

Supporting Information for

Synthesis and Side-Chain Isomeric Effect of 4,9-/5,10-Dialkylated- β -Angular-Shaped Naphthodithiophenes-based Donor-Acceptor Copolymers for Polymer Solar Cells and Field-Effect Transistors

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Jianquan Zhang,^d He Yan,^d Chun-Jen Su^c, Yen-Ju Cheng^{a*}

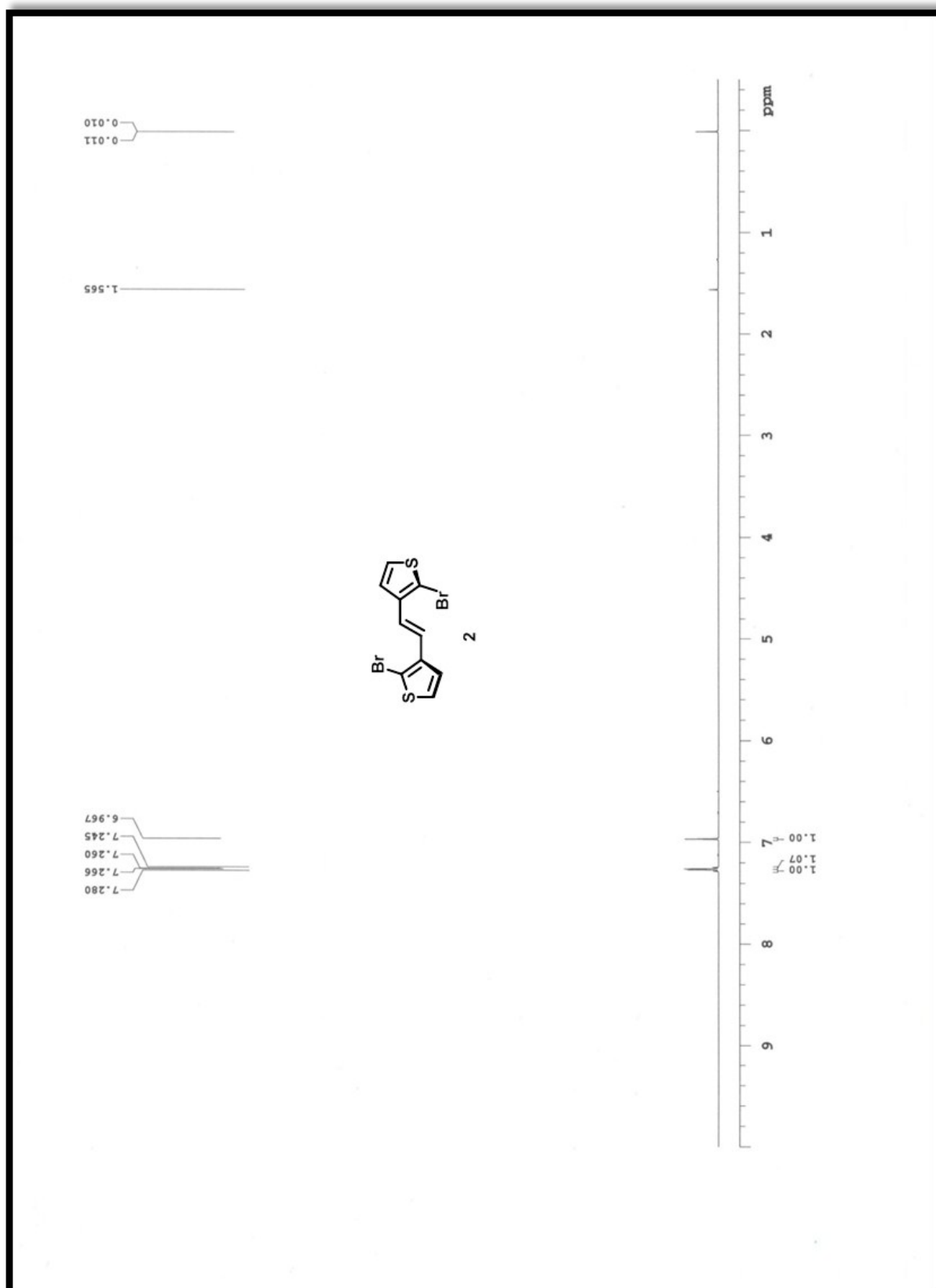
Department of Applied Chemistry, National Chiao Tung University 1001 University Road, Hsin-Chu Taiwan

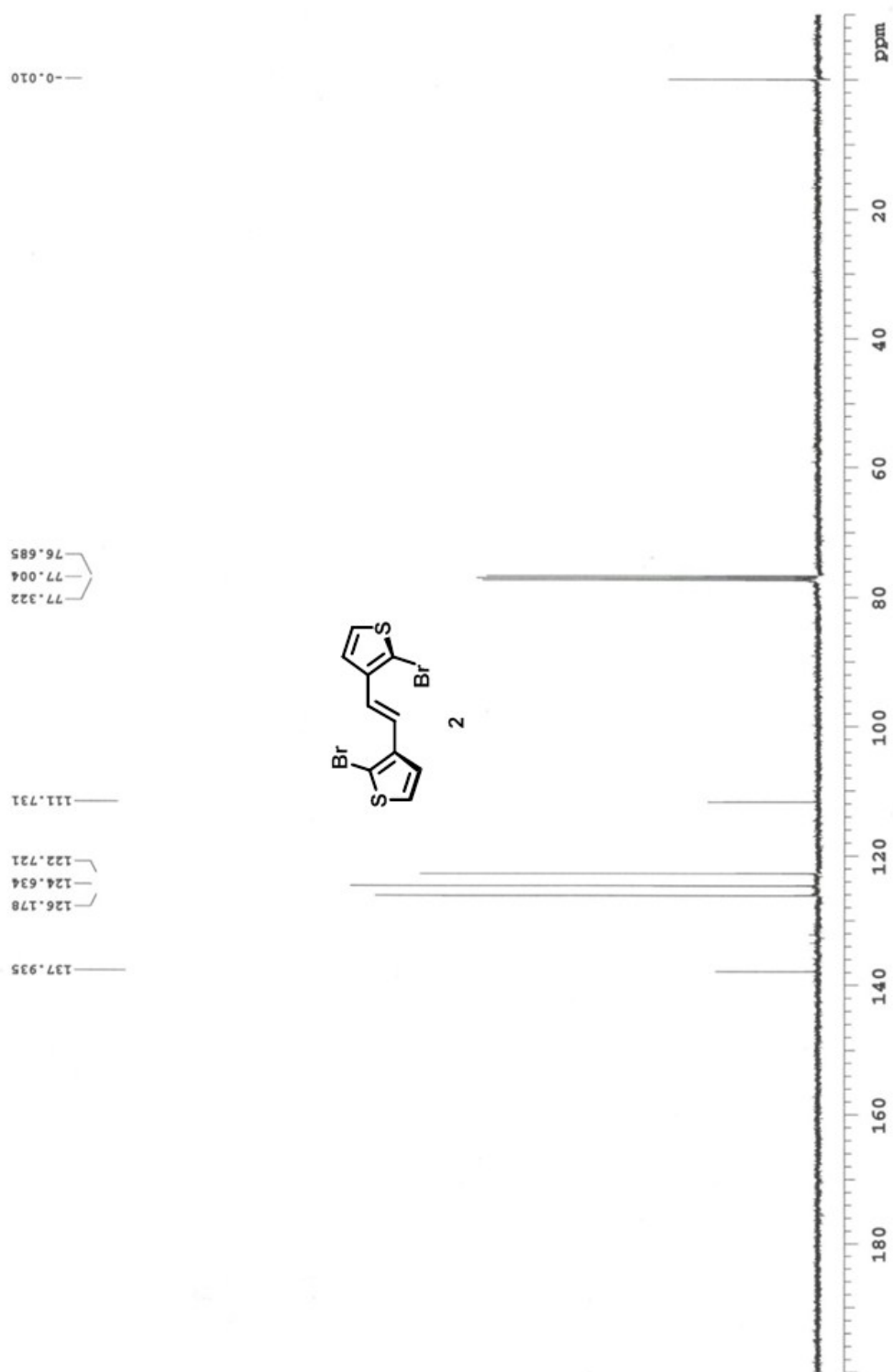
Email: yjcheng@mail.nctu.edu.tw

Table of Contents

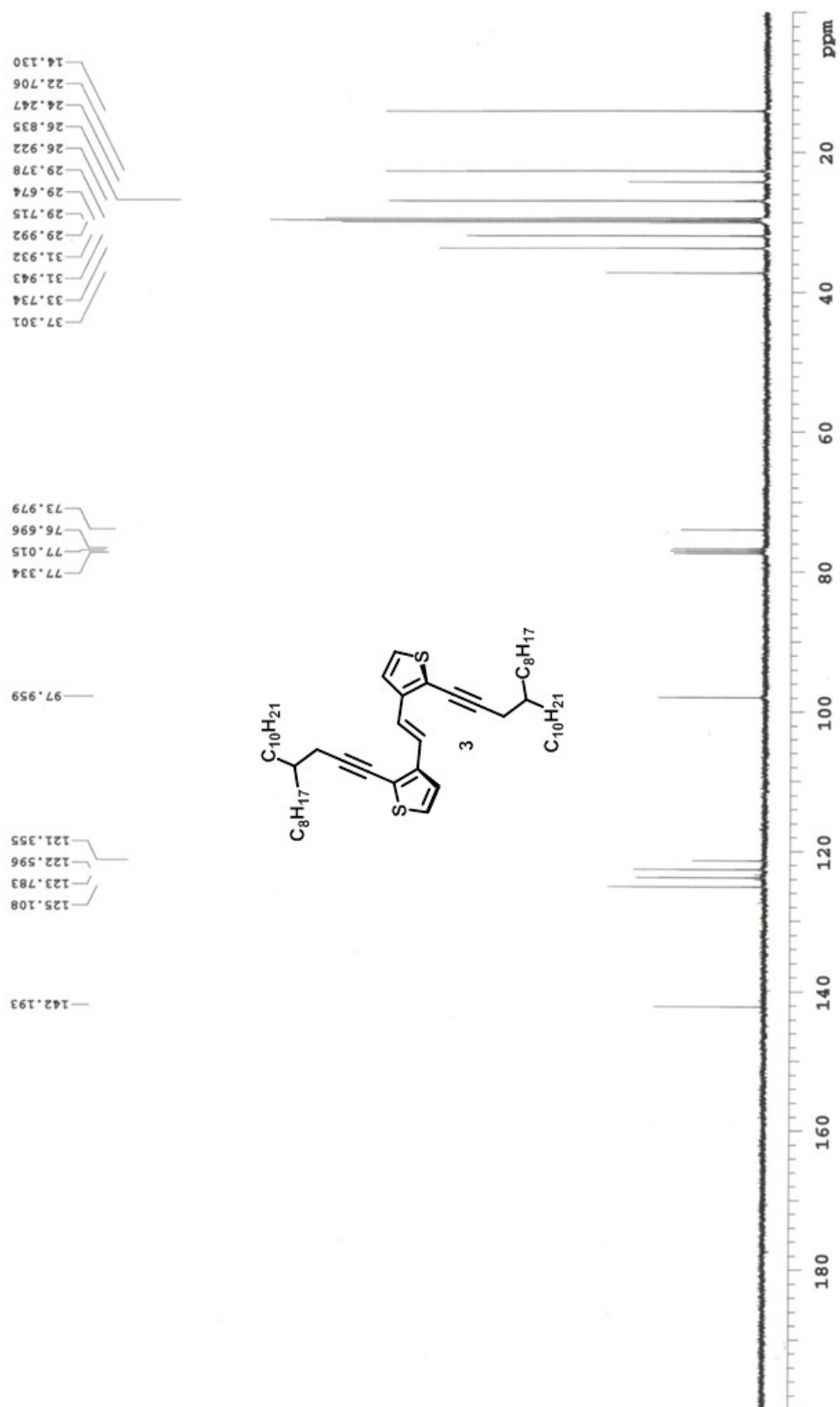
1. ¹ H and ¹³ C NMR Spectra.	S1
2. Computational Details.	S21
3. The HT-GPC Distribution Plots.	S30
4. 1D- GIWAXS Profiles.....	S31
5. Solubility Test Table.....	S31

