**SUPPORTING INFORMATION**

Bridging Molecular Docking to Molecular Dynamics to Enlighten Recognition Processes of Tailored D-A/D-A-D Types' AIEgens with HSA/BSA

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**Figure S3.** Binding poses and residue interactions of the investigated ligands with HSA (PDB ID: 4L9Q)

**Table S1.** Molecular structures and IUPAC names of the studied photosensitizers

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| **D1A1**  2-(2-(4-(diphenylamino)phenyl)-9H-fluoren-9-ylidene)malononitrile |
| **D1A2**  2-(3-(4-(diphenylamino)phenyl)-5H-cyclopenta[2,1-b:3,4-b']dipyridin-5-ylidene)malononitrile |
| **D2A1**  2-(2-(4-(bis(4-methoxyphenyl)amino)phenyl)-9H-fluoren-9-ylidene)malononitrile |
| **D2A2**  2-(3-(4-(bis(4-methoxyphenyl)amino)phenyl)-5H-cyclopenta[2,1-b:3,4-b']dipyridin-5-ylidene)malononitrile |

**Table S1 *(cont.)*.** Molecular structures and IUPAC names of the studied photosensitizers

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| **D1A1D1**  2-(2,7-bis(4-(diphenylamino)phenyl)-9H-fluoren-9-ylidene)malononitrile |
| **D1A2D1**  2-(3,7-bis(4-(diphenylamino)phenyl)-5H-cyclopenta[2,1-b:3,4-b']dipyridin-5-ylidene)malononitrile |
| **D2A1D2**  2-(2,7-bis(4-(bis(4-methoxyphenyl)amino)phenyl)-9H-fluoren-9-ylidene)malononitrile |
| **D2A2D2**  2-(3,7-bis(4-(bis(4-methoxyphenyl)amino)phenyl)-5H-cyclopenta[2,1-b:3,4-b']dipyridin-5-ylidene)malononitrile |

**Table S2.** Interaction data of the studied ligands with BSA (PDB ID: 4F5S)

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| **Ligands** | **Distance** | **Category** | **Type of Interactions** | **Residue Information** |
| **D1-A1** | 2.69 | HB | C-HB | LYS136 |
| 4.50 | E | Pi-Ca | LYS136 |
| 4.15 | E | Pi-Ca | ARG185 |
| 3.41 | E | Pi-An | GLU125 |
| 3.13 | E | Pi-An | GLU125 |
| 4.87 | Other | Pi-S | MET184 |
| 5.13 | Hyd | Pi-Pi-T-Sh | TYR137 |
| 4.99 | Hyd | Am-Pi-St | MET184, ARG185 |
| 3.72 | Hyd | Pi-Al | LYS136 |
| 5.31 | Hyd | Pi-Al | LEU122 |
| 4.62 | Hyd | Pi-Al | LYS136 |
| 3.72 | Hyd | Pi-Al | LYS136 |
| 4.76 | Hyd | Pi-Al | LEU115 |
| 5.29 | Hyd | Pi-Al | PRO117 |
| 5.24 | Hyd | Pi-Al | LEU115 |
| 4.24 | Hyd | Pi-Al | PRO117 |
| 5.38 | Hyd | Pi-Al | ILE181 |
| 4.04 | Hyd | Pi-Al | ARG185 |
| 5.48 | Hyd | Pi-Al | VAL188 |
| **D1-A2** | 2.92 | HB | CON-HB | LYS116 |
| 2.40 | HB | CON-HB | ASP118 |
| 2.78 | HB | C-HB | LEU115 |
| 3.78 | E | Pi-Ca | LYS132 |
| 3.49 | E | Pi-Ca | LYS136 |
| 3.30 | HB; E | Pi-Ca; Pi-Do HB | LYS136 |
| 3.16 | E | Pi-An | GLU125 |
| 5.81 | Hyd | Pi-Pi-St | TYR160 |
| 4.45 | Hyd | Pi-Al | LEU115 |
| 4.84 | Hyd | Pi-Al | LEU122 |
| 5.42 | Hyd | Pi-Al | LEU122 |
| 4.60 | Hyd | Pi-Al | LYS136 |
| 4.13 | Hyd | Pi-Al | LEU115 |
| 4.88 | Hyd | Pi-Al | PRO117 |
| 4.19 | Hyd | Pi-Al | LYS136 |
| **D2-A1** | 4.89 | E | Pi-An | GLU424 |
| 3.91 | E | Pi-An | GLU424 |
| 3.96 | E | Pi-An | GLU424 |
| 3.86 | Hyd | Al | ALA193 |
| 5.12 | Hyd | Pi-Al | PRO420 |
| 5.23 | Hyd | Pi-Al | ILE522 |
| 5.21 | Hyd | Pi-Al | VAL423 |
| 4.46 | Hyd | Pi-Al | ILE522 |
| 4.14 | Hyd | Pi-Al | PRO420 |
| 4.69 | Hyd | Pi-Al | LEU189 |
| 4.83 | Hyd | Pi-Al | LEU189 |
| **D2-A2** | 2.73 | HB; E | Pi-Ca; Pi-Do HB | LYS116 |
| 3.07 | E | Pi-An | GLU125 |
| 4.60 | Hyd | Al | LYS132 |
| 5.09 | Hyd | Al | LEU115 |
| 4.91 | Hyd | Pi-Al | TYR137 |
| 5.38 | Hyd | Pi-Al | LEU115 |
| 5.46 | Hyd | Pi-Al | LEU122 |
| 3.65 | Hyd | Pi-Al | LYS136 |
| 4.43 | Hyd | Pi-Al | LEU115 |
| ***Abbreviations:*** Hydrophobic: Hyd, Electrostatic: E, Hydrogen Bond: HB, Conventional Hydrogen Bond: CON-HB, Carbon Hydrogen Bond: C-HB, Pi- Cation: Pi-Ca, Pi-Anion: Pi-An, Pi-Donor: Pi-Do, Alkyl: Al, Pi-Alkyl: Pi-Al, Pi-Pi T-Shaped: Pi-Pi T, Pi-Pi Stacked: Pi-Pi-St, Pi-Sulfur: Pi-S, Pi-Sigma: Pi-  Sg, Amide-Pi Stacked: Am-Pi-St | | | | |

