Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.


**Supplementary material for**

# Evolutionary *de novo* design of phenothiazine derivatives for dye-sensitized solar cells

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*Table S1: QSPR predictions for the molecules used in the calibration and validation. In the "Molecule" column, names starting with "C" indicate the calibration data while those starting with "T" are the test data. The "QSPR" column contains the predicted $PCE$ with calculated uncertainties. $h_i$ is the leverage value for each prediction. The last column contains the 6 ADAN categories $D_1$-$D_6$ (see the main text), where a "0" indicates no violation and "1" otherwise.*

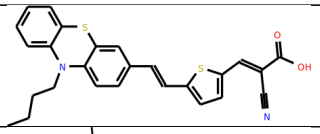
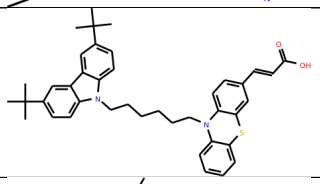
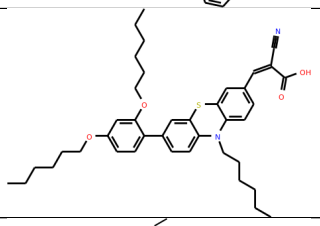
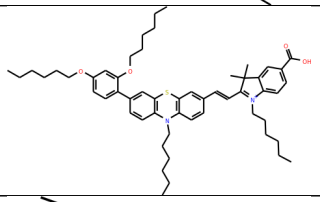
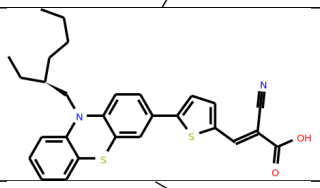
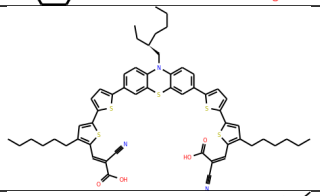
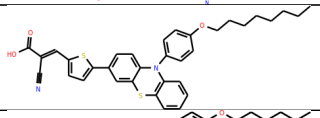
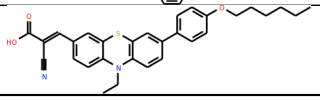
| **Molecule** | **Structure** | $PCE$ | **QSPR** | $h_i$ | **ADAN** |
|---|---|---|---|---|---|
| C01[29] |  | 6.40 | 5.94±0.53 | 0.07 | 0,0,0,0,0,0 |
| C02[9] |  | 2.40 | 2.39±0.57 | 0.04 | 0,0,0,0,0,0 |
| C03[7] |  | 5.80 | 6.15±0.45 | 0.03 | 0,0,0,0,0,0 |
| C04[7] |  | 4.90 | 5.14±0.44 | 0.07 | 0,0,0,0,0,0 |
| C05[16] |  | 4.91 | 5.35±0.41 | 0.04 | 0,0,0,0,0,0 |
| C06[16] |  | 7.31 | 6.76±1.27 | 0.09 | 0,0,0,0,0,0 |
| C07[18] |  | 6.34 | 6.08±0.64 | 0.03 | 0,0,0,0,0,0 |
| C08[13] |  | 6.87 | 7.37±0.43 | 0.04 | 0,0,0,0,0,0 |

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Table S1 – *Continued from previous page*

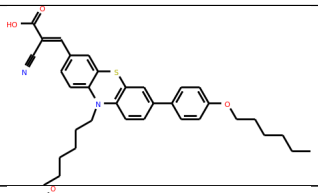
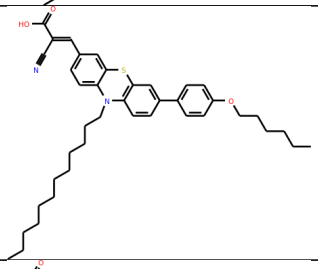
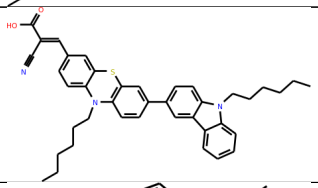
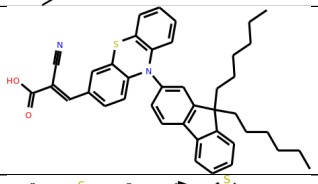
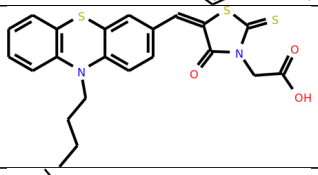
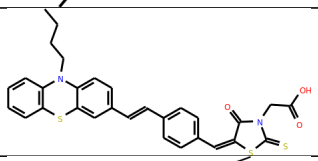
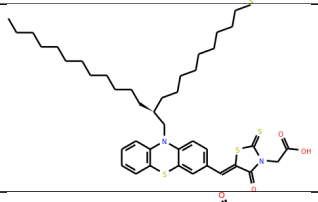
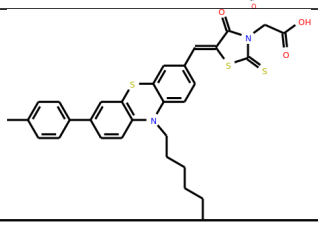
| **Molecule** | **Structure** | *PCE* | **QSPR** | $h_i$ | **ADAN** |
|---|---|---|---|---|---|
| C09[13] |  | 8.18 | 8.08±0.47 | 0.05 | 0,0,0,0,0,0 |
| C10[13] |  | 7.57 | 7.44±0.46 | 0.06 | 0,0,0,0,0,0 |
| C11[14] |  | 6.72 | 6.86±0.33 | 0.02 | 0,0,0,0,0,0 |
| C12[14] |  | 3.98 | 4.46±0.48 | 0.00 | 0,0,0,0,0,0 |
| C13[28] |  | 1.90 | 2.00±0.46 | 0.08 | 0,0,0,0,0,0 |
| C14[28] |  | 2.40 | 1.85±0.48 | 0.08 | 0,0,0,0,0,0 |
| C15[26] |  | 0.70 | 0.45±0.56 | 0.13 | 0,0,0,1,0,0 |
| C16[26] |  | 1.20 | 2.01±0.93 | 0.05 | 0,0,0,0,0,1 |

