SUPPORTING INFORMATIONS

1. Methodology

1.1 Chosen descriptors:

VolSurf+[a]

a. Size and shape descriptors: molecular volume (V), molecular surface (S), rugosity (R), molecular globularity (G), flexibility parameters (Flex, Flex_RB)
b. Descriptors of hydrophilic regions: hydrophilic volumes (W1 - W8), capacity factors (CW1 - CW8)
c. Descriptors of hydrophobic regions: hydrophobic volumes (D1 - D8), capacity factors (CD1 - CD8), differences of the hydrophobic volumes (DD1 - DD8)
d. INTEraction enerGY (= INTEGY) moments: unbalance between the centre of mass of a molecule and the barycenter of its hydrophilic or hydrophobic regions (IW1 - IW4, ID1 - ID4)
e. Descriptors of H-bond donor / acceptor regions: H-bond donor volumes (WO1 - WO6), H-bond acceptor volumes (WN1 - WN6)
f. Charge State descriptors: number of charged centers (NCC), available uncharged species (AUS7.4), % unionised species (%FU4 - %FU10)
g. Mixed descriptors: molecular Weight (MW), hydrophilic-lipophilic balance (HL1, HL2), amphiphilic moments (A), critical packing parameter (CP), polarizability (POL), diffusivity (DIFF), LogP octanol/water (LOGP n-Oct), LogP cyclohexane/water (LOGP c-Hex), LogD (LgD5 - LgD10), polar and hydrophobic surface areas (PSA, HSA, PSAR, PHSAR), intrinsic solubility (SOLY)

Semi-empirical calculated from the G09 package

h. HOMO (USR1)
i. LUMO (USR2)
j. BANDGAP (USR3)

Specifically designed

k. Undesirable moieties from experimental knowledge (USR6)
l. Molecular electrostatic potential (USR 8) and minimum electrostatic potential center (USR7)

[a] further details on ref. 26.

1.2 Modelled dyes (labelled as in ref. 33):

1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 19, 20, 21, 22, 23, 24, 25, 26, 27, 30, 32, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 53, 54, 55, 56, 57, 58, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82

Labels in red represent the subgroup of 54 dyes chosen to model the effect of Li+ ions used to build the solar device; dyes structures given below in Table 1.