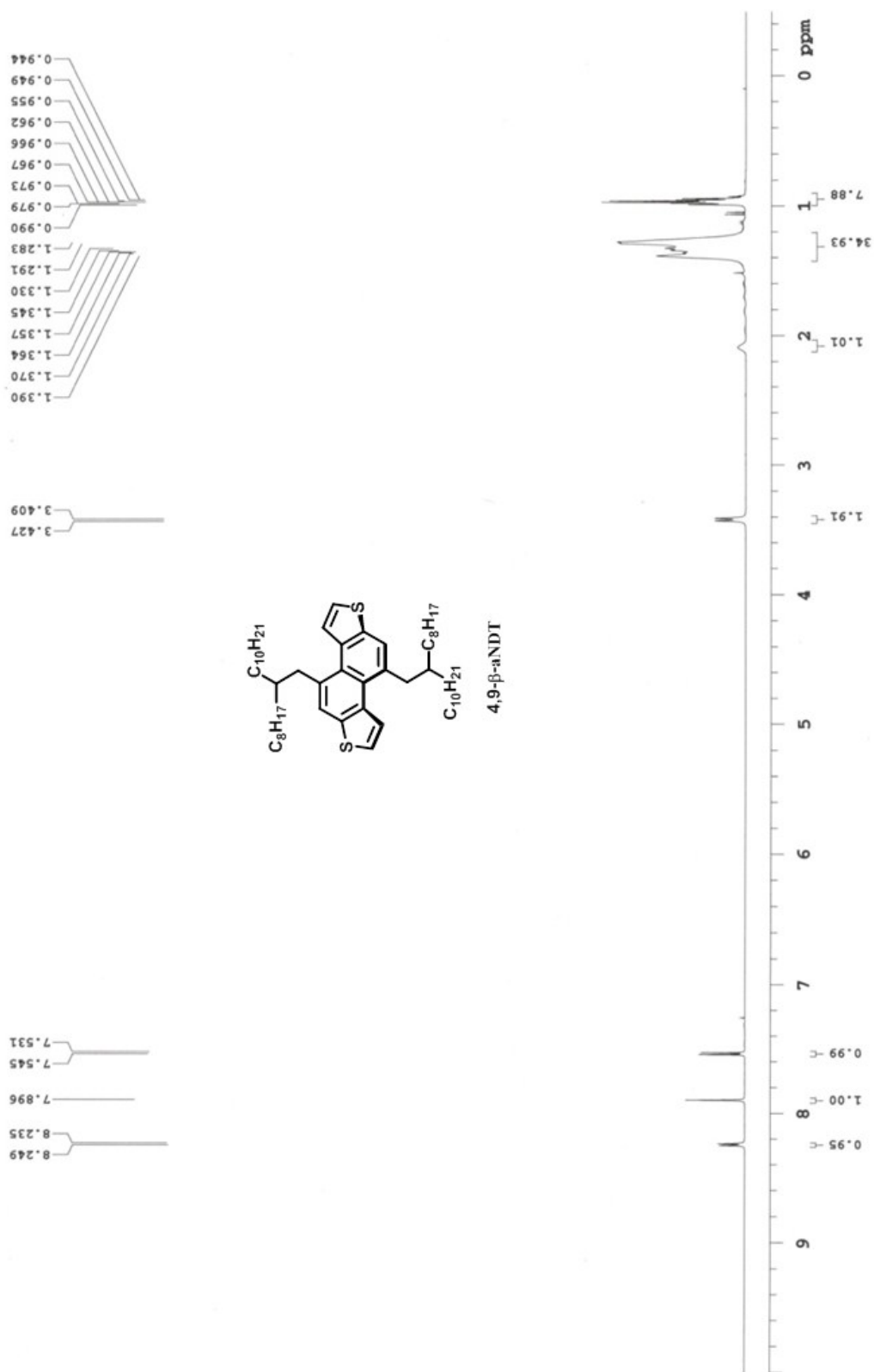
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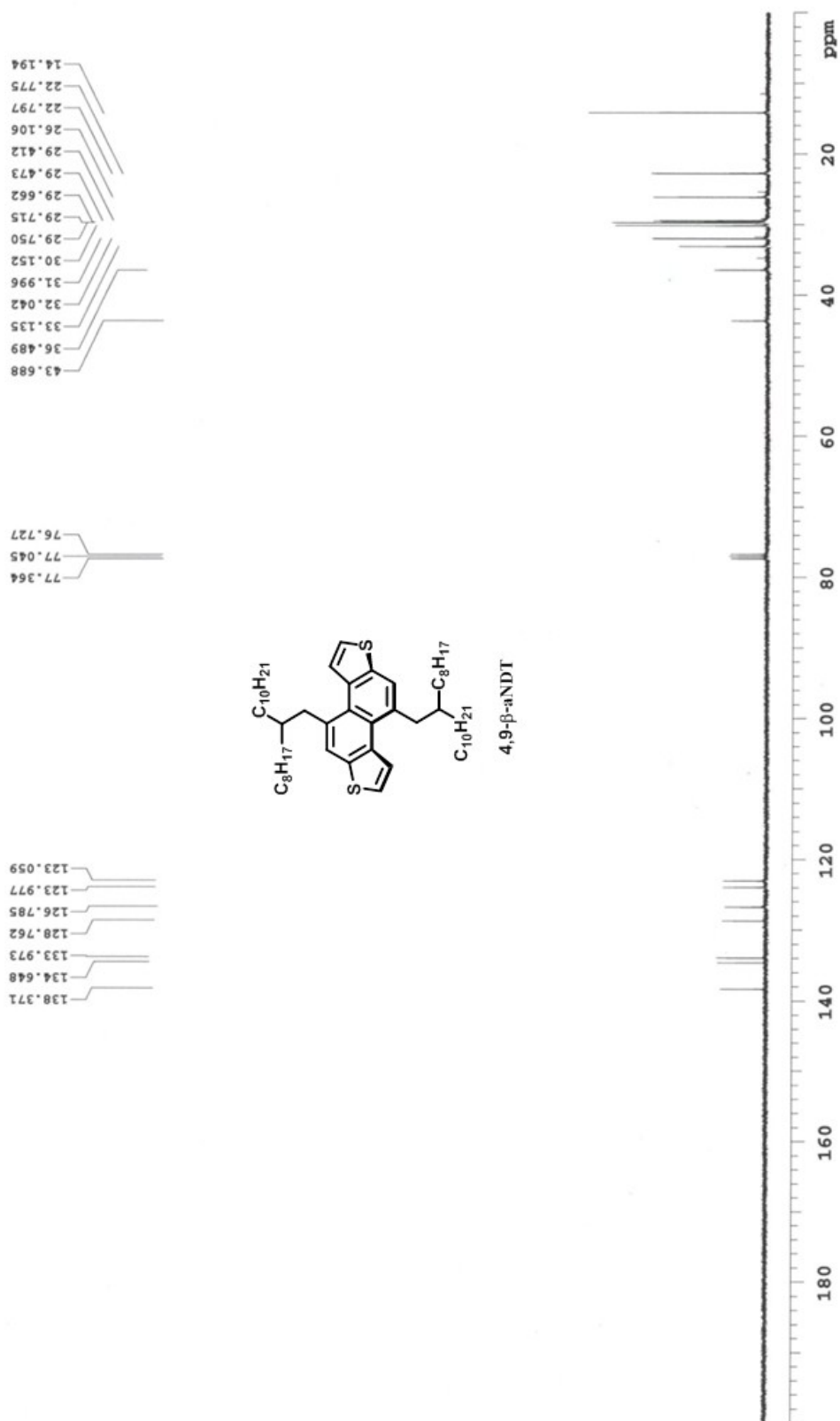


