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Cyclopenta[*c*]selenophene based cooligomers and their polymers: comparative study with thiophene analogues

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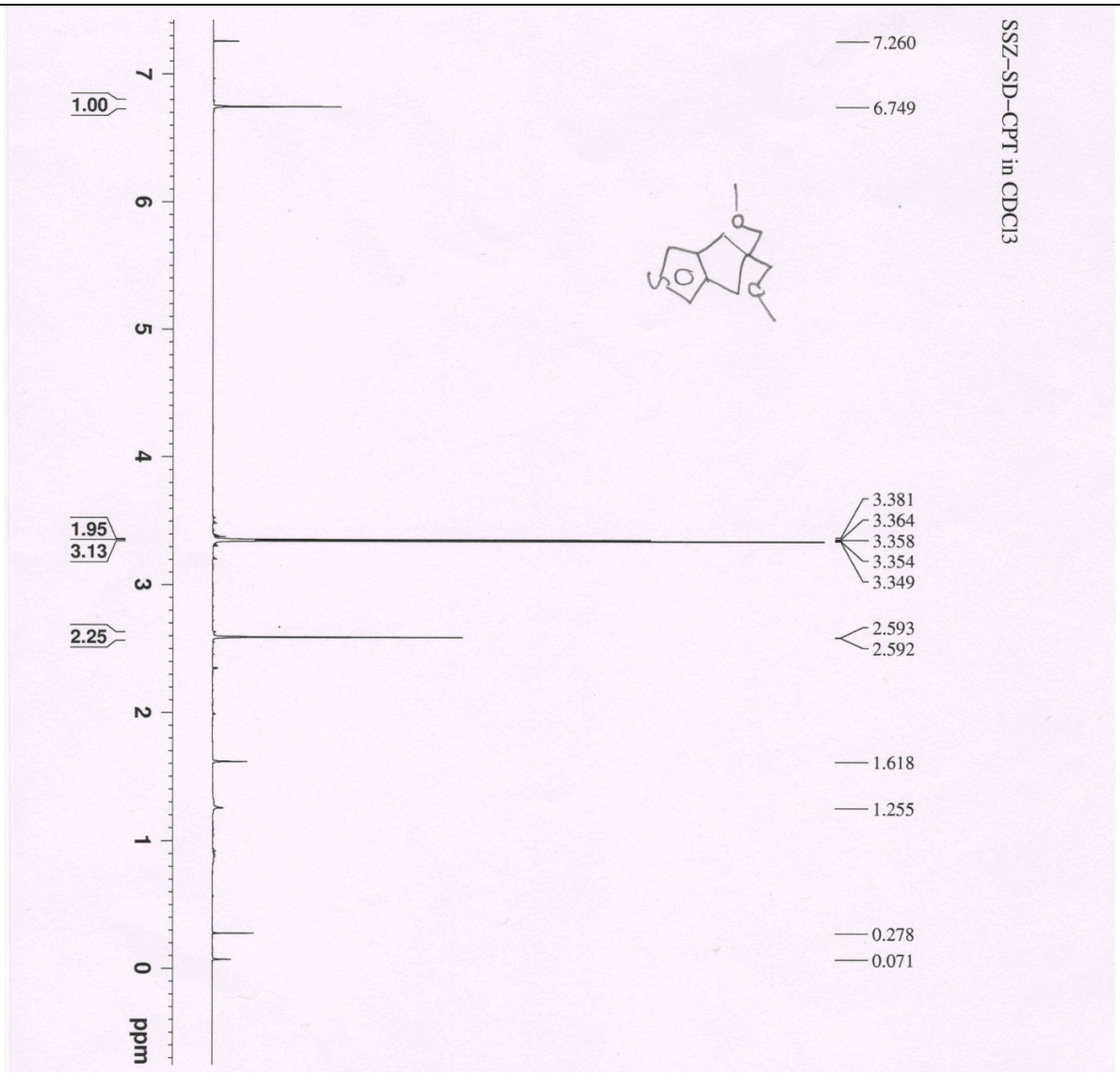