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Table S1 – *Continued from previous page*

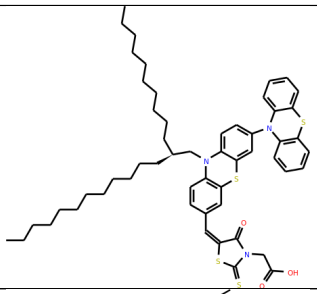
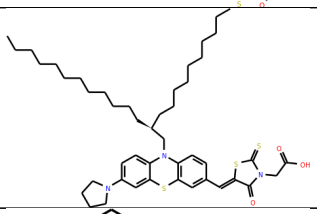
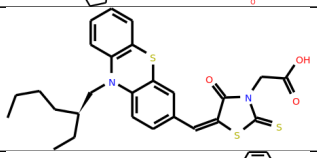
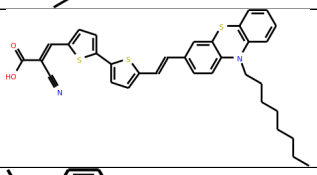
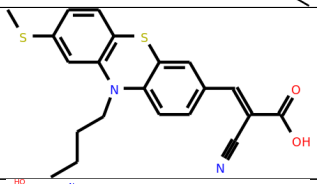
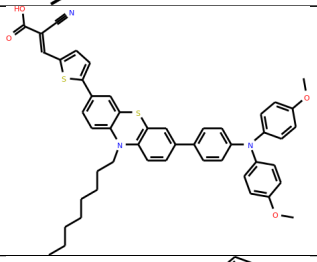
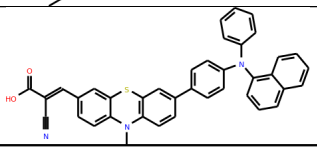
| **Molecule** | **Structure** | $PCE$ | **QSPR** | $h_i$ | **ADAN** |
|---|---|---|---|---|---|
| C17[26] |  | 1.80 | 1.16±0.67 | 0.12 | 0,0,0,0,0,0 |
| C18[26] |  | 0.50 | 0.56±0.79 | 0.14 | 1,0,0,1,0,0 |
| C19[27] |  | 0.40 | 0.89±0.82 | 0.09 | 0,0,0,1,0,0 |
| C20[36] |  | 5.40 | 5.33±0.28 | 0.03 | 0,0,0,0,0,0 |
| C21[24] |  | 6.53 | 6.08±0.58 | 0.03 | 0,0,0,0,0,0 |
| C22[35] |  | 3.78 | 3.62±0.43 | 0.01 | 0,0,0,0,0,0 |
| C23[37] |  | 4.60 | 4.58±0.34 | 0.03 | 0,0,0,0,0,0 |

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Table S1 – *Continued from previous page*

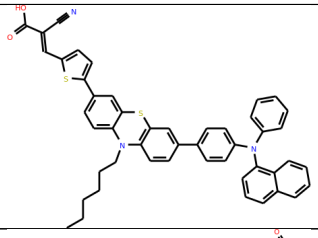
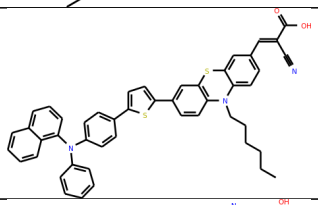
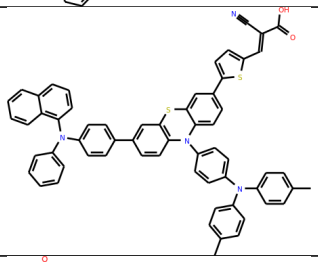
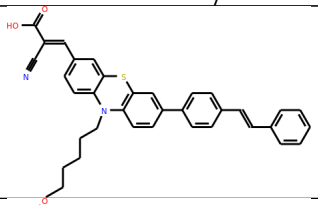
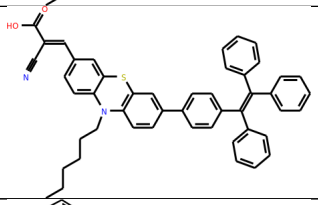
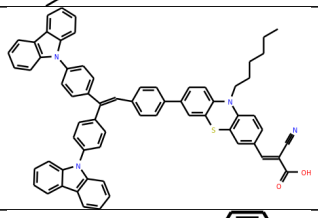
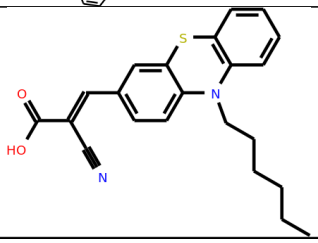
| **Molecule** | **Structure** | $PCE$ | **QSPR** | $h_i$ | **ADAN** |
|---|---|---|---|---|---|
| C24[37] |  | 2.04 | 3.28±1.12 | 0.03 | 0,0,0,0,0,1 |
| C25[37] |  | 6.22 | 5.35±0.64 | 0.03 | 0,0,0,0,0,0 |
| C26[37] |  | 4.24 | 3.20±0.92 | 0.04 | 0,0,1,0,0,1 |
| C27[4] |  | 5.84 | 6.04±0.21 | 0.02 | 0,0,0,0,0,0 |
| C28[4] |  | 5.76 | 5.47±0.30 | 0.05 | 0,0,0,0,0,0 |
| C29[5] |  | 5.51 | 5.72±0.69 | 0.05 | 0,0,0,0,0,0 |
| C30[3] |  | 5.43 | 5.42±0.33 | 0.02 | 0,0,0,0,0,0 |

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Table S1 – *Continued from previous page*