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| **Ligands** | **Distance** | **Category** | **Type of Interactions** | **Residue Information** |
| **D1-A2-D1** | 2.93 | HB | CON-HB | LYS294 |
| 3.43 | E | Pi-Ca | ARG217 |
| 4.00 | E | Pi-Ca | LYS294 |
| 3.65 | E | Pi-Ca | LYS294 |
| 4.16 | Hyd | Pi-Al | ALA290 |
| 5.30 | Hyd | Pi-Al | LYS187 |
| **D2-A1-D2** | 3.63 | HB | C-HB | GLU182 |
| 4.86 | E | Pi-Ca | LYS114 |
| 4.90 | E | Pi-An | GLU424 |
| 4.24 | E | Pi-An | GLU424 |
| 4.48 | E | Pi-An | GLU424 |
| 2.65 | Hyd | Pi-Sg | LEU189 |
| 2.84 | Hyd | Pi-Sg | ILE522 |
| 4.03 | Hyd | Al | ARG185 |
| 4.08 | Hyd | Al | LYS504 |
| 4.77 | Hyd | Pi-Al | HIS145 |
| 5.13 | Hyd | Pi-Al | VAL423 |
| 5.10 | Hyd | Pi-Al | PRO420 |
| 5.28 | Hyd | Pi-Al | VAL423 |
| 4.88 | Hyd | Pi-Al | ILE522 |
| 4.08 | Hyd | Pi-Al | PRO420 |
| 4.92 | Hyd | Pi-Al | VAL423 |
| 4.69 | Hyd | Pi-Al | LEU189 |
| 5.03 | Hyd | Pi-Al | PRO420 |
| ***Abbreviations:*** Hydrophobic: Hyd, Electrostatic: E, Hydrogen Bond: HB, Conventional Hydrogen Bond: CON-HB, Carbon Hydrogen Bond: C-HB, Pi-Cation: Pi-Ca, Pi-Anion: Pi-An, Pi-Donor: Pi-Do, Alkyl: Al, Pi-Alkyl: Pi- Al, Pi-Pi T-Shaped: Pi-Pi T, Pi-Pi Stacked: Pi-Pi-St, Pi-Sulfur: Pi-S, Pi-  Sigma: Pi-Sg, Amide-Pi Stacked: Am-Pi-St | | | | |

