

SUPPORTING INFORMATION

Donor Conjugated Polymers-based on Alkyl chain Substituted Oligobenzo[c]thiophene derivatives with Well-balanced Energy Levels for Bulk Heterojunction Solar Cells

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Fig.S7 XRD patterns of drop-cast (a) CN-PHTBTPB and (b) CN-POTBTPB polymer film.

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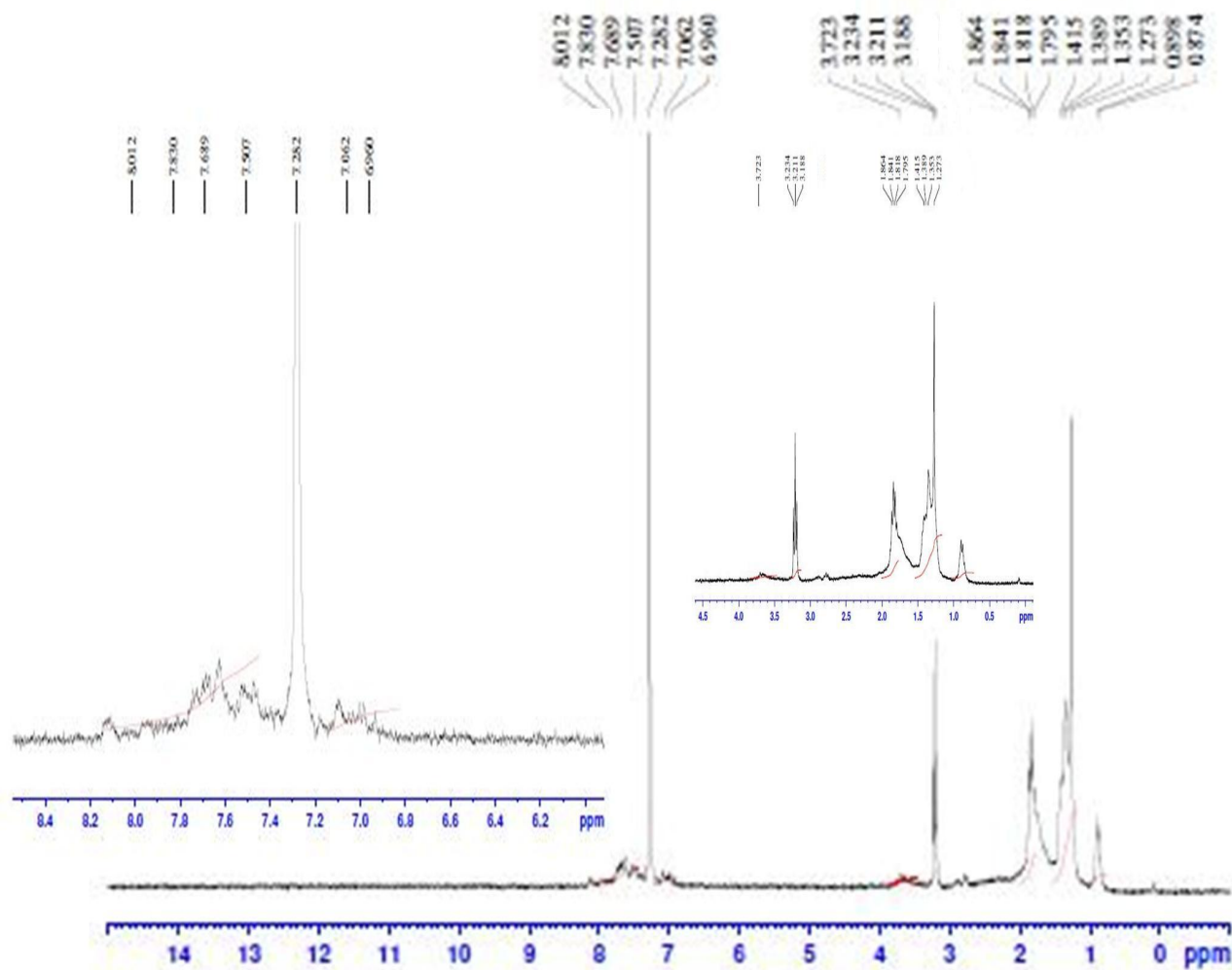


Fig. S1. ^1H -NMR spectrum of monomer (10) in CDCl_3 as solvent.

