Electronic Supplementary Material (ESI) for Energy & Environmental Science

SUPPLEMENTARY INFORMATION:

Effect of Synthetic Accessibility on the Commercial Viability of Organic Photovoltaics

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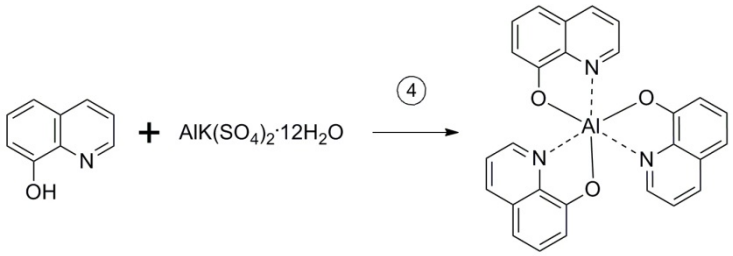
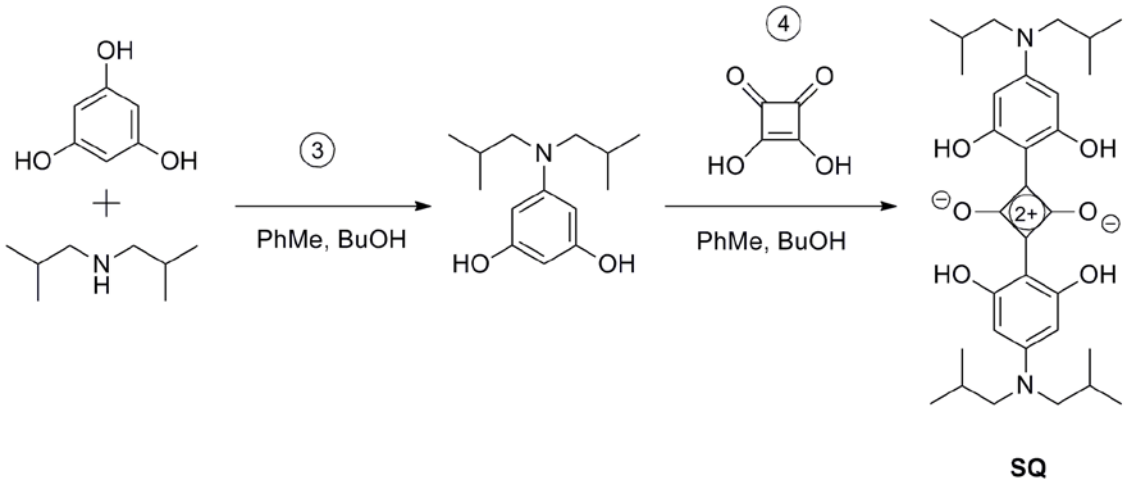
1. Synthetic Procedures for OPV Active Layer Materials



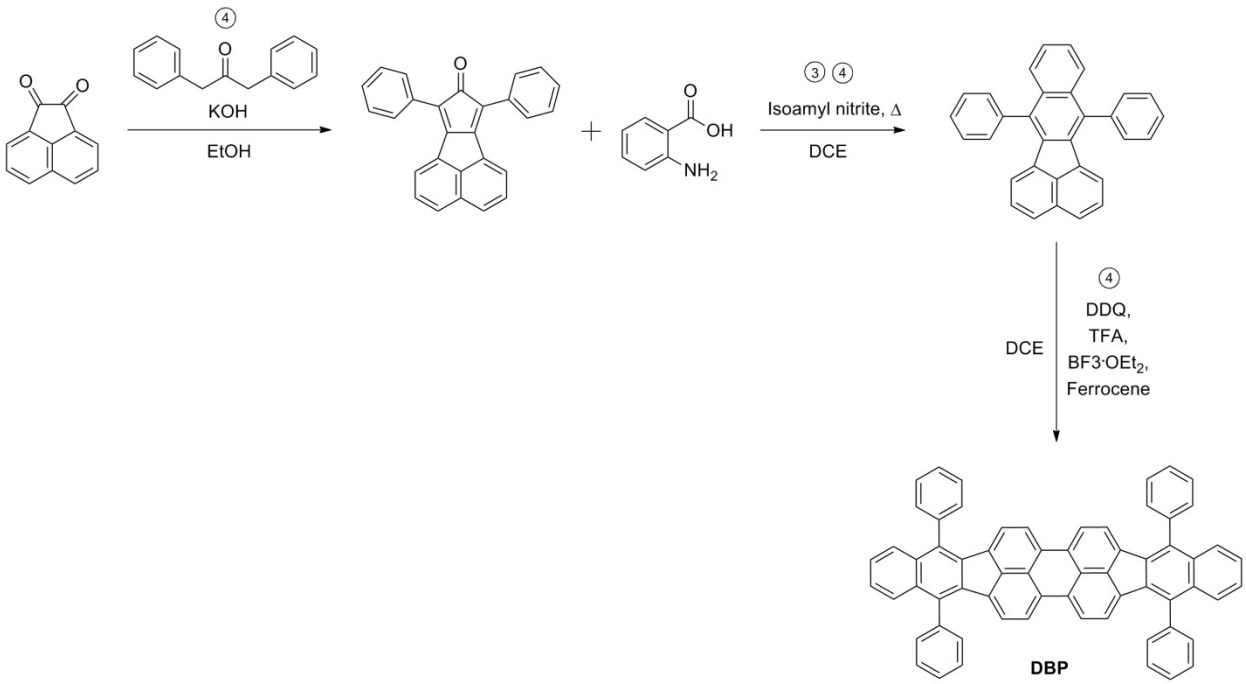
Alq3

Scheme S1. Synthesis procedure for **Alq3**.

