Supporting Information

New Alternating Electron Donor-Acceptor Conjugated Polymers Entailing (*E*)-[4,4'-biimidazolylidene]-5,5'(1*H*,1'*H*)-dione Moieties

Jianguo Wang, Xin Chen, Zhengxu Cai, Hewei Luo, Yonghai Li, Zitong Liu,* Guanxin Zhang, Deqing Zhang*

Beijing National Laboratory for Molecular Sciences, Organic Solids Laboratory, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China.
E-mail: dqzhang@iccas.ac.cn

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1. TGA analysis

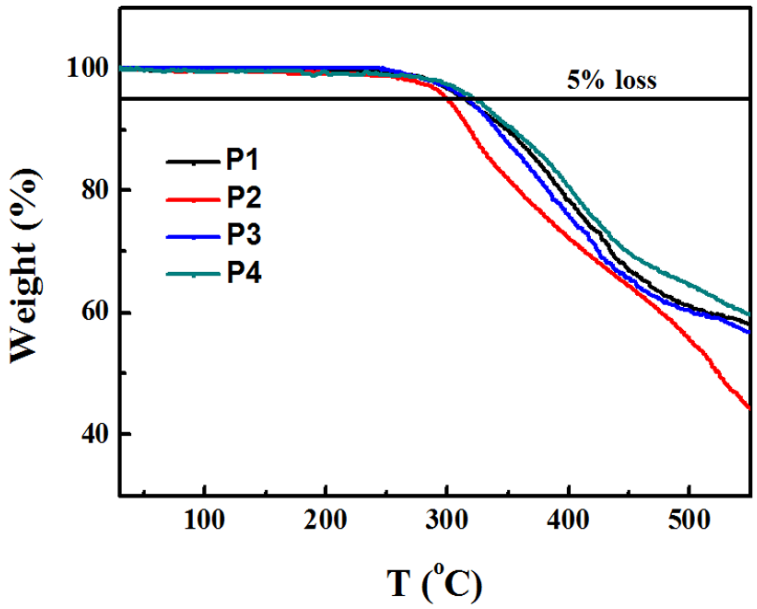
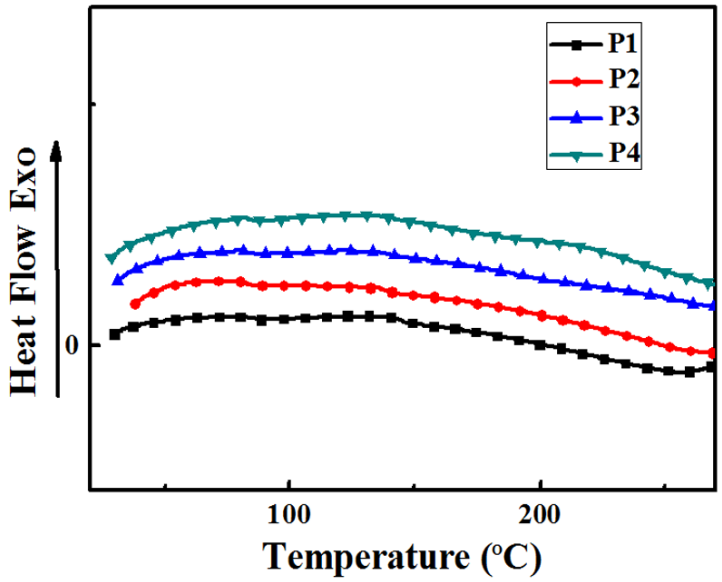


Figure S1. TGA curves of **P1-P4**: heating rate: 10 °C/min. from 16 °C to 550 °C under nitrogen atmosphere.

2. DSC analysis



Figures S2. DSC curves of **P1-P4**: heating rate: 10 °C /min. from 16 °C to 300 °C under nitrogen atmosphere.

3. Absorption spectra for P1-P4 in different solvents

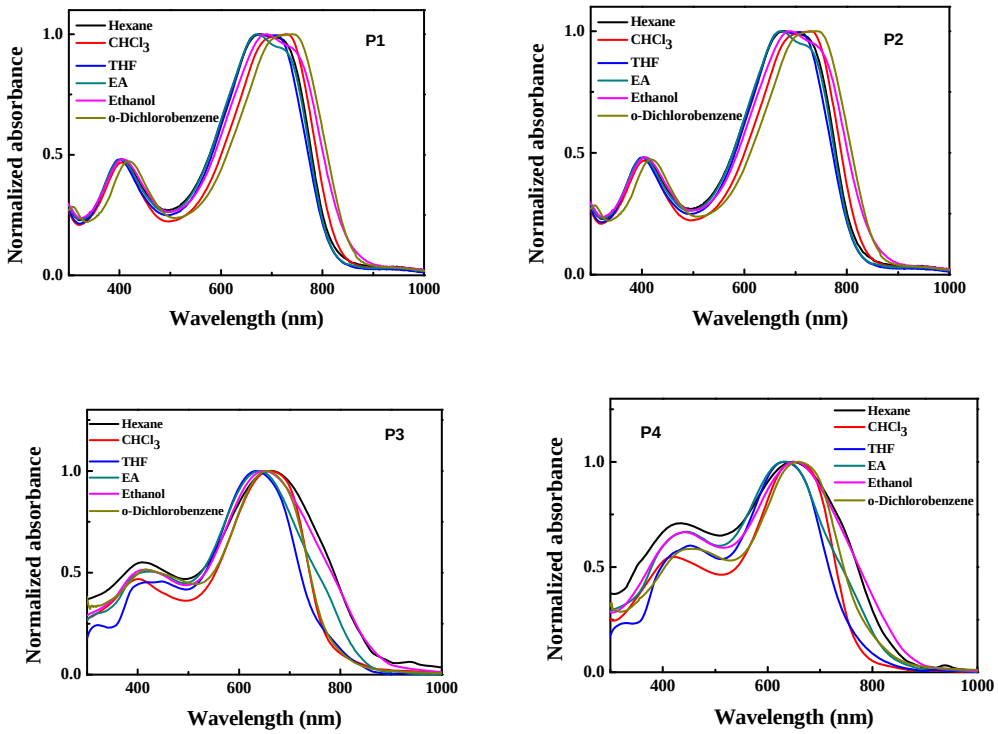


Figure S3. Normalized absorption spectra for **P1**-**P4** in different solvents (the concentration for each polymer was 1.0×10^{-5} M).

4. Density Funtional Theory Calculations

Geometries optimization and frequency analysis were performed at the level of B3LYP /6-31G(d) by using Gaussian09 (revision A.02)[S1]. Table S1-Table S4 listed the coordinates and energies at the optimized geometries for **P1-P4**, and there were no any imaginary frequencies. Then the molecular orbitals were analyzed, the energy gaps between HOMO and LUMO were obtained.

HOMO/LUMO energies were calculated to be -4.99 eV/-3.04 eV, -4.94 eV/-3.01 eV, -4.98 eV/-3.09 eV and -4.94 eV/-3.05 eV, respectively, for the respective two repeated units in **P1**-**P4**. Note that solvent effects were not included in the calculations and the alkyl groups in **P1**-**P4** were replaced with methyl groups for simplifying the calculations.

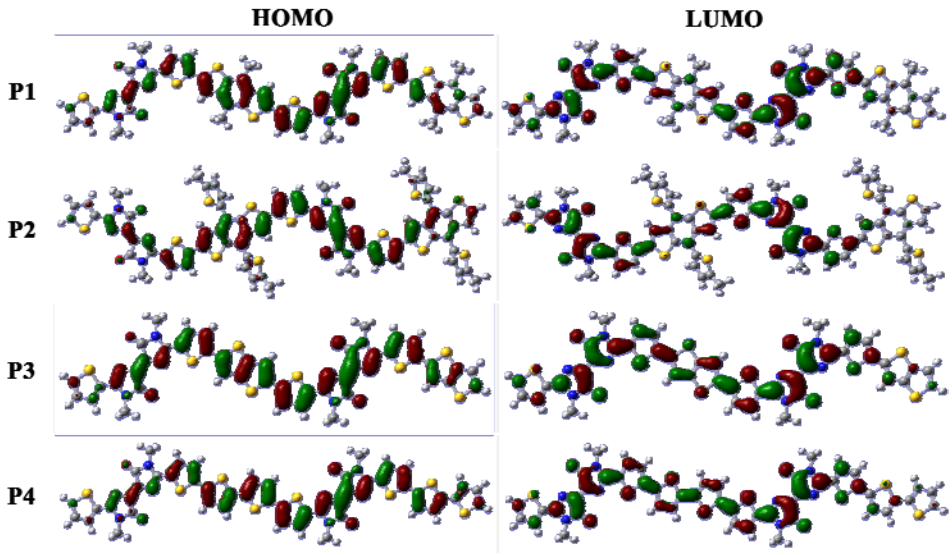


Figure S4. Calculated molecular orbitals of two repeated units of **P1-P4** at the B3LYP/6-31G(d) level; the alkyl chains are replaced with methyl groups for computational simplicity.