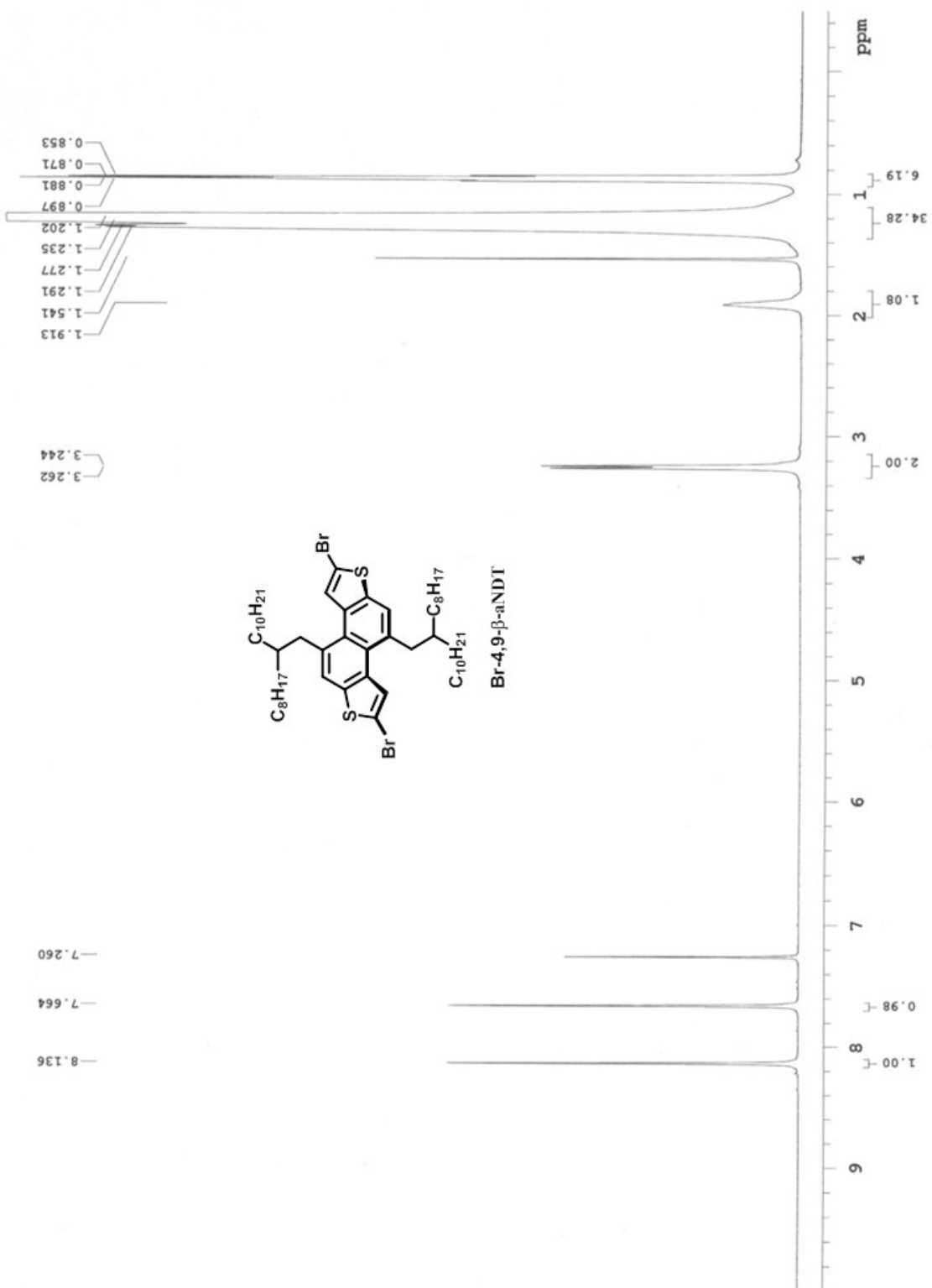


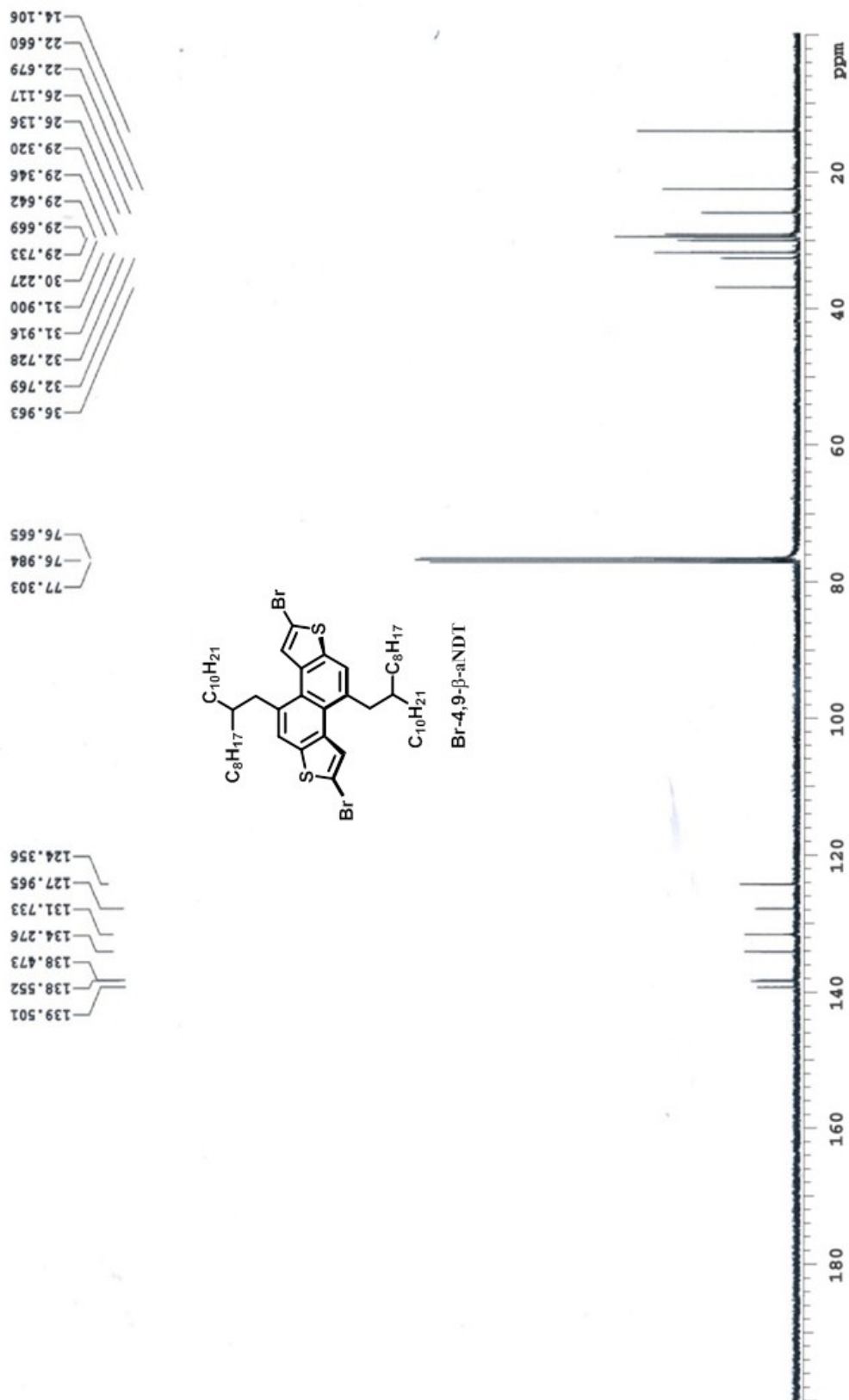


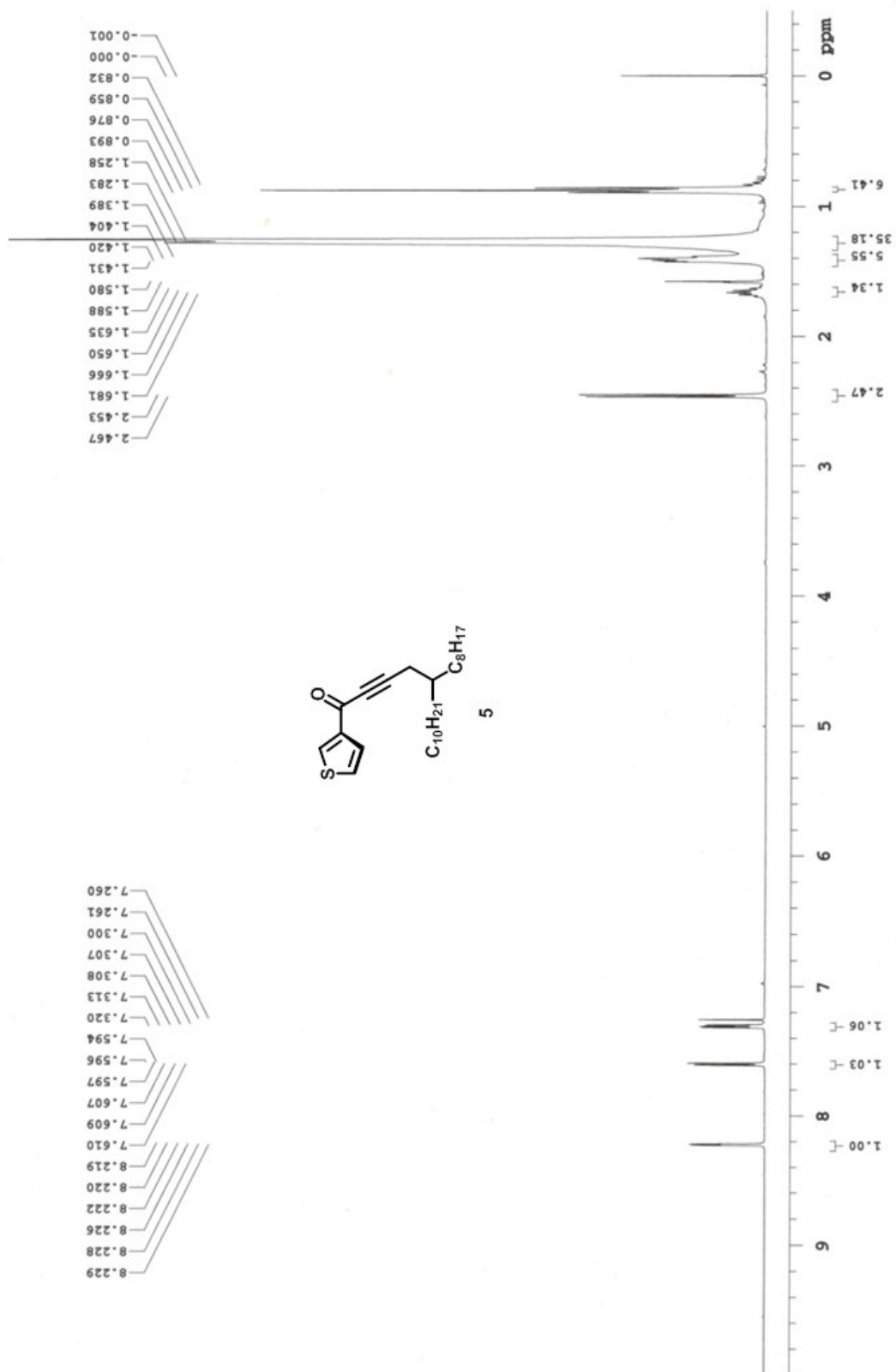


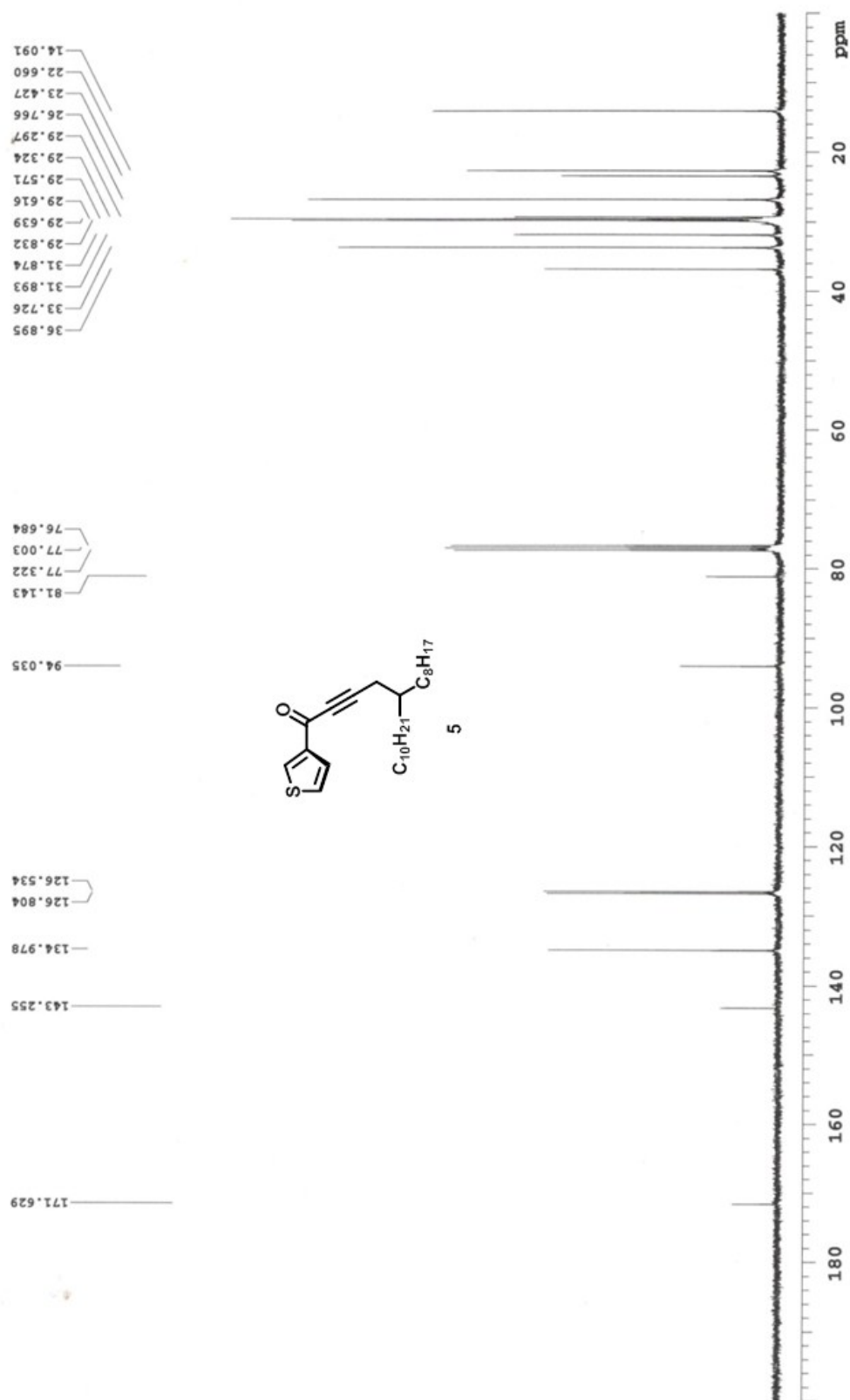


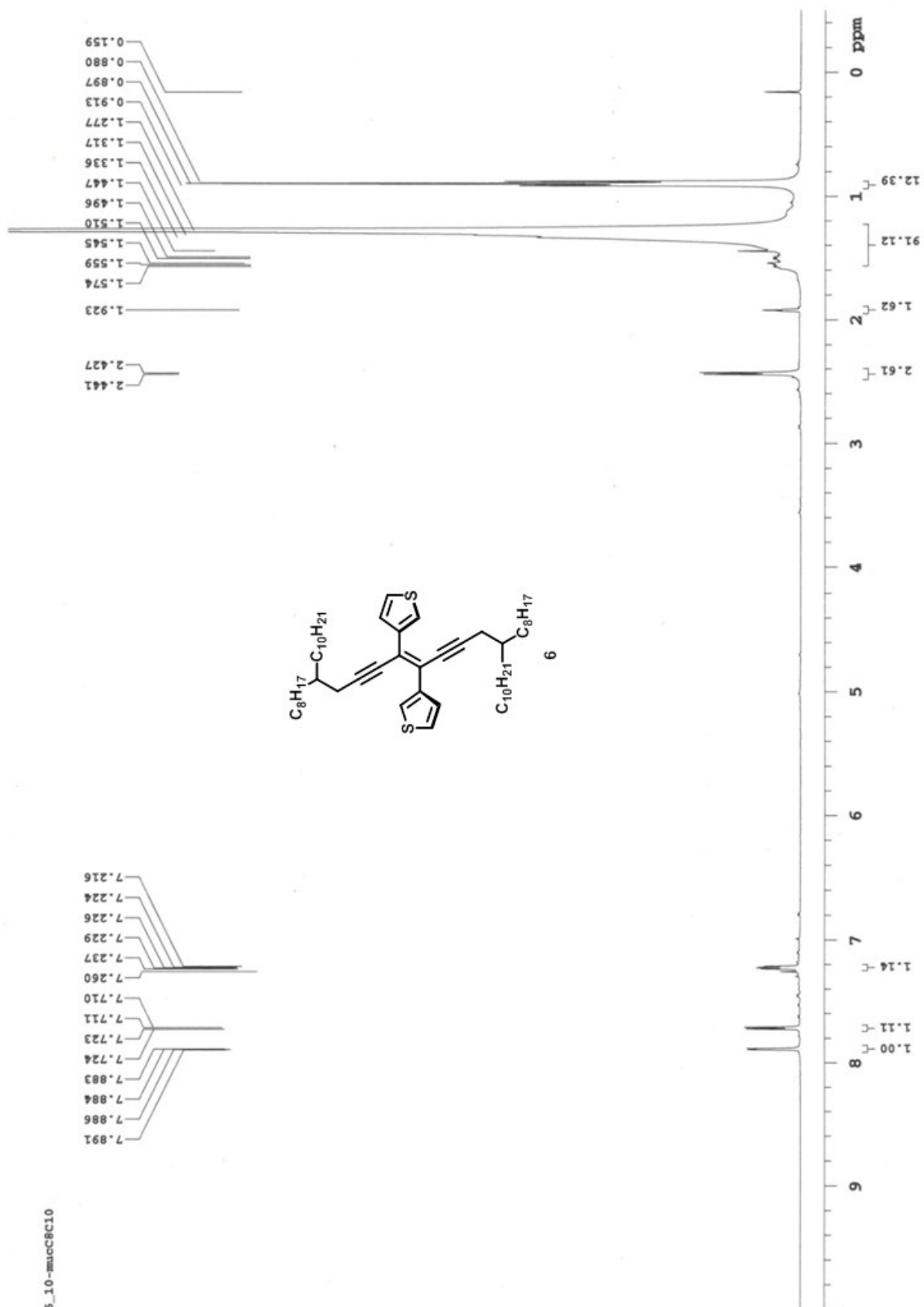


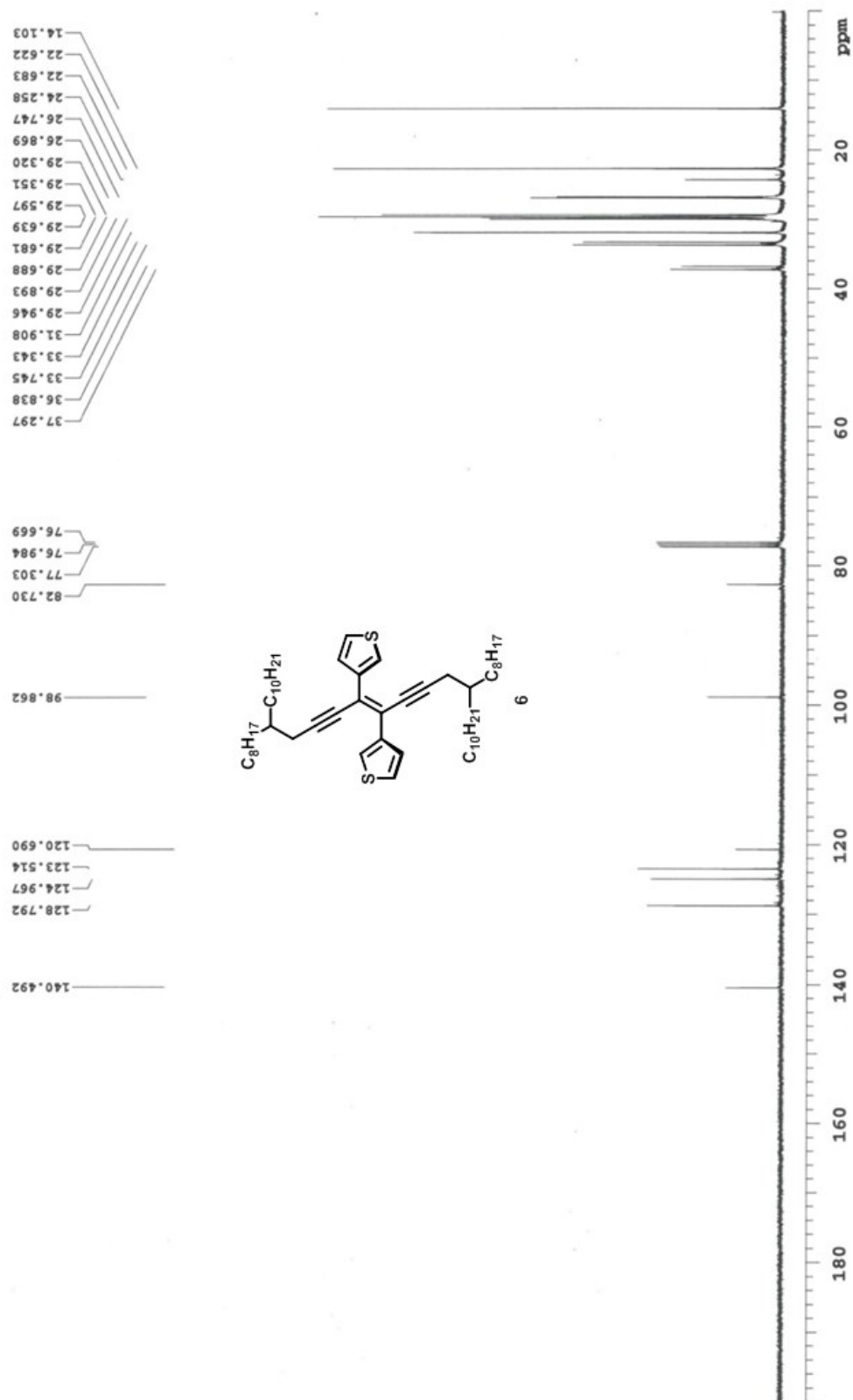


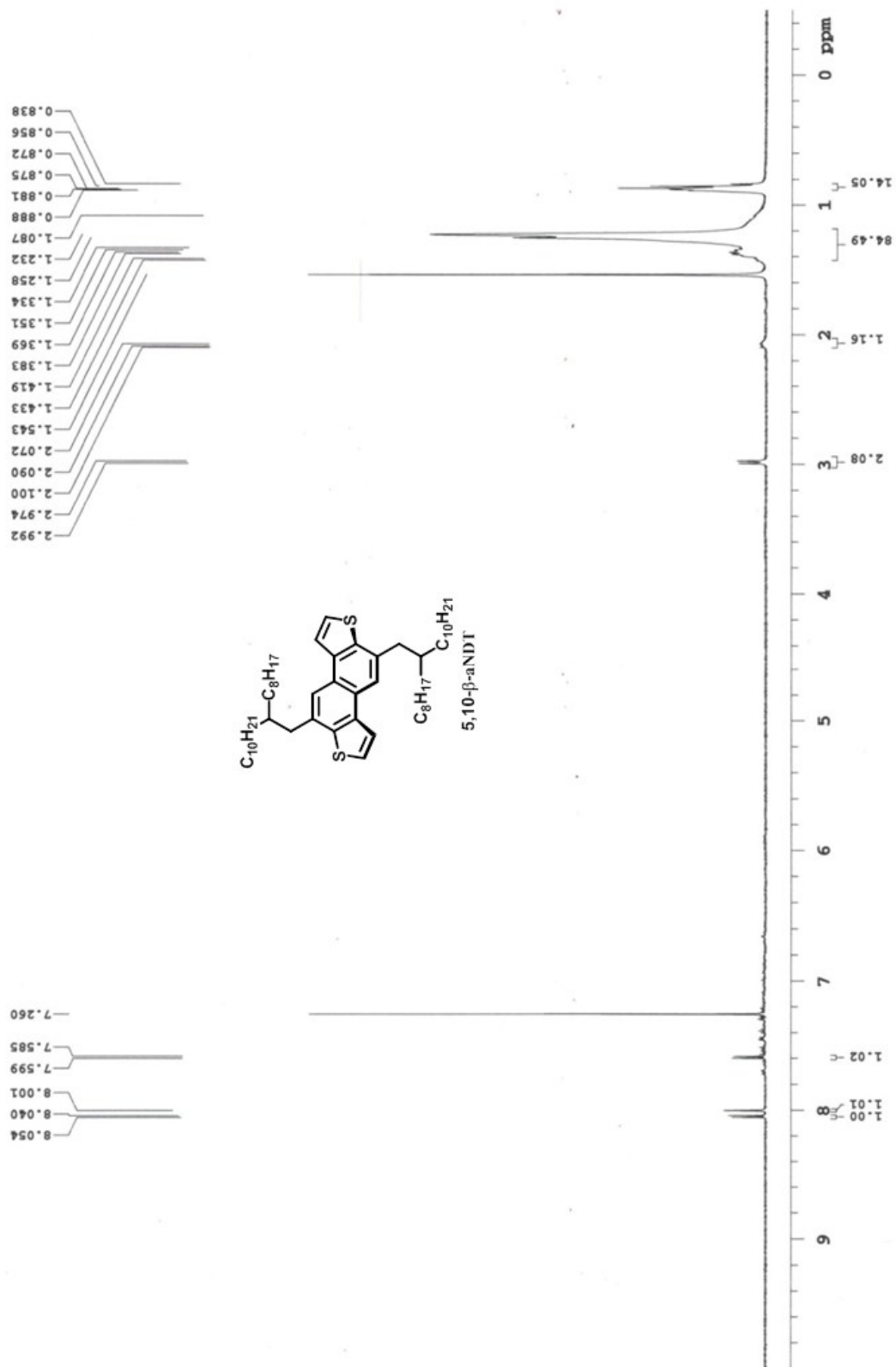


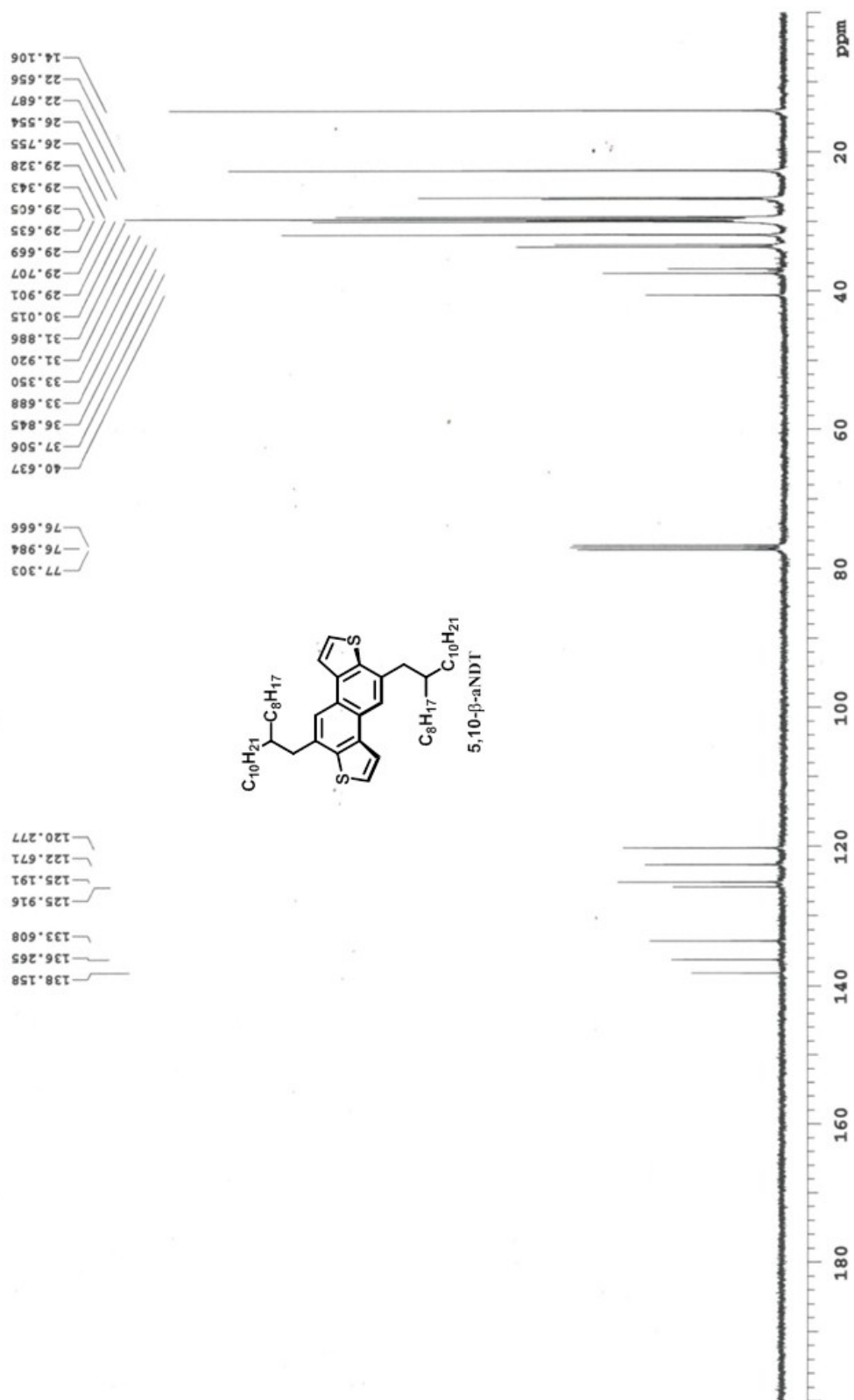


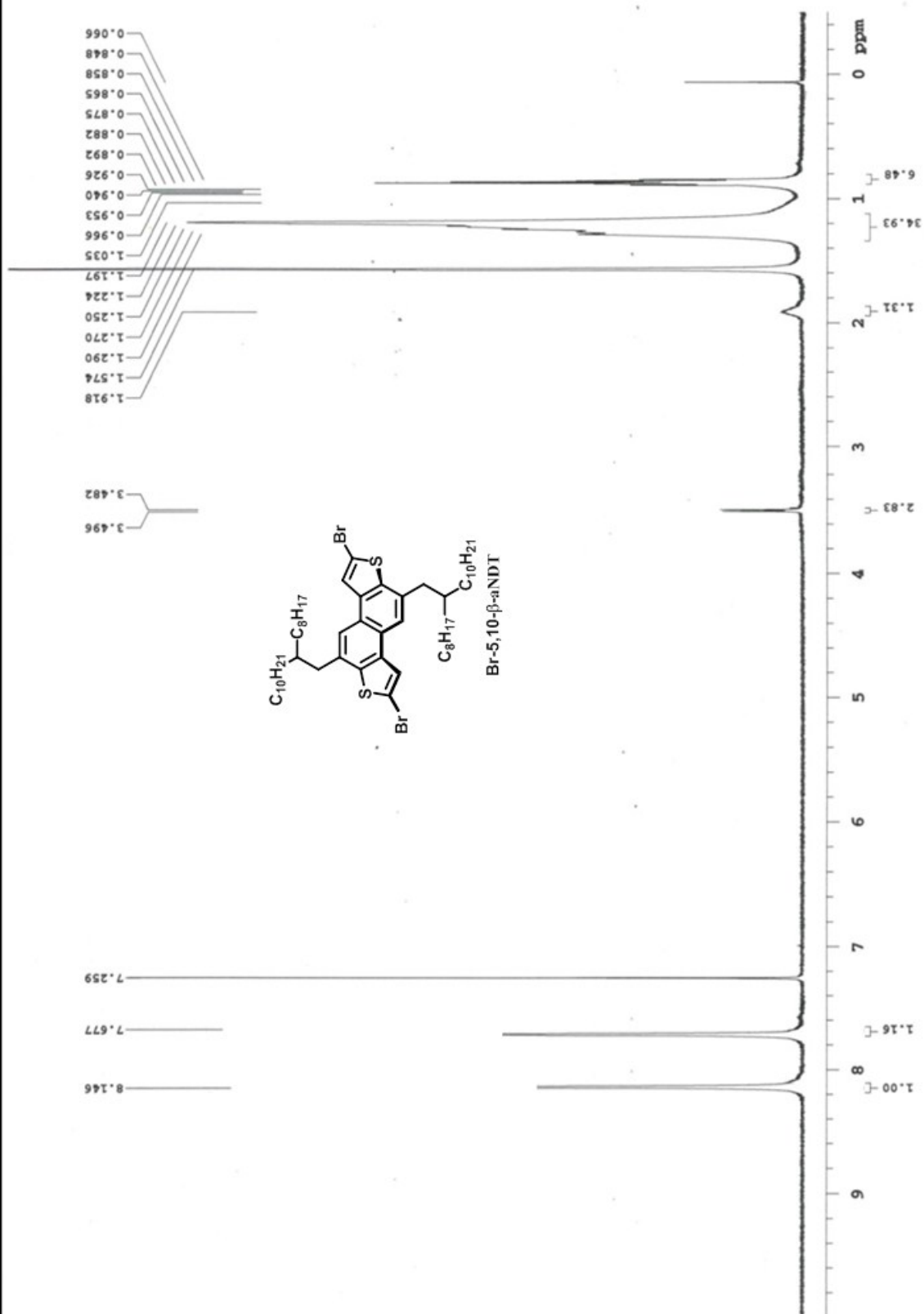


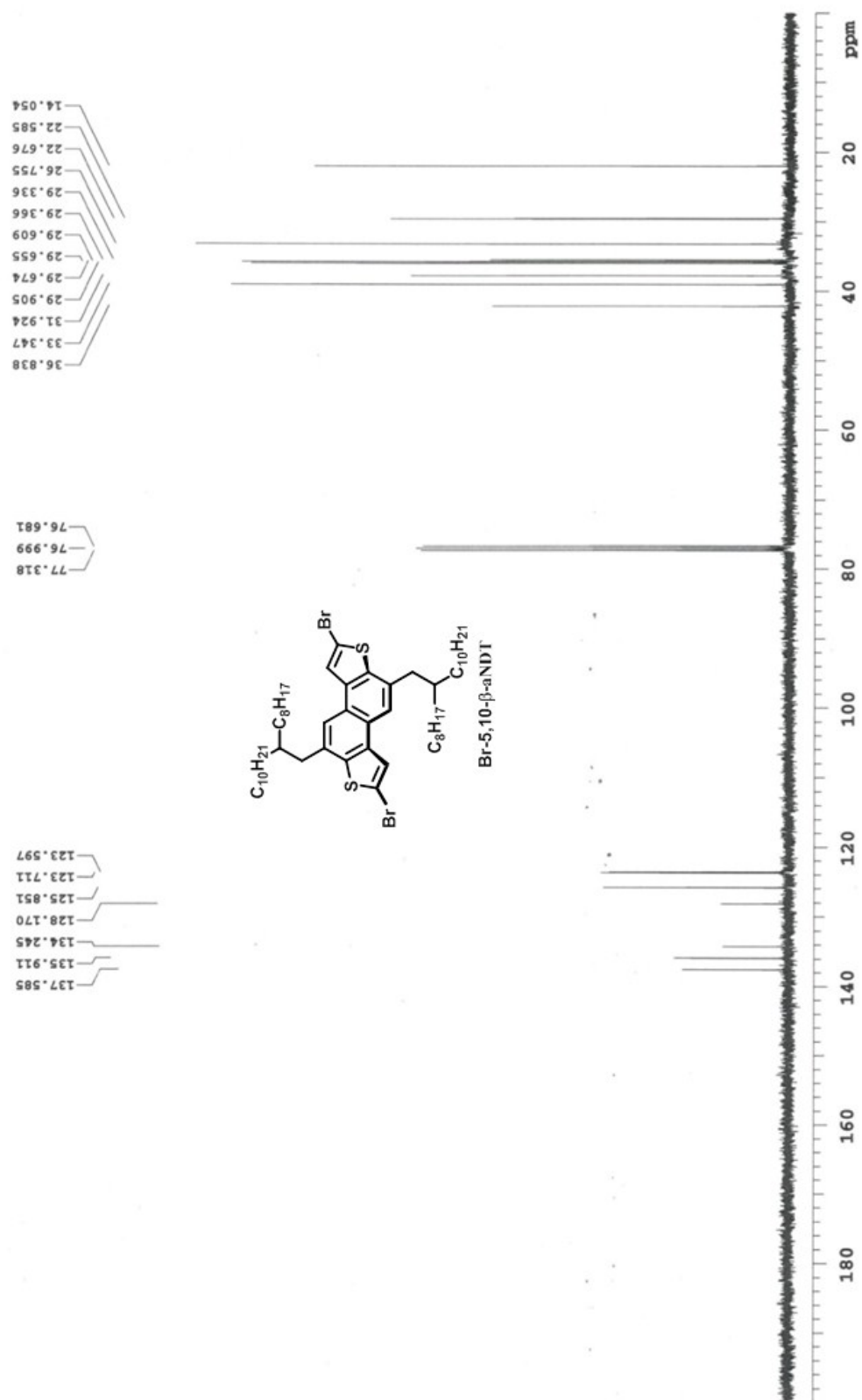




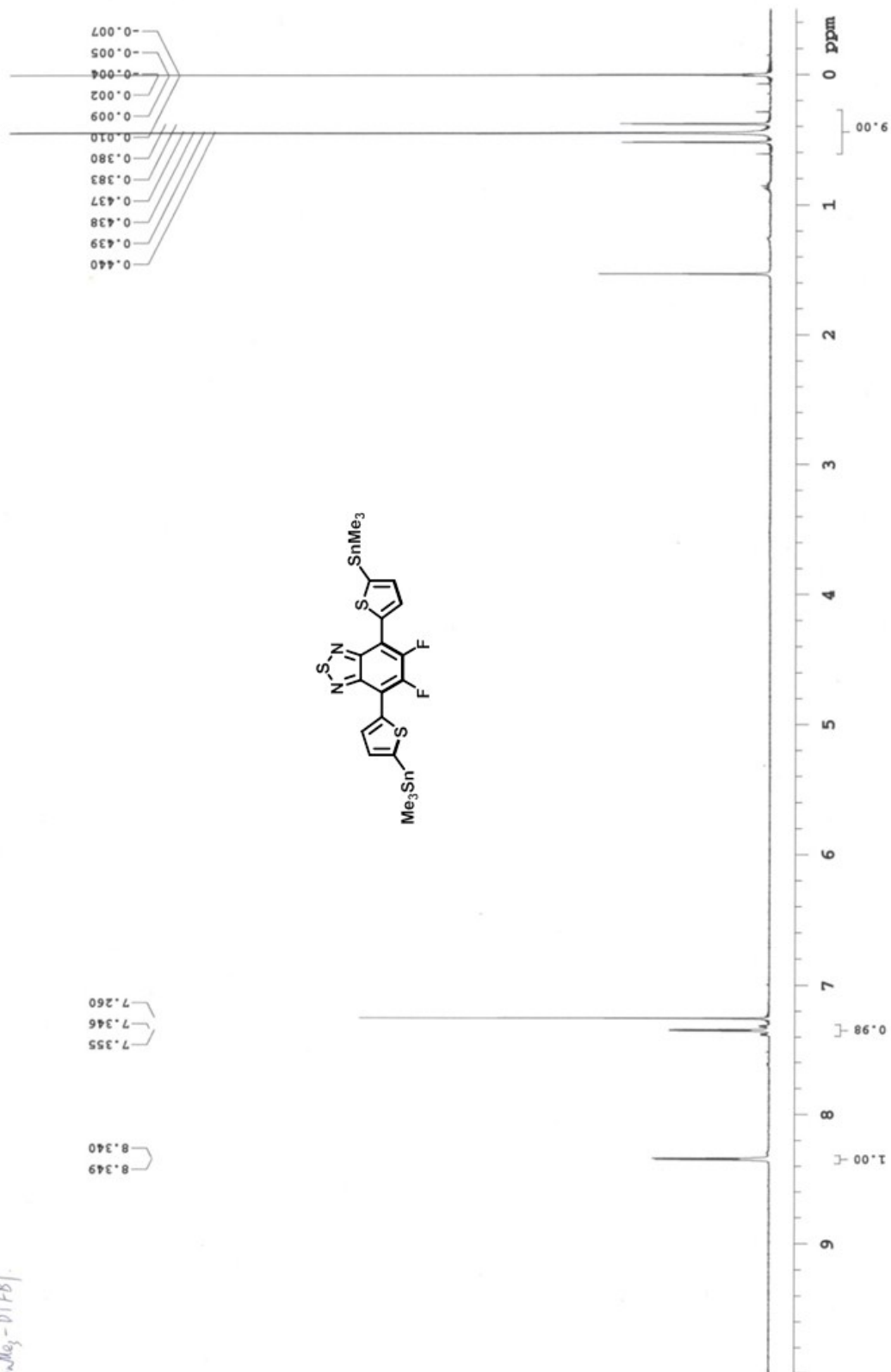


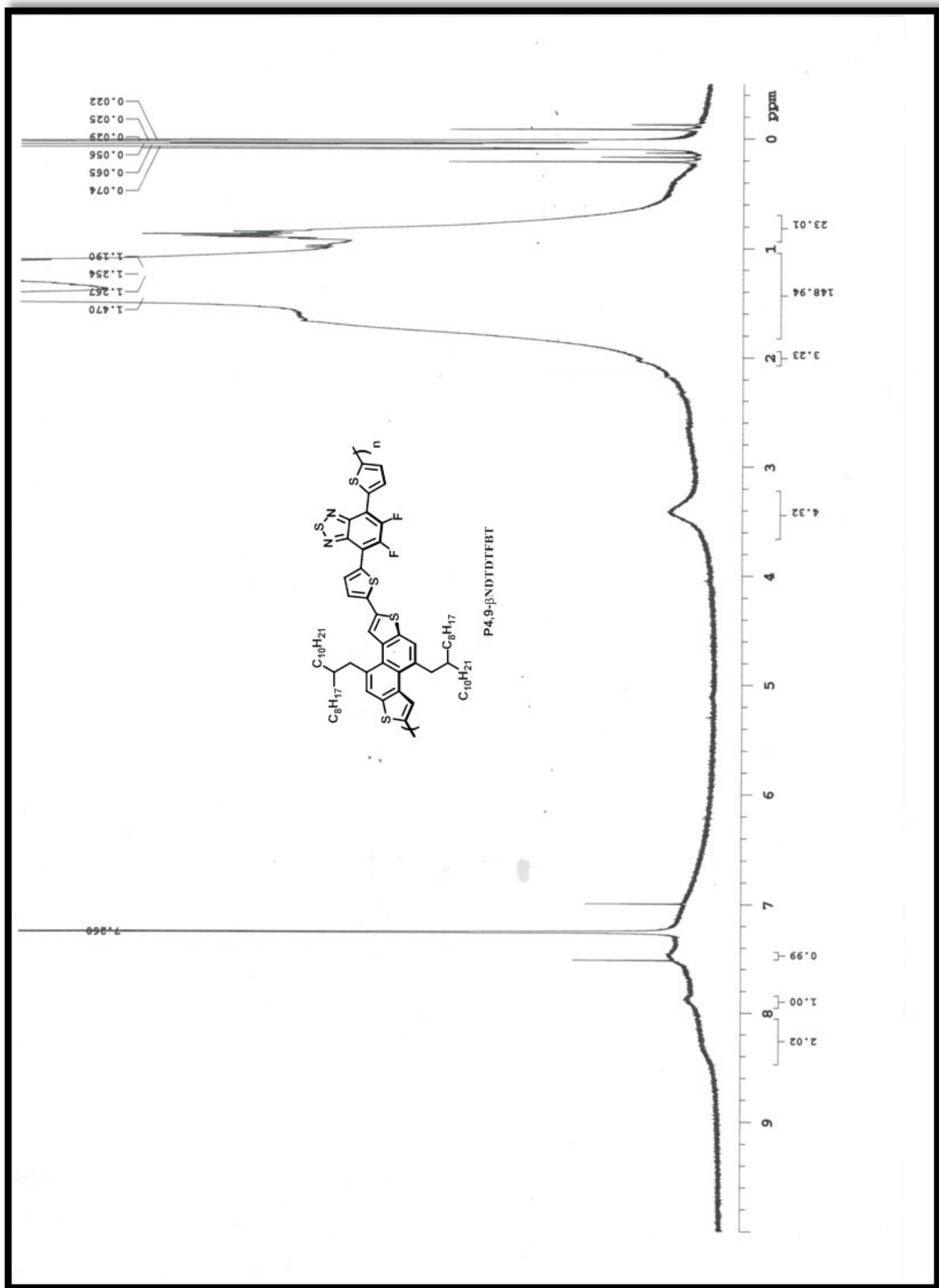


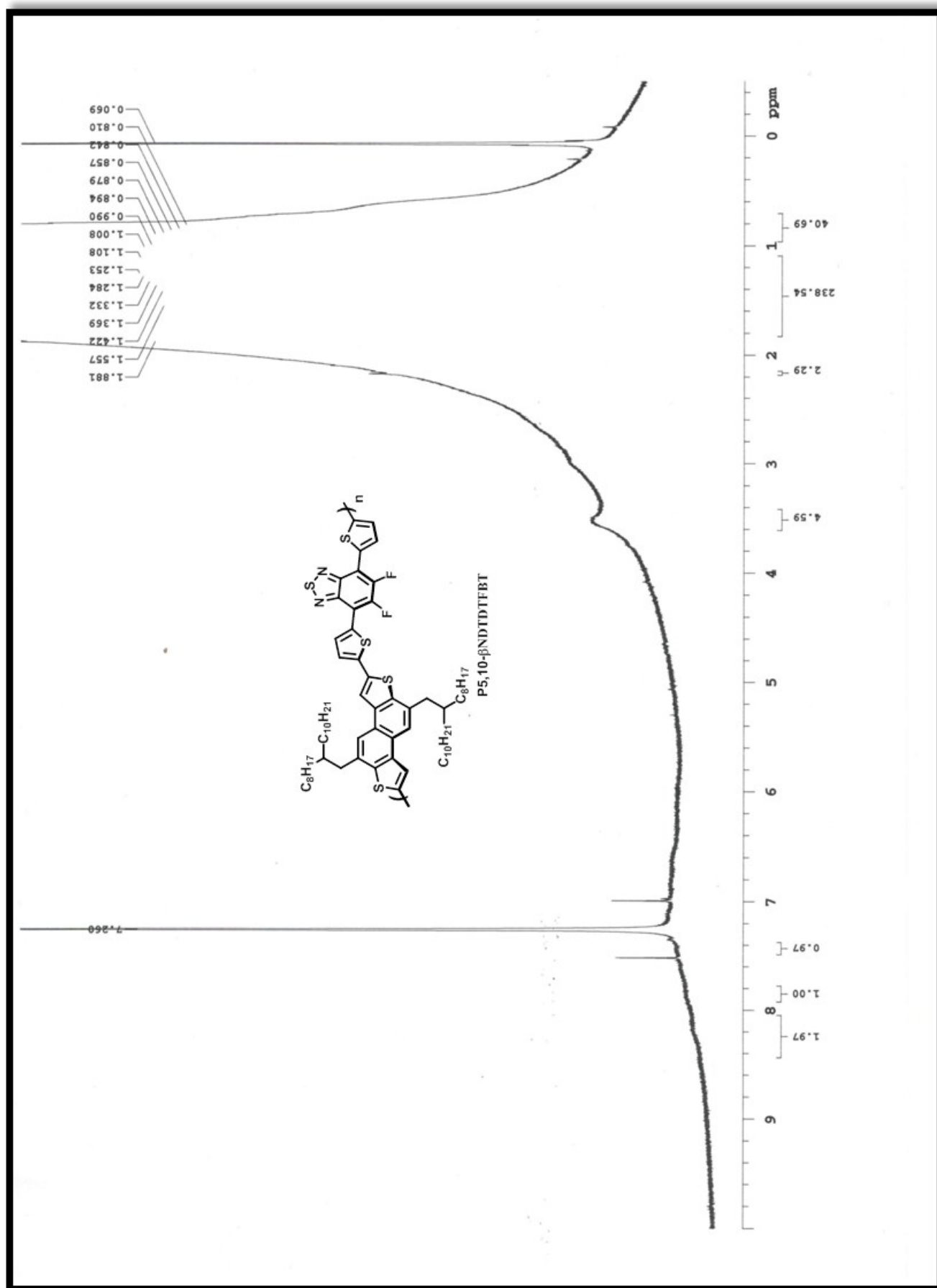




