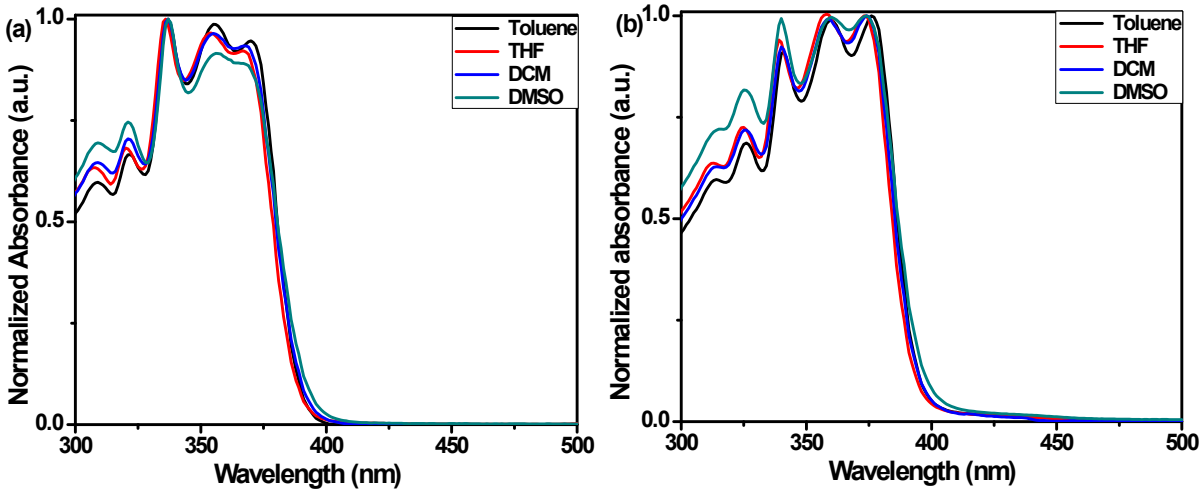


Figure S3. Solution state absorption spectra of compound (a) **6** and compound (b) **7**.

Scan rate dependence of polymer

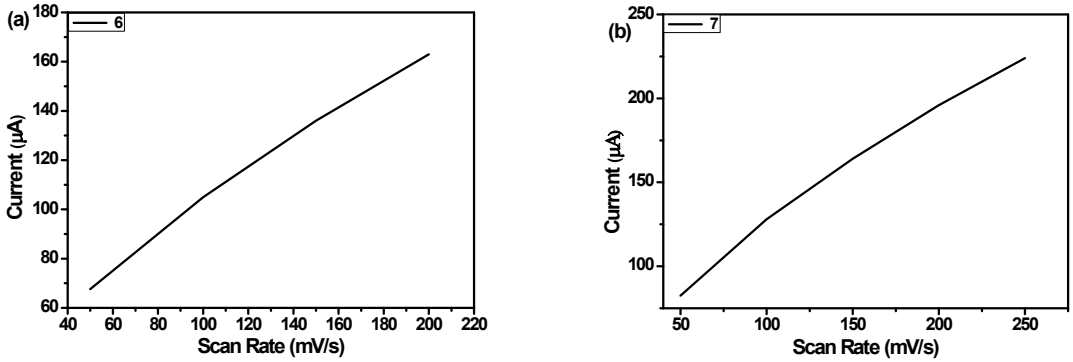


Figure S4. Linear increase in current with the scan rate for (a) **6** and (b) **7**.

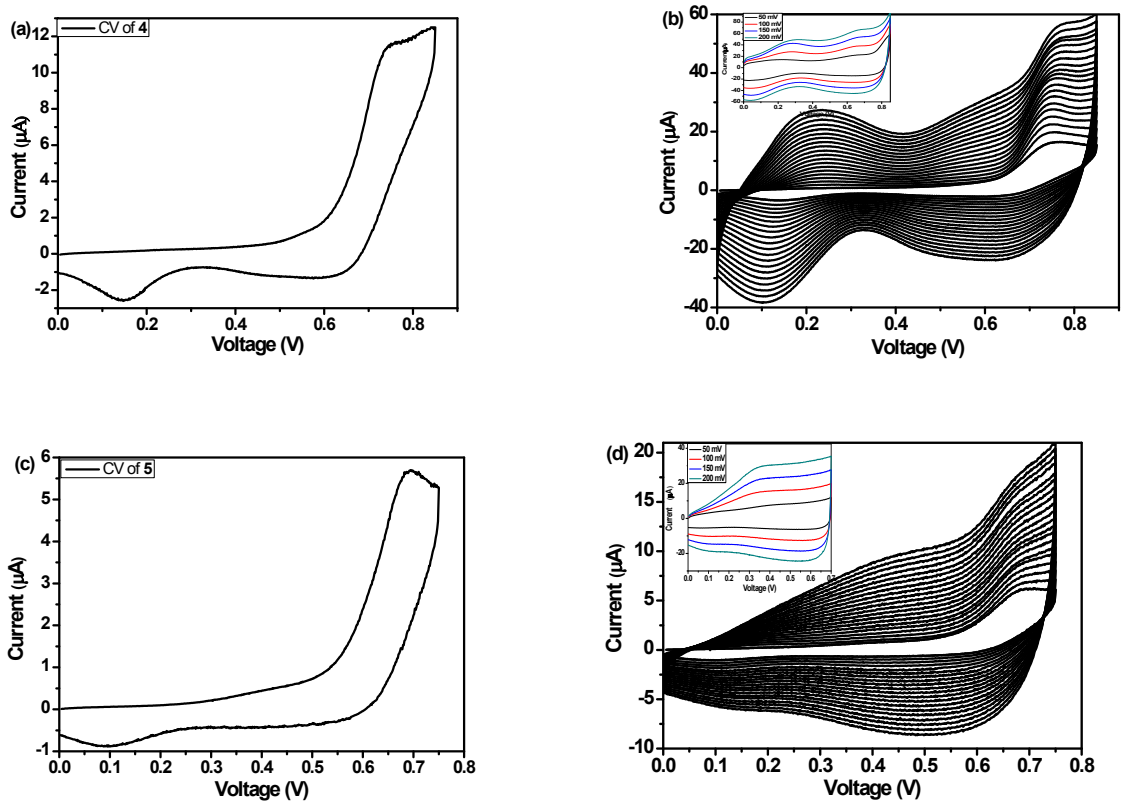


Figure S5. CV of (a) **4** and (c) **5** in ACN and 0.1 M TBAPC on a Pt electrode at a scan rate of 50 mV/s vs Ag/AgCl wire. Multisweep electrochemical polymerization of (b) **4** and (d) **5** on a Pt electrode in ACN and 0.1 M TBAPC at a scan rate of 50 mV/s vs Ag/AgCl wire. (Inset) CV of (b) **P4** and (d) **P5** produced in monomer free ACN and 0.1 M TBAPC as a function of scan rate.