Table S1. Coordinates and energy of two repeated units of **P1**

		X	Y	Z
1	C	-18.336335	-1.764014	0.324906
2	C	-16.927165	-1.459201	0.272189
3	N	-16.506571	-0.214805	0.139355
4	C	-15.136122	-0.257959	0.120849
5	C	-14.676190	-1.677557	0.256649
6	N	-15.897508	-2.385638	0.348921
7	C	-14.314117	0.839768	-0.003212
8	O	-13.576207	-2.193582	0.290285
9	C	-14.773744	2.260753	-0.136541
10	N	-13.552628	2.968696	-0.227980
11	C	-12.522908	2.041580	-0.154980
12	N	-12.944774	0.795893	-0.023585
13	O	-15.873490	2.776419	-0.168895
14	C	-11.117005	2.339913	-0.211296
15	C	-15.925516	-3.827331	0.495332
16	C	-13.523143	4.410415	-0.373254
17	C	-19.022776	-2.958315	0.461040
18	C	-20.431414	-2.792615	0.463172
19	C	-20.805152	-1.478990	0.329037
20	S	-19.452275	-0.416142	0.197902
21	C	-10.422575	3.532098	-0.343784
22	C	-9.023579	3.363472	-0.356901
23	C	-8.625544	2.040860	-0.235388
24	S	-10.011453	0.982557	-0.094597

25	C	-7.280726	1.516363	-0.222316
26	S	-5.895304	2.620798	-0.227450
27	C	-4.763229	1.266848	-0.220456
28	C	-5.461806	0.021002	-0.203999
29	C	-6.880741	0.205009	-0.205605
30	C	-3.365034	-1.095722	-0.191188
31	C	-2.666445	0.150012	-0.209016
32	C	-1.247453	-0.034028	-0.210120
33	C	-0.847620	-1.345472	-0.193565
34	S	-2.233163	-2.449441	-0.164764
35	C	-3.375690	1.371334	-0.230018
36	C	-4.752576	-1.200453	-0.194689
37	C	-5.471559	-2.525187	-0.170537
38	C	-2.655806	2.695743	-0.243100
39	C	2.988156	-2.172138	-0.173793
40	C	4.394430	-1.875275	-0.124687
41	N	4.819181	-0.629257	-0.002764
42	C	6.188053	-0.675067	0.008770
43	C	6.645250	-2.096345	-0.119478
44	N	5.422876	-2.803734	-0.198126
45	C	7.013283	0.423054	0.121639
46	O	7.744495	-2.613856	-0.156290
47	C	6.556737	1.844228	0.259085
48	N	7.779360	2.550577	0.339310
49	C	8.807558	1.622867	0.252680
50	N	8.381658	0.377258	0.126381
51	O	5.457655	2.361559	0.301358
52	C	10.213691	1.920121	0.284626
53	C	5.391246	-4.245978	-0.336495
54	C	7.812531	3.992853	0.476926
55	C	2.292247	-3.365241	-0.290575
56	C	0.893457	-3.195398	-0.303938
57	C	0.496782	-1.871032	-0.198744
58	S	1.883908	-0.812450	-0.071142
59	C	10.911640	3.109229	0.427026
60	C	12.310560	2.940681	0.403527
61	C	12.705532	1.621436	0.242262
62	S	11.316680	0.565922	0.112957
63	C	14.050059	1.098584	0.176151
64	S	15.435388	2.204788	0.161284
65	C	16.565230	0.851961	0.087453
66	C	15.869538	-0.394140	0.056352
67	C	14.449370	-0.210328	0.115010
68	C	17.974930	-1.493209	-0.043057

69	C	18.669958	-0.246821	-0.012801
70	C	20.098527	-0.435851	-0.069527
71	C	20.466493	-1.740289	-0.129174
72	S	19.109967	-2.843851	-0.120992
73	C	17.953112	0.965860	0.058514
74	C	16.585757	-1.607734	-0.013390
75	C	15.896258	-2.947923	-0.027735
76	C	18.638396	2.308622	0.076029
77	H	-14.883114	-4.151842	0.504528
78	H	-16.441300	-4.304520	-0.343297
79	H	-16.400461	-4.125074	1.435044
80	H	-13.007244	4.886597	0.465996
81	H	-14.565173	4.736145	-0.382338
82	H	-13.047848	4.708507	-1.312773
83	H	-18.543328	-3.922203	0.557111
84	H	-21.134170	-3.611697	0.559806
85	H	-21.809032	-1.077284	0.300516
86	H	-10.897101	4.499127	-0.432735
87	H	-8.324435	4.185093	-0.461263
88	H	-7.587153	-0.616810	-0.199424
89	H	-0.540940	0.787497	-0.229379
90	H	-4.803576	-3.350523	-0.429477
91	H	-6.301856	-2.540637	-0.883235
92	H	-5.887738	-2.735734	0.822061
93	H	-2.224049	2.925238	0.738539
94	H	-3.326942	3.516563	-0.507918
95	H	-1.836534	2.696109	-0.968737
96	H	6.433002	-4.572316	-0.353058
97	H	4.907502	-4.548169	-1.270382
98	H	4.882490	-4.718147	0.509403
99	H	8.330021	4.462763	-0.364813
100	H	8.288715	4.295039	1.414768
101	H	6.771378	4.321395	0.484889
102	H	2.765674	-4.333758	-0.368226
103	H	0.193380	-4.017435	-0.398411
104	H	10.439565	4.073781	0.550009
105	H	13.012371	3.759851	0.509026
106	H	13.741816	-1.030975	0.124548
107	H	20.815331	0.376037	-0.071341
108	H	21.470441	-2.139824	-0.177692
109	H	16.476660	-3.684448	-0.591764
110	H	14.906856	-2.890098	-0.487589
111	H	15.766939	-3.341852	0.988039
112	H	19.645438	2.244037	0.494243

113	H	18.078485	3.029118	0.680946
114	H	18.724324	2.727984	-0.934214

Total energy: -6081.39464962 Hartrees

Table S2. Coordinates and energy of two repeated units of **P2**

		X	Y	Z
1	C	-19.857139	1.447628	-0.083326
2	C	-18.440721	1.172830	-0.075940
3	N	-17.989533	-0.065354	-0.150512
4	C	-16.620211	0.007505	-0.122262
5	C	-16.195467	1.440466	-0.019062
6	N	-17.434092	2.124048	0.005041
7	C	-15.772993	-1.076508	-0.180247
8	O	-15.108626	1.982046	0.036652
9	C	-16.202072	-2.510015	-0.279326
10	N	-14.966238	-3.196968	-0.304709
11	C	-13.956199	-2.248211	-0.229714
12	N	-14.404981	-1.006905	-0.155988
13	O	-17.290640	-3.047490	-0.330599
14	C	-12.544523	-2.523102	-0.229505
15	C	-17.497833	3.568719	0.100299
16	C	-14.906807	-4.642074	-0.397937
17	C	-20.573238	2.630210	-0.015591
18	C	-21.977351	2.432950	-0.055785
19	C	-22.318085	1.107278	-0.153601
20	S	-20.938961	0.071213	-0.198590
21	C	-11.828734	-3.708604	-0.294848
22	C	-10.433107	-3.518475	-0.268933
23	C	-10.058816	-2.185870	-0.184147
24	S	-11.463560	-1.145152	-0.127690
25	C	-8.721856	-1.642285	-0.143439
26	S	-7.324081	-2.727798	-0.079693
27	C	-6.215700	-1.358870	-0.091596
28	C	-6.927789	-0.122422	-0.117756
29	C	-8.343481	-0.325027	-0.161228
30	C	-4.827843	1.020449	-0.087981
31	C	-4.115780	-0.216152	-0.067071
32	C	-2.699425	-0.014328	-0.063687
33	C	-2.320911	1.302981	-0.055708
34	S	-3.719529	2.389444	-0.061484
35	C	-4.820683	-1.446927	-0.056837
36	C	-6.223199	1.108654	-0.104639
37	C	-6.906160	2.413226	-0.107848
38	C	-4.138408	-2.751058	-0.011635

39	C	1.504376	2.176426	-0.036922
40	C	2.914728	1.897427	-0.000886
41	N	3.357671	0.654959	0.087753
42	C	4.725816	0.719587	0.094755
43	C	5.162568	2.149954	0.000368
44	N	3.930152	2.841790	-0.055142
45	C	5.566300	-0.369891	0.175687
46	O	6.254253	2.683928	-0.028574
47	C	5.128760	-1.800086	0.275807
48	N	6.360641	-2.492532	0.328723
49	C	7.376786	-1.549395	0.264570
50	N	6.934083	-0.306418	0.176105
51	O	4.036728	-2.332917	0.310907
52	C	8.786539	-1.830786	0.283387
53	C	3.878133	4.286300	-0.157603
54	C	6.412026	-3.937242	0.428685
55	C	0.793111	3.363736	-0.117926
56	C	-0.603257	3.176583	-0.129693
57	C	-0.982653	1.844707	-0.058752
58	S	0.418118	0.800622	0.031436
59	C	9.496644	-3.017992	0.375882
60	C	10.893438	-2.834500	0.356785
61	C	11.274444	-1.505519	0.249892
62	S	9.875143	-0.459845	0.163772
63	C	12.614224	-0.967912	0.204193
64	S	14.006812	-2.059897	0.120527
65	C	15.121734	-0.695618	0.128232
66	C	14.416273	0.543718	0.168398
67	C	12.998482	0.346388	0.226486
68	C	16.524083	1.674645	0.120316
69	C	17.228173	0.435259	0.084460
70	C	18.655134	0.634079	0.056545
71	C	19.009134	1.943639	0.048349
72	S	17.645458	3.035609	0.085189
73	C	16.516413	-0.788882	0.077676
74	C	15.126601	1.769546	0.154053
75	C	14.451570	3.077743	0.171378
76	C	17.188444	-2.099138	0.016922
77	C	-6.720474	3.467693	-0.968773
78	C	-7.526543	4.603185	-0.664375
79	C	-8.330071	4.433232	0.431688
80	S	-8.094803	2.843138	1.115822
81	C	-4.291763	-3.820615	-0.860240
82	C	-3.497403	-4.949941	-0.506219

83	C	-2.735267	-4.760201	0.615841
84	S	-2.996027	-3.158472	1.262723
85	C	14.667660	4.134335	1.022680
86	C	13.862141	5.274546	0.735598
87	C	13.028828	5.106913	-0.338347
88	S	13.234139	3.512693	-1.022276
89	C	17.050961	-3.165636	0.871080
90	C	17.818557	-4.306094	0.492205
91	C	18.544202	-4.127766	-0.655176
92	S	18.282899	-2.522160	-1.294376
93	C	-9.305128	5.400194	1.033036
94	C	-1.783094	-5.715543	1.270065
95	C	12.045656	6.079214	-0.917439
96	C	19.455185	-5.099852	-1.342862
97	H	-16.463474	3.916173	0.138017
98	H	-18.015191	3.887634	1.010235
99	H	-17.990304	4.006011	-0.773430
100	H	-14.413672	-5.079411	0.475439
101	H	-14.392718	-4.963789	-1.308779
102	H	-15.942159	-4.986834	-0.432623
103	H	-20.118088	3.607569	0.060493
104	H	-22.700329	3.238980	-0.014040
105	H	-23.311535	0.682176	-0.201647
106	H	-12.285661	-4.685709	-0.362323
107	H	-9.718839	-4.332173	-0.318551
108	H	-9.054875	0.489278	-0.216435
109	H	-1.987152	-0.829586	-0.077728
110	H	4.915357	4.626841	-0.173379
111	H	3.369417	4.730767	0.703231
112	H	3.383354	4.604803	-1.080227
113	H	6.904055	-4.257712	1.352142
114	H	6.923410	-4.379819	-0.431460
115	H	5.374721	-4.277647	0.441282
116	H	1.253787	4.340090	-0.169299
117	H	-1.314116	3.992265	-0.194234
118	H	9.034856	-3.991631	0.459316
119	H	11.603909	-3.649916	0.427899
120	H	12.291121	1.163068	0.296286
121	H	19.370515	-0.177662	0.047028
122	H	20.010523	2.352524	0.033129
123	H	-6.041126	3.420195	-1.811950
124	H	-7.518548	5.518155	-1.246934
125	H	-4.939005	-3.788513	-1.729022
126	H	-3.483362	-5.874917	-1.072615

