Supporting Information

Conjugated electron donor-acceptor molecules with (*E*)-[4,4'-biimidazolylidene]-5,5'(1*H*,1'*H*)-dione toward new organic semiconductors

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1. TGA analysis

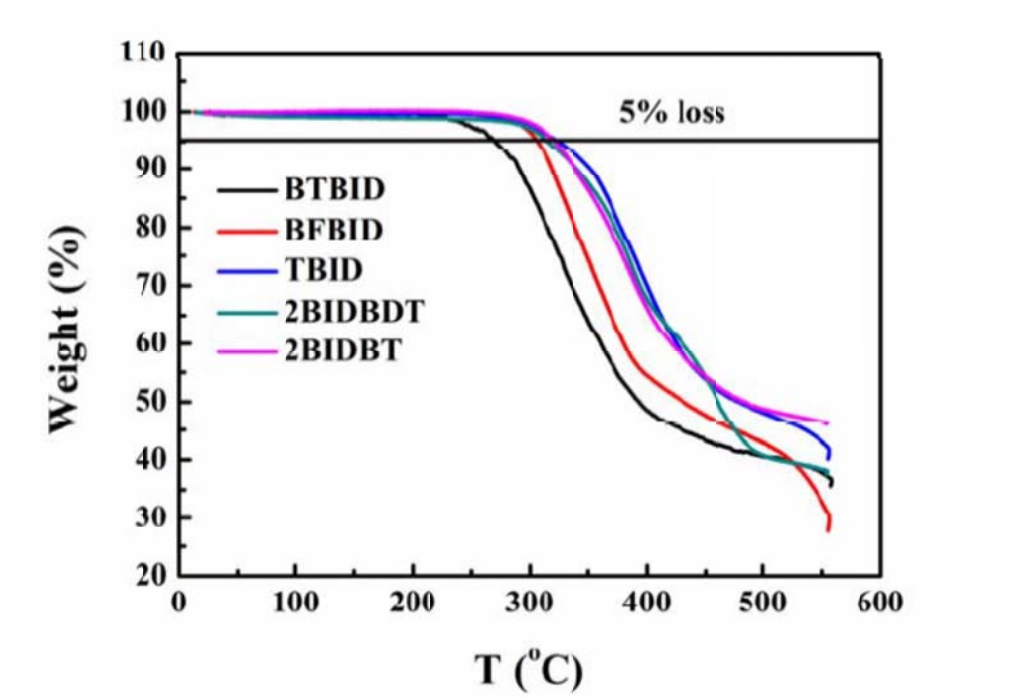
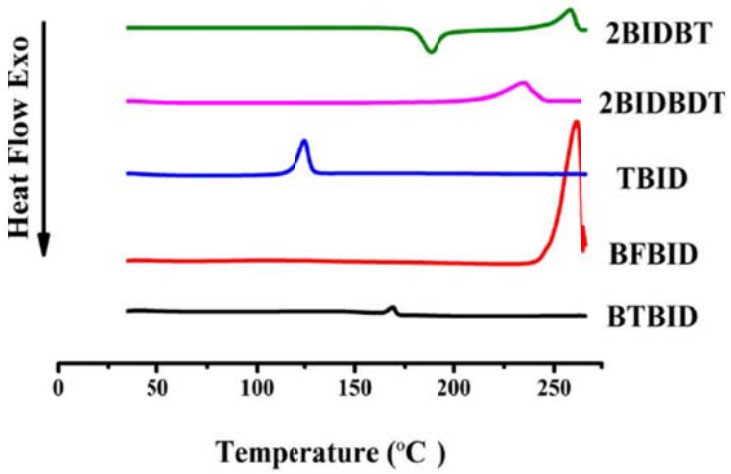


Figure S1 TGA curves of **BTBID**, **BFBID**, **TBID**, **2BIDBDT** and **2BIDBT**.

2. DSC analysis



Figures S2. DSC curves of **BTBID**, **BFBID**, **TBID**, **2BIDBDT** and **2BIDBT**: heating rate: 10 °C /min. from 25 °C to 270 °C under nitrogen atmosphere. All data were collected from the first heating cycle.

3. Density Funtional Theory Calculations

Table S1. Coordinates and energy of compound **BTBID**

		X	Y	Z
1	C	-0.000003861	-0.000003314	0.000000736
2	C	0.000000849	-0.000004160	-0.000000026
3	N	-0.000001904	0.000001999	0.000002003
4	C	0.000001127	-0.000002811	-0.000000668
5	C	0.000003890	0.000002232	-0.000003473
6	N	-0.000000317	0.000002445	0.000001827
7	C	0.000000840	0.000003048	0.000001869
8	O	-0.000000924	-0.000000623	0.000000822
9	C	-0.000003440	-0.000002773	-0.000000825
10	N	0.000002830	0.000000551	-0.000002696
11	C	-0.000000040	0.000001705	-0.000000412
12	N	-0.000000241	-0.000001997	-0.000000936
13	O	0.000001959	0.000001683	-0.000000218
14	C	-0.000000964	0.000002707	0.000008010
15	C	-0.000001385	0.000000777	0.000001574
16	C	0.000000890	-0.000001158	0.000000245
17	C	0.000002533	0.000003208	-0.000003304
18	C	-0.000002488	-0.000002562	0.000002712
19	C	0.000000514	0.000003107	-0.000000690
20	S	0.000001728	0.000000571	-0.000000258
21	C	0.000002240	0.000000570	-0.000006431
22	C	-0.000002662	-0.000003126	0.000000568
23	C	0.000001366	0.000002271	0.000000939
24	S	-0.000001116	-0.000002174	-0.000002947
25	C	-0.000002317	-0.000001382	0.000001376
26	C	-0.000002198	0.000002280	-0.000000400
27	C	0.000002815	0.000001164	-0.000002274
28	C	-0.000001479	-0.000000188	-0.000000011
29	C	0.000001051	0.000000093	0.000000872
30	S	0.000001035	0.000000455	-0.000001213
31	C	0.000001550	-0.000001050	-0.000001232
32	C	-0.000001017	-0.000001498	0.000000984
33	C	-0.000000293	0.000000860	-0.000000608
34	S	-0.000000329	-0.000001571	0.000002169
35	C	-0.000000850	-0.000000774	-0.000000408
36	C	0.000000069	0.000002291	-0.000000567
37	C	0.000001263	-0.000001096	0.000000240
38	C	-0.000002079	-0.000000270	-0.000000776
39	C	0.000001632	0.000001011	0.000000780
40	C	-0.000000285	-0.000002387	0.000000442

41	C	-0.000001237	0.000001175	0.000000214
42	C	0.000001213	0.000000108	0.000000169
43	H	-0.000000101	-0.000000808	0.000000997
44	H	0.000000563	-0.000000552	-0.000000264
45	H	0.000000737	0.000000437	-0.000000053
46	H	0.000000554	0.000000472	-0.000000780
47	H	-0.000000646	0.000000085	-0.000000319
48	H	0.000000124	0.000000284	0.000000166
49	H	-0.000000842	-0.000000911	0.000000881
50	H	0.000000062	-0.000000088	0.000000469
51	H	-0.000000589	-0.000000740	0.000001111
52	H	-0.000000270	0.000000229	-0.000000859
53	H	-0.000000298	-0.000000142	-0.000000126
54	H	0.000000600	0.000000485	0.000000534
55	H	0.000000519	0.000000185	0.000000203
56	H	0.000000234	-0.000000518	-0.000000296
57	H	0.000000004	0.000000417	-0.000000861
58	H	0.000000416	0.000000117	-0.000000621
59	H	-0.000000585	-0.000000117	0.000000148
60	H	-0.000000145	0.000000452	0.000000096
61	H	0.000000045	-0.000000483	0.000000694
62	H	-0.000000352	-0.000000198	0.000000704

Total energy: -3193.71665950 Hartrees

Table S2. Coordinates and energy of compound **BFBID**

		X	Y	Z
1	C	3.751488	-1.796857	0.000359
2	C	2.326759	-1.596971	0.000432
3	N	1.813403	-0.378733	0.000493
4	C	0.451003	-0.520873	0.000532
5	C	0.096908	-1.977002	0.000498
6	N	1.367145	-2.599564	0.000439
7	C	-0.451006	0.520903	0.000591
8	O	-0.962346	-2.572900	0.000522
9	C	-0.096918	1.977031	0.000688
10	N	-1.367163	2.599591	0.000747
11	C	-2.326768	1.596989	0.000649
12	N	-1.813406	0.378755	0.000574
13	O	0.962332	2.572935	0.000706
14	C	-3.751498	1.796868	0.000622
15	C	1.499810	-4.042502	0.000358
16	C	-1.499836	4.042527	0.000641
17	C	4.526013	-2.948489	0.000429
18	C	5.909530	-2.687831	0.000293