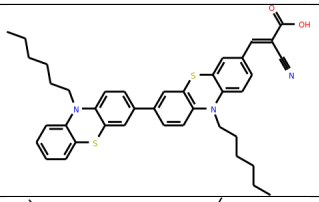
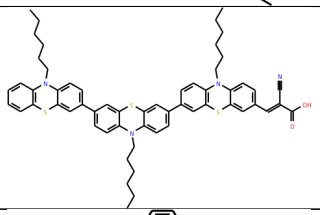
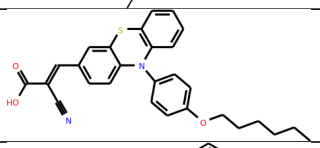
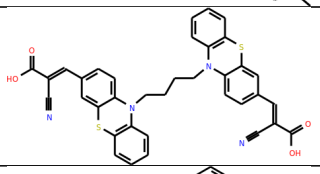
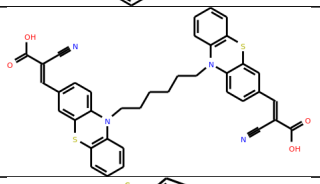
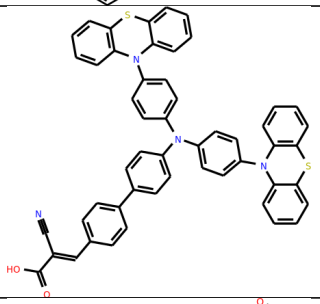
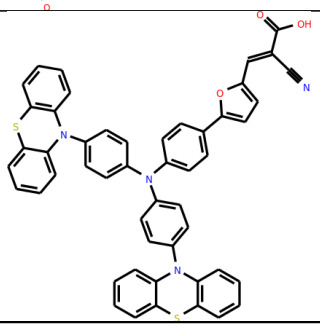
| **Molecule** | **Structure** | $PCE$ | **QSPR** | $h_i$ | **ADAN** |
|---|---|---|---|---|---|
| C31[3] |  | 5.44 | 5.57±0.25 | 0.01 | 0,0,0,0,0,0 |
| C32[3] |  | 5.05 | 4.89±0.29 | 0.07 | 0,0,0,0,0,0 |
| C33[3] |  | 6.52 | 6.17±0.53 | 0.02 | 0,0,0,0,0,0 |
| C34[2] |  | 4.13 | 4.14±0.46 | 0.05 | 0,0,0,0,0,0 |
| C35[2] |  | 4.22 | 4.20±0.39 | 0.05 | 0,0,0,0,0,0 |
| C36[31] |  | 4.90 | 4.99±0.37 | 0.03 | 0,0,0,0,0,0 |
| C37[31] |  | 6.79 | 6.43±0.52 | 0.03 | 0,0,0,0,0,0 |

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Table S1 – *Continued from previous page*

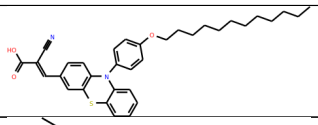
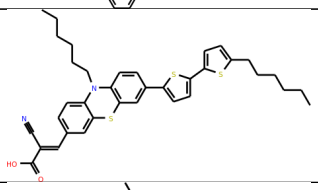
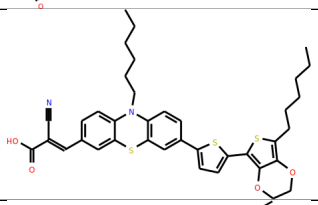
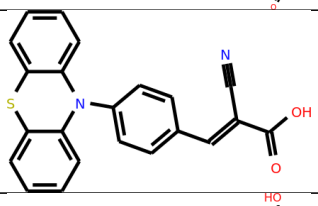
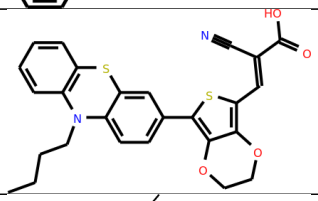
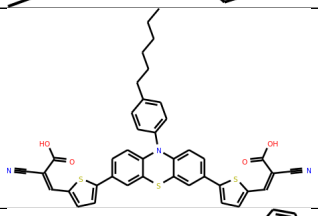
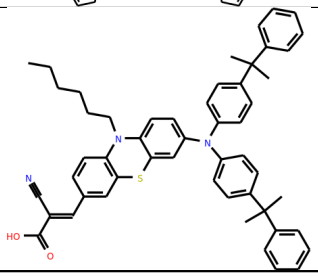
| **Molecule** | **Structure** | *PCE* | **QSPR** | $h_i$ | **ADAN** |
|---|---|---|---|---|---|
| C38[17] |  | 4.54 | 5.05±0.40 | 0.01 | 0,0,0,0,0,0 |
| C39[12] |  | 7.87 | 7.63±0.55 | 0.04 | 0,0,0,0,0,0 |
| C40[12] |  | 5.62 | 6.35±0.51 | 0.01 | 0,0,0,0,0,0 |
| C41[22] |  | 6.10 | 6.12±0.20 | 0.02 | 0,0,0,0,0,0 |
| C42[33] |  | 1.83 | 4.14±1.63 | 0.05 | 0,0,0,0,1,1 |
| C43[21] |  | 5.43 | 4.93±0.54 | 0.04 | 0,0,0,0,0,1 |
| C44[19] |  | 6.04 | 5.98±0.66 | 0.01 | 0,0,1,0,0,0 |
| C45[34] |  | 6.14 | 5.43±0.71 | 0.00 | 0,0,0,0,0,0 |

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Table S1 – *Continued from previous page*