127	H	15.369464	4.085511	1.847083
128	H	13.892892	6.191663	1.314029
129	H	16.430237	-3.125409	1.758694
130	H	17.837526	-5.231488	1.057955
131	H	-10.326778	5.004561	1.027673
132	H	-9.301831	6.330917	0.459334
133	H	-9.052482	5.644047	2.070990
134	H	-0.762481	-5.318200	1.297651
135	H	-1.763092	-6.655515	0.712000
136	H	-2.075383	-5.942893	2.301343
137	H	12.271192	6.315545	-1.963361
138	H	12.073195	7.012850	-0.349117
139	H	11.021104	5.692691	-0.881450
140	H	20.479800	-4.718561	-1.417283
141	H	19.116612	-5.329637	-2.359398
142	H	19.486146	-6.036989	-0.780458

Total energy: -8288.65078147 Hartrees

Table S3. Coordinates and energy of two repeated units of **P3**

		X	Y	Z
1	C	-16.014003	-1.458547	-0.006163
2	C	-14.586450	-1.250157	-0.008547
3	N	-14.078867	-0.031390	0.010882
4	C	-12.714680	-0.168552	0.002759
5	C	-12.355992	-1.623127	-0.024780
6	N	-13.624589	-2.249408	-0.030447
7	C	-11.817203	0.875787	0.017981
8	O	-11.294748	-2.215504	-0.040111
9	C	-12.176244	2.331296	0.045035
10	N	-10.908191	2.958010	0.051454
11	C	-9.945710	1.958847	0.030825
12	N	-10.453991	0.738729	0.010854
13	O	-13.237468	2.922923	0.059420
14	C	-8.522485	2.161970	0.031382
15	C	-13.754122	-3.692741	-0.055879
16	C	-10.777840	4.401114	0.077837
17	C	-16.783839	-2.608876	-0.022199
18	C	-18.177487	-2.345149	-0.012008
19	C	-18.456737	-1.001777	0.011693
20	S	-17.031451	-0.029557	0.022138
21	C	-7.744553	3.309233	0.046111
22	C	-6.361030	3.045577	0.040060
23	C	-6.056429	1.691975	0.020783
24	S	-7.515228	0.725049	0.011539

25	C	-4.754228	1.074550	0.009835
26	S	-3.291033	2.077706	0.073643
27	C	-2.279325	0.659452	0.023114
28	C	-3.054155	-0.500852	-0.036830
29	C	-4.447510	-0.273606	-0.045060
30	C	3.189350	-2.002771	-0.027147
31	C	4.612398	-1.799365	-0.026925
32	N	5.120646	-0.578787	-0.032225
33	C	6.483417	-0.715592	-0.028596
34	C	6.843361	-2.170055	-0.020007
35	N	5.575685	-2.797833	-0.020201
36	C	7.381001	0.330478	-0.032145
37	O	7.905247	-2.761565	-0.014032
38	C	7.020650	1.785539	-0.042797
39	N	8.287921	2.413375	-0.041550
40	C	9.251671	1.415239	-0.031239
41	N	8.743142	0.194195	-0.025897
42	O	5.958538	2.376504	-0.051122
43	C	10.674040	1.619625	-0.026689
44	C	5.446325	-4.241145	-0.012367
45	C	8.417329	3.856664	-0.052514
46	C	2.411638	-3.150371	-0.023151
47	C	1.028004	-2.886942	-0.021724
48	C	0.723014	-1.533388	-0.024706
49	S	2.181680	-0.565982	-0.033316
50	C	11.451299	2.767249	-0.021492
51	C	12.835514	2.504224	-0.010509
52	C	13.140626	1.151295	-0.007983
53	S	11.683723	0.183435	-0.028266
54	C	14.444638	0.532617	0.009156
55	S	15.904564	1.524425	-0.184018
56	C	16.919905	0.115099	-0.045251
57	C	16.151223	-1.033762	0.130787
58	C	14.754230	-0.804061	0.163375
59	C	-0.885937	0.432250	0.033239
60	C	-0.579211	-0.915966	-0.019993
61	S	-2.042282	-1.919145	-0.086330
62	C	18.323235	-0.119775	-0.072409
63	C	18.602056	-1.449879	0.084530
64	S	17.172755	-2.442220	0.268355
65	H	-12.736752	-4.088749	-0.068037
66	H	-14.280064	-4.031445	-0.953549
67	H	-14.271258	-4.063774	0.834090
68	H	-10.251536	4.739136	0.975686

69	H	-11.794962	4.797772	0.090698
70	H	-10.261204	4.772841	-0.812284
71	H	-16.373971	-3.608790	-0.040474
72	H	-18.936909	-3.117978	-0.021789
73	H	-19.429694	-0.529358	0.023671
74	H	-8.149885	4.311092	0.059287
75	H	-5.606775	3.824108	0.046665
76	H	-5.200997	-1.050655	-0.090928
77	H	6.463760	-4.637208	-0.007872
78	H	4.927074	-4.601501	-0.905656
79	H	4.923039	-4.591468	0.882567
80	H	8.947683	4.203922	-0.944407
81	H	8.930003	4.219564	0.843556
82	H	7.400071	4.252953	-0.065668
83	H	2.817296	-4.152179	-0.019197
84	H	0.273947	-3.665678	-0.013713
85	H	11.045496	3.769067	-0.019094
86	H	13.589778	3.282498	0.007531
87	H	14.004175	-1.573265	0.303455
88	H	-0.132496	1.209178	0.081469
89	H	19.081946	0.642299	-0.199577
90	H	19.575206	-1.920578	0.103954

Total energy: -5616.79702968 Hartrees

Table S4. Coordinates and energy of two repeated units of **P4**

		X	Y	Z
1	C	-17.930956	-1.354402	0.051440
2	C	-16.495277	-1.211953	0.031789
3	N	-15.930764	-0.019121	0.072070
4	C	-14.574636	-0.219619	0.037846
5	C	-14.285177	-1.688041	-0.030450
6	N	-15.581712	-2.254119	-0.029666
7	C	-13.628529	0.780698	0.062354
8	O	-13.253395	-2.328907	-0.077965
9	C	-13.917246	2.250552	0.130397
10	N	-12.620896	2.816152	0.127960
11	C	-11.707378	1.773419	0.066139
12	N	-12.273839	0.579578	0.027179
13	O	-14.948647	2.891140	0.178991
14	C	-10.276392	1.909141	0.044611
15	C	-15.779232	-3.688590	-0.089296
16	C	-12.421100	4.250119	0.188684
17	C	-18.753324	-2.467502	0.022866
18	C	-20.133032	-2.140315	0.058783

19	C	-20.349651	-0.786389	0.114178
20	S	-18.880796	0.118857	0.124236
21	C	-9.444367	3.017956	0.064196
22	C	-8.075405	2.689266	0.025782
23	C	-7.836098	1.323280	-0.023339
24	S	-9.339089	0.426788	-0.019241
25	C	-6.567711	0.641368	-0.073356
26	S	-5.054702	1.531996	0.011719
27	C	-4.107491	0.059302	-0.122057
28	C	-4.943875	-1.039301	-0.212699
29	C	-6.316430	-0.714215	-0.185316
30	C	3.499439	-1.759194	-0.048298
31	C	4.930946	-1.628255	-0.038310
32	N	5.501618	-0.435694	-0.056301
33	C	6.855493	-0.642327	-0.041218
34	C	7.140115	-2.112936	-0.010091
35	N	5.841920	-2.674647	-0.010433
36	C	7.805799	0.356218	-0.054382
37	O	8.170082	-2.758296	0.011728
38	C	7.520499	1.827484	-0.086086
39	N	8.818139	2.389423	-0.090496
40	C	9.729893	1.343478	-0.063781
41	N	9.159015	0.150311	-0.042100
42	O	6.490091	2.472099	-0.104559
43	C	11.160478	1.475380	-0.058897
44	C	5.638553	-4.108932	0.018825
45	C	9.021186	3.823828	-0.115846
46	C	2.664688	-2.866182	-0.043394
47	C	1.296267	-2.533447	-0.062160
48	C	1.059836	-1.166366	-0.081227
49	S	2.565329	-0.273604	-0.073301
50	C	11.995018	2.582292	-0.088636
51	C	13.363629	2.250409	-0.076227
52	C	13.601042	0.883804	-0.036001
53	S	12.096523	-0.009111	-0.008393
54	C	14.869630	0.199395	-0.015804
55	S	16.380315	1.092205	0.094208
56	C	17.329587	-0.381978	0.035768
57	C	16.498624	-1.482741	-0.043168
58	C	15.123801	-1.157941	-0.071244
59	C	-2.667569	0.104007	-0.125343
60	C	-1.830637	1.203846	-0.191266
61	C	-0.458148	0.877000	-0.180033
62	C	-0.207630	-0.481349	-0.105600

63	S	-1.721030	-1.372543	-0.036241
64	C	18.774455	-0.332465	0.077421
65	C	19.613285	0.741303	-0.139711
66	C	20.993007	0.418145	-0.018631
67	C	21.205988	-0.897890	0.288554
68	S	19.715286	-1.768926	0.448701
69	H	-14.781972	-4.131134	-0.130184
70	H	-16.335956	-3.978710	-0.985408
71	H	-16.297773	-4.058519	0.800340
72	H	-11.859285	4.538125	1.082405
73	H	-13.417417	4.694229	0.235383
74	H	-11.906981	4.621062	-0.703274
75	H	-18.390311	-3.484555	-0.021770
76	H	-20.927426	-2.877081	0.044154
77	H	-21.299455	-0.270119	0.150113
78	H	-9.801390	4.037511	0.101354
79	H	-7.284500	3.430588	0.028382
80	H	-4.573330	-2.053249	-0.310956
81	H	-7.105913	-1.453801	-0.256001
82	H	6.634098	-4.556626	0.042798
83	H	5.112439	-4.457385	-0.875237
84	H	5.086894	-4.416760	0.912311
85	H	9.561467	4.167043	0.771643
86	H	8.025567	4.271917	-0.122672
87	H	9.559006	4.136336	-1.016189
88	H	3.019414	-3.887101	-0.029921
89	H	0.503591	-3.272901	-0.066613
90	H	11.640016	3.602673	-0.123113
91	H	14.156351	2.989223	-0.104008
92	H	16.873969	-2.498002	-0.101004
93	H	14.337178	-1.900254	-0.146491
94	H	-2.200656	2.220421	-0.260283
95	H	0.331701	1.617521	-0.234828
96	H	19.248094	1.728865	-0.398147
97	H	21.793865	1.134042	-0.161961
98	H	22.146080	-1.411584	0.432506