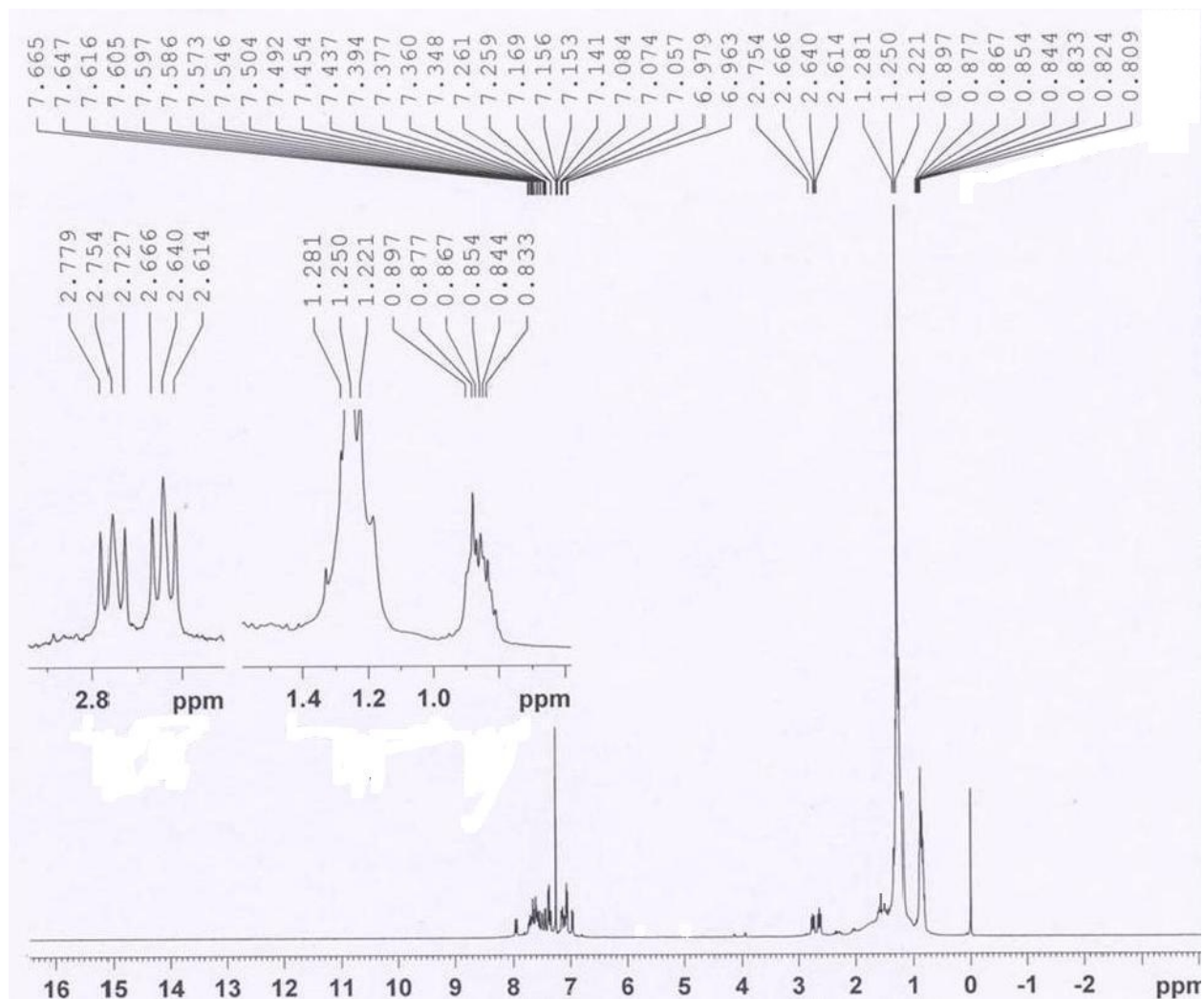


Fig. S2. ^1H -NMR spectrum of monomer (11) in CDCl_3 as solvent.