19	C	6.205646	-1.333398	0.000095
20	S	4.758639	-0.361127	0.000108
21	C	-4.526025	2.948498	0.000991
22	C	-5.909541	2.687835	0.000812
23	C	-6.205649	1.333399	0.000310
24	S	-4.758639	0.361133	0.000103
25	C	7.508646	-0.725111	-0.000081
26	C	-7.508645	0.725103	-0.000058
27	C	8.775742	-1.247794	0.000579
28	C	9.679130	-0.133319	-0.000054
29	C	8.861544	1.015121	-0.001046
30	O	7.541835	0.655054	-0.001060
31	C	-8.775745	1.247776	-0.000497
32	C	-9.679123	0.133292	-0.000780
33	C	-8.861527	-1.015141	-0.000488
34	O	-7.541821	-0.655062	-0.000042
35	C	11.074651	0.031249	0.000102
36	C	11.587017	1.323932	-0.000745
37	C	10.740150	2.449429	-0.001732
38	C	9.352420	2.313558	-0.001903
39	C	-11.074643	-0.031289	-0.001265
40	C	-11.586996	-1.323979	-0.001432
41	C	-10.740118	-2.449467	-0.001130
42	C	-9.352389	-2.313583	-0.000650
43	H	0.483123	-4.440614	0.000262
44	H	2.021717	-4.396931	0.894471
45	H	2.021833	-4.396810	-0.893733
46	H	-2.021512	4.397002	0.894874
47	H	-2.022093	4.396789	-0.893330
48	H	-0.483150	4.440644	0.000290
49	H	4.118263	-3.949392	0.000550
50	H	6.666996	-3.462603	0.000276
51	H	-4.118276	3.949403	0.001412
52	H	-6.667010	3.462602	0.001080
53	H	9.029135	-2.297866	0.001451
54	H	-9.029147	2.297846	-0.000658
55	H	11.735985	-0.829686	0.000853
56	H	12.662517	1.472444	-0.000646
57	H	11.175837	3.443632	-0.002376
58	H	8.685942	3.168669	-0.002656
59	H	-11.735985	0.829638	-0.001500
60	H	-12.662495	-1.472501	-0.001804
61	H	-11.175795	-3.443676	-0.001276
62	H	-8.685902	-3.168687	-0.000419

Total energy: -2547.76754419 Hartrees

Table S3. Coordinates and energy of compound **TBID**

		X	Y	Z
1	C	0.000000116	0.000003616	-0.000000898
2	C	-0.000001373	-0.000002586	-0.000003141
3	N	0.000000411	0.000000015	0.000000031
4	C	0.000001560	0.000000234	0.000000087
5	C	-0.000004961	0.000002911	0.000000735
6	N	0.000004078	-0.000000838	0.000003789
7	C	0.000000075	0.000000660	0.000002564
8	O	0.000001309	-0.000000277	0.000000417
9	C	0.000006239	-0.000002809	-0.000003949
10	N	-0.000003400	0.000002608	-0.000002665
11	C	0.000000905	0.000000893	0.000007191
12	N	-0.000001327	-0.000001176	-0.000003331
13	O	-0.000002291	-0.000000383	0.000001410
14	C	-0.000000199	-0.000005676	-0.000003911
15	C	0.000000676	-0.000000640	-0.000003795
16	C	0.000000298	0.000000876	0.000001295
17	C	0.000000839	-0.000000329	0.000001332
18	C	-0.000000734	-0.000001533	0.000000889
19	C	0.000001061	0.000001408	0.000001250
20	S	-0.000000173	-0.000001233	-0.000001088
21	C	-0.000004109	0.000001463	0.000002531
22	C	0.000002346	0.000002087	-0.000000752
23	C	-0.000004019	-0.000003897	0.000003413
24	S	0.000001091	0.000002506	-0.000001588
25	C	-0.000001343	-0.000000794	0.000000560
26	C	0.000005040	-0.000000089	0.000000767
27	C	0.000000590	-0.000000190	-0.000000417
28	C	-0.000001236	-0.000001450	0.000001713
29	C	0.000001064	0.000000935	0.000000553
30	S	-0.000001008	0.000000392	-0.000001998
31	C	-0.000002490	-0.000000670	0.000000149
32	C	0.000002310	0.000003178	-0.000001067
33	C	-0.000002301	-0.000001986	0.000002472
34	S	0.000000468	-0.000000030	-0.000002582
35	C	-0.000001594	0.000001289	0.000001151
36	C	0.000002370	-0.000000768	0.000000594
37	C	-0.000001921	0.000001185	-0.000000137
38	C	0.000000589	-0.000000554	-0.000000041
39	C	0.000000060	0.000000542	-0.000000424
40	C	-0.000000245	-0.000000309	-0.000000324
41	C	0.000000097	-0.000000194	0.000000134

42	S	0.000000127	0.000000354	0.000001270
43	C	-0.000000032	-0.000000178	0.000000434
44	C	0.000002226	-0.000000362	0.000000926
45	C	-0.000000486	-0.000000348	-0.000000340
46	C	-0.000000304	0.000000299	0.000001512
47	C	0.000000747	-0.000000201	-0.000001253
48	C	-0.000000633	0.000000803	0.000001660
49	S	0.000000040	-0.000000180	-0.000001435
50	C	-0.000000047	-0.000000342	0.000000472
51	H	0.000000023	0.000000171	0.000000386
52	H	0.000000227	0.000001017	0.000001192
53	H	-0.000001372	-0.000000821	0.000000792
54	H	0.000000554	-0.000000561	-0.000000415
55	H	-0.000000273	-0.000000211	0.000000691
56	H	-0.000000013	0.000000580	-0.000000445
57	H	0.000000449	0.000000490	-0.000000109
58	H	0.000000157	0.000000093	-0.000001261
59	H	-0.000000362	-0.000000151	-0.000001179
60	H	0.000000975	0.000001251	-0.000000832
61	H	0.000000041	0.000000140	0.000000508
62	H	0.000000642	0.000000065	-0.000001492
63	H	-0.000001715	-0.000000197	-0.000000257
64	H	-0.000000093	-0.000000075	-0.000000220
65	H	0.000000102	-0.000000139	-0.000000116
66	H	-0.000000279	0.000000236	0.000000029
67	H	0.000000665	0.000000122	-0.000000477
68	H	0.000000052	-0.000000069	-0.000000125
69	H	0.000000124	-0.000000159	0.000000094
70	H	0.000000303	-0.000000109	-0.000000617
71	H	-0.000000027	-0.000000153	0.000000457
72	H	-0.000000432	0.000000274	-0.000000567
73	H	-0.000000569	-0.000000358	-0.000000952
74	H	0.000000180	-0.000000210	-0.000000816
75	H	-0.000000126	0.000000214	0.000000076
76	H	-0.000000004	-0.000000039	-0.000000189
77	H	0.000000149	0.000000285	-0.000000307
78	H	0.000000117	0.000000082	-0.000000014

Total energy: -4223.50881658 Hartrees

Table S4. Coordinates and energy of compound **2BIDBDT**

		X	Y	Z
1	C	-0.000000911	-0.000000200	0.000001805
2	C	0.000000935	-0.000001897	-0.000001789
3	N	-0.000001295	0.000000471	0.000000240

