*Electronic Supplementary Information for*

# Design of potential singlet fission chromophores based on diketofurofuran: an alternative to diketopyrrolopyrrole

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Because of the donor-acceptor-donor structures for all the compounds, different functionals were used to evaluate the effect of charge-transfer character on SF relevant excited states. These functionals include B3LYP, CAM-B3LYP, ωB97XD, M06-2X and tuned LC-BLYP. The solvation effects were evaluated by polarizable continuum model (PCM) with toluene and chloroform used as solvents. Compared to available experimental results, the functional CAM-B3LYP, ωB97XD, M06-2X and tuned LC-BLYP overestimate $E(S_1)_v$ and give larger $E(S_1)$ simultaneously (Table S1). The range separating parameters μ were tuned for DFF derivatives (Table S2) with Quantum program optDFTw.[a] The functional CAM-B3LYP and ωB97XD show similar results and larger $E(T_1)$ than the functional B3LYP. The calculated $E(S_1)_v$ with functional B3LYP are more close to the experimental values for both ***1*B-DFF** and **Br-1F-DFF**.[b] Moreover, the basis set was extended to larger basis set, including 6-311G** and cc-pVTZ. The calculated results show that solvation effects affect the SF relevant excited state energies (Table S3), while the excitation energies are insensitive to the extension of basis set (Table S4).

Singlet fission is an intrinsically multi-molecular process, and electronic coupling among adjacent molecules may affect the SF relevant excited energies. We took four dimers in which the two monomer units show different distances and relative orientations in 1B-DFF crystal. We calculated $E(S_1)_v$ and $E(T_1)_v$ for these dimers at the theoretical level of ωB97xd/6-311G* based on the original geometries without optimizations. Due to electronic coupling, $S_1$ state in the monomer splits into a higher and a lower excited states in dimers. Compared to 1B-DFF monomer, the energy shift caused by molecular interactions is rather small (Table S5). The maximum energy shifts are ~0.09 eV for $E(S_1)_v$ and ~ 0.03 eV for $E(T_1)$v. Likewise, in a covalent TDPP dimer with H-aggregate character, the energy difference of $S_1$ state between monomer and dimer is only 0.03 eV.[c] It is reasonable that molecular interactions make negligible effect on SF relevant excited energies in DFF dimers. In addition, the functional ωB97XD was also used to obtain the relaxed geometries of $S_1$, $T_1$ and $T_2$ states of αMeO-1F-DFF and α$Me_2$N-1F-DFF in toluene. Changing from B3LYP to ωB97XD, there exists negligible variations in bond length (< 0.007 Å) and dihedral angles (< 0.3°) (Fig. 1S, Table S6). As a result, it is reasonable to evaluate SF feasibility of DFF derivatives at the theoretical level of B3LYP/6-311G*.

