

## Supplementary Materials

### N-Annulation of the BTI Rylene Imide Organic Building Block: Impact on the Optoelectronic Properties of $\pi$ -Extended Molecular Structures

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## General information

All reagents and chemicals were procured from commercial sources and used without further purification. Solvents were dried and purified using standard techniques. Flash chromatography was performed with analytical-grade solvents using Aldrich silica gel technical grade, pore size 60 Å, 230-400 mesh particle size (Saint Louis, MO, USA). Flexible plates ALUGRAM® Xtra SIL G UV254 from MACHEREY-NAGEL (Düren, Deutschland) were used for TLC. Compounds were detected by UV irradiation (Thermo Fisher Scientific, Waltham, MA, USA) or staining with I<sub>2</sub>, unless stated otherwise. NMR spectra were recorded with a Bruker (Billerica, MA, USA) AVANCE III 300 (<sup>1</sup>H, 300 MHz and <sup>13</sup>C, 75 MHz) or a Bruker AVANCE DRX500 (<sup>1</sup>H, 500 MHz; <sup>13</sup>C, 125 MHz). Chemical shifts are given in ppm relative to TMS and coupling constants J in Hz. Matrix Assisted Laser Desorption/Ionization was performed on MALDI-TOF MS BIFLEX III Bruker Daltonics spectrometer using DCTB+ as matrix (Bruker, Billerica, MA, USA). Photoelectron spectroscopy in air (PESA) measurements were carried out using a Riken AC-2 photoelectron spectrometer (Riken Keiki, Tokyo, Japan). UV-vis spectra were recorded on a Shimadzu UV-1800 spectrometer (Shimadzu, Kyoto, Japan).

## Synthetic procedures

The syntheses of **DPP** [1], **BTI-Br** [2] and **TCI-Br** [3] (Figure S1) were successfully reproduced using procedures previously reported in the literature or by our group.

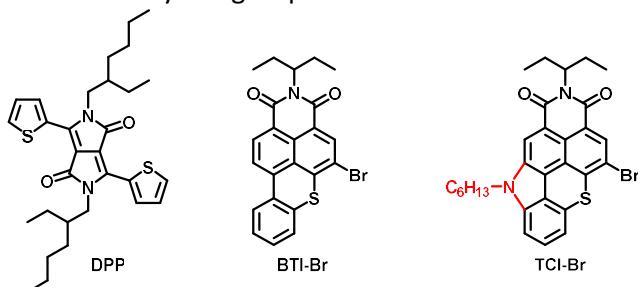
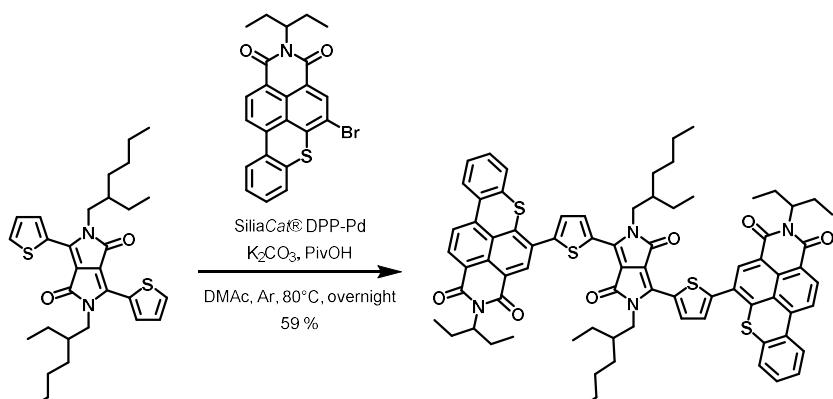


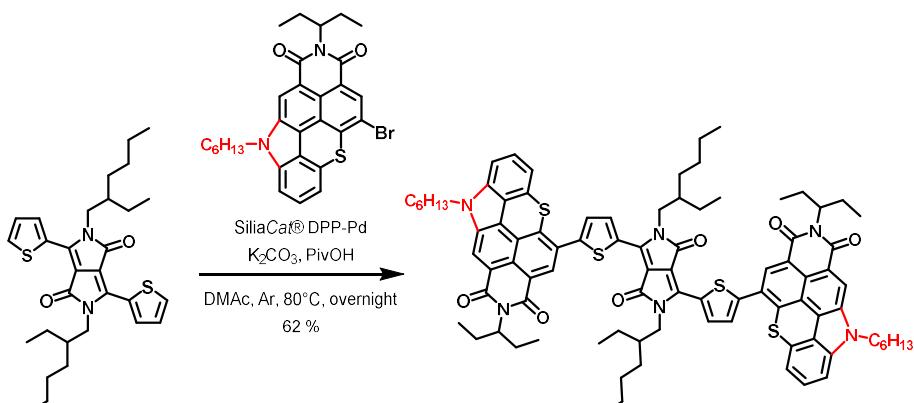
Figure S1. Chemical structures of **DPP**, **BTI-Br** and **TCI-Br**.



Scheme S1. Synthesis of **DPP-BTI**.

**Synthesis of DPP-BTI:** **DPP** (75 mg, 1 eq), **BTI-Br** (135 mg, 2.1 eq), pivalic acid (9 mg, 0.6 eq), potassium carbonate (30 mg, 1.5 eq) and SiliaCat® DPP-Pd (57 mg, 0.25 mmol Pd/g, 0.1 eq) were placed into a Schlenk tube and degassed under vacuum for 30 minutes. Dry and degassed DMAc was then added to the powders and the reaction mixture was stirred at 80 °C under an argon atmosphere for 16 hours. After the complete disappearance of the starting **DPP** and mono-substituted product (monitored by TLC), the mixture was

allowed to cool to room temperature. The solvent was then removed by rotary evaporation and the crude was filtered over a pad of Celite® to remove baseline impurities and catalysts (eluent: dichloromethane). After concentration of the filtrate under vacuum, the crude was subjected to silica gel column chromatography using dichloromethane as eluent to afford pure **DPP-BT1** as a dark purple powder (107 mg, 59 % yield). **<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>) δ = 9.15 (d, *J* = 4.0 Hz, 1H), 8.63 (d, *J* = 8.0 Hz, 1H), 8.52 (s, 1H), 8.24 (d, *J* = 8.2 Hz, 1H), 8.18 (m, 1H), 7.60 (d, *J* = 4.1 Hz, 1H), 7.43 – 7.30 (m, 3H), 5.07 (m, 6.0 Hz, 1H), 4.08 (m, 2H), 2.26 (m, 2H), 1.92 (m, 2H), 1.50 – 1.22 (m, 8H), 0.90 (m, 12H). **<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ = 161.81, 144.61, 140.24, 140.14, 136.93, 136.42, 131.39, 131.12, 130.19, 130.14, 129.83, 128.05, 127.61, 126.87, 126.25, 126.03, 125.17, 120.13, 108.79, 57.70, 46.35, 39.47, 30.44, 28.58, 25.06, 23.77, 23.27, 14.17, 11.48, 10.72. **HRMS (FAB+, Ar)** calculated for C<sub>76</sub>H<sub>74</sub>N<sub>4</sub>O<sub>6</sub>S<sub>4</sub> 1266.4491, found 1266.4486.