4	C	0.000001562	0.000000018	0.000000200
5	C	-0.000002221	-0.000000658	-0.000000586
6	N	0.000002373	0.000000989	0.000001083
7	C	-0.000001640	0.000000231	-0.000000434
8	O	0.000000230	0.000000012	-0.000000120
9	C	0.000002869	-0.000000439	0.000000140
10	N	-0.000002206	-0.000001247	-0.000000520
11	C	-0.000000207	0.000002072	0.000000959
12	N	0.000001105	-0.000001138	0.000000595
13	O	-0.000000406	-0.000000313	-0.000000268
14	C	0.000000766	-0.000002039	-0.000000090
15	C	-0.000000938	-0.000000841	-0.000000321
16	C	0.000000535	-0.000000802	0.000000710
17	C	0.000001126	-0.000000400	-0.000000968
18	C	-0.000001355	-0.000000057	-0.000000371
19	C	0.000002068	0.000000497	-0.000000539
20	S	-0.000000670	-0.000000262	-0.000000142
21	C	-0.000002632	0.000000664	-0.000000198
22	C	0.000002453	0.000000764	-0.000000012
23	C	-0.000000371	-0.000002350	-0.000000126
24	S	-0.000000142	0.000001553	-0.000000077
25	C	-0.000001345	-0.000000894	-0.000000604
26	C	0.000000811	0.000000860	0.000000231
27	C	-0.000000148	-0.000001090	0.000000177
28	C	-0.000000270	-0.000000397	-0.000000424
29	S	0.000001022	-0.000000382	0.000000921
30	C	0.000000105	-0.000000037	0.000000059
31	C	-0.000000131	-0.000001224	-0.000000185
32	C	-0.000000332	-0.000000353	-0.000000114
33	C	-0.000000087	-0.000000330	-0.000000464
34	C	0.000001008	-0.000000470	-0.000000241
35	C	0.000000379	-0.000000009	-0.000000665
36	C	-0.000000113	0.000002548	-0.000000993
37	N	0.000001770	0.000000800	0.000000167
38	C	-0.000003699	0.000000007	0.000000646
39	C	0.000003080	0.000000329	-0.000001627
40	N	-0.000003244	-0.000002664	0.000002397
41	C	0.000001865	-0.000000394	-0.000000154
42	O	-0.000000503	0.000000030	0.000000648
43	C	-0.000001344	0.000001639	-0.000000046
44	N	0.000001872	0.000001575	0.000003595
45	C	0.000000594	-0.000002269	-0.000002364
46	N	-0.000001263	0.000001300	0.000000625
47	O	-0.000000676	-0.000000507	-0.000000235

48	C	-0.000001550	-0.000000193	-0.000000782
49	C	0.000000551	0.000001288	-0.000001512
50	C	-0.000000070	0.000000151	-0.000002235
51	C	-0.000000815	-0.000000344	0.000000591
52	C	0.000001545	0.000000846	0.000001022
53	C	0.000001073	-0.000000416	-0.000000938
54	S	-0.000000735	0.000001292	0.000000957
55	C	0.000002263	0.000000778	-0.000000069
56	C	-0.000002138	-0.000001154	0.000000255
57	C	0.000001799	0.000003698	-0.000000725
58	S	-0.000000448	0.000000273	0.000001361
59	C	-0.000000460	0.000000810	-0.000000422
60	C	-0.000000405	-0.000000474	0.000000022
61	C	0.000000408	0.000001361	0.000000558
62	C	-0.000000404	0.000000581	0.000000095
63	S	0.000000216	0.000000381	0.000000301
64	C	-0.000000756	-0.000000575	-0.000000260
65	C	0.000000382	0.000001092	0.000000423
66	C	0.000000660	0.000000074	-0.000000548
67	C	-0.000000973	0.000000287	-0.000000011
68	S	0.000000341	0.000001129	0.000000683
69	C	-0.000006399	0.000001731	0.000000050
70	C	0.000000884	-0.000007181	-0.000000124
71	C	0.000000299	0.000002738	-0.000000409
72	C	-0.000005781	-0.000000647	-0.000000142
73	C	-0.000000788	-0.000005837	-0.000002373
74	C	0.000001881	0.000003428	0.000001473
75	C	-0.000000604	-0.000005652	-0.000001354
76	S	0.000000121	0.000003467	0.000001211
77	C	0.000005237	0.000003487	-0.000000130
78	C	0.000003490	0.000005040	0.000001442
79	C	-0.000000188	-0.000003591	-0.000000427
80	C	-0.000000008	0.000000302	0.000001507
81	H	-0.000000307	-0.000000309	-0.000000257
82	H	0.000000015	-0.000000319	-0.000000579
83	H	0.000000329	-0.000000168	-0.000000157
84	H	-0.000000089	-0.000000281	0.000000093
85	H	0.000000342	-0.000000027	-0.000000120
86	H	-0.000000215	0.000000398	-0.000000307
87	H	0.000000043	-0.000000371	0.000000066
88	H	-0.000000038	-0.000000884	-0.000000004
89	H	0.000000262	-0.000000219	0.000000576
90	H	-0.000000142	0.000000015	0.000000219
91	H	0.000000436	-0.000000526	-0.000000306

92	H	0.000000041	-0.000000535	-0.000000245
93	H	0.000000336	-0.000000390	-0.000000127
94	H	0.000000408	-0.000000279	0.000000037
95	H	-0.000000027	-0.000000383	0.000000249
96	H	0.000000226	0.000000347	-0.000000022
97	H	-0.000000489	-0.000000248	0.000000527
98	H	0.000000321	0.000000438	0.000000808
99	H	-0.000000419	-0.000000270	0.000000475
100	H	-0.000000489	0.000000051	-0.000000514
101	H	0.000000574	0.000000510	-0.000000165
102	H	0.000000201	0.000000148	0.000000232
103	H	-0.000000370	0.000000139	-0.000000075
104	H	-0.000000151	-0.000000646	0.000000257
105	H	0.000000049	-0.000000326	-0.000000535
106	H	0.000000403	0.000000468	0.000000509
107	H	-0.000000080	0.000000674	0.000000343
108	H	-0.000000287	0.000000424	0.000000097
109	H	-0.000000380	0.000000424	0.000000137
110	H	0.000000192	0.000000300	-0.000000092
111	H	-0.000000309	-0.000001550	0.000000252
112	H	-0.000000148	0.000000360	-0.000000149
113	H	0.000001079	0.000000873	-0.000000234
114	H	0.000000167	0.000000937	-0.000000245
115	H	0.000000130	0.000000914	-0.000000182
116	H	-0.000000410	-0.000000515	-0.000000525
117	H	-0.000000376	0.000000015	0.000000457
118	H	0.000000166	-0.000000056	-0.000000509

Total energy: -6233.81975804 Hartrees

Table S5. Coordinates and energy of compound **2BIDBT**

		X	Y	Z
1	C	0.000000123	-0.000000406	0.000001020
2	C	-0.000001113	0.000001344	0.000000246
3	N	0.000000784	-0.000001257	-0.000000214
4	C	-0.000000540	-0.000000721	-0.000000709
5	C	-0.000006528	0.000000247	-0.000000121
6	N	0.000005847	-0.000002327	-0.000001130
7	C	0.000000263	-0.000001121	-0.000000227
8	O	0.000001739	0.000001216	-0.000000703
9	C	0.000000274	0.000000399	0.000002680
10	N	-0.000000516	0.000000583	-0.000003231
11	C	0.000000041	-0.000002617	-0.000001039
12	N	-0.000000645	0.000000949	0.000001811
13	O	0.000000140	-0.000000242	0.000000174
14	C	0.000000767	0.000002994	0.000001997

15	C	-0.000002407	0.000001143	-0.000000522
16	C	0.000000781	-0.000001041	0.000003112
17	C	0.000002186	-0.000000433	-0.000001335
18	C	-0.000001388	-0.000000145	0.000000018
19	C	0.000000546	0.000001206	-0.000000392
20	S	0.000000638	-0.000001833	0.000000673
21	C	-0.000000730	-0.000001293	-0.000000347
22	C	0.000001150	0.000000575	0.000000679
23	C	-0.000000676	0.000000198	-0.000000439
24	S	-0.000000094	-0.000002245	0.000001124
25	C	-0.000000938	0.000000077	-0.000000077
26	C	0.000000598	0.000000702	0.000000674
27	C	-0.000000796	-0.000001703	-0.000000611
28	C	0.000002752	0.000000003	0.000001520
29	S	-0.000000766	-0.000000999	0.000000152
30	C	-0.000000281	0.000000040	0.000000264
31	C	-0.000000587	-0.000000220	0.000000183
32	C	0.000000908	-0.000000815	0.000001398
33	C	-0.000001419	-0.000000739	0.000000736
34	C	-0.000000400	-0.000000441	0.000001271
35	C	0.000002337	0.000000928	0.000000133
36	C	-0.000001346	0.000000249	0.000001695
37	N	0.000001245	0.000000201	-0.000000241
38	C	-0.000001181	0.000000511	-0.000000133
39	C	0.000003215	-0.000000631	0.000000876
40	N	-0.000003148	0.000000594	-0.000000671
41	C	0.000000130	-0.000000550	-0.000000482
42	O	-0.000000557	-0.000000024	0.000000210
43	C	-0.000001091	0.000000421	0.000001902
44	N	0.000002228	0.000000169	-0.000002361
45	C	-0.000000238	0.000001722	-0.000000421
46	N	-0.000000035	-0.000000470	-0.000000352
47	O	0.000000040	0.000000486	-0.000001433
48	C	-0.000001039	-0.000001741	-0.000001847
49	C	0.000000745	-0.000000718	0.000001727
50	C	-0.000000920	0.000000828	-0.000001597
51	C	-0.000003181	0.000000154	-0.000000099
52	C	0.000002570	0.000000003	0.000001787
53	C	-0.000004730	-0.000000556	-0.000000462
54	S	0.000001203	-0.000000266	-0.000000368
55	C	0.000001921	0.000001054	-0.000000339
56	C	-0.000001898	-0.000000805	-0.000000729
57	C	0.000000545	0.000000642	-0.000001203
58	S	0.000000645	0.000000590	0.000001543