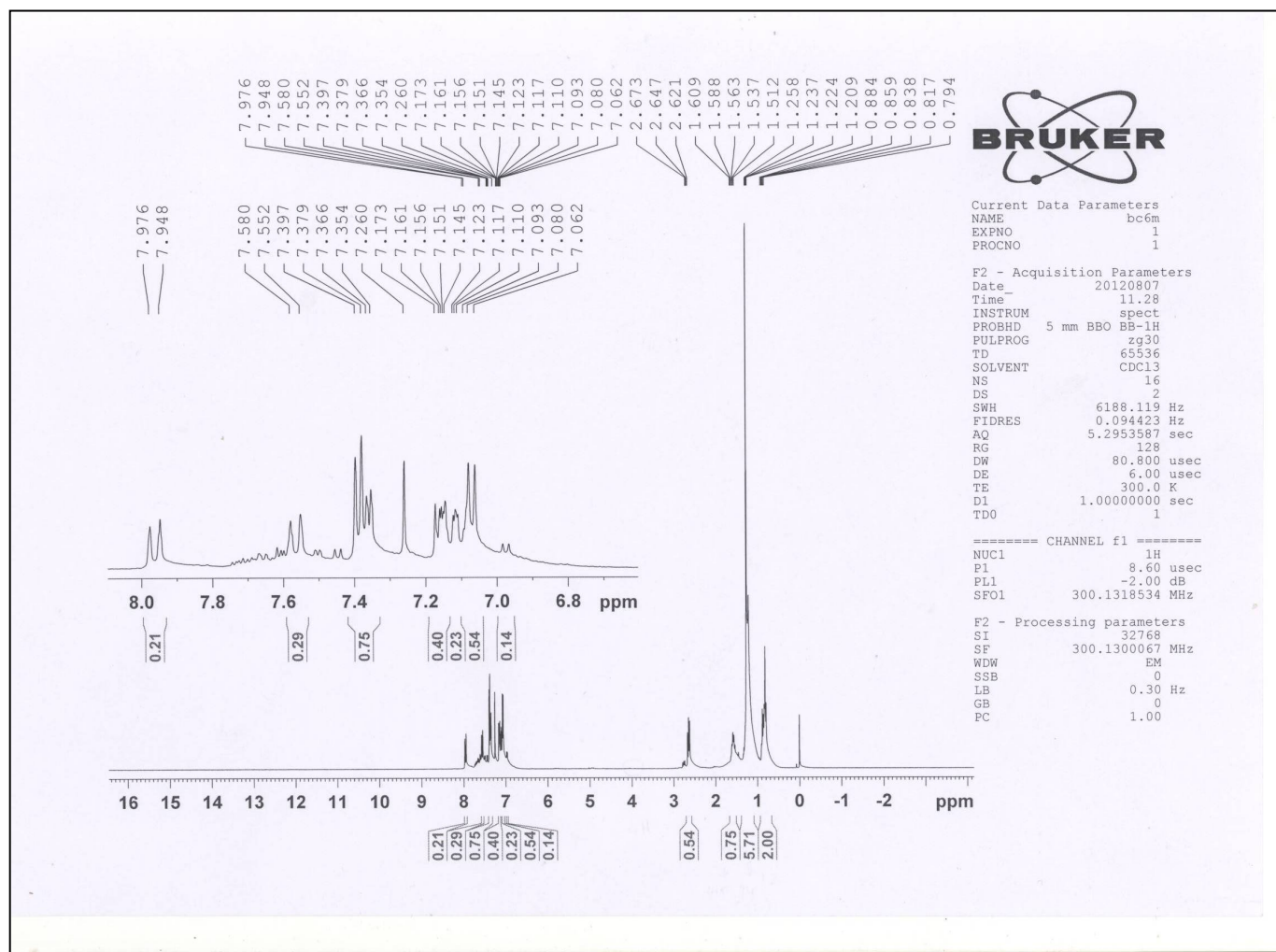


Fig. S3. ^1H -NMR spectrum of CN-PHTBTPB polymer in CDCl_3 and TMS as internal standard.

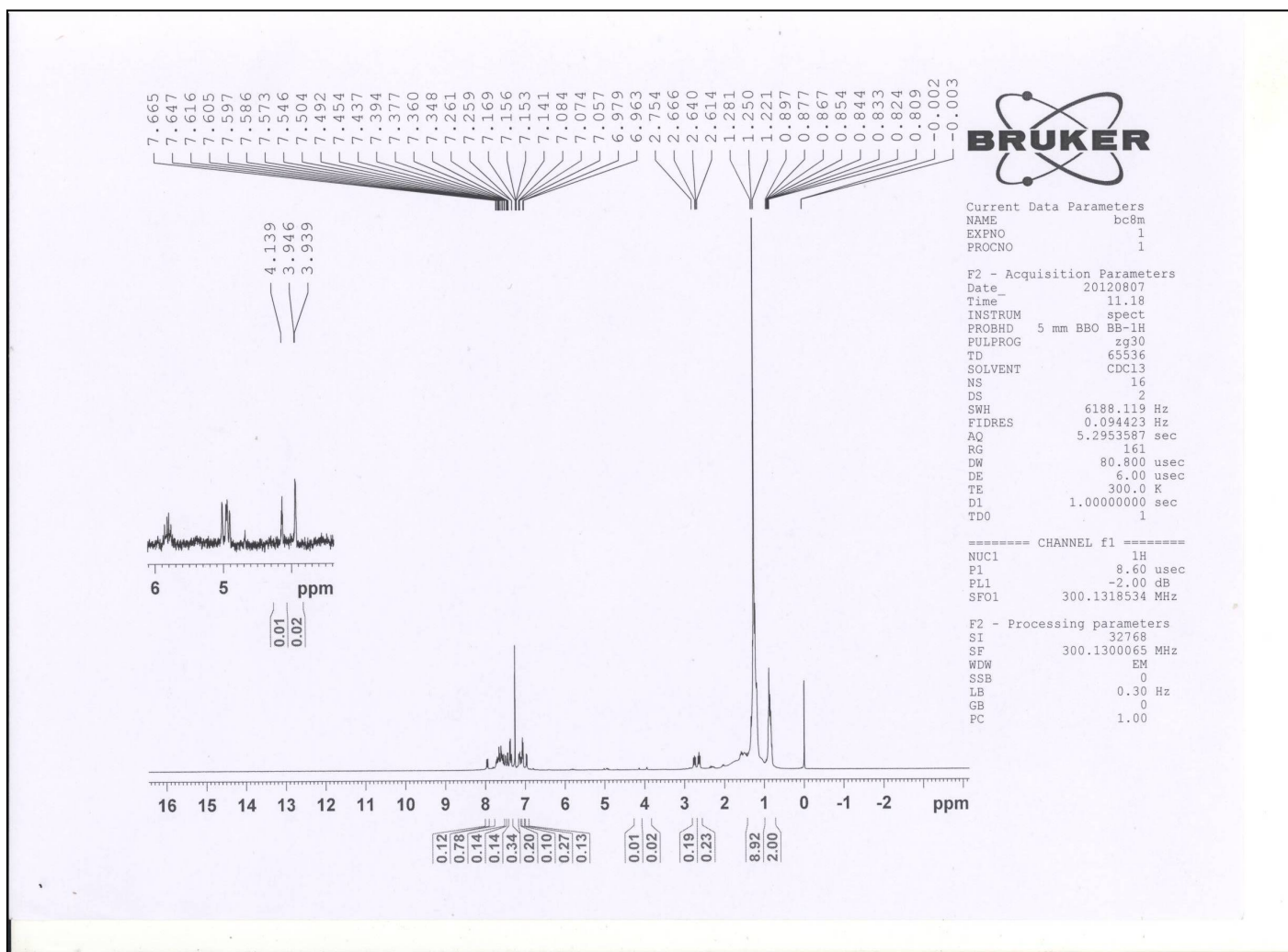


Fig. S4. ^1H -NMR spectrum of CN-POTBTPB polymer in CDCl_3 and TMS as internal standard.