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| **Ligands** | **Distance** | **Category** | **Type of Interactions** | **Residue Information** |
| **D2-A2-D2** | 2.91 | HB | C-HB | THR526 |
| 3.58 | HB | C-HB | LEU189 |
| 3.54 | HB | C-HB | GLU182 |
| 4.54 | E | Pi-Ca | LYS114 |
| 5.00 | E | Pi-An | GLU424 |
| 4.80 | E | Pi-An | GLU424 |
| 2.65 | Hyd | Pi-Sg | LEU189 |
| 2.72 | Hyd | Pi-Sg | ILE522 |
| 3.91 | Hyd | Al | ALA193 |
| 4.87 | Hyd | Al | LEU189 |
| 4.46 | Hyd | Al | ARG185 |
| 5.09 | Hyd | Pi-Al | VAL423 |
| 5.22 | Hyd | Pi-Al | PRO420 |
| 5.31 | Hyd | Pi-Al | VAL423 |
| 4.80 | Hyd | Pi-Al | ILE522 |
| 4.15 | Hyd | Pi-Al | PRO420 |
| 4.94 | Hyd | Pi-Al | VAL423 |
| 4.87 | Hyd | Pi-Al | LEU189 |
| 4.92 | Hyd | Pi-Al | PRO420 |
| ***Abbreviations:*** Hydrophobic: Hyd, Electrostatic: E, Hydrogen Bond: HB, Conventional Hydrogen Bond: CON-HB, Carbon Hydrogen Bond: C-HB, Pi-Cation: Pi-Ca, Pi-Anion: Pi-An, Pi-Donor: Pi-Do, Alkyl: Al, Pi-Alkyl: Pi-Al, Pi-Pi T-Shaped: Pi-Pi T, Pi-Pi Stacked: Pi-Pi-St, Pi-  Sulfur: Pi-S, Pi-Sigma: Pi-Sg, Amide-Pi Stacked: Am-Pi-St | | | | |

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| **Ligands** | **Distance** | **Category** | **Type of Interactions** | **Residue Information** |
| **D1-A2** | 2.20 | HB | CON-HB | TYR160 |
| 2.61 | HB | C-HB | PHE133 |
| 4.65 | E | Pi-Ca | LYS136 |
| 5.84 | Other | Pi-S | MET122 |
| 5.27 | Hyd | Pi-Al | LEU114 |
| 5.13 | Hyd | Pi-Al | PRO117 |
| 4.99 | Hyd | Pi-Al | LYS136 |
| 5.24 | Hyd | Pi-Al | LYS136 |
| 4.92 | Hyd | Pi-Al | LEU114 |
| 5.46 | Hyd | Pi-Al | LEU181 |
| 4.47 | Hyd | Pi-Al | ARG185 |
| 4.34 | Hyd | Pi-Al | ARG185 |
| **D2-A1** | 2.56 | HB | CON-HB | ARG116 |
| 2.55 | HB | C-HB | PRO117 |
| 2.44 | HB | C-HB | GLY188 |
| 4.15 | HB; E | Pi-Ca; Pi-Do, HB | ARG185 |
| 5.23 | Hyd | Pi-Pi-St | PHE133 |
| 5.28 | Hyd | Pi-Pi-St | PHE133 |
| 5.32 | Hyd | Pi-Pi-St | PHE133 |
| 5.65 | Hyd | Pi-Pi-T-Sh | TYR137 |
| 3.89 | Hyd | Al | ILE141 |
| 4.06 | Hyd | Pi-Al | HIS145 |
| 5.08 | Hyd | Pi-Al | PHE148 |
| 5.13 | Hyd | Pi-Al | LYS136 |
| 4.43 | Hyd | Pi-Al | LYS136 |
| 4.03 | Hyd | Pi-Al | LYS136 |
| 4.86 | Hyd | Pi-Al | ILE141 |
| 4.00 | Hyd | Pi-Al | ARG185 |
| 4.04 | Hyd | Pi-Al | ARG185 |
| ***Abbreviations:*** Hydrophobic: Hyd, Electrostatic: E, Hydrogen Bond: HB, Conventional Hydrogen Bond: CON-HB, Carbon Hydrogen Bond: C-HB, Pi- Cation: Pi-Ca, Pi-Anion: Pi-An, Pi-Donor: Pi-Do, Alkyl: Al, Pi-Alkyl: Pi-Al, Pi-Pi T-Shaped: Pi-Pi T, Pi-Pi Stacked: Pi-Pi-St, Pi-Sulfur: Pi-S, Pi-Sigma: Pi-  Sg, Amide-Pi Stacked: Am-Pi-St | | | | |