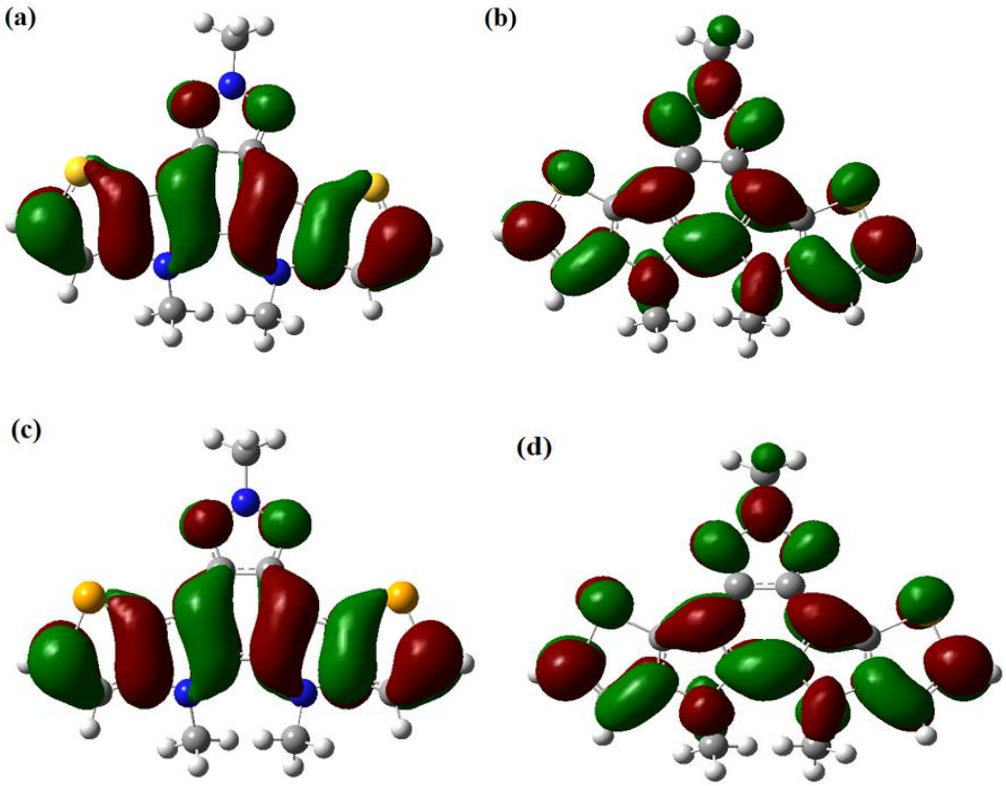


Figure S6. (a) HOMO, (b) LUMO for **6**; (c) HOMO and (d) LUMO for **7**.

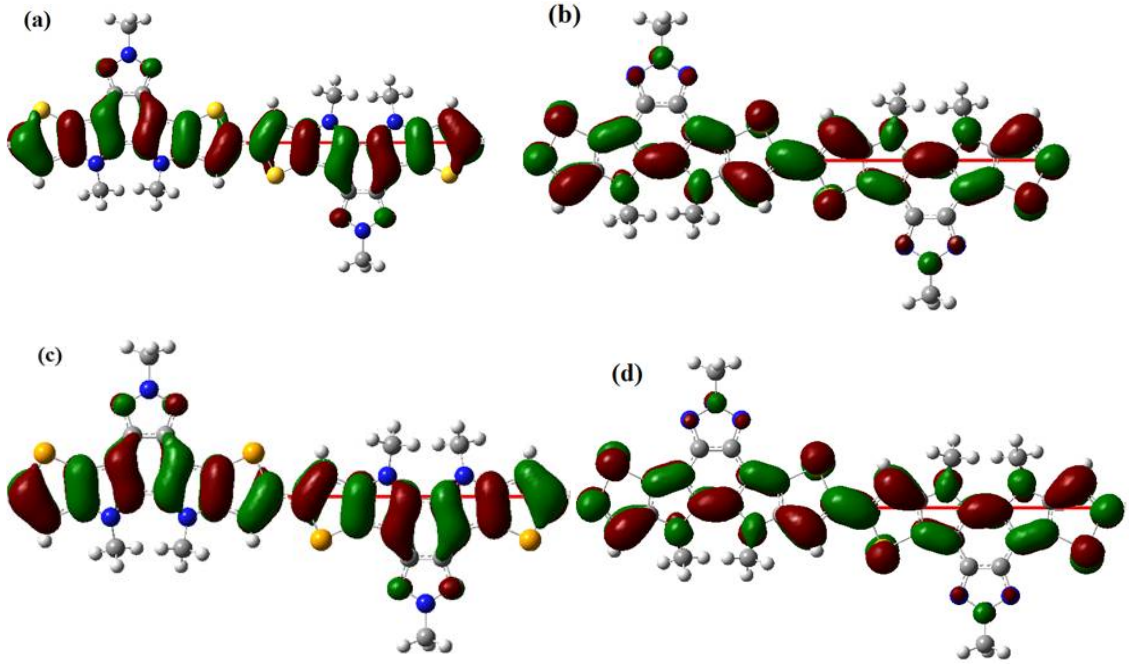
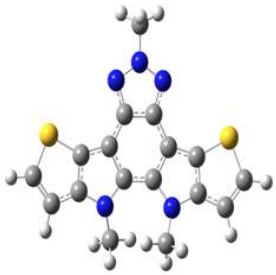
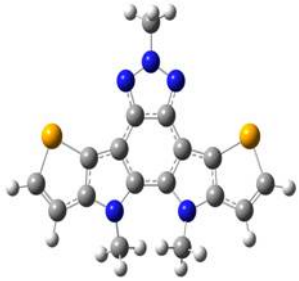
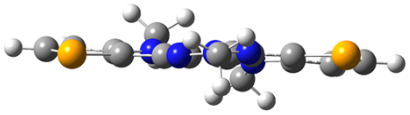


Figure S7. (a) HOMO, (b) LUMO for **P6**; (c) HOMO and (d) LUMO for **P7**.

Table S2. Optimized structures of **6** and **7**.

