Electronic Supplementary Information

Selection of green solvents for organic photovoltaics by reverse engineering

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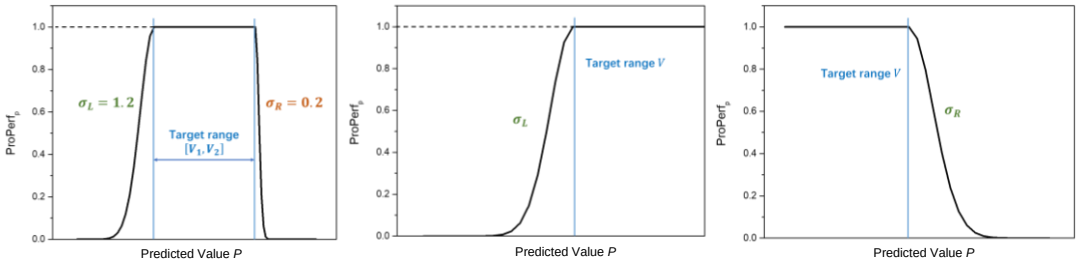
Table S1. Physico-chemical properties of P3HT[2] and PF2[1].

Polymers	HOMO (eV)	LUMO (eV)	M_n (kg mol^{-1})	M_w (kg mol^{-1})	Đ
P3HT	-5.0	-3.0		70-90	
PF2	-5.4	-3.8	35	63	1.8

Fig. S1 Gaussian function of $ProPerf_p(P)$ for target value V with different σ values of the property P.



$$ProPerf_p(P) = \begin{cases} 1, & V_1 \le P \le V_2 \\ exp\left[-\left(\frac{V_1 - P}{\sigma_L}\right)^2\right] < 1, & P < V_1 \\ exp\left[-\left(\frac{V_2 - P}{\sigma_R}\right)^2\right] < 1, & P > V_2 \end{cases}$$

$$ProPerf_p(P) = \begin{cases} 1, & P \ge V \\ exp\left[-\left(\frac{V - P}{\sigma_L}\right)^2\right] < 1, & P < V \end{cases}$$

$$ProPerf_p(P) = \begin{cases} 1, & P \le V \\ exp\left[-\left(\frac{V - P}{\sigma_R}\right)^2\right] < 1, & P > V \end{cases}$$

Hansen parameters determination

The HSPs of a solvent can be determined by solubility experiments. Firstly, the solubility of a solute is tested in a list of solvents. The solvents are ranked into 1 ("good" solvents), 0 ("bad" solvents) and 2 (between "good" and "bad" solvents), depending on their capacity to solubilize the solute. The software HSPiP uses the scores to build a solubility sphere which separates good and bad solvents. The center of the HSP solubility sphere yield the HSP parameters of the solute. The radius of the sphere, R_0, defines the region in HSP space corresponding to the solvents that are able to solubilize the solute. The larger R_0 the more easily soluble is the solute.

In this work, 36 solutions were prepared with a solute concentration of 2 mg/ml. Commonly available laboratory solvents are chosen, as well as these solvents should be covered the entire Hansen space. The prepared solutions were annealed at 40 °C overnight. The Hansen parameters of PF2 were found to be δ_D=19.15, δ_P=3.87, δ_H=2.83, and R_0 was estimated to 4.0. And the Hansen parameters of EH-IDTBR were defined to be 18.8 ± 0.3, 4.4 ± 0.75, 4.3 ± 0.80, and R_0 was found to be 6.1. The error margins correspond to the standard deviation of the mean values.

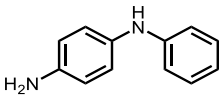
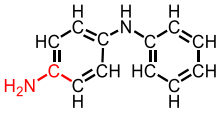
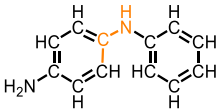
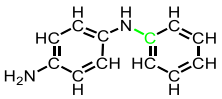
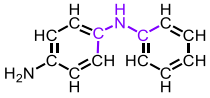
The solubility experiments of P3HT were done by Dr. Markus Kohlstädt from the Albert Ludwigs Universität Freiburg. The HSPs of P3HT were estimated to δ_D=18.5, δ_P=4.7, δ_H=5.0, and R_0=4.7. The HSPs of $PC_{71}BM$ have been reported in literature and are given by δ_D=20.2, δ_P=5.4, δ_H=4.5, R_0=8.4.[3]

Table S2. The physicochemical properties and corresponding values of o-DCB and CB.

Physicochemical properties	Values	
	o-DCB	CB
Non-polar interactions (δ_D, $MPa^{1/2}$)	19.2	19.0
Polar interactions (δ_P, $MPa^{1/2}$)	6.3	4.3
Hydrogen bonds (δ_H, $MPa^{1/2}$)	3.3	2.0
Distance (R_a, $MPa^{1/2}$) with P3HT	2.83	3.19
Distance (R_a, $MPa^{1/2}$) with PF2	2,48	
Relative energy difference (*RED*) with P3HT (defined by R_a/R_o)	0.64	0.68
Relative energy difference (*RED*) with PF2 (defined by R_a/R_o)	0.62	
Boiling Point (T_b, K)	453	405
Vaporization enthalpy (ΔH_{vap}, kJ/mol)	49.08	40.76
Density (ρ, g/cm^3)	1.31	1.11
Viscosity (η, mPa s)	1.30	0.76
Flash Point (T_f, K)	339	301
Melting Point (T_m, K)	256	228
Safety information (GHS label)	 [a]	 [a]

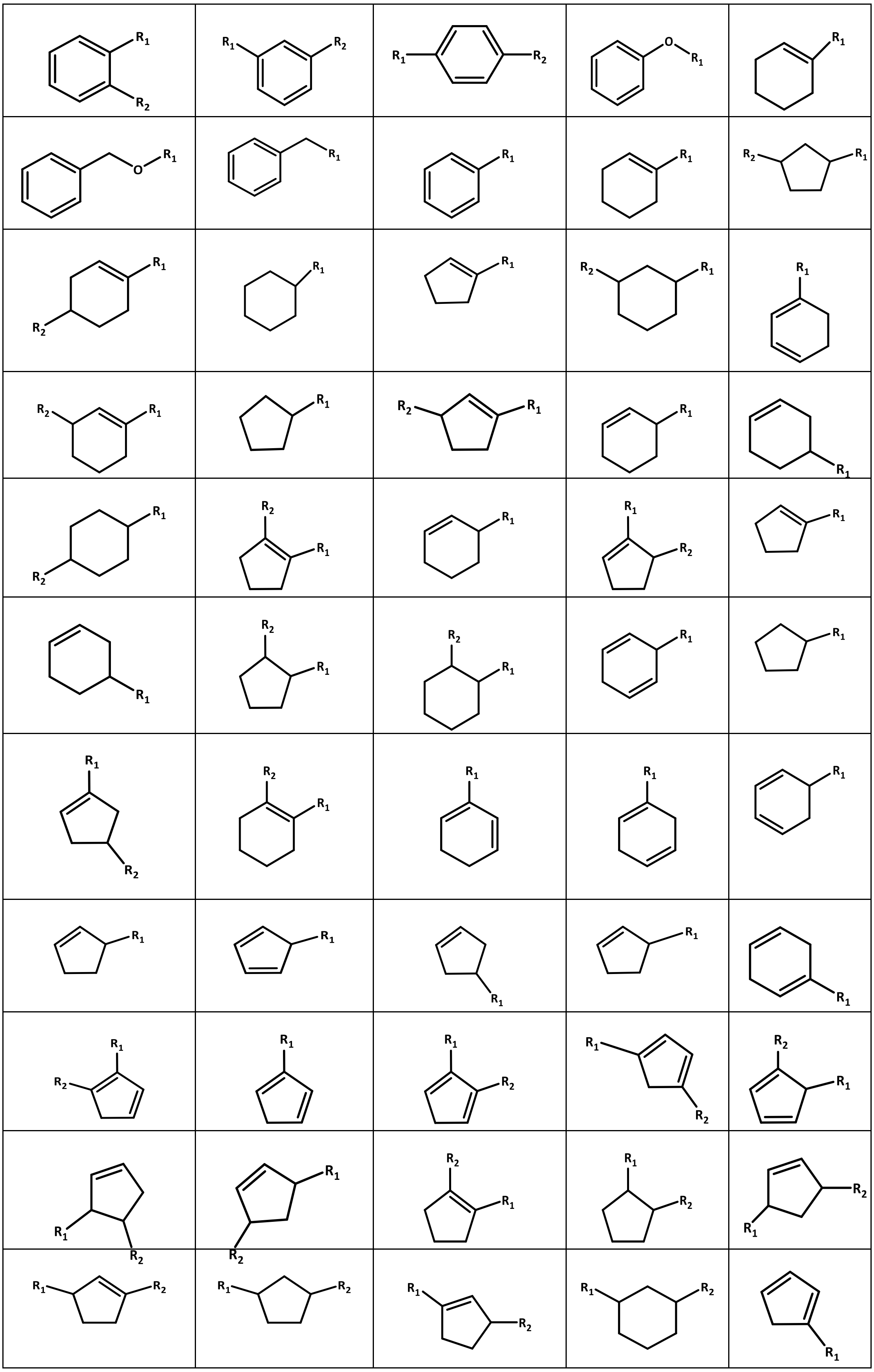
[a] ECHA, https://echa.europa.eu/home

Table S3. Estimation of normal boiling point of N-phenyl-1,4-benzenediamine. [4]

N-phenyl-1,4-benzenediamine (Experimental value: T_b = 627 K)			Molecular structure 	
First order groups	n_{1k}		A_k	$\sum n_{1k}A_k$
-C–NH_2	1		3.8298	15.8281
-C–NH	1		2.9230	
-C	1		1.5468	
-CH	9		0.8365	
Second order groups	n_{2k}		B_k	$\sum n_{2k}B_k$
AROMRINGs[1]s[4] (1,4-substituted aromatic ring)	1		0.1007	0.1007
Third order groups	n_{3k}		C_k	$\sum n_{3k}C_k$
-C–NH–C-	1		0.5768	0.5768
$T_b^{est} = 222.543 \ln P = 222.543 \ln(15.8281 + 0.1007 + 0.5768) = 624K$ (error = 627-624 = 3K)				

Taking N-phenyl-1,4-benzenediamine as an example, the boiling point of this solvent can be estimated using the parameters given in Table S3, leading to an estimation which matches well the experimental value. The related parameters including n_{1k}, A_k, n_{2k}, B_k, n_{3k}, C_k, and universal constants for the target properties can be found in Ref. 4.

Table S4. List of chemical groups for molecular design by IBSS®CAMD.



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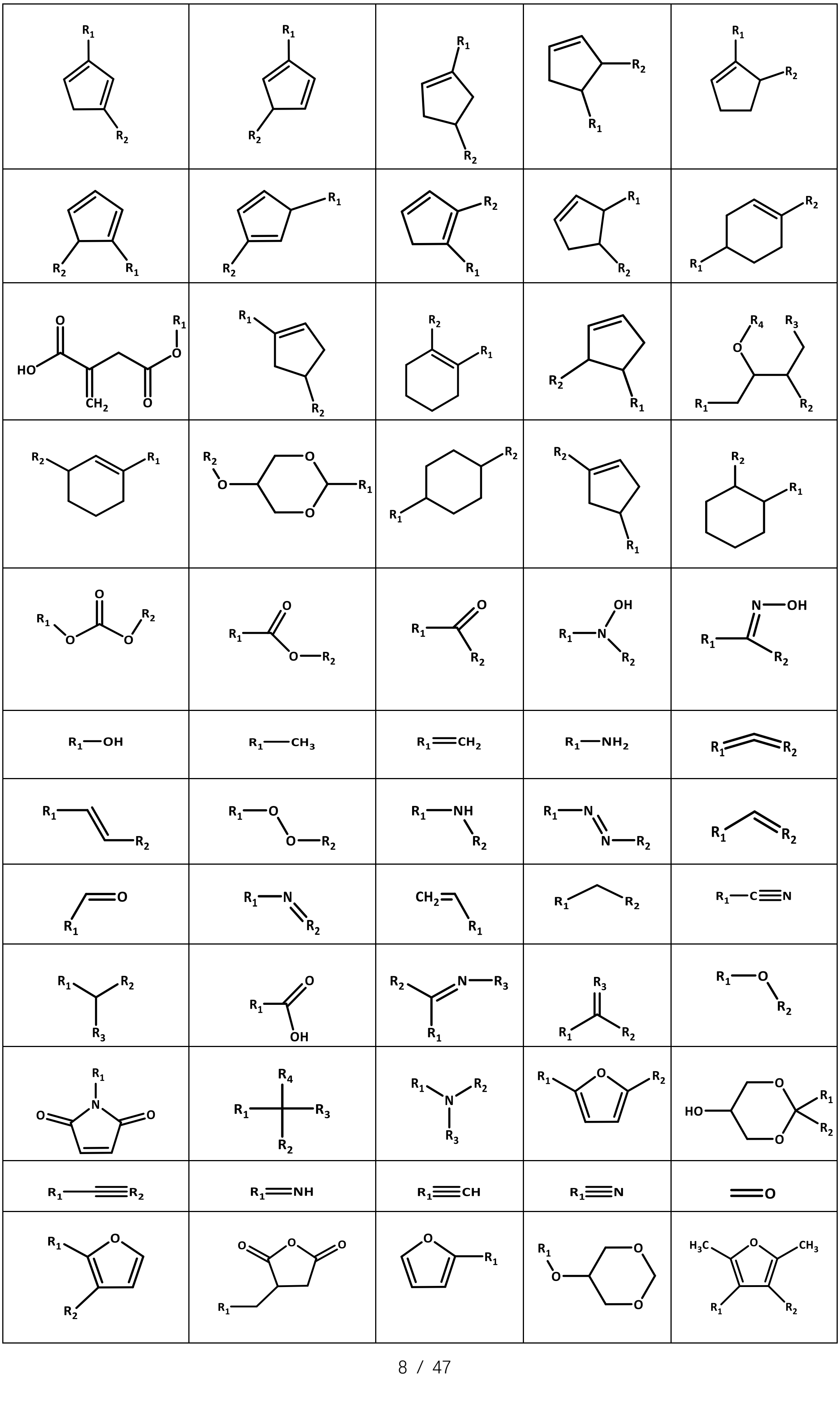