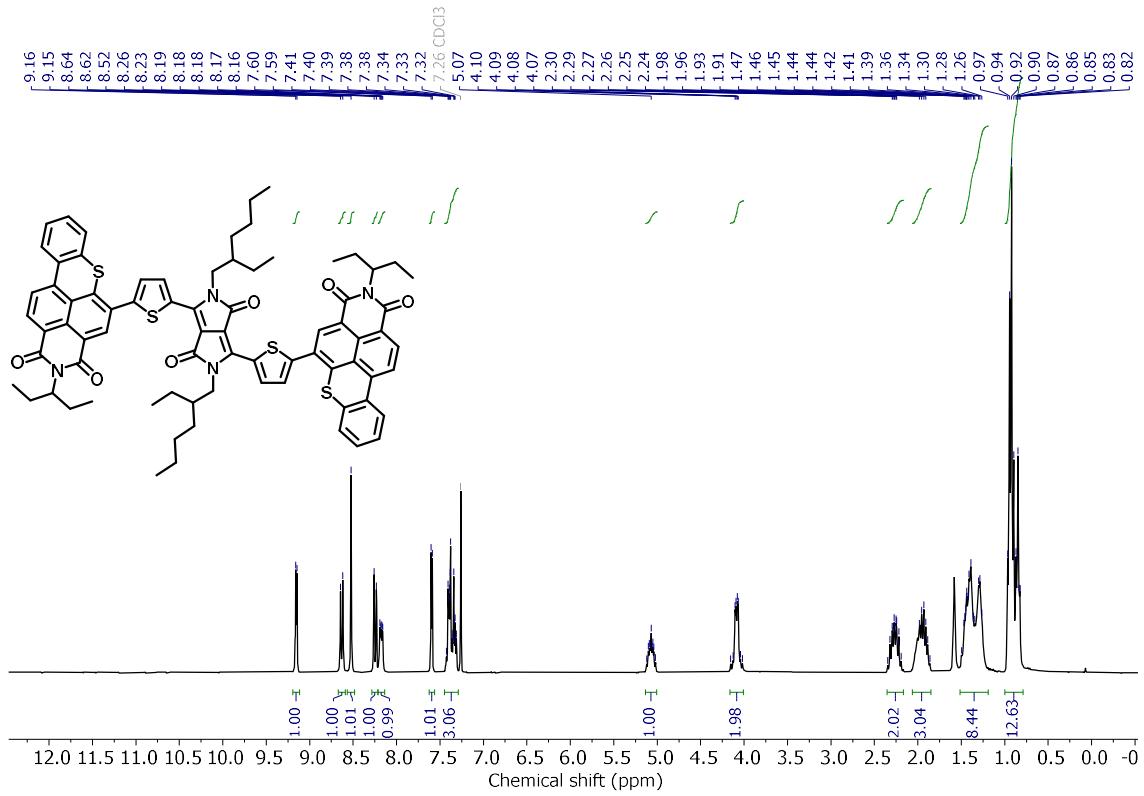


**Scheme S2.** Synthesis of **DPP-TCI**.

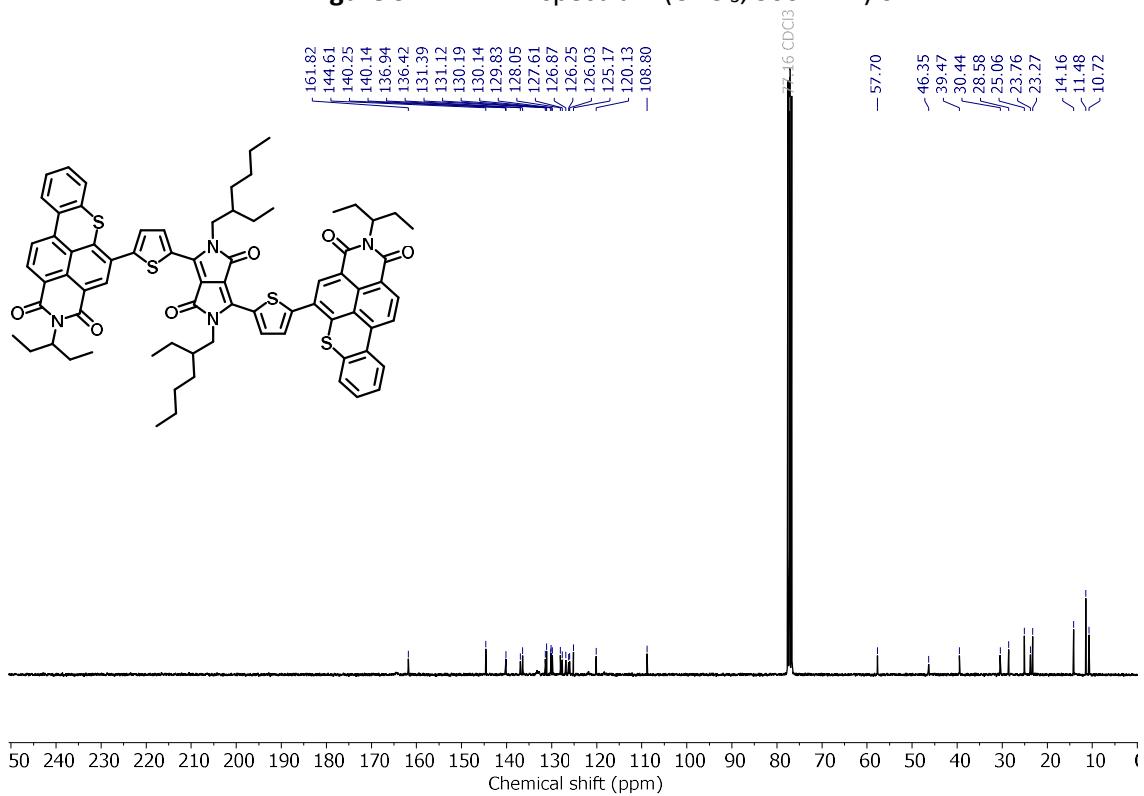
**Synthesis of DPP-TCI:** **DPP** (75 mg, 1 eq), **TCI-Br** (165 mg, 2.1 eq), pivalic acid (9 mg, 0.6 eq), potassium carbonate (30 mg, 1.5 eq) and **SiliaCat® DPP-Pd** (57 mg, 0.25 mmol Pd/g, 0.1 eq) were placed into a Schlenk tube and degassed under vacuum for 30 minutes. Dry and degassed DMAc was then added to the powders and the reaction mixture was stirred at 80 °C under an argon atmosphere for 16 hours. After complete disappearance of the starting **DPP** and mono-substituted product (monitored by TLC), the mixture was allowed to cool to room temperature. The solvent was then removed by rotary evaporation and the crude was filtered over a pad of Celite® to remove baseline impurities and catalysts (eluent: dichloromethane). After concentration of the filtrate under vacuum, the crude was subjected to silica gel column chromatography using dichloromethane as eluent to afford pure **DPP-TCI** as a dark purple powder (130 mg, 62 % yield).