Monomer	Top View	Side View	HOMO (eV)	LUMO (eV)
6			−4.72	−1.00
7			−4.69	−1.01

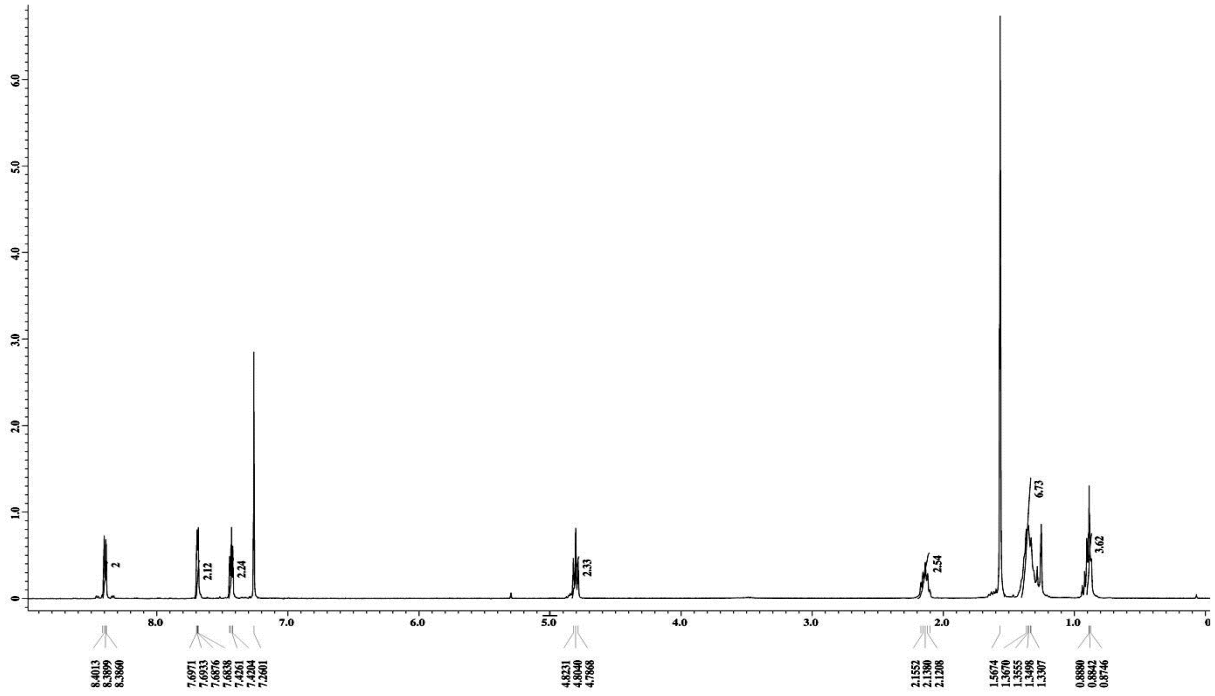


Figure S8. ^{1}H NMR of compound **3.**

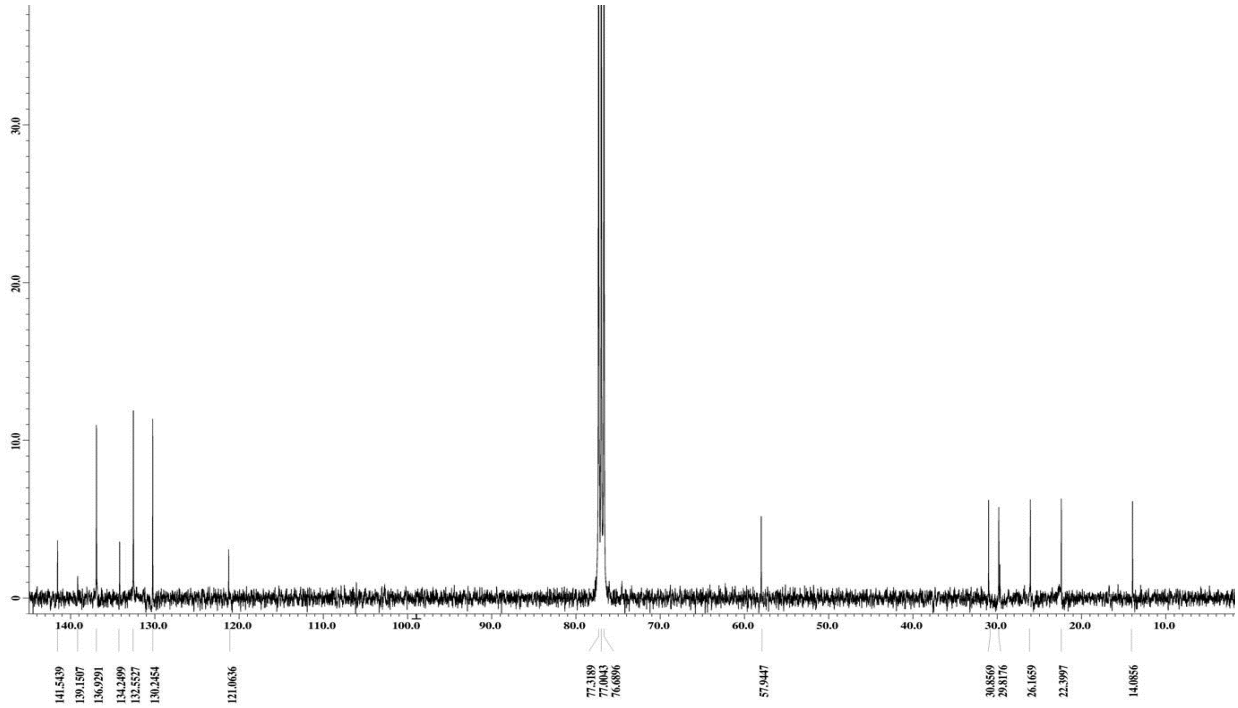


Figure S9. ^{13}C NMR of compound **3**.