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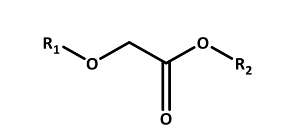	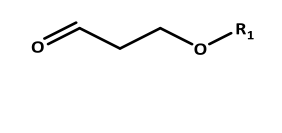	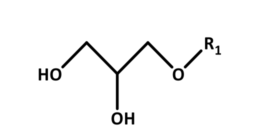	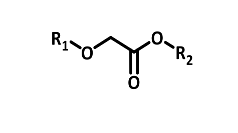
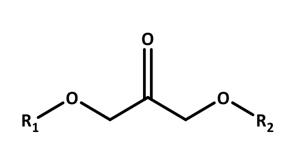	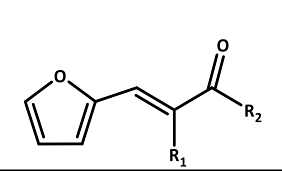	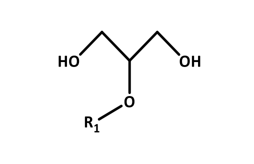	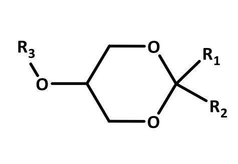
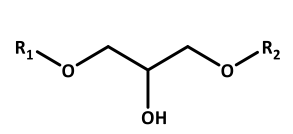	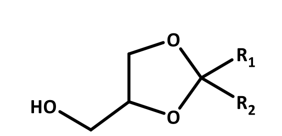	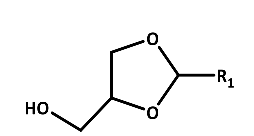	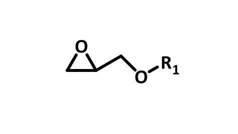
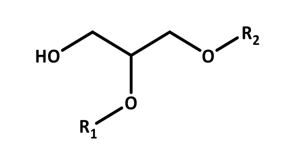	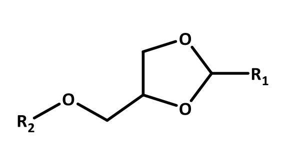	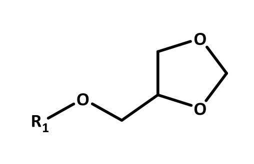	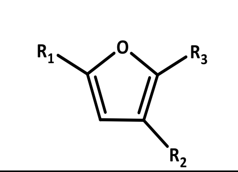
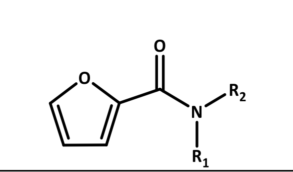	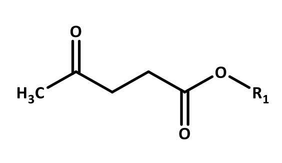	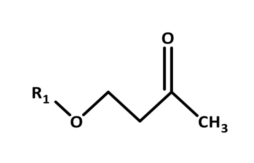	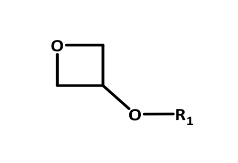
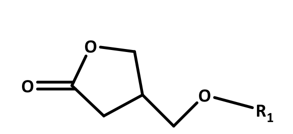	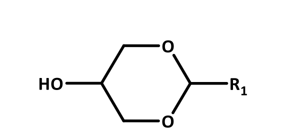	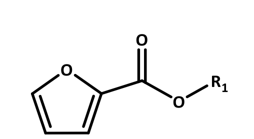	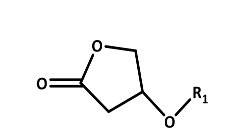
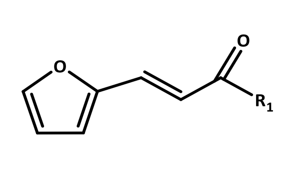	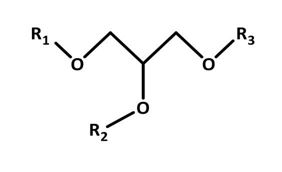	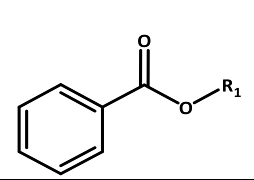	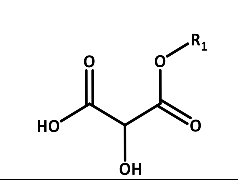
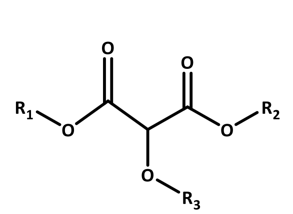	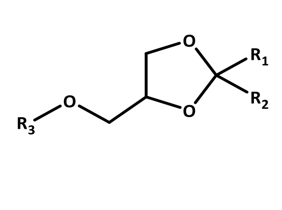	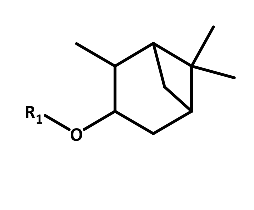	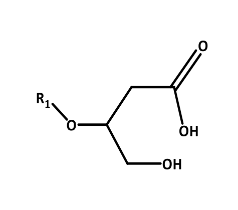
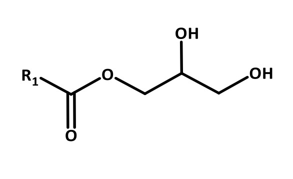	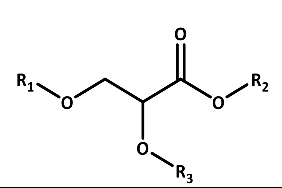	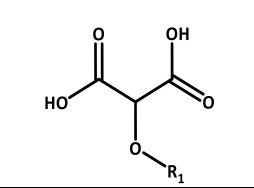	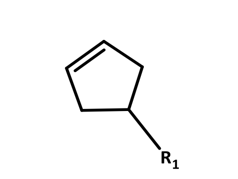
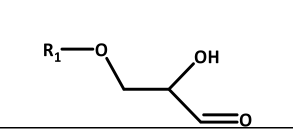	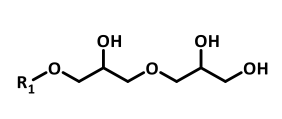	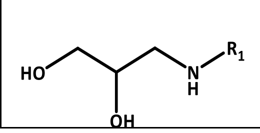	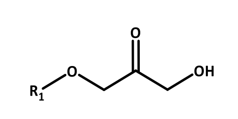

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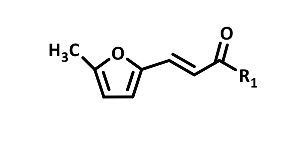	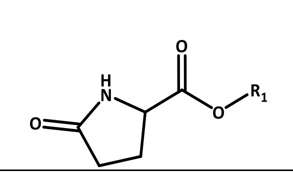	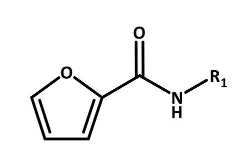	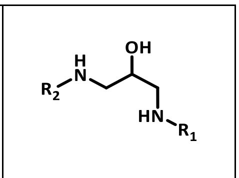
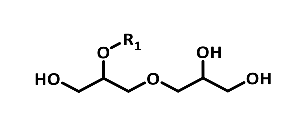	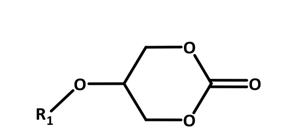	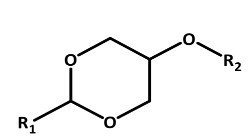	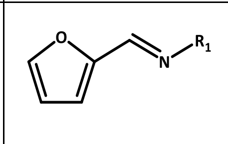
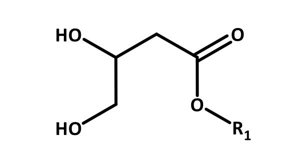	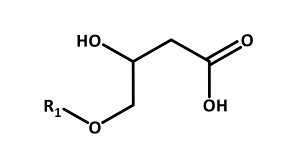	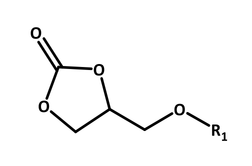	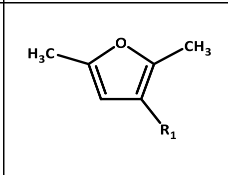
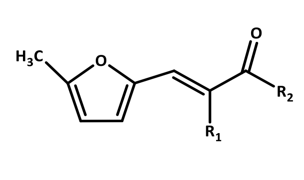	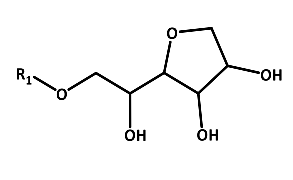	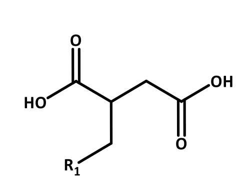	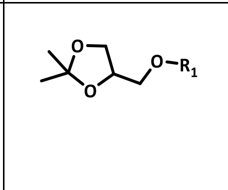
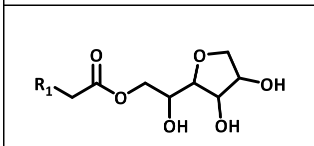	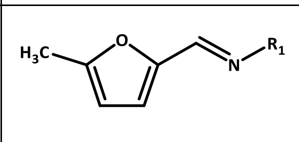	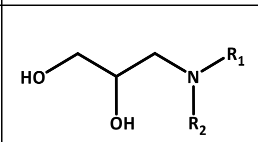	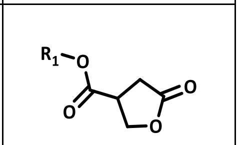
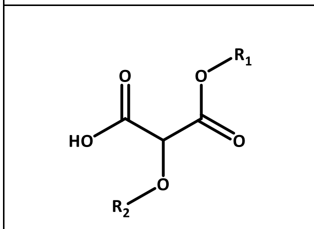	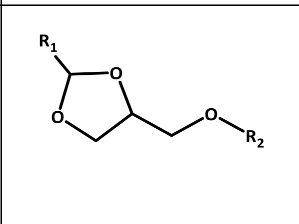	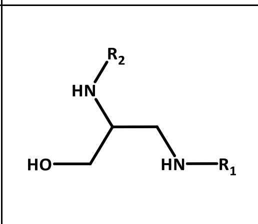	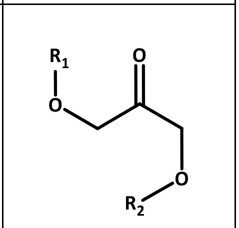
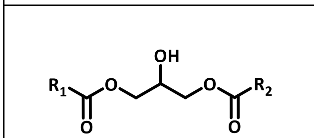	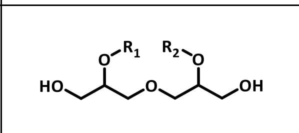	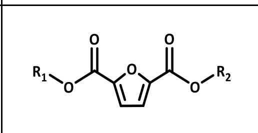	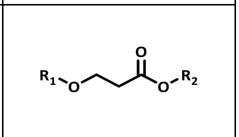
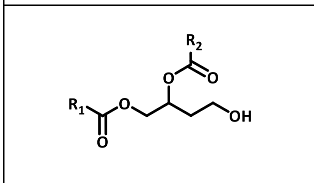	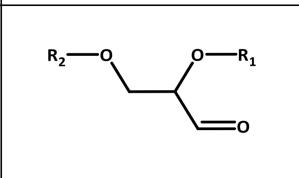	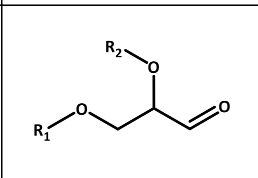	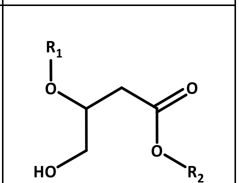
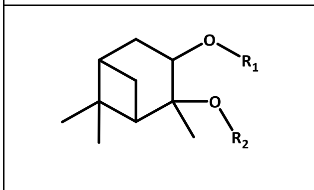	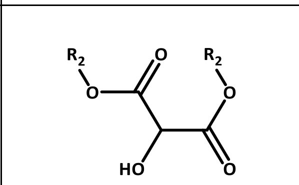	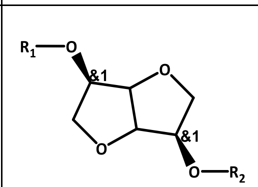	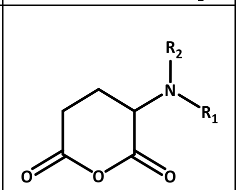
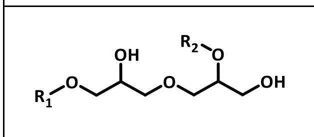	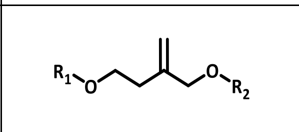	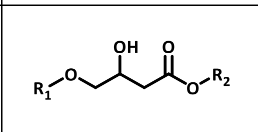	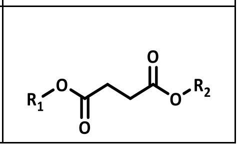