SnMe₃-DTFBT

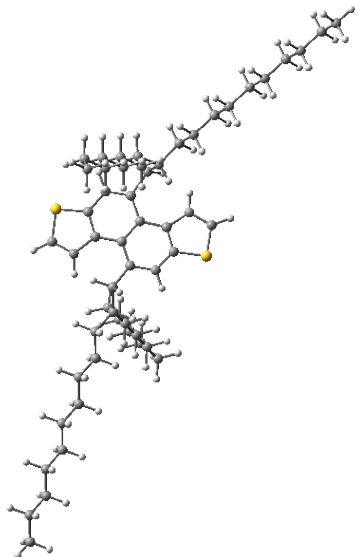






Computational Details

**Cartesian coordinates (Å) of the Gaussian B3LYP/6–311G(d,p) optimized structures:
4,9-b-aNDT**



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Will use up to 8 processors via shared memory.

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Symbolic Z-matrix:

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C	-2.23436	0.61919	0.00528
C	-2.95328	1.84244	0.00629
C	-4.37467	1.81186	0.00757
C	-5.04515	0.61331	0.00775
C	-0.81266	0.64995	0.00389
C	-2.23157	3.06778	0.0059
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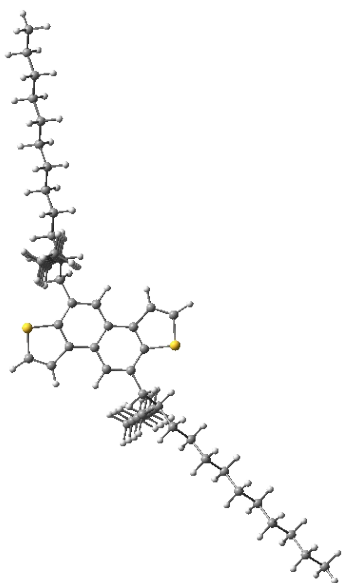
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H	-6.07668	3.02114	0.51336
C	-0.04545	-0.68534	0.00324
H	0.88937	-0.55932	-0.50187
H	-0.62566	-1.42981	-0.50076
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H	-0.25335	4.72673	-8.70606
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H	1.37058	-4.99651	2.40876
C	2.22834	-4.70884	4.35723
H	2.82924	-3.97601	4.85399
H	1.29449	-4.8111	4.86945
C	2.96437	-6.06157	4.35675
H	3.89822	-5.95931	3.84452
H	2.36346	-6.79439	3.85998
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H	3.35635	-8.59228	5.31121
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H	3.28025	-8.40687	7.7719
C	4.95013	-9.65734	7.2592
H	4.34813	-10.39076	6.76464
H	5.88284	-9.5557	6.74479
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H	5.7221	-11.04036	8.71052
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H	0.3685	-0.6302	4.13714
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H	3.07321	0.69331	3.8523
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C	2.39524	0.12213	5.80912
H	1.46042	-0.00388	6.31423
H	2.9283	-0.80563	5.80866
C	3.23031	1.19362	6.53449
H	4.16513	1.31963	6.02938
H	2.69725	2.12138	6.53495
C	3.48716	0.74845	7.9862
H	4.02022	-0.17931	7.98575
H	2.55235	0.62244	8.49131
C	4.32224	1.81994	8.71158
H	5.25705	1.94595	8.20647
H	3.78917	2.7477	8.71203
C	4.57908	1.37477	10.16329
H	5.1593	2.11925	10.66728
H	3.64427	1.24876	10.6684
H	5.11215	0.44701	10.16283

5,10-b-aNDT



%mem=24GB

%nprocshared=8

Will use up to 8 processors via shared memory.