Figure S1. ^{1}H NMR of compound **2**

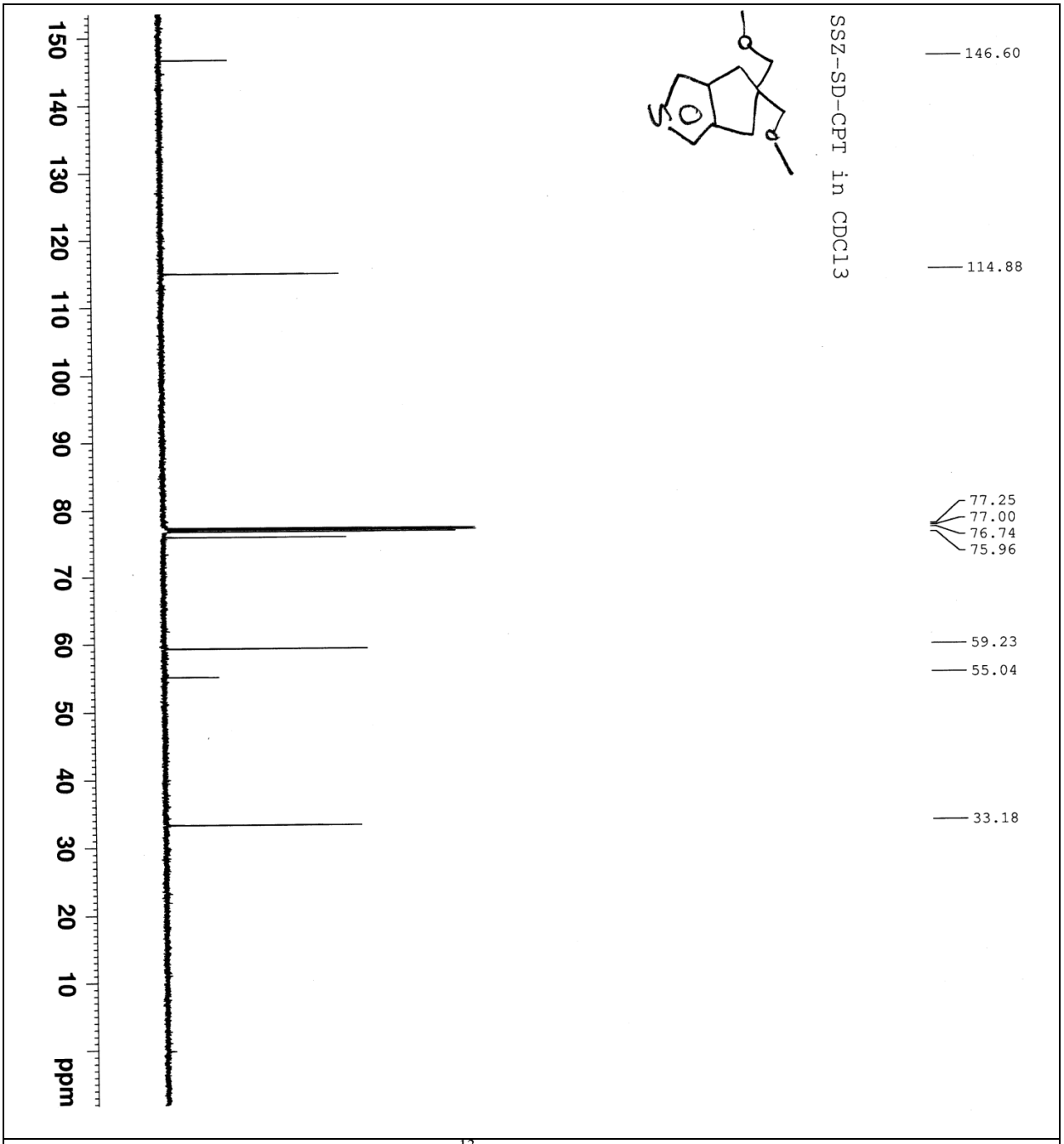


Figure S2. ^{13}C NMR of compound **2**

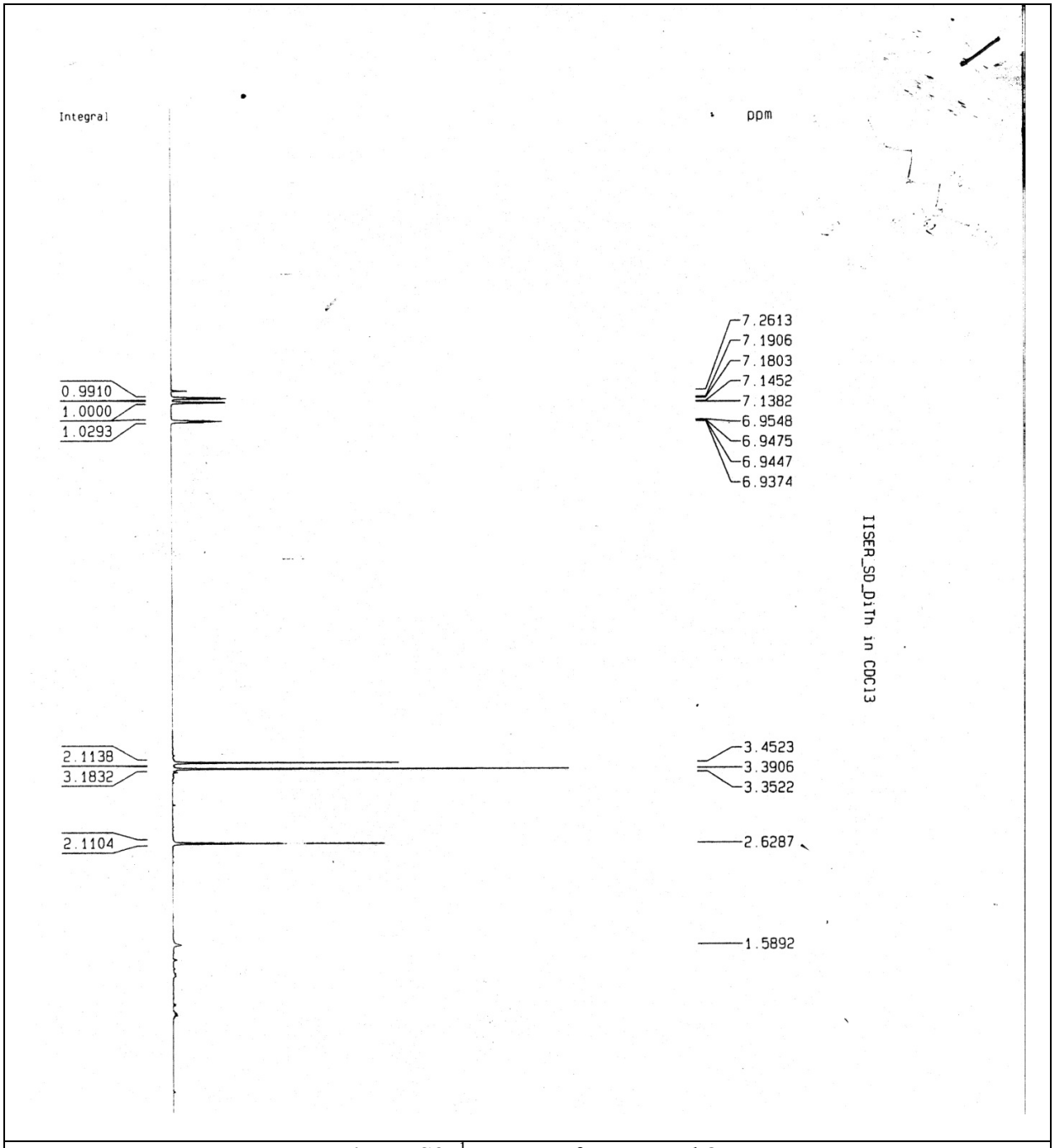


Figure S3. ^{1}H NMR of compound **8**

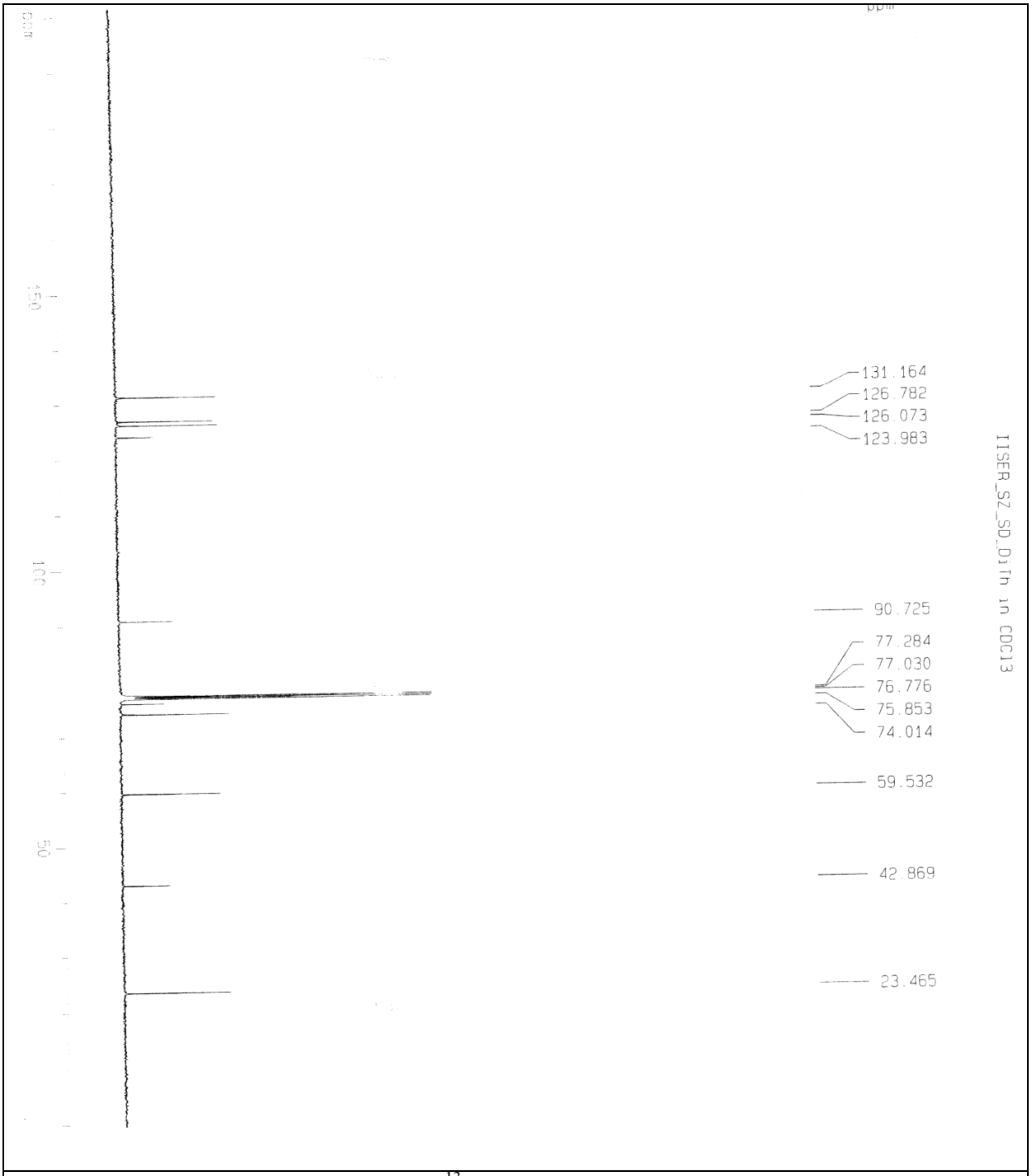


Figure S4. ^{13}C NMR of compound **8**

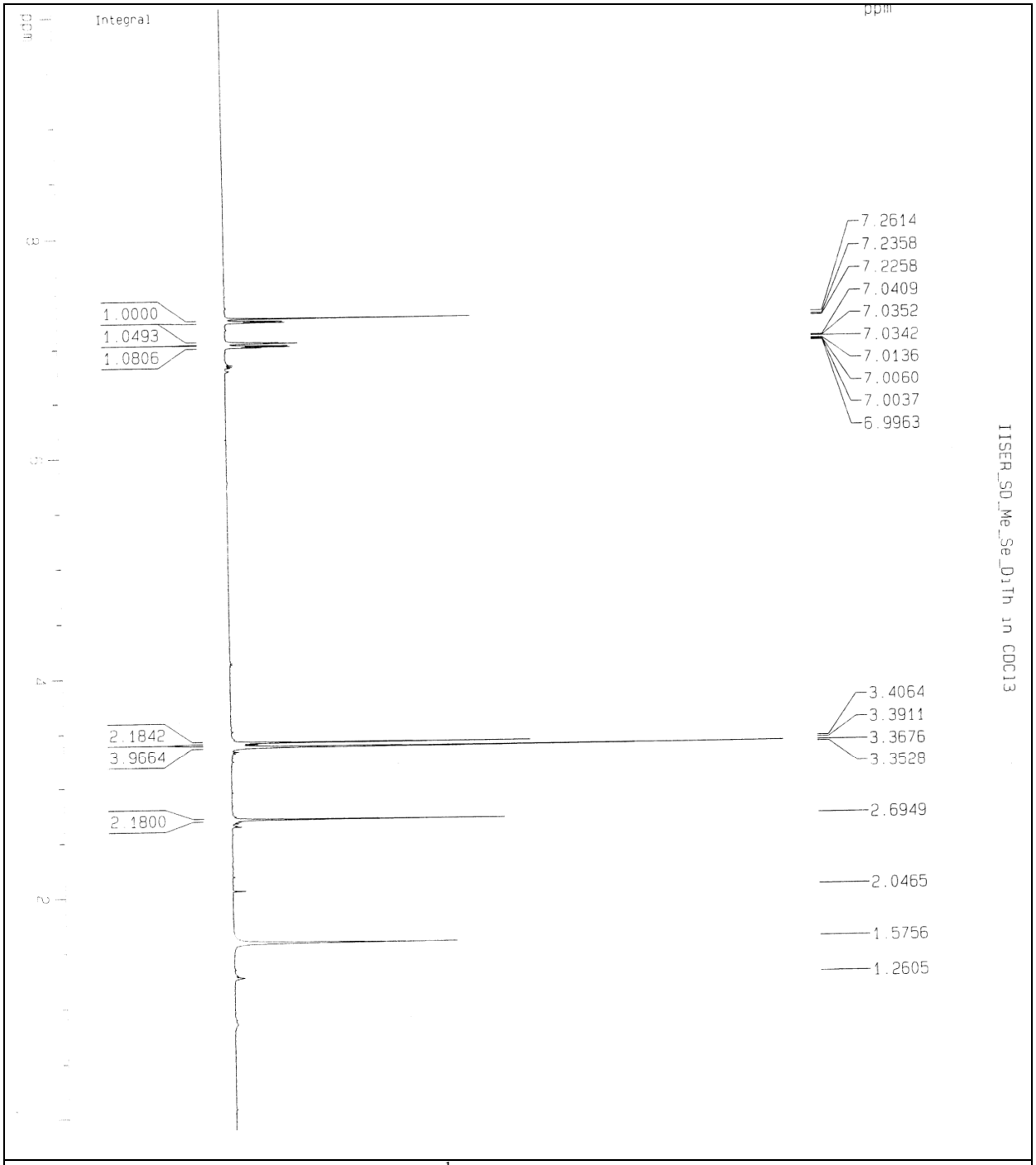


Figure S5. ^{1}H NMR of compound **10**

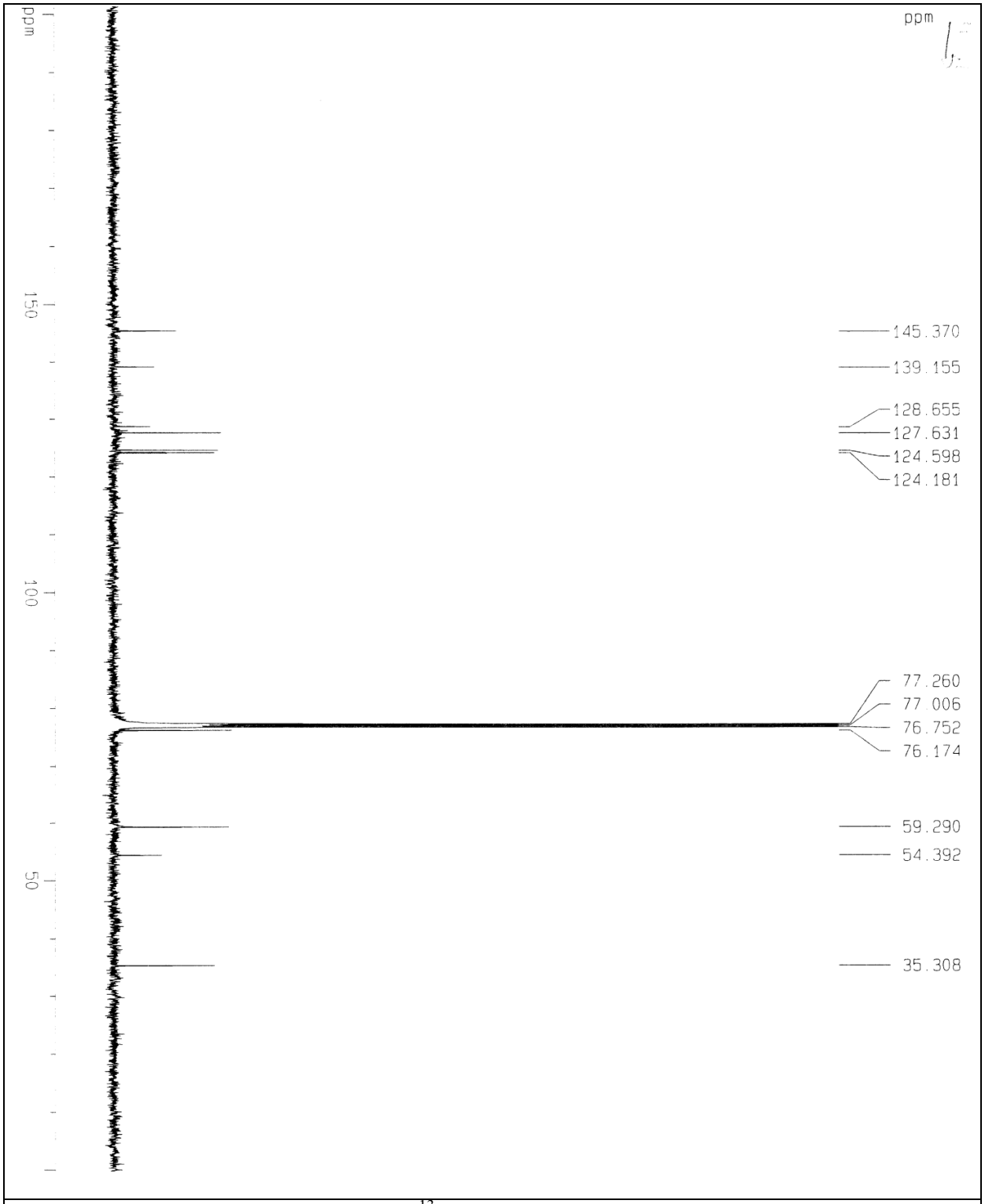


Figure S6. ^{13}C NMR of compound **10**

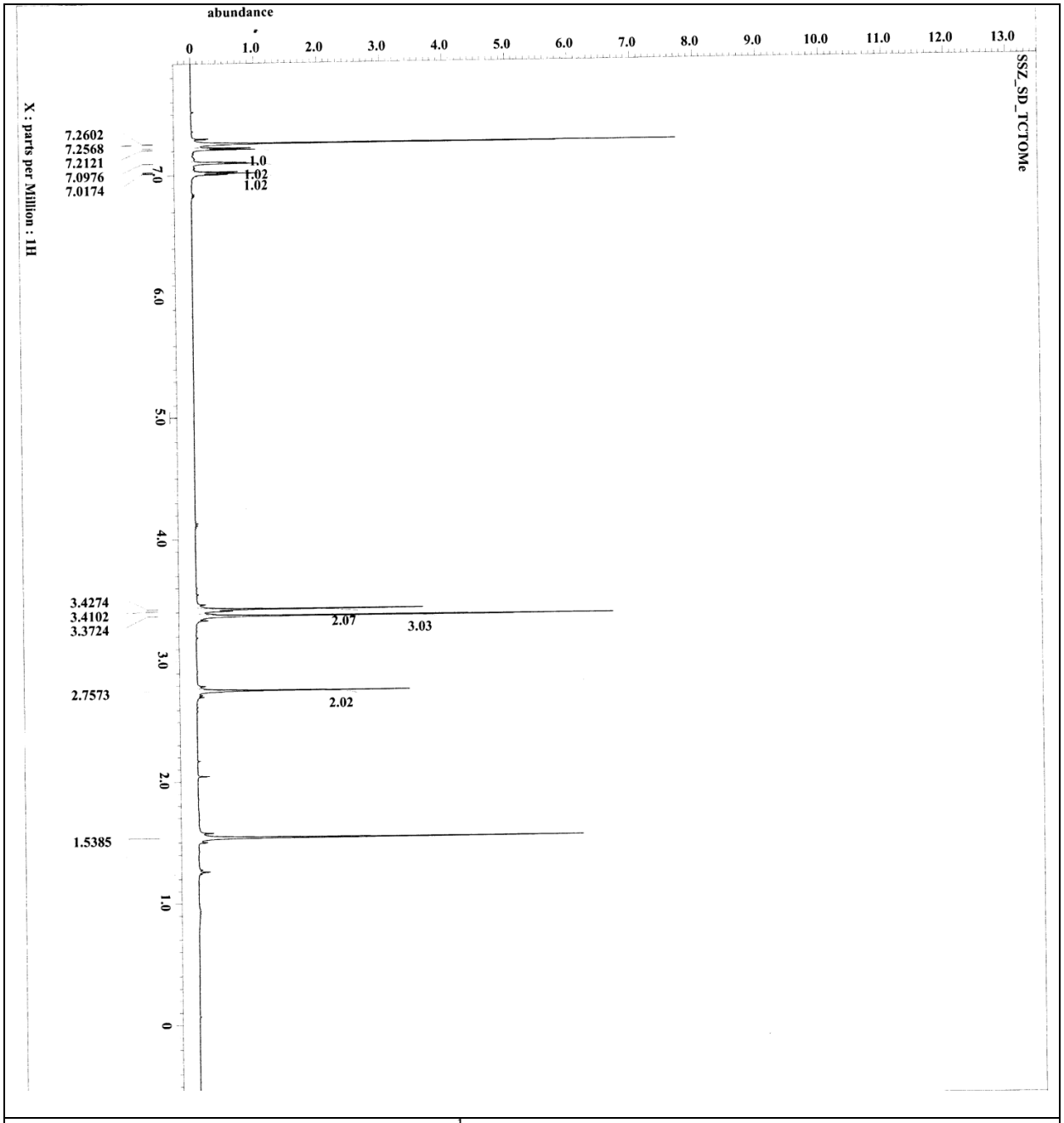


Figure S7. ^{1}H NMR of compound **11**

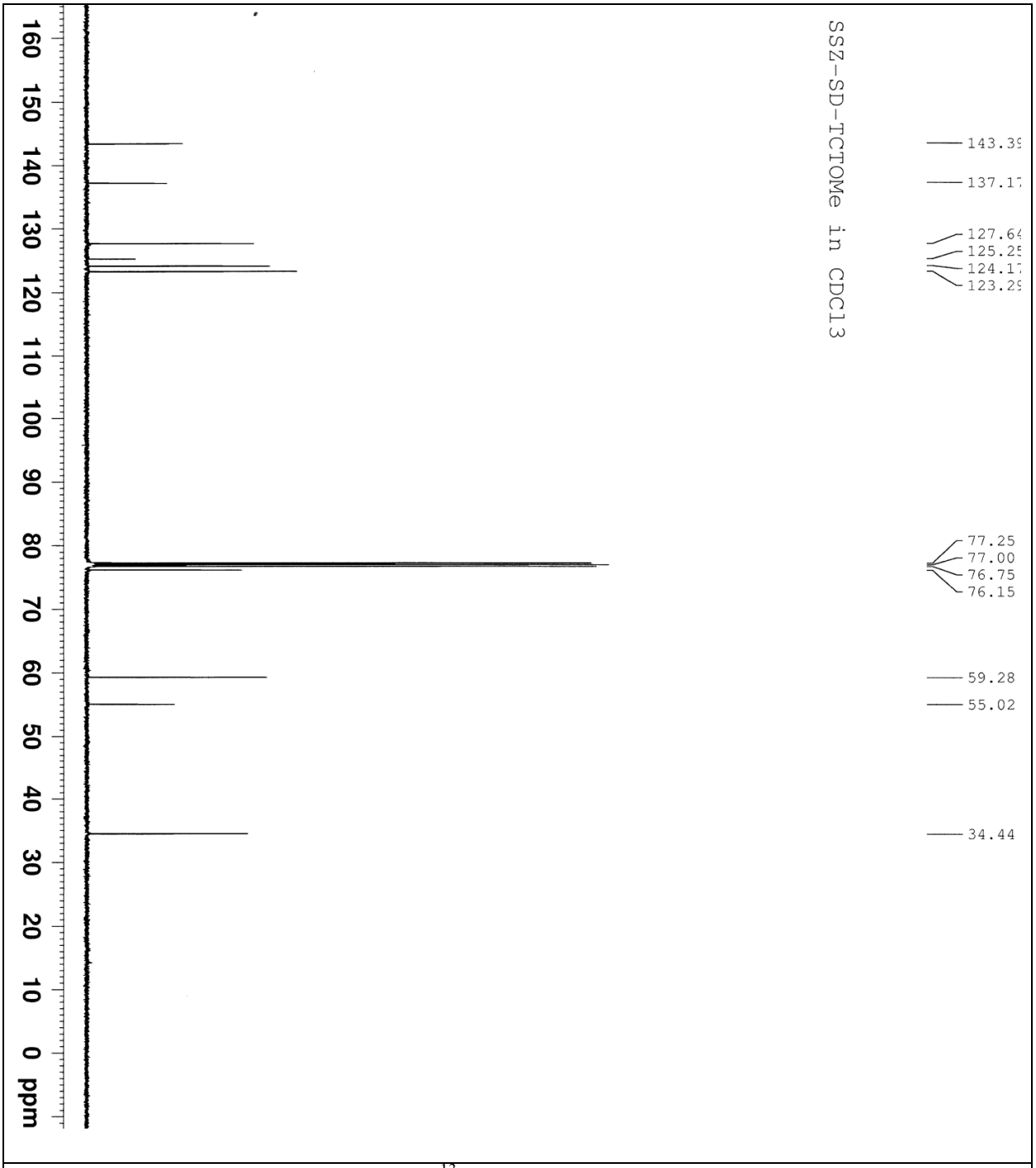


Figure S8. ^{13}C NMR of compound **11**

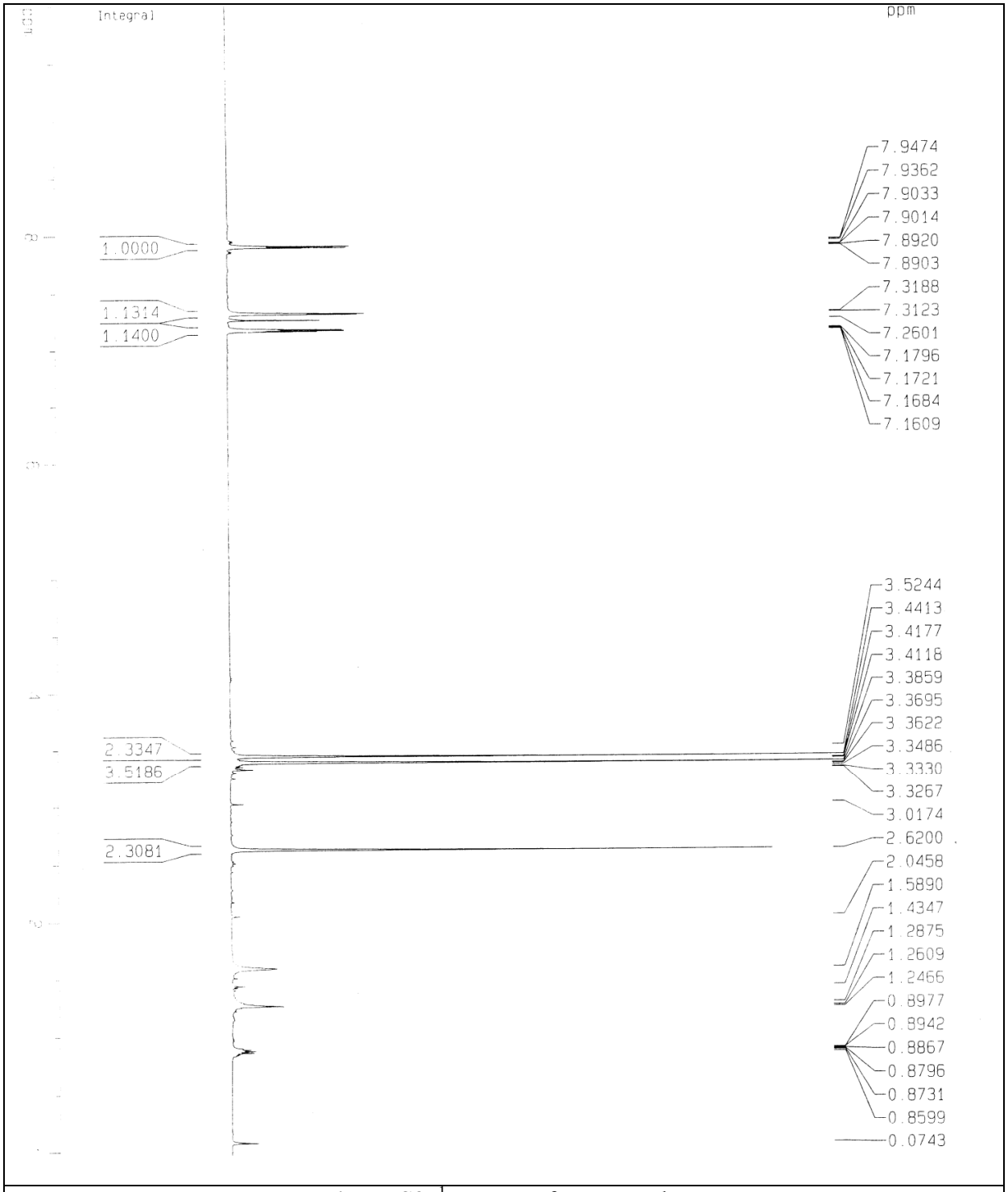


Figure S9. ^{1}H NMR of compound **7**

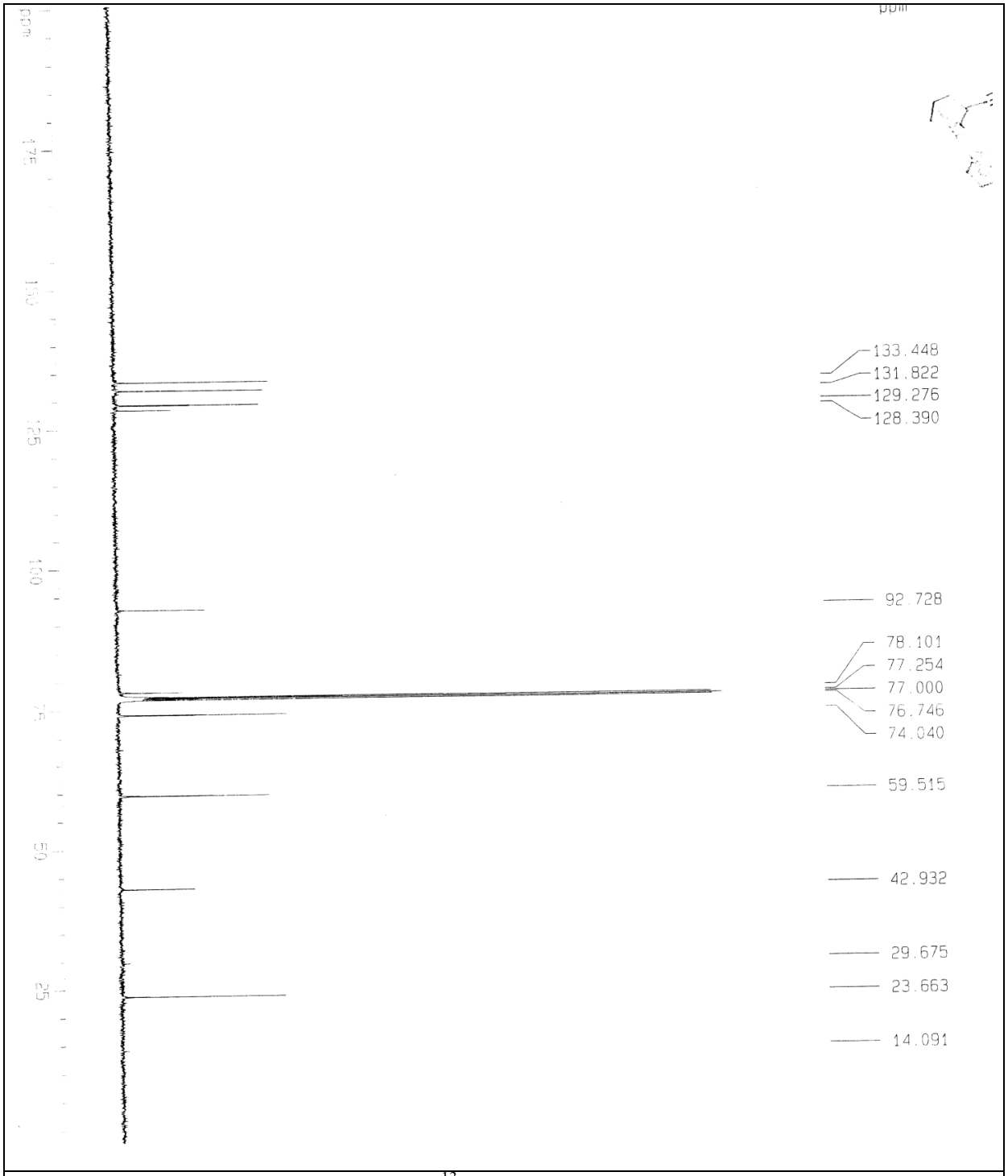


Figure S10. ^{13}C NMR of compound **7**

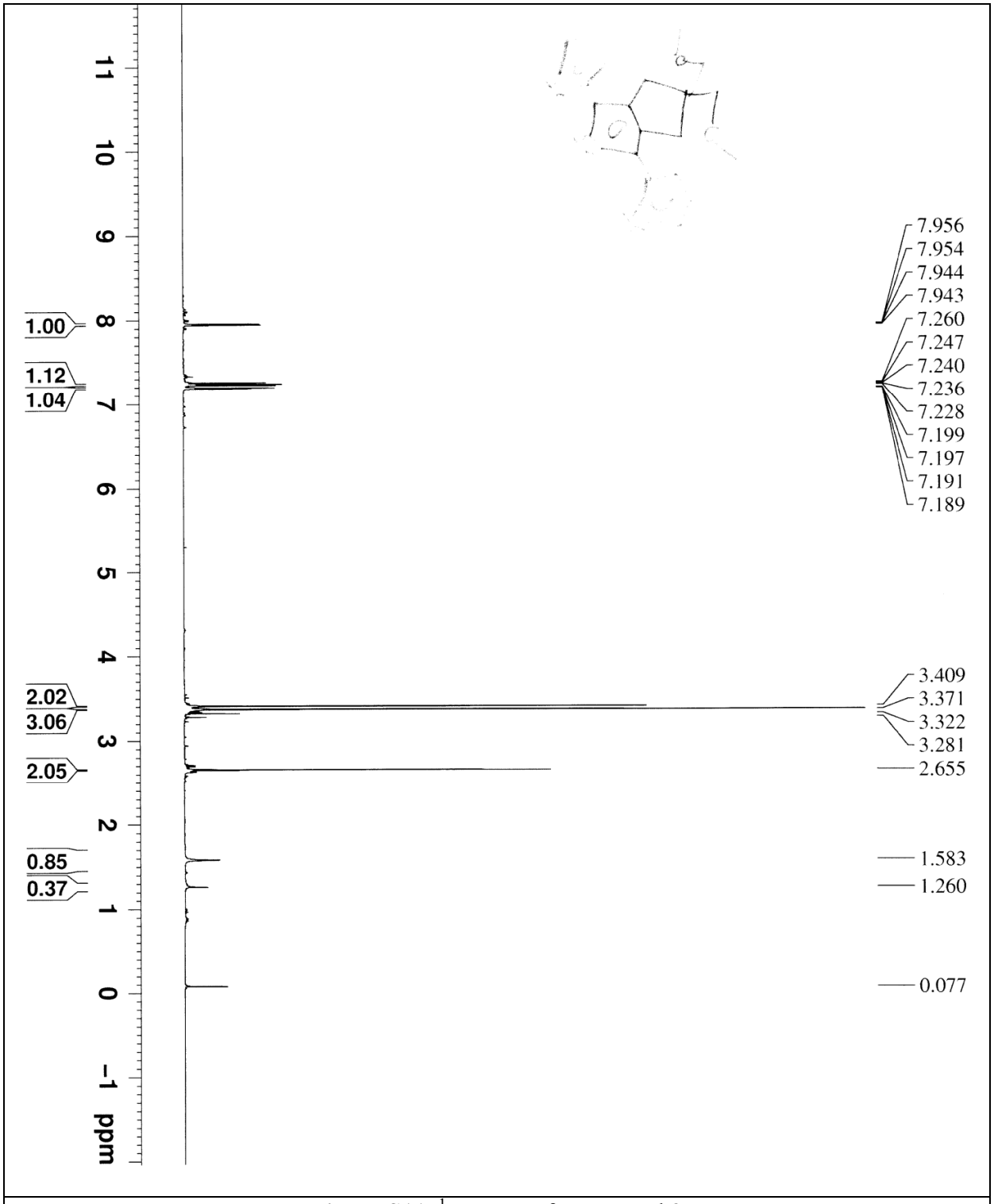


Figure S11. ^{1}H NMR of compound **9**

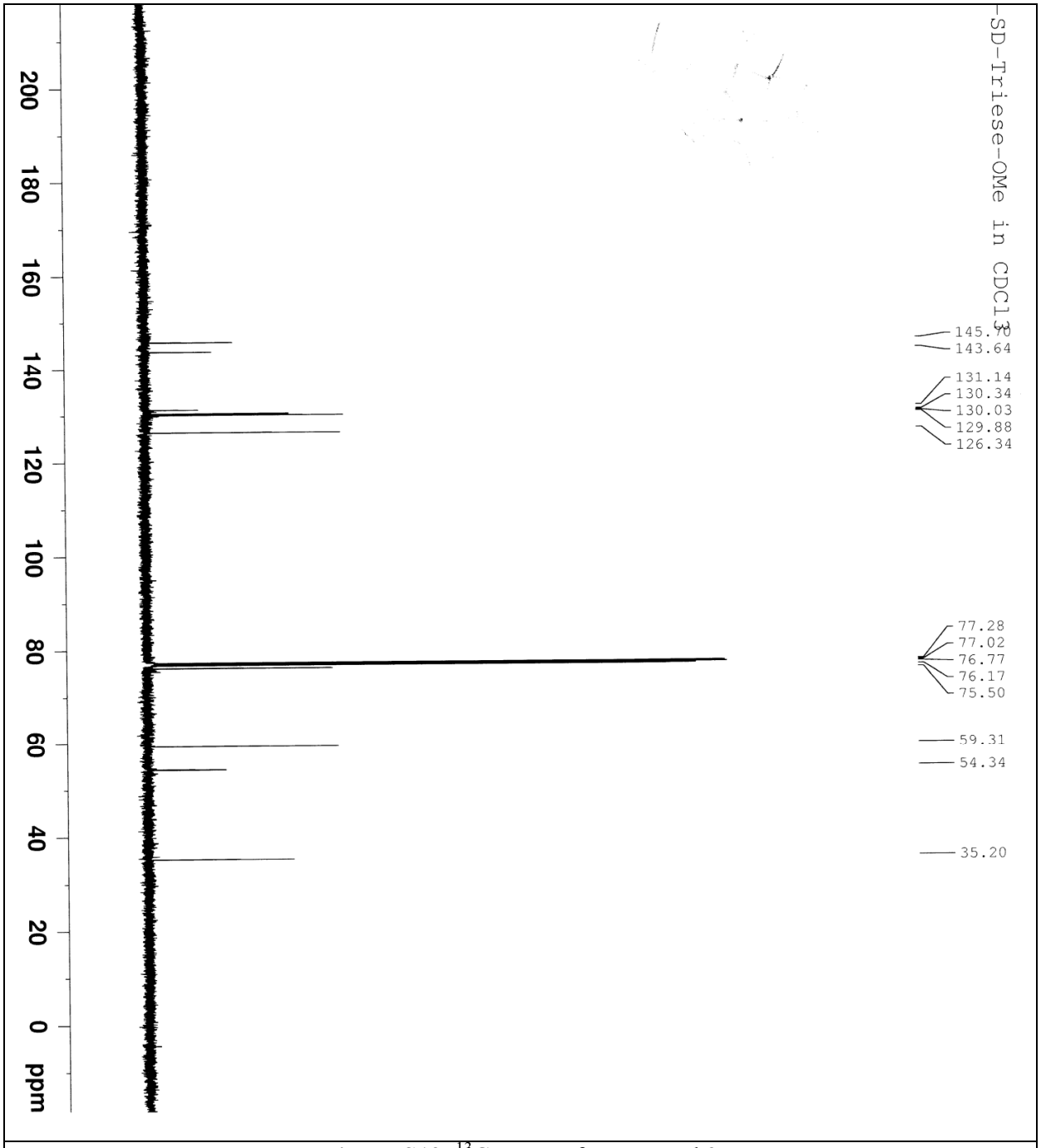


Figure S12. ^{13}C NMR of compound **9**

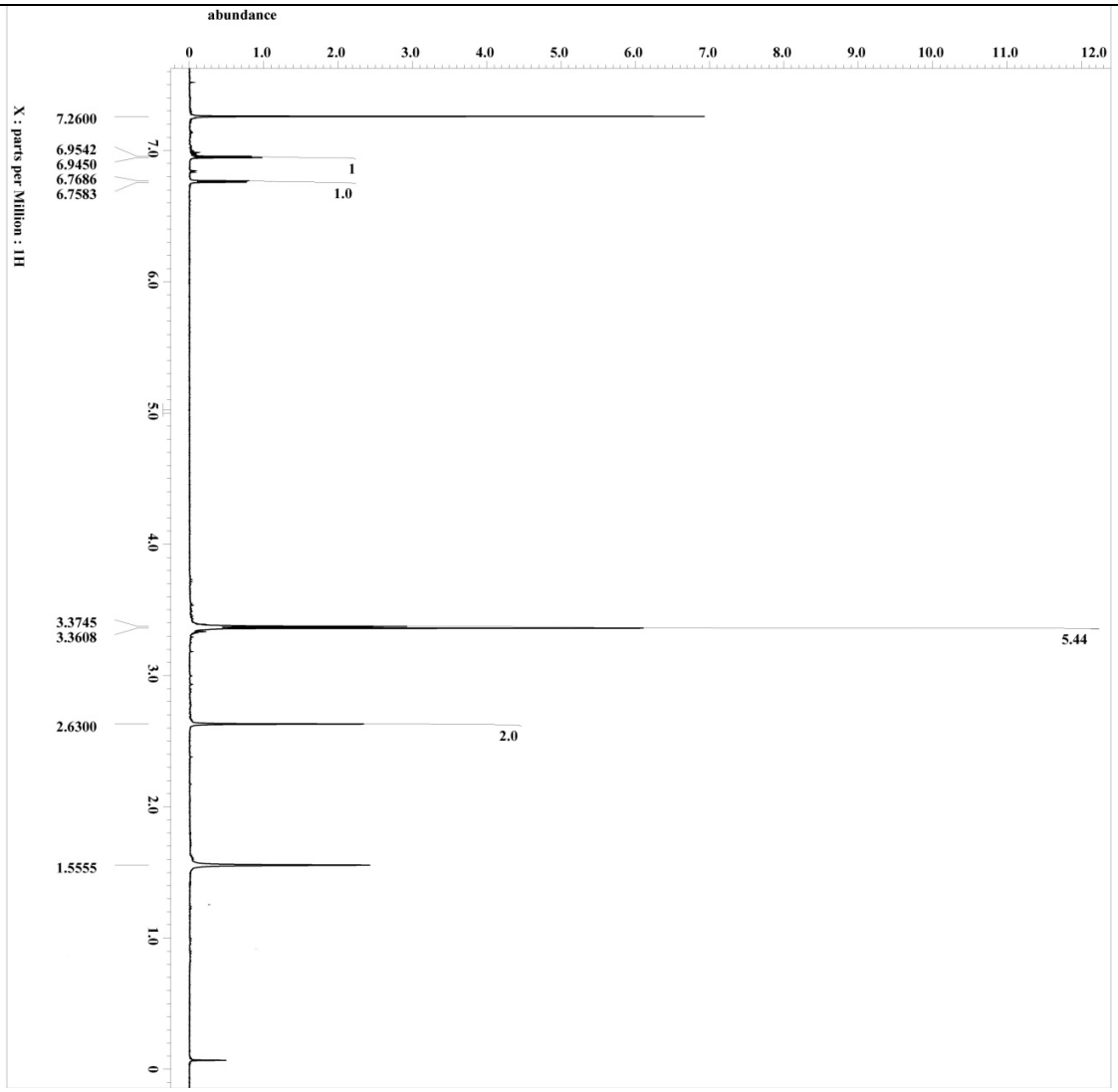


Figure S13. ^{1}H NMR of compound **12**

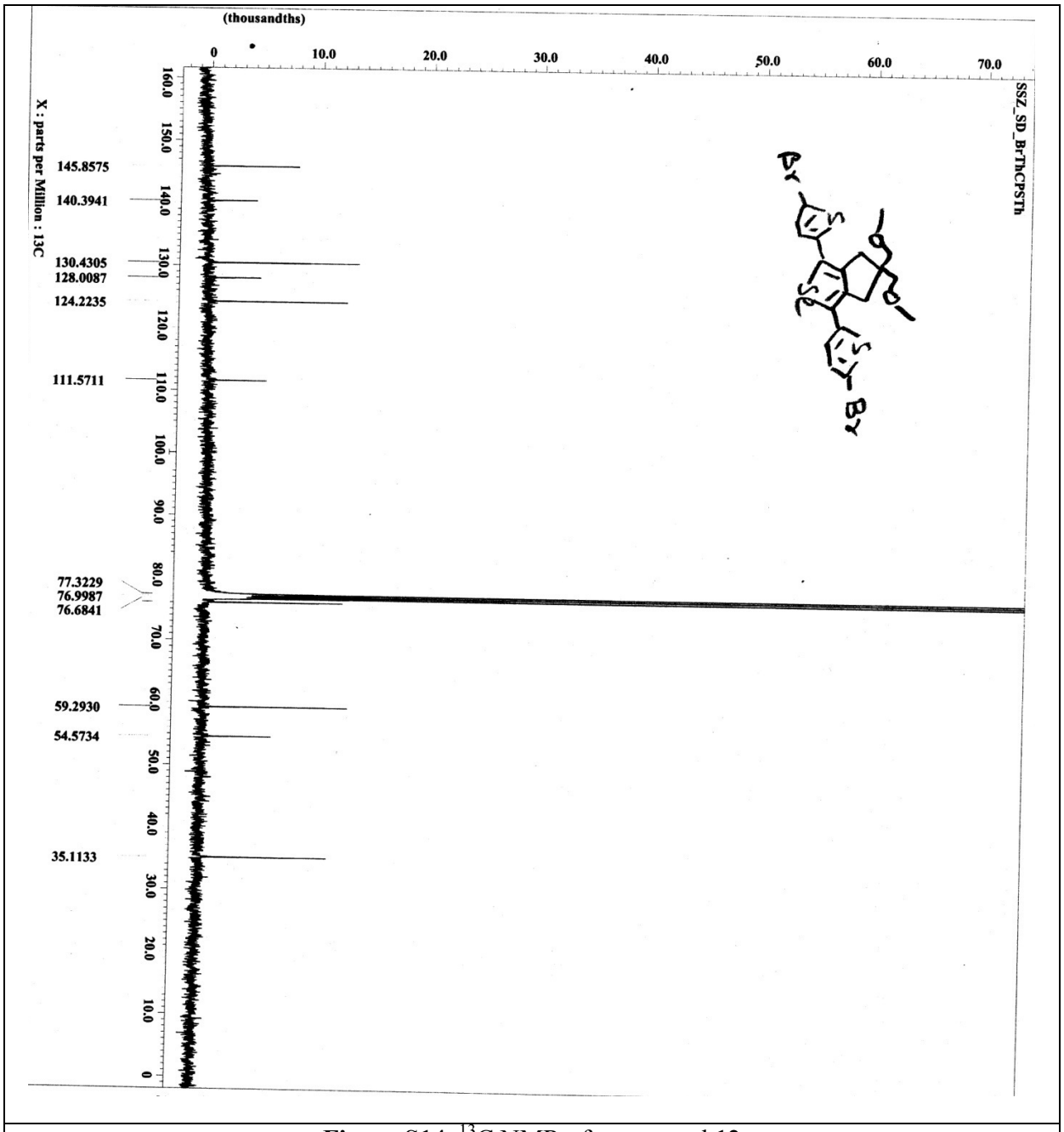


Figure S14. ^{13}C NMR of compound **12**

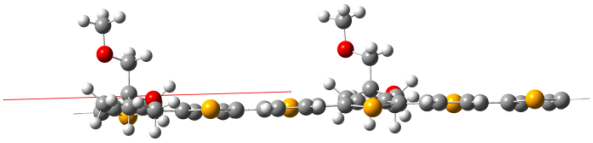
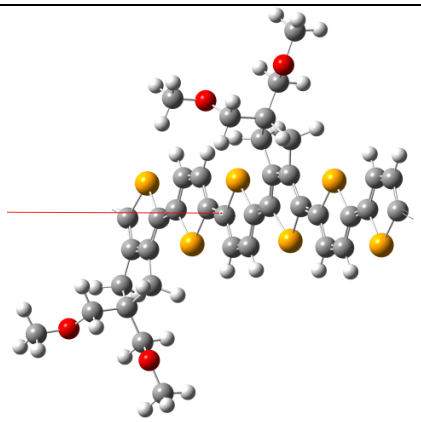
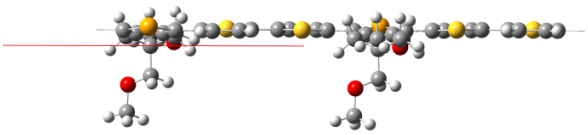
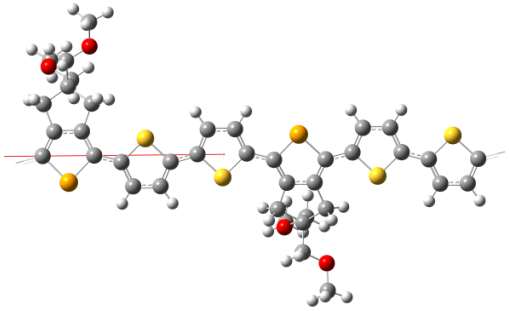
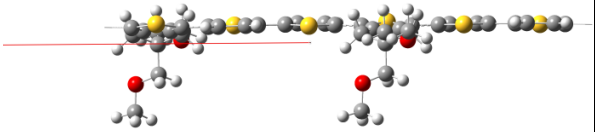
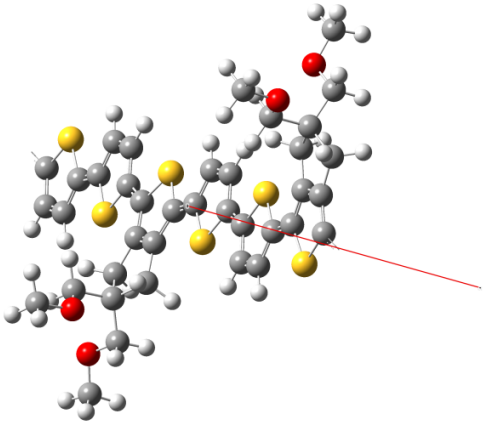
P9		
P10		
P11		

Figure S15. Optimized structures of polymers P9, P10 and P11

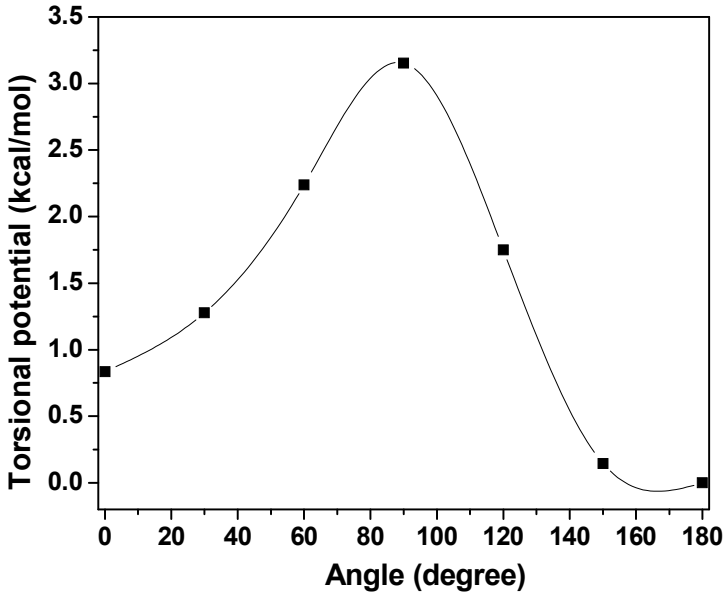


Figure S16. Point-wise calculated energy curve for rotation of one of the capped thiophene ring in **11** at B3LYP/6-31G(d).

Table S1 Energies of **P9-P11**

Polymer	Absolute energy at PBC/B3LYP/6-31G(d)
P9	–16166.8289242
P10	–8162.0611561
P11	–4159.6792288