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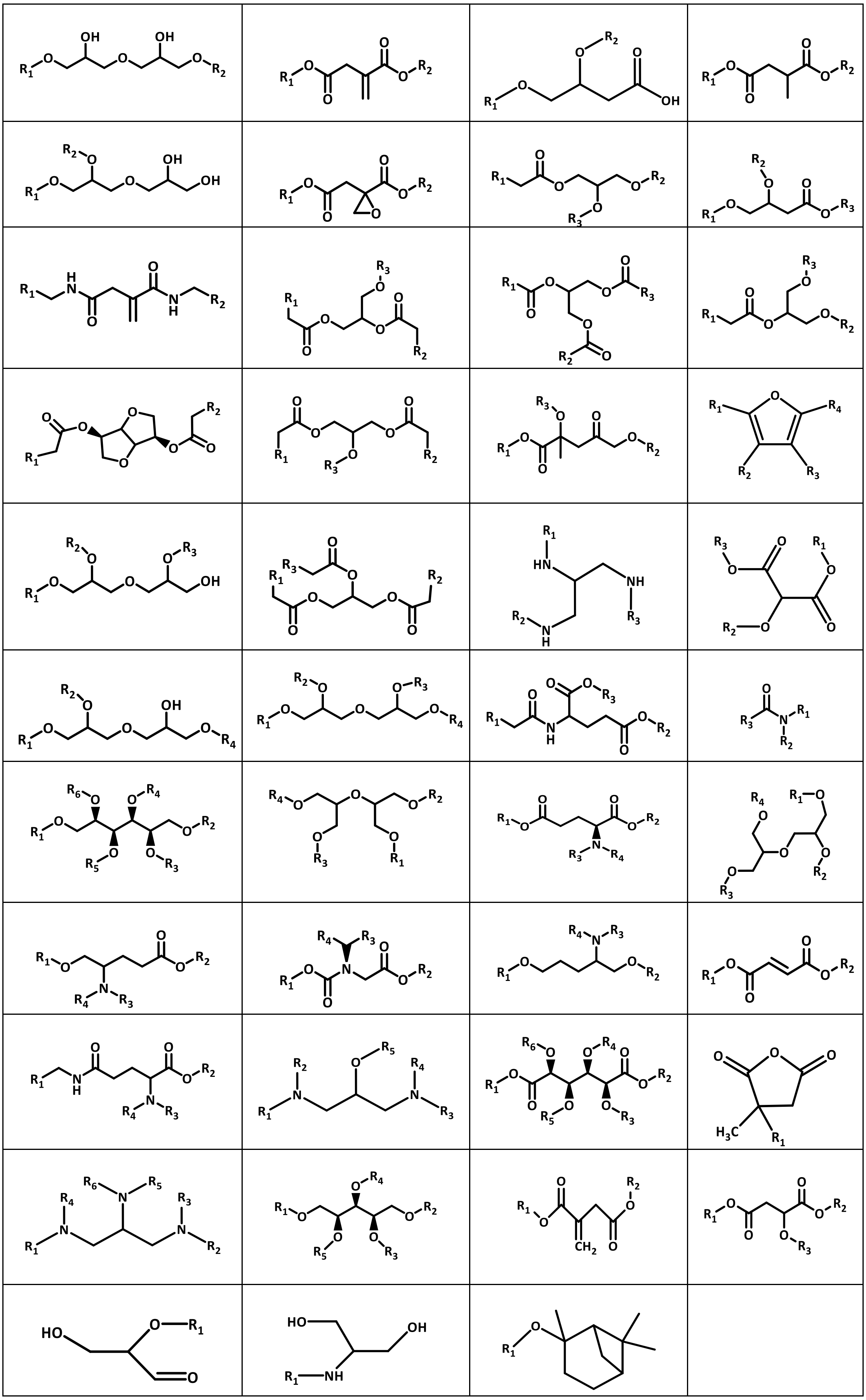


Fig. S2 Examples of chemical groups and connection types for building alternative solvents using IBSS®CAMD tool. (R1 and R2 are randomly selected chemical groups from the IBSS ®CAMD data base that are connected to other chemical groups by either simple or double bonds).

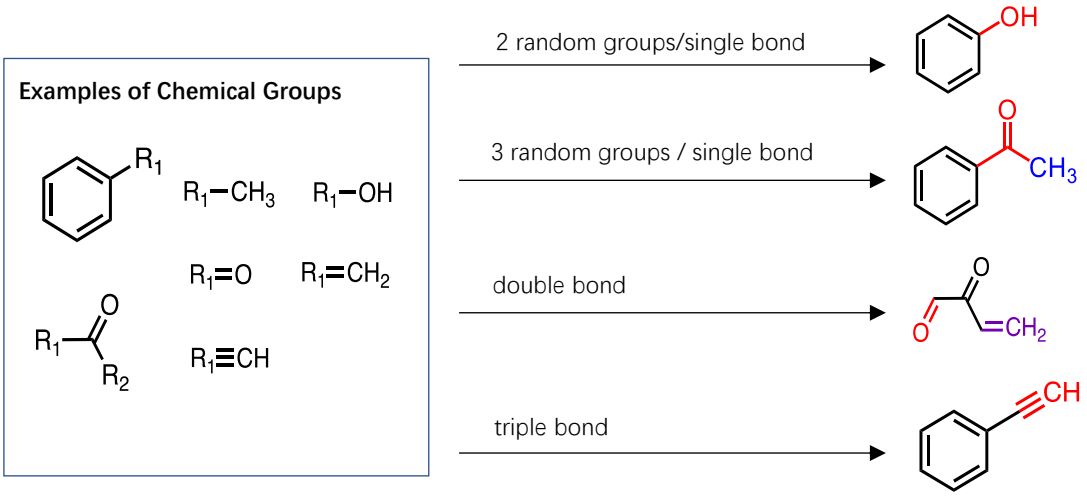


Table S5. List of selected known green solvents.

N.	Name	N.	Name
1	Anisole	2	Methyl 9,12-octadecadienoate
3	Methyl 9,12-octadecadienoate	4	Geranyl acetate
5	p-Xylene	6	Dimethyl Adipate
7	Isoamyl acetate	8	Nopol
9	Benzyl Benzoate	10	Methyl myristate
11	p-Cymene	12	2-Octanol
13	Terpinolene	14	2-Furylmethanol
15	Butyl acetate	16	1,3-Dioxolan-4-ylmethanol
17	Tetrahydrofuran	18	Ethyl myristate
19	d-Limonene	20	Ethyl palmitate
21	Cyclopentyl methyl ether	22	Bis(2-ethylhexyl) succinate
23	Isobutyl acetate	24	Methyl palmitate
25	2-Methyltetrahydrofuran	26	Dimethyl sulfoxide
27	Propylene carbonate	28	Dimethyl isosorbide
29	Ethylene carbonate	30	Butyl laurate
31	Glycerol -1,2,3-triethyl ether	32	9,12-Octadecadienoic acid (9Z,12Z)-, ethyl ester
33	Dimethyl Succinate	34	Propionic acid
35	1,2,3-Trimethoxypropane	36	Methyl 9-octadecenoate
37	Diethyl carbonate	38	Dioctyl-succinate
39	Furfural	40	N,N-Dimethyldec-9-enamide
41	5-Methyldihydro-2(3H)-furanone	42	Methyl stearate
43	1,2-Ethanediyl diacetate	44	p-Anisaldehyde
45	alpha-Pinene	46	Glycerol 1,3-diethyl ether
47	2-(4-Methylcyclohexyl)-2-propanyl acetate	48	Isopropyl myristate
49	Dimethyl Glutarate	50	Oleic Acid
51	1 – Butanol	52	1,3-Dioxan-5-ol
53	Pinane	54	Ethyl 9-octadecenoate
55	Isobutanol	56	2,6-Dimethyl-7-octen-2-ol
57	β-Myrcene	58	Tetrahydro-2-furanylmethanol
59	Isosorbide dioctanoate	60	Menthanol
61	Methyl linolenate	62	N,N-Dimethylactanamide
63	Isoamyl alcohol	64	Butyl palmitate
65	Isopropyl palmitate	66	Methyl 12-hydroxy-9-octadecenoate
67	2-Furanamine	68	Butyl myristate
69	Dimethyl 2-methylglutarate	70	Ethylene glycol
71	Bis(3-methylbutyl) succinate	72	Ethyl 2-hydroxypropanoate
73	Diisopropyl Adipate	74	3-Methoxy-1,2-propanediol
75	Ethyl linolenate	76	1,3-Dimethoxy-2-propanol
77	1,3-Dioxolane	78	Propylene glycol

Table S5 (continued):

79	β –Pinene	80	Glycerol-1,2,3-tributhyl ether
81	Methyl laurate	82	Glycerol -1,3-dibutyl ether (Dibuprol)
83	Ethyl Laurate	84	1-Octanol
85	N,N-Dimethyldecanamide	86	beta-Terpineol
87	Dibutyl ether	88	1,3-Propanediol
89	Terpineol acetate	90	Methanol
91	6,8-Dioxabicyclo[3.2.1]octan-4-one	92	1,1,1,3,3-Pentafluorobutane
93	Isopropyl Acetate	94	2,3-Dibutoxy-1-propanol
95	Diethoxymethane	96	5-(Hydroxymethyl)-2-furaldehyde
97	Acetic acid	98	4-(Hydroxymethyl)-1,3-dioxolan-2-one
99	Tributyl citrate acetate	100	Triethyl citrate
101	1,4-Butanediol	102	Hexamethyldisiloxane
103	2,3-Dimethoxy-1-propanol	104	Ethyl acetate
105	2-Methoxy-1,3-propanediol	106	Tributyl citrate
107	2-Hydroxypropanoic acid	108	3-Ethoxy-1,2-propanediol
109	1,2,3-Propanetriyl triacetate	110	2-Ethoxy-2-methylpropane
111	Alpha-Terpineol	112	2-(2-Butoxyethoxy)ethanol
113	2,3-Diethoxy-1-propanol	114	3-Butoxy-1,2-propanediol
115	2-Methoxy-2-methylbutane	116	Acetone
117	(2,2-Dimethyl-1,3-dioxolan-4-yl)methanol	118	2-Hydroxy-N,N-dimethylpropanamide
119	2-Ethylhexyl lactate	120	3-Hydroxypropanoic acid
121	Geraniol	122	2-Ethoxy-1,3-propanediol
123	O-Acetylcholine	124	Glycerol
125	1-Decanol	126	1,4-Bis(aminooxy)-1,4-butanedione
127	1,2-Pentanediol	128	N,N-Bis(2-hydroxyethyl)octanamide
129	Cyclademol	130	2-Butoxy-1,3-propanediol
131	Butyl stearate	132	Dimethyl carbonate
133	12-Hydroxy-9-octadecenoic acid	134	Methoxy(trimethyl)silane
135	9-Octadecen-1-ol	136	Isopropanol
137	Ethanol	138	Butyl 3-hydroxybutanoate

Table S6. Calculated property values of list of the solvent candidates selected from the results of molecular design provided by IBSS®CAMD for P3HT:$PC_{71}BM$.

name	CAS	$GloPerf$	Melting Point (T_m) [K]	Boiling Point (T_b) [K]	Flash Point (T_f) [K]	ΔH_{vap} [kJ/mol]	Density [g/cm^3]	δ_D [$MPa^{1/2}$]	δ_P [$MPa^{1/2}$]	δ_H [$MPa^{1/2}$]	R_a [$MPa^{1/2}$]	*RED*	Viscosity [mPa s]
4-Ethynyltoluene	766-97-2	1	246	442	325	47.91	0.923	18.8	4	3.5	1.755	0.37	0.721
Anisole	100-66-3	0.997	239	427	314	46.52	0.974	18.1	4.9	6.1	1.392	0.296	0.569
(Vinyloxy)benzene	766-94-9	0.989	246	450	322	50.33	0.982	17.8	4.9	5.3	1.502	0.32	0.655
2-Methylanisole	578-58-5	0.946	234	448	329	52.276	0.964	18.6	4.4	6.6	1.560	0.34	0.668
methylbenzoate	93-58-3	0.923	246	465	343	55.57	1.068	18.7	7.5	5.3	2.863	0.609	1.34
4-Methoxycyclohexene	15766-93-5	0.916	210	416	301	41.72	0.892	17.1	3.7	5.2	3.025	0.644	0.611
Cyclopentyl acetate	933-05-1	0.907	226	419	313	50.86	0.974	16.9	4.5	5.5	3.298	0.702	1.182
Cyclopentyl formate	62781-99-1	0.901	209	404	302	46.94	1.001	17	5.4	6.1	3.323	0.707	0.944
benzyl ethyl ether	539-30-0	0.899	243	484	352	55.11	0.934	17.9	4	3.9	1.82	0.387	0.902
Formylcyclohexane	2043-61-0	0.895	254	442	326	46.61	0.932	17.8	7.6	4.6	3.302	0.702	1.3
Benzyl vinyl ether	935-04-6	0.889	251	486	352	54.38	0.956	18	4.4	5.1	1.096	0.233	0.82
1-(2-Cyclopenten-1-yl)ethanone	73113-00-5	0.884	253	435	318	47.18	0.948	17.4	6.7	5	3.038	0.646	1.026
3-Methoxycyclohexene	2699-13-0	0.877	210	416	301	41.72	0.89	16.8	4.6	5.2	3.465	0.737	0.611
Vinylxylene	3333-13-9	0.867	219	459	328	51.03	0.887	18.1	3.1	2.6	3.018	0.642	0.822
2-Propylfuran	4229-91-8	0.865	197	402	293	43.59	0.896	16.9	4.9	5.1	3.269	0.696	0.862
1-Acetylcyclohexane	823-76-7	0.863	262	465	337	49.43	0.917	17.2	5.4	3.6	3.107	0.661	1.676
1-(1-Cyclohexen-1-yl)ethanone	932-66-1	0.863	279	472	334	47.46	0.953	17.1	5.3	4.1	3.073	0.654	1.809
Acetyl cyclopentane	6004-60-0	0.859	249	437	319	46.09	0.916	17.1	6.1	3.5	3.545	0.754	1.187
Benzyl formate	104-57-4	0.855	257	470	346	57.55	1.079	18.7	6.3	6.7	2.358	0.502	1.348
p-xylene	106-42-3	0.853	229	419	301	43.35	0.873	18.6	3.8	1.6	3.541	0.753	0.568