%chk=b510NDTRegularR.chk

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C	-2.95309	1.83357	-0.02659
C	-4.37446	1.80227	-0.02775
C	-5.04843	0.76688	0.57208
H	-0.27086	-0.00708	1.09359
C	-0.81615	0.81314	0.60312
C	-2.22781	2.89214	-0.63956
H	-4.91965	2.6225	-0.51811
C	-0.85505	2.89791	-0.62419
C	-0.14166	1.84774	0.00344
C	-3.01497	4.02815	-1.31886
H	-4.08477	4.00797	-1.32167
C	-2.35736	5.05333	-1.91311
H	-2.90978	5.84915	-2.36742
S	-0.6593	4.43878	-1.55344
C	-2.17467	-1.41284	1.89462
C	-2.92946	-2.57435	2.56753
S	-4.4356	-1.73755	2.05424
H	-1.23318	-1.39953	1.89988
H	-2.67461	-3.46846	3.09716
C	1.39786	1.88611	0.00196
H	1.74119	2.39194	-0.8762
H	1.77956	0.88654	0.01001
C	-6.58796	0.72858	0.57339
H	-6.96961	1.72817	0.56533
H	-6.9314	0.22274	1.4515
C	1.89389	2.6351	1.25279
H	1.55056	2.12927	2.13095
C	3.43341	2.67347	1.25131

H	3.81512	1.6742	1.27705
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C	3.92888	3.44427	2.48904
H	3.56803	2.9656	3.37536
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C	5.46876	3.45721	2.50326
H	5.83358	2.45192	2.53784
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C	5.96424	4.22602	3.74222
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H	5.59953	5.23135	3.70757
C	7.50412	4.23879	3.75654
H	7.86505	4.72038	2.87184
H	7.86884	3.2334	3.78942
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H	7.63968	4.52312	5.88159
H	7.63387	6.01045	4.9646
C	9.53948	5.01968	5.01025
H	9.89939	5.50267	4.1259
H	9.90521	4.01462	5.04172
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C	11.57483	5.80056	6.26397
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H	11.94121	4.79571	6.29472
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H	-13.06247	-0.61741	-3.20881
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H	-12.83388	-1.89341	-5.30921
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C	-15.22508	-3.16277	-5.68071
H	-14.85445	-4.16624	-5.65691
H	-14.87015	-2.67228	-6.56295
C	-16.7649	-3.18435	-5.68961
H	-17.11983	-3.67512	-4.80753
H	-17.13554	-2.18086	-5.71308
C	-17.26046	-3.94385	-6.93427
H	-16.88934	-4.94716	-6.9111
H	-18.33033	-3.95935	-6.94015
H	-16.90601	-3.45275	-7.81637
C	1.34453	4.07373	1.24121
H	1.68786	4.57956	0.36305
H	0.27487	4.04708	1.24223
C	1.84056	4.82272	2.49204
H	1.49723	4.31689	3.37019
H	2.91023	4.84938	2.49101
C	1.2912	6.26136	2.48045
H	1.63453	6.76719	1.60229
H	0.22154	6.2347	2.48148
C	1.78723	7.01034	3.73128
H	2.8569	7.037	3.73026
H	1.4439	6.50452	4.60944
C	1.23787	8.44898	3.7197

H	1.5812	8.95481	2.84154
H	0.16821	8.42232	3.72072
C	1.7339	9.19797	4.97053
H	2.80357	9.22463	4.9695
H	1.39057	8.69214	5.84868
C	1.18454	10.6366	4.95894
H	0.11546	10.61045	4.99473
H	1.49945	11.13145	4.06403
C	1.72063	11.40068	6.18385
H	2.78911	11.43833	6.14115
H	1.32834	12.39618	6.18297
H	1.4169	10.89842	7.07849
C	-6.58958	0.70767	-1.94133
H	-5.51991	0.73428	-1.94224
H	-6.97123	1.70725	-1.94939
C	-7.0855	-0.04127	-3.19223
H	-6.70385	-1.04086	-3.18416
H	-8.15517	-0.06788	-3.19132
C	-6.5912	0.68676	-4.45605
H	-6.97285	1.68634	-4.46412
H	-5.52153	0.71337	-4.45696
C	-7.08712	-0.06218	-5.70695
H	-6.70205	-1.06047	-5.70102
H	-8.15669	-0.09244	-5.7039
C	-6.59788	0.66923	-6.97079
H	-6.98239	1.66774	-6.97638
H	-5.5283	0.69888	-6.97419
C	-7.09465	-0.07915	-8.22169
H	-8.16426	-0.10789	-8.21882
H	-6.71099	-1.07798	-8.21558
C	-6.60415	0.65142	-9.48553
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H	-5.53451	0.67883	-9.48916
C	-7.10275	-0.09573	-10.73643
H	-8.17242	-0.12206	-10.73343
H	-6.76092	0.41118	-11.61455
H	-6.72135	-1.09542	-10.73045

The HT-GPC Distribution Plots

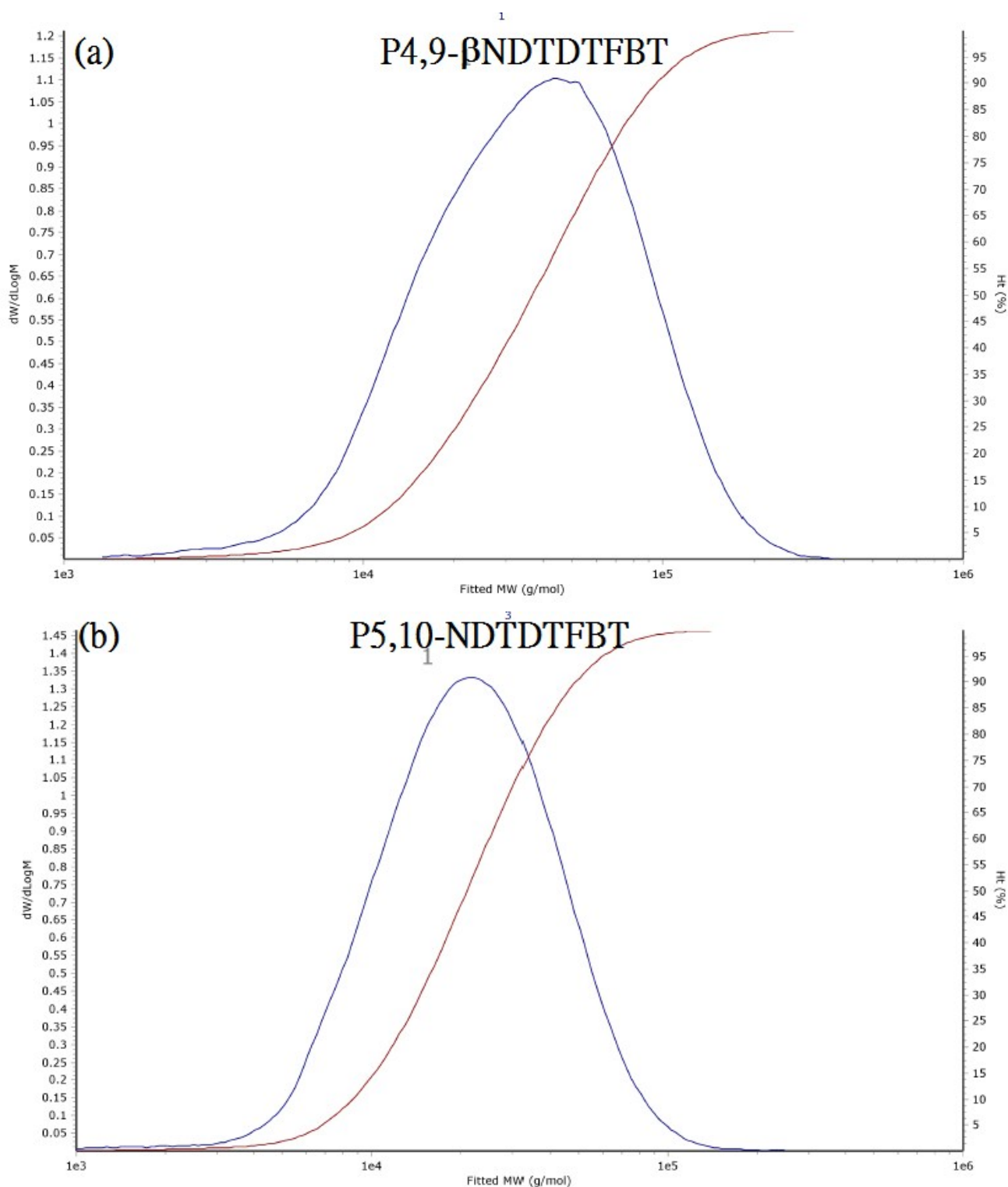


Figure S1. The HT-GPC distribution plots of (a) **P4,9- β NDTDTFBT** and (b) **P5,10- β NDTDTFBT** with a Angilent PL-GPC 220 using 1,2,4-trichlorobenzene (1,2,4-TCB) as eluent under 160 °C and calibrated with polystyrene standards..

1D- GIWAXS Profiles

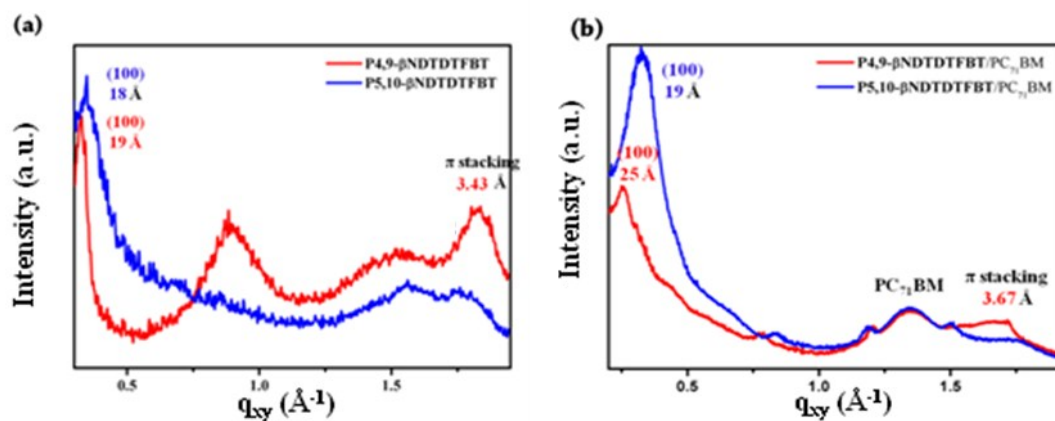


Figure S2. 1-D in-plane GIWAXS profiles of **P4,9- β NDTDTFBT** and **P5,10- β NDTDTFBT** (a); out-of-plane of **P4,9- β NDTDTFBT:PC₇₁BM** and **P5,10- β NDTDTFBT:PC₇₁BM** blend films (b).