Table S2. Energies of compound **11** at different rotational angle

0	–2081.023998
30	–2081.023294
60	–2081.021763
90	–2081.020304
120	–2081.02254

150	–2081.025097
180	–2081.025329
TS-rotation	–2081.020304

Single crystal X-ray data for compound :

Single crystals suitable for X-ray diffraction of the compounds were grown from hexane. The crystals were carefully chosen using a stereo zoom microscope supported by a rotatable polarizing stage. The data was collected at 296(2) and 100 (2)K on Bruker's KAPPA APEX II CCD Duo with graphite monochromated Mo-Kα radiation (0.71073 Å). The crystals were glued to a thin glass fibre using FOMBLIN immersion oil and mounted on the diffractometer. The intensity data were processed using Bruker's suite of data processing programs (SAINT), and absorption corrections were applied using SADABS.[1] The crystal structure was solved by direct methods using SHELXS-97 and the data was refined by full matrix least-squares refinement on F^2 with anisotropic displacement parameters for non-H atoms, using SHELXL-97.[2]

Table S3. Contact details of compound **11**:

	D-H	**H···A**	**D···A**	**D-H···A angle**
C7 -- H7A .. O2	0.97	2.44	2.874(6)	107
C9 -- H9B .. O2	0.97	2.54	2.883(6)	100
C11 -- H11C .. O4	0.96	2.49	3.311(7)	143
C12 -- H12B .. O1	0.97	2.57	2.895(6)	100
C19 -- H19 .. O4	0.93	2.41	3.296(6)	159
C20 -- H20 .. O2	0.93	2.58	3.489(7)	166
C26 -- H26B .. S4	0.97	2.85	3.271(5)	107
C26 -- H26B .. O3	0.97	2.52	2.926(6)	105
C31 -- H31A .. O3	0.97	2.53	2.860(6)	100

C38 -- H38 .. O1	0.93	2.52	3.419(7)	162

The detailed contact analysis report:

		D-H	H···A	D···A	D-H···A angle
C7 -- H7A .. O2	[ ]	0.97	2.44	2.874(6)	107
C9 -- H9B .. O2	[ ]	0.97	2.54	2.883(6)	100
C11 -- H11C .. O4	[1565.02]	0.96	2.49	3.311(7)	143