Table S6 (continued):

name	CAS	$GloPerf$	Melting Point (T_m) [K]	Boiling Point (T_b) [K]	Flash Point (T_f) [K]	ΔH_{vap} [kJ/mol]	Density [g/cm^3]	δ_D [MPa$^{1/2}$]	δ_P [MPa$^{1/2}$]	δ_H [MPa$^{1/2}$]	R_a [MPa$^{1/2}$]	*RED*	Viscosity [mPa s]
1-Phenyl-2-butene	935-00-2	0.837	220	459	329	51.81	0.888	18.2	1.9	3.2	3.385	0.72	0.815
3-Methyl-2-cyclohexen-1-yl acetate	75411-49-3	0.829	248	463	339	54.9	0.983	16.9	4.2	5.7	3.361	0.715	1.632
2-Ethylfuran	3208-16-0	0.827	186	373	273	38.68	0.908	17	5.1	5.4	3.112	0.662	0.67
Cyclohexylacetone	103-78-6	0.826	255	479	346	54.13	0.912	17.2	5	5.1	2.681	0.57	2.089
Allylbenzene	300-57-2	0.824	197	435	311	46.1	0.888	18.1	2	3.1	3.405	0.724	0.707
3-(Vinyloxy)cyclohexene	80816-25-7	0.823	214	461	332	47.82	0.904	16.7	4.6	5.7	3.721	0.792	0.701
2-(3-Buten-1-yl)-5-methylfuran	5312-85-6	0.812	207	441	316	46.96	0.907	16.7	4.3	5.9	3.78	0.804	1.146
(2E)-2,4-Pentadien-1-ylbenzene	91166-39-1	0.811	234	481	344	57.19	0.9	18	2.2	3.8	2.956	0.629	0.921
2-Cyclopenten-1-yl acetate	20657-21-0	0.807	231	417	312	51.94	1.007	17.1	4.9	7	3.48	0.741	1.024
2-Cyclohexen-1-yl acetate	14447-34-8	0.802	246	447	331	55.28	0.996	17	5.2	6.7	3.526	0.75	1.428
1-Cyclohexyl-2-propen-1-one	2177-34-6	0.794	247	462	332	59.15	0.928	17.1	5.4	4.2	3.066	0.652	1.7
2-Methyl-5-propylfuran	1456-16-2	0.792	200	422	303	43.21	0.889	16.6	4.7	5.5	3.889	0.827	1.009
Allyl Benzyl Ether	14593-43-2	0.791	248	500	362	58.86	0.947	17.9	4.1	4.9	1.389	0.296	1.016
[(2E)-2-Buten-1-yloxy]benzene	14503-58-3	0.79	267	490	357	60.89	0.961	17.8	4	6.1	1.93	0.411	0.933
3-Cyclohexene-1-carbaldehyde	100-50-5	0.777	258	441	325	47.69	0.965	18.1	8.3	6.2	3.91	0.832	1.124

Table S6 (continued):

name	CAS	$GloPerf$	Melting Point (T_m) [K]	Boiling Point (T_b) [K]	Flash Point (T_f) [K]	ΔH_{vap} [kJ/mol]	Density [g/cm^3]	δ_D [MPa$^{1/2}$]	δ_P [MPa$^{1/2}$]	δ_H [MPa$^{1/2}$]	R_a [MPa$^{1/2}$]	*RED*	Viscosity [mPa s]
3-Methyl-1-cyclohexene-1-carbaldehyde	63282-01-9	0.772	242	460	330	48.03	0.953	17.5	7.8	5.1	3.748	0.797	1.316
Benzyl acetate	140-11-4	0.767	259	484	356	61.47	1.044	18.3	5.2	6.1	1.28	0.272	1.658
[(3-Buten-1-yloxy)methyl]benzene	70388-33-9	0.765	255	518	375	63.77	0.937	17.8	3.7	4.7	1.784	0.379	1.248
Isopropoxybenzene	2741-16-4	0.761	243	494	358	57.98	0.922	18.7	3.5	4.2	1.474	0.314	1.107
Acetophenone	98-86-2	0.758	268	471	346	55.4	1.018	19.1	8.6	4.8	4.098	0.872	1.357
1-Acetoxycyclohexene	1424-22-2	0.748	241	455	332	51.61	1.005	16.9	3.5	5.9	3.571	0.76	1.779
4-Methoxycyclopentene	40955-64-4	0.744	191	382	279	38.38	0.887	17.1	3.8	5.6	3.043	0.648	0.426
propenylfuran	10599-55-0	0.741	235	408	289	43.29	0.931	17.3	4.9	7.5	3.494	0.743	0.717
(Vinyloxy)cyclohexane	2182-55-0	0.739	209	463	332	46.74	0.88	16.7	3.4	4.4	3.925	0.835	0.808
2-Methylcyclohexyl acetate	5726-19-2	0.739	247	466	343	57.58	0.949	16.7	3.8	4.6	3.786	0.806	1.507
2-Methyl-4-phenyl-1-butene	1647-06-9	0.738	207	46	335	54.34	0.881	17.6	1.6	3.4	3.942	0.839	1.093
Methyl 4-methylbenzoate	99-75-2	0.728	261	488	358	60.5	1.047	18.7	7.6	4.6	2.981	0.634	1.535
1-Cyclohexyl-2-propen-1-one	2177-34-6	0.727	251	460	331	60.23	0.955	17.3	5.8	3.2	3.268	0.695	1.649
2-Isopropyl-5-methylfuran	10504-05-9	0.727	219	413	295	41.17	0.889	16.4	4.1	5.5	4.324	0.92	1.001
2-Isopropylfuran	10599-59-4	0.725	216	392	285	41.55	0.896	16.6	4.3	5.1	3.878	0.825	0.855
Methyl 3-allylbenzoate	61463-60-3	0.724	232	517	374	65.93	1.032	18.3	5.3	4.8	0.813	0.173	2.092
α-benzylacrolein	37442-55-0	0.723	256	486	346	67.04	1.002	18.4	6.4	4.8	1.764	0.375	1.917

Table S6 (continued):

name	CAS	$GloPerf$	Melting Point (T_m) [K]	Boiling Point (T_b) [K]	Flash Point (T_f) [K]	ΔH_{vap} [kJ/mol]	Density [g/cm^3]	δ_D [MPa$^{1/2}$]	δ_P [MPa$^{1/2}$]	δ_H [MPa$^{1/2}$]	R_a [MPa$^{1/2}$]	*RED*	Viscosity [mPa s]
1-Ethoxy-1,4-cyclohexadiene	55983-17-0	0.723	218	423	303	43.57	0.919	16.7	3.2	5	3.944	0.839	0.833
Cyclopentylformaldehyde	872-53-7	0.718	240	42	307	43.27	0.933	17.6	8.4	4.7	4.181	0.89	0.906
Phenylacetone	103-79-7	0.717	266	488	353	56.92	0.997	18.6	6.5	4.3	1.975	0.42	1.7
Isopropoxybenzene	2741-16-4	0.717	247	462	337	54.3	0.941	18.7	3.8	0.3	4.821	1.026	0.895
3-Isopropylbenzaldehyde	34246-57-6	0.714	258	498	369	NA	0.972	18.3	5.2	3.4	1.775	0.378	1.894
n-propylbenzene	103-65-1	0.711	200	439	316	47.26	0.862	18	2	2.3	3.963	0.843	0.779
2-Ethyl-5-methylfuran	1703-52-2	0.706	189	395	284	38.3	0.898	16.7	4.7	5.8	3.74	0.796	0.798
3-methylacetophenone	585-74-0	0.701	265	491	356	58.09	1.003	19.1	6.6	3.9	2.51	0.534	1.574
Tetrahydrobenzaldehyde	42540-33-0	0.696	258	441	325	47.69	0.964	17.8	9.3	6.2	4.994	1.062	1.124
1-Methoxycyclopentene	1072-59-9	0.695	199	376	273	34.71	0.9	16.7	4.5	5.3	3.674	0.782	0.531
Vinylfuran	1487-18-9	0.691	215	377	266	37.58	0.937	17	5.6	6.5	3.52	0.749	0.606
1-(2-Cyclopenten-1-yl)acetone	105-24-8	0.682	245	451	328	51.87	0.939	15.9	6.1	4.8	5.456	1.161	1.298
Ethylbenzene	100-41-4	0.68	189	415	298	42.35	0.867	18.2	1.6	2.2	4.227	0.899	0.614
Allyl 3-butenoate	1745-31-9	0.679	186	416	307	45.69	0.919	15.8	5.1	5.8	5.531	1.177	0.751
1-(3-Methylphenyl)-2-propen-1-one	51594-61-7	0.679	271	509	362	61.9	1.008	18.8	6.5	4.5	1.98	0.421	1.776
3-(Allyloxy)oxetane	6777-00-0	0.677	198	397	294	45.68	0.957	16.9	5.6	7.2	4.025	0.856	0.694
Methyl cyclohexanecarboxylate	4630-82-4	0.676	235	462	338	NA	0.969	16.7	3.9	5.4	3.758	0.8	1.645
2-(3-Buten-2-yl)furan	61503-24-0	0.675	221	416	300	45.76	0.917	16.7	4.1	7.2	4.293	0.913	0.982

Table S6 (continued):

name	CAS	$GloPerf$	Melting Point (T_m) [K]	Boiling Point (T_b) [K]	Flash Point (T_f) [K]	ΔH_{vap} [kJ/mol]	Density [g/cm^3]	δ_D [MPa$^{1/2}$]	δ_P [MPa$^{1/2}$]	δ_H [MPa$^{1/2}$]	R_a [MPa$^{1/2}$]	*RED*	Viscosity [mPa s]
1-Cyclohexenylacetone	768-50-3	0.674	246	474	340	51.97	0.944	16.4	4.9	5.6	4.304	0.916	2.258
2-Cyclopentene-1-carbaldehyde	29329-02-0	0.674	244	410	306	44.35	0.972	18	9.3	6.5	4.972	1.058	0.781
Cumene	98-82-8	0.672	203	425	306	45.13	0.862	19.1	1.5	2.3	4.336	0.923	0.773
2-Propylcyclohexanecarbaldehyde	89543-81-7	0.67	269	501	366	59.29	0.897	17.4	5.4	3.6	2.772	0.59	1.875
Butylbenzene	104-51-8	0.669	211	461.81	332	52.17	0.858	17.7	2.2	2.2	4.107	0.874	0.976
3-Cyclopentene-1-carbaldehyde	20145-35-1	0.664	244	410	306	44.35	0.972	18.3	8.8	6.9	4.557	0.97	0.781
1-Ethoxycyclohexene	1122-84-5	0.66	213	425	304	42.48	0.892	16.5	2.8	3.7	4.664	0.992	0.961
(2E)-2-Buten-1-ylcyclohexane	5860-28-6	0.658	214	456	326	49.01	0.822	16.9	1.4	4	4.731	1.007	1.002
3-(2-Cyclopenten-1-yl)propanal	64504-73-0	0.657	249	452	332	54.36	0.943	16.7	7.7	5.6	4.786	1.018	1.27
Benzyl methyl carbonate	13326-10-8	0.655	284	500	368	63.96	1.123	18	7.2	5.3	2.756	0.586	1.874
3-Vinylcyclopentanecarboxylic acid	89730-32-5	0.651	317	521	371	55.62	1.025	17.3	3.5	6	2.892	0.615	3.211
3-Cyclohexen-1-ylacetaldehyde	24480-99-7	0.641	255	457	334	52.79	0.954	16.5	7.7	5.9	5.14	1.094	1.421
Phenylacetaldehyde	122-78-1	0.64	262	468	342	54.5	1.024	18.8	10.6	5.5	5.973	1.271	1.328

Table S6 (continued):

name	CAS	$GloPerf$	Melting Point (T_m) [K]	Boiling Point (T_b) [K]	Flash Point (T_f) [K]	ΔH_{vap} [kJ/mol]	Density [g/cm^3]	δ_D [MPa$^{1/2}$]	δ_P [MPa$^{1/2}$]	δ_H [MPa$^{1/2}$]	R_a [MPa$^{1/2}$]	*RED*	Viscosity [mPa s]
Tetrahydrobenzaldehyde	42540-33-0	0.639	237	442	319	44.64	0.975	17.1	9	5.3	5.196	1.106	1.4
Methyl phenyl carbonate	13509-27-8	0.632	293	497	366	58.8	1.154	18.2	8	5.5	3.427	0.729	1.529
Acrylophenone	768-03-6	0.629	274	490	353	59.22	1.022	18.8	8.2	5.3	3.581	0.762	1.545
p-Cymene	99-87-6	0.628	224	450	323	50.06	0.864	17.4	2.3	2.4	4.2	0.89	0.897
5-Ethoxy-1,3-cyclopentadiene	90125-26-1	0.619	192	395	288	43.9	0.905	16.5	3.9	5.5	4.159	0.885	0.4724
1-Methoxycyclohexene	931-57-7	0.614	217	411	295	38.05	0.899	16.6	3	4.3	4.269	0.908	0.761
Methyl (2E)-2,4-pentadienoate	1515-75-9	0.608	220	410	298	46.19	0.93	16	5.4	7.2	5.554	1.182	0.547
Methyl 2-allylbenzoate	61463-59-0	0.606	232	515	377	69	1.032	18.1	8	5.1	3.44	0.732	2.092
Methyl o-methylbenzoate	89-71-4	0.605	241	484	356	61.33	1.048	18.5	8.6	4.8	3.937	0.838	1.535
d-Limonene	138-86-3	0.598	189	452	311	44.443	0.843	16.7	2.2	4.9	4.417	0.94	1.675
Cyclopentyl methyl ether	5614-37-9	0.592	184	384	280	37.296	0.857	16.6	3.7	3.7	4.196	0.893	0.494
Isobutyl acetate	110-19-0	0.589	190	392	293	43.982	0.868	15.7	4.3	6.3	5.813	1.237	0.718

Table S7. *ProPerf*$_p$ values of list of the solvent candidates selected from the results of molecular design provided by IBSS®CAMD for P3HT:$PC_{71}BM$.