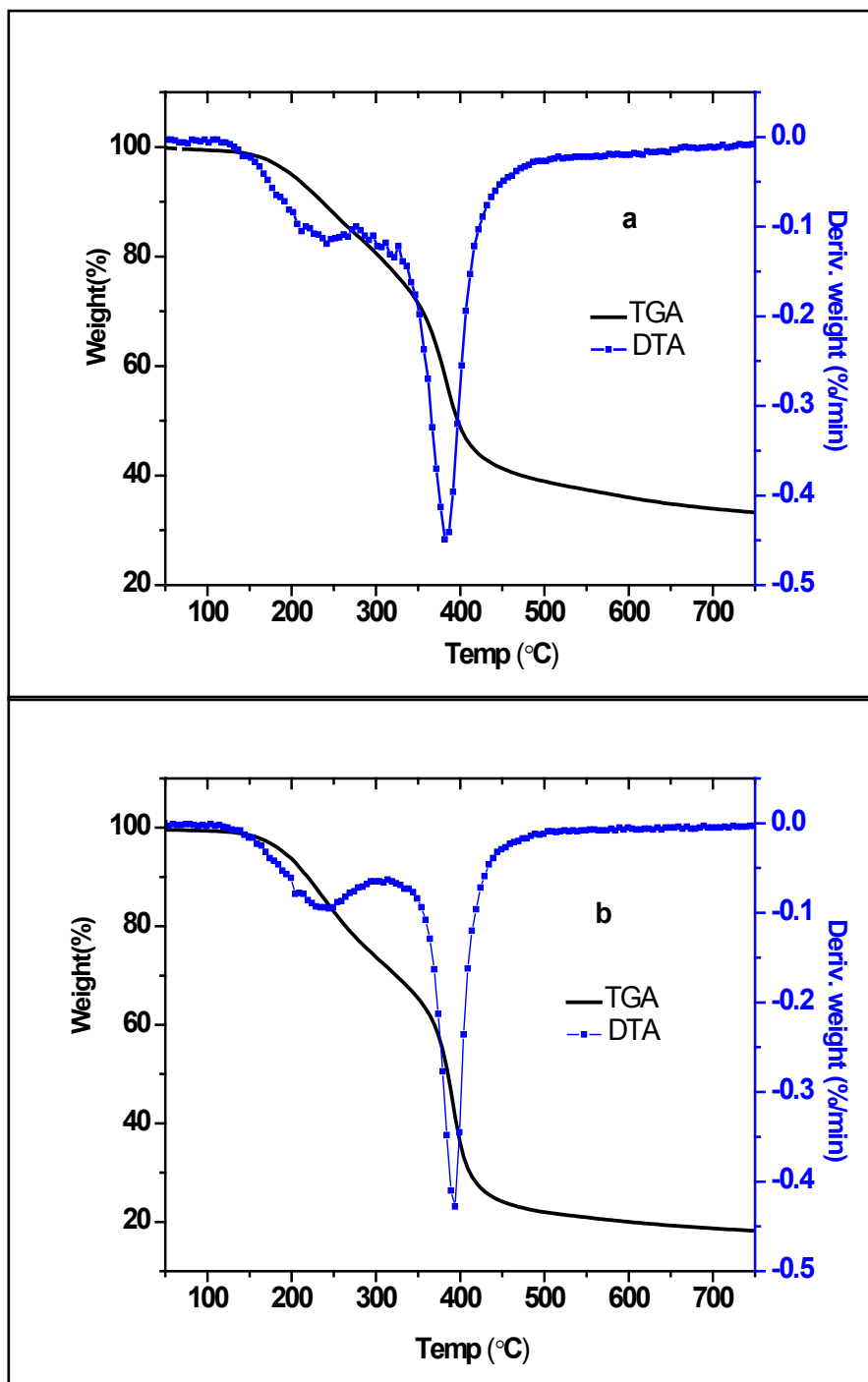


Fig. S5. Thermogravimetric (black) and its corresponding derivative weight (blue) curve for (a) CN-PHTBTPB and (b) CN-POTBTPB polymer.