C12 -- H12B .. O1	[ ]	0.97	2.57	2.895(6)	100
C19 -- H19 .. O4	[2756.02]	0.93	2.41	3.296(6)	159
C20 -- H20 .. O2	[3667.01]	0.93	2.58	3.489(7)	166
C26 -- H26B .. S4	[ ]	0.97	2.85	3.271(5)	107
C26 -- H26B .. O3	[ ]	0.97	2.52	2.926(6)	105
C31 -- H31A .. O3	[ ]	0.97	2.53	2.860(6)	100
C38 -- H38 .. O1	[2746.01]	0.93	2.52	3.419(7)	162

Table S4. Compound **11**: Bond Lengths (Angstrom) for Residue-1. - (Bonds are ordered on the first label, left to right and top to bottom) - su in last digit in ().

S(1) - C(1) 1.604(5)	S(1) - C(4) 1.684(5)	S(2) - C(5) 1.745(5)	S(2) - C(15) 1.748(5)
>S(3) - C(16) 1.724(5)	>S(3) - C(19) 1.698(5)	O(1) - C(9) 1.408(6)	O(1) - C(10) 1.408(7)
O(2) - C(11) 1.428(7)	O(2) - C(12) 1.416(6)	C(1) - C(2) 1.392(7)	C(2) > C(3) 1.509(6)
C(3) > C(4) 1.556(7)	C(4) > C(5) 1.484(6)	C(5) - C(6) 1.365(7)	C(6) - C(7) 1.502(7)
C(6) - C(14) 1.413(7)	C(7) - C(8) 1.555(7)	C(8) - C(9) 1.508(7)	C(8) - C(12) 1.533(7)
C(8) - C(13) 1.558(7)	C(13) - C(14) 1.512(7)	C(14) - C(15) 1.377(7)	C(15) - C(16) 1.470(7)
C(16) - <C(17) 1.380(15)	C(18) > C(19) 1.382(7)	<C(17) - C(18)1.392(12)	

C(1) - H(1) 0.93	C(2) - H(2) 0.93	C(3) - H(3) 0.93	C(7) - H(7A) 0.97
C(7) - H(7B) 0.97	C(9) - H(9A) 0.97	C(9) - H(9B) 0.97	C(10) - H(10A) 0.96
C(10) - H(10B) 0.96	C(10) - H(10C) 0.96	C(11) - H(11A) 0.96	C(11) - H(11B) 0.96
C(11) - H(11C) 0.96	C(12) - H(12A) 0.97	C(12) - H(12B) 0.97	C(13) - H(13A) 0.97
C(13) - H(13B) 0.97	C(18) - H(18) 0.93	C(19) - H(19) 0.93	<C(17) - <H(17) 0.93

Table S5. Compound **11**: Bond Lengths (Angstrom) for residue-2. - (Bonds are ordered on the first label, left to right and top to bottom) - su in last digit in ().

S(4) - C(20) 1.669(5)	S(4) - C(23) 1.729(6)	S(5) - C(24) 1.745(5)	S(5) - C(34) 1.748(5)