**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>): δ (ppm) 9.16 (d, *J* = 4.1 Hz, 2H), 8.57 (d, *J* = 10.0 Hz, 2H), 8.45 (d, *J* = 2.8 Hz, 2H), 7.74 (dd, *J* = 4.1, 1.7 Hz, 2H), 7.47 – 7.36 (m, 2H), 7.12 (t, *J* = 8.1 Hz, 2H), 6.98 (t, *J* = 7.7 Hz, 2H), 5.22 – 5.06 (m, 2H), 4.33 (t, *J* = 7.1 Hz, 4H), 4.14 – 4.04 (m, 4H), 2.44 – 2.18 (m, 4H), 2.06 – 1.84 (m, 10H), 1.52 – 1.19 (m, 28H), 0.96 (t, *J* = 7.4 Hz, 18H), 0.92 – 0.78 (m, 12H). **<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>): δ (ppm) 161.4, 145.1, 140.5, 139.6, 136.4, 134.0, 130.4, 129.6, 129.2, 128.9, 126.0, 122.5, 122.0, 121.9, 119.3, 118.2, 115.4, 113.5, 108.6, 107.1, 57.7, 46.3, 44.8, 39.6, 31.5, 30.4, 29.8, 28.6, 26.9, 25.2, 23.8, 23.3, 22.6, 14.2, 14.1, 11.7, 10.8. **HRMS (FAB+, Ar)**: *m/z* calculated for C<sub>88</sub>H<sub>96</sub>N<sub>6</sub>O<sub>6</sub>S<sub>4</sub>: 1460.6269, found: 1460.6297.

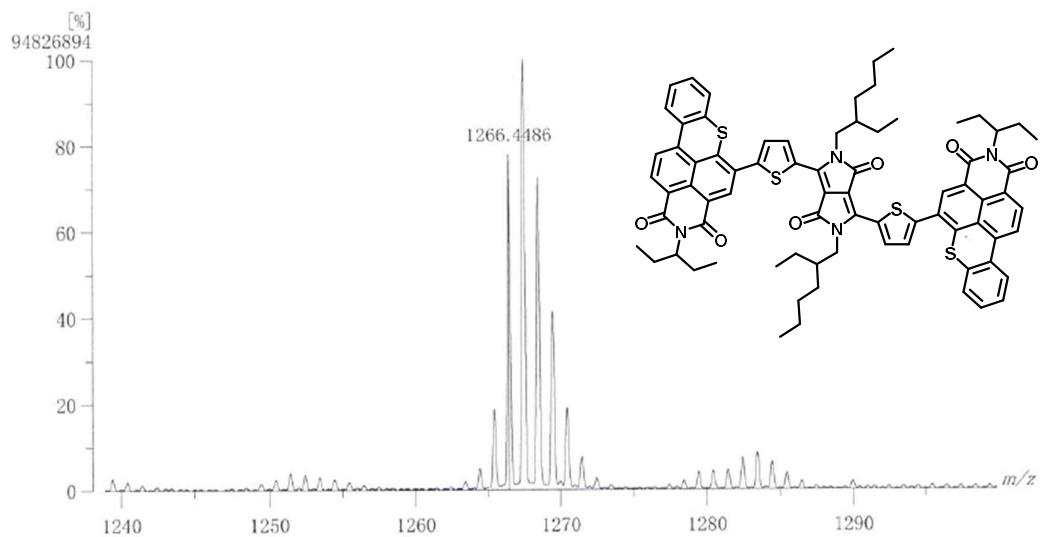
### Spectroscopic data



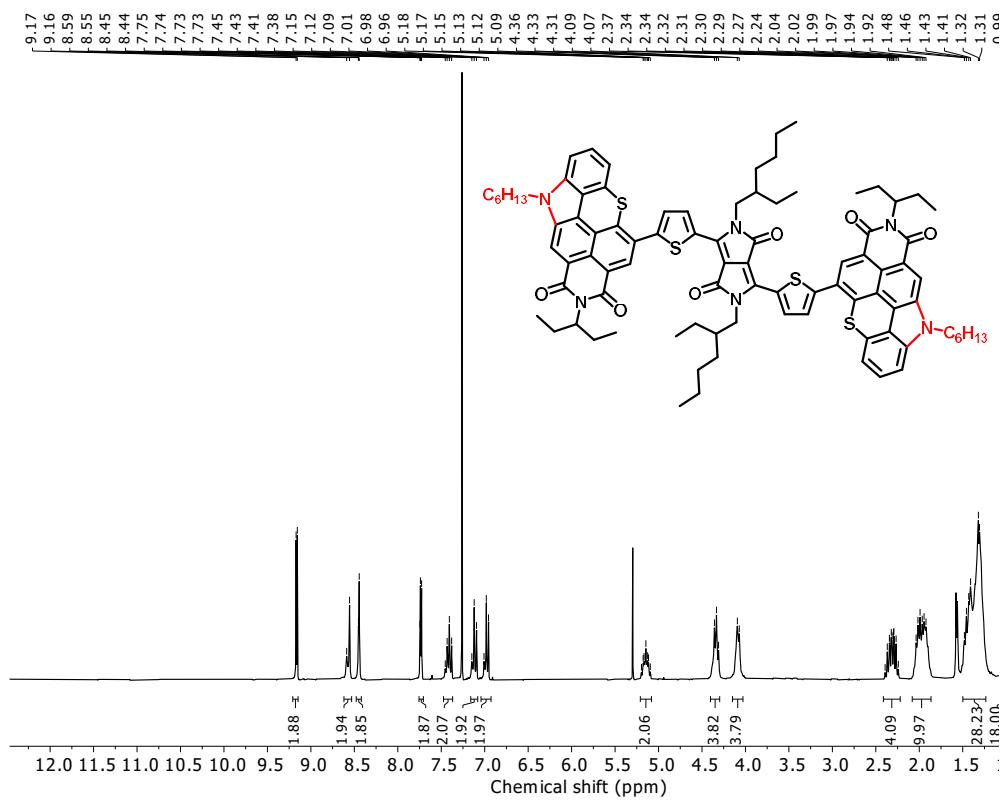
**Figure S2.**  $^1\text{H}$  NMR spectrum ( $\text{CDCl}_3$ , 300 MHz) of DPP-BTI.