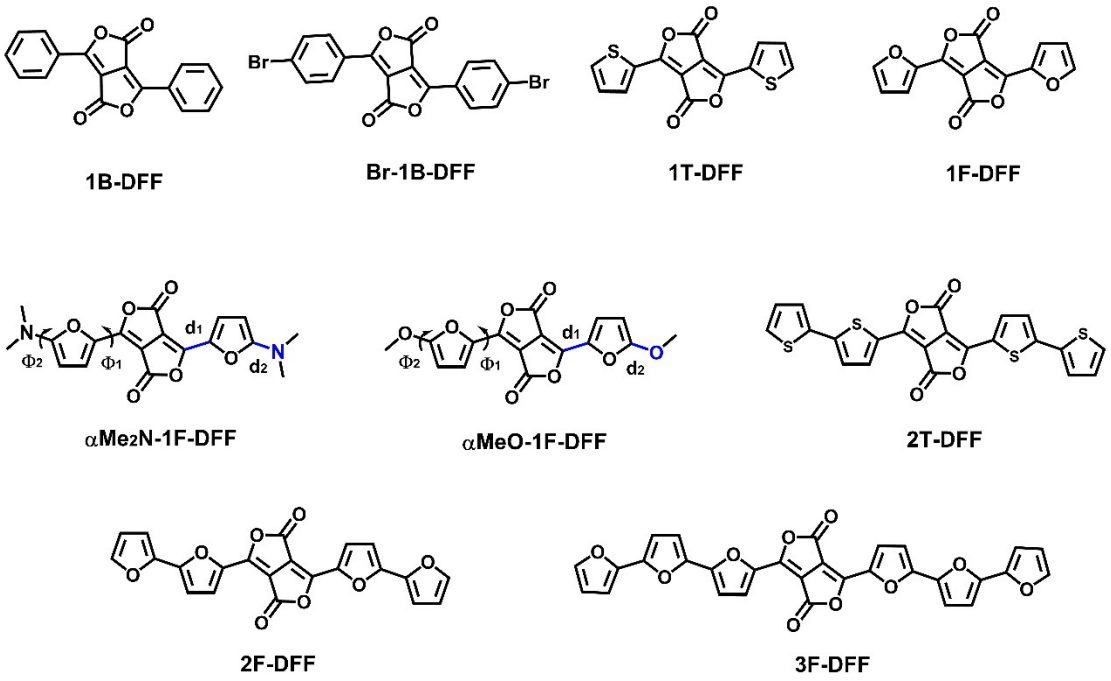


Fig. S1 Molecular structures of the involved molecules for test.

**Table S1** Vertical and adiabatic excitation energies with different functionals in toluene.

| | | B3LYP | Cam-B3LYP | M06-2X | ωB97XD | Tuned-LC-BLYP[1] | Exp[b] |
|---|---|---|---|---|---|---|---|
| ***1*B-DFF** | $E(S_1)_v$ | 2.720 | 3.051 | 3.055 | 3.062 | 2.849 | 2.725 |
| | $E(S_1)$ | 2.548 | 2.804 | 2.808 | 2.815 | | |
| | $E(T_1)$ | 1.385 | 1.419 | 1.599 | 1.457 | | |
| | $E(T_2)_v$ | 2.739 | 2.808 | 3.115 | 2.902 | | |
| | $E(T_2)$ | 2.529 | 2.600 | 2.862 | 2.692 | | |
| **Br-*1*B-DFF** | $E(S_1)_v$ | 2.610 | 2.888 | 2.968 | 2.994 | 2.743 | 2.638 |
| | $E(S_1)$ | 2.447 | 2.726 | 2.722 | 2.743 | | |
| | $E(T_1)$ | 1.355 | 1.394 | 1.572 | 1.433 | | |
| | $E(T_2)_v$ | 2.674 | 2.647 | 3.055 | 2.845 | | |
| | $E(T_2)$ | 2.481 | 2.554 | 2.819 | 2.643 | | |
| ***1*F-DFF** | $E(S_1)_v$ | 2.565 | 2.853 | 2.848 | 2.858 | 2.706 | |
| | $E(S_1)$ | 2.435 | 2.650 | 2.652 | 2.658 | | |
| | $E(T_1)$ | 1.210 | 1.234 | 1.417 | 1.279 | | |
| | $E(T_2)_v$ | 2.476 | 2.545 | 2.816 | 2.615 | | |
| | $E(T_2)$ | 2.284 | 2.327 | 2.593 | 2.405 | | |
| ***1*T-DFF** | $E(S_1)_v$ | 2.519 | 2.836 | 2.833 | 2.850 | 2.656 | |
| | $E(S_1)$ | 2.370 | 2.612 | 2.616 | 2.629 | | |
| | $E(T_1)$ | 1.216 | 1.252 | 1.443 | 1.301 | | |
| | $E(T_2)_v$ | 2.392 | 2.476 | 2.782 | 2.558 | | |
| | $E(T_2)$ | 2.191 | 2.248 | 2.549 | 2.342 | | |
| ***2*T-DFF** | $E(S_1)_v$ | 2.027 | 2.466 | 2.432 | 2.529 | 2.187 | |
| | $E(S_1)$ | 1.880 | 2.209 | 2.195 | 2.266 | | |
| | $E(T_1)$ | 1.000 | 1.092 | 1.262 | 1.162 | | |
| | $E(T_2)_v$ | 1.906 | 2.067 | 2.347 | 2.184 | | |
| | $E(T_2)$ | 1.706 | 1.731 | 2.086 | 1.838 | | |