S(6) - C(35) 1.732(5)	S(6) - C(38) 1.705(6)	O(3) - C(28) 1.409(6)	O(3) - C(29) 1.411(6)
O(4) - C(30) 1.422(7)	O(4) - C(31) 1.415(6)	C(20) - C(21) 1.378(8)	C(21) > C(22) 1.450(7)
C(22) > C(23) 1.504(7)	C(23) > C(24) 1.483(7)	C(24) - C(25) 1.384(7)	C(25) - C(26) 1.506(7)
C(25) - C(33) 1.413(7)	C(26) - C(27) 1.566(7)	C(27) - C(28) 1.533(7)	C(27) - C(31) 1.525(7)
C(27) - C(32) 1.556(7)	C(32) - C(33) 1.515(7)	C(33) - C(34) 1.368(7)	C(34) > C(35) 1.448(7)
C(35) - C(36) 1.405(7)	C(36) - C(37) 1.426(8)	C(37) - C(38) 1.344(8)	
C(20) - H(20) 0.93	C(21) - H(21) 0.93	C(22) - H(22) 0.93	C(26) - H(26A) 0.97
C(26) - H(26B) 0.97	C(28) - H(28A) 0.97	C(28) - H(28B) 0.97	C(29) - H(29A) 0.96
C(29) - H(29B) 0.96	C(29) - H(29C) 0.96	C(30) - H(30A) 0.96	C(30) - H(30B) 0.96
C(30) - H(30C) 0.96	C(31) - H(31A) 0.97	C(31) - H(31B) 0.97	C(32) - H(32A) 0.97
C(32) - H(32B) 0.97	C(36) - H(36) 0.93	C(37) - H(37) 0.93	C(38) - H(38) 0.93

Table S6. Complete crystallographic information of compound **11** and compound **12**

Formula	$C_{19}H_{20}O_2S_3$	$C_{19}H_{18}Br_2O_2S_2Se$
Crystal System	Monoclinic	Monoclinic
Space group	P 21/c	P 21/c
a [Å]	5.8122(4)	5.7974(7)
b [Å]	17.1465(14)	17.042(2)
c [Å]	36.266(3)	41.927(5)
α [^{0}]	90.00	90.00
β [^{0}]	93.2950(10)	90.920(5)
γ [^{0}]	90.00	90.00
V [Å ^{3}]	3608.3(5)	4141.9(9)
Z	8	**8**
λ [Å]	0.71073	0.71073
ρ_{calcd} [gcm^{-3}]	1.353	1.864
F[000]	1547.0	2272
μ [mm^{-1}]	0.419	5.885
θ [^{0}]	2.25-30.83	2.28-23.91
index ranges	$-8 \le h \le 8$ $-24 \le k \le 24$ $-52 \le l \le 49$	$-7 \le h \le 7$ $-21 \le k \le 21$ $-53 \le l \le 53$
T [K]	100(2)	296(2)
*R*1	0.1515	0.0467
*wR*2	0.4817	0.1240
R_{merge}	0.1638	0.0983
Parameters	385	473
GOF	2.401	0.937
reflns total	58663	59499
unique reflns	11215	8987
obsd reflns	9727	5631
CCDC[a]		