name	CAS	$GloPerf$	Melting Point (T_m)	Boiling Point (T_b)	Flash Point (T_f)	ΔH_{vap}	Density	δ_D	δ_P	δ_H	R_a	*RED*	Viscosity
4-Ethynyltoluene	766-97-2	1	1	1	1	1	1	1	1	1	1	1	1
Anisole	100-66-3	0.997	1	1	1	1	1	1	1	0.96	1	1	1
(Vinyloxy)benzene	766-94-9	0.989	1	1	1	1	1	0.84	1	1	1	1	1
2-Methylanisole	578-58-5	0.946	1	1	1	1	1	1	1	0.21	1	1	1
methylbenzoate	93-58-3	0.923	1	1	1	0.89	1	1	0	1	1	1	1
4-Methoxycyclohexene	15766-93-5	0.916	1	1	1	1	1	0.03	0.75	1	1	1	1
Cyclopentyl acetate	933-05-1	0.907	1	1	1	1	1	0.01	1	1	0.88	1	1
Cyclopentyl formate	62781-99-1	0.901	1	1	1	1	1	0.01	1	0.96	0.86	1	1
benzyl ethyl ether	539-30-0	0.899	1	0.29	1	1	1	0.96	1	1	1	1	1
Formylcyclohexane	2043-61-0	0.895	1	1	1	1	1	0.84	0	1	0.88	1	1
Benzyl vinyl ether	935-04-6	0.889	1	0.2	1	1	1	1	1	1	1	1	1
1-(2-Cyclopenten-1-yl)ethanone	73113-00-5	0.884	1	1	1	1	1	0.21	0.12	1	1	1	1
3-Methoxycyclohexene	2699-13-0	0.877	1	1	1	1	1	0	1	1	0.74	1	1
Vinylxylene	3333-13-9	0.867	1	1	1	1	1	1	0.08	0	1	1	1
2-Propylfuran	4229-91-8	0.865	1	1	0.34	1	1	0.01	1	1	0.90	1	1
1-Acetylcyclohexane	823-76-7	0.863	1	1	1	1	1	0.06	1	1	0.98	1	0
1-(1-Cyclohexen-1-yl)ethanone	932-66-1	0.863	1	1	1	1	1	0.03	1	1	0.99	1	0
Acetyl cyclopentane	6004-60-0	0.859	1	1	1	1	1	0.03	0.96	1	0.66	1	1
Benzyl formate	104-57-4	0.855	1	1	1	0.1	1	1	0.68	0.12	1	1	1
p-xylene	106-42-3	0.853	1	1	1	1	1	1	0.88	0	0.66	1	1

Table S7 (continued):

name	CAS	$GloPerf$	Melting Point (T_m)	Boiling Point (T_b)	Flash Point (T_f)	ΔH_{vap}	Density	δ_D	δ_P	δ_H	R_a	*RED*	Viscosity
1-Phenyl-2-butene	935-00-2	0.837	1	1	1	1	1	1	0	0.21	0.81	1	1
3-Methyl-2-cyclohexen-1-yl acetate	75411-49-3	0.829	1	1	1	1	1	0.01	1	1	0.83	1	0.02
2-Ethylfuran	3208-16-0	0.827	1	1	0	0.53	1	0.01	1	1	0.98	1	1
Cyclohexylacetone	103-78-6	0.826	1	0.71	1	1	1	0.06	1	1	1	1	0
Allylbenzene	300-57-2	0.824	1	1	1	1	1	1	0	0.06	0.79	1	1
3-(Vinyloxy)cyclohexene	80816-25-7	0.823	1	1	1	1	1	0	1	1	0.48	1	1
2-(3-Buten-1-yl)-5-methylfuran	5312-85-6	0.812	1	1	1	1	1	0	1	1	0.42	1	1
(2E)-2,4-Pentadien-1-ylbenzene	91166-39-1	0.811	1	0.54	1	0.18	1	1	0	1	1	1	1
2-Cyclopenten-1-yl acetate	20657-21-0	0.807	1	1	1	1	1	0.03	1	0.01	0.72	1	1
2-Cyclohexen-1-yl acetate	14447-34-8	0.802	1	1	1	0.97	1	0.01	1	0.12	0.68	1	1
1-Cyclohexyl-2-propen-1-one	2177-34-6	0.794	1	1	1	0	1	0.03	1	1	0.99	1	0
2-Methyl-5-propylfuran	1456-16-2	0.792	1	1	1	1	1	0	1	1	0.33	1	1
Allyl Benzyl Ether	14593-43-2	0.791	1	0	1	0	1	0.96	1	1	1	1	1
[(2E)-2-Buten-1-yloxy]benzene	14503-58-3	0.79	1	0.08	1	0	1	0.84	1	0.96	1	1	1
3-Cyclohexene-1-carbaldehyde	100-50-5	0.777	1	1	1	1	1	1	0	0.84	0.31	1	1

Table S7 (continued):

name	CAS	$GloPerf$	Melting Point (T_m)	Boiling Point (T_b)	Flash Point (T_f)	ΔH_{vap}	Density	δ_D	δ_P	δ_H	R_a	*RED*	Viscosity
3-Methyl-1-cyclohexene-1-carbaldehyde	63282-01-9	0.772	1	1	1	1	1	0.34	0	1	0.45	1	1
Benzyl acetate	140-11-4	0.767	1	0.33	1	0	1	1	1	0.96	1	1	0
[(3-Buten-1-yloxy)methyl]benzene	70388-33-9	0.765	1	0	1	0	1	0.84	0.75	1	1	1	1
Isopropoxybenzene	2741-16-4	0.761	1	0.02	1	0.04	1	1	0.45	1	1	1	1
Acetophenone	98-86-2	0.758	1	1	1	0.94	1	1	0	1	0.18	1	1
1-Acetoxycyclohexene	1424-22-2	0.748	1	1	1	1	1	0.01	0.45	1	0.63	1	0
4-Methoxycyclopentene	40955-64-4	0.744	1	1	0	0.39	1	0.03	0.88	1	1	1	0
propenylfuran	10599-55-0	0.741	1	1	0	1	1	0.12	1	0	0.71	1	1
(Vinyloxy)cyclohexane	2182-55-0	0.739	1	1	1	1	1	0	0.32	1	0.3	1	1
2-Methylcyclohexyl acetate	5726-19-2	0.739	1	1	1	0.09	1	0	0.88	1	0.42	1	0.99
2-Methyl-4-phenyl-1-butene	1647-06-9	0.738	1	1	1	1	1	0.5	0	0.84	0.28	1	1
Methyl 4-methylbenzoate	99-75-2	0.728	1	0.16	1	0	1	1	0	1	1	1	0.75
1-Cyclohexyl-2-propen-1-one	2177-34-6	0.727	1	1	1	0	1	0.12	1	0.21	0.9	1	0.01
2-Isopropyl-5-methylfuran	10504-05-9	0.727	1	1	0.79	1	1	0	1	1	0.08	1	1
2-Isopropylfuran	10599-59-4	0.725	1	1	0	1	1	0	1	1	0.34	1	1
Methyl 3-allylbenzoate	61463-60-3	0.724	1	0	1	0	1	1	1	1	1	1	0
α-benzylacrolein	37442-55-0	0.723	1	0.24	1	0	1	1	0.5	1	1	1	0

Table S7 (continued):

name	CAS	$GloPerf$	Melting Point (T_m)	Boiling Point (T_b)	Flash Point (T_f)	ΔH_{vap}	Density	δ_D	δ_P	δ_H	R_a	*RED*	Viscosity
1-Ethoxy-1,4-cyclohexadiene	55983-17-0	0.723	1	1	1	1	1	0	0.13	1	0.28	1	1
Cyclopentylformaldehyde	872-53-7	0.718	1	1	1	1	1	0.5	0	1	0.14	1	1
Phenylacetone	103-79-7	0.717	1	0.15	1	0.27	1	1	0.34	1	1	1	0
Isopropoxybenzene	2741-16-4	0.717	1	1	1	1	1	1	0.88	0	0.01	0.99	1
3-Isopropylbenzaldehyde	34246-57-6	0.714	1	0	1	0	1	1	1	0.84	1	1	0
n-propylbenzene	103-65-1	0.711	1	1	1	1	1	1	0	0	0.27	1	1
2-Ethyl-5-methylfuran	1703-52-2	0.706	1	1	0	0.35	1	0	1	1	0.46	1	1
3-methylacetophenone	585-74-0	0.701	1	0.07	1	0.03	1	1	0.21	1	1	1	0.28
Tetrahydrobenzaldehyde	42540-33-0	0.696	1	1	1	1	1	0.84	0	0.84	0	0.95	1
1-Methoxycyclopentene	1072-59-9	0.695	1	1	0	0	1	0	1	1	0.53	1	1
Vinylfuran	1487-18-9	0.691	1	1	0	0.12	1	0.01	1	0.34	0.68	1	1
1-(2-Cyclopenten-1-yl)acetone	105-24-8	0.682	1	1	1	1	1	0	0.96	1	0	0.72	1
Ethylbenzene	100-41-4	0.68	1	1	1	1	1	1	0	0	0.12	1	1
Allyl 3-butenoate	1745-31-9	0.679	1	1	1	1	1	0	1	1	0	0.67	1
1-(3-Methylphenyl)-2-propen-1-one	51594-61-7	0.679	1	0	1	0	1	1	0.34	1	1	1	0
3-(Allyloxy)oxetane	6777-00-0	0.677	1	1	0.62	1	1	0.01	1	0	0.23	1	1
Methyl cyclohexanecarboxylate	4630-82-4	0.676	1	1	1	0	1	0	0.97	1	0.44	1	0.01
2-(3-Buten-2-yl)furan	61503-24-0	0.675	1	1	1	1	1	0	1	0	0.09	1	1

Table S7 (continued):

name	CAS	$GloPerf$	Melting Point (T_m)	Boiling Point (T_b)	Flash Point (T_f)	ΔH_{vap}	Density	δ_D	δ_P	δ_H	R_a	*RED*	Viscosity
1-Cyclohexenylacetone	768-50-3	0.674	1	1	1	1	1	0	1	1	0.09	1	0
2-Cyclopentene-1-carbaldehyde	29329-02-0	0.674	1	1	1	1	1	1	0	0.34	0	0.96	1
Cumene	98-82-8	0.672	1	1	1	1	1	1	0	0	0.08	1	1
2-Propylcyclohexanecarbaldehyde	89543-81-7	0.67	1	0	1	0	1	0.21	1	1	1	1	0
Butylbenzene	104-51-8	0.669	1	1	1	1	1	0.68	0	0	0.18	1	1
3-Cyclopentene-1-carbaldehyde	20145-35-1	0.664	1	1	1	1	1	1	0	0.03	0.03	1	1
1-Ethoxycyclohexene	1122-84-5	0.66	1	1	1	1	1	0	0.01	1	0.02	1	1
(2E)-2-Buten-1-ylcyclohexane	5860-28-6	0.658	1	1	1	1	1	0.01	0	1	0.01	1	1
3-(2-Cyclopenten-1-yl)propanal	64504-73-0	0.657	1	1	1	1	1	0	0	1	0.01	1	1
Benzyl methyl carbonate	13326-10-8	0.655	0.97	0	1	0	1	1	0	1	1	1	0
3-Vinylcyclopentanecarboxylic acid	89730-32-5	0.651	0	0	1	0.87	1	0.12	0.45	1	1	1	0
3-Cyclohexen-1-ylacetaldehyde	24480-99-7	0.641	1	1	1	1	1	0	0	1	0	0.89	1
Phenylacetaldehyde	122-78-1	0.64	1	1	1	1	1	1	0	1	0	0.39	1

Table S7 (continued):

name	CAS	$GloPerf$	Melting Point (T_m)	Boiling Point (T_b)	Flash Point (T_f)	ΔH_{vap}	Density	δ_D	δ_P	δ_H	R_a	*RED*	Viscosity
Tetrahydrobenzaldehyde	42540-33-0	0.639	1	1	1	1	1	0.03	0	1	0	0.87	1
Methyl phenyl carbonate	13509-27-8	0.632	0.01	0.01	1	0.01	1	1	0	1	0.77	1	0.82
Acrylophenone	768-03-6	0.629	1	0.07	1	0	1	1	0	1	0.62	1	0.62
p-Cymene	99-87-6	0.628	1	1	1	1	1	0.21	0	0	0.13	1	1
5-Ethoxy-1,3-cyclopentadiene	90125-26-1	0.619	1	1	0	1	1	0	0.97	1	0.15	1	0.06
1-Methoxycyclohexene	931-57-7	0.614	1	1	0.79	0.26	1	0	0.04	1	0.1	1	1
Methyl (2E)-2,4-pentadienoate	1515-75-9	0.608	1	1	1	1	1	0	1	0	0	0.66	1
Methyl 2-allylbenzoate	61463-59-0	0.606	1	0	1	0	1	1	0	1	0.76	1	0
Methyl o-methylbenzoate	89-71-4	0.605	1	0.33	1	0	1	1	0	1	0.29	1	0.75
d-Limonene	138-86-3	0.598	1	1	1	1	1	0	0	1	0.06	1	0
Cyclopentyl methyl ether	5614-37-9	0.592	1	1	0	0.07	1	0	0.75	1	0.13	1	0.87
Isobutyl acetate	110-19-0	0.589	1	1	0.39	1	1	0	1	0.677	0	0.49	1

Table S8. Calculated property values of list of the solvent candidates selected from the results of molecular design provided by IBSS®CAMD for PF2:$PC_{71}BM$.