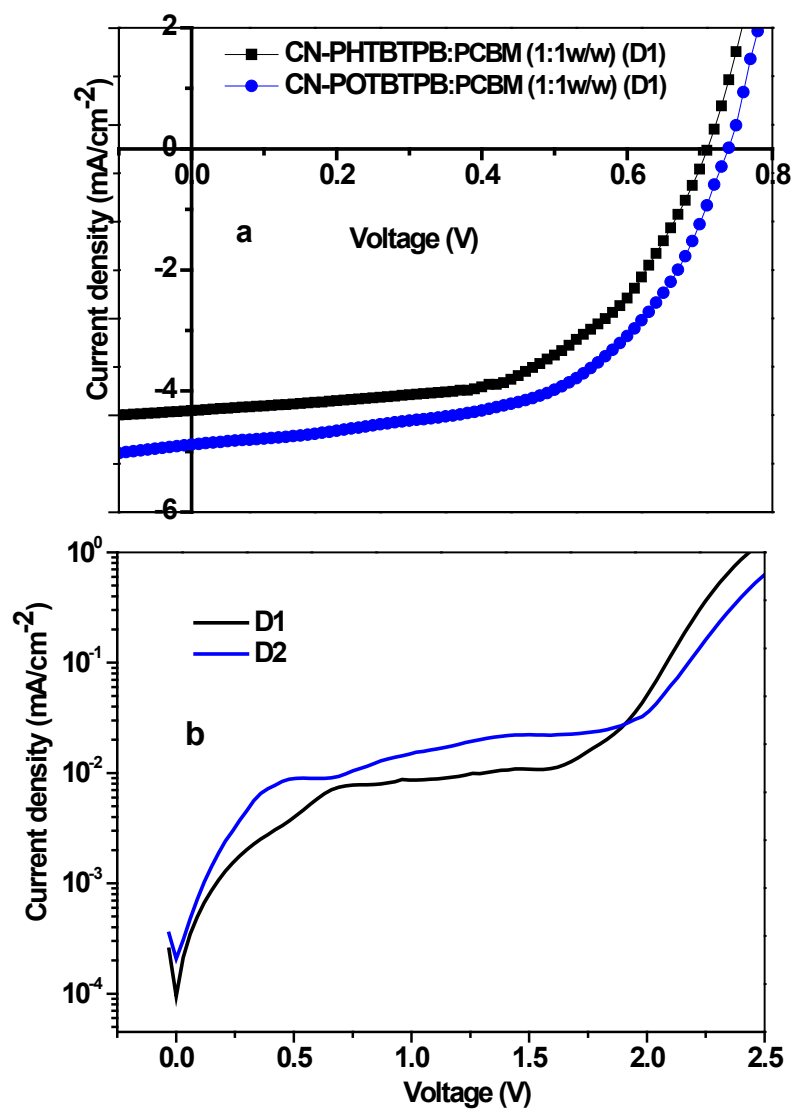


Fig. S6 The current density–voltage (J-V) characteristic curves of (a) ITO/PEDOT:PSS (40nm)/CN-PHTBTPB:PCBM (100nm) (1:1 w/w)/LiF(5nm)/Al(110nm) (**D1**) and ITO/PEDOT:PSS/CN-POTBTPB:PCBM (100nm) (1:1 w/w)/LiF(5nm)/Al (110nm) (**D2**) under AM 1.5G condition; (b) Semi-logarithmic J-V characteristic curves under dark conditions.

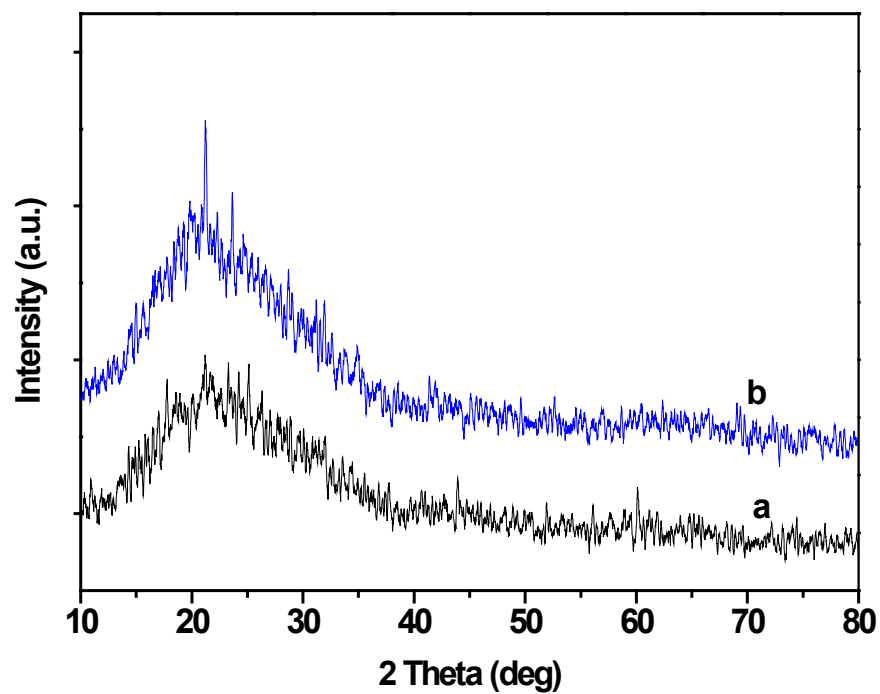


Fig. S7. XRD patterns of drop-cast (a) CN-PHTBTPB and (b) CN-POTBTPB polymer film.

DATA: XYZ coordinates of **CN-PHTBTPB** polymer optimized at B3LYP/6-31G(d) level using G09 package.

S	13.21565	-2.51018	-0.59293
C	12.16028	-1.53798	0.43362
C	12.89775	-0.82608	1.3632
C	14.30259	-1.07852	1.24082
C	14.62291	-1.95723	0.246
H	15.04296	-0.61584	1.88583
H	15.60376	-2.31256	-0.04146
C	12.32926	0.05597	2.44909
H	11.28115	0.28953	2.23754
H	12.86573	1.01526	2.45304
C	12.42822	-0.57981	3.85134
H	13.47611	-0.83218	4.06584
H	11.87944	-1.53131	3.84877
C	11.88323	0.32958	4.95956
H	10.83634	0.58471	4.73846
H	12.43538	1.28129	4.95409
C	11.96803	-0.29825	6.35674
H	13.01453	-0.55808	6.57626
H	11.41265	-1.24789	6.36227
C	11.42904	0.60874	7.47054
H	10.38411	0.86978	7.25065
H	11.98589	1.55664	7.46682
C	11.51428	-0.02794	8.86149
H	11.12275	0.64366	9.63402