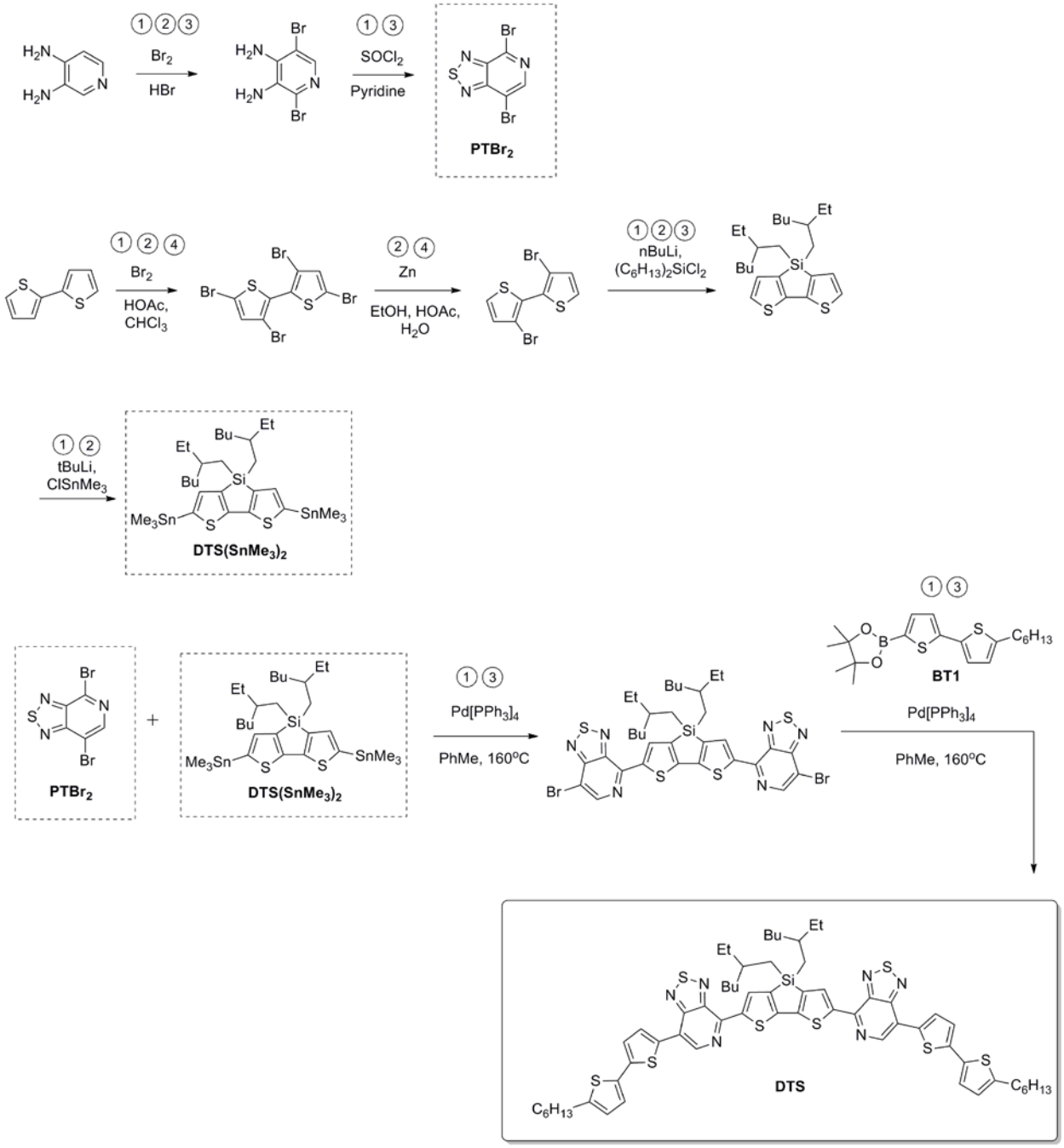


SQ

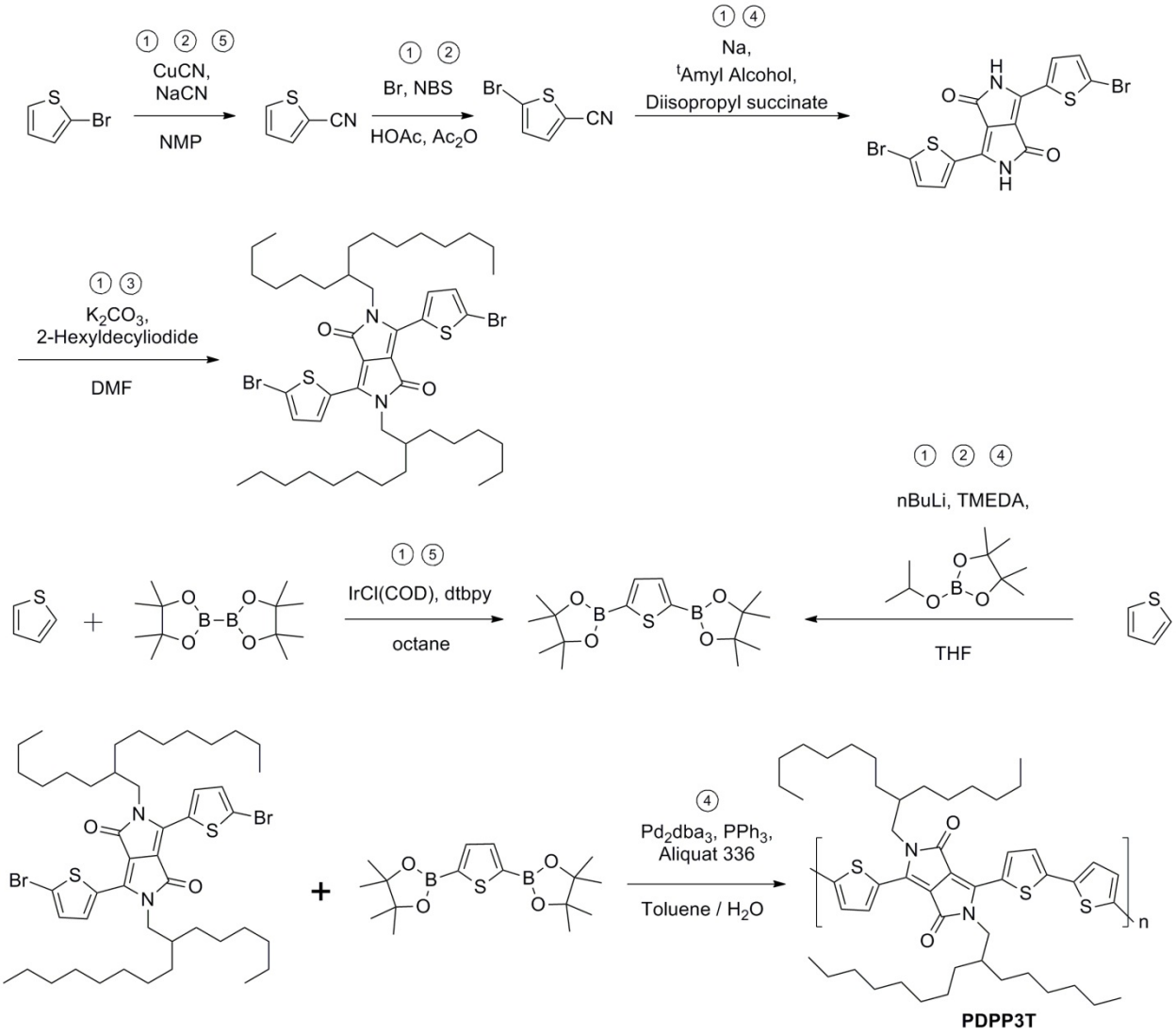
Scheme S2. Synthesis procedure for **SQ**.