name	CAS	$GloPerf$	Melting Point (T_m) [K]	Boiling Point (T_b) [K]	Flash Point (T_f) [K]	ΔH_{vap} [kJ/mol]	Density [g/cm^3]	δ_D [$MPa^{1/2}$]	δ_P [$MPa^{1/2}$]	δ_H [$MPa^{1/2}$]	R_a [$MPa^{1/2}$]	*RED*	Viscosity [mPa s]
4-Allytoluene	222-063-5	0.957	219	459	328	51.03	0.887	18.1	3.1	2.6	2.317	0.579	0.822
p-Xylene	106-42-3	0.931	229	419	301	43.35	0.873	18.6	3.8	1.6	1.697	0.424	0.568
Cumene	98-82-8	0.931	203	425	306	45.13	0.862	19.1	1.5	2.3	2.362	0.591	0.773
Isopropoxybenzene	2741-16-4	0.931	247	462	337	54.3	0.941	18.7	3.8	0.3	2.693	0.673	0.895
Ethyl phenyl ether	103-73-1	0.899	247	451	330	51.43	0.957	17.8	4.4	4.5	3.33	0.833	0.721
Ethylbenzene	100-41-4	0.897	189	415	298	42.35	0.867	18.2	1.6	2.2	3.033	0.758	0.614
Allylbenzene	300-57-2	0.897	197	435	311	46.1	0.888	18.1	2	3.1	2.858	0.715	0.707
n-propylbenzene	103-65-1	0.885	200	439	316	47.26	0.862	18	2	2.3	3.041	0.76	0.779
3-Butenylbenzene	768-56-9	0.884	207	458	328	51.01	0.883	18	1.9	3	3.068	0.767	0.888
4-Ethyltoluene	622-96-8	0.882	212	441	316	47.27	0.869	18.2	2.9	1.8	2.41	0.603	0.722
3-Vinylcyclopentanecarbaldehyde	16668-88-5	0.854	245	454	333	50.37	0.93	18.1	6.4	2.8	3.406	0.851	0.99
2-Ethyltoluene	611-14-3	0.851	183	437	314	48.11	0.87	18.1	2.5	2	2.678	0.669	0.722
(3R)-3-Methylcyclopentanecarbaldehyde	1822302-16-8	0.829	245	432	319	46.66	0.917	18.3	6.4	4.5	3.59	0.898	0.863
2-Methylcyclohexanecarbaldehyde	13076-15-8	0.815	258	460	337	50	0.914	17.8	5.8	3.8	3.583	0.896	1.219

Table S8 (continued):

name	CAS	$GloPerf$	Melting Point (T_m) [K]	Boiling Point (T_b) [K]	Flash Point (T_f) [K]	ΔH_{vap} [kJ/mol]	Density [g/cm^3]	δ_D [MPa$^{1/2}$]	δ_P [MPa$^{1/2}$]	δ_H [MPa$^{1/2}$]	R_a [MPa$^{1/2}$]	*RED*	Viscosity [mPa s]
3-Ethylcyclopentanecarbaldehyde	1497771-39-7	0.814	249	457	336	51.04	0.908	18	6	4.3	3.585	0.896	1.09
(Isopropoxymethyl)benzene	22921-10-4	0.799	243	494	358	57.98	0.922	18.7	3.5	4.2	1.746	0.437	1.107
2-Methylanisole	578-58-5	0.77	234	449	329	52.28	0.964	18.6	4.4	6.6	4.03	1.007	0.668
(2E)-2,4-Pentadien-1-ylbenzene	91166-39-1	0.766	234	481	344	57.19	0.9	18	2.2	3.8	3.053	0.763	0.921
Benzyl vinyl ether	935-04-6	0.741	251	487	352	54.38	0.956	18	4.4	5.1	3.378	0.844	0.82
3-Phenylbut-1-ene	934-10-1	0.741	203	442	315	47.92	0.883	17.7	1.5	3.3	3.813	0.953	0.881
Allyl Phenyl Ether	1746-13-0	0.728	252	469	342	55.18	0.969	17.7	4.4	5.2	3.888	0.972	0.82
(Vinyloxy)benzene	766-94-9	0.728	246	451	322	50.33	0.982	17.8	4.9	5.3	3.912	0.978	0.655
Toluene	108-88-3	0.725	209	390	282	38.43	0.872	18.6	1.5	2.1	2.687	0.672	0.475
Anisole	100-66-3	0.724	239	428	314	46.52	0.974	18.1	4.9	6.1	4.116	1.029	0.569
2-Methyl-4-phenyl-1-butene	6683-51-8	0.718	207	469	335	54.34	0.881	17.6	1.6	3.4	3.929	0.982	1.093
p-Cymene	99-87-6	0.693	224	450	323	50.06	0.864	17.4	2.3	2.4	4.10	1.026	0.897
Isobutylbenzene	538-93-2	0.667	201	451	323	50.13	0.853	17.4	1.5	2.5	4.283	1.071	0.969
Phenylacetone	103-79-7	0.667	266	488	353	56.92	0.997	18.6	6.5	4.3	3.314	0.828	1.7
Methoxycyclohexane	931-56-6	0.653	204	419	302	40.64	0.864	16.8	3.2	3.8	4.94	1.235	0.707
1-Acetylcyclohexane	823-76-7	0.651	262	465	337	49.43	0.917	17.2	5.4	3.6	4.382	1.095	1.676
Allyl Benzyl Ether	14593-43-2	0.651	248	500	362	58.86	0.947	17.9	4.1	4.9	3.356	0.839	1.016

Table S8 (continued):

name	CAS	$GloPerf$	Melting Point (T_m) [K]	Boiling Point (T_b) [K]	Flash Point (T_f) [K]	ΔH_{vap} [kJ/mol]	Density [g/cm^3]	δ_D [MPa$^{1/2}$]	δ_P [MPa$^{1/2}$]	δ_H [MPa$^{1/2}$]	R_a [MPa$^{1/2}$]	*RED*	Viscosity [mPa s]
2-Methylcyclopentanecarbaldehyde	20106-44-9	0.626	245	432	319	46.66	0.916	18	7.3	4.6	4.61	1.152	0.863
methylbenzoate	93-58-3	0.623	246	466	343	55.57	1.068	18.7	7.5	5.3	4.576	1.144	1.34
(Vinyloxy)cyclohexane	2182-55-0	0.622	209	463	332	46.74	0.88	16.7	3.4	4.4	5.265	1.316	0.808
1-(3-Methylphenyl)-2-propen-1-one	51594-61-7	0.621	271	509	362	61.9	1.008	18.8	6.5	4.5	3.289	0.822	1.776
1-(1-Cyclohexen-1-yl)ethanone	932-66-1	0.621	279	473	334	47.46	0.953	17.1	5.3	4.1	4.645	1.161	1.809
3,3-Dimethyl-1,5-hexadiene	24253-25-6	0.604	221	434	306	46.9	0.778	16.8	3.3	3.9	4.95	1.237	0.745
Acetyl cyclopentane	6004-60-0	0.602	249	438	319	46.09	0.916	17.1	6.1	3.5	4.839	1.21	1.187
4-Methoxycyclohexene	15766-93-5	0.6	210	416	301	41.72	0.892	17.1	3.7	5.2	4.838	1.21	0.611

Table S9. *ProPerf*$_p$ values of list of the solvent candidates selected from the results of molecular design provided by IBSS®CAMD for PF2:$PC_{71}BM$.

name	CAS	$GloPerf$	Melting Point (T_m)	Boiling Point (T_b)	Flash Point (T_f)	ΔH_{vap}	Density	δ_D	δ_P	δ_H	R_a	*RED*	Viscosity
4-Alltoluene	222-063-5	0.957	1	1	1	1	1	0.5	0.88	1	1	1	1
p-xylene	106-42-3	0.931	1	1	1	1	1	1	1	0	1	1	1
Cumene	98-82-8	0.931	1	1	1	1	1	1	0	1	1	1	1
Isopropoxybenzene	2741-16-4	0.931	1	1	1	1	1	1	1	0	1	1	1
Ethyl phenyl ether	103-73-1	0.899	1	1	1	1	1	0.12	1	0.84	0.86	1	1
Ethylbenzene	100-41-4	0.897	1	1	1	1	1	0.68	0	0.84	1	1	1
Allylbenzene	300-57-2	0.897	1	1	1	1	1	0.5	0	1	1	1	1
n-propylbenzene	103-65-1	0.885	1	1	1	1	1	0.34	0	1	1	1	1
3-Butenylbenzene	768-56-9	0.884	1	1	1	1	1	0.34	0	1	0.99	1	1
4-Ethyltoluene	622-96-8	0.882	1	1	1	1	1	0.68	0.6	0.01	1	1	1
3-Vinylcyclopentanecarbaldehyde	16668-88-5	0.854	1	1	1	1	1	0.5	0.01	1	0.79	1	1
2-Ethyltoluene	611-14-3	0.851	1	1	1	1	1	0.5	0.13	0.21	1	1	1
(3R)-3-Methylcyclopentanecarbaldehyde	1822302-16-8	0.829	1	1	1	1	1	0.84	0.01	0.84	0.61	1	1
2-Methylcyclohexanecarbaldehyde	13076-15-8	0.815	1	1	1	1	1	0.12	0.34	1	0.62	1	1
3-Ethylcyclopentanecarbaldehyde	1497771-39-7	0.814	1	1	1	1	1	0.34	0.12	1	0.62	1	1
(Isopropoxymethyl)benzene	22921-10-4	0.799	1	0.02	1	0.04	1	1	1	1	1	1	1
2-Methylanisole	578-58-5	0.770	1	1	1	1	1	1	1	0	0.22	1	1

Table S9 (continued):

name	CAS	$GloPerf$	Melting Point (T_m)	Boiling Point (T_b)	Flash Point (T_f)	ΔH_{vap}	Density	δ_D	δ_P	δ_H	R_a	*RED*	Viscosity
(2E)-2,4-Pentadien-1-ylbenzene	91166-39-1	0.766	1	0.54	1	0.18	1	0.34	0.02	1	1	1	1
Benzyl vinyl ether	935-04-6	0.741	1	0.2	1	1	1	0.34	1	0.06	0.82	1	1
3-Phenylbut-1-ene	934-10-1	0.741	1	1	1	1	1	0.06	0	1	0.39	1	1
Allyl Phenyl Ether	1746-13-0	0.728	1	1	1	0.99	1	0.06	1	0.03	0.33	1	1
(Vinyloxy)benzene	766-94-9	0.728	1	1	1	1	1	0.12	1	0.01	0.31	1	1
Toluene	108-88-3	0.725	1	1	0	0.41	1	1	0	0.5	1	1	0.1
Anisole	100-66-3	0.724	1	1	1	1	1	0.5	1	0	0.17	0.99	1
2-Methyl-4-phenyl-1-butene	6683-51-8	0.718	1	1	1	1	1	0.03	0	1	0.29	1	1
p-Cymene	99-87-6	0.693	1	1	1	1	1	0.01	0.02	1	0.18	0.99	1
Isobutylbenzene	538-93-2	0.667	1	1	1	1	1	0.01	0	1	0.1	0.94	1
Phenylacetone	103-79-7	0.667	1	0.15	1	0.27	1	1	0	1	0.87	1	0
Methoxycyclohexane	931-56-6	0.653	1	1	1	1	1	0	0.97	1	0	0.49	1
1-Acetylcyclohexane	823-76-7	0.651	1	1	1	1	1	0	0.96	1	0.07	0.89	0
Allyl Benzyl Ether	14593-43-2	0.651	1	0	1	0	1	0.21	1	0.21	0.84	1	1
2-Methylcyclopentanecarbaldehyde	20106-44-9	0.626	1	1	1	1	1	0.34	0	0.68	0.03	0.74	1
methylbenzoate	93-58-3	0.623	1	1	1	0.89	1	1	0	0.01	0.03	0.77	1
(Vinyloxy)cyclohexane	2182-55-0	0.622	1	1	1	1	1	0	1	0.96	0	0.28	1
1-(3-Methylphenyl)-2-propen-1-one	51594-61-7	0.621	1	0	1	0	1	1	0	0.84	0.89	1	0
1-(1-Cyclohexen-1-yl)ethanone	932-66-1	0.621	1	1	1	1	1	0	1	1	0.02	0.72	0

Table S9 (continued):

name	CAS	$GloPerf$	Melting Point (T_m)	Boiling Point (T_b)	Flash Point (T_f)	ΔH_{vap}	Density	δ_D	δ_P	δ_H	R_a	*RED*	Viscosity
3,3-Dimethyl-1,5-hexadiene	24253-25-6	0.604	1	1	1	1	0.28	0	1	1	0	0.49	1
Acetyl cyclopentane	6004-60-0	0.602	1	1	1	1	1	0	0.06	1	0.01	0.57	1
4-Methoxycyclohexene	15766-93-5	0.6	1	1	1	1	1	0	1	0.03	0.01	0.57	1

Table S10. The selected candidates (*GloPerf*>0.5) from the results of evaluation mode provided by IBSS®CAMD for P3HT:$PC_{71}BM$.