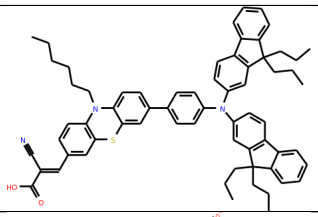
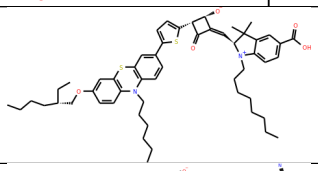
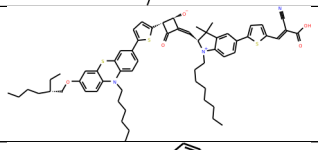
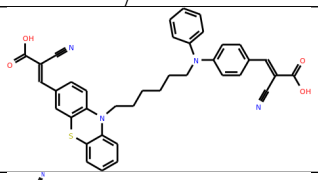
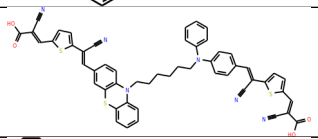
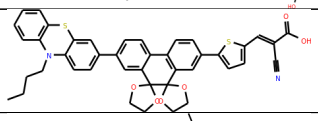
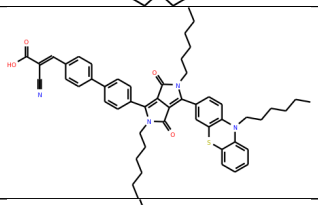
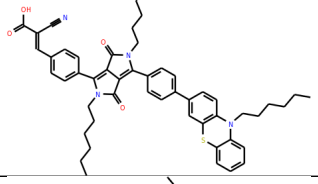
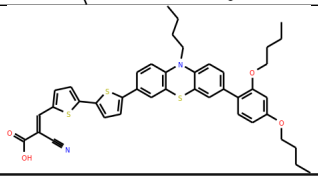
| **Molecule** | **Structure** | $PCE$ | **QSPR** | $h_i$ | **ADAN** |
|---|---|---|---|---|---|
| C46[34] |  | 6.49 | 7.00±0.51 | 0.08 | 0,0,0,0,0,0 |
| C47[1] |  | 0.90 | 0.49±0.99 | 0.13 | 0,0,0,1,0,0 |
| C48[1] |  | 0.90 | 1.67±1.49 | 0.10 | 0,0,0,0,0,0 |
| C49[11] |  | 4.66 | 4.77±0.40 | 0.02 | 0,0,0,0,0,0 |
| C50[11] |  | 5.19 | 4.81±0.46 | 0.01 | 0,0,0,0,0,0 |
| C51[40] |  | 6.00 | 4.89±0.99 | 0.02 | 0,0,0,0,0,0 |
| C52[39] |  | 5.16 | 4.08±0.93 | 0.01 | 0,0,0,0,0,0 |
| C53[39] |  | 3.26 | 3.54±0.62 | 0.02 | 0,0,0,0,0,0 |
| C54[38] |  | 7.50 | 7.40±0.93 | 0.07 | 0,0,0,0,0,0 |

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Table S1 – *Continued from previous page*

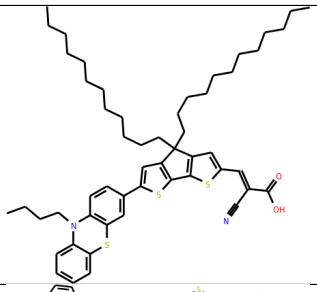
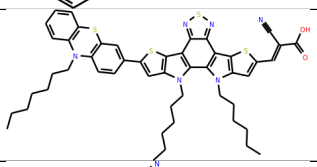
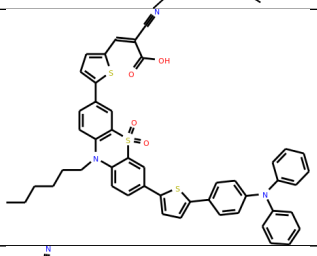
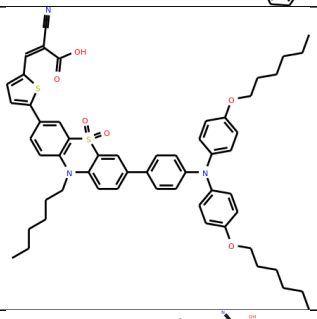
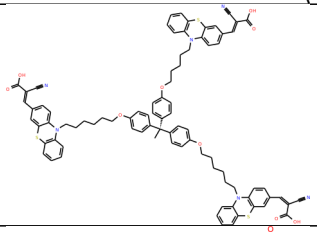
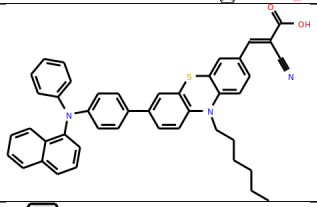
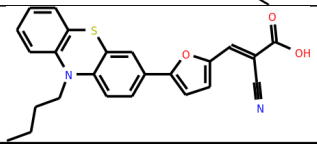
| **Molecule** | **Structure** | $PCE$ | **QSPR** | $h_i$ | **ADAN** |
|---|---|---|---|---|---|
| C55[25] |  | 7.00 | 7.65±0.91 | 0.19 | 1,0,0,0,0,0 |
| C56[15] |  | 5.02 | 5.67±0.55 | 0.02 | 0,0,0,0,0,0 |
| C57[23] |  | 5.44 | 5.16±0.32 | 0.01 | 0,0,0,0,0,0 |
| C58[23] |  | 6.80 | 6.94±0.33 | 0.06 | 0,0,0,0,0,0 |
| C59[20] |  | 4.90 | 4.32±1.17 | 0.26 | 1,0,1,0,0,0 |
| T01[37] |  | 5.60 | 4.40±0.46 | 0.05 | 0,0,0,0,0,0 |
| T02[21] |  | 6.02 | 5.75±0.44 | 0.05 | 0,0,0,0,0,0 |

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Table S1 – *Continued from previous page*