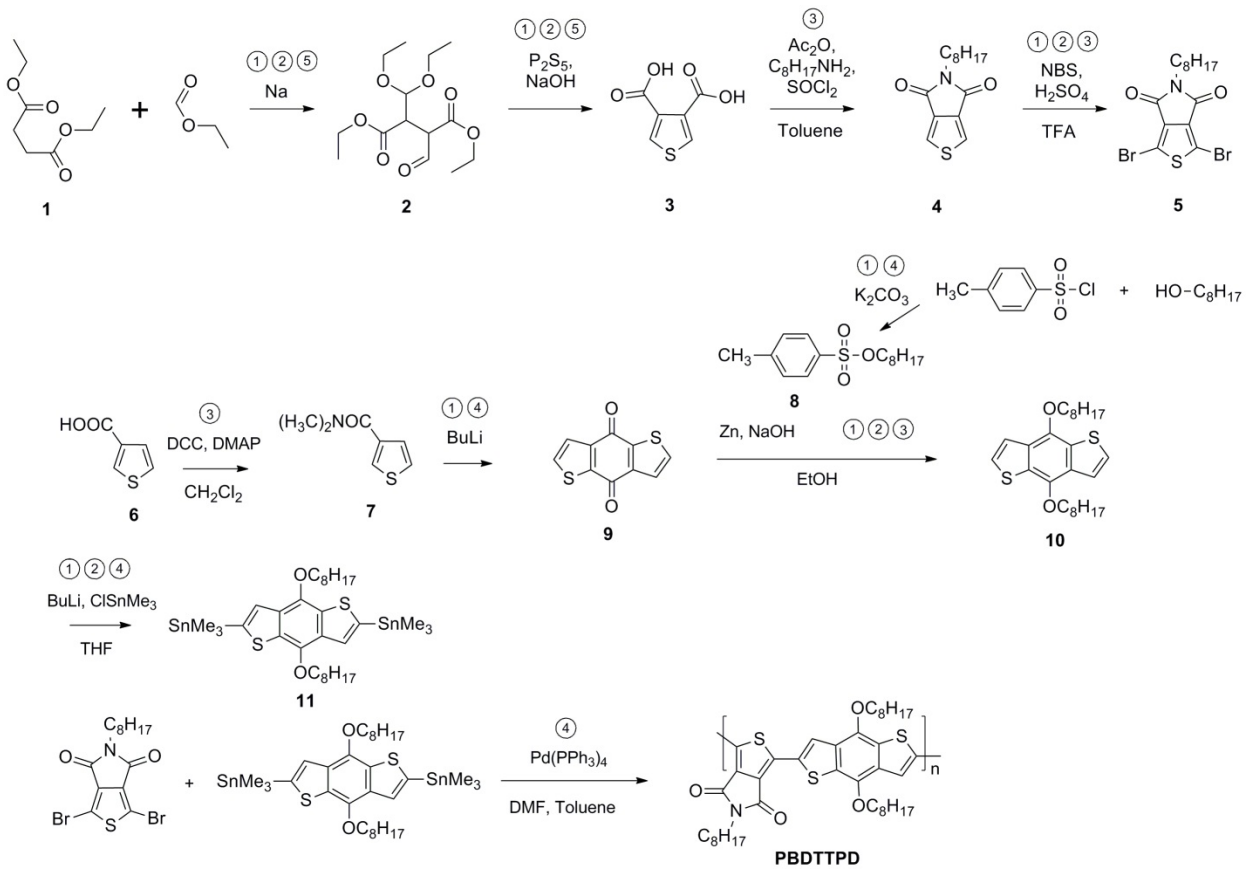
Scheme S3. Synthesis procedure for **DBP**.



Scheme S4. Synthesis procedure for **DBP**.



Scheme S5. Synthesis procedure for **PDPP3T**.



Scheme S6. Synthesis procedure for **PBDTTPD**.

2. Isolation and Purification Procedures

There are generally three phases associated with a particular synthetic step: the reaction itself, isolation (often termed "work-up"), and purification. For example, after a particular synthetic operation is conducted using the necessary reaction conditions and reagents, an aqueous quenching or neutralization step is often necessary to either pacify reactive intermediates or reagents, or neutralize the pH of the reaction from an otherwise acidic or basic state. Such aqueous quenching/neutralization operations are often also accompanied by extraction steps, wherein the desired products of the reaction are isolated, in crude, from the aqueous medium with the use of organic solvents; common organic solvents used for extraction are ethyl acetate, diethyl ether and dichloromethane. The organic solvents are then also dried over a drying agent, such as sodium or magnesium sulfate, to remove major traces of residual water from the quenching/neutralization operation.

The product that is isolated after the aforementioned isolation operations is often crude and must be purified. Depending on the particular molecule, a variety of purification procedures may be employed: distillation or sublimation, recrystallization, or chromatography. Products that are oils at ambient conditions and are thermally-stable are best purified by distillation. Products that have high molecular mass and are thermally-stable may be purified by a combination of recrystallization and sublimation. All other products are usually purified by chromatography using, most often, a gel consisting of micron-sized silica particles.

3. Synthesis Flowcharts for OPV Active Layer Materials

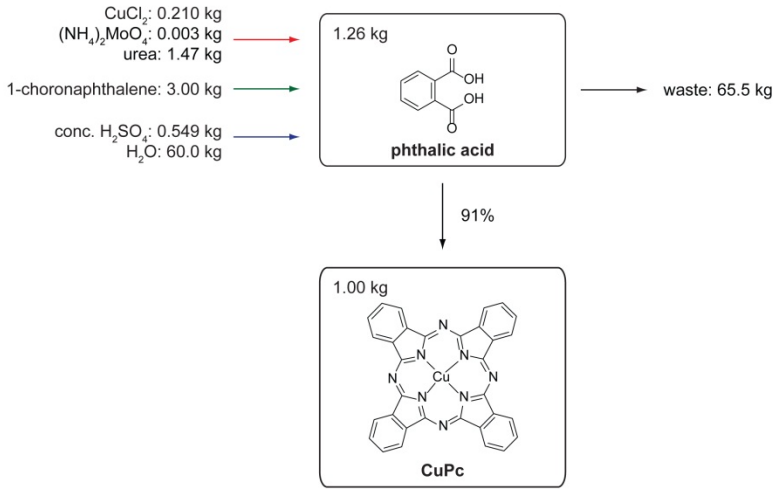


Figure S1. Flowchart describing the synthesis of 1 kg of **CuPc**. The requisite quantities of reagent (red arrow), solvents (green arrow) and work-up materials (blue arrow) are indicated for each step.