Table S7. Contact details of compound **12**

	D-H	H···A	D···A	D-H···A angle
C7 -- H7B .. S1	0.97	2.81	3.216(5)	106
C7 -- H7B .. O1	0.97	2.46	2.884(6)	106
C11 -- H11A .. O1	0.97	2.53	2.862(7)	100
C17 -- H17 .. Se1	0.93	2.96	3.278(6)	102
C22 -- H22 .. Se2	0.93	2.97	3.278(6)	101
C26 -- H26A .. S3	0.97	2.86	3.280(5)	107
C26 -- H26A .. O3	0.97	2.47	2.892(6)	106
C26 -- H26A .. Br1	0.97	2.83	3.749(5)	158
C30 -- H30B .. O3	0.97	2.53	2.864(6)	100
C32 -- H32B .. S4	0.97	2.81	3.253(5)	108
C36 -- H36 .. Se2	0.93	2.94	3.263(6)	102

The detailed contact analysis report:

		D-H	H···A	D···A	D-H···A angle
C7 -- H7B .. S1	[ ]	0.97	2.81	3.216(5)	106
C7 -- H7B .. O1	[ ]	0.97	2.46	2.884(6)	106
C11 -- H11A .. O1	[ ]	0.97	2.53	2.862(7)	100
C17 -- H17 .. Se1	[ ]	0.93	2.96	3.278(6)	102
C22 -- H22 .. Se2	[ ]	0.93	2.97	3.278(6)	101
C26 -- H26A .. S3	[ ]	0.97	2.86	3.280(5)	107
C26 -- H26A .. O3	[ ]	0.97	2.47	2.892(6)	106
C26 -- H26A .. Br1	[3665.01]	0.97	2.83	3.749(5)	158

C30	--	H30B	..	O3	[	]	0.97	2.53	2.864(6)	100
C32	--	H32B	..	S4	[	]	0.97	2.81	3.253(5)	108
C36	--	H36	..	Se2	[	]	0.93	2.94	3.263(6)	102

Table S8. Compound **12**: Bond Lengths (Angstrom) for residue-1. - (Bonds are ordered on the first label, left to right and top to bottom) - su in last digit in ().

Br(1) - C(1) 1.867(6)	Br(2) - C(19) 1.850(6)	Se(1) - C(5) 1.876(5)	Se(1) - C(15) 1.876(5)
S(1) - C(1) 1.689(6)	S(1) - C(4) 1.726(6)	S(2) - C(16) 1.731(6)	S(2) - C(19) 1.708(6)
O(1) - C(9) 1.403(6)	O(1) - C(10) 1.411(8)	O(2) - C(11) 1.406(7)	O(2) - C(12) 1.412(8)
C(1) - C(2) 1.334(9)	C(2) - C(3) 1.390(9)	C(3) - C(4) 1.396(8)	C(4) - C(5) 1.432(7)
C(5) - C(6) 1.349(7)	C(6) - C(7) 1.489(7)	C(6) - C(14) 1.419(7)	C(7) - C(8) 1.553(7)
C(8) - C(9) 1.529(7)	C(8) - C(11) 1.487(7)	C(8) - C(13) 1.543(7)	C(13) - C(14) 1.485(7)
C(14) - C(15) 1.368(7)	C(15) > C(16) 1.441(8)	C(16) - C(17) 1.365(8)	C(17) - C(18) 1.395(9)
C(18) - C(19) 1.341(8)			
C(2) - H(2) 0.93	C(3) - H(3) 0.93	C(7) - H(7A) 0.97	C(7) - H(7B) 0.97
C(9) - H(9A) 0.97	C(9) - H(9B) 0.97	C(10) - H(10A) 0.96	C(10) - H(10B) 0.96
C(10) - H(10C) 0.96	C(11) - H(11A) 0.97	C(11) - H(11B) 0.97	C(12) - H(12A) 0.96
C(12) - H(12B) 0.96	C(12) - H(12C) 0.96	C(13) - H(13A) 0.97	C(13) - H(13B) 0.97
C(17) - H(17) 0.93	C(18) - H(18) 0.93		

Table S9. Compound **12**: Bond Lengths (Angstrom) for residue-2. - (Bonds are ordered on the first label, left to right and top to bottom) - su in last digit in ().

Br(3) - C(20)	1.851(6)	Br(4) - C(38)	1.845(6)	Se(2) - C(24)	1.869(5)	Se(2) - C(34)	1.885(5)
S(3) - C(20)	1.715(6)	S(3) - C(23)	1.724(6)	S(4) - C(35)	1.726(5)	S(4) - C(38)	1.698(6)
O(3) - C(28)	1.404(6)	O(3) - C(29)	1.403(8)	O(4) - C(30)	1.405(6)	O(4) - C(31)	1.399(8)
C(20) - C(21)	1.345(9)	C(21) - C(22)	1.368(8)	C(22) - C(23)	1.370(8)	C(23) > C(24)	1.454(8)
C(24) - C(25)	1.335(7)	C(25) - C(26)	1.493(7)	C(25) - C(33)	1.423(7)	C(26) - C(27)	1.542(7)
C(27) - C(28)	1.511(7)	C(27) - C(30)	1.495(7)	C(27) - C(32)	1.538(7)	C(32) - C(33)	1.479(7)
C(33) - C(34)	1.373(7)	C(34) - C(35)	1.419(7)	C(35) - C(36)	1.368(8)	C(36) - C(37)	1.391(9)
C(37) - C(38)	1.344(9)						
C(21) - H(21)	0.93	C(22) - H(22)	0.93	C(26) - H(26A)	0.97	C(26) - H(26B)	0.97
C(28) - H(28A)	0.97	C(28) - H(28B)	0.97	C(29) - H(29A)	0.96	C(29) - H(29B)	0.96
C(29) - H(29C)	0.96	C(30) - H(30A)	0.97	C(30) - H(30B)	0.97	C(31) - H(31A)	0.96
C(31) - H(31B)	0.96	C(31) - H(31C)	0.96	C(32) - H(32A)	0.97	C(32) - H(32B)	0.97
C(36) - H(36)	0.93	C(37) - H(37)	0.93				

1. Bruker. SADABS V2008-1, Bruker AXS: Madison, WI, USA, 2008.

2. G. M. Sheldrick, *SHELX 97, Program for Crystal Structure Determination*, University of Göttingen, Göttingen, Germany, 1997.

Coordinates for optimized geometry of **P9** at PBC/B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.372311	0.782170	-0.005530
2	6	0	-4.740588	1.105859	-1.187527
3	6	0	-3.321125	1.102931	-1.173152
4	6	0	-2.714763	0.774118	0.020588
5	6	0	-2.770292	1.473407	-2.527261
6	6	0	-5.261669	1.472134	-2.554590
7	6	0	-4.005126	1.377604	-3.480899
8	1	0	-2.355368	2.492957	-2.513302
9	1	0	-1.967104	0.814362	-2.873862
10	1	0	-5.681686	2.487597	-2.566069
11	1	0	-6.065740	0.810732	-2.901189
12	6	0	-3.978166	2.492173	-4.528459
13	6	0	-4.020446	0.002753	-4.169427
14	8	0	-5.158642	2.417723	-5.308198
15	8	0	-2.826118	-0.163450	-4.913221
16	6	0	-2.761744	-1.408859	-5.574971
17	1	0	-3.585058	-1.529282	-6.296930
18	1	0	-1.809959	-1.440998	-6.111879
19	1	0	-2.799716	-2.249501	-4.863696
20	6	0	-5.203664	3.390216	-6.329936
21	1	0	-6.142633	3.247506	-6.871477
22	1	0	-5.179542	4.413207	-5.920452
23	1	0	-4.363315	3.280412	-7.033879
24	1	0	-4.895731	-0.061602	-4.832838
25	1	0	-4.108459	-0.792232	-3.408891
26	1	0	-3.087339	2.384995	-5.166593
27	1	0	-3.918038	3.473303	-4.025144
28	6	0	-1.324682	0.672410	0.348211
29	6	0	-0.749787	0.216544	1.519688
30	6	0	0.661181	0.225914	1.569498
31	1	0	-1.354168	-0.137747	2.349956
32	6	0	1.311251	0.691643	0.443352
33	1	0	1.208914	-0.117286	2.442911
34	6	0	-6.769303	0.691181	0.295139
35	6	0	-7.371395	0.221074	1.447106
36	6	0	-8.782880	0.249204	1.471916
37	1	0	-6.786879	-0.158278	2.280530
38	6	0	-9.406297	0.745206	0.343630
39	1	0	-9.350953	-0.103051	2.328562
40	6	0	2.722006	0.795750	0.210124
41	6	0	3.372184	1.296773	-0.900714
42	6	0	4.783244	1.259295	-0.871305
43	1	0	2.824301	1.693999	-1.750815
44	6	0	5.358623	0.723400	0.265573
45	1	0	5.387267	1.621494	-1.698418
46	6	0	-10.810948	0.873974	0.086966
47	6	0	-11.432852	1.409012	-1.024225
48	6	0	-12.844562	1.392482	-1.021159
49	1	0	-10.863584	1.817662	-1.854649

50	6	0	-13.448614	0.840630	0.093018
51	1	0	-13.427707	1.784080	-1.849859
52	6	0	6.748552	0.555842	0.565042
53	6	0	7.353891	-0.078262	1.629558
54	6	0	8.772871	-0.087194	1.642436
55	6	0	9.405912	0.538969	0.589562
56	6	0	9.296108	-0.808234	2.858953
57	6	0	6.800892	-0.794926	2.835717
58	6	0	8.039395	-1.524572	3.453365
59	1	0	10.081248	-1.538485	2.634620
60	1	0	9.729080	-0.096068	3.578053
61	1	0	6.003441	-1.505854	2.584217
62	1	0	6.359285	-0.091174	3.554751
63	6	0	8.011017	-2.989966	2.990310
64	6	0	8.043824	-1.451379	4.981493
65	8	0	6.847335	-2.028048	5.473860
66	8	0	9.188455	-3.644450	3.428467
67	6	0	6.779769	-2.031572	6.883585
68	1	0	6.812489	-1.009893	7.295706
69	1	0	5.829271	-2.495148	7.160961
70	1	0	7.604572	-2.610091	7.329354
71	6	0	9.235955	-5.002195	3.044564
72	1	0	9.212399	-5.115787	1.948905
73	1	0	10.175432	-5.412819	3.423988
74	1	0	8.396509	-5.574855	3.469935
75	1	0	7.940983	-3.028769	1.889411
76	1	0	7.121113	-3.485438	3.406314
77	1	0	8.920881	-1.985101	5.378957
78	1	0	8.115060	-0.396567	5.300527
79	34	0	-12.116351	0.264307	1.313839
80	34	0	-8.102867	1.253353	-0.930585
81	34	0	-4.057636	0.430708	1.323582
82	34	0	0.037893	1.191641	-0.864066
83	34	0	3.995677	0.196276	1.474950
84	34	0	8.092427	1.251076	-0.587850
85	-2	0	24.251916	-0.150353	0.224966

Lengths of translation vectors: 24.253425

Coordinates for optimized geometry of **P10** at PBC/B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.297274	0.811385	0.083163
2	6	0	-4.663285	1.128860	-1.098027
3	6	0	-3.239988	1.123417	-1.078379
4	6	0	-2.641191	0.799507	0.119306
5	6	0	-2.690056	1.477146	-2.438377
6	6	0	-5.171649	1.484037	-2.473873
7	6	0	-3.917585	1.326498	-3.392193
8	1	0	-2.313384	2.511291	-2.444983

9	1	0	-1.863985	0.838646	-2.765232
10	1	0	-5.543103	2.517892	-2.504207
11	1	0	-6.002970	0.854046	-2.809817
12	6	0	-3.881394	2.373788	-4.506304
13	6	0	-3.935775	-0.088337	-3.994780
14	8	0	-5.057925	2.256708	-5.287316
15	8	0	-2.741942	-0.302252	-4.727637
16	6	0	-2.680073	-1.585767	-5.311618
17	1	0	-3.505918	-1.750395	-6.021964
18	1	0	-1.730199	-1.651258	-5.848986
19	1	0	-2.715514	-2.381290	-4.550025
20	6	0	-5.089217	3.161667	-6.369507
21	1	0	-6.026246	2.991919	-6.906666
22	1	0	-5.058949	4.208761	-6.026643
23	1	0	-4.245756	3.000236	-7.059703
24	1	0	-4.810887	-0.191532	-4.653539
25	1	0	-4.025552	-0.835308	-3.187395
26	1	0	-2.987699	2.223995	-5.131555
27	1	0	-3.820151	3.383952	-4.064270
28	6	0	-1.252630	0.677604	0.469720
29	6	0	-0.702280	0.191374	1.643793
30	6	0	0.708151	0.202513	1.669400
31	1	0	-1.309689	-0.180102	2.462782
32	6	0	1.285480	0.698824	0.514423
33	1	0	1.290937	-0.155928	2.511450
34	6	0	-6.695937	0.702144	0.395701
35	6	0	-7.283217	0.201946	1.545698
36	6	0	-8.693617	0.233985	1.535659
37	1	0	-6.702336	-0.195325	2.371805
38	6	0	-9.234038	0.760829	0.376335
39	1	0	-9.302938	-0.131940	2.355384
40	6	0	2.680443	0.834580	0.181482
41	6	0	3.258122	1.288669	-0.990580
42	6	0	4.668590	1.261472	-0.980461
43	1	0	2.675353	1.622062	-1.842869
44	6	0	5.218682	0.785564	0.197932
45	1	0	5.276270	1.568171	-1.825653
46	6	0	-10.617752	0.923346	0.010093
47	6	0	-11.157575	1.415928	-1.164465
48	6	0	-12.567953	1.407624	-1.192549
49	1	0	-10.547922	1.765335	-1.991161
50	6	0	-13.155819	0.908389	-0.042303
51	1	0	-13.148312	1.746952	-2.044446
52	6	0	6.607016	0.625200	0.533394
53	6	0	7.205371	0.001551	1.606406
54	6	0	8.628549	-0.002822	1.627493
55	6	0	9.262882	0.615875	0.572464
56	6	0	9.138790	-0.724934	2.850357
57	6	0	6.655884	-0.719808	2.812915
58	6	0	7.887647	-1.489967	3.387977
59	1	0	9.960321	-1.418450	2.647727
60	1	0	9.507952	-0.005456	3.596907
61	1	0	5.827278	-1.397239	2.577284
62	1	0	6.265668	-0.010041	3.555520
63	6	0	7.869741	-2.919984	2.823245
64	6	0	7.881821	-1.526373	4.917460
65	8	0	6.683953	-2.141215	5.358564