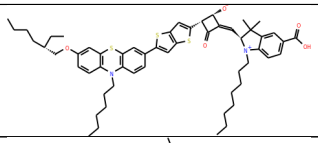
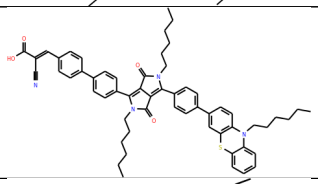
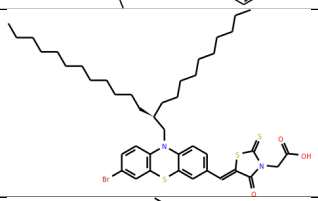
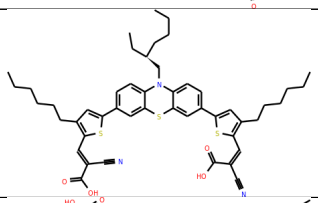
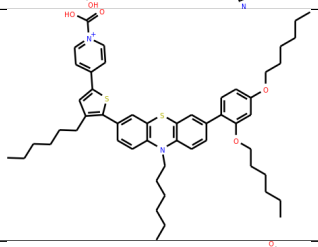
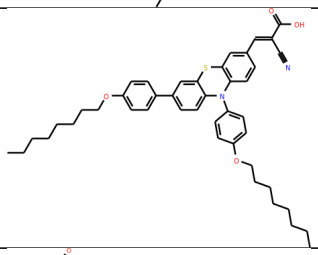
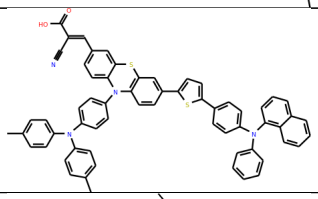
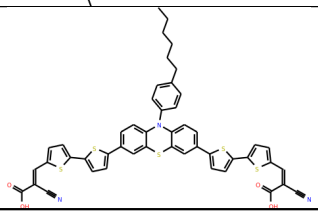
| **Molecule** | **Structure** | $PCE$ | **QSPR** | $h_i$ | **ADAN** |
|---|---|---|---|---|---|
| T03[1] |  | 0.80 | 1.68±0.95 | 0.09 | 0,0,0,0,0,0 |
| T04[39] |  | 4.56 | 3.80±0.64 | 0.03 | 0,0,0,0,0,0 |
| T05[26] |  | 0.60 | 0.97±0.56 | 0.10 | 0,0,0,0,0,0 |
| T06[16] |  | 6.85 | 6.27±0.80 | 0.05 | 0,0,0,0,0,0 |
| T07[8] |  | 6.70 | 5.94±0.48 | 0.08 | 0,0,0,0,0,0 |
| T08[17] |  | 5.73 | 5.50±0.38 | 0.01 | 0,0,0,0,0,0 |
| T09[37] |  | 4.80 | 3.68±0.77 | 0.05 | 0,0,0,0,0,0 |
| T10[19] |  | 7.30 | 6.63±0.45 | 0.02 | 0,0,0,0,0,0 |

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Table S1 – *Continued from previous page*

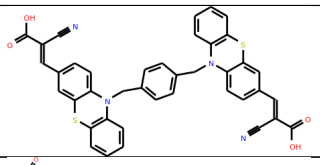
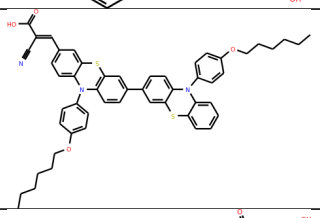
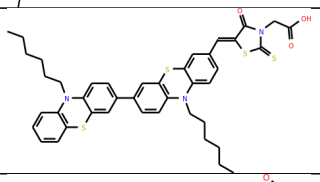
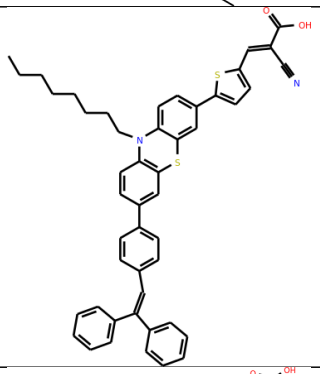
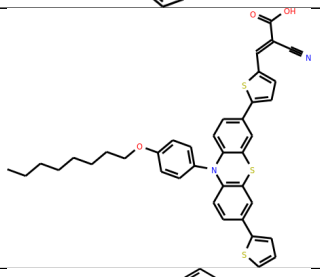
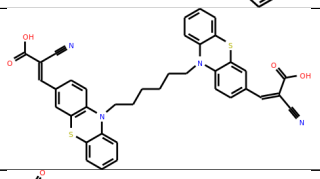
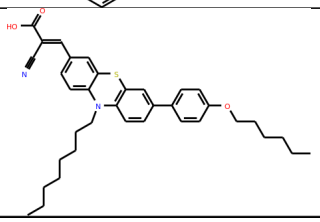
| **Molecule** | **Structure** | *PCE* | **QSPR** | $h_i$ | **ADAN** |
|---|---|---|---|---|---|
| T11[2] |  | 3.56 | 4.28±0.46 | 0.03 | 0,0,0,0,0,0 |
| T12[3] |  | 7.38 | 7.47±0.45 | 0.04 | 0,0,0,0,0,0 |
| T13[26] |  | 1.90 | 2.06±0.64 | 0.04 | 0,0,0,0,0,0 |
| T14[35] |  | 2.48 | 4.29±0.43 | 0.00 | 0,0,0,0,0,0 |
| T15[18] |  | 5.12 | 5.15±0.43 | 0.01 | 0,0,0,0,0,0 |
| T16[20] |  | 3.91 | 4.01±0.35 | 0.03 | 0,0,0,0,0,0 |
| T17[13] |  | 8.08 | 7.37±0.41 | 0.04 | 0,0,0,0,0,0 |

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Table S1 – *Continued from previous page*