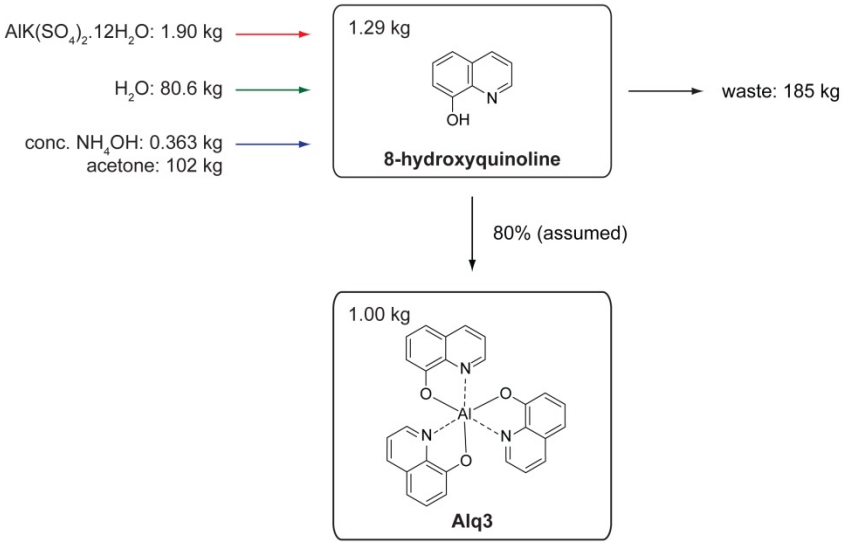


Figure S2. Flowchart describing the synthesis of 1 kg of **Alq3**. The requisite quantities of reagent (red arrow), solvents (green arrow) and work-up materials (blue arrow) are indicated for each step.

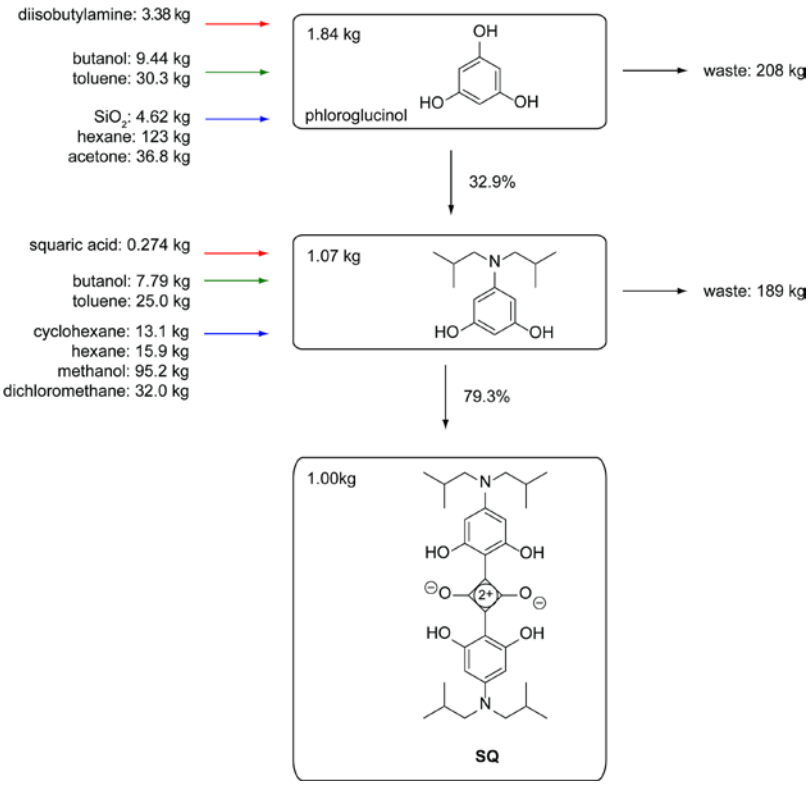


Figure S3. Flowchart describing the synthesis of 1 kg of **SQ**. The requisite quantities of reagent (red arrow), solvents (green arrow) and work-up materials (blue arrow) are indicated for each step.

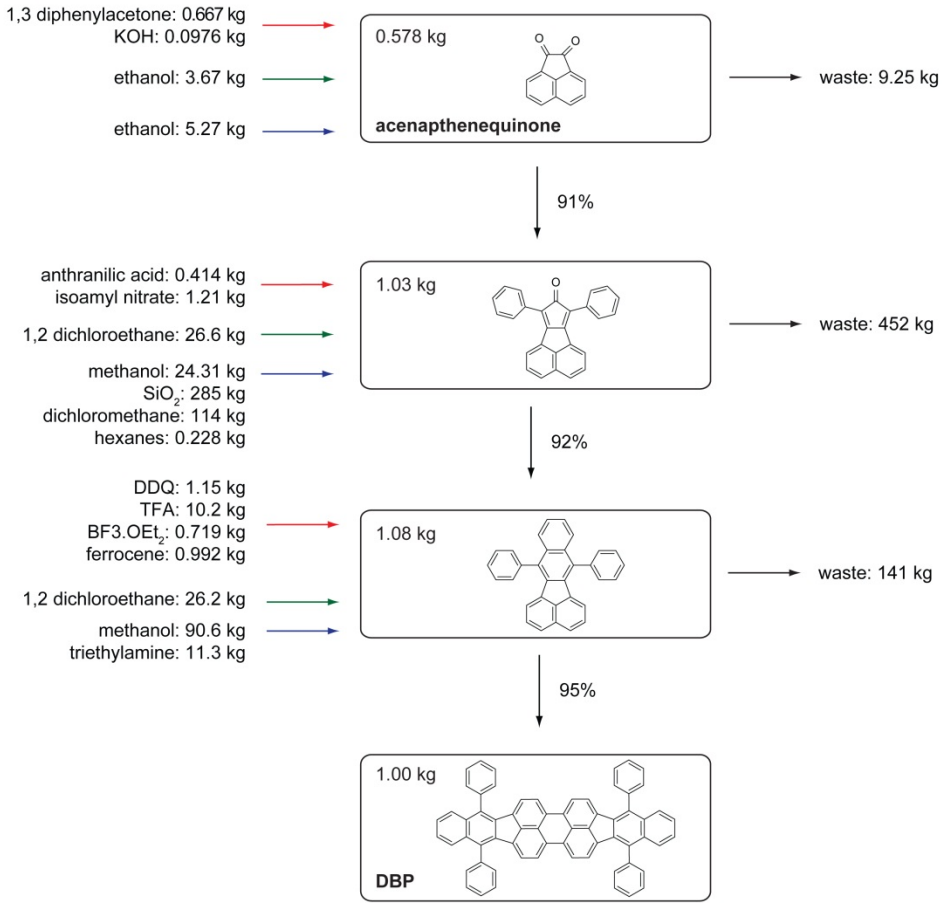


Figure S4. Flowchart describing the synthesis of 1 kg of **DBP**. The requisite quantities of reagent (red arrow), solvents (green arrow) and work-up materials (blue arrow) are indicated for each step.