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| **Ligands** | **Distance** | **Category** | **Type of Interactions** | **Residue Information** |
| **D2-A2** | 2.77 | HB | CON-HB | ARG221 |
| 2.25 | HB | CON-HB | ARG221 |
| 4.17 | E | Pi-Ca | LYS194 |
| 4.19 | E | Pi-Ca | LYS194 |
| 4.21 | E | Pi-An | ASP450 |
| 4.66 | Hyd | Pi-Pi-St | TYR451 |
| 4.57 | Hyd | Al | LYS189 |
| 5.37 | Hyd | Al | LYS431 |
| 5.39 | Hyd | Pi-Al | LYS194 |
| 4.52 | Hyd | Pi-Al | LYS194 |
| 5.29 | Hyd | Pi-Al | VAL342 |
| 5.10 | Hyd | Pi-Al | ALA190 |
| 3.87 | Hyd | Pi-Al | LYS435 |
| 4.55 | Hyd | Pi-Al | ALA190 |
| 5.42 | Hyd | Pi-Al | LYS431 |
| 5.18 | Hyd | Pi-Al | LYS435 |
| **D1-A1-D1** | 2.52 | HB | C-HB | MET122 |
| 4.24 | E | Pi-Ca | ARG185 |
| 3.55 | E | Pi-An | ASP128 |
| 4.32 | Hyd | Pi-Pi-St | PHE133 |
| 5.29 | Hyd | Pi-Pi-St | PHE133 |
| 4.58 | Hyd | Pi-Pi-St | PHE133 |
| 5.30 | Hyd | Pi-Pi-T-Sh | TYR137 |
| 4.88 | Hyd | Pi-Al | ALA125 |
| 4.62 | Hyd | Pi-Al | LYS136 |
| 4.48 | Hyd | Pi-Al | LYS136 |
| 4.24 | Hyd | Pi-Al | ALA125 |
| 4.82 | Hyd | Pi-Al | LYS136 |
| 5.26 | Hyd | Pi-Al | LEU181 |
| 4.85 | Hyd | Pi-Al | ARG185 |
| 5.19 | Hyd | Pi-Al | LEU114 |
| 4.65 | Hyd | Pi-Al | ARG116 |
| 5.13 | Hyd | Pi-Al | ALA125 |
| ***Abbreviations:*** Hydrophobic: Hyd, Electrostatic: E, Hydrogen Bond: HB, Conventional Hydrogen Bond: CON-HB, Carbon Hydrogen Bond: C-HB, Pi-Cation: Pi-Ca, Pi-Anion: Pi-An, Pi-Donor: Pi-Do, Alkyl: Al, Pi-Alkyl: Pi-Al, Pi-Pi T-Shaped: Pi-Pi T, Pi-Pi Stacked: Pi-Pi-St, Pi-  Sulfur: Pi-S, Pi-Sigma: Pi-Sg, Amide-Pi Stacked: Am-Pi-St | | | | |

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| **Ligands** | **Distance** | **Category** | **Type of Interactions** | **Residue Information** |
| **D1-A2-D1** | 2.46 | HB | C-HB | MET122 |
| 1.86 | HB | C-HB | PHE133 |
| 4.18 | E | Pi-Ca | ARG185 |
| 5.73 | Hyd | Pi-Pi-St | TYR160 |
| 5.08 | Hyd | Pi-Al | ALA125 |
| 4.53 | Hyd | Pi-Al | LYS136 |
| 4.48 | Hyd | Pi-Al | LYS136 |
| 4.37 | Hyd | Pi-Al | ALA125 |
| 4.59 | Hyd | Pi-Al | LYS136 |
| 4.86 | Hyd | Pi-Al | ARG116 |
| 5.24 | Hyd | Pi-Al | LEU181 |
| 5.36 | Hyd | Pi-Al | LEU114 |
| 5.11 | Hyd | Pi-Al | ILE141 |
| 5.10 | Hyd | Pi-Al | ARG185 |
| 4.89 | Hyd | Pi-Al | ALA125 |
| **D2-A1-D2** | 2.33 | HB | C-HB | ARG116 |
| 2.68 | HB | C-HB | PRO117 |
| 3.40 | E | Pi-Ca | ARG185 |
| 4.55 | E | Pi-An | ASP128 |
| 5.04 | Hyd | Pi-Pi-St | PHE133 |
| 5.02 | Hyd | Pi-Pi-St | PHE133 |
| 5.03 | Hyd | Pi-Pi-St | PHE133 |
| 3.75 | Hyd | Al | ILE141 |
| 4.35 | Hyd | Pi-Al | HIS145 |
| 5.19 | Hyd | Pi-Al | PHE148 |
| 4.81 | Hyd | Pi-Al | LYS136 |
| 4.21 | Hyd | Pi-Al | LYS136 |
| 4.08 | Hyd | Pi-Al | LYS136 |
| 5.18 | Hyd | Pi-Al | LEU114 |
| 4.91 | Hyd | Pi-Al | ILE141 |
| 4.10 | Hyd | Pi-Al | ARG185 |
| 4.96 | Hyd | Pi-Al | ARG185 |
| 5.03 | Hyd | Pi-Al | ALA125 |
| ***Abbreviations:*** Hydrophobic: Hyd, Electrostatic: E, Hydrogen Bond: HB, Conventional Hydrogen Bond: CON-HB, Carbon Hydrogen Bond: C-HB, Pi-Cation: Pi-Ca, Pi-Anion: Pi-An, Pi-Donor: Pi-Do, Alkyl: Al, Pi-Alkyl:  Pi-Al, Pi-Pi T-Shaped: Pi-Pi T, Pi-Pi Stacked: Pi-Pi-St, Pi-Sulfur: Pi-S, Pi- Sigma: Pi-Sg, Amide-Pi Stacked: Am-Pi-St | | | | |