59	C	0.000003306	0.000003693	0.000000578
60	C	-0.000000623	-0.000001514	-0.000001168
61	C	0.000001388	0.000001660	0.000000957
62	C	-0.000001066	-0.000000096	-0.000000822
63	S	-0.000000838	-0.000001835	-0.000000455
64	C	-0.000000291	-0.000000180	-0.000000124
65	C	0.000000685	0.000000081	-0.000000169
66	C	-0.000000805	0.000000925	-0.000000318
67	C	0.000000970	0.000000545	-0.000001273
68	S	0.000000689	0.000000588	0.000000164
69	C	0.000000525	-0.000002805	0.000000049
70	C	0.000000831	0.000001363	-0.000000833
71	C	-0.000000902	-0.000000413	-0.000001548
72	C	-0.000002729	0.000002823	0.000000816
73	C	0.000001248	-0.000000847	-0.000000610
74	C	-0.000000326	-0.000001092	0.000000482
75	C	0.000001905	0.000000726	0.000000747
76	C	-0.000004663	-0.000002346	-0.000000951
77	C	0.000005602	-0.000003053	-0.000000853
78	N	0.000000584	0.000001683	-0.000001376
79	S	-0.000000871	0.000000920	-0.000000177
80	N	-0.000002440	0.000003200	-0.000000638
81	C	0.000000006	-0.000000453	-0.000001178
82	C	-0.000001606	0.000000340	-0.000000393
83	C	0.000001463	0.000000628	0.000001486
84	C	-0.000001474	0.000000147	-0.000001290
85	S	0.000001493	0.000000095	0.000001038
86	H	-0.000000272	-0.000000232	-0.000000878
87	H	-0.000000516	-0.000000135	-0.000001332
88	H	0.000000560	-0.000000062	-0.000000847
89	H	0.000000051	0.000000138	0.000000896
90	H	-0.000000268	-0.000000528	0.000001308
91	H	0.000000301	-0.000000085	0.000001325
92	H	-0.000000045	0.000001048	-0.000000334
93	H	-0.000000022	-0.000000436	-0.000000972
94	H	0.000000259	-0.000000267	0.000001545
95	H	-0.000000378	-0.000000388	0.000000526
96	H	0.000000547	-0.000000318	-0.000000171
97	H	0.000000521	-0.000000580	0.000000225
98	H	0.000000261	-0.000000959	0.000000539
99	H	0.000000101	-0.000000271	0.000001042
100	H	0.000000009	-0.000000161	0.000001046
101	H	0.000000233	0.000000419	0.000001139
102	H	-0.000000253	0.000000545	0.000000492

103	H	-0.000000163	0.000000172	0.000000984
104	H	0.000000013	-0.000000694	-0.000000608
105	H	-0.000000300	0.000000104	-0.000001426
106	H	0.000000285	0.000000970	-0.000001096
107	H	0.000000527	0.000000422	0.000000771
108	H	0.000000161	0.000000842	0.000000754
109	H	-0.000000586	0.000000163	-0.000000846
110	H	0.000000529	0.000000356	-0.000001399
111	H	-0.000000624	0.000000088	0.000001094
112	H	-0.000000253	0.000000173	0.000000354
113	H	-0.000000240	0.000000404	-0.000000119
114	H	-0.000000114	0.000000117	-0.000000833
115	H	-0.000000119	0.000000237	-0.000000850
116	H	-0.000000345	0.000000165	-0.000000803
117	H	0.000000553	0.000000371	-0.000000173
118	H	0.000000310	0.000000004	0.000000447
119	H	0.000000031	-0.000000131	0.000001007
120	H	0.000000521	-0.000000051	-0.000000404
121	H	-0.000000511	-0.000000094	-0.000000317

Total energy: -6816.47029612 Hartrees

4. X-ray Crystallographic Data

Table S6 Crystallographic data of **BTBID**

Name	**BTBID**
Empirical formula	$C_{46}H_{48}N_4O_2S_4$
Formular weight	816.266
T/K	173 (2)
Wavelength, Å	0.71073
Crystal system	Monoclinic
Space group	P2(1)/n
a, Å	11.408(2)
b, Å	19.620(4)
c, Å	11.720(2)
α,deg	90
β, deg	106.43(3)
γ, deg	90
Volume, $Å^3$	2516.1(9)
Z	2
Calculated density, Mg/m^3	1.394
Absorption coefficient, mm^{-1}	0.550
F (000)	1096
Crystal size, mm	0.31 x 0.12 x 0.07
θ range, deg	2.38-25.00
Limiting indices	-13<=h<=13, -22<=k<=23, -13<=l<=13
Reflections collected/ unique	14143 / 4406 [R(int) = 0.0567]
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	4406/311/375
Goddness-of-fit on F^2	1.202
Final R indices [I>2σ(I)]	R1 = 0.0969, wR2 = 0.2495
R indices (all data)	R1 = 0.1088, wR2 = 0.2682
Largest diff. peak and hole, $e.A^{-3}$	0.807 and -0.611

5. Thin film characterizations

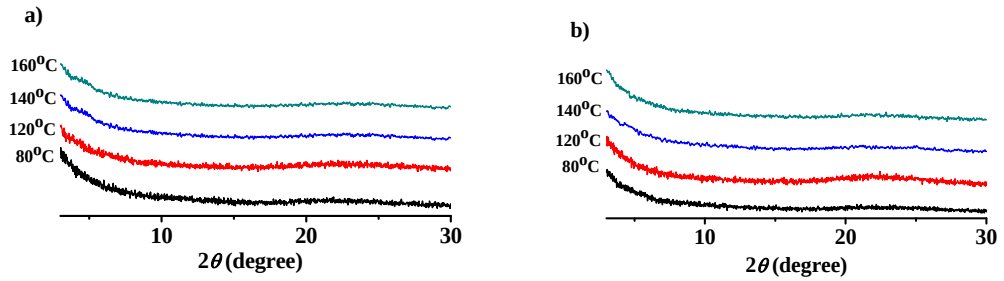


Figure S3. XRD patterns of thin film of **2BIDBDT**(a) and **2BIDBT**(b) after annealing at different temperatures.