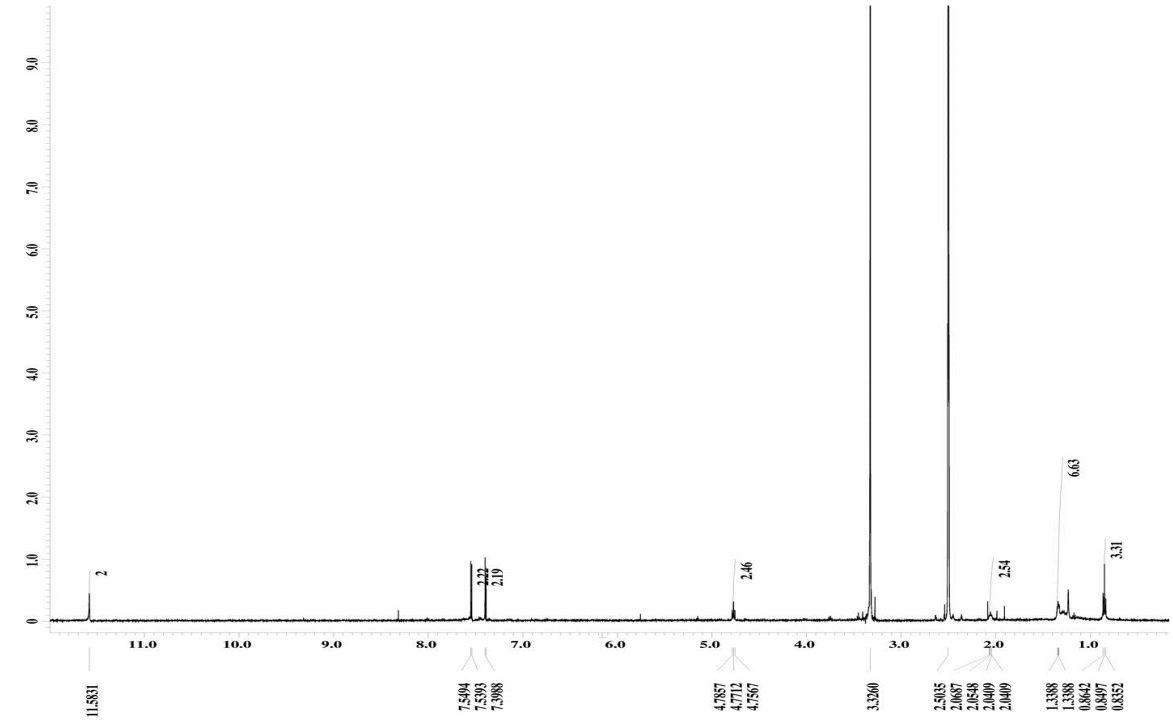


Figure S10. ^{1}H NMR of compound **4.**

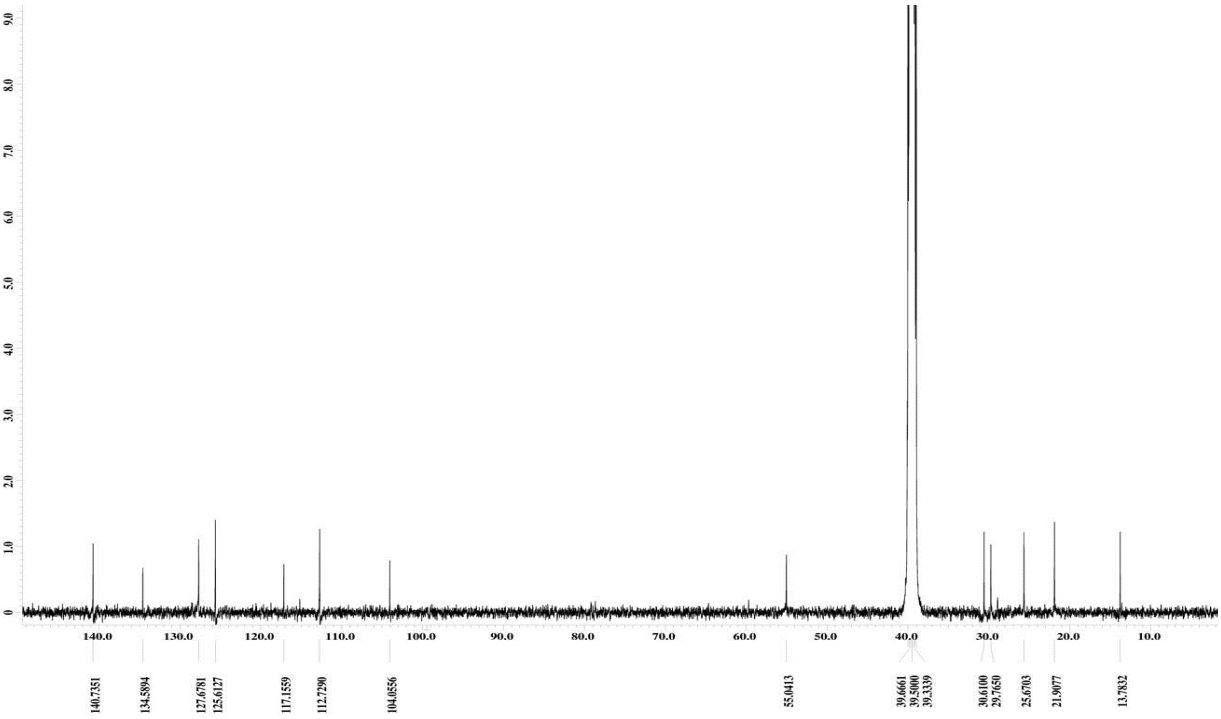


Figure S11. ^{13}C NMR of compound **4**.