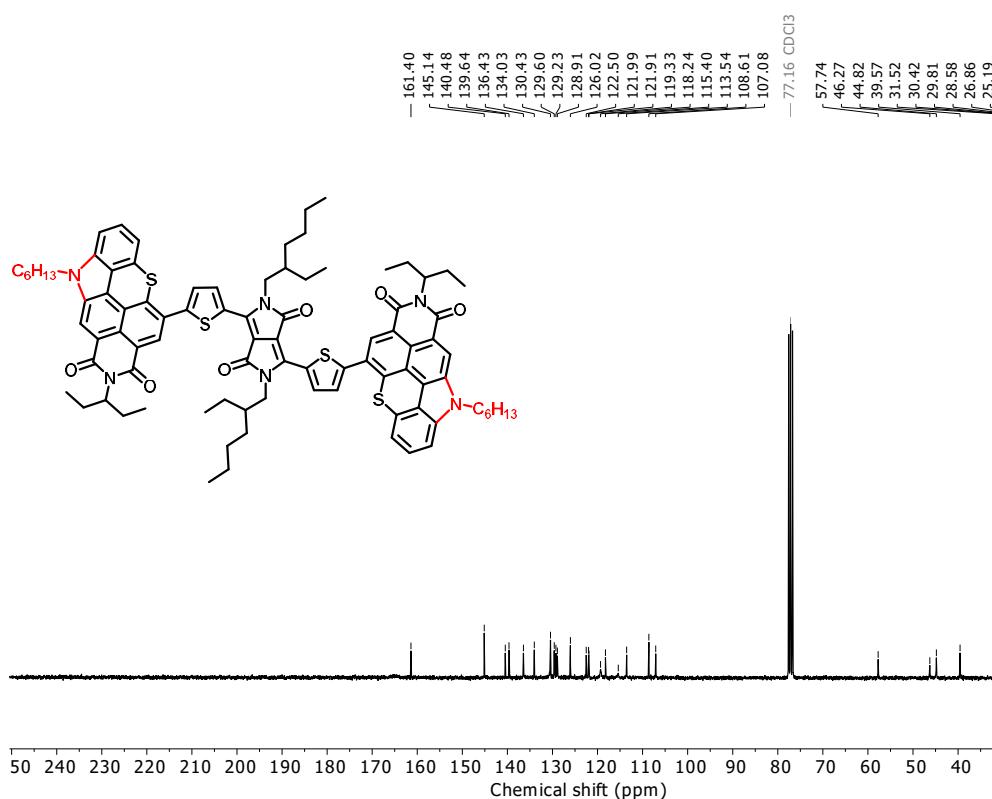
**Figure S3.**  $^{13}\text{C}$  NMR spectrum ( $\text{CDCl}_3$ , 75 MHZ) of DPP-BTI.



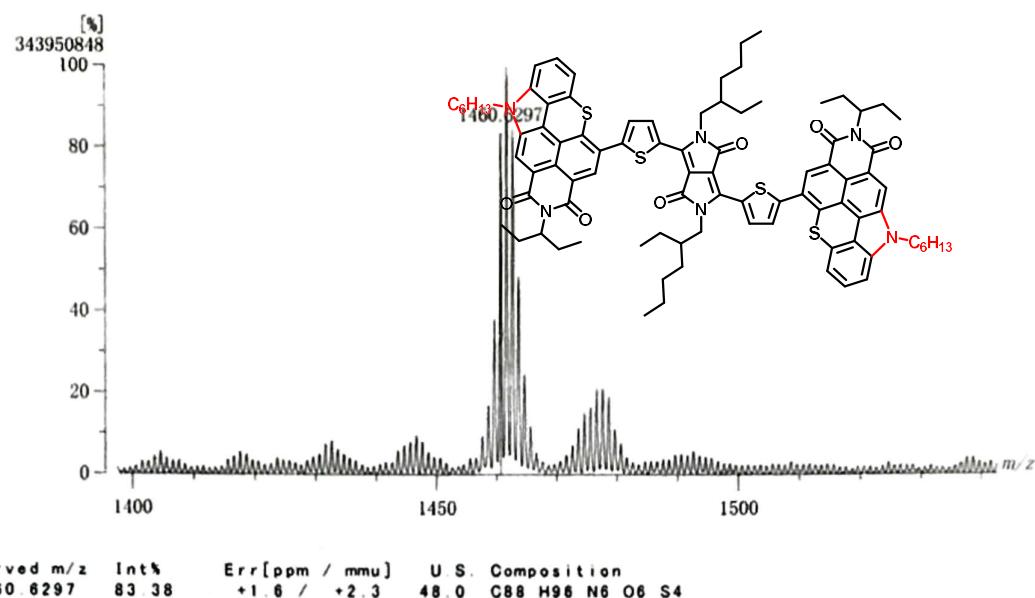
**Figure S4.** HRMS spectrum (FAB+, Ar) of **DPP-BTI**.  $m/z$  calculated for C<sub>76</sub>H<sub>74</sub>N<sub>4</sub>O<sub>6</sub>S<sub>4</sub> 1266.4491, found 1266.4486.



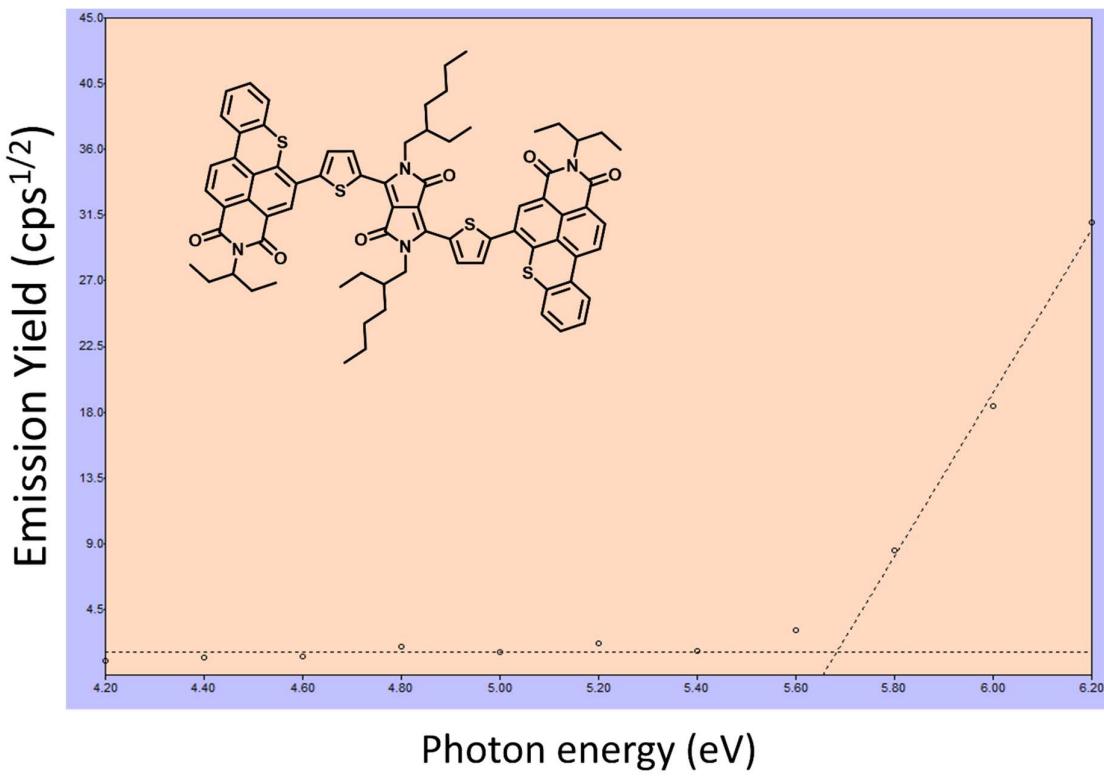
**Figure S5.**  $^1\text{H}$  NMR spectrum (CDCl<sub>3</sub>, 300 MHz) of **DPP-TCl**.