Total energy: -5771.63388466 Hartrees

[S1]. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, 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.; 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. and Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

5. Transfer and output characteristics of FETs with thin-films of P3 and P4

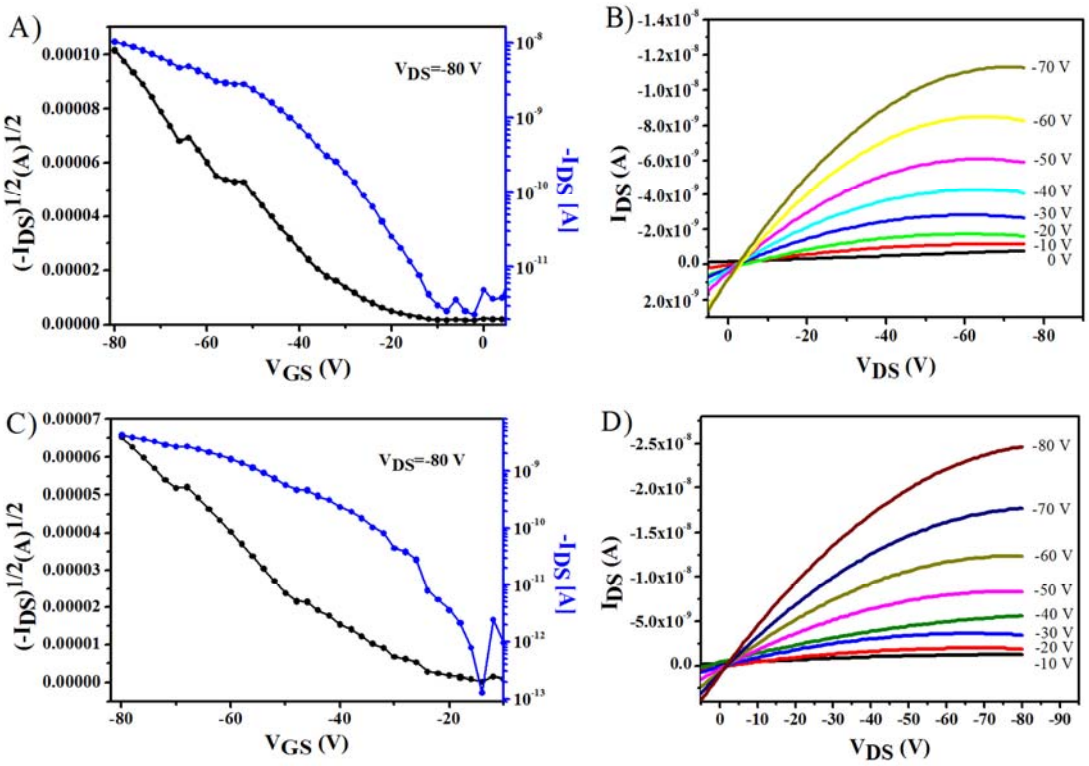
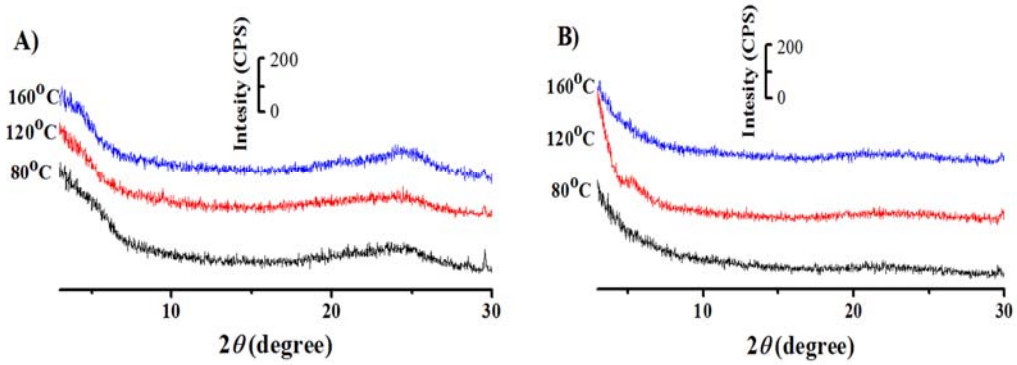


Figure S5. The transfer and output characteristics for FETs with thin-films of **P3** (up) and **P4** (bottom) after annealing at 80 °C; the channel width (W) and length (L) were 1440 nm and 50 nm, respectively.

6. XRD and AFM studies of thin films



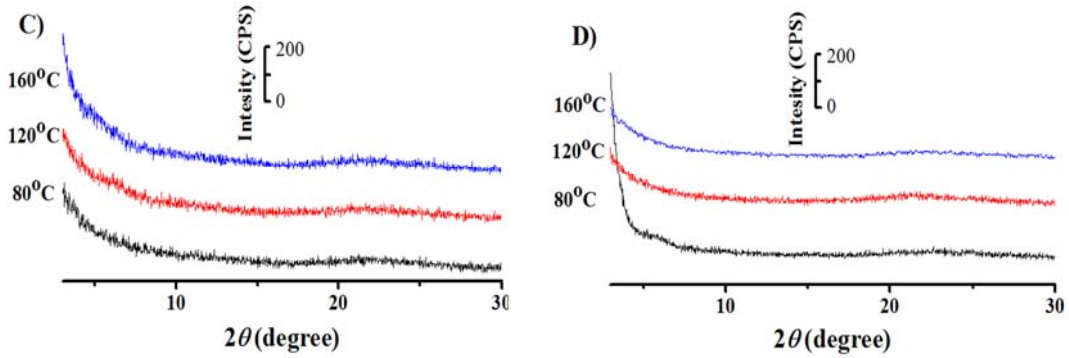


Figure S6. XRD patterns of thin films of **P1**(A), **P2**(B), **P3**(C) and **P4**(D) after annealing at different temperatures.

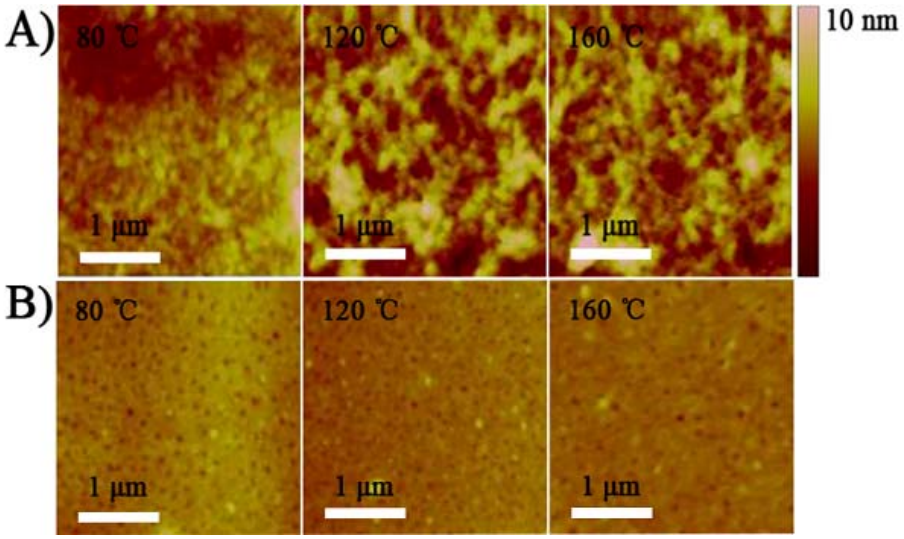
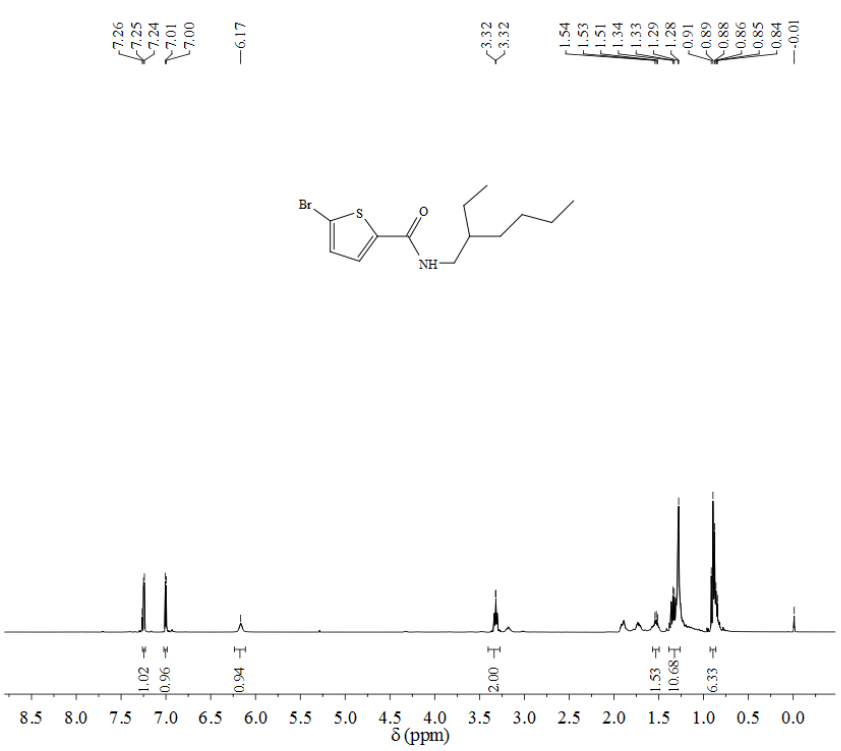
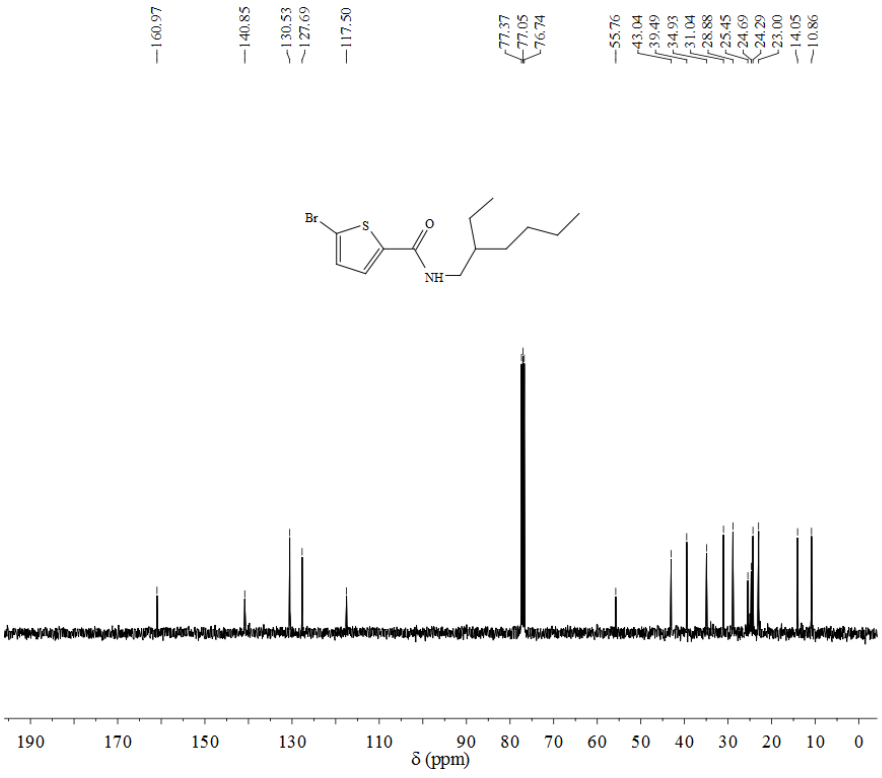