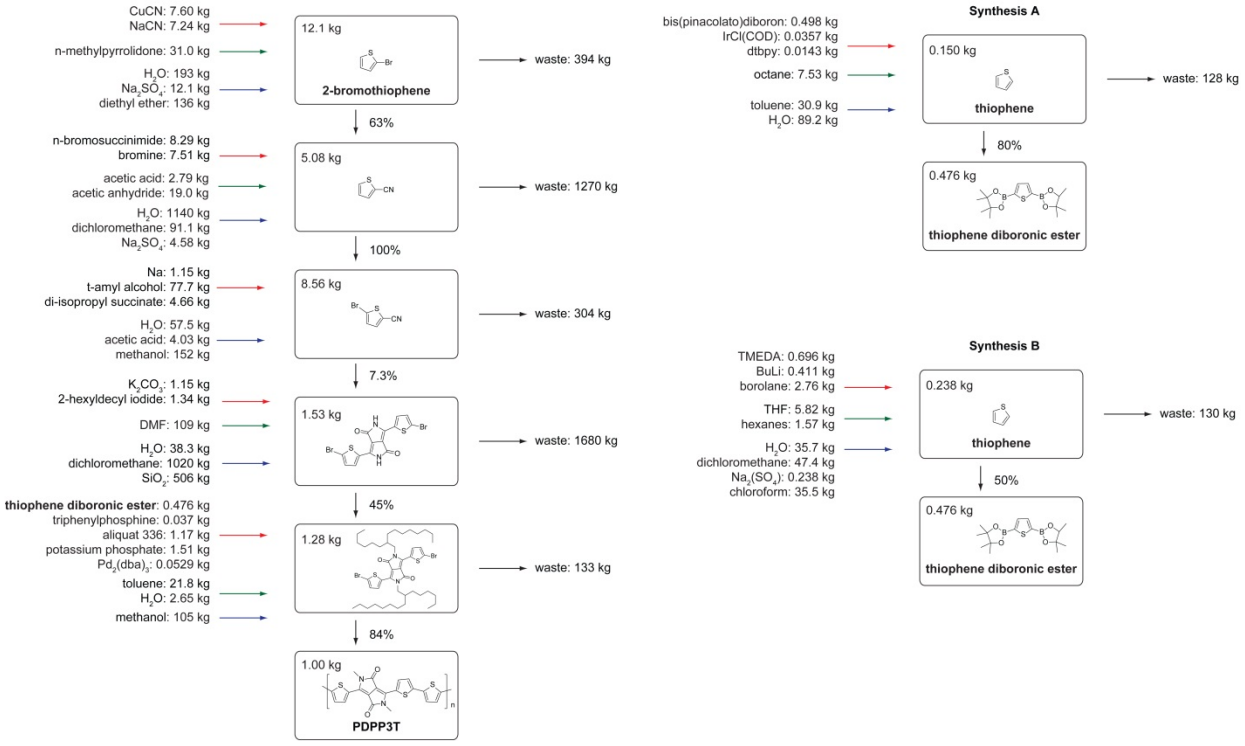


Figure S5. Flowchart describing the synthesis of 1 kg of **PDPP3T**. The requisite quantities of reagent (red arrow), solvents (green arrow) and work-up materials (blue arrow) are indicated for each step.

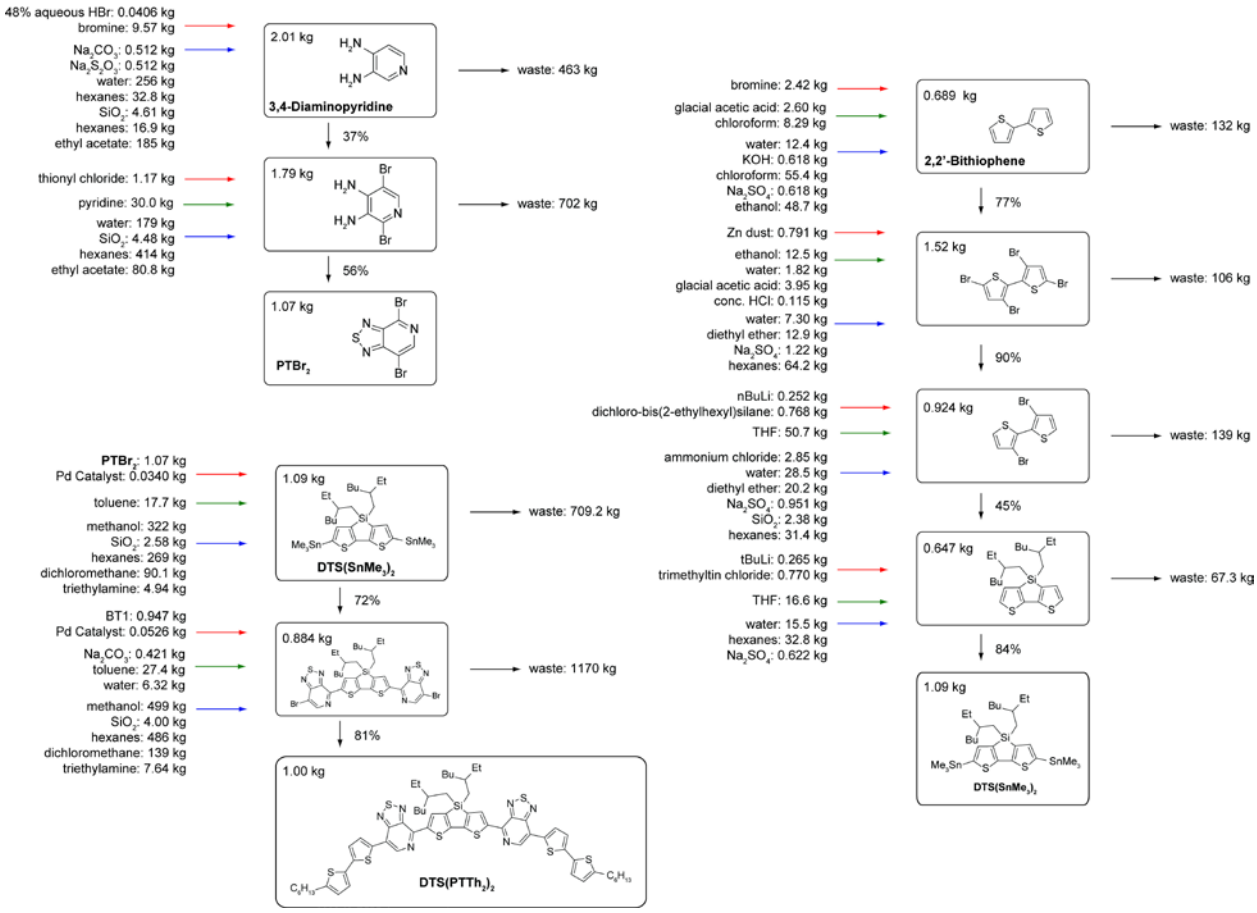


Figure S6. Flowchart describing the synthesis of 1 kg of **DTS**. The requisite quantities of reagent (red arrow), solvents (green arrow) and work-up materials (blue arrow) are indicated for each step.