66	8	0	9.048143	-3.597912	3.222787
67	6	0	6.608366	-2.250625	6.763362
68	1	0	6.633452	-1.262587	7.251242
69	1	0	5.658667	-2.738091	6.999623
70	1	0	7.433615	-2.856959	7.169776
71	6	0	9.101143	-4.927851	2.752965
72	1	0	9.081137	-4.971700	1.652146
73	1	0	10.040803	-5.359234	3.108278
74	1	0	8.262226	-5.529222	3.138086
75	1	0	7.806039	-2.884285	1.722149
76	1	0	6.980642	-3.447478	3.199527
77	1	0	8.757960	-2.084291	5.282535
78	1	0	7.947032	-0.497361	5.313197
79	34	0	-3.988754	0.479482	1.420976
80	34	0	7.954351	1.328562	-0.607436
81	16	0	3.930067	0.372850	1.327775
82	16	0	0.035769	1.171409	-0.627288
83	16	0	-7.948549	1.237013	-0.723455
84	16	0	-11.903559	0.446913	1.109257
85	-2	0	23.817533	-0.141497	0.321420

Lengths of translation vectors: 23.820122

Coordinates for optimized geometry of **P11** at PBC/B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.170637	1.032079	0.003433
2	6	0	-4.655065	0.991350	-1.276676
3	6	0	-3.238930	0.951623	-1.336634
4	6	0	-2.615591	0.959432	-0.104731
5	16	0	-3.840500	1.036827	1.168004
6	6	0	-2.762319	0.900773	-2.765699
7	6	0	-5.251761	0.967693	-2.660523
8	6	0	-4.053538	0.544300	-3.574946
9	1	0	-2.361531	1.877261	-3.076862
10	1	0	-1.974164	0.164203	-2.948591
11	1	0	-5.627291	1.958345	-2.951461
12	1	0	-6.100367	0.281366	-2.760694
13	6	0	-4.075086	1.270099	-4.921576
14	6	0	-4.127516	-0.976354	-3.790787
15	8	0	-5.302447	0.993299	-5.572775
16	8	0	-2.985060	-1.404971	-4.511093
17	6	0	-2.980665	-2.795335	-4.754916
18	1	0	-3.850366	-3.106070	-5.355550
19	1	0	-2.066008	-3.023657	-5.308581
20	1	0	-2.984334	-3.372874	-3.816564
21	6	0	-5.398868	1.600736	-6.842948
22	1	0	-6.370821	1.324892	-7.260698
23	1	0	-5.338139	2.699172	-6.775145
24	1	0	-4.604477	1.252688	-7.522343
25	1	0	-5.043604	-1.219942	-4.349218

26	1	0	-4.175708	-1.488240	-2.814249
27	1	0	-3.227176	0.937702	-5.540210
28	1	0	-3.969983	2.357348	-4.758925
29	6	0	-1.219811	0.908720	0.245006
30	6	0	-0.645880	0.806573	1.500299
31	16	0	0.040508	0.974270	-0.983349
32	6	0	0.765432	0.776120	1.486243
33	1	0	-1.233020	0.746927	2.410508
34	6	0	1.316041	0.854040	0.220051
35	1	0	1.367090	0.694315	2.385445
36	6	0	-6.532559	1.059143	0.469794
37	6	0	-7.005887	0.946389	1.765447
38	16	0	-7.882780	1.259058	-0.643204
39	6	0	-8.412136	1.011922	1.871144
40	1	0	-6.350751	0.808665	2.619035
41	6	0	-9.059356	1.176143	0.660083
42	1	0	-8.941748	0.934627	2.814949
43	6	0	2.702024	0.831195	-0.172945
44	6	0	3.252924	0.938182	-1.436915
45	16	0	3.974993	0.624026	1.021435
46	6	0	4.661796	0.850707	-1.457607
47	1	0	2.652433	1.070309	-2.330877
48	6	0	5.233476	0.674506	-0.209658
49	1	0	5.248168	0.903655	-2.368712
50	6	0	-10.471481	1.262536	0.387163
51	6	0	-11.117588	1.454601	-0.820398
52	16	0	-11.650839	1.099707	1.680320
53	6	0	-12.525724	1.468034	-0.721194
54	1	0	-10.586533	1.578799	-1.758372
55	6	0	-13.001537	1.286836	0.565756
56	1	0	-13.181046	1.599666	-1.575585
57	6	0	6.626244	0.545083	0.131784
58	6	0	7.236632	0.209294	1.323752
59	16	0	7.864235	0.826201	-1.098570
60	6	0	8.652376	0.159281	1.262747
61	6	0	9.180484	0.455948	0.022156
62	6	0	9.235342	-0.224370	2.598631
63	6	0	6.746670	-0.135522	2.706844
64	6	0	8.003162	-0.760507	3.401059
65	1	0	10.021377	-0.983407	2.542086
66	1	0	9.677398	0.652155	3.095889
67	1	0	5.894672	-0.824927	2.711582
68	1	0	6.414648	0.761038	3.247945
69	6	0	7.918599	-2.289553	3.262179
70	6	0	8.098295	-0.369632	4.877158
71	8	0	6.919084	-0.789472	5.541009
72	8	0	9.107235	-2.873711	3.765890
73	6	0	6.935337	-0.501659	6.922438
74	1	0	7.018142	0.580892	7.112237
75	1	0	5.991669	-0.863279	7.339648
76	1	0	7.770464	-1.006457	7.433881
77	6	0	9.105012	-4.282650	3.679214
78	1	0	9.014871	-4.626045	2.636128
79	1	0	10.056846	-4.633178	4.087150
80	1	0	8.280836	-4.725008	4.261208
81	1	0	7.782045	-2.559661	2.200956
82	1	0	7.046252	-2.656832	3.822892

83	1	0	8.984167	-0.838718	5.332564
84	1	0	8.212192	0.725328	4.964921
85	-2	0	23.546633	-0.791453	-1.001296

Lengths of translation vectors: 23.581199

Coordinates for optimized geometry of **11** at 0° calculated at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.376357	-4.256901	-0.379979
2	1	0	4.384575	-4.609301	-0.550835
3	6	0	2.286743	-4.965474	0.046924
4	1	0	2.314651	-6.026189	0.271987
5	6	0	1.118218	-4.164706	0.171715
6	1	0	0.160996	-4.549455	0.507328
7	6	0	1.314973	-2.839091	-0.161386
8	6	0	0.357022	-1.756085	-0.164616
9	6	0	0.533036	-0.396218	-0.299800
10	6	0	1.724542	0.504346	-0.502479
11	1	0	2.082642	0.446135	-1.541304
12	1	0	2.578891	0.266948	0.138429
13	6	0	1.168870	1.932728	-0.185718
14	6	0	1.449271	2.285347	1.284531
15	1	0	1.052394	3.288954	1.498682
16	1	0	0.934311	1.565626	1.943789
17	6	0	3.186072	2.573517	2.850757
18	1	0	2.737371	1.867534	3.568004
19	1	0	2.861249	3.591570	3.118948
20	1	0	4.274979	2.515358	2.929749
21	6	0	1.746187	5.278726	-1.628172
22	1	0	1.609015	5.095770	-2.706433
23	1	0	2.823140	5.407242	-1.434657
24	1	0	1.223425	6.199610	-1.355864
25	6	0	1.794547	2.980822	-1.107669
26	1	0	2.881160	3.028744	-0.937376
27	1	0	1.629443	2.694585	-2.161395
28	6	0	-0.382364	1.831519	-0.375263
29	1	0	-0.915980	2.447870	0.357952
30	1	0	-0.677123	2.208895	-1.364424
31	6	0	-0.667669	0.359157	-0.237560
32	6	0	-1.806330	-0.397038	-0.054617
33	6	0	-3.187894	0.029534	0.016738
34	6	0	-3.697318	1.311215	-0.082948
35	1	0	-3.078823	2.179924	-0.269751
36	6	0	-5.111226	1.375836	0.061211
37	1	0	-5.677898	2.299102	0.004604
38	6	0	-5.684777	0.152624	0.273881
39	1	0	-6.730289	-0.088043	0.410437
40	8	0	2.846204	2.250970	1.519458
41	8	0	1.196335	4.239311	-0.848056
42	16	0	2.988838	-2.586654	-0.643013

43	16	0	-1.362748	-2.102736	0.029054
44	16	0	-4.495965	-1.110127	0.304436

Coordinates for optimized geometry of **11** at 30° calculated at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.229835	4.369503	-0.360156
2	1	0	-4.227173	4.749996	-0.534616
3	6	0	-2.109894	5.056657	0.020479
4	1	0	-2.096794	6.126652	0.197879
5	6	0	-0.968206	4.220917	0.163307
6	1	0	0.007675	4.587158	0.464196
7	6	0	-1.215634	2.890077	-0.109067
8	6	0	-0.295757	1.774156	-0.075469
9	6	0	-0.515507	0.421456	-0.222532
10	6	0	-1.727240	-0.432276	-0.496845
11	1	0	-2.051676	-0.320542	-1.542369
12	1	0	-2.593711	-0.194405	0.127713
13	6	0	-1.226257	-1.888957	-0.221515
14	6	0	-1.561139	-2.288110	1.225350
15	1	0	-1.196899	-3.309157	1.413608
16	1	0	-1.049170	-1.607018	1.926826
17	6	0	-3.352242	-2.582232	2.728173
18	1	0	-2.908980	-1.911855	3.482112
19	1	0	-3.061147	-3.616541	2.971802
20	1	0	-4.441317	-2.498845	2.776099
21	6	0	-1.869582	-5.157696	-1.805398
22	1	0	-1.689933	-4.941258	-2.871123
23	1	0	-2.956254	-5.254698	-1.651737
24	1	0	-1.388133	-6.105712	-1.550589
25	6	0	-1.858117	-2.880121	-1.200366
26	1	0	-2.950502	-2.896644	-1.064364
27	1	0	-1.650529	-2.561284	-2.237056
28	6	0	0.331663	-1.831262	-0.364121
29	1	0	0.820561	-2.512987	0.339186
30	1	0	0.642077	-2.155452	-1.366814
31	6	0	0.658006	-0.376041	-0.139620
32	6	0	1.813996	0.340700	0.072046
33	6	0	3.184330	-0.123310	0.178780
34	6	0	3.647759	-1.336092	0.645092
35	1	0	2.989647	-2.107473	1.027107
36	6	0	5.065526	-1.458106	0.606010
37	1	0	5.601922	-2.340575	0.938115
38	6	0	5.684424	-0.339475	0.118973
39	1	0	6.743000	-0.159002	-0.010753
40	8	0	-2.963311	-2.224958	1.419460
41	8	0	-1.310978	-4.167179	-0.969972
42	16	0	-2.905072	2.676760	-0.554658
43	16	0	1.425567	2.057878	0.188326
44	16	0	4.536623	0.883364	-0.321783

Coordinates for optimized geometry of **11** at 60° calculated at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.082804	-3.611520	-0.366492
2	1	0	5.133191	-3.776610	-0.564977
3	6	0	3.149316	-4.505660	0.081172
4	1	0	3.372563	-5.544862	0.297407
5	6	0	1.859164	-3.927908	0.238870
6	1	0	0.994937	-4.480229	0.592530
7	6	0	1.806225	-2.588463	-0.089808
8	6	0	0.668720	-1.692877	-0.059081
9	6	0	0.597603	-0.327229	-0.227719
10	6	0	1.592776	0.767132	-0.521430
11	1	0	1.917317	0.727244	-1.572186
12	1	0	2.499718	0.723391	0.089411
13	6	0	0.791224	2.082724	-0.237500
14	6	0	1.035775	2.537443	1.210768
15	1	0	0.464728	3.458105	1.403079
16	1	0	0.679962	1.761161	1.909983
17	6	0	2.725422	3.204070	2.712128
18	1	0	2.433319	2.456778	3.467523
19	1	0	2.223170	4.154404	2.954167
20	1	0	3.807674	3.351838	2.759648
21	6	0	0.706785	5.416377	-1.814419
22	1	0	0.567677	5.166921	-2.879018
23	1	0	1.748496	5.745232	-1.670686
24	1	0	0.034889	6.238355	-1.552911
25	6	0	1.193791	3.190706	-1.212226
26	1	0	2.257220	3.441977	-1.077081
27	1	0	1.058374	2.838749	-2.250144
28	6	0	-0.716750	1.689660	-0.381809
29	1	0	-1.357884	2.256704	0.300400
30	1	0	-1.074130	1.915123	-1.395734
31	6	0	-0.718998	0.203416	-0.131766
32	6	0	-1.688062	-0.731260	0.130748
33	6	0	-3.129929	-0.555838	0.258805
34	6	0	-3.816310	0.229304	1.156297
35	1	0	-3.312180	0.831426	1.904391
36	6	0	-5.232716	0.151837	1.016497
37	1	0	-5.930952	0.703206	1.637127
38	6	0	-5.621445	-0.708193	0.026061
39	1	0	-6.626285	-0.962020	-0.284527
40	8	0	2.420117	2.770605	1.404435
41	8	0	0.382388	4.328616	-0.976458
42	16	0	3.395089	-2.037843	-0.608325
43	16	0	-0.949819	-2.330420	0.236800
44	16	0	-4.259282	-1.428174	-0.767650