[1]Calcualted $E(S_1)_v$ based on the optimized $S_0$ geometries at the theoretical level of B3LYP/6-311G*

**Table S2** Tuned range separating parameters μ [bohr$^{-1}$] in LC-BLYP/6-31G* for DPP derivatives with Quantum program optDFTw.

| | ***1*B-DFF** | **Br-*1*B-DFF** | ***1*F-DFF** | ***1*T-DFF** | ***2*T-DFF** |
|---|---|---|---|---|---|
| μ | 0.2160 | 0.2012 | 0.2324 | 0.2181 | 0.1754 |

**Table S3** Solvation effects on $E(S_1)$ and $E(T_1)$ of DFF derivatives (in eV).

| | vacuum | toluene | $CHCl_3$ |
|---|---|---|---|
| ***1*F-DFF** | 2.618/1.211 | 2.435/1.210 | 2.341/1.209 |
| ***2*F-DFF** | 2.181/1.029 | 1.967/1.023 | 1.862 /1.018 |
| ***3*F-DFF** | 1.929/0.970 | 1.725/0.961 | 1.626/0.953 |

**Table S4** Basis set effects on $E(S_1)$ and $E(T_1)$ of DFF derivatives in toluene (in eV).

| | 6-311G* | 6-311G** | cc-pVTZ |
|---|---|---|---|
| ***1*F-DFF** | 2.435/1.210 | 2.433/1.210 | 2.414/1.200 |
| ***2*F-DFF** | 1.967/1.023 | 1.967/1.024 | 1.949/1.012 |
| ***3*F-DFF** | 1.725/0.961 | 1.725/0.961 | 1.709/0.948 |

**Table S5**. Effect of electronic coupling in ***1*B-DFF** dimers on $E(S_1)_v$ and $E(T_1)_v$ in vacuum (oscillator strengths are listed in parentheses) (in eV).

| | Monomer | Dimer1 | Dimer2 | Dimer3 | Dimer4 |
|---|---|---|---|---|---|
| $S_1$ | 3.208(0.750) | 3.160(1.477) | 3.117(0.000) | 3.171(1.635) | 3.192(1.455) |
| $S_2$ | 4.388(0.001) | 3.218(0.071) | 3.227(1.298) | 3.237(0.000) | 3.207(0.083) |
| $S_3$ | 4.473(0.000) | 4.263(0.003) | 4.059(0.030) | 4.382(0.001) | 4.432(0.000) |
| $S_4$ | 4.677(0.000) | 4.318(0.003) | 4.060(0.000) | 4.382(0.000) | 4.434(0.001) |
| $T_1$ | 1.284 | 1.294 | 1.258 | 1.282 | 1.296 |
| $T_2$ | 2.895 | 1.300 | 1.263 | 1.282 | 1.300 |
| $T_3$ | 3.745 | 2.893 | 2.883 | 2.895 | 2.889 |
| $T_4$ | 3.891 | 2.896 | 2.890 | 2.895 | 2.893 |

**Table S6** Bond lengths (Å) and torsion Angles (deg) of along the conjugated backbones of **αMe$_2$N-*1*F-DFF** and **αMeO-*1*F-DFF**.