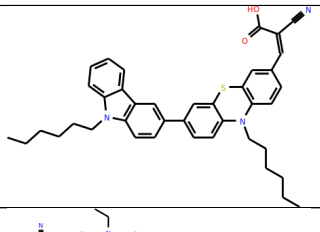
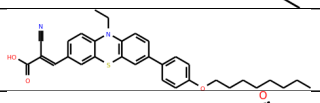
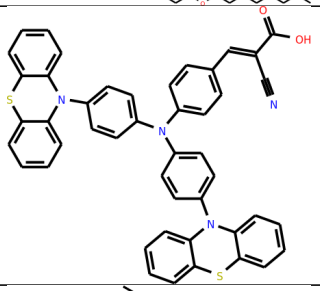
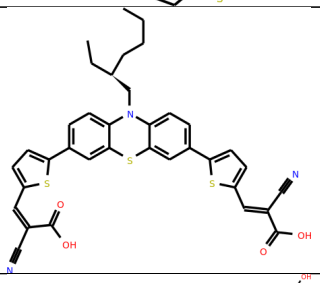
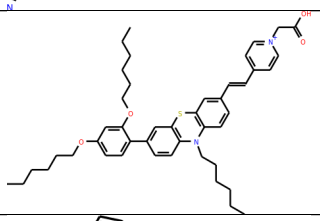
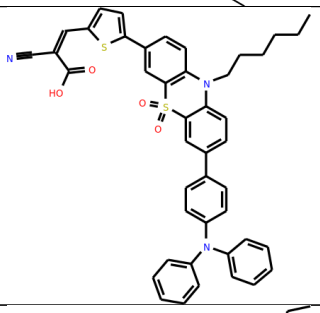
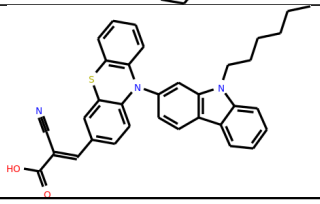
| **Molecule** | **Structure** | $PCE$ | **QSPR** | $h_i$ | **ADAN** |
|---|---|---|---|---|---|
| T18[34] |  | 7.13 | 5.82±0.33 | 0.00 | 0,0,0,0,0,0 |
| T19[17] |  | 6.32 | 6.32±0.40 | 0.02 | 0,0,0,0,0,0 |
| T20[31] |  | 4.40 | 4.40±0.96 | 0.03 | 0,0,0,0,0,0 |
| T21[16] |  | 5.53 | 5.52±0.44 | 0.02 | 0,0,0,0,0,0 |
| T22[7] |  | 6.80 | 6.21±0.49 | 0.04 | 0,0,0,0,0,0 |
| T23[23] |  | 6.37 | 6.12±0.35 | 0.01 | 0,0,0,0,0,0 |
| T24[14] |  | 5.12 | 4.56±0.32 | 0.01 | 0,0,0,0,0,0 |

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Table S1 – *Continued from previous page*

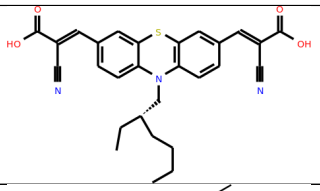
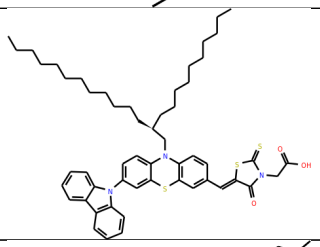
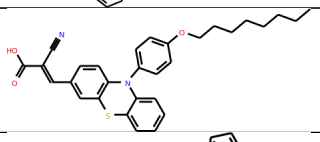
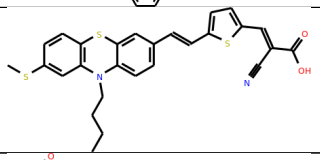
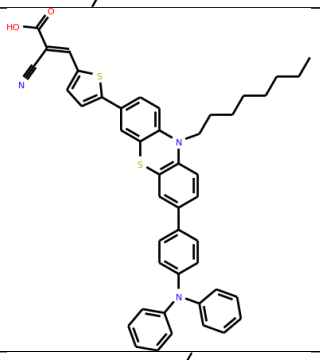
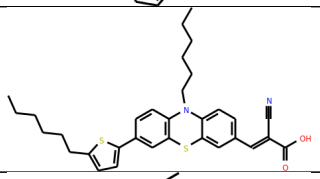
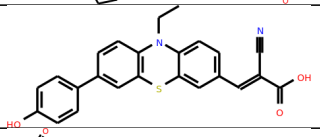
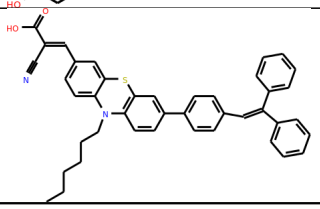
| **Molecule** | **Structure** | *PCE* | **QSPR** | $h_i$ | **ADAN** |
|---|---|---|---|---|---|
| T25[27] |  | 6.80 | 6.06±0.47 | 0.01 | 0,0,0,0,0,0 |
| T26[26] |  | 1.30 | 1.85±0.52 | 0.10 | 0,0,0,0,0,0 |
| T27[17] |  | 4.79 | 5.17±0.46 | 0.02 | 0,0,0,0,0,0 |
| T28[24] |  | 7.44 | 5.32±0.52 | 0.04 | 0,0,0,0,0,0 |
| T29[35] |  | 4.41 | 5.35±0.52 | 0.00 | 0,0,0,0,0,0 |
| T30[12] |  | 8.07 | 6.88±0.40 | 0.02 | 0,0,0,0,0,0 |
| T31[17] |  | 5.23 | 5.87±0.53 | 0.03 | 0,0,0,0,0,0 |
| T32[4] |  | 6.29 | 6.03±0.31 | 0.03 | 0,0,0,0,0,0 |

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Table S1 – *Continued from previous page*

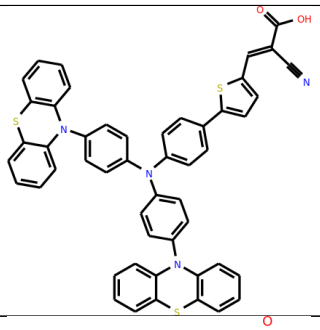
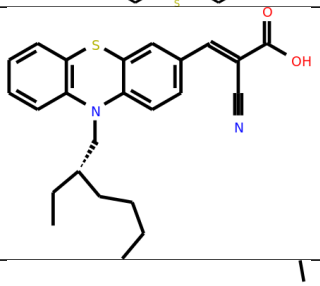
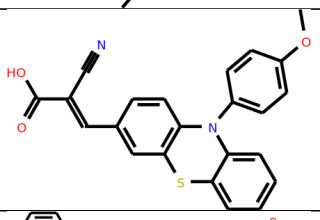
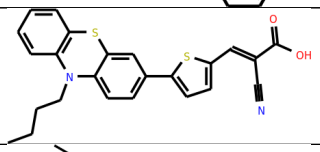
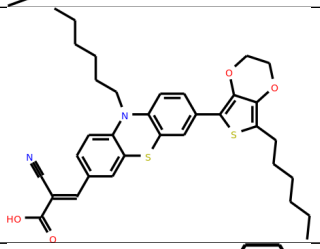
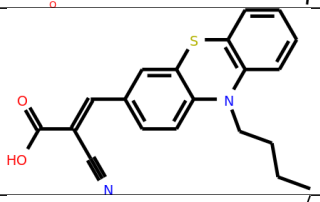
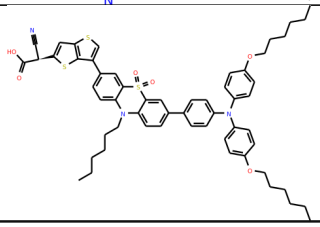
| **Molecule** | **Structure** | $PCE$ | **QSPR** | $h_i$ | **ADAN** |
|---|---|---|---|---|---|
| T33[31] |  | 6.02 | 5.56±0.38 | 0.03 | 0,0,0,0,0,0 |
| T34[27] |  | 5.60 | 4.98±0.36 | 0.01 | 0,0,0,0,0,0 |
| T35[17] |  | 4.53 | 5.44±0.43 | 0.04 | 0,0,0,0,0,0 |
| T36[21] |  | 5.36 | 5.66±0.46 | 0.07 | 0,0,0,0,0,0 |
| T37[12] |  | 7.98 | 5.66±0.37 | 0.00 | 0,0,0,0,0,0 |
| T38[28] |  | 5.39 | 6.08±0.34 | 0.04 | 0,0,0,0,0,0 |
| T39[23] |  | 3.94 | 6.40±0.51 | 0.04 | 0,0,1,0,0,0 |