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| **Ligands** | **Distance** | **Category** | **Type of Interactions** | **Residue Information** |
| **D2-A2-D2** | 2.25 | HB | CON-HB | MET297 |
| 2.69 | HB | C-HB | GLU293 |
| 2.81 | HB | C-HB | CYS447 |
| 3.54 | HB | C-HB | GLU291 |
| 4.35 | E | Pi-An | GLU187 |
| 3.34 | HB | Pi-Do, HB | ASN294 |
| 3.88 | Hyd | Al | ALA442 |
| 5.37 | Hyd | Al | MET297 |
| 4.83 | Hyd | Pi-Al | ALA190 |
| 4.90 | Hyd | Pi-Al | PRO338 |
| 4.95 | Hyd | Pi-Al | LYS443 |
| 5.39 | Hyd | Pi-Al | PRO338 |
| 5.43 | Hyd | Pi-Al | ALA442 |
| 5.48 | Hyd | Pi-Al | MET297 |
| 5.11 | Hyd | Pi-Al | PRO338 |
| ***Abbreviations:*** Hydrophobic: Hyd, Electrostatic: E, Hydrogen Bond: HB, Conventional Hydrogen Bond: CON-HB, Carbon Hydrogen Bond: C-HB, Pi-Cation: Pi-Ca, Pi-Anion: Pi-An, Pi-Donor: Pi-Do, Alkyl: Al, Pi-Alkyl: Pi-Al, Pi-Pi T-Shaped: Pi-Pi T, Pi-Pi Stacked: Pi-Pi-St, Pi-  Sulfur: Pi-S, Pi-Sigma: Pi-Sg, Amide-Pi Stacked: Am-Pi-St | | | | |

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| **D1A2** | **D2A1** | **D2A2** |
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| **D1A1D1** | **D1A2D1** | **D2A1D2** |
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|  | **D2A2D2** |  |

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| **D1-A1 (binding score: -9.10 kcal/mol || binding domain: IB)** |
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| **D1-A2 (binding score: -11.40 kcal/mol || binding domain: IA & IB)** |
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| **D2-A1 (binding score: -8.90 kcal/mol || binding domain: IB & IIIA)** |
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| **D2-A2 (binding score: -8.50 kcal/mol || binding domain: IB)** |
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| **D1-A2-D1 (binding score: -10.90 kcal/mol || binding domain: IB & IIIA)** |
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| **D2-A1-D2 (binding score: -8.80 kcal/mol || binding domain: IB & IIIA & IIIB)** |
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| **D2-A2-D2 (binding score: -8.50 kcal/mol || binding domain: IB & IIIA & IIIB)** |
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| **D1-A2 (binding score: -9.90 kcal/mol || binding domain: IB)** |
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| **D2-A1 (binding score: -10.00 kcal/mol || binding domain: IB)** |
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| **D2-A2 (binding score: -9.40 kcal/mol || binding domain: IB & IIIA)** |
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| **D1-A1-D1 (binding score: -10.10 kcal/mol || binding domain: IB)** |
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| **D1-A2-D1 (binding score: -9.70 kcal/mol || binding domain: IB)** |
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| **D2-A1-D2 (binding score: -8.80 kcal/mol || binding domain: IB)** |
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| **D2-A2-D2 (binding score: -8.40 kcal/mol || binding domain: IB & IIIA)** |
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