Target properties with performance	1,2-dichlorobenzene	Anisole	p-Xylene	Isoamyl Acetate	Benzyl Benzoate	p-Cymene
CAS	95-50-1	100-66-3	106-42-3	123-92-2	120-51-4	99-87-6
$GloPerf$	1	0.997	0.853	0.674	0.667	0.628
Melting Point (T_m) [K]	255	239	229	202	307	224
$ProPerf_p$ (T_m)	1	1	1	1	≈ 0	1
Boiling Point (T_b) [K]	449	428	419	420	573	450
$ProPerf_p$ (T_b)	1	1	1	1	≈ 0	1
Flash Point (T_f) [K]	332	314	301	312	420	323
$ProPerf_p$ (T_f)	1	1	1	1	1	1
ΔH_{vap}(kJ/mol)	50.1	46.5	43.4	48.9	85.8	50.1
$Properf_p$ (ΔH_{vap})	1	1	1	1	≈ 0	1
Density (g/cm^3)	1.280	0.974	0.873	0.868	1.123	0.864
$Properf_p$*(Density)*	1	1	1	1	1	1
δ_D (MPa$^{1/2}$)	19.5	18.1	18.6	15.8	19.8	17.4
$Properf_p$ (δ_D)	1	1	1	≈ 0	1	0.21
δ_P (MPa$^{1/2}$)	5.1	4.9	3.8	4	6.3	2.3
$Properf_p$ (δ_P)	1	1	0.88	1	0.68	≈ 0
δ_H (MPa$^{1/2}$)	3.1	6.1	1.6	6	4.7	2.4
$Properf_p$ (δ_H)	1	0.96	≈ 0	1	1	≈ 0
R_a (MPa$^{1/2}$)	2.77	1.39	3.54	5.59	3.04	4.20
$Properf_p$ (R_a)	1	1	0.66	≈ 0	0.99	0.13
RED	0.59	0.30	0.75	1.19	0.65	0.89
$Properf_p$*(RED)*	1	1	1	0.64	1	1
Viscosity (mPa s)	1.089	0.569	0.568	0.903	5.224	0.897
$Properf_p$*(Viscosity)*	1	1	1	1	≈ 0	1

Table S10 (continued):

Target properties with performance values	Terpinolene	Butyl Acetate	Tetrahydrofuran	d-Limonene	Cyclopentyl methyl ether
CAS	586-62-9	123-86-4	109-99-9	138-86-3	5614-37-9
$GloPerf$	0.626	0.621	0.609	0.598	0.592
Melting Point (T_m) [K]	221	201	179	189	185
$ProPerf_p$ (T_m)	1	1	1	1	1
Boiling Point (T_b) [K]	448	407	323	452	385
$ProPerf_p$ (T_b)	1	1	≈ 0	1	1
Flash Point (T_f) [K]	308	305	243	311	281
$ProPerf_p$ (T_f)	1	1	≈ 0	1	0
ΔH_{vap} (kJ/mol)	38.3	46.0	32.0	44.44	37.30
$Properf_p$ (ΔH_{vap})	0.34	1	≈ 0	1.00	0.07
Density (g/cm^3)	0.855	0.873	0.872	0.843	0.857
$Properf_p$*(Density)*	1	1	1	1	1
δ_D (MPa$^{1/2}$)	16.9	15.8	16.9	16.7	16.6
$Properf_p$ (δ_D)	0.005	≈ 0	0.005	0	0
δ_P (MPa$^{1/2}$)	1.8	5.1	4.2	2.2	3.7
$Properf_p$ (δ_P)	≈ 0	1	1	0.00	0.75
δ_H (MPa$^{1/2}$)	4.8	6.5	4.1	4.9	3.7
$Properf_p$ (δ_H)	1	0.34	1	1	1
R_a (MPa$^{1/2}$)	4.35	5.67	3.42	4.42	4.20
$Properf_p$ (R_a)	0.08	≈ 0	0.78	0.06	0.13
RED	0.93	1.21	0.73	0.94	0.89
$Properf_p$*(RED)*	1	0.58	1	1	1
Viscosity (mPa s)	0.748	0.724	0.557	1.675	0.494
$Properf_p$*(Viscosity)*	1	1	1	0	0.87

Table S10 (continued):

Target properties with performance values	Isobutyl acetate	2-Methyl tetrahydrofuran	Propylene carbonate	Ethylene carbonate	Glycerol -1,2,3-triethyl ether
CAS	110-19-0	96-47-9	108-32-7	96-49-1	162614-45-1
$GloPerf$	0.589	0.568	0.566	0.564	0.553
Melting Point (T_m) [K]	191	187	287	283	210
$ProPerf_p$ (T_m)	1	1	0.50	1	1
Boiling Point (T_b) [K]	393	351	433	413	467
$ProPerf_p$ (T_b)	1	0	1	1	1
Flash Point (T_f) [K]	293	261	334	324	343
$ProPerf_p$ (T_f)	0.39	0.00	1.00	1.00	1.00
ΔH_{vap} (kJ/mol)	43.98	35.36	52.68	49.29	60.16
$Properf_p$ (ΔH_{vap})	1	0	1	1	0
Density (g/cm^3)	0.868	0.861	1.195	1.303	0.893
$Properf_p$*(Density)*	1	1	1	1	1
δ_D (MPa$^{1/2}$)	15.7	16.8	17.9	18.4	15.5
$Properf_p$ (δ_D)	0	0	0.96	1	0
δ_P (MPa$^{1/2}$)	4.3	5	18.3	21.2	4.8
$Properf_p$ (δ_P)	1	1	0	0	1
δ_H (MPa$^{1/2}$)	6.3	4	5	6.3	3.6
$Properf_p$ (δ_H)	0.68	1	1	0.68	1
R_a (MPa$^{1/2}$)	5.81	3.63	13.69	16.58	6.23
$Properf_p$ (R_a)	0	0.58	0	0	0
RED	1.24	0.77	2.91	3.53	1.33
$Properf_p$*(RED)*	0.49	1.00	0.00	0.00	0.26
Viscosity (mPa s)	0.718	0.554	0.797	0.824	0.962
$Properf_p$*(Viscosity)*	1	1	1	1	1

Table S10 (continued):

Target properties with performance values	Dimethyl Succinate	1,2,3-Trimethoxypropane	Diethyl carbonate	Furfural	5-Methyldihydro-2(3H)-furanone
CAS	106-65-0	20637-49-4	105-58-8	35796.00	108-29-2
$GloPerf$	0.552	0.533	0.531	0.517	0.509
Melting Point (T_m) [K]	234	222	228	249	270
$ProPerf_p$ (T_m)	1	1	1	1	1
Boiling Point (T_b) [K]	452	430	404	417	425
$ProPerf_p$ (T_b)	1	1	1	1	1
Flash Point (T_f) [K]	341	320	303	310	322
$ProPerf_p$ (T_f)	1	1	1	1	1
ΔH_{vap} (kJ/mol)	54.37	46.86	43.60	45.92	49.15
$Properf_p$ (ΔH_{vap})	1	1	1	1	1
Density (g/cm^3)	1.067	0.912	0.985	1.113	1.029
$Properf_p$(Density)	1	1	1	1	1
δ_D (MPa$^{1/2}$)	16.30	15.50	15.30	18.00	17.10
$Properf_p$ (δ_D)	0	0	0	1	0.03
δ_P (MPa$^{1/2}$)	6.00	5.70	6.80	12.50	11.90
$Properf_p$ (δ_P)	1	1	0.06	0	0
δ_H (MPa$^{1/2}$)	9.20	7.50	5.70	8.80	6.20
$Properf_p$ (δ_H)	0	0	1	0	0.84
R_a (MPa$^{1/2}$)	6.25	6.62	6.84	8.75	7.86
$Properf_p$ (R_a)	0	0	0	0	0
RED	1.33	1.41	1.45	1.86	1.67
$Properf_p$(RED)	0.25	0.12	0.07	0	0
Viscosity (mPa s)	1.550	0.519	0.670	1.142	0.586
$Properf_p$(Viscosity)	1	1	1	1	1

Table S11. The selected candidates (*GloPerf*>0.5) from the results of evaluation mode provided by IBSS®CAMD for P3HT:EH-IDTBR.

Target properties with performance	Chlorobenzene	Anisole	p-Xylene	p-Cymene	Isoamyl acetate	Terpinolene
CAS	108-90-7	100-66-3	106-42-3	99-87-6	123-92-2	586-62-9
$GloPerf$	0.931	0.997	0.861	0.680	0.674	0.640
Melting Point (T_m) [K]	226	239	229	224	202	221
$ProPerf_p$ (T_m)	1	1	1	1	1	1
Boiling Point (T_b) [K]	410	428	419	450	420	448
$ProPerf_p$ (T_b)	1	1	1	1	1	1
Flash Point (T_f) [K]	300	314	301	323	312	308
$ProPerf_p$ (T_f)	1	1	1	1	1	1
ΔH_{vap} (kJ/mol)	41.37	46.52	43.35	50.06	48.89	38.26
$Properf_p$ (ΔH_{vap})	1	1	1	1	1	0.34
Density (g/cm^3)	1.099	0.974	0.873	0.864	0.868	0.855
$Properf_p$*(Density)*	1	1	1	1	1	1
δ_D (MPa$^{1/2}$)	19.30	18.10	18.60	17.40	15.80	16.90
$Properf_p$ (δ_D)	1	1	1	0.96	0	0.21
δ_P (MPa$^{1/2}$)	4.80	4.90	3.80	2.30	4.00	1.80
$Properf_p$ (δ_P)	1	1	1	0.01	1	0
δ_H (MPa$^{1/2}$)	2.70	6.10	1.60	2.40	6.00	4.80
$Properf_p$ (δ_H)	0.00	0.96	0.00	0.00	1	1
R_a (MPa$^{1/2}$)	1.58	1.39	3.54	4.20	5.59	4.35
$Properf_p$ (R_a)	1	1	0.66	0.13	0	0.08
RED	0.41	0.30	0.75	0.89	1.19	0.93
$Properf_p$*(RED)*	1	1	1	1	0.64	1
Viscosity (mPa s)	0.682	0.569	0.568	0.897	0.903	0.748
$Properf_p$*(Viscosity)*	1	1	1	1	1	1

Table S11 (continued):

Target properties with performance	Tetrahydrofuran	Butyl acetate	Cyclopentyl methyl ether	d-Limonene	Isobutyl acetate	2-Methyltetrahydrofuran
CAS	109-99-9	123-86-4	5614-37-9	138-86-3	110-19-0	96-47-9
$GloPerf$	0.624	0.621	0.612	0.603	0.589	0.576
Melting Point (T_m) [K]	179	201	185	189	191	187
$ProPerf_p$ (T_m)	1	1	1	1	1	1
Boiling Point (T_b) [K]	323	407	385	452	393	351
$ProPerf_p$ (T_b)	0	1	1	1	1	0
Flash Point (T_f) [K]	243	305	281	311	293	261
$ProPerf_p$ (T_f)	0	1	0	1	0.39	0
ΔH_{vap} (kJ/mol)	31.97	46.02	37.30	44.44	43.98	35.36
$Properf_p$ (ΔH_{vap})	0	1	0.07	1	1	0
Density (g/cm^3)	0.872	0.873	0.857	0.843	0.868	0.861
$Properf_p$*(Density)*	1	1	1	1	1	1
δ_D (MPa$^{1/2}$)	16.90	15.80	16.60	16.70	15.70	16.80
$Properf_p$ (δ_D)	0.21	0	0.03	0.06	0	0.12
δ_P (MPa$^{1/2}$)	4.20	5.10	3.70	2.20	4.30	5.00
$Properf_p$ (δ_P)	1	1	1	0	1	1
δ_H (MPa$^{1/2}$)	4.10	6.50	3.70	4.90	6.30	4.00
$Properf_p$ (δ_H)	1	0.34	1.00	1.00	0.68	1.00
R_a (MPa$^{1/2}$)	3.42	5.67	4.20	4.42	5.81	3.63
$Properf_p$ (R_a)	0.78	0	0.13	0.06	0	0.58
RED	0.73	1.21	0.89	0.94	1.24	0.77
$Properf_p$*(RED)*	1	0.58	1	1	0.49	1
Viscosity (mPa s)	0.557	0.724	0.494	1.675	0.718	0.554
$Properf_p$*(Viscosity)*	1	1	0.87	0	1	1

Table S11 (continued):

Target properties with performance values	Propylene carbonate	Benzyl Benzoate	Ethylene carbonate	Glycerol -1,2,3-triethyl ether	5-Methyldihydro-2(3H)-furanone
CAS	108-32-7	120-51-4	96-49-1	162614-45-1	108-29-2
$GloPerf$	0.569	0.564	0.564	0.553	0.541
Melting Point (T_m) [K]	287	307	283	210	270
$ProPerf_p$ (T_m)	0.50	0	1	1	1
Boiling Point (T_b) [K]	433	573	413	467	425
$ProPerf_p$ (T_b)	1	0	1	1	1
Flash Point (T_f) [K]	334	420	324	343	322
$ProPerf_p$ (T_f)	1	1	1	1	1
ΔH_{vap} (kJ/mol)	52.68	85.75	49.29	60.16	49.15
$Properf_p$ (ΔH_{vap})	1	0	1	0	1
Density (g/cm^3)	1.195	1.123	1.303	0.893	1.029
$Properf_p$*(Density)*	1	1	1	1	1
δ_D (MPa$^{1/2}$)	17.90	19.80	18.40	15.50	17.10
$Properf_p$ (δ_D)	1	0.13	1	0	0.50
δ_P (MPa$^{1/2}$)	18.30	6.30	21.20	4.80	11.90
$Properf_p$ (δ_P)	0	0.06	0	1	0
δ_H (MPa$^{1/2}$)	5.00	4.70	6.30	3.60	6.20
$Properf_p$ (δ_H)	1	1	0.68	1	0.84
R_a (MPa$^{1/2}$)	13.69	3.04	16.58	6.23	7.86
$Properf_p$ (R_a)	0	1	0	0	0
RED	2.91	0.65	3.53	1.33	1.67
$Properf_p$*(RED)*	0	1	0	0.26	0
Viscosity (mPa s)	0.797	5.224	0.824	0.962	0.586
$Properf_p$*(Viscosity)*	1	0	1	1	1

Table S11 (continued):

Target properties with performance values	Diethyl carbonate	1,2,3-Trimethoxypropane	Furfural	Dimethyl Succinate	alpha-Pinene
CAS	105-58-8	20637-49-4	98-01-1	106-65-0	80-56-8
$GloPerf$	0.527	0.522	0.517	0.506	0.501
Melting Point (T_m) [K]	228	222	249	234	227
$ProPerf_p$ (T_m)	1	1	1	1	1
Boiling Point (T_b) [K]	404	430	417	452	430
$ProPerf_p$ (T_b)	1	1	1	1	1
Flash Point (T_f) [K]	303	320	310	341	301
$ProPerf_p$ (T_f)	1	1	1	1	1
ΔH_{vap} (kJ/mol)	43.60	46.86	45.92	54.37	47.70
$Properf_p$ (ΔH_{vap})	1	1	1	1	1
Density (g/cm^3)	0.985	0.912	1.113	1.067	0.872
$Properf_p$*(Density)*	1	1	1	1	1
δ_D (MPa$^{1/2}$)	15.30	15.50	18.00	16.30	17.00
$Properf_p$ (δ_D)	0	0	1	0	0.34
δ_P (MPa$^{1/2}$)	6.80	5.70	12.50	6.00	1.30
$Properf_p$ (δ_P)	0	0.84	0	0.34	0
δ_H (MPa$^{1/2}$)	5.70	7.50	8.80	9.20	2.00
$Properf_p$ (δ_H)	1	0	0	0	0
R_a (MPa$^{1/2}$)	6.84	6.62	8.75	6.25	5.47
$Properf_p$ (R_a)	0	0	0	0	0
RED	1.45	1.41	1.86	1.33	1.16
$Properf_p$*(RED)*	0.07	0.12	0	0.25	0.71
Viscosity (mPa s)	0.670	0.519	1.142	1.550	/
$Properf_p$*(Viscosity)*	1	1	1	1	0

Table S12. The candidates form the molecules evaluation results provided by IBSS®CAMD with a *GloPerf* > 0.5 for PF2:EH-IDTBR.