H	12.55172	-0.26915	9.12442
C	10.9373	-0.95983	8.90671
S	10.72254	-1.54539	0.18812
C	9.8849	-0.08864	-0.24307
H	8.34348	-0.87975	-0.42521
C	6.4735	-3.03359	-0.54388
C	7.48503	-3.27848	-0.23982
C	10.13646	-3.9885	0.49631
C	8.4801	-2.25682	-0.17092
C	7.81707	-4.57571	0.05698
C	9.14541	-4.93207	0.43984
H	9.83553	-2.62845	0.18001
H	7.05762	-5.35047	-0.00185
H	9.36784	-5.96738	0.68266
C	11.14885	-4.25634	0.78071
C	7.19123	-0.08655	-0.77411
C	7.18211	1.14798	-1.41607
C	5.90426	1.71078	-1.57924
S	4.87756	0.92265	-1.07189
H	5.55297	-0.54053	-0.35618
H	8.0881	1.6193	-1.78195
C	5.73465	2.65927	-2.0716
H	3.45021	1.06493	-1.03726
C	2.9097	0.23015	-0.60615
C	2.66404	2.10373	-1.4699
N	3.2701	3.2757	-2.02647
C	3.7518	4.23653	-2.47752

C	1.18523	2.13578	-1.36231
C	-1.65694	2.34247	-1.13981
C	0.53416	3.3862	-1.33411
C	0.3745	0.98224	-1.2858
C	-1.00902	1.10333	-1.17908
H	-0.8497	3.50351	-1.2187
H	1.13955	4.28262	-1.38192
O	-1.59439	0.18938	-1.15515
O	0.91302	-0.29141	-1.31168
C	-1.504	4.68923	-1.13471
H	0.94042	-0.91026	-2.61275
H	-0.08105	-0.9476	-3.01757
C	1.54975	-0.30162	-3.29571
H	1.51786	-2.30944	-2.46007
H	0.91906	-2.85536	-1.71933
C	2.53263	-2.23078	-2.04781
H	1.55239	-3.08434	-3.78429
H	0.53218	-3.17025	-4.18608
C	2.12722	-2.51504	-4.5292
H	2.16032	-4.48561	-3.64039
H	1.59361	-5.05048	-2.8856
C	3.18387	-4.39605	-3.24767
H	2.18816	-5.27988	-4.95263
H	1.16335	-5.37572	-5.34115
C	2.74777	-4.71122	-5.71003
H	2.80764	-6.67555	-4.80752
H	2.25161	-7.24299	-4.04615

C	3.83424	-6.57899	-4.42332
H	2.83179	-7.47652	-6.11591
H	1.806	-7.57548	-6.49857
C	3.38617	-6.90937	-6.87714
H	3.4552	-8.86738	-5.96119
H	3.45859	-9.41293	-6.91172
H	2.90089	-9.47156	-5.23232
C	4.49312	-8.79977	-5.61222
H	-0.79345	5.91137	-1.36001
H	-0.29113	5.86992	-2.33653
C	-0.0224	6.03892	-0.58652
H	-1.80634	7.04645	-1.30915
H	-2.30079	7.02975	-0.3293
C	-2.58534	6.85379	-2.05684
H	-1.1579	8.41605	-1.54868
H	-0.66603	8.42326	-2.5324
C	-0.36076	8.58072	-0.80849
H	-2.16027	9.57542	-1.47605
H	-2.65413	9.56544	-0.49326
C	-2.95622	9.41331	-2.21723
H	-1.51984	10.94987	-1.70817
H	-1.02862	10.96029	-2.69254
C	-0.72008	11.10703	-0.96904
H	-2.51793	12.11199	-1.62809
H	-3.01112	12.10053	-0.64449
C	-3.31682	11.9575	-2.36866
H	-1.87773	13.48751	-1.8554

H	-1.38589	13.49977	-2.83852
C	-1.07961	13.64175	-1.11521
H	-2.88082	14.64265	-1.77283
H	-3.36302	14.67982	-0.78808
H	-3.67311	14.53369	-2.52378
C	-2.39332	15.6098	-1.94124
C	-3.13201	2.41868	-1.01299
N	-3.83209	3.35549	-1.83816
C	-4.43118	4.08116	-2.52533
H	-3.81392	1.57323	-0.17898
C	-3.18655	0.9236	0.42765
C	-5.22761	1.41712	0.02758
C	-6.33687	2.03402	-0.53605
C	-7.56126	1.58372	-0.0087
S	-7.4413	0.60537	0.97141
H	-5.74834	0.23513	1.22597
H	-6.26374	2.80022	-1.29663
S	-8.5222	1.98096	-0.31791
C	-10.05628	-0.22577	0.87084
C	-10.76936	-1.13593	2.16513
C	-8.50878	-0.08241	1.656
C	-9.83631	-1.31672	3.19342
C	-7.74925	-1.47835	5.06645
C	-8.54833	-0.71663	2.91042
C	-10.03065	-2.02393	4.41948
C	-9.00672	-2.10306	5.32557
H	-7.51746	-0.80479	3.89469