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Table S1 – *Continued from previous page*

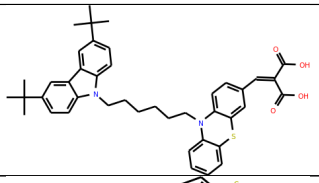
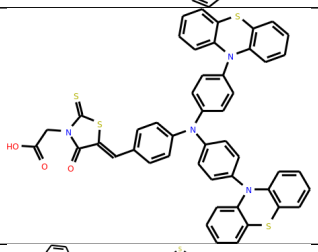
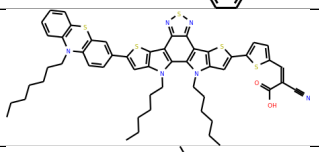
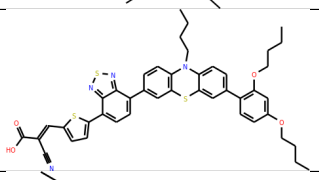
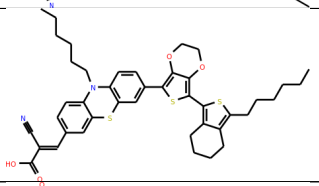
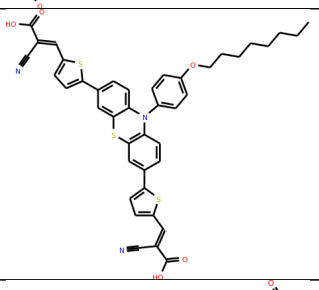
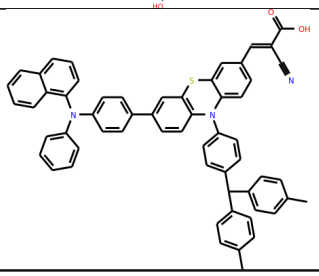
| **Molecule** | **Structure** | $PCE$ | **QSPR** | $h_i$ | **ADAN** |
|---|---|---|---|---|---|
| T40[9] |  | 3.60 | 3.44±0.54 | 0.02 | 0,0,1,0,0,0 |
| T41[32] |  | 2.10 | 3.90±0.59 | 0.03 | 0,0,0,0,0,1 |
| T42[15] |  | 3.54 | 4.83±0.35 | 0.01 | 0,0,0,0,0,1 |
| T43[38] |  | 6.40 | 6.14±0.86 | 0.03 | 0,0,1,0,0,0 |
| T44[12] |  | 2.24 | 5.27±0.38 | 0.01 | 0,0,0,0,0,1 |
| T45[18] |  | 6.82 | 3.86±0.69 | 0.02 | 0,0,1,0,0,0 |
| T46[37] |  | 5.22 | 4.20±0.55 | 0.03 | 0,0,1,0,0,0 |

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Table S1 – *Continued from previous page*

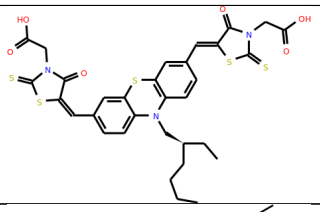
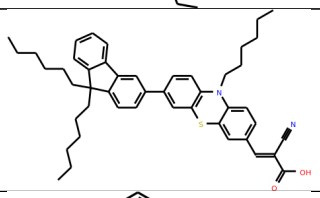
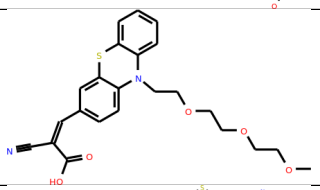
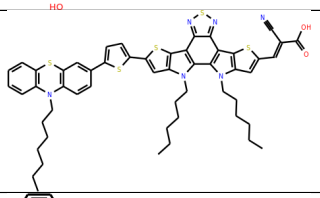
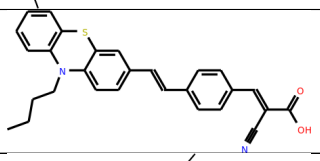
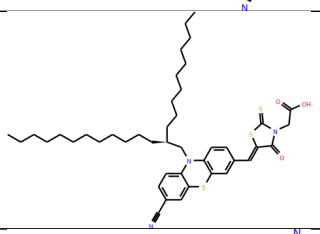
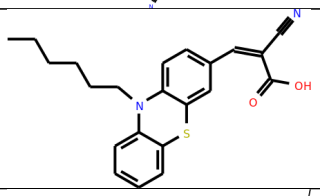
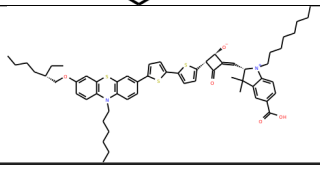
| **Molecule** | **Structure** | $PCE$ | **QSPR** | $h_i$ | **ADAN** |
|---|---|---|---|---|---|
| T47[27] |  | 1.30 | 0.87±0.66 | 0.08 | 0,0,0,1,0,0 |
| T48[14] |  | 6.13 | 5.26±0.44 | 0.02 | 0,0,0,0,0,1 |
| T49[10] |  | 4.07 | 4.25±0.36 | 0.02 | 0,0,0,0,0,1 |
| T50[15] |  | 4.39 | 5.41±0.41 | 0.02 | 0,0,0,0,0,1 |
| T51[28] |  | 4.80 | 4.61±0.40 | 0.03 | 0,0,0,0,0,1 |
| T52[26] |  | 0.40 | 2.67±0.61 | 0.07 | 0,0,1,0,0,0 |
| T53[14] |  | 4.43 | 4.49±0.37 | 0.02 | 0,0,0,0,0,1 |
| T54[1] |  | 0.50 | 1.90±1.09 | 0.09 | 0,0,1,0,0,0 |