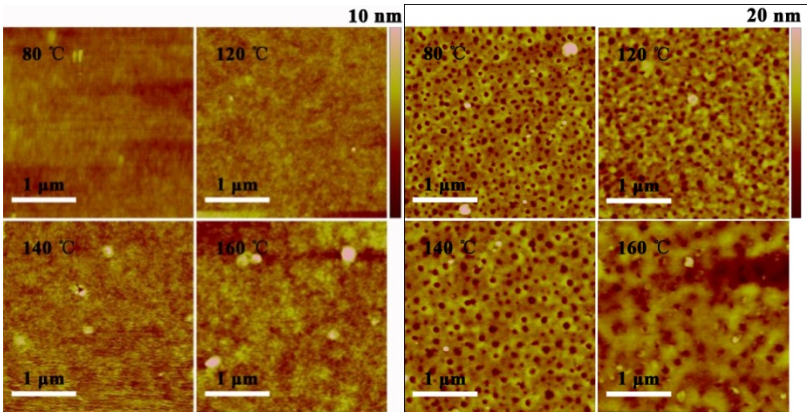
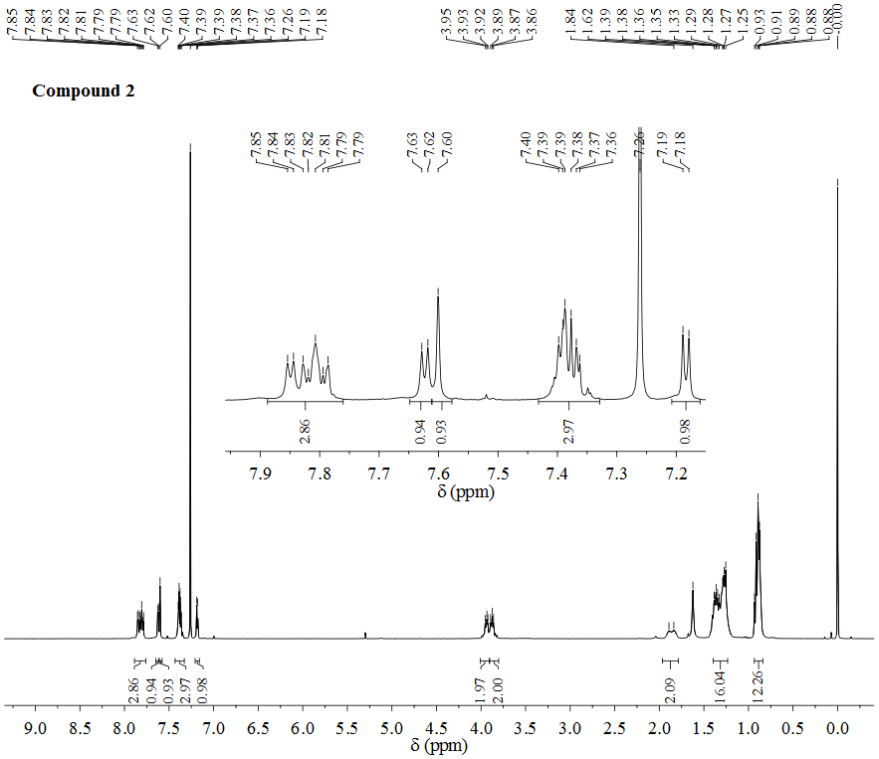
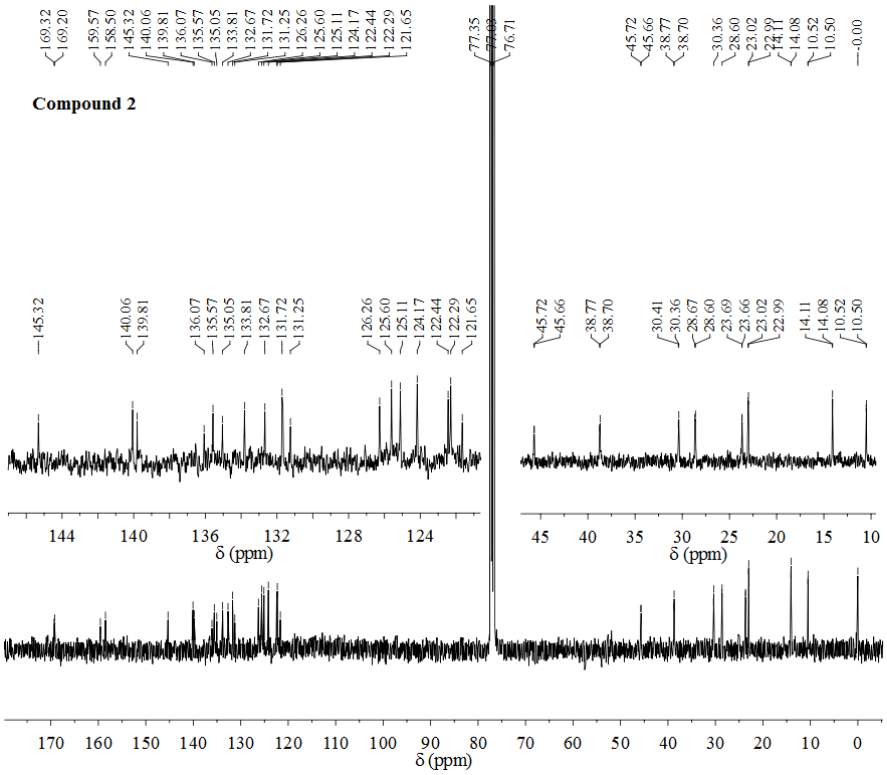


Figure S4. AFM images of thin film of **2BIDBDT**(a) and **2BIDBT**(b) after annealing at different temperatures.

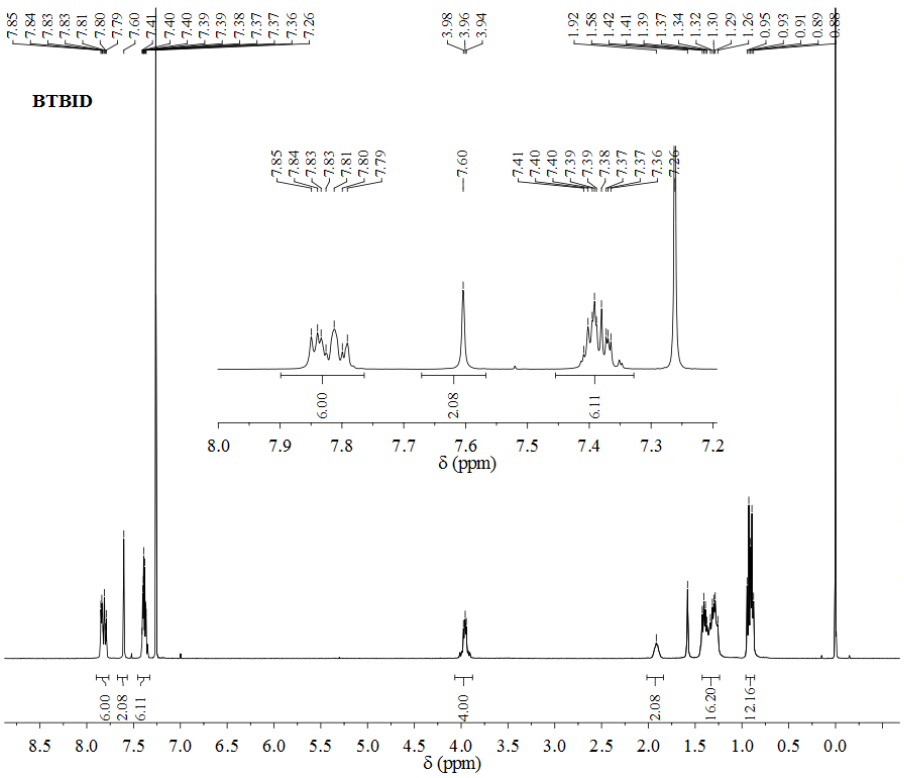
6. ^{1}HNMR and ^{13}CNMR spectra



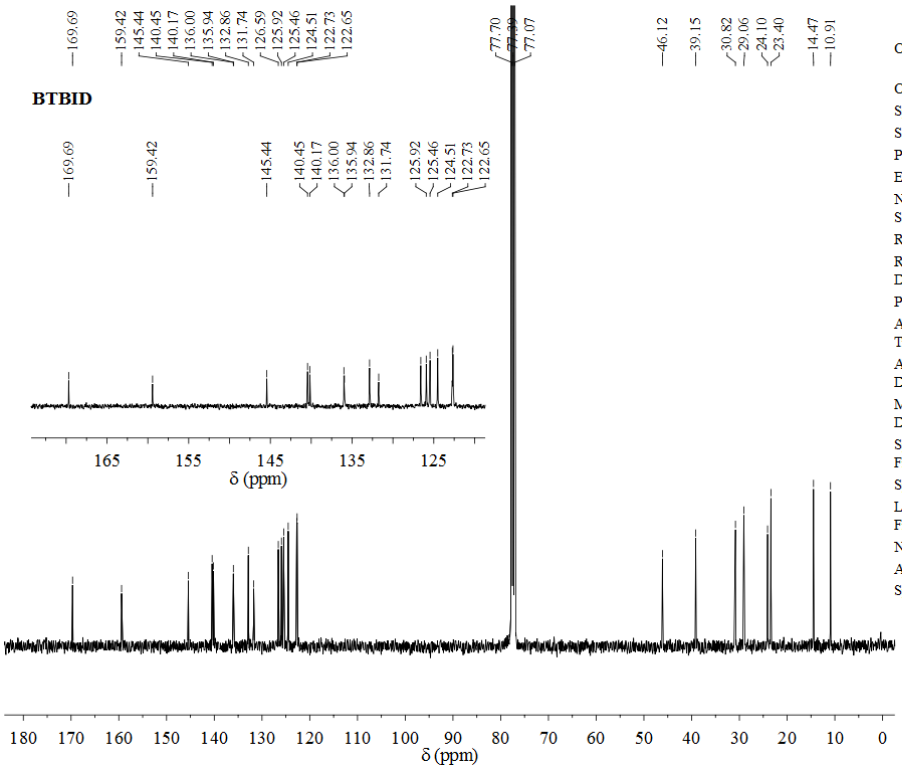
Parameter	Value
Origin	Bruker BioSpin GmbH
Owner	nmrsu
Spectrometer	AV400
Solvent	CDCl3
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	256
Relaxation Delay	1.0000
Pulse Width	12.1000
Acquisition Time	2.7329
Acquisition Date	2012-06-26T08:06:00
Modification Date	2012-06-26T08:06:18
Spectrometer Frequency	400.13
Spectral Width	11990.4
Lowest Frequency	-3533.1
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