| | | **αMe$_2$N-*1*F-DFF** | | | | **αMeO-*1*F-DFF** | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | $d_1$ | $d_2$ | $\Phi_1$ | $\Phi_2$ | $d_1$ | $d_2$ | $\Phi_1$ | $\Phi_2$ |
| B3LYP | $S_0$ | 1.405 | 1.353 | -0.582 | -9.176 | 1.412 | 1.321 | 0 | 0 |
| | $S_1$ | 1.392 | 1.351 | -0.193 | -7.524 | 1.393 | 1.318 | 0 | 0 |
| | $T_1$ | 1.384 | 1.352 | -0.316 | -7.959 | 1.386 | 1.320 | 0 | 0 |
| | $T_2$ | 1.378 | 1.347 | -0.126 | -7.208 | 1.381 | 1.317 | 0 | 0 |
| ωB97XD | $S_0$ | 1.409 | 1.352 | -0.535 | -9.298 | 1.416 | 1.316 | 0 | 0 |
| | $S_1$ | 1.388 | 1.345 | 0.090 | -7.366 | 1.390 | 1.311 | 0 | 0 |
| | $T_1$ | 1.379 | 1.350 | -0.249 | -8.019 | 1.383 | 1.315 | 0 | 0 |
| | $T_2$ | 1.383 | 1.344 | 0.131 | -7.109 | 1.385 | 1.311 | 0 | 0 |

**Table S7** Comparisons of the calculated results for **F3B-DFF**, **Pa-DFF** and **3B-DFF**.[1]

| | HOMO | LUMO | HLG | $y_0$ | $y_1$ | $E(S_1)$ | $E(T_1)$ | $E(T_2)$ |
|---|---|---|---|---|---|---|---|---|
| **F*3*B-DFF** | -5.606 | -3.249 | 2.356 | 0.273 | 0.141 | 2.018 | 1.194 | 1.520 |
| **Pa-DFF** | -5.893 | -3.183 | 2.710 | 0.193 | 0.056 | 2.290 | 1.347 | 2.322 |
| ***3*B-DFF** | -5.822 | -3.175 | 2.647 | 0.186 | 0.044 | 2.191 | 1.319 | 2.276 |

[1] Energies are evaluated in toluene (in eV).

**Table S8** Hammett constant ($\sigma_p$) of the introduced terminal substituents.[d]

| | -F | -Cl | -Br | -COOMe | -COOH | -$CF_3$ | -CHO |
|---|---|---|---|---|---|---|---|
| $\sigma_p$ | 0.06 | 0.23 | 0.23 | 0.45 | 0.45 | 0.54 | 0.42 |
| | -CN | -$NO_2$ | -Me | -OH | -OMe | -$NH_2$ | -$NMe_2$ |
| $\sigma_p$ | 0.66 | 0.78 | -0.17 | -0.37 | -0.27 | -0.66 | -0.83 |

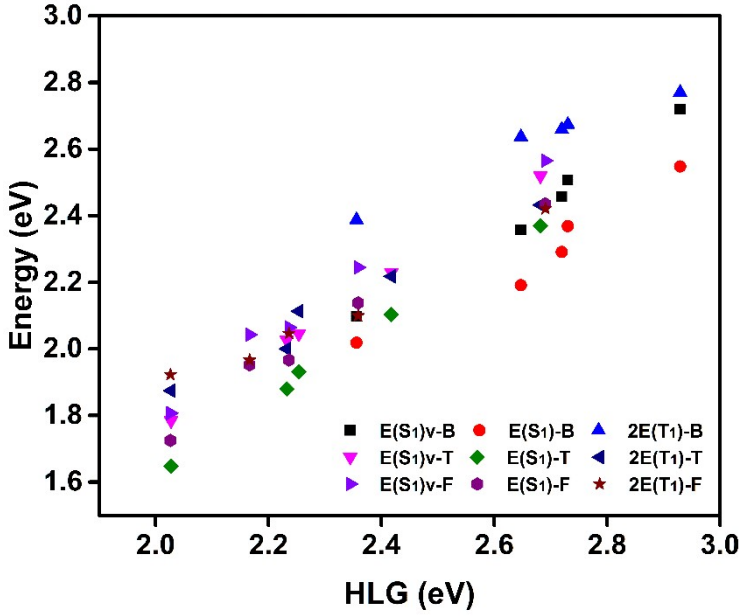


**Fig. S2** $E(S_1)_v$, $E(S_1)$ and $E(T_1)$ as a function of HLG in DFF derivatives with different aromatic substituents in toluene.