Target properties with performance values	1,2-dichlorobenzene	p-Xylene	Anisole	p-Cymene	Benzyl Benzoate	Glycerol -1,2,3-triethyl ether
CAS	95-50-1	106-42-3	100-66-3	99-87-6	120-51-4	162614-45-1
$GloPerf$	1	0.931	0.758	0.714	0.564	0.517
Melting Point (T_m) [K]	255	229	239	224	307	210
$ProPerf_p$ (T_m)	1	1	1	1	≈ 0	1
Boiling Point (T_b) [K]	449	419	428	450	573	467
$ProPerf_p$ (T_b)	1	1	1	1	≈ 0	1
Flash Point (T_f) [K]	332	301	314	323	420	343
$ProPerf_p$ (T_f)	1	1	1	1	1	1
ΔH_{vap} (kJ/mol)	50.1	43.4	46.5	50.1	85.8	60.2
$Properf_p$ (ΔH_{vap})	1	1	1	1	≈ 0	≈ 0
Density (g/cm^3)	1.280	0.873	0.974	0.864	1.123	0.893
$Properf_p$*(Density)*	1	1	1	1	1	1
δ_D (MPa$^{1/2}$)	19.5	18.6	18.1	17.4	19.8	15.5
$Properf_p$ (δ_D)	1	1	1	0.21	1	0.00
δ_P (MPa$^{1/2}$)	5.1	3.8	4.9	2.3	6.3	4.8
$Properf_p$ (δ_P)	1	1	1	0.13	≈ 0	1
δ_H (MPa$^{1/2}$)	3.1	1.6	6.1	2.4	4.7	3.6
$Properf_p$ (δ_H)	1	0.00	0.00	1	0.68	1
R_a (MPa$^{1/2}$)	1.51	1.70	4.12	4.10	3.36	7.51
$Properf_p$ (R_a)	1	1	0.17	0.18	0.83	≈ 0
RED	0.38	0.42	1.03	1.03	0.84	1.88
$Properf_p$*(RED)*	1	1.00	0.99	0.99	1	≈ 0
Viscosity (mPa s)	1.089	0.568	0.569	0.897	5.224	0.962
$Properf_p$*(Viscosity)*	1	1	1	1	0	1

Table S12 (continued):

Target properties with performance	Isoamyl acetate	Butyl acetate	Ethylene carbonate	2-Furaldehyde	Dibutyl ether	Propylene carbonate
CAS	123-92-2	123-86-4	96-49-1	98-01-1	142-96-1	108-32-7
$GloPerf$	0.517	0.517	0.517	0.517	0.516	0.511
Melting Point (T_m)	202	201	283	249	187	287
$ProPerf_p$ (T_m)	1	1	1	1	1	0.50
Boiling Point (T_b) [K]	420	407	413	417	426	433
$ProPerf_p$ (T_b)	1	1	1	1	1	1
Flash Point (T_f) [K]	312	305	324	310	311	334
$ProPerf_p$ (T_f)	1	1	1	1	1	1
ΔH_{vap} (kJ/mol)	48.9	46.0	49.3	45.9	46.7	52.7
$Properf_p$ (ΔH_{vap})	1	1	1	1	1	1
Density (g/cm^3)	0.868	0.873	1.303	1.113	0.770	1.195
$Properf_p$(Density)	1	1	1	1	0.10	1
δ_D (MPa$^{1/2}$)	15.8	15.8	18.4	18	15.4	17.9
$Properf_p$ (δ_D)	0.00	0.00	1	1	0.00	0.96
δ_P (MPa$^{1/2}$)	4	5.1	21.2	12.5	2.9	18.3
$Properf_p$ (δ_P)	1	1	≈ 0	≈ 0	0.88	≈ 0
δ_H (MPa$^{1/2}$)	6	6.5	6.3	8.8	2.7	5
$Properf_p$ (δ_H)	0.00	0.00	0.00	0.00	1	0.21
R_a (MPa$^{1/2}$)	7.52	7.85	17.82	10.84	7.65	14.89
$Properf_p$ (R_a)	≈ 0	≈ 0	≈ 0	≈ 0	≈ 0	≈ 0
RED	1.88	1.96	4.46	2.71	1.91	3.72
$Properf_p$(RED)	≈ 0	≈ 0	≈ 0	≈ 0	≈ 0	≈ 0
Viscosity (mPa s)	0.903	0.724	0.824	1.142	0.612	0.797
$Properf_p$(Viscosity)	1	1	1	1	1	1

Fig. S3 Pictures of PF2 solutions in (a) PX, (b) 2-MA, (c) AN and (d) PC. (PF2 solubility testing from 40 °C to 120 °C.)

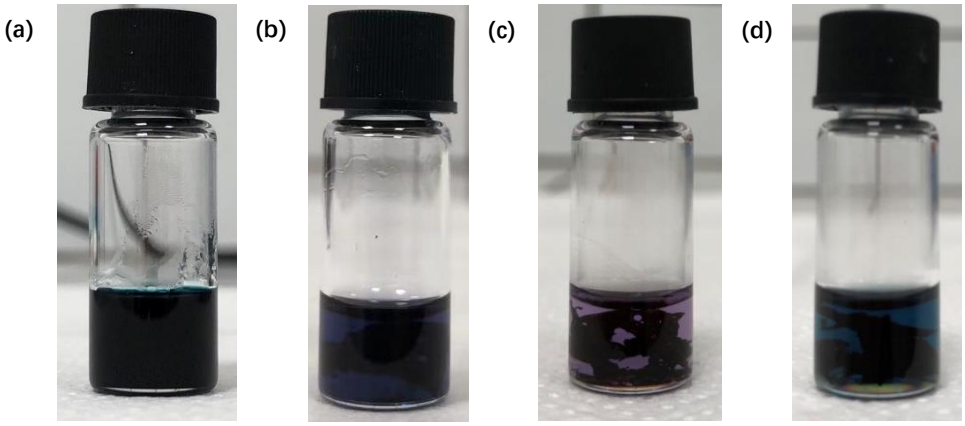


Fig. S4 Current-Voltage characteristics of P3HT:$PC_{71}BM$ based OPV devices processed from various solvents without additive.

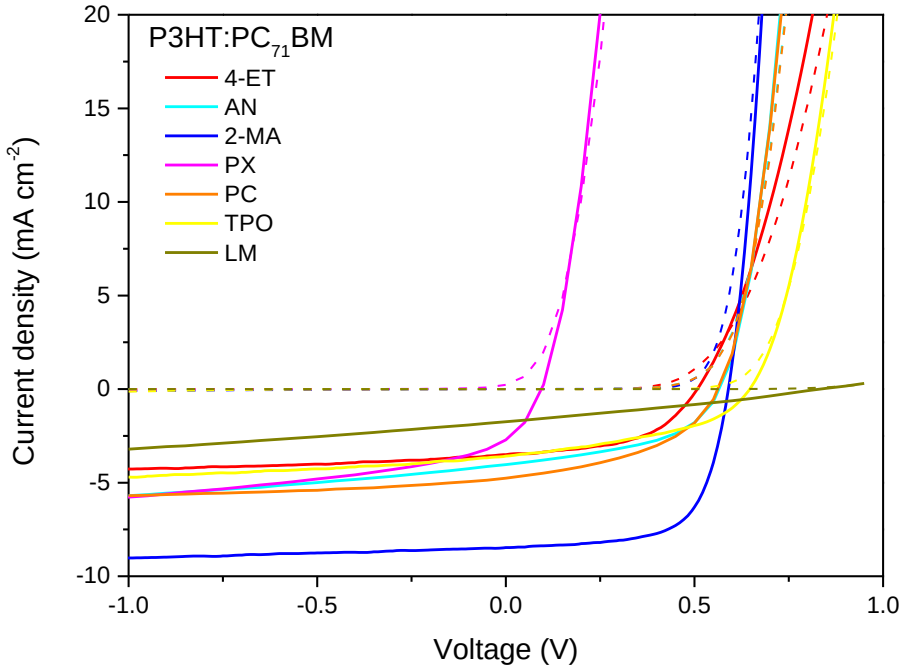


Table S13. Average photovoltaic parameters of P3HT:$PC_{71}BM$ based devices fabricated without additives.

Processing solvents	V_{oc} (mV)	J_{sc} (mA/cm^2)	*FF* (%)	*PCE* (%)
4-Ethynyltoluene (4-ET)	540±4	3.3±0.3	49±2	0.9±0.1
Anisole (AN)	571±1	4.2±0.3	46±2	1.1±0.2
2-Methylanisole (2-MA)	587±2	8.3±0.1	64±1	3.1±0.2
p-Xylene (PX)	585±2	4.5±0.2	51±4	1.1±0.1
p-Cymene (PC)	555±4	5.0±0.1	43±2	1.2±0.3
Terpinolene (TPO)	645±7	3.5±0.3	42±2	1.0±0.2
d-Limonene (LM)	846±9	1.7±0.1	28±4	0.4±0.1

Table S14. R_a and *RED* values between various solvents and two acceptor materials.

Processing solvents	$PC_{71}BM$		EH-IDTBR	
	Ra	RED	Ra	RED
o-DCB	2.50	0.30	2.11	0.35
AN	4.52	0.54	2.24	0.37
PX	4.61	0.55	2.85	0.47
PC	6.74	0.80	3.93	0.64
TPO	7.52	0.90	4.51	0.74

Fig. S5 The JV curves of PF2 based devices processed from *PX/DPE* mixture solvents at different processing temperature.

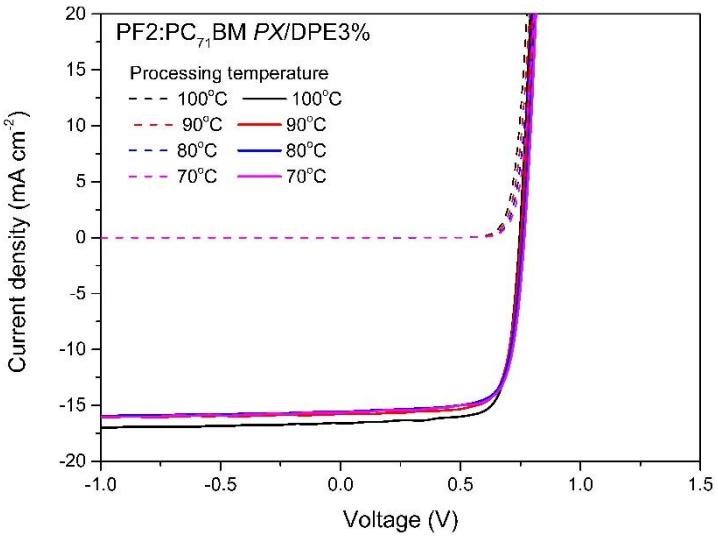
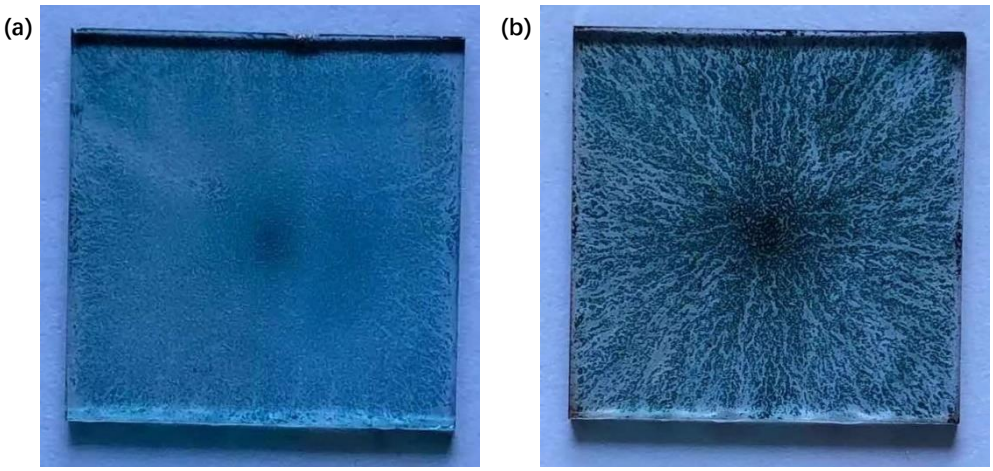


Table S15. Summary of PF2:$PC_{71}BM$ device performance from o-DCB and PX/DPE (3%).

Processing solvents	Processing temperature	V_{oc} (mV)	J_{sc} (mA cm^{-2})	FF (%)	PCE (%)	Thickness (nm)
o-DCB	100°C	754±5	17.9±1.3	74±0.5	9.8±0.7	~160
PX/DPE	100°C	753±3	15.9±0.6	76±1	9.1±0.4	~130
PX/DPE	90°C	753±5	15.3±0.5	76±1	8.8±0.2	~120
PX/DPE	80°C	758±3	15.4±0.2	75±1	8.8±0.1	~125
PX/DPE	70°C	761±6	15.3±0.4	75±1	8.8±0.2	~135

Fig. S6 Photographs of (a) PF2 and (b) PF2:$PC_{71}BM$ layers deposited on glass/ITO substrates from o-DCB solution at 70°C.



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