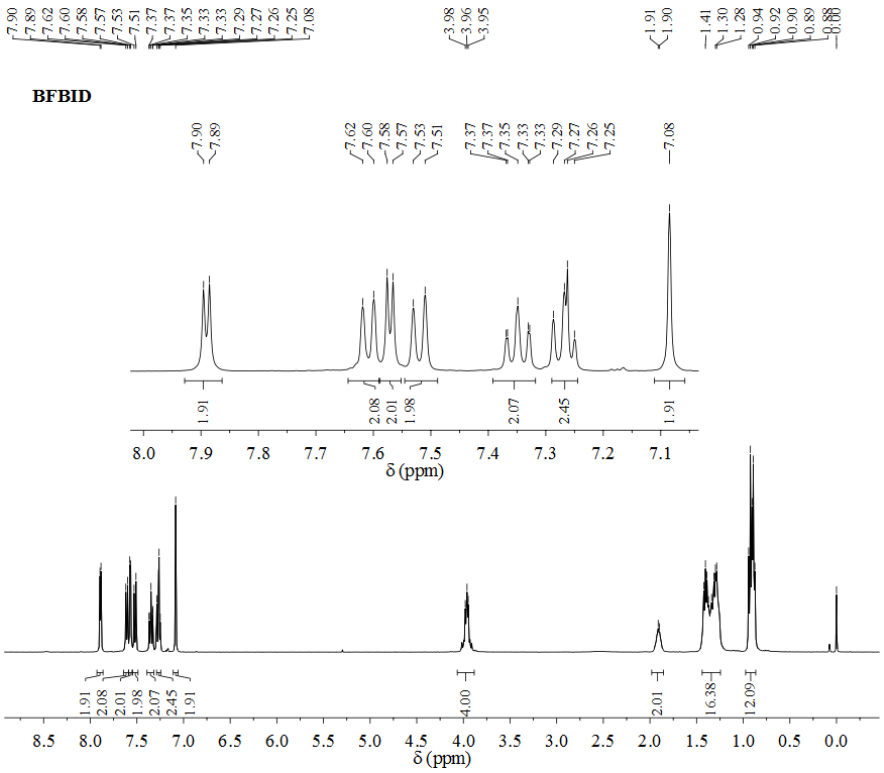
Parameter	Value
Origin	Bruker BioSpin GmbH
Owner	nmrsu
Spectrometer	AV400
Solvent	CDCl3
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	6704
Receiver Gain	6502
Relaxation Delay	2.0000
Pulse Width	12.2000
Acquisition Time	1.3665
Acquisition Date	2013-01-03T16:19:00
Modification Date	2013-01-03T21:12:14
Spectrometer Frequency	100.61
Spectral Width	23980.8
Lowest Frequency	-1931.3
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



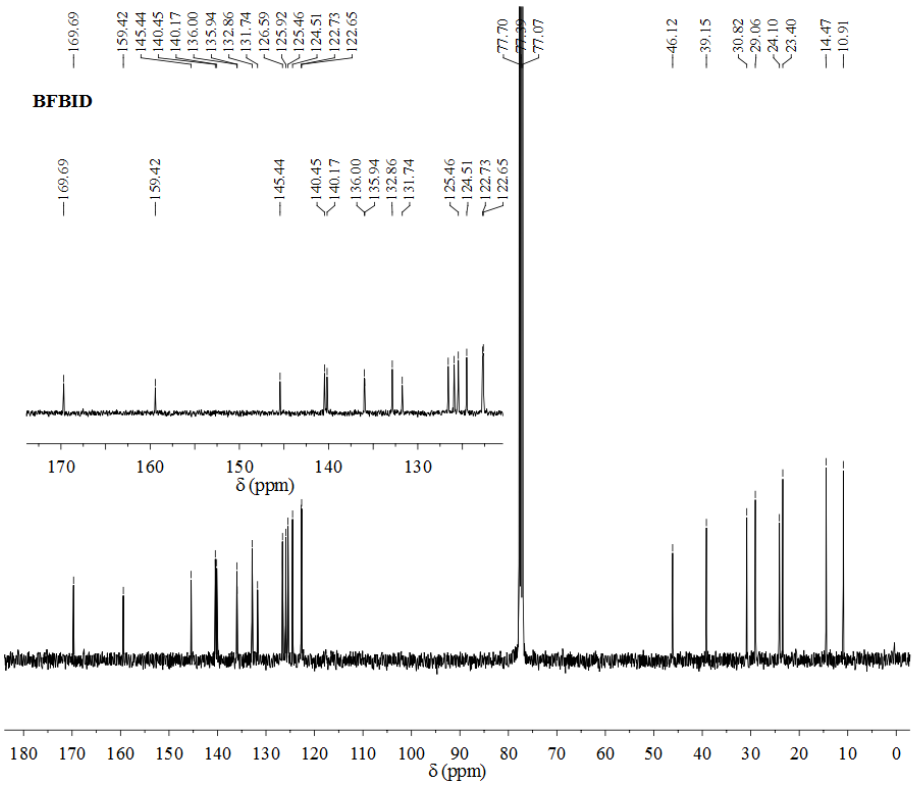
Parameter	Value
Origin	Bruker BioSpin GmbH
Owner	nmrsu
Spectrometer	AV400
Solvent	CDCl3
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	362
Relaxation Delay	1.0000
Pulse Width	12.1000
Acquisition Time	2.7329
Acquisition Date	2012-06-15T15:22:00
Modification Date	2012-06-15T15:23:04
Spectrometer Frequency	400.13
Spectral Width	11990.4
Lowest Frequency	-3532.9
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