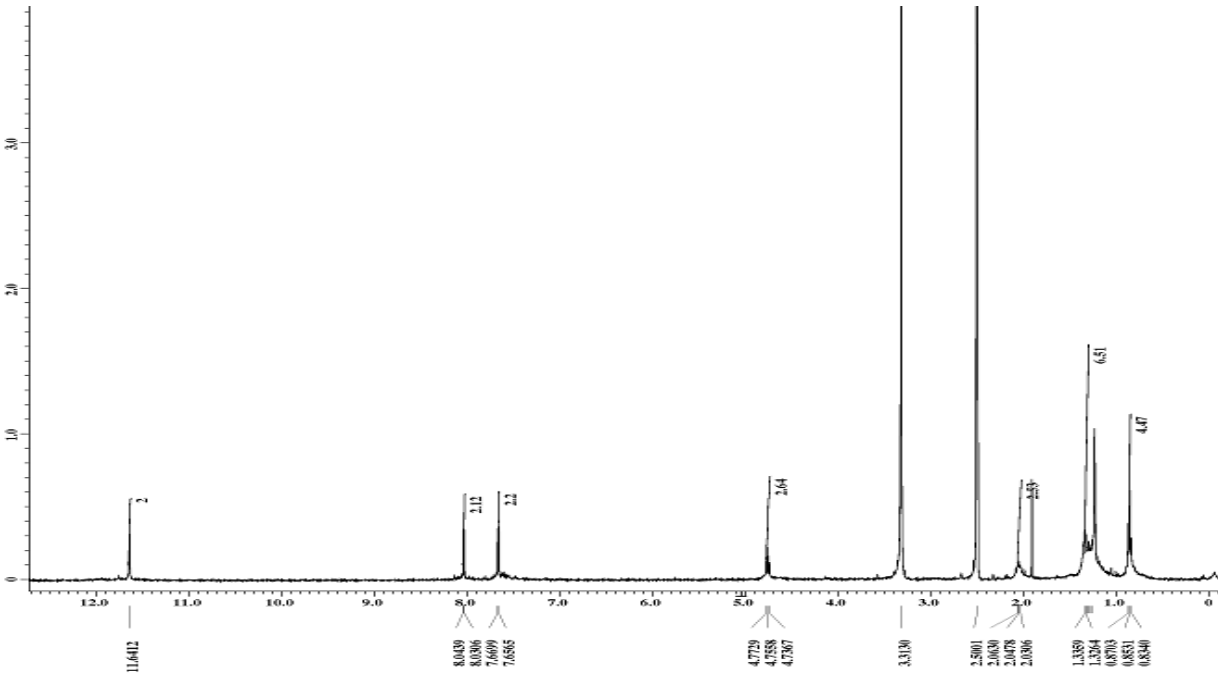


Figure S12. ^{1}H NMR of compound **5.**

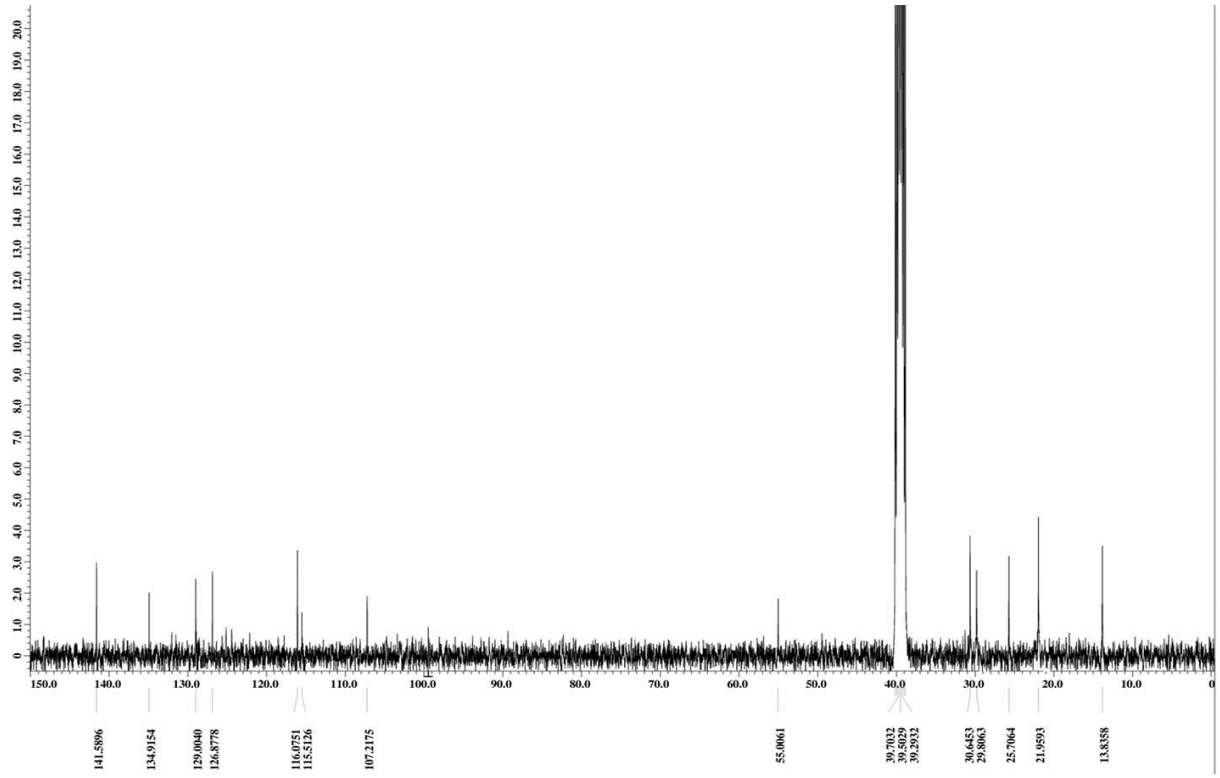


Figure S13. ^{13}C NMR of compound **5**.