H	-10.98925	-2.49248	4.61699
H	-9.14901	-2.64179	6.25826
H	-6.56063	-0.32381	3.72408
C	-6.9646	-1.53734	5.81566
C	-12.16983	-1.53944	2.11321
C	-12.84073	-2.29914	1.17068
C	-14.23537	-2.42227	1.47437
S	-14.61322	-1.77492	2.61562
H	-13.27664	-0.9754	3.36654
H	-14.92649	-2.98505	0.85484
C	-15.59878	-1.72357	3.05946
H	-12.20839	-2.99743	-0.0096
H	-11.18532	-2.63778	-0.15646
C	-12.76174	-2.73661	-0.92307
H	-12.18298	-4.53267	0.13868
H	-13.20602	-4.9042	0.29031
C	-11.62557	-4.79283	1.04871
H	-11.55668	-5.23663	-1.07152
H	-12.11223	-4.96109	-1.98048
C	-10.53205	-4.86426	-1.21779
H	-11.52702	-6.76469	-0.93927
H	-12.55213	-7.13748	-0.79456
C	-10.9733	-7.04027	-0.02942
H	-10.89847	-7.47199	-2.14696
H	-11.45058	-7.19485	-3.05634
C	-9.87335	-7.10176	-2.28977
H	-10.87585	-8.99766	-2.00863

H	-11.89023	-9.40076	-1.89856
C	-10.30055	-9.30736	-1.12737
H	-10.42233	-9.47286	-2.88596

DATA: XYZ coordinates of **CN-POTBTPB** polymer optimized at B3LYP/6-31G(d) level using G09 package.

S	13.09374300	-2.80882800	-1.39448500
C	12.10007000	-1.83080700	-0.31367900
C	12.88588100	-1.16535200	0.61033700
C	14.27819100	-1.45647100	0.43937700
C	14.54166600	-2.31909100	-0.58575900
H	15.05126200	-1.03260200	1.07255100
H	15.50223100	-2.69622200	-0.91142100
C	12.37499200	-0.29590300	1.73428200
H	11.32645900	-0.03326500	1.56215800
H	12.93437300	0.65017900	1.74311200
C	12.50374000	-0.96816200	3.11691900
H	13.55226800	-1.24683200	3.29227100
H	11.93558700	-1.90819200	3.10821100
C	12.01222800	-0.07702500	4.26429500
H	10.96407100	0.20328100	4.08354000
H	12.58247000	0.86393600	4.26495100
C	12.12948900	-0.74313400	5.64144300
H	13.17753300	-1.02676300	5.81946900
H	11.55770800	-1.68285900	5.63878200
C	11.64227800	0.14283800	6.79535700
H	10.59474600	0.42770400	6.61686900
H	12.21518700	1.08212400	6.79911100
C	11.75786200	-0.52624300	8.17093800
H	12.80517400	-0.81309200	8.34920300

H	11.18366100	-1.46486000	8.16789900
C	10.65585000	-1.78706200	-0.51517900
S	9.85699000	-0.29856400	-0.90925200
C	8.28415700	-1.03406800	-1.04870800
H	6.33588700	-3.11922400	-1.12046400
C	7.34751000	-3.40228900	-0.85160600
C	9.99505000	-4.21068000	-0.20681000
C	8.37971200	-2.41665500	-0.80725000
C	7.64336100	-4.71274100	-0.57550700
C	8.97019400	-5.11855300	-0.23874000
C	9.73175700	-2.83823400	-0.50250000
H	6.85580900	-5.46017400	-0.61545200
H	9.16377000	-6.16320200	-0.01170700
H	11.00624400	-4.51571200	0.04240500
C	7.15070100	-0.19868800	-1.35982800
C	7.16515800	1.02954800	-2.01308800
C	5.90489900	1.64128300	-2.13198000
C	4.86888600	0.89941400	-1.57621300
S	5.51393100	-0.58357600	-0.87294100
H	8.07405700	1.46087600	-2.41887200
H	5.75373000	2.59166600	-2.62656000
C	3.45111200	1.10079300	-1.48344700
H	2.89676200	0.29854100	-1.01016200
C	2.68923500	2.16196500	-1.90509400
C	3.31721800	3.29359900	-2.51823800
N	3.81702400	4.22201300	-3.01509600
C	1.21978200	2.26114700	-1.73017900

C	-1.59603500	2.60097800	-1.37356100
C	0.62465700	3.53929900	-1.71276200
C	0.36517500	1.14767800	-1.57540300
C	-1.00449000	1.33362000	-1.40333600
C	-0.74538300	3.72179000	-1.53457300
H	1.26477600	4.40605800	-1.81909600
H	-1.62621600	0.44785300	-1.31743500
O	0.84610900	-0.14909700	-1.58376700
O	-1.34305000	4.93788800	-1.46278200
C	0.80270500	-0.80287600	-2.86727400
H	-0.23511600	-0.82058700	-3.22970900
H	1.40113200	-0.23175500	-3.59096300
C	1.34641400	-2.21374800	-2.69850200
H	0.76144300	-2.72358400	-1.92189400
H	2.37777700	-2.15282400	-2.32607000
C	1.31129000	-3.02286200	-4.00200500
H	0.27521100	-3.09092100	-4.36464700
H	1.87347100	-2.48876200	-4.78180900
C	1.88686700	-4.43614100	-3.84284200
H	1.33083600	-4.96750600	-3.05644900
H	2.92465600	-4.36430600	-3.48541700
C	1.85175000	-5.26191000	-5.13527100
H	0.81283900	-5.34019400	-5.48866700
H	2.40078100	-4.72618900	-5.92378200
C	2.44008000	-6.66946800	-4.97560600
H	1.89397600	-7.20464800	-4.18429000
H	3.48018500	-6.59045300	-4.62527100