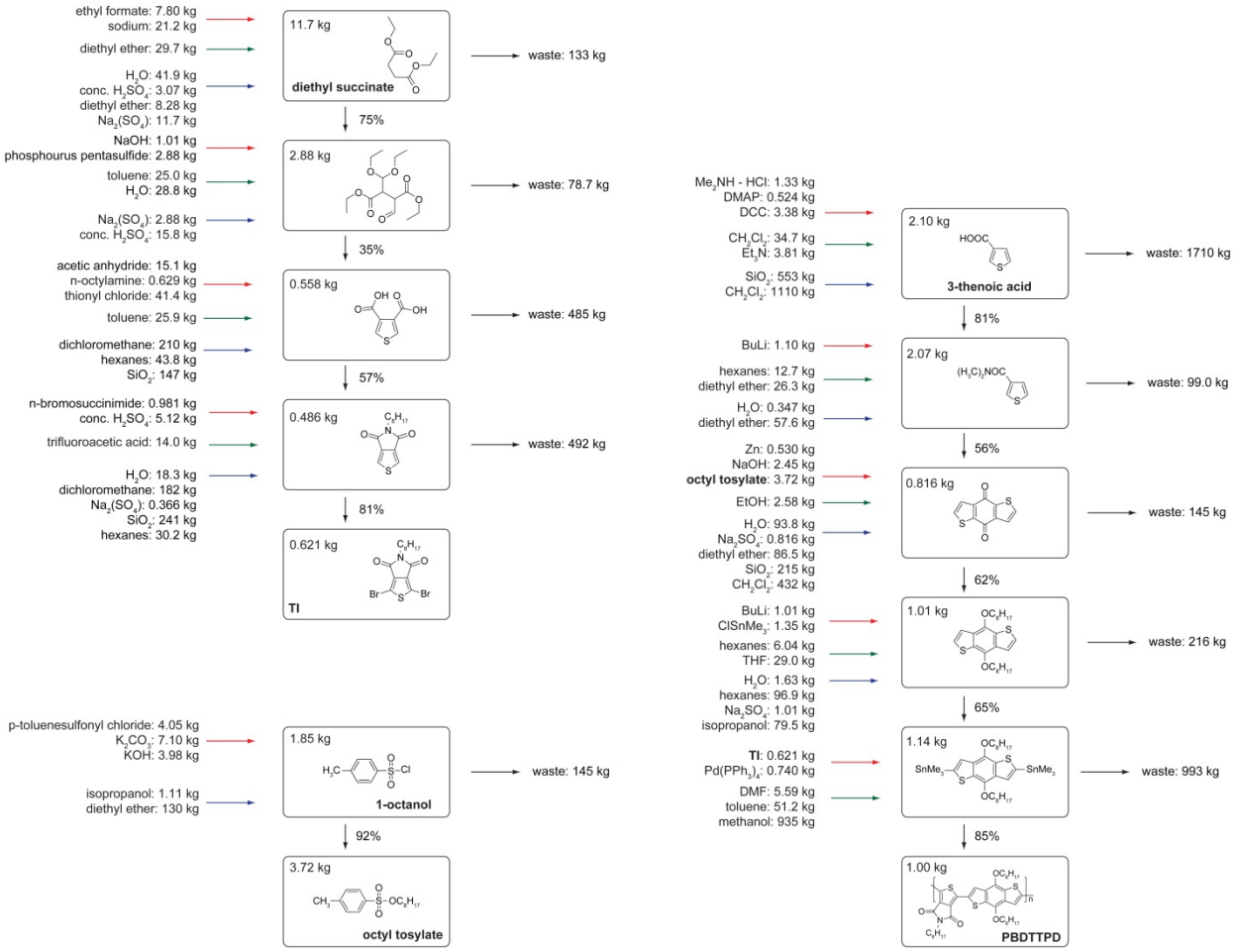


Figure S7. Flowchart describing the synthesis of 1 kg of **PBDTTPD**. The requisite quantities of reagent (red arrow), solvents (green arrow) and work-up materials (blue arrow) are indicated for each step.