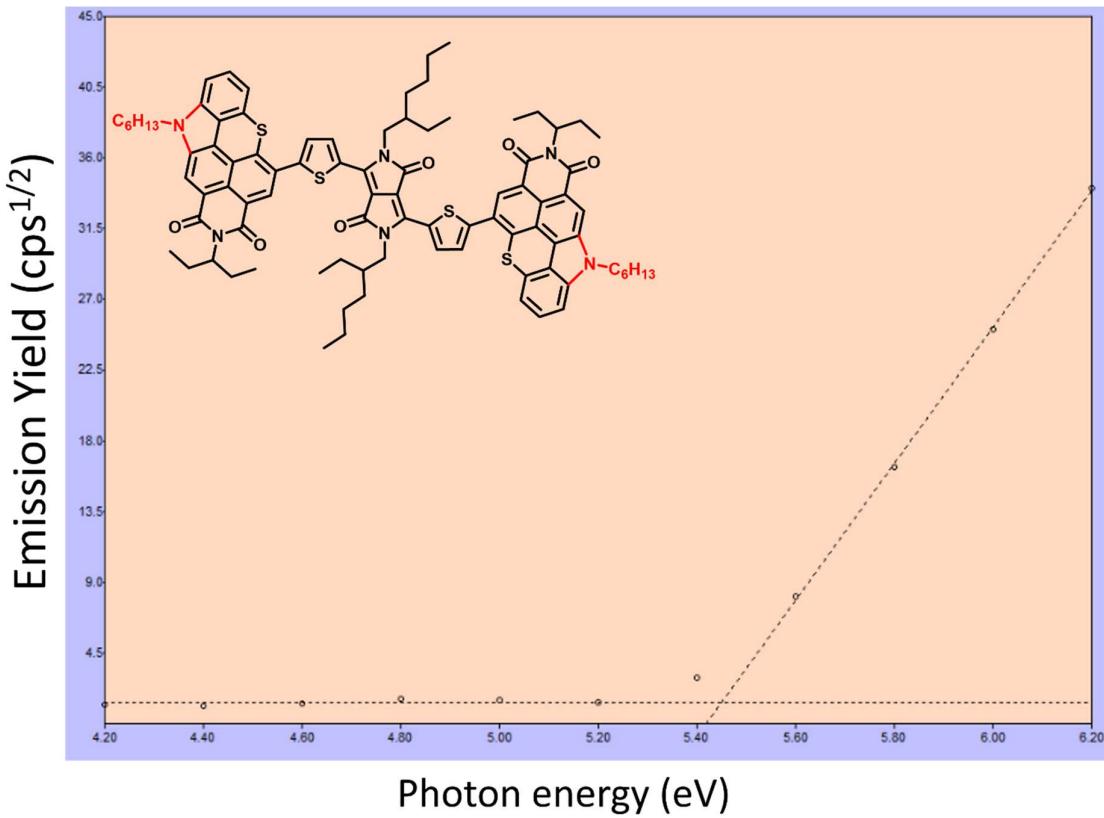
**Figure S6.**  $^{13}\text{C}$  NMR spectrum ( $\text{CDCl}_3$ , 75 MHz) of DPP-TCl.



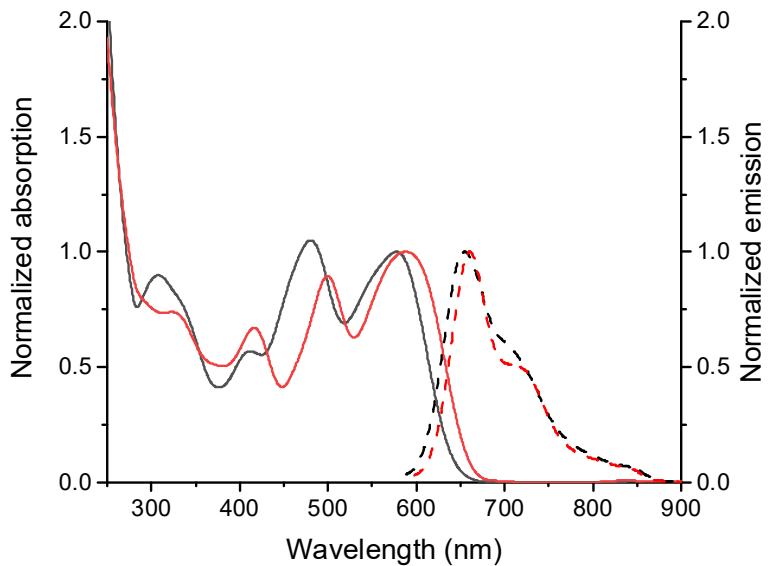
**Figure S7.** HRMS spectrum (FAB+, Ar) of DPP-TCl.  $m/z$  calculated for  $\text{C}_{88}\text{H}_{96}\text{N}_6\text{O}_6\text{S}_4$  1460.6269, found 1460.6297.



**Figure S8.** PESA spectrum of **DPP-BTI**.



**Figure S9.** PESA spectrum of **DPP-TCI**.



**Figure S10.** Absportion (full line) and fluorescence spectra (dash line) of **DPP-BTI** (black) and **DPP-TCI** (red). **Photovoltaic devices fabrication and characterization**

ITO-coated glass substrates were first cleaned by surfactant/water scrubbing, followed by sequentially ultrasonicing in de-ionized water, acetone and isopropanol (10+ minutes each) before use. ITO substrates were then dried with pressurized air and UV-Ozone treated for 30 minutes. An aqueous solution of poly(3,4-ethylenedioxythiophene)-poly(styrenesulfonate) (PEDOT:PSS; Clevios P VP. AI 4083), filtered through a 0.45 µm RC membrane (Millex®), was spun-cast onto the patterned ITO surface at 5000 rpm for 40 s before being baked at 140 °C for 30 min. Then, blends of **DPP-BTI** or **DPP-TCI** and PC<sub>71</sub>BM (1:3 w:w donor:PC<sub>71</sub>BM ratio) dissolved in chloroform (10 mg/mL), stirred at 35 °C for 10 minutes, were spun-cast at 1000 rpm onto the PEDOT:PSS layer. Finally, devices were completed by the successive thermal deposition of lithium fluoride (1 nm) and aluminum (120 nm) at a pressure of  $1.5 \times 10^{-5}$  Torr through a shadow mask defining six cells of 27 mm<sup>2</sup> each (13.5 mm x 2 mm).

Current density-voltage (J-V) characteristics were measured using a Keithley 2420 Source Measure Unit. Solar cell performance used an Air Mass 1.5 Global (AM 1.5G) Solar Simulator (Newport, Model 92251A-1000) with an irradiation intensity of 100 mW.cm<sup>-2</sup>, which was measured by a calibrated silicon solar cell and a readout meter (Newport, Model 91150V).