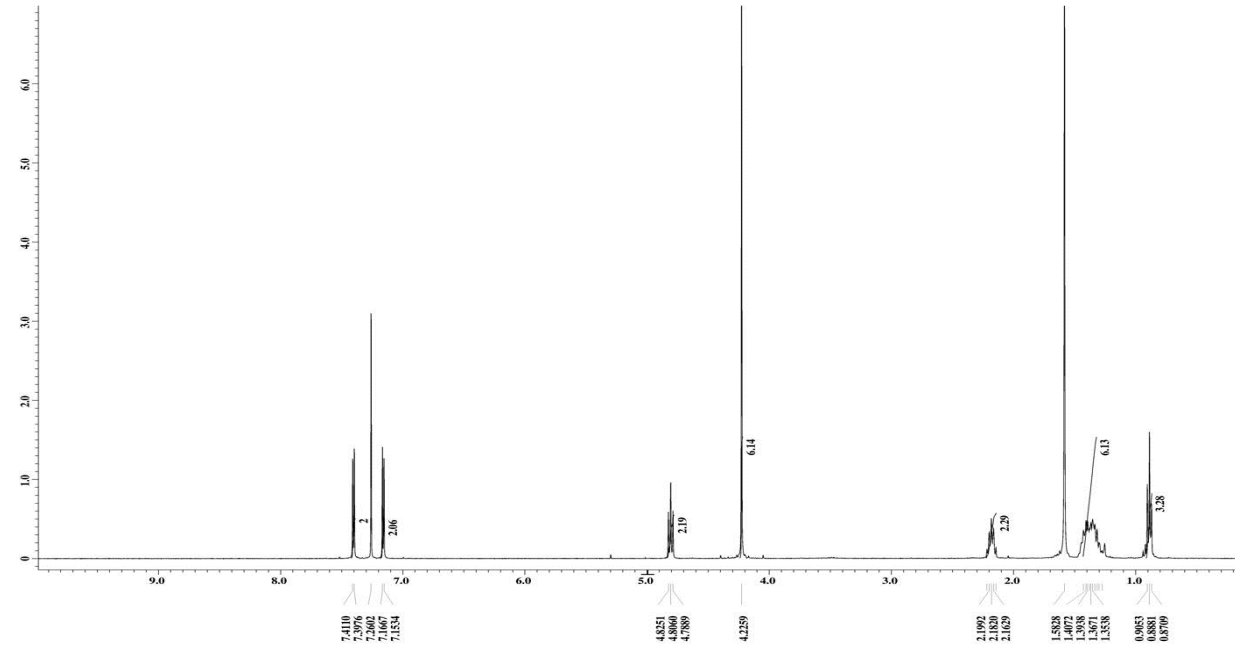


Figure S14. ^{1}H NMR of compound **6.**

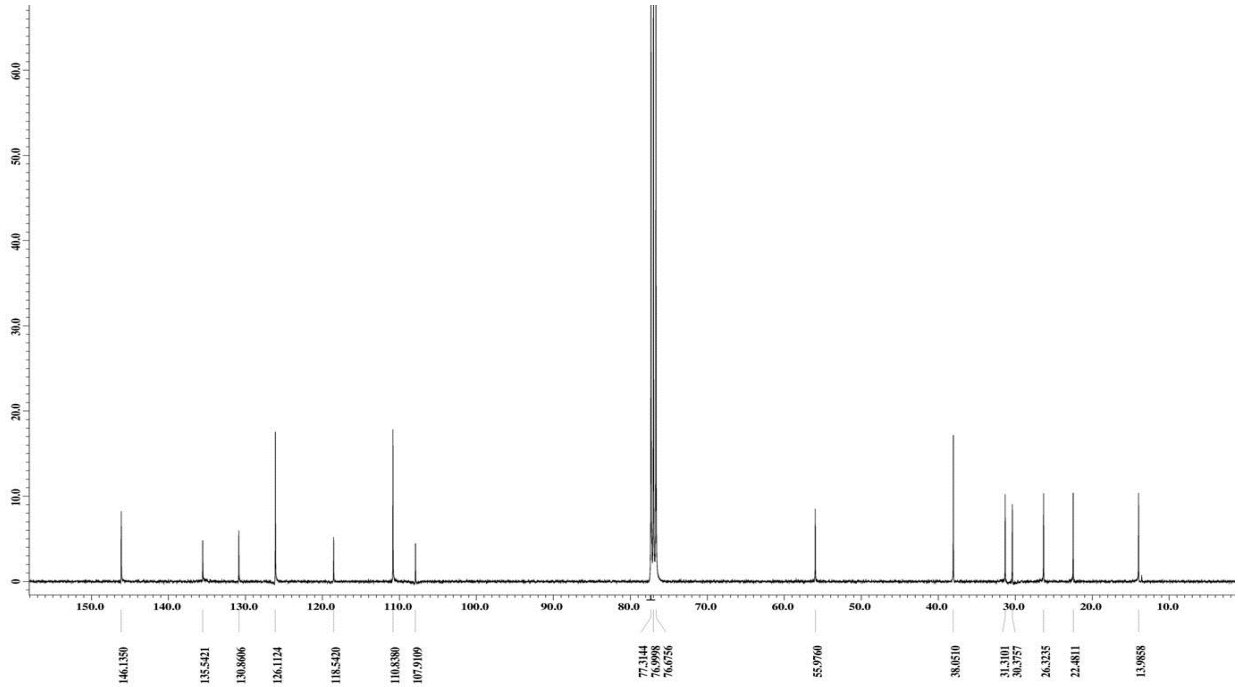


Figure S15. ^{13}C NMR of compound **6**.