Coordinates for optimized geometry of **11** at 90° calculated at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.864029	-2.516609	-0.427335
2	1	0	5.917652	-2.419345	-0.651864
3	6	0	4.198923	-3.594939	0.088537
4	1	0	4.684399	-4.531236	0.341914
5	6	0	2.807657	-3.355902	0.264277
6	1	0	2.119751	-4.090007	0.670321
7	6	0	2.408831	-2.091712	-0.118871
8	6	0	1.080369	-1.513411	-0.092680
9	6	0	0.667850	-0.210611	-0.264771
10	6	0	1.354177	1.105095	-0.532728
11	1	0	1.665472	1.175176	-1.585949
12	1	0	2.250171	1.273741	0.072315
13	6	0	0.251177	2.170130	-0.209022
14	6	0	0.385742	2.630454	1.251661
15	1	0	-0.400169	3.367901	1.473081
16	1	0	0.247197	1.769428	1.927914
17	6	0	1.861701	3.665808	2.768823
18	1	0	1.781654	2.847395	3.502503
19	1	0	1.132095	4.445524	3.040274
20	1	0	2.868772	4.088669	2.818090
21	6	0	-0.664445	5.425065	-1.684041
22	1	0	-0.742076	5.182365	-2.756458
23	1	0	0.265056	5.995193	-1.526025
24	1	0	-1.516818	6.047933	-1.399473
25	6	0	0.357650	3.370234	-1.151478
26	1	0	1.327104	3.872869	-1.010818
27	1	0	0.304994	3.024869	-2.199150
28	6	0	-1.112246	1.416554	-0.362674
29	1	0	-1.869073	1.776940	0.342177
30	1	0	-1.526244	1.578964	-1.366745
31	6	0	-0.740287	-0.028862	-0.159580
32	6	0	-1.442051	-1.176192	0.098650
33	6	0	-2.881077	-1.366073	0.294023
34	6	0	-3.601814	-1.314341	1.462680
35	1	0	-3.133690	-1.127865	2.423277
36	6	0	-5.000312	-1.529227	1.283203
37	1	0	-5.720963	-1.522072	2.093919
38	6	0	-5.338500	-1.746162	-0.024598
39	1	0	-6.320371	-1.934146	-0.438800
40	8	0	1.666185	3.204856	1.449671
41	8	0	-0.707659	4.265292	-0.881872
42	16	0	3.792928	-1.183073	-0.713654
43	16	0	-0.324897	-2.538761	0.198960
44	16	0	-3.952241	-1.691872	-1.061389

Coordinates for optimized geometry of **11** at 120° calculated at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.252513	-1.624921	-0.437776
2	1	0	6.274477	-1.340712	-0.649378
3	6	0	4.786919	-2.795714	0.095122
4	1	0	5.431219	-3.621057	0.378421
5	6	0	3.372681	-2.812019	0.246936
6	1	0	2.823448	-3.649270	0.664457
7	6	0	2.756084	-1.650408	-0.171809
8	6	0	1.344831	-1.325385	-0.175587
9	6	0	0.702824	-0.117045	-0.336255
10	6	0	1.144661	1.310361	-0.538957
11	1	0	1.436315	1.483795	-1.585823
12	1	0	1.996601	1.607021	0.080213
13	6	0	-0.130983	2.144300	-0.177493
14	6	0	-0.090774	2.538609	1.308040
15	1	0	-0.996128	3.112755	1.555024
16	1	0	-0.080110	1.630570	1.935004
17	6	0	1.168112	3.732550	2.902489
18	1	0	1.225541	2.873800	3.590750
19	1	0	0.311720	4.357988	3.201472
20	1	0	2.085831	4.320170	2.991717
21	6	0	-1.611424	5.257143	-1.490678
22	1	0	-1.638157	5.063358	-2.575483
23	1	0	-0.802745	5.977915	-1.289267
24	1	0	-2.564711	5.697618	-1.186284
25	6	0	-0.234899	3.395317	-1.051861
26	1	0	0.627151	4.054831	-0.867373
27	1	0	-0.217774	3.105659	-2.117509
28	6	0	-1.337030	1.170468	-0.395494
29	1	0	-2.154328	1.353894	0.310655
30	1	0	-1.761405	1.311732	-1.398305
31	6	0	-0.715329	-0.194893	-0.253230
32	6	0	-1.199916	-1.460786	-0.039687
33	6	0	-2.562261	-1.921983	0.195428
34	6	0	-3.069352	-2.592099	1.285748
35	1	0	-2.449423	-2.886157	2.125825
36	6	0	-4.470769	-2.836874	1.202990
37	1	0	-5.039003	-3.349931	1.971483
38	6	0	-5.030472	-2.340579	0.057314
39	1	0	-6.066236	-2.377143	-0.253108
40	8	0	1.066830	3.317531	1.557730
41	8	0	-1.445928	4.066939	-0.751446
42	16	0	3.960405	-0.516949	-0.771160
43	16	0	0.144820	-2.598023	0.055410
44	16	0	-3.846599	-1.576206	-0.952013

Coordinates for optimized geometry of **11** at 150° calculated at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.331838	-1.359377	-0.424085
2	1	0	6.339378	-1.017410	-0.618625
3	6	0	4.922560	-2.569087	0.066480
4	1	0	5.605921	-3.370038	0.327377
5	6	0	3.510278	-2.661599	0.206775
6	1	0	3.001947	-3.538977	0.592440
7	6	0	2.837903	-1.518921	-0.178529
8	6	0	1.413518	-1.265789	-0.182796
9	6	0	0.708938	-0.091441	-0.331574
10	6	0	1.080618	1.356667	-0.525670
11	1	0	1.373180	1.547243	-1.569275
12	1	0	1.911433	1.692848	0.101918
13	6	0	-0.236851	2.124527	-0.171794
14	6	0	-0.225367	2.519218	1.314165
15	1	0	-1.162151	3.042157	1.557725
16	1	0	-0.167232	1.612378	1.940182
17	6	0	0.962454	3.774298	2.916116
18	1	0	1.067922	2.917056	3.600494
19	1	0	0.071338	4.348364	3.216564
20	1	0	1.844975	4.412984	3.009218
21	6	0	-1.860209	5.162050	-1.492294
22	1	0	-1.865872	4.971420	-2.577952
23	1	0	-1.089966	5.920660	-1.279668
24	1	0	-2.837088	5.554080	-1.196608
25	6	0	-0.398396	3.369012	-1.046440
26	1	0	0.427492	4.071471	-0.855177
27	1	0	-0.358354	3.081409	-2.111987
28	6	0	-1.391097	1.091220	-0.396340
29	1	0	-2.218579	1.233803	0.307876
30	1	0	-1.820848	1.214740	-1.399755
31	6	0	-0.702631	-0.242416	-0.256294
32	6	0	-1.122740	-1.536120	-0.050304
33	6	0	-2.452015	-2.079796	0.138714
34	6	0	-2.835689	-3.190111	0.862392
35	1	0	-2.127769	-3.803133	1.409782
36	6	0	-4.238422	-3.428913	0.839156
37	1	0	-4.716801	-4.252486	1.358291
38	6	0	-4.925824	-2.499953	0.106691
39	1	0	-5.991684	-2.433255	-0.065263
40	8	0	0.886653	3.360203	1.569249
41	8	0	-1.644161	3.978472	-0.755408
42	16	0	3.987713	-0.306641	-0.730357
43	16	0	0.280334	-2.604080	0.024442
44	16	0	-3.861819	-1.316500	-0.583117

Coordinates for optimized geometry of **11** at 180° calculated at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.348368	-1.310197	-0.389950
2	1	0	6.352439	-0.951889	-0.572591
3	6	0	4.950842	-2.540480	0.057219
4	1	0	5.641910	-3.343582	0.289632
5	6	0	3.539658	-2.652044	0.192785
6	1	0	3.040527	-3.548419	0.545365
7	6	0	2.855671	-1.503083	-0.152276
8	6	0	1.429766	-1.263422	-0.145871
9	6	0	0.711801	-0.097100	-0.289704
10	6	0	1.070418	1.349530	-0.513474
11	1	0	1.373443	1.517825	-1.557823
12	1	0	1.891394	1.709036	0.114230
13	6	0	-0.256006	2.114260	-0.190462
14	6	0	-0.246964	2.572702	1.277152
15	1	0	-1.189159	3.095198	1.499841
16	1	0	-0.177749	1.693715	1.940827
17	6	0	0.929522	3.907388	2.821985
18	1	0	1.046155	3.080846	3.541367
19	1	0	0.032447	4.483336	3.100157
20	1	0	1.804803	4.559454	2.885818
21	6	0	-1.917233	5.074150	-1.634609
22	1	0	-1.923795	4.837625	-2.711176
23	1	0	-1.155018	5.849560	-1.456618
24	1	0	-2.897666	5.467327	-1.352569
25	6	0	-0.433831	3.318187	-1.117454
26	1	0	0.384569	4.037478	-0.959068
27	1	0	-0.393026	2.985429	-2.169723
28	6	0	-1.401180	1.061014	-0.367559
29	1	0	-2.208684	1.216716	0.357086
30	1	0	-1.862999	1.154825	-1.360060
31	6	0	-0.697449	-0.263040	-0.211812
32	6	0	-1.106121	-1.563161	-0.010013
33	6	0	-2.430599	-2.131965	0.104507
34	6	0	-2.789104	-3.450120	0.307826
35	1	0	-2.060662	-4.245441	0.425211
36	6	0	-4.194527	-3.661594	0.352677
37	1	0	-4.650944	-4.633298	0.507639
38	6	0	-4.913078	-2.510589	0.179532
39	1	0	-5.986883	-2.381124	0.170718
40	8	0	0.855738	3.436063	1.493808
41	8	0	-1.685667	3.925276	-0.848923
42	16	0	3.994202	-0.260269	-0.659364
43	16	0	0.312172	-2.612923	0.077251
44	16	0	-3.876461	-1.137931	-0.044158

Coordinates for optimized geometry of TS for the rotation of one of the capped thiophene ring of **11** calculated at B3LYP/6-31G(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.819170	-2.597070	-0.423723
2	1	0	5.874337	-2.518068	-0.648166
3	6	0	4.135049	-3.664461	0.090022
4	1	0	4.603834	-4.609742	0.341460
5	6	0	2.748233	-3.401163	0.266239
6	1	0	2.047508	-4.123902	0.670761
7	6	0	2.371823	-2.129396	-0.114493
8	6	0	1.053758	-1.527820	-0.087202
9	6	0	0.663884	-0.218269	-0.260591
10	6	0	1.372192	1.084620	-0.534340
11	1	0	1.682913	1.145515	-1.588307
12	1	0	2.271820	1.240501	0.068702
13	6	0	0.287952	2.169341	-0.212702
14	6	0	0.432235	2.631694	1.246432
15	1	0	-0.340951	3.382807	1.466676
16	1	0	0.280322	1.775080	1.925415
17	6	0	1.927533	3.646661	2.758441
18	1	0	1.834559	2.831885	3.494638
19	1	0	1.211670	4.439475	3.028544
20	1	0	2.941706	4.052493	2.805115
21	6	0	-0.577278	5.433536	-1.697449
22	1	0	-0.660495	5.187836	-2.768759
23	1	0	0.361201	5.989849	-1.543235
24	1	0	-1.419408	6.070652	-1.413935
25	6	0	0.413282	3.364777	-1.158851
26	1	0	1.390903	3.852033	-1.020779
27	1	0	0.353775	3.017178	-2.205419
28	6	0	-1.088244	1.438750	-0.362556
29	1	0	-1.838255	1.814857	0.341300
30	1	0	-1.499920	1.604321	-1.367059
31	6	0	-0.740834	-0.012062	-0.154321
32	6	0	-1.462051	-1.146364	0.107694
33	6	0	-2.904997	-1.310716	0.296867
34	6	0	-3.635531	-1.198963	1.455184
35	1	0	-3.174142	-0.973144	2.410572
36	6	0	-5.034269	-1.410152	1.272978
37	1	0	-5.761984	-1.359232	2.075778
38	6	0	-5.362493	-1.686484	-0.026105
39	1	0	-6.342105	-1.886521	-0.440013
40	8	0	1.722375	3.185196	1.440926
41	8	0	-0.637113	4.277698	-0.890667
42	16	0	3.771910	-1.244103	-0.707133
43	16	0	-0.368713	-2.528101	0.208266
44	16	0	-3.966690	-1.692532	-1.051415