## Density Functional Theory Calculations

DFT calculations were performed using Gaussian 09 Revision D.01 (Win64) [4]. Alkyl chains were truncated to methyl groups to aid in convergence on minimum energy structure and geometries were optimized to minimum energies using global hybrid generalized gradient approximation (GH-GGA) density functional B3LYP and the 6-311G basis set [5,6]. Atomic coordinates of input structures and optimized structures for both **DPP-BTI** and **DPP-TCI** are included below. **DPP-BTI** reached an optimal energy of -4338.8956 Hartree while **DPP-TCI** reached an optimal energy of -4525.8227 Hartree.

DPP- BTI	In- put Sym- bol	X	Y	Z	DPP- BTI	Opti- mized Sym- bol	X	Y	Z
1	C	1.638806	-0.57967	2.3133	1	C	1.441839	-1.24918	0.22745
2	N	0.685196	-1.60678	2.453676	2	N	0.496677	-2.01107	0.941625
3	C	1.027794	0.589394	2.767519	3	C	0.715805	-0.35616	-0.55936
4	C	-0.55106	-1.10033	2.996613	4	C	-0.84968	-1.61425	0.610774
5	C	-0.31032	0.308318	3.175377	5	C	-0.68201	-0.56519	-0.36199
6	C	1.267495	1.998526	2.94502	6	C	0.883583	0.695403	-1.52931
7	N	0.017915	2.511918	3.448804	7	N	-0.46274	1.058974	-1.89648
8	C	-0.93827	1.485876	3.580867	8	C	-1.40835	0.2917	-1.18847
9	C	-2.28416	1.694017	4.037098	9	C	-2.82968	0.418308	-1.34998
10	S	-3.36609	0.259497	4.389493	10	S	-3.96477	-0.43966	-0.19718
11	C	-2.98251	2.866166	4.271456	11	C	-3.56827	1.116778	-2.28908
12	C	-4.70776	1.38386	4.853302	12	C	-5.38571	0.246398	-1.08549
13	C	-4.31543	2.691637	4.718948	13	C	-4.97403	1.018678	-2.14162
14	C	2.959601	-0.77326	1.782047	14	C	2.863703	-1.42846	0.334433
15	S	4.173612	0.597982	1.821382	15	S	4.001049	-0.20549	-0.41539
16	C	3.535012	-1.88017	1.182014	16	C	3.597746	-2.43367	0.937872
17	C	5.400551	-0.46468	1.019515	17	C	5.417917	-1.16213	0.176012
18	C	4.878164	-1.70654	0.76416	18	C	5.005373	-2.28495	0.845824
19	C	-6.0171	0.829938	5.239	19	C	-6.75037	-0.11073	-0.66016
20	C	-6.61401	1.103838	6.478259	20	C	-7.68696	0.853542	-0.26081
21	C	-6.68182	-0.02697	4.338395	21	C	-7.1183	-1.47091	-0.63122
22	C	-7.88866	0.570322	6.840622	22	C	-9.01085	0.502471	0.144652
23	C	-7.89819	-0.59711	4.652402	23	C	-8.37325	-1.86731	-0.21664
24	C	-8.51751	-0.32025	5.898774	24	C	-9.33229	-0.90116	0.184376
25	C	6.756846	0.053992	0.764865	25	C	6.785941	-0.71184	-0.13935
26	C	7.897243	-0.51716	1.347226	26	C	7.677599	-0.29214	0.855995
27	C	6.913495	1.142975	-0.11476	27	C	7.209132	-0.70808	-1.48276
28	C	9.209887	-0.01161	1.09857	28	C	9.006283	0.133401	0.553066
29	C	8.160845	1.652112	-0.41334	29	C	8.497305	-0.35118	-1.82684
30	C	9.322976	1.08685	0.173054	30	C	9.416101	0.060441	-0.82647
31	O	-1.53066	-1.83781	3.235459	31	O	-1.85238	-2.12816	1.150276
32	O	2.268586	2.725153	2.769301	32	O	1.886345	1.270082	-2.00281
33	S	7.622679	-2.04012	2.30825	33	S	7.065511	-0.39653	2.569027
34	C	9.250794	-2.32139	3.077205	34	C	8.359543	0.484121	3.504001
35	C	10.41413	-0.53903	1.69642	35	C	9.95153	0.619231	1.531263
36	C	10.40084	-1.58341	2.74796	36	C	9.58484	0.884286	2.942922
37	C	9.272342	-3.33318	4.045225	37	C	8.04282	0.73088	4.845475
38	C	10.44593	-3.62353	4.72832	38	C	8.940893	1.401807	5.665097
39	C	11.56907	-1.88026	3.492551	39	C	10.4606	1.596395	3.799419
40	C	11.59904	-2.87856	4.456176	40	C	10.15543	1.845392	5.130205
41	C	11.63927	-0.01963	1.266003	41	C	11.25872	0.874883	1.104544
42	C	10.59493	1.602076	-0.18254	42	C	10.74455	0.384071	-1.20086
43	C	11.73549	1.028934	0.349855	43	C	11.65389	0.760921	-0.22933
44	C	8.260554	2.786466	-1.34823	44	C	8.900346	-0.41953	-3.24237
45	N	9.544796	3.258867	-1.65553	45	N	10.22654	-0.08378	-3.55262
46	C	10.73008	2.72512	-1.12804	46	C	11.18371	0.311135	-2.60624
47	O	7.259037	3.328742	-1.86277	47	O	8.118737	-0.76947	-4.15243
48	O	11.84442	3.190652	-1.45229	48	O	12.35335	0.586397	-2.95187
49	C	9.630991	4.390026	-2.59864	49	C	10.62047	-0.16451	-4.97216
50	C	0.813034	-3.03675	2.198813	50	C	0.706812	-3.02635	1.967267
51	C	-0.07493	3.92143	3.81046	51	C	-0.67036	2.158637	-2.83136
52	S	-5.59555	2.035107	7.669466	52	S	-7.06801	2.56264	-0.12595
53	C	-6.7842	2.406053	9.000536	53	C	-8.59695	3.515992	0.146804
54	C	-8.56746	0.852543	8.083558	54	C	-10.0267	1.455279	0.526454
55	C	-8.07246	1.84789	9.063541	55	C	-9.84481	2.920864	0.399601
56	C	-6.32146	3.31045	9.96436	56	C	-8.44056	4.905583	0.074568
57	C	-7.14595	3.699276	11.01211	57	C	-9.53705	5.742673	0.235208
58	C	-8.89942	2.299376	10.12141	58	C	-10.9467	3.803475	0.518052
59	C	-8.45093	3.198166	11.07926	59	C	-10.8021	5.181903	0.445167
60	C	-9.75346	0.162245	8.353169	60	C	-11.2386	0.958324	1.015976
61	C	-9.74863	-0.94919	6.212406	61	C	-10.6	-1.33786	0.644572
62	C	-10.3384	-0.71867	7.441966	62	C	-11.527	-0.40611	1.075202
63	C	-8.53795	-1.4922	3.672115	63	C	-8.69585	-3.30509	-0.20182
64	N	-9.75791	-2.08098	4.035878	64	N	-9.96706	-3.67667	0.259801
65	C	-10.4049	-1.86555	5.26175	65	C	-10.9455	-2.77036	0.694744
66	O	-8.03957	-1.73596	2.552612	66	O	-7.89051	-4.18267	-0.57913
67	O	-11.4892	-2.43034	5.524105	67	O	-12.0575	-3.17112	1.102804
68	C	-10.3836	-2.98237	3.049717	68	C	-10.2739	-5.11974	0.278878
69	H	-2.56841	3.84412	4.10325	69	H	-3.12367	1.674458	-3.09375