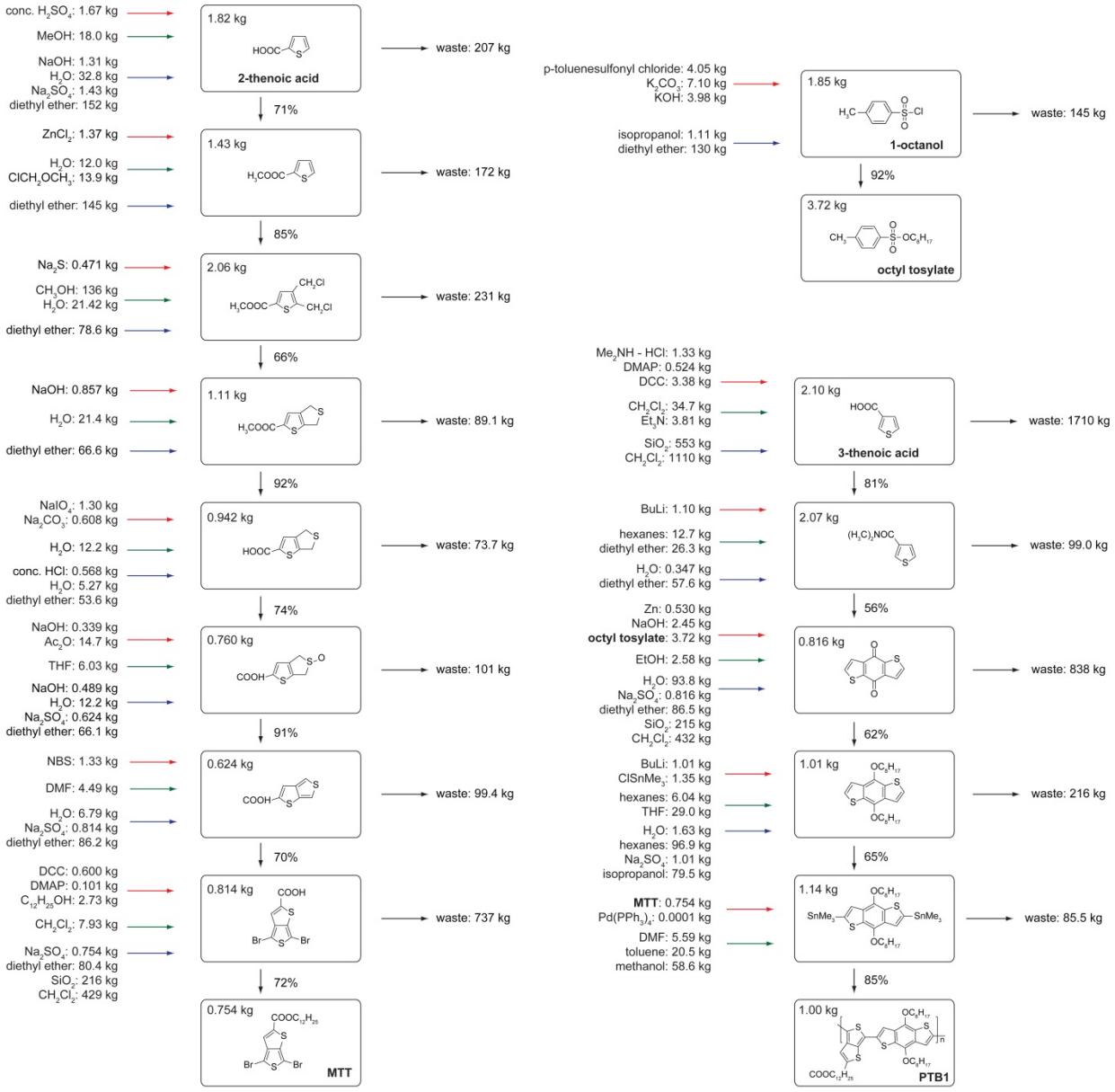


Figure S8. Flowchart describing the synthesis of 1 kg of **PTB1**. The requisite quantities of reagent (red arrow), solvents (green arrow) and work-up materials (blue arrow) are indicated for each step.

4. Material Costs Used in this Work

Table S1. Material costs used in this work.

Chemical Name	Active Layer Material	Quantity [kg]	Cost [$/kg]
(1,3-diphenylphosphinopropane)nickel (II) chloride	P3HT	0.025	$8,640.00
1-chloronaphthalene	CuPc	1	$209.00
1-octanol	PBDTTPD, PTB1	8.27	$28.30
1,2 dichloroethane	DBP	12.54	$11.24
1,3 diphenylacetone	DBP	0.1	$1,140.00
2-aminobenzoic acid	DBP	2	$61.50
2-bromothiophene	PDPP3T (1), PDPP3T (2)	1	$379.00
2-hexyldecyl iodide	PDPP3T (1), PDPP3T (2)	0.06685	$2,468.21
2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane	PDPP3T (2)	0.456	$1,085.53
2-thiophenecarboxylic acid	PTB1	0.5	$152.00
2,2'-bithiophene	DTS	0.025	$9,280.00
2,3-dichloro-5,6-dicyanobenzoquinone	DBP	0.25	$2,120.00
2M hexylmagnesium bromide in ether	P3HT	0.772	$195.60
3-bromothiophene	P3HT	0.5	$350.00
3-thiophenecarboxylic acid	PBDTTPD, PTB1	0.1	$1,130.00
3,4-Diaminopyridine	DTS	0.025	$17,000.00
4,4′-di-tert-butyl-2,2′-dipyridyl	PDPP3T (1)	0.025	$8,020.00
8-hydroxyquinoline	Alq3	2.5	$151.60
acenaphthenequinone	DBP	0.1	$1,735.00
acetic acid	PDPP3T (1), PDPP3T (2), DTS	21	$18.87
acetic anhydride	PDPP3T (1), PDPP3T (2), PBDTTPD, PTB1	2.16	$41.44
acetone	Alq3, SQ	12.7	$36.93
aliquat 336	PDPP3T (1), PDPP3T (2)	0.884	$170.81
aluminum potassium sulfate dodecahydrate	Alq3	2.5	$130.80
ammonium chloride	DTS	0.5	$699.00
ammonium molybdate	CuPc	0.5	$310.66
amyl alcohol	PDPP3T (1)	20	$13.05
bis(pinacolato)diboron	PDPP3T (1)	0.5	$7,080.00
boron trifluoride diethyl etherate	DBP	0.02875	$1,266.09
bromine	PDPP3T (1), PDPP3T (2), DTS	0.5	$1,650.00
BT1	DTS	0.005	$45,000.00
Butanol	SQ	16.2	$31.48

chloro-1,5-cyclooctadiene iridium(I) dimer	PDPP3T (1)	0.01	$86,500.00
chloroform	PDPP3T (2), DTS	2.98	$31.21
chloromethyl methyl ether	PTB1	0.025	$2,712.00
chlorotrimethyltin	PBDTTPD, PTB1	0.05	$5,290.00
conc. Ammonium hydroxide	Alq3	3	$351.78
copper (I) cyanide	PDPP3T (1), PDPP3T (2)	5	$52.80
copper (II) chloride	CuPc	1	$145.00
cyclohexane	SQ	1.56	$72.76
decanol	PTB1	2.07	$25.75
di-isopropyl succinate	PDPP3T (1)	0.495	$409.58
dichloro-bis(2-ethylhexyl)silane	DTS	10.7	$7.06
dichloromethane	DBP, PDPP3T (1), PDPP3T (2), PBDTTPD, PTB1, DTS, SQ	270	$9.09
dicyclohexylcarbodiimide	PBDTTPD, PTB1	2.5	$155.40
diethyl ether	P3HT, PDPP3T (1), PDPP3T (2), PBDTTPD, PTB1, DTS	4.24	$78.66
diethyl succinate	PBDTTPD	1	$61.80
diisobutylamine	SQ	0.74	$72.03
dimethylamine hydrochloride	PBDTTPD, PTB1	1	$68.60
dimethylformamide	PDPP3T (1), PDPP3T (2), PBDTTPD, PTB1	192.6	$20.23
ethanol	PBDTTPD, PTB1, DTS	12.6	$11.42
ethyl acetate	DTS	18	$38.61
ethyl formate	PBDTTPD	1.84	$69.57
ferrocene	DBP	2	$140.00
hexanes	PDPP3T (2), PBDTTPD, PTB1, DTS, SQ	135	$7.60
hydrobromic acid 48 wt% in water	P3HT, DTS	2.69	$40.52
hydrochloric acid	P3HT, PTB1, DTS	4.4	$38.77
hydrogen peroxide	P3HT	5.13	$17.19
isoamyl nitrite	DBP	0.5	$245.04
isopropanol	PBDTTPD, PTB1	163	$8.49
methanol	P3HT, DBP, PDPP3T (1), PDPP3T (2), PBDTTPD, PTB1, DTS	15	$6.24
N-bromosuccinimide	PDPP3T (1), PDPP3T (2), PBDTTPD, PTB1	5	$81.60