Figure S7. AFM images of thin films of **P3 (A)** and **P4 (B)** after annealing at different temperatures.

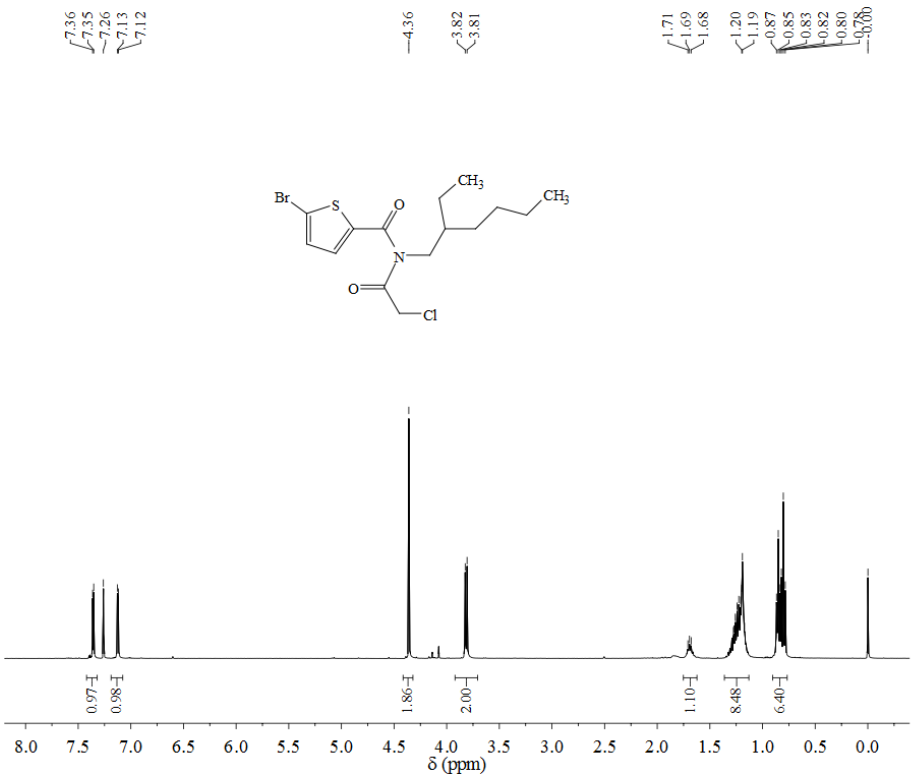
7. ^{1}HNMR and ^{13}CNMR spectra



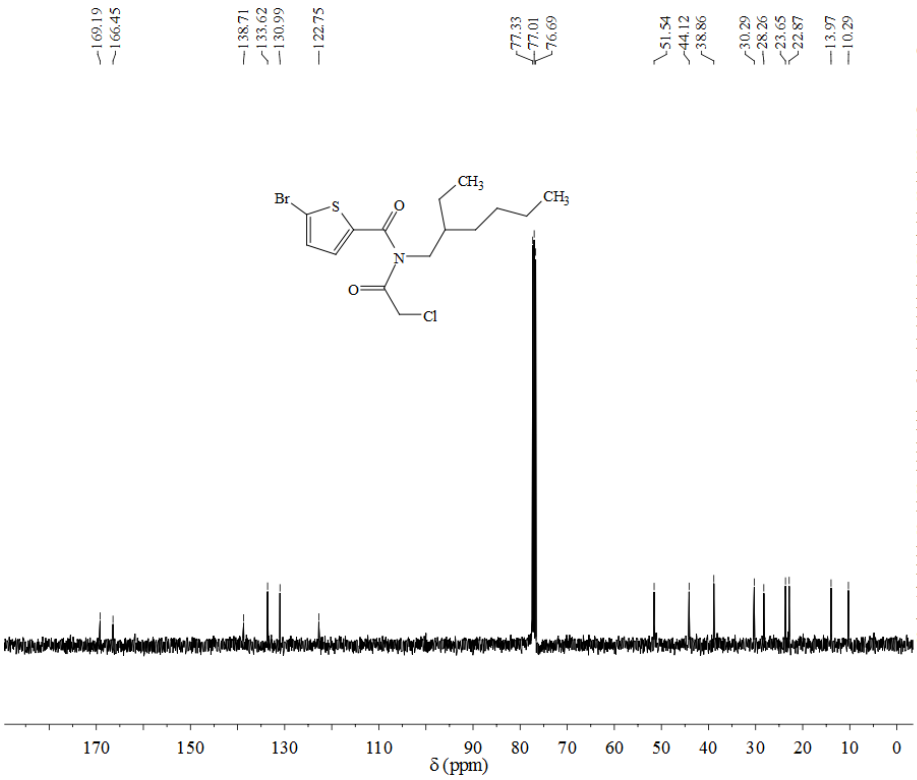
Parameter	Value
Origin	Bruker BioSpin GmbH
Owner	nmrsu
Spectrometer	AV400
Solvent	CDCl3
Pulse Sequence	zg30
Experiment	1D
Number of Scans	4
Receiver Gain	90
Relaxation Delay	1.0000
Pulse Width	12.1000
Acquisition Time	2.7329
Acquisition Date	2012-05-31T08:02:00
Modification Date	2012-05-31T08:03:06
Spectrometer Frequency	400.13
Spectral Width	11990.4
Lowest Frequency	-3531.9
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



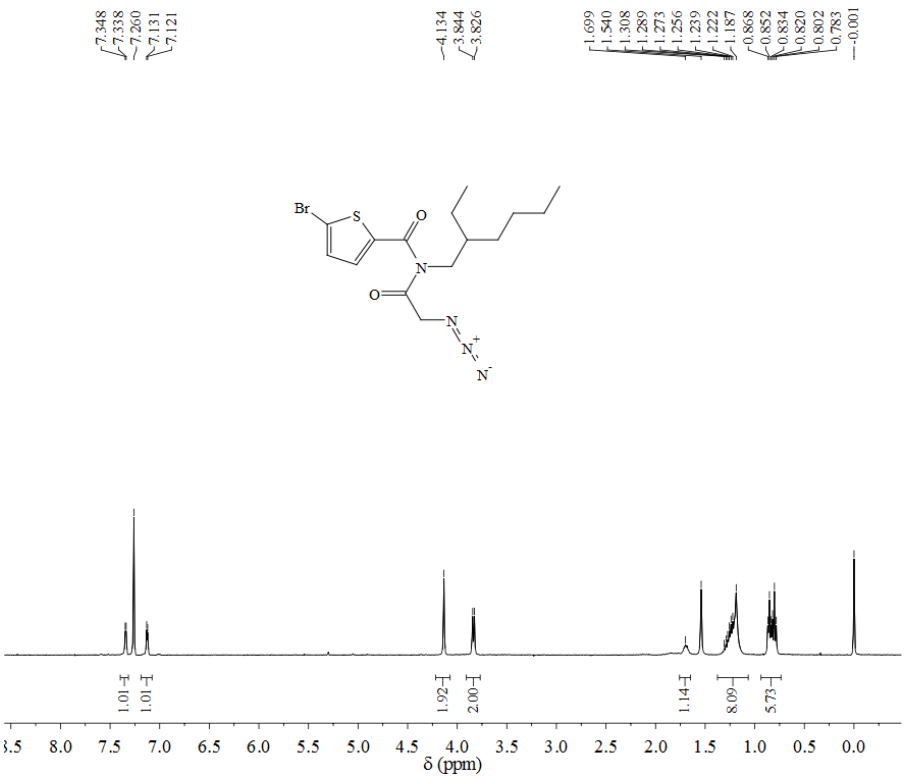
Parameter	Value
Origin	Bruker BioSpin GmbH
Owner	nmrsu
Spectrometer	AV400
Solvent	CDCl3
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	48
Receiver Gain	14596
Relaxation Delay	2.0000
Pulse Width	12.2000
Acquisition Time	1.3665
Acquisition Date	2012-05-31T08:06:00
Modification Date	2012-05-31T08:07:44
Spectrometer Frequency	100.61
Spectral Width	23980.8
Lowest Frequency	-1929.6
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