70	H	-4.97784	3.519466	4.921672	70	H	-5.66825	1.499817	-2.81384
71	H	3.01448	-2.80858	1.029965	71	H	3.149508	-3.28536	1.417534
72	H	5.44997	-2.48987	0.289867	72	H	5.699041	-3.00551	1.252808
73	H	-6.23887	-0.24865	3.378373	73	H	-6.41091	-2.22767	-0.93774
74	H	6.045988	1.596858	-0.5712	74	H	6.528873	-1.01496	-2.26391
75	H	8.365356	-3.88057	4.262524	75	H	7.088088	0.405046	5.235014
76	H	10.4578	-4.40567	5.474489	76	H	8.691039	1.592071	6.699509
77	H	12.46768	-1.30768	3.328149	77	H	11.3916	1.979339	3.413761
78	H	12.51359	-3.07079	4.999539	78	H	10.85569	2.391884	5.746326
79	H	12.55854	-0.43593	1.643013	79	H	12.00623	1.174684	1.819973
80	H	12.69826	1.412614	0.045213	80	H	12.67014	0.974605	-0.5268
81	H	9.086889	5.243426	-2.19968	81	H	10.01492	0.520346	-5.56205
82	H	10.67891	4.631425	-2.72879	82	H	11.66886	0.099831	-5.03825
83	H	9.181028	4.111274	-3.5491	83	H	10.45443	-1.17384	-5.34206
84	H	-0.10299	-3.49364	2.566543	84	H	-0.2712	-3.23316	2.395972
85	H	0.900279	-3.25122	1.13307	85	H	1.098704	-3.95316	1.546337
86	H	1.663045	-3.46015	2.732809	86	H	1.373919	-2.66505	2.748926
87	H	-0.73923	4.469242	3.140923	87	H	-1.08343	1.812252	-3.77925
88	H	-0.40587	4.043608	4.841145	88	H	-1.31702	2.924632	-2.40423
89	H	0.92803	4.328971	3.705324	89	H	0.312196	2.584615	-3.02213
90	H	-5.32029	3.710744	9.881128	90	H	-7.46058	5.321362	-0.11579
91	H	-6.78431	4.39729	11.75417	91	H	-9.41133	6.814963	0.179681
92	H	-9.91914	1.955025	10.18619	92	H	-11.9392	3.403986	0.651921
93	H	-9.11678	3.514493	11.86994	93	H	-11.6712	5.817333	0.542242
94	H	-10.2484	0.300441	9.300104	94	H	-11.9927	1.641223	1.370042
95	H	-11.2604	-1.22974	7.677943	95	H	-12.477	-0.75661	1.451607
96	H	-9.70943	-3.80616	2.825236	96	H	-9.53998	-5.64208	0.888363
97	H	-11.3069	-3.35086	3.47997	97	H	-11.2689	-5.23992	0.689577
98	H	-10.5796	-2.43951	2.127527	98	H	-10.2266	-5.51967	-0.73201

DPP- TCI	In- put Sym-		DPP- TCI	Opti- mized Sym-					
Tag	bol	X	Y	Z	Tag	bol	X	Y	Z
1	C	1.473459	-0.97828	-0.29328	1	C	1.414519	0.416623	-1.11525
2	N	0.596529	-2.06533	-0.2457	2	N	0.458009	0.254819	-2.13698
3	C	0.685258	0.168619	-0.3631	3	C	0.696261	0.598279	0.068073
4	C	-0.79211	-1.62684	-0.28174	4	C	-0.8833	0.332049	-1.61387
5	C	-0.69044	-0.19334	-0.35559	5	C	-0.7036	0.551722	-0.20233
6	C	0.786868	1.60258	-0.42766	6	C	0.875877	0.808824	1.481079
7	N	-0.60184	2.041494	-0.45495	7	N	-0.46549	0.879962	2.005001
8	C	-1.47876	0.954348	-0.40938	8	C	-1.42175	0.721451	0.98273
9	C	-2.90507	1.044985	-0.408	9	C	-2.84188	0.735157	1.195859
10	S	-3.91318	-0.47992	-0.33897	10	S	-3.98482	0.583465	-0.22899
11	C	-3.72774	2.152478	-0.45368	11	C	-3.57748	0.836383	2.364718
12	C	-5.42084	0.524992	-0.3704	12	C	-5.40269	0.684639	0.894504
13	C	-5.11357	1.86277	-0.43014	13	C	-4.98341	0.808069	2.196116
14	C	2.899531	-1.0673	-0.26207	14	C	2.834705	0.383677	-1.32536
15	S	3.907564	0.457819	-0.32707	15	S	3.976936	0.593035	0.093005
16	C	3.722009	-2.17337	-0.1875	16	C	3.571431	0.202402	-2.48388
17	C	5.414853	-0.54426	-0.23826	17	C	5.395704	0.419293	-1.02059
18	C	5.107538	-1.88172	-0.1719	18	C	4.977094	0.222292	-2.31346
19	C	-6.77105	-0.03389	-0.2561	19	C	-6.76393	0.650203	0.344214
20	C	-7.943	0.716534	-0.08265	20	C	-7.76381	-0.20319	0.834649
21	C	-6.8838	-1.4537	-0.29569	21	C	-7.08778	1.511251	-0.74102
22	C	-9.18578	0.046695	0.053741	22	C	-9.05511	-0.17599	0.244958
23	C	-8.08906	-2.1125	-0.16378	23	C	-8.34695	1.55394	-1.31658
24	C	-9.27405	-1.37026	0.01426	24	C	-9.36483	0.700186	-0.83065
25	C	6.76363	0.024087	-0.15913	25	C	6.756346	0.52595	-0.47906
26	C	7.946275	-0.71891	-0.0327	26	C	7.765439	-0.40781	-0.75978
27	C	6.864047	1.445172	-0.18346	27	C	7.071316	1.618607	0.376329
28	C	9.187513	-0.04076	0.073285	28	C	9.056851	-0.23012	-0.19715
29	C	8.067719	2.112033	-0.08089	29	C	8.32994	1.806685	0.922942
30	C	9.263483	1.377259	0.04983	30	C	9.357491	0.87527	0.644573
31	O	-1.73979	-2.42799	-0.24812	31	O	-1.89322	0.218533	-2.34077
32	O	1.734521	2.403871	-0.45822	32	O	1.885689	0.922932	2.208003
33	S	7.872806	-2.57886	0.020509	33	S	7.378363	-1.89517	-1.83302
34	C	9.631211	-3.09975	0.230917	34	C	8.969736	-2.84822	-1.87063
35	C	10.40109	-0.71737	0.221455	35	C	10.09712	-1.13956	-0.42052
36	C	10.58958	-2.10654	0.291927	36	C	10.04746	-2.32002	-1.17922
37	C	10.05262	-4.4202	0.324994	37	C	9.153622	-4.04918	-2.54775
38	C	11.43382	-4.68186	0.480036	38	C	10.42382	-4.67111	-2.49616