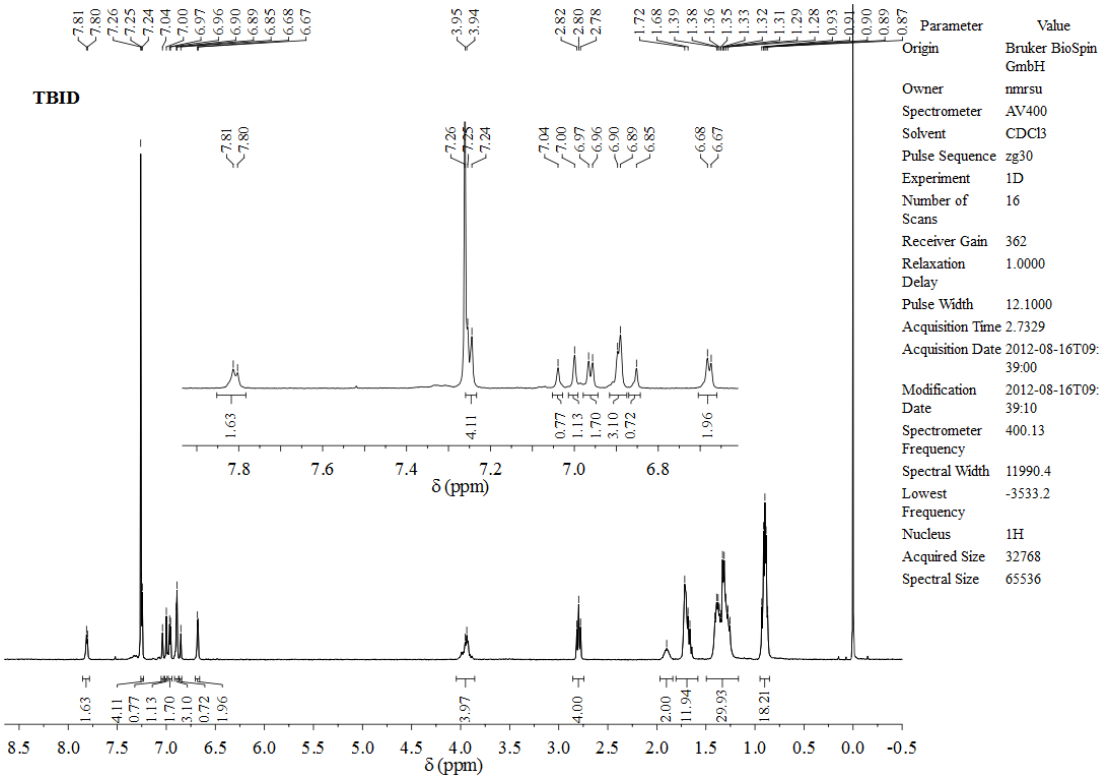
Parameter	Value
Origin	Bruker BioSpin GmbH
Owner	nmrsu
Spectrometer	AV400
Solvent	CDCl3
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	2167
Receiver Gain	9195
Relaxation Delay	2.0000
Pulse Width	12.2000
Acquisition Time	1.3665
Acquisition Date	2012-11-23T22:07:00
Modification Date	2012-11-24T00:09:10
Spectrometer Frequency	100.61
Spectral Width	23980.8
Lowest Frequency	-1894.6
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	456
Relaxation Delay	1.0000
Pulse Width	12.1000
Acquisition Time	2.7329
Acquisition Date	2012-11-27T20:14:00
Modification Date	2012-11-27T20:15:00
Spectrometer Frequency	400.13
Spectral Width	11990.4
Lowest Frequency	-3532.8
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	2167
Receiver Gain	9195
Relaxation Delay	2.0000
Pulse Width	12.2000
Acquisition Time	1.3665
Acquisition Date	2012-11-23T2 2:07:00
Modification Date	2012-11-24T0 0:09:10
Spectrometer Frequency	100.61
Spectral Width	23980.8
Lowest Frequency	-1894.6
Nucleus	13C
Acquired Size	32768
Spectral Size	65536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7.24
7.04
7.00
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6.96
6.90
6.89
6.85
6.68
6.67
3.95
3.94
2.82
2.80
2.78
1.72
1.68
1.39
1.38
1.36
1.35
1.33
1.32
1.31
1.29
1.28
0.93
0.91
0.90
0.89
0.87
1.63
4.11
0.77
1.13
1.70
3.10
0.72
1.96
3.97
4.00
2.00
11.94
29.93
18.21
δ (ppm)
Parameter Value
Origin Bruker BioSpin GmbH
Owner nmrsu
Spectrometer AV400
Solvent CDCl3
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 362
Relaxation Delay 1.0000
Pulse Width 12.1000
Acquisition Time 2.7329
Acquisition Date 2012-08-16T09:39:00
Modification Date 2012-08-16T09:39:10
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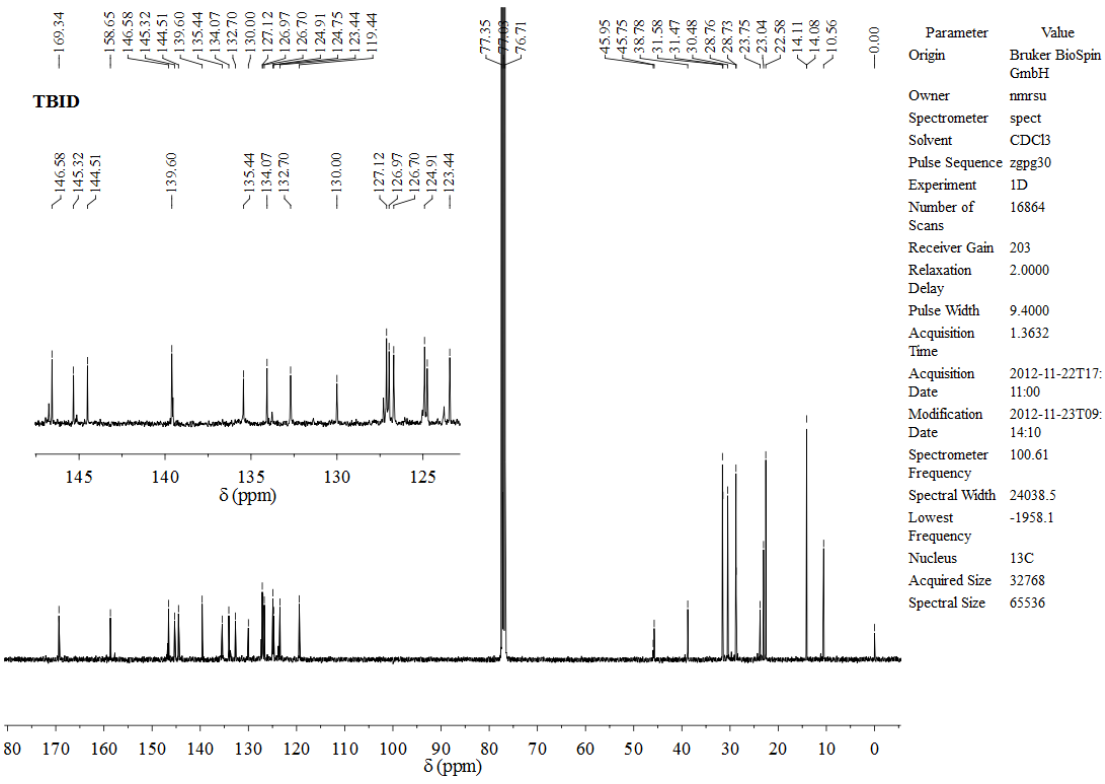
Spectral Width 11990.4
Lowest Frequency -3533.2
Nucleus 1H
Acquired Size 32768
Spectral Size 65536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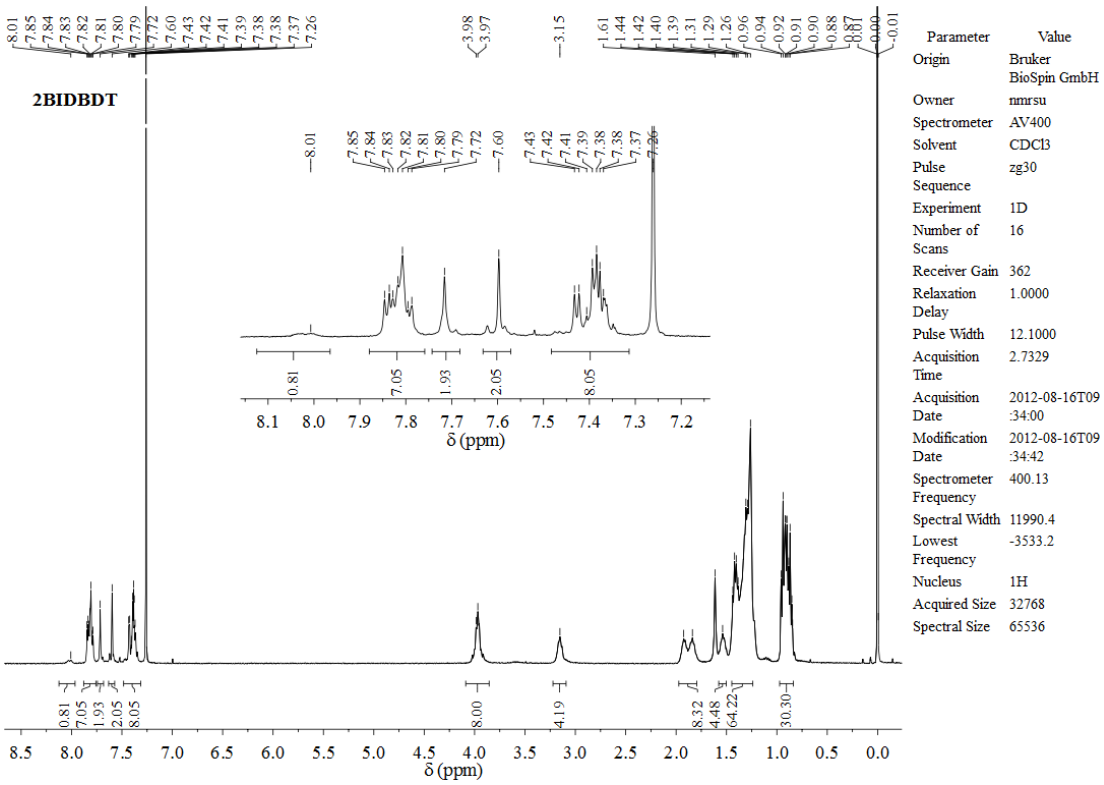
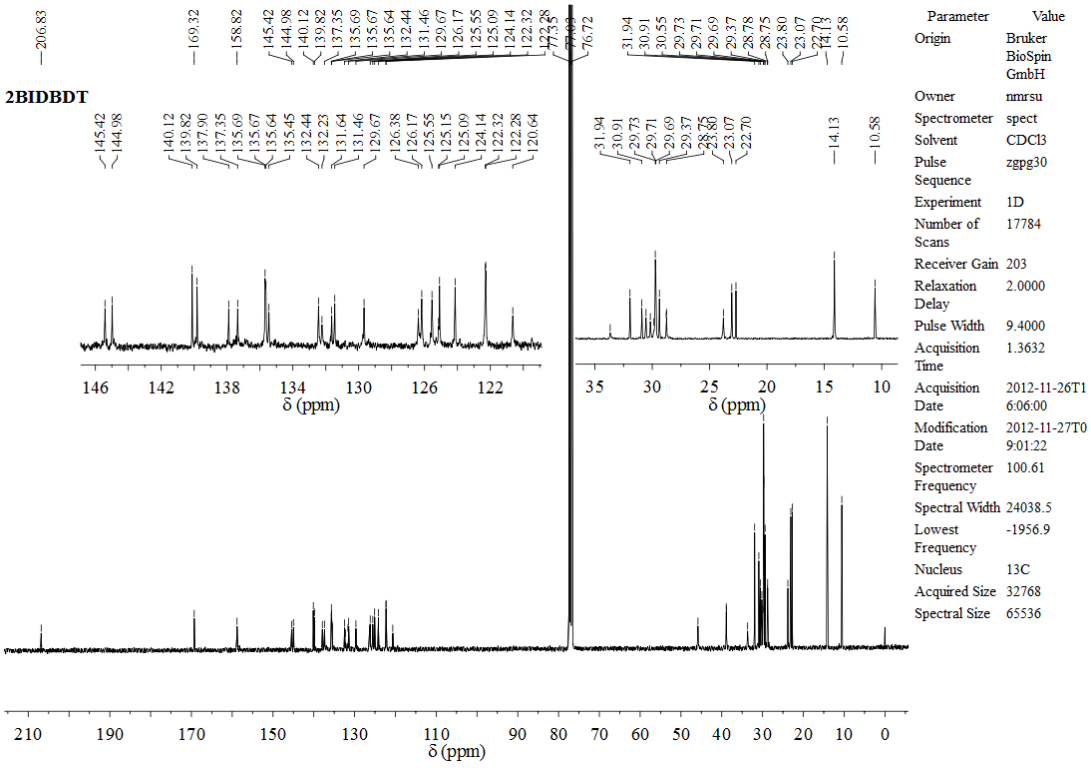
124.91
124.75
123.44
119.44
77.35
77.03
76.71
45.95
45.75
38.78
31.58
31.47
30.48
28.76
28.73
23.75
23.04
22.58
14.11
14.08
10.56
0.00
δ (ppm)
Parameter Value
Origin Bruker BioSpin GmbH
Owner nmrsu
Spectrometer spect
Solvent CDCl3
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 16864
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.4000
Acquisition Time 1.3632
Acquisition Date 2012-11-22T17:11:00
Modification Date 2012-11-23T09:14:10
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1958.1
Nucleus 13C
Acquired Size 32768
Spectral Size 65536