C	2.40362100	-7.50071000	-6.26465300
H	1.36420700	-7.58275300	-6.61305000
H	2.94737400	-6.96516900	-7.05584800
C	2.99738100	-8.90294100	-6.09622100
H	2.95682700	-9.47033500	-7.03299700
H	2.45194800	-9.47565200	-5.33591300
H	4.04727500	-8.85362600	-5.78180100
C	-0.59037100	6.11806900	-1.76228700
H	-0.12401800	6.01563800	-2.75200300
H	0.21152500	6.24294000	-1.02031700
C	-1.55122100	7.29818000	-1.72812100
H	-2.01931900	7.34073600	-0.73624200
H	-2.35784200	7.11351400	-2.44800500
C	-0.84787900	8.62627100	-2.03694600
H	-0.36887300	8.56751900	-3.02531600
H	-0.03481100	8.78890600	-1.31391800
C	-1.79749000	9.83112200	-2.00762000
H	-2.28341400	9.88618500	-1.02241300
H	-2.60560600	9.67306500	-2.73635900
C	-1.09695700	11.16341100	-2.30360600
H	-0.60646500	11.10510000	-3.28667500
H	-0.29043000	11.31967100	-1.57171400
C	-2.04197800	12.37155700	-2.28064100
H	-2.53676600	12.42835800	-1.29945000
H	-2.84573000	12.21891500	-3.01628800
C	-1.33909200	13.70441400	-2.56920500
H	-0.84310300	13.64716500	-3.54865800

H	-0.53785100	13.85754100	-1.83218400
C	-2.28928200	14.90609000	-2.54769900
H	-2.77408600	15.01069900	-1.56912200
H	-3.08202000	14.79760500	-3.29822400
H	-1.75790500	15.84151200	-2.75749100
C	-3.05698300	2.74764300	-1.16873500
C	-3.76250500	3.68637800	-1.98690400
N	-4.36875600	4.41409600	-2.66560000
C	-3.72486400	1.96484000	-0.26504300
H	-3.09198700	1.30696900	0.32681600
C	-5.12821900	1.88804600	0.03465800
C	-6.23953900	2.54469100	-0.47780900
C	-7.44658100	2.18267800	0.14778200
C	-7.31182400	1.23467900	1.15585000
S	-5.62752800	0.77893300	1.30941900
H	-6.17841100	3.27865400	-1.27056200
H	-8.40362800	2.62283700	-0.11129500
S	-9.97735800	0.59051400	1.28583300
C	-10.64723400	-0.22822800	2.66154000
C	-8.36473500	0.63953300	1.94175000
C	-9.64934600	-0.45182500	3.61795200
C	-7.43519900	-0.72314700	5.32428400
C	-8.34828400	0.04215800	3.21499800
C	-9.79510200	-1.11080800	4.87711300
C	-8.70972600	-1.24426000	5.70162300
C	-7.25059900	-0.09861900	4.11741500
H	-10.76634700	-1.50063100	5.16379700

H	-8.81488200	-1.74703800	6.65897800
H	-6.27795700	0.30433700	3.85798500
H	-6.59860600	-0.82232800	6.01038600
C	-12.07400100	-0.52019900	2.73615300
C	-12.87954200	-1.24403400	1.87446400
C	-14.24974400	-1.24400100	2.29289800
C	-14.47857900	-0.54077000	3.44062500
S	-13.02448700	0.16298100	4.05699100
H	-15.03270800	-1.76239300	1.74847800
H	-15.41670100	-0.39776000	3.96065000
C	-12.40569300	-2.02122700	0.66920400
H	-11.36736200	-1.76392100	0.43834600
H	-12.99930700	-1.72653000	-0.20803100
C	-12.51439800	-3.54850800	0.85647600
H	-13.55199300	-3.81513800	1.10135500
H	-11.91047100	-3.84407800	1.72508400
C	-12.06339400	-4.33547900	-0.38028500
H	-12.66533000	-4.02618300	-1.24785500
H	-11.02388700	-4.06924500	-0.62194600
C	-12.17074000	-5.85584500	-0.20437900
H	-13.21018900	-6.12001700	0.04111600
H	-11.56733800	-6.16414100	0.66218100
C	-11.72548000	-6.64908200	-1.43986100
H	-12.32768000	-6.33902700	-2.30690700
H	-10.68541300	-6.38674700	-1.68438000
C	-11.83651200	-8.16896300	-1.26396800
H	-12.87669500	-8.43168000	-1.01934500

H	-11.23446200	-8.47972100	-0.39694000
C	-11.39191300	-8.96443300	-2.49815200
H	-10.35244300	-8.70240100	-2.74200000
H	-11.99370300	-8.65469800	-3.36450400
C	-11.50604500	-10.48105900	-2.31348500
H	-12.54128400	-10.77839600	-2.10515900
H	-11.17927500	-11.01986200	-3.21026300
H	-10.88895700	-10.82575000	-1.47447600
C	11.27342200	0.35780700	9.32735300
H	11.84830900	1.29490500	9.33192100
H	10.22720500	0.64484800	9.14962200
C	11.39113400	-0.31975600	10.69643800
H	12.43164300	-0.58767900	10.91816700
H	11.03804700	0.33641000	11.50020800
H	10.79803900	-1.24185800	10.73459000