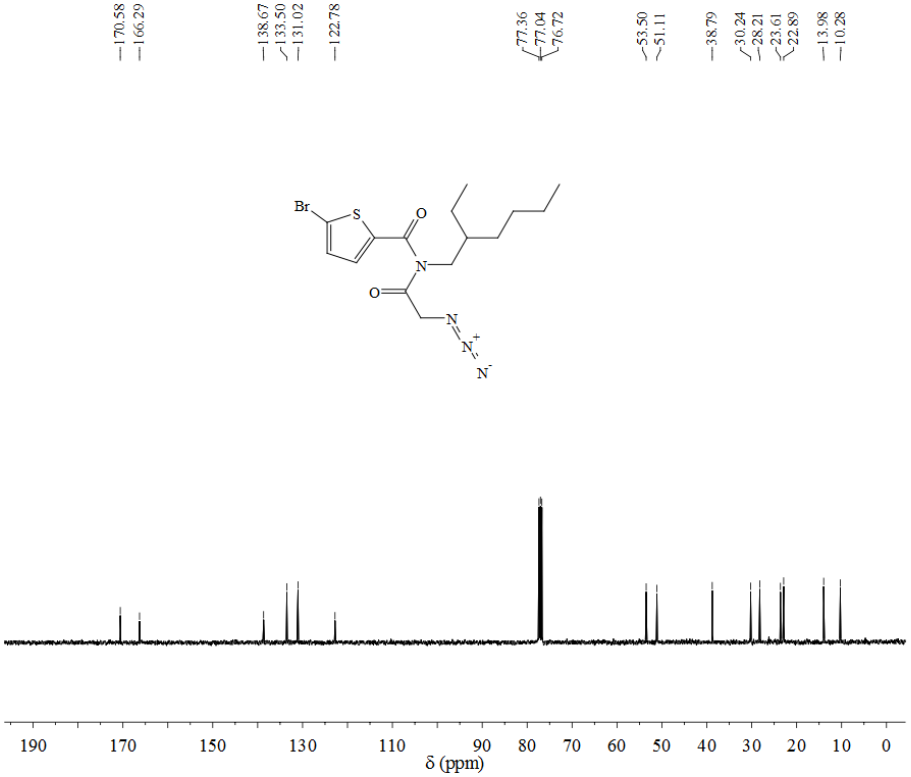
Parameter	Value
Origin	Bruker BioSpin GmbH
Owner	nmrsu
Spectrometer	AV400
Solvent	CDCl3
Pulse Sequence	zg30
Experiment	1D
Number of Scans	8
Receiver Gain	575
Relaxation Delay	1.0000
Pulse Width	12.1000
Acquisition Time	2.7329
Acquisition Date	2012-05-29T07:51:00
Modification Date	2012-05-29T07:51:28
Spectrometer Frequency	400.13
Spectral Width	11990.4
Lowest Frequency	-3533.2
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



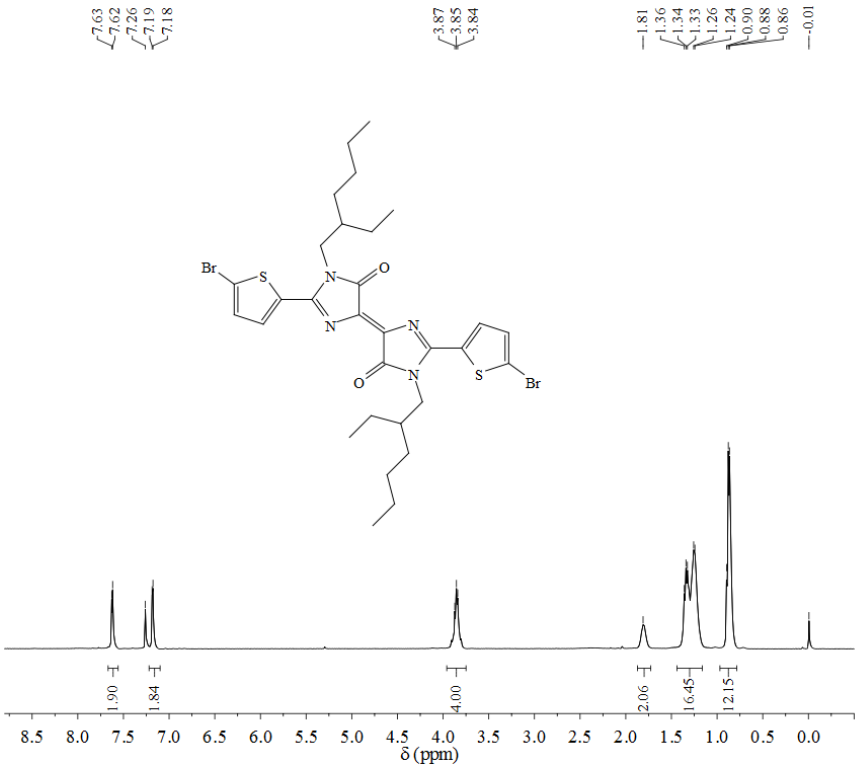
Parameter	Value
Origin	Bruker BioSpin GmbH
Owner	nmrsu
Spectrometer	AV400
Solvent	CDCl3
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	107
Receiver Gain	14596
Relaxation Delay	2.0000
Pulse Width	12.2000
Acquisition Time	1.3665
Acquisition Date	2012-05-29T07:53:00
Modification Date	2012-05-29T07:58:12
Spectrometer Frequency	100.61
Spectral Width	23980.8
Lowest Frequency	-1929.6
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



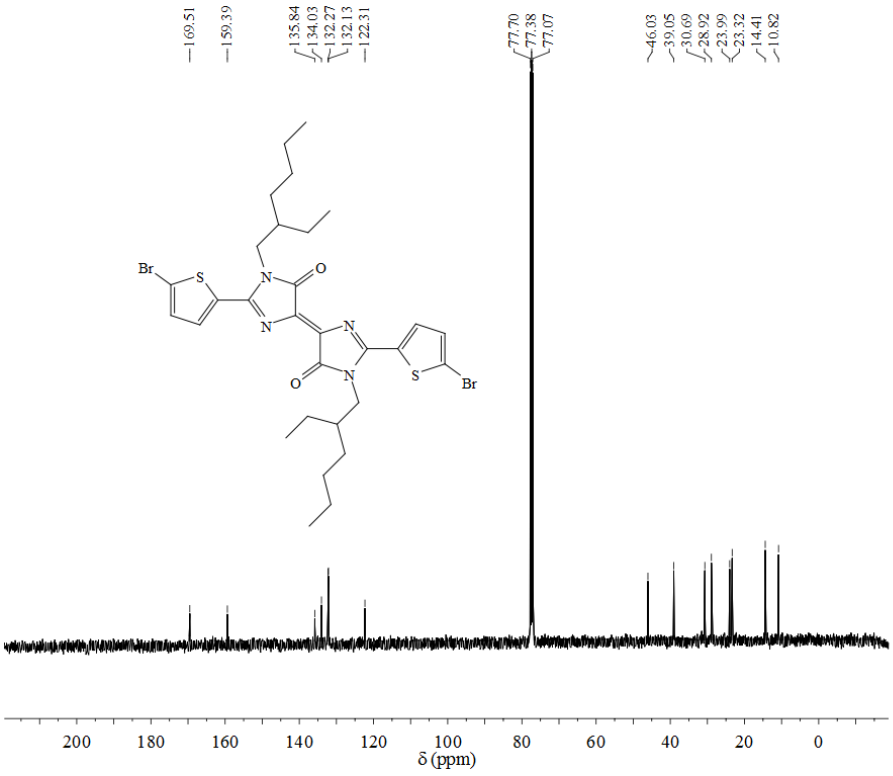
Parameter	Value
Origin	Bruker BioSpin GmbH
Owner	nmrsu
Spectrometer	AV400
Solvent	CDCl3
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	575
Relaxation Delay	1.0000
Pulse Width	12.1000
Acquisition Time	2.7329
Acquisition Date	2012-05-25T08:09:00
Modification Date	2012-05-25T08:09:28
Spectrometer Frequency	400.13
Spectral Width	11990.4
Lowest Frequency	-3533.3
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



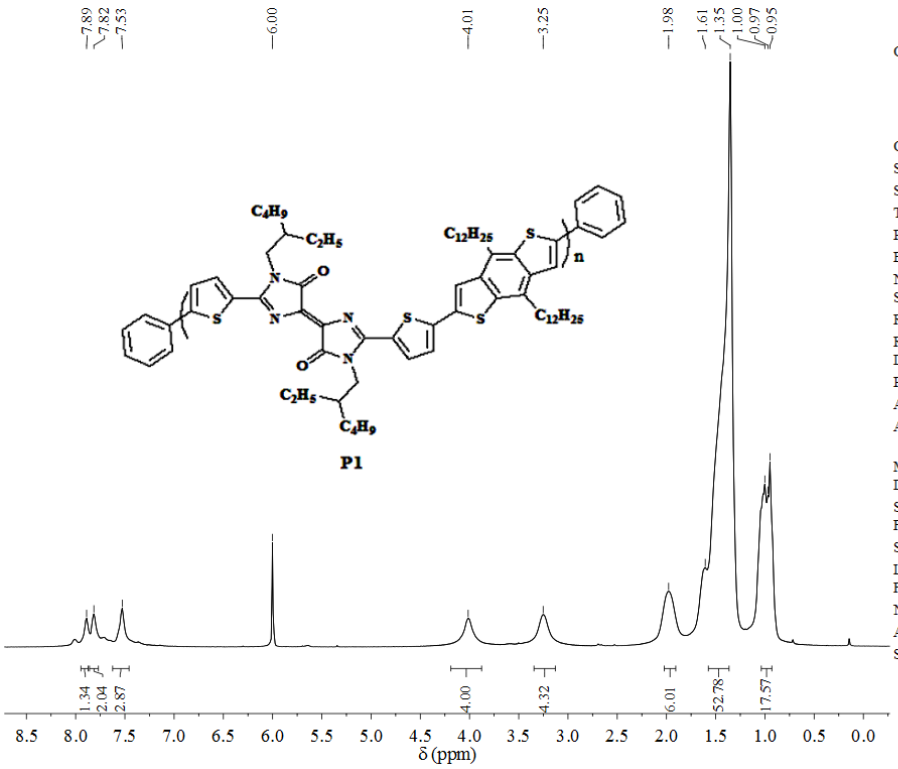
Parameter	Value
Origin	Bruker BioSpin GmbH
Owner	nmrsu
Spectrometer	AV400
Solvent	CDCl3
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	147
Receiver Gain	14596
Relaxation Delay	2.0000
Pulse Width	12.2000
Acquisition Time	1.3665
Acquisition Date	2012-05-25T21:06:00
Modification Date	2012-05-25T21:07:12
Spectrometer Frequency	100.61
Spectral Width	23980.8
Lowest Frequency	-1929.6
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