n-butyllithium in hexanes	PDPP3T (2), PBDTTPD, PTB1, DTS	0.0102	$3,654.90
N-methylpyrrolidone	PDPP3T (1)	18.504	$54.58
n-octylamine	PBDTTPD	0.5	$127.08
N,N,-dimethylaminopyridine	PBDTTPD, PTB1	0.25	$1,120.00
Na2S2O3 sodium thiosulfate	DTS	2.5	$62.40
octane	PDPP3T (1)	14.1	$98.94
p-toluenesulfonyl chloride	PBDTTPD, PTB1	5	$40.40
Phloroglucinol	SQ	0.1	$717.00
phosphorus pentasulfide	PBDTTPD	0.5	$63.02
phthalic acid	CuPc	1	$69.30
potassium carbonate	PDPP3T (1), PDPP3T (2), PBDTTPD, PTB1	2.5	$38.18
potassium hydroxide	PBDTTPD, PTB1, DTS	450	$17.06
potassium phosphate	PDPP3T (1), PDPP3T (2)	5	$70.20
pyridine	DTS	19.6	$59.95
silica 60 um particles	DBP, PDPP3T (1), PDPP3T (2), PBDTTPD, PTB1, DTS, SQ	1	$275.56
sodium	PDPP3T (1), PBDTTPD	0.05	$1,498.00
sodium carbonate	PTB1, DTS	1	$115.50
sodium cyanide	PDPP3T (1), PDPP3T (2)	1	$53.60
sodium hydroxide	PBDTTPD, PTB1	12	$27.58
sodium metaperiodate	PTB1	0.5	$590.00
sodium sulfate	P3HT, PDPP3T (1), PDPP3T (2), PBDTTPD, PTB1, DTS	12	$30.92
sodium sulfide	PTB1	0.05	$7,020.00
squaric acid	SQ	0.1	$6,860.00
sulfuric acid	CuPc, PBDTTPD, PTB1	5.49	$36.07
t-butylmagnesium chloride in ether	P3HT	0.144	$1,680.56
tBuLi	DTS	1.09	$833.94
tetrahydrofuran	P3HT, PDPP3T (2), PBDTTPD, PTB1, DTS	16.9	$40.82
tetrakis(triphenylphosphine)palladium	PBDTTPD, PTB1, DTS	0.025	$16,800.00
N,N’-tetramethylethylenediamine	PDPP3T (2)	0.775	$166.45
thionyl chloride	PBDTTPD, DTS	2	$128.00
thiophene	PDPP3T (1), PDPP3T (2)	0.5	$84.80

toluene	PDPP3T (1), PDPP3T (2), PBDTTPD, PTB1, DTS, SQ	176	$4.89
triethylamine	DBP, PBDTTPD, PTB1, DTS	1	$118.00
trifluoroacetic acid	DBP, PBDTTPD	2.5	$163.20
trimethyltin chloride	DTS	0.05	$264.50
triphenylphosphine	PDPP3T (1), PDPP3T (2)	2	$97.50
tris(dibenzylideneacetone)dipalladium	PDPP3T (2)	0.025	$28,320.00
urea	CuPc	10	$8.31
water	CuPc, Alq3, P3HT, PDPP3T (1), PDPP3T(2), PBDTTPD, PTB1, DTS	0	$0.00
zinc (II) chloride	PTB1	6	$235.83
zinc dust	PBDTTPD, PTB1, DTS	1	$83.50

5. Cost-per-Peak-Watt for Several OPV Active Layer Materials

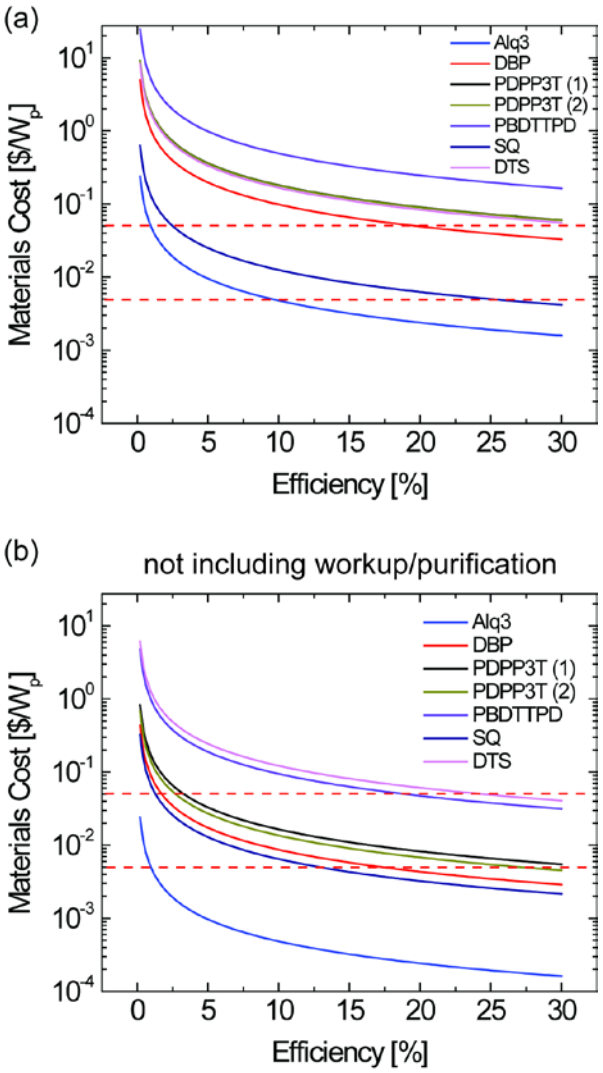


Figure S9. Calculated material cost-per-peak-Watt ($/$W_p$) as a function of solar cell efficiency for hypothetical devices incorporating **Alq3**,**DBP**, **PDPP3T**, **PBDTTPD, SQ and DTS**. (a) Includes the cost of reagents, solvents and work-up procedures. (b) Includes only the cost of reagents and solvents. The red dashed lines indicate 0.005 and 0.050-dollars-per-peak-Watt.