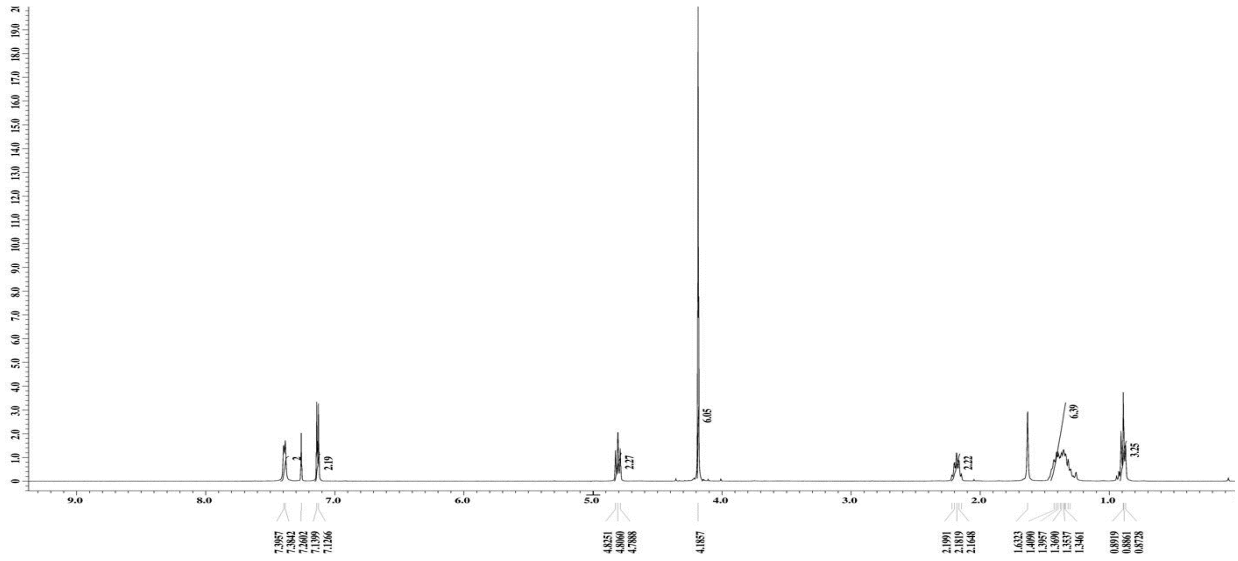


Figure S16. ^{1}H NMR of compound **7.**

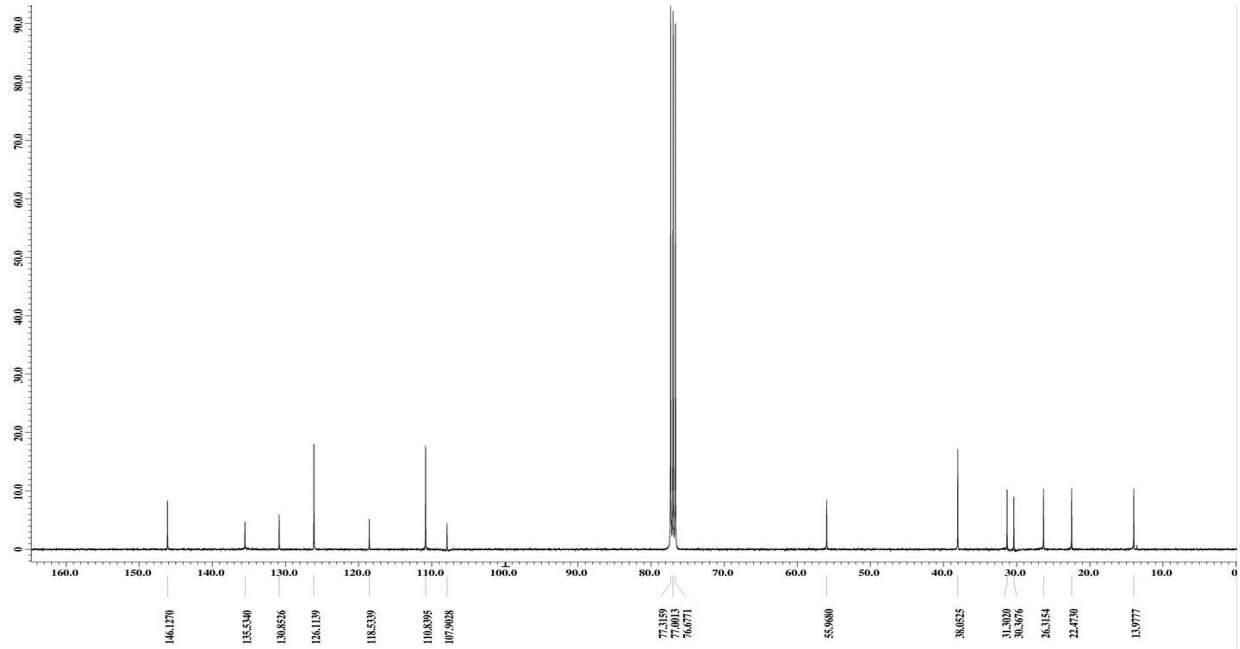


Figure S17. ^{13}C NMR of compound **7**.

Reference

T. L. Tam, H. Li, Y. M. Lam, S. G. Mhaisalkar and A. C. Grimsdale, *Org. Lett.*, 2011, **13**, 4613.

Coordinates for optimized geometry

6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.133492	2.831711	-0.124909
2	7	0	-1.133939	2.832765	0.097281
3	7	0	-0.001169	3.526997	-0.026602
4	16	0	4.382166	0.721874	-0.159349
5	16	0	-4.382454	0.724836	0.146267
6	7	0	1.635056	-1.945685	0.099189
7	7	0	-1.636272	-1.945656	-0.090545
8	6	0	5.138738	-0.852914	0.006244
9	1	0	6.218369	-0.920269	0.008480
10	6	0	-5.139530	-0.850629	-0.010278
11	1	0	-6.219188	-0.917495	-0.013839
12	6	0	4.242005	-1.885106	0.094984
13	1	0	4.532094	-2.925372	0.189454
14	6	0	-4.243159	-1.883816	-0.091074
15	1	0	-4.533590	-2.924531	-0.179306
16	6	0	-2.809271	-0.011334	0.099568
17	6	0	-2.908279	-1.392737	-0.022831
18	6	0	-0.716170	-0.890448	-0.004390
19	6	0	-1.433039	0.333669	0.087250
20	6	0	0.715330	-0.890628	0.007454

21	6	0	1.432616	0.332586	-0.093016
22	6	0	2.808707	-0.013176	-0.105354
23	6	0	2.907251	-1.393837	0.025721
24	6	0	0.707430	1.556419	-0.073573
25	6	0	-0.707145	1.557067	0.065587
26	6	0	-1.409545	-3.261445	-0.673136
27	1	0	-2.226001	-3.488899	-1.365079
28	1	0	-0.478587	-3.259910	-1.242305
29	1	0	-1.366728	-4.052865	0.083867
30	6	0	1.408729	-3.257261	0.691475
31	1	0	0.477644	-3.251888	1.260487
32	1	0	1.366259	-4.054161	-0.059757
33	1	0	2.225156	-3.479424	1.385175
34	6	0	0.006315	4.975642	0.043467
35	1	0	0.112220	5.309653	1.081207
36	1	0	0.847643	5.342491	-0.545336
37	1	0	-0.936752	5.342065	-0.363218

7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.135507	2.693608	-0.103393
2	7	0	-1.136592	2.694161	0.078510
3	7	0	-0.001347	3.389079	-0.024435
4	7	0	1.644300	-2.074971	0.117016
5	7	0	-1.644766	-2.075456	-0.106995
6	6	0	5.197268	-1.076938	0.065142
7	1	0	6.267954	-1.229642	0.083373
8	6	0	-5.197626	-1.076522	-0.067000
9	1	0	-6.268307	-1.229133	-0.086304
10	6	0	4.237103	-2.046460	0.136396
11	1	0	4.471837	-3.102079	0.226061
12	6	0	-4.237536	-2.046613	-0.131142
13	1	0	-4.472329	-3.102698	-0.214966
14	6	0	-2.806455	-0.134901	0.059195
15	6	0	-2.915924	-1.515020	-0.057752
16	6	0	-0.716521	-1.030525	-0.010550
17	6	0	-1.431327	0.195580	0.065397
18	6	0	0.716073	-1.030446	0.015964
19	6	0	1.430950	0.195115	-0.068197
20	6	0	2.806042	-0.135659	-0.063112
21	6	0	2.915468	-1.515077	0.061902
22	6	0	0.707189	1.418865	-0.060156
23	6	0	-0.707355	1.419204	0.054547
24	6	0	-1.419101	-3.405575	-0.654244
25	1	0	-2.241417	-3.653618	-1.331454
26	1	0	-0.494177	-3.417357	-1.233372
27	1	0	-1.366790	-4.176705	0.122910
28	6	0	1.419514	-3.401417	0.673562
29	1	0	0.494777	-3.409656	1.253035
30	1	0	1.367272	-4.177869	-0.098277
31	1	0	2.242177	-3.644468	1.352187
32	6	0	0.004565	4.837490	0.046095
33	1	0	0.090283	5.171807	1.085665

34	1	0	0.856946	5.204878	-0.526292
35	1	0	-0.930344	5.204302	-0.378766
36	34	0	-4.485795	0.666386	0.098925
37	34	0	4.485456	0.665105	-0.109954

P6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-4.748244	3.726213	-0.278968
2	7	0	-7.010957	3.735429	-0.015107
3	7	0	-5.881043	4.425276	-0.183439
4	16	0	-1.507516	1.621351	-0.308804
5	16	0	-10.250180	1.636414	0.180199
6	7	0	-4.240823	-1.042214	0.100165
7	7	0	-7.514708	-1.048193	-0.032341
8	6	0	-0.720834	0.038825	-0.080372
9	6	0	-11.035321	0.040407	0.071448
10	6	0	-1.646483	-0.981890	0.058131
11	1	0	-1.364215	-2.017834	0.207885
12	6	0	-10.108685	-0.986722	0.007637
13	1	0	-10.389675	-2.031282	-0.064285
14	6	0	-8.680490	0.894415	0.119416
15	6	0	-8.783893	-0.492579	0.044935
16	6	0	-6.592072	0.007772	-0.000095
17	6	0	-7.309764	1.237330	0.064626
18	6	0	-5.164184	0.007624	-0.011296
19	6	0	-4.447064	1.229476	-0.166595
20	6	0	-3.076224	0.884272	-0.194822
21	6	0	-2.971885	-0.493292	-0.017259
22	6	0	-5.172916	2.454051	-0.176119
23	6	0	-6.584241	2.459783	-0.011414
24	6	0	-7.301692	-2.384417	-0.573540
25	1	0	-8.131324	-2.632575	-1.242135
26	1	0	-6.381292	-2.404372	-1.159107
27	1	0	-7.247391	-3.148595	0.209845
28	6	0	-4.454025	-2.337670	0.732520
29	1	0	-5.374293	-2.317261	1.318347
30	1	0	-4.508621	-3.153995	0.003630
31	1	0	-3.624231	-2.539298	1.416364
32	6	0	-5.872820	5.875453	-0.163483
33	1	0	-5.749908	6.245182	0.860165
34	1	0	-5.041568	6.221374	-0.778663
35	1	0	-6.822457	6.228043	-0.567112
36	6	0	0.716795	-0.053174	-0.075147
37	16	0	1.505834	-1.647475	-0.180797
38	6	0	1.640967	0.976263	-0.012561
39	6	0	3.073709	-0.901607	-0.120635
40	1	0	1.357503	2.020291	0.057354
41	6	0	2.966941	0.485242	-0.048429
42	6	0	4.445237	-1.241155	-0.064697
43	7	0	4.234768	1.044072	0.028527
44	6	0	5.159924	-0.009800	-0.001507
45	6	0	5.173662	-2.461748	0.013455