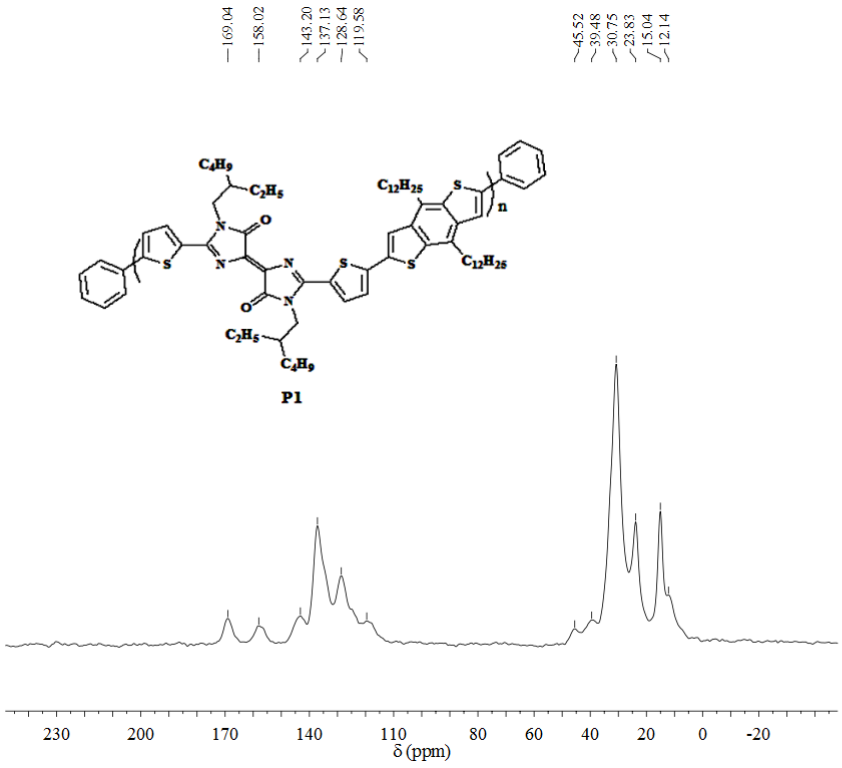
Parameter	Value
Origin	Bruker BioSpin GmbH
Owner	nmrsu
Spectrometer	AV400
Solvent	CDCl3
Pulse Sequence	zg30
Experiment	1D
Number of Scans	8
Receiver Gain	362
Relaxation Delay	1.0000
Pulse Width	12.1000
Acquisition Time	2.7329
Acquisition Date	2012-11-23T21:45:00
Modification Date	2012-11-23T21:45:22
Spectrometer Frequency	400.13
Spectral Width	11990.4
Lowest Frequency	-3533.7
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



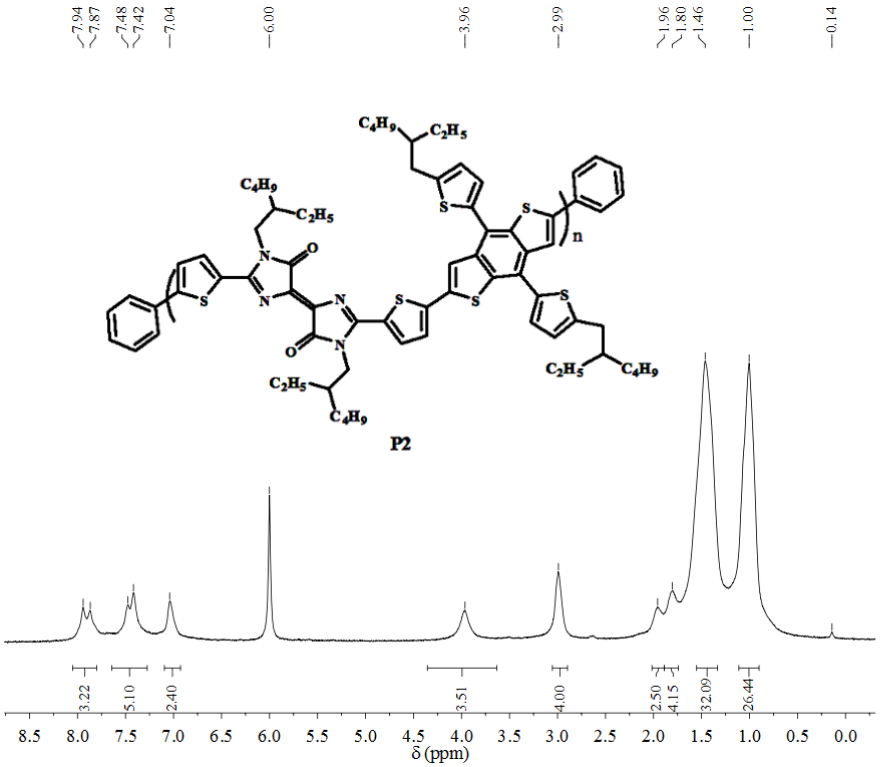
Parameter	Value
Origin	Bruker BioSpin GmbH
Owner	nmrsu
Spectrometer	AV400
Solvent	CDCl3
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	302
Receiver Gain	9195
Relaxation Delay	2.0000
Pulse Width	12.2000
Acquisition Time	1.3665
Acquisition Date	2012-11-23T21:51:00
Modification Date	2012-11-23T22:03:24
Spectrometer Frequency	100.61
Spectral Width	23980.8
Lowest Frequency	-1894.6
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



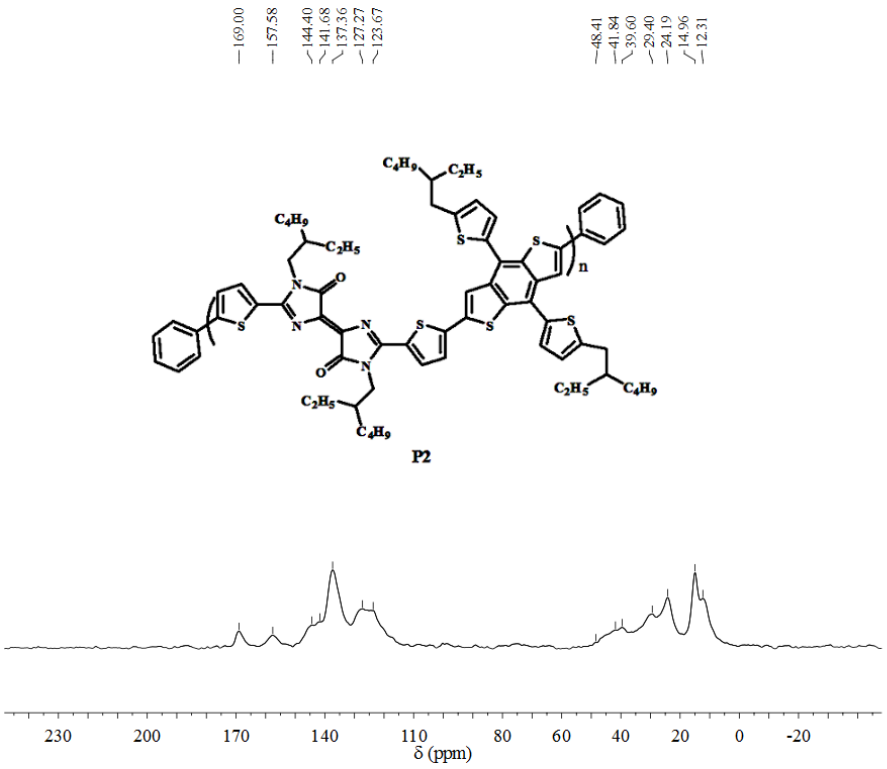
Parameter	Value
Origin	UXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Spectrometer	spect
Solvent	CDCl2CDCl2
Temperature	364.7
Pulse Sequence	zg30
Experiment	1D
Number of Scans	64
Receiver Gain	2048
Relaxation Delay	2.0000
Pulse Width	13.8000
Acquisition Time	3.0409
Acquisition Date	2012-10-30T12:58:00
Modification Date	2012-10-30T13:00:20
Spectrometer Frequency	300.13
Spectral Width	5387.9
Lowest Frequency	-969.8
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



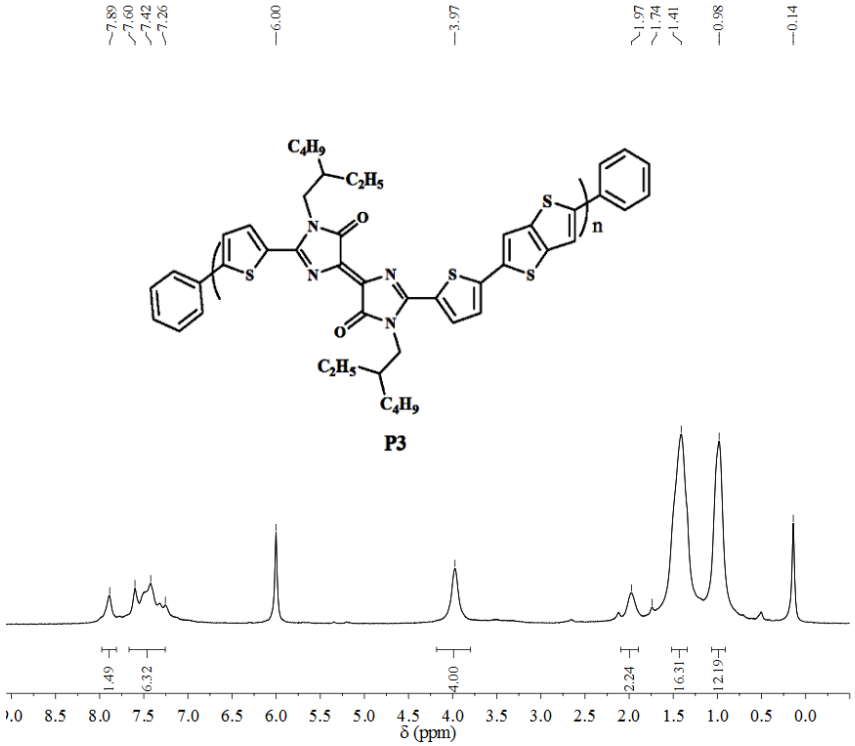
Parameter	Value
Origin	Bruker BioSpin GmbH
Owner	hp
Spectrometer	spect
Solvent	None
Temperature	298.2
Pulse Sequence	cptoss
Experiment	1D
Number of Scans	2000
Receiver Gain	1620
Relaxation Delay	2.0000
Pulse Width	2.5000
Acquisition Time	0.0344
Acquisition Date	2013-02-06T09:33:00
Modification Date	2013-02-07T02:41:22
Spectrometer Frequency	100.37
Spectral Width	29761.9
Lowest Frequency	-4844.1
Nucleus	13C
Acquired Size	1024
Spectral Size	2048