Table 1. Modelled dyes smiles

1	c1(ncccc1)c1ncccc1
2	c1(nccc(c1)C)c1nccc(c1)C
3	c1(nccc(c1)CCCCCC)c1nccc(c1)CCCCCC
4	c1(nccc(c1)CCCCCCCCC)c1nccc(c1)CCCCCCCCC
5	c1(nccc(c1)CCCCCCCCCCCCC)c1nccc(c1)CCCCCCCCCCCCC
6	c1(nccc(c1)CCCCCCCCCCCCCCCCC)c1nccc(c1)CCCCCCCCCCCCCCCCC
7	c1(nccc(c1)c1ccc(cc1)C)c1nccc(c1)c1ccc(cc1)C
8	c1(nccc(c1)c1ccc(cc1)C#N)c1nccc(c1)c1ccc(cc1)C#N
9	c1(nccc(c1)c1ccc(cc1)F)c1nccc(c1)c1ccc(cc1)F
10	c1(nccc(c1)c1ccccc1)c1nccc(c1)c1ccccc1
11	c1(nccc(c1)c1ccc(cc1)OC)c1nccc(c1)c1ccc(cc1)OC
12	c1(nccc(c1)c1ccc(cc1)N(C)C)c1nccc(c1)c1ccc(cc1)N(C)C
13	c1(nccc(c1)/C=C/c1ccc(cc1)OC)c1nccc(c1)/C=C/c1ccc(cc1)OC
14	c1(nccc(c1)/C=C/c1ccc(cc1)OCCCCCC)c1nccc(c1)/C=C/c1ccc(cc1)OCCCCCC
15	c1(nccc(c1)/C=C/c1ccc(cc1)OC(C)(C)C)c1nccc(c1)/C=C/c1ccc(cc1)OC(C)(C)C
16	c1(nccc(c1)/C=C/c1c(cc(cc1)OCC)OC)c1nccc(c1)/C=C/c1ccc(cc1OC)OCC
19	c1(nccc(c1)C(=O)NCCCNC(=O)O[C@@H]1CC[C@]2(C)[C@@H]3[C@@H]([C@H](C[C@@H]2C1)C)[C@@H]1CC[C@@H]([C@]1(CC3)C)[C@@H](CCCC(C)C)C)c1nccc(c1)C(=O)NCCCNC(=O)O[C@@H]1CC[C@]2([C@H](C1)C[C@H]([C@H]1[C@H]2CC[C@@]2([C@H](CC[C@H]12)[C@H](C)CCCC(C)C)C)C)C
20	c1(nccc(c1)CCCCCCCCCCCCO)c1nccc(c1)CCCCCCCCCCCCO
21	c1(nccc(c1)C(=O)NCCCCCCCC)c1nccc(c1)C(=O)NCCCCCCCC
22	c1(nccc(c1)/C=C/c1ccc(cc1)SCCCCCC)c1nccc(c1)/C=C/c1ccc(cc1)SCCCCCC
23	c1(nccc(c1)COCCOCCOCCOC)c1nccc(c1)COCCOCCOCCOC
24	c1(nccc(c1)/C=C/c1ccc(cc1)OCCOCCOCCOC)c1nccc(c1)/C=C/c1ccc(cc1)OCCOCCOCCOC
25	c1(nccc(c1)COCC(C(F)F)(F)F)c1nccc(c1)COCC(C(F)F)(F)F
26	c1(nccc(c1)COCC(C(C(F)(F)F)(F)F)(F)F)c1nccc(c1)COCC(C(F)(F)C(F)(F)F)(F)F
27	c1(nccc(c1)COCC(C(C(F)(C(F)F)F)(F)F)(F)F)c1nccc(c1)COCC(C(F)(F)C(F)(F)C(F)F)(F)F
30	c1(nccc(c1)/C=C/c1ccc(cc1)N(c1ccc(cc1)C)c1ccc(cc1)C)c1nccc(c1)/C=C/c1ccc(cc1)N(c1ccc(cc1)C)c1ccc(cc1)C
32	c1(nccc(c1)/C=C/c1ccc(cc1)/C=C/c1ccc(cc1)N(CCCC)CCCC)c1nccc(c1)/C=C/c1ccc(cc1)/C=C/c1ccc(cc1)N(CCCC)CCCC
34	c1(nccc(c1)/C=C/c1sc(cc1)CCCCCC)c1nccc(c1)/C=C/c1sc(cc1)CCCCCC
35	c1(nccc(c1)c1sc(cc1)c1ccc(CCCCCCCC)s1)c1nccc(c1)c1sc(cc1)c1sc(CCCCCCCC)cc1
36	c1(nccc(c1)c1sc(cc1)CCCCCCCC)c1nccc(c1)c1sc(cc1)CCCCCCCC
37	c1(nccc(c1)c1sc(c2c1OCCO2)CCCCCCCC)c1nccc(c1)c1sc(c2c1OCCO2)CCCCCCCC
38	c1(nccc(c1)/C=C/c1scc2c1OCCO2)c1nccc(c1)/C=C/c1scc2c1OCCO2
39	c1(nccc(c1)c1sc(cc1)c1ccc(SCCCCCC)s1)c1nccc(c1)c1sc(cc1)c1sc(SCCCCCC)cc1
40	c1(nccc(c1)c1sc(cc1)CCCCCC)c1nccc(c1)c1sc(cc1)CCCCCC
41	c1(nccc(c1)c1oc(cc1)CCCCCC)c1nccc(c1)c1oc(cc1)CCCCCC
42	c1(nccc(c1)c1sc2c(c1)sc(c2)CCCCCCCC)c1nccc(c1)c1sc2c(c1)sc(c2)CCCCCCCC
43	c1(nccc(c1)c1sc(c2c1OCCO2)CCCCCC)c1nccc(c1)c1sc(c2c1OCCO2)CCCCCC
44	c1(nccc(c1)c1sc(c2c1OCCO2)c1sc(CCCCCC)c2OCCOc12)c1nccc(c1)c1sc(c2c1OCCO2)c1sc(c2c1OCCO2)CCCCCC
45	c1(nccc(c1)c1[se]c(cc1)CCCCCC)c1nccc(c1)c1[se]c(cc1)CCCCCC
46	c1(nccc(c1)c1sc(cc1)SCCCCCC)c1nccc(c1)c1sc(cc1)SCCCCCC
47	c1(nccc(c1)c1cc(c2sccc2)c(c2cccs2)s1)c1nccc(c1)c1sc(c(c1)c1cccs1)c1cccs1
48	c1(nccc(c1)c1oc(cc1)SC[C@H](CCCC)CC)c1nccc(c1)c1oc(cc1)SC[C@@H](CCCC)CC
49	c1(nccc(c1)c1cc2c(C(C)(C)c3c2sc(CCCCCC)c3)cc1)c1nccc(c1)c1cc2c(cc1)c1c(C2(C)C)cc(s1)CCCCCC
50	c1(nccc(c1)c1cc2c(c3sc(cc3C2(C)C)CCCCCC)s1)c1nccc(c1)c1sc2c(C(c3c2sc(c3)CCCCCC)(C)C)c1
53	c1(nccc(c1)c1ccc(n2c3ccc(cc3c3cc(C(C)(C)C)ccc23)C(C)(C)C)s1)c1nccc(c1)c1sc(cc1)n1c2c(c3c1ccc(c3)C(C)(C)C)cc(cc2)C(C)(C)C
54	c1(nccc(c1)c1ccc(n2c3ccc(cc3c3cc(CCCCCCC)ccc23)CCCCCCC)s1)c1nccc(c1)c1sc(cc1)n1c2c(c3c1ccc(c3)CCCCCCC)cc(cc2)CCCCCCC