46	6	0	4.444189	2.381140	0.569184
47	6	0	6.587801	-0.006171	0.010237
48	7	0	4.749991	-3.738401	0.018921
49	6	0	6.584902	-2.452382	0.178709
50	1	0	3.613852	2.627453	1.237591
51	1	0	5.364468	2.403786	1.154827
52	1	0	4.496603	3.145065	-0.214573
53	7	0	7.508705	1.045595	-0.102851
54	6	0	7.307819	-1.226082	0.167621
55	7	0	5.881494	-4.425290	0.188694
56	7	0	7.012578	-3.723374	0.283596
57	6	0	8.778904	0.499958	0.015847
58	6	0	7.292411	2.340152	-0.735856
59	6	0	8.677814	-0.877572	0.195633
60	6	0	5.893202	-5.875470	0.170982
61	6	0	10.103171	0.991609	-0.059932
62	1	0	6.372573	2.317014	-1.322276
63	1	0	7.235202	3.156688	-0.007402
64	1	0	8.122107	2.543668	-1.419250
65	16	0	10.248251	-1.610694	0.311384
66	1	0	6.018809	-6.246477	-0.851877
67	1	0	6.724164	-6.218542	0.788158
68	1	0	4.943674	-6.229630	0.573474
69	6	0	11.031184	-0.026673	0.080473
70	1	0	10.383082	2.027920	-0.211559
71	-2	0	23.503919	0.028375	0.004392

Lengths of translation vectors: 23.503937

P7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-4.796571	3.891524	-0.066709
2	7	0	-7.061229	3.887590	0.187599
3	7	0	-5.930144	4.585386	0.060257
4	7	0	-4.281817	-0.881773	0.052144
5	7	0	-7.574150	-0.880153	-0.064759
6	6	0	-0.711354	0.102307	-0.090802
7	6	0	-11.145018	0.099504	0.097075
8	6	0	-1.703621	-0.855008	-0.006315
9	1	0	-1.474087	-1.912535	0.079533
10	6	0	-10.152571	-0.855068	-0.012520
11	1	0	-10.382028	-1.909603	-0.129677
12	6	0	-8.727139	1.059442	0.176147
13	6	0	-8.841791	-0.321770	0.038404
14	6	0	-6.642416	0.162648	0.018672
15	6	0	-7.357313	1.389512	0.139201
16	6	0	-5.213672	0.163113	0.001524
17	6	0	-4.499093	1.393024	-0.084697
18	6	0	-3.129372	1.064145	-0.135949
19	6	0	-3.014424	-0.320458	-0.038509
20	6	0	-5.223262	2.616496	-0.032389
21	6	0	-6.633031	2.614008	0.127242

22	6	0	-7.369187	-2.203568	-0.637139
23	1	0	-8.212593	-2.439662	-1.292174
24	1	0	-6.462305	-2.209369	-1.243942
25	1	0	-7.296367	-2.984453	0.128195
26	6	0	-4.484797	-2.219405	0.591530
27	1	0	-5.391344	-2.241289	1.198419
28	1	0	-4.557255	-2.981007	-0.193017
29	1	0	-3.640762	-2.470747	1.240071
30	6	0	-5.921873	6.032311	0.156389
31	1	0	-5.803117	6.348006	1.198517
32	1	0	-5.088199	6.410185	-0.436340
33	1	0	-6.869736	6.406213	-0.232001
34	34	0	-10.403694	1.859505	0.290007
35	34	0	-1.453041	1.867113	-0.230959
36	6	0	0.709325	-0.097284	-0.095957
37	6	0	1.702155	0.856939	0.013253
38	34	0	1.449957	-1.857574	-0.288887
39	1	0	1.473125	1.911580	0.130297
40	6	0	3.012725	0.323146	-0.037888
41	6	0	3.126830	-1.058125	-0.175459
42	7	0	4.280604	0.881093	0.064908
43	6	0	4.496542	-1.388716	-0.138684
44	6	0	5.211912	-0.162104	-0.018515
45	6	0	4.486164	2.204281	0.637653
46	6	0	5.220383	-2.613472	-0.126699
47	6	0	6.640653	-0.163072	-0.001696
48	1	0	3.643101	2.440408	1.293123
49	1	0	5.393306	2.209629	1.244067
50	1	0	4.558882	2.985388	-0.127463
51	7	0	4.791720	-3.886911	-0.186790
52	6	0	6.630190	-2.616441	0.032622
53	7	0	7.572851	0.881480	-0.052654
54	6	0	7.354817	-1.393224	0.084577
55	7	0	5.922582	-4.585092	-0.059610
56	7	0	7.056435	-3.891617	0.066990
57	6	0	8.840070	0.319746	0.037770
58	6	0	7.370168	2.219189	-0.591952
59	6	0	8.724663	-1.064814	0.135374
60	6	0	5.930309	-6.032033	-0.155556
61	6	0	10.151053	0.853828	0.005169
62	1	0	6.463429	2.241406	-1.198542
63	1	0	7.298239	2.980805	0.192630
64	1	0	8.214079	2.470243	-1.240768
65	34	0	10.400733	-1.868359	0.230029
66	1	0	6.048303	-6.347901	-1.197717
67	1	0	6.764235	-6.410087	0.436699
68	1	0	4.982572	-6.405588	0.233481
69	6	0	11.143001	-0.103830	0.089502
70	1	0	10.380936	1.911264	-0.080850
71	-2	0	23.708769	-0.004252	-0.002805

Lengths of translation vectors: 23.708770