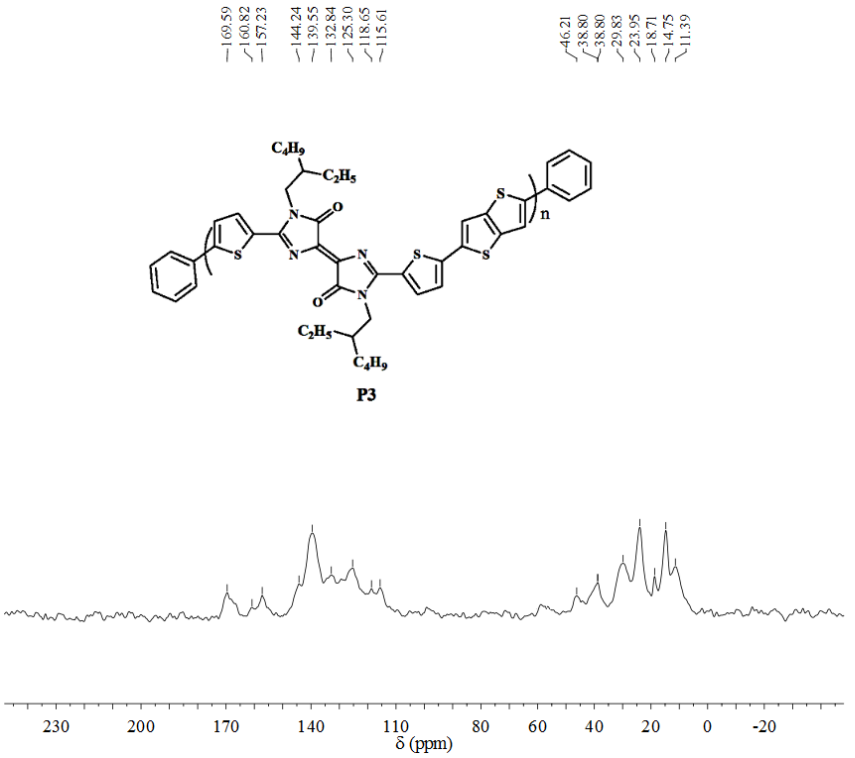
Parameter	Value
Origin	UXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Spectrometer	spect
Solvent	CDCl2CDCl2
Temperature	361.7
Pulse Sequence	zg30
Experiment	1D
Number of Scans	42
Receiver Gain	8192
Relaxation Delay	2.0000
Pulse Width	13.8000
Acquisition Time	3.0409
Acquisition Date	2012-10-30T13:31:00
Modification Date	2012-10-30T13:33:02
Spectrometer Frequency	300.13
Spectral Width	5387.9
Lowest Frequency	-969.5
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



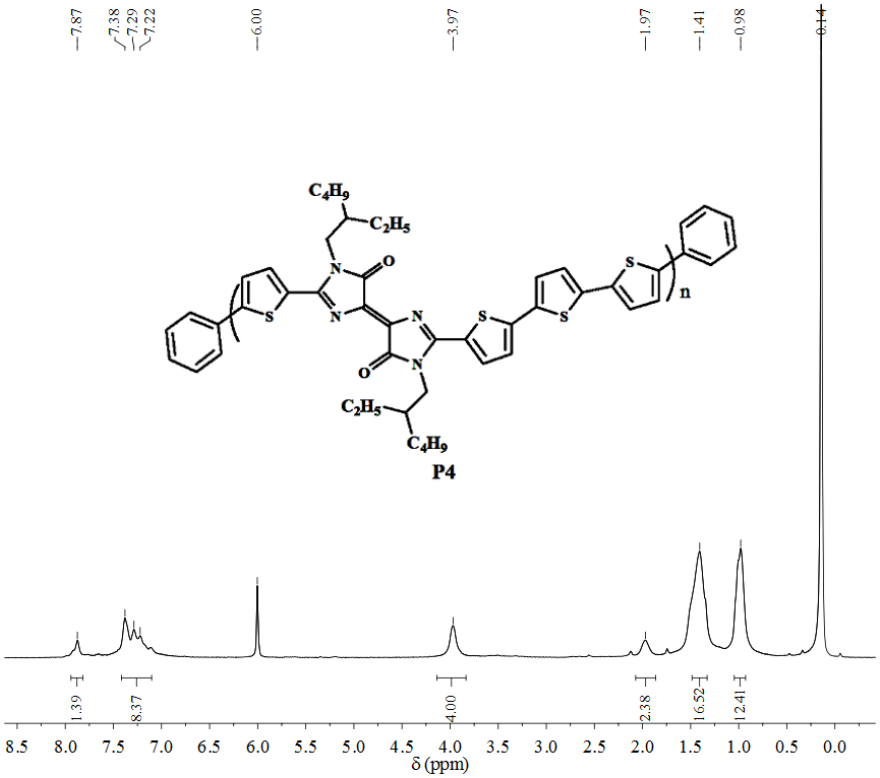
Parameter	Value
Origin	Bruker BioSpin GmbH
Owner	hp
Spectrometer	spect
Solvent	None
Temperature	298.2
Pulse Sequence	cptoss
Experiment	1D
Number of Scans	6357
Receiver Gain	1620
Relaxation Delay	2.0000
Pulse Width	2.5000
Acquisition Time	0.0344
Acquisition Date	2013-02-06T11:06:00
Modification Date	2013-02-07T06:21:04
Spectrometer Frequency	100.37
Spectral Width	29761.9
Lowest Frequency	-4844.1
Nucleus	13C
Acquired Size	1024
Spectral Size	2048



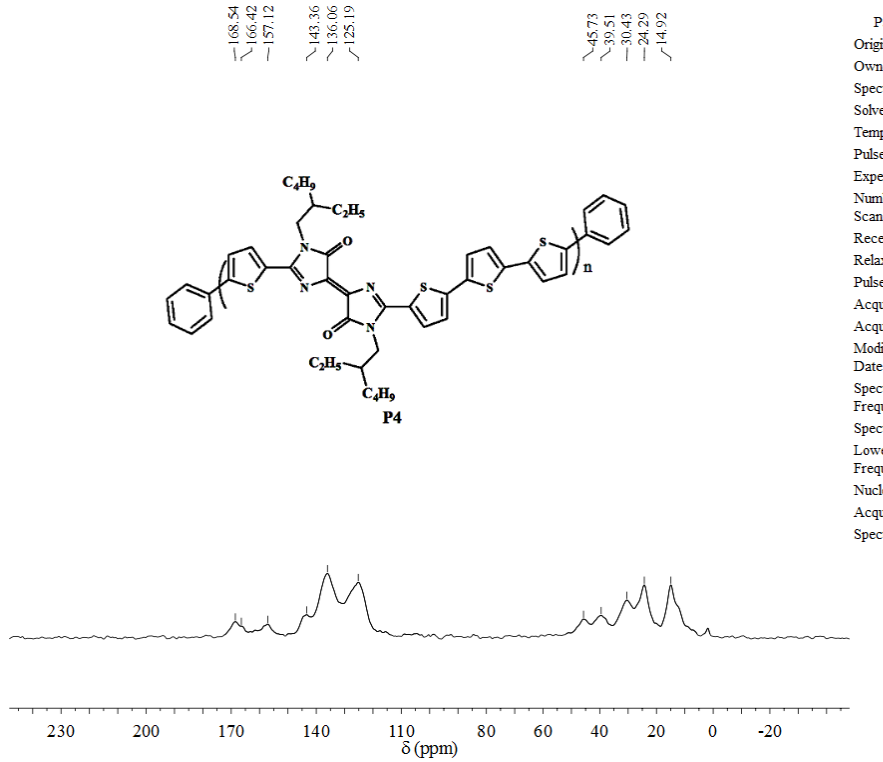
Parameter	Value
Origin	UXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Spectrometer	spect
Solvent	CDCl2CDCl2
Temperature	361.5
Pulse Sequence	zg30
Experiment	1D
Number of Scans	53
Receiver Gain	8192
Relaxation Delay	2.0000
Pulse Width	13.8000
Acquisition Time	3.0409
Acquisition Date	2012-10-30T13:46:00
Modification Date	2012-10-30T13:47:34
Spectrometer Frequency	300.13
Spectral Width	5387.9
Lowest Frequency	-969.5
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



Parameter	Value
Origin	Bruker BioSpin GmbH
Owner	hp
Spectrometer	spect
Solvent	None
Temperature	298.2
Pulse Sequence	cptoss
Experiment	1D
Number of Scans	5347
Receiver Gain	1620
Relaxation Delay	2.0000
Pulse Width	2.5000
Acquisition Time	0.0344
Acquisition Date	2013-02-06T17:25:00
Modification Date	2013-02-07T09:25:10
Spectrometer Frequency	100.37
Spectral Width	29761.9
Lowest Frequency	-4844.1
Nucleus	13C
Acquired Size	1024
Spectral Size	2048



Parameter	Value
Origin	UXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Spectrometer	spect
Solvent	CDCl2CDCl2
Temperature	359.2
Pulse Sequence	zg30
Experiment	1D
Number of Scans	26
Receiver Gain	8192
Relaxation Delay	2.0000
Pulse Width	13.8000
Acquisition Time	3.0409
Acquisition Date	2012-10-30T13:57:00
Modification Date	2012-10-30T13:58:02
Spectrometer Frequency	300.13
Spectral Width	5387.9
Lowest Frequency	-969.5
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



Parameter	Value
Origin	Bruker BioSpin GmbH
Owner	hp
Spectrometer	spect
Solvent	None
Temperature	298.2
Pulse Sequence	cptoss
Experiment	1D
Number of Scans	20480
Receiver Gain	1620
Relaxation Delay	2.0000
Pulse Width	2.5000
Acquisition Time	0.0344
Acquisition Date	2013-02-07T05:08:00
Modification Date	2013-02-07T21:08:54
Spectrometer Frequency	100.37
Spectral Width	29761.9
Lowest Frequency	-4844.1
Nucleus	13C
Acquired Size	1024
Spectral Size	2048