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Table S1 – *Continued from previous page*

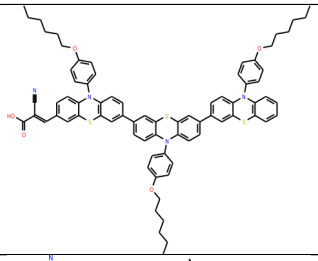
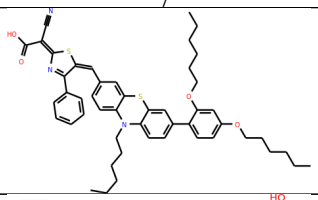
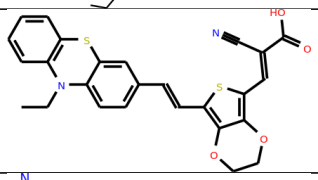
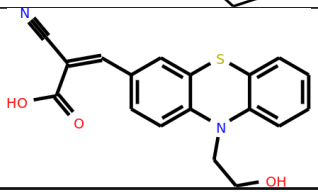
| **Molecule** | **Structure** | $PCE$ | **QSPR** | $h_i$ | **ADAN** |
|---|---|---|---|---|---|
| T55[3] |  | 6.44 | 7.26±0.74 | 0.11 | 1,0,1,0,0,0 |
| T56[6] |  | 5.40 | 4.49±0.59 | 0.01 | 0,0,1,0,0,1 |
| T57[30] |  | 6.72 | 4.22±0.41 | 0.03 | 0,0,0,0,1,1 |
| T58[10] |  | 3.88 | 4.12±0.60 | 0.04 | 0,0,0,0,1,1 |

*Table S2: The compatibility matrix for attachment point classes. Each fragment is a small molecule with explicitly modeled attachment points (AP). Each AP is further annotated with a "class" (R#) that contains additional information in the form of dummy atoms used for the identification of compatible bond types. In addition to the 16 classes derived from BRICS cleavage rules, the class "me" is used to refer to the methyl group.*

| **Definition** | **Class** | **Compatible Class** |
|---|---|---|
| C (carbonyl from amides/esters) | R1 | R2,R3,R10 |
| N (amide) | R2 | R12,R14,R16 |
| O (ether/ester) | R3 | R4,R13,R15,R16,me |
| C (alkyl from amines/(thio)ethers) | R4 | R5,R11 |
| N (amine) | R5 | R13,R15,me |
| C (carbonyl from acylated rings) | R6 | R13,R14,R15,R16,me |
| C (olefin) | R7 | R7 |
| C (alkyl from ring substitutions) | R8 | R9,R10,R13,R14,R15,R16 |
| n (aromatic) | R9 | R13,R14,R15,R16,me |
| N (lactame) | R10 | R13,R14,R15,R16,me |
| S (sulfur from thioethers/sulfoxides) | R11 | R13,R14,R15,R16,me |
| S (sulfone from sulfonamides) | R12 | me |
| C ('activated' aliphatic ring C, next to N/O/S) | R13 | R13,R14,R15,R16 |
| c ('activated' aromatic ring c, next to N/O/S) | R14 | R14,R15,R16 |
| C (aliphatic ring C, not next to N/O/S) | R15 | R15,R16 |
| c (aromatic ring c, not next to N/O/S) | R16 | R16 |

*Figure F1: The phenothiazine scaffold to which different fragments are attached as dictated by the compatibility rules.*

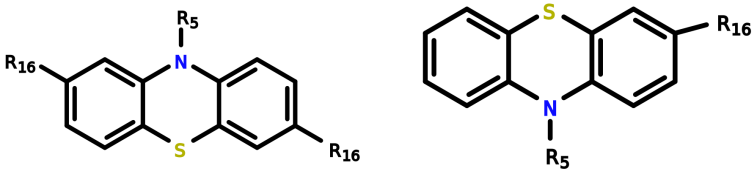
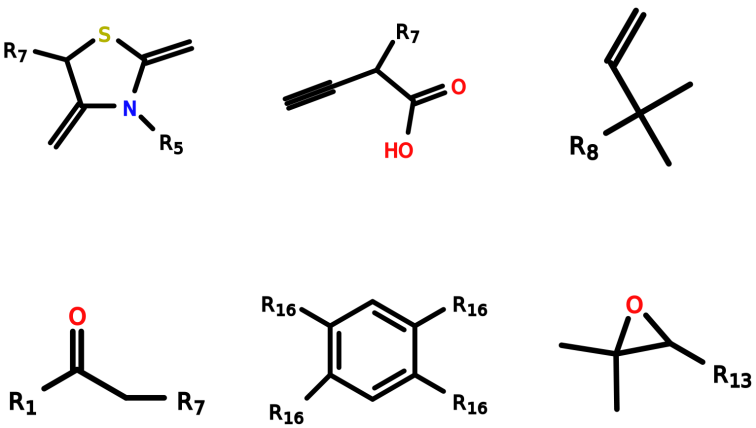



*Figure F2: A subset of the fragments obtained by applying the BRICS rules to existing dyes. The R# correspond to the class of the attachment point. Connecting two fragments with compatible attachment points requires the addition of a single bond (only class R7 has a double bond) between the participating atoms of the respective fragments.*



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