2BIDBDT
δ (ppm)
Parameter Value
Origin Bruker BioSpin GmbH
Owner nmrsu
Spectrometer AV400
Solvent CDCl3
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 362
Relaxation Delay 1.0000
Pulse Width 12.1000
Acquisition Time 2.7329
Acquisition Date 2012-08-16T09:34:00
Modification Date 2012-08-16T09:34:42
Spectrometer Frequency 400.13
Spectral Width 11990.4
Lowest Frequency -3533.2
Nucleus 1H
Acquired Size 32768
Spectral Size 65536


2BIDBDT
δ (ppm)
Parameter Value
Origin Bruker BioSpin GmbH
Owner nmrsu
Spectrometer spect
Solvent CDCl3
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 17784
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.4000
Acquisition Time 1.3632
Acquisition Date 2012-11-26T16:06:00
Modification Date 2012-11-27T09:01:22
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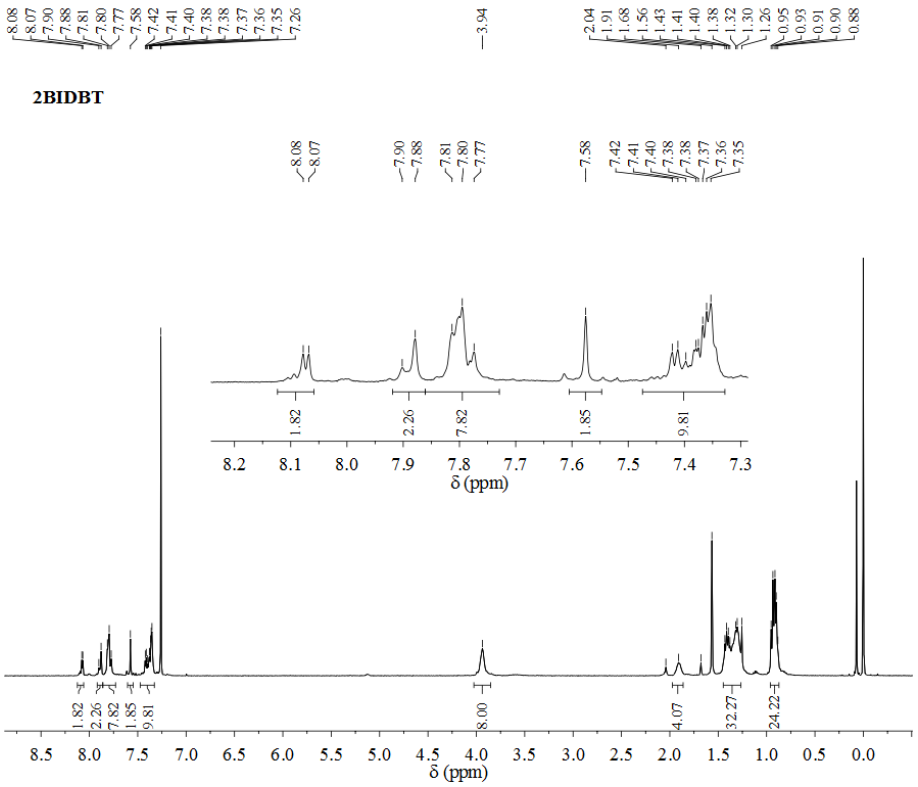
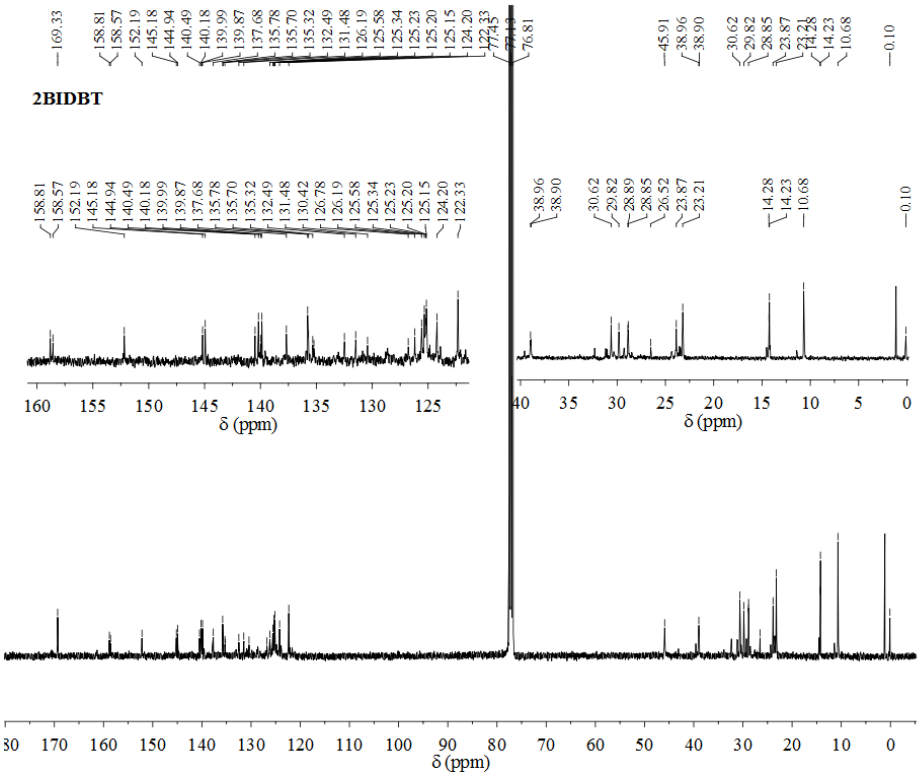
Lowest Frequency -1956.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536



Parameter	Value
Origin	Bruker BioSpin GmbH
Owner	nmrsu
Spectrometer	AV400
Solvent	CDCl3
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	362
Relaxation Delay	1.0000
Pulse Width	12.1000
Acquisition Time	2.7329
Acquisition Date	2012-08-16T 09:24:00
Modification Date	2012-08-16T 09:24:50
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	nmr
Spectrometer	spect
Solvent	CDCl3
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	17936
Receiver Gain	206
Relaxation Delay	2.0000
Pulse Width	8.7000
Acquisition Time	1.2976
Acquisition Date	2012-11-29T1 7:08:12
Modification Date	2012-11-30T0 9:22:06
Spectrometer Frequency	100.64
Spectral Width	25252.5
Lowest Frequency	-2551.5
Nucleus	13C
Acquired Size	32768
Spectral Size	65536