39	C	11.9749	-2.35239	0.446135	39	C	11.31941	-2.93388	-1.12037
40	C	12.40943	-3.67938	0.545163	40	C	11.51798	-4.14538	-1.79585
41	C	11.65522	-0.09083	0.332618	41	C	11.38736	-1.01087	0.116621
42	C	10.52786	2.019049	0.158309	42	C	10.6692	1.011529	1.192461
43	C	11.71885	1.309788	0.298797	43	C	11.68496	0.08569	0.939314
44	C	8.093245	3.586549	-0.11883	44	C	8.60382	2.969808	1.783716
45	N	9.370547	4.174736	-0.01312	45	N	9.911271	3.072239	2.3047
46	C	10.5935	3.493767	0.125507	46	C	10.957	2.164245	2.062412
47	O	7.067678	4.277505	-0.23327	47	O	7.740844	3.832119	2.049523
48	O	11.65777	4.128501	0.213574	48	O	12.07949	2.357144	2.581128
49	C	9.450075	5.65454	-0.04746	49	C	10.22779	4.220736	3.176521
50	C	0.871871	-3.50093	-0.16271	50	C	0.645496	0.041262	-3.56688
51	C	-0.87735	3.478153	-0.51614	51	C	-0.65384	1.117968	3.43097
52	S	-7.85264	2.574977	-0.00752	52	S	-7.36417	-1.39225	2.226514
53	C	-9.5992	3.106672	0.265337	53	C	8.94426	-2.33066	2.481935
54	C	-10.3885	0.730685	0.249101	54	C	-10.0856	-1.02145	0.671934
55	C	-10.5633	2.120211	0.343684	55	C	-10.0251	-1.99239	1.684432
56	C	-10.0066	4.428978	0.390023	56	C	-9.11695	-3.34281	3.420213
57	C	-11.38	4.699277	0.592197	57	C	-10.3793	-3.97583	3.512727
58	C	-11.941	2.374754	0.54497	58	C	-11.2892	-2.61938	1.767707
59	C	-12.3613	3.703632	0.675087	59	C	-11.4764	-3.64208	2.707105
60	C	-11.6436	0.112488	0.391793	60	C	-11.3748	-1.03742	0.117411
61	C	-10.5396	-2.00359	0.154352	61	C	-10.6762	0.690309	-1.39634
62	C	-11.7197	-1.28702	0.341732	62	C	-11.6818	-0.16477	-0.93716
63	C	-8.12783	-3.58613	-0.2201	63	C	-8.63078	2.482796	-2.42333
64	N	-9.40594	-4.16573	-0.08169	64	N	-9.93765	2.446946	-2.95438
65	C	-10.6183	-3.47719	0.10443	65	C	-10.9742	1.608103	-2.50872
66	O	-7.11207	-4.28344	-0.37592	66	O	-7.77645	3.269923	-2.88121
67	O	-11.6844	-4.10477	0.217867	67	O	-12.0977	1.664395	-3.05733
68	C	-9.49865	-5.64429	-0.13271	68	C	-10.2644	3.359795	-4.06756
69	N	-12.5968	1.134737	0.565215	69	N	-12.1201	-2.02005	0.806039
70	N	12.62144	-1.10741	0.462146	70	N	12.1443	-2.11703	-0.32881
71	C	14.06481	-0.90611	0.625421	71	C	13.53045	-2.40613	0.017282
72	C	-14.036	0.942614	0.771461	72	C	-13.5017	-2.39895	0.536674
73	H	-3.35781	3.162407	-0.50917	73	H	-3.13269	0.934649	3.338196
74	H	-5.87536	2.629112	-0.47279	74	H	-5.67036	0.900518	3.023073
75	H	3.352231	-3.18417	-0.14978	75	H	3.127663	0.066964	-3.45327
76	H	5.869336	-2.64801	-0.12848	76	H	5.664369	0.116895	-3.13852
77	H	-5.9954	-2.05045	-0.45872	77	H	-6.32892	2.176809	-1.12686
78	H	5.966325	2.036696	-0.31048	78	H	6.305617	2.347739	0.59962
79	H	9.348799	-5.24128	0.281553	79	H	8.35157	-4.51302	-3.10353
80	H	11.7507	-5.7157	0.553966	80	H	10.55162	-5.60594	-3.02543
81	H	13.45225	-3.93885	0.671055	81	H	12.46297	-4.669	-1.78381
82	H	12.63852	1.874953	0.380409	82	H	12.65073	0.252111	1.394486
83	H	9.912239	6.018995	0.872484	83	H	10.53354	3.865286	4.158363
84	H	10.06192	5.970639	-0.89527	84	H	11.0485	4.792063	2.748367
85	H	8.429591	6.019447	-0.1449	85	H	9.336179	4.830889	3.253439
86	H	-0.11257	-3.97654	-0.14791	86	H	-0.35203	-0.02737	-3.99509
87	H	1.431653	-3.85238	-1.03477	87	H	1.169159	0.876614	-4.03199
88	H	1.409652	-3.75283	0.756321	88	H	1.177837	-0.88873	-3.76682
89	H	-1.42394	3.742664	-1.42643	89	H	-1.22144	2.030638	3.611457
90	H	-1.42847	3.817902	0.365968	90	H	-1.1422	0.274094	3.919087
91	H	0.107107	3.953664	-0.53316	91	H	0.342384	1.23314	3.852118
92	H	-9.2978	5.245074	0.335052	92	H	-8.3121	-3.6541	4.070309
93	H	-11.6859	5.734474	0.68966	93	H	-10.4985	-4.7631	4.245129
94	H	-13.3974	3.969482	0.837332	94	H	-12.4152	-4.16553	2.816693
95	H	-12.6409	-1.84607	0.445062	95	H	-12.6476	-0.11983	-1.41967
96	H	-9.93472	-6.01728	0.796494	96	H	-10.5993	2.784783	-4.928
97	H	-10.1393	-5.94438	-0.9649	97	H	-11.0676	4.031238	-3.77095
98	H	-8.48474	-6.01578	-0.26696	98	H	-9.36906	3.920415	-4.30689
99	H	14.36766	-1.01656	1.672545	99	H	13.59991	-3.17015	0.794693
100	H	14.6085	-1.63132	0.01285	100	H	14.07207	-2.74785	-0.86466
101	H	14.32388	0.097812	0.282695	101	H	14.0108	-1.49906	0.376036
102	H	-14.3049	1.043629	1.828733	102	H	-13.5595	-3.33848	-0.01724
103	H	-14.5929	1.678725	0.184253	103	H	-14.0507	-2.50494	1.472465
104	H	-14.3135	-0.05543	0.426121	104	H	-13.9829	-1.61961	-0.0491

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