55	c1(nccc(c1)c1c2c(c(n3c4ccc(cc4c4cc(C(C)(C)C)ccc34)C(C)(C)C)s1)OCCO2)c1nccc(c1)c1sc(c2c1OCCO2)n1c2c(c3c1ccc(c3)C(C)(C)C)cc(cc2)C(C)(C)C
56	c1cnc(cc1c1sc(cc1)c1ccc(s1)n1c2c(c3c1ccc(c3)CCCCCCC)cc(cc2)CCCCCCC)c1cc(ccn1)c1ccc(s1)c1sc(n2c3ccc(cc3c3cc(ccc23)CCCCCCC)CCCCCCC)cc1
57	c12ncccc1ccc1c2nccc1
58	c12ncccc1[C@H]1[C@H](c3c2nccc3)N=c2c(=N1)cccc2
60	c12ncccc1c(cc1c2nccc1)N
61	c12ncccc1c(c(c1c2nccc1)N)N
62	c12ncccc1c(c(c1c2nccc1)N)[N+](=O)[O-]
63	c12ncccc1c(c(c1c2nccc1)[N+](=O)[O-])[N+](=O)[O-]
64	c12ncc(cc1ccc1c2ncc(c1)c1ccc(s1)CCCCCCCC)c1ccc(s1)CCCCCCCC
65	c12ncc(cc1ccc1c2ncc(c1)c1sc(c(c1)CCCCCCCC)c1scc(c1)CCCCCCCC)c1cc(c(s1)c1scc(c1)CCCCCCCC)CCCCCCCC
66	c12ncccc1c1c(c3c2nccc3)n(c(n1)c1cc2c(cc1)n(c1c2cccc1)CC)CC
67	c12ncccc1c1c(c3c2nccc3)n(c(n1)c1ccccc1)CC
68	c12ncccc1c1c(c3c2nccc3)n(c(n1)c1ccc(cc1)OC)CC
69	c12ncccc1c1c(c3c2nccc3)[nH]c(n1)c1ccc(cc1)CCCCCCCC
70	c12ncccc1c1c(c3c2nccc3)[nH]c(n1)c1sc(CCCCCCCC)cc1
71	c12ncccc1c1c(c3c2nccc3)[nH]c(n1)c1sc(cc1)c1ccc(CCCCCCCC)s1
72	c12ncccc1c1c(c3c2nccc3)[nH]c(n1)c1sc(cc1)c1ccc(s1)c1ccc(s1)CCCCCCCC
73	c12ncccc1c1c(c3c2nccc3)[nH]c(n1)c1sc(c(c1)c1ccc(s1)CCCCCCCC)c1sc(cc1)CCCCCCCC
74	c12ncccc1c1c(c3c2nccc3)[nH]c(n1)c1sc(c(c1)N1c2c(Sc3c1cccc3)cccc2)CCCCCCCC
75	c12ncccc1c1c(c3c2nccc3)[nH]c(n1)c1sc(c(c1)N(c1ccccc1)c1ccccc1)CCCCCCCC
76	c12ncccc1c1c(c3c2nccc3)[nH]c(n1)c1ccc(N(c2ccccc2)c2ccccc2)cc1
77	c12ncccc1c1c(c3c2nccc3)[nH]c(n1)c1ccccc1
78	c1ncccc1N(c1cnccc1)CCCCCCCCCCCCCC
79	c1ncccc1N(c1cnccc1)c1ccc(cc1)OCCCC
80	c1ncccc1N(c1cnccc1)c1ccc(cc1)OCCCCCCCC
81	c1ncc(cc1N(c1cncc(c1)c1ccc(CCCCCC)s1)CCCCCC)c1ccc(s1)CCCCCC
82	c1ncc(cc1N(c1cncc(c1)c1cc2sc(CCCCCC)cc2s1)CCCCCC)c1cc2c(s1)cc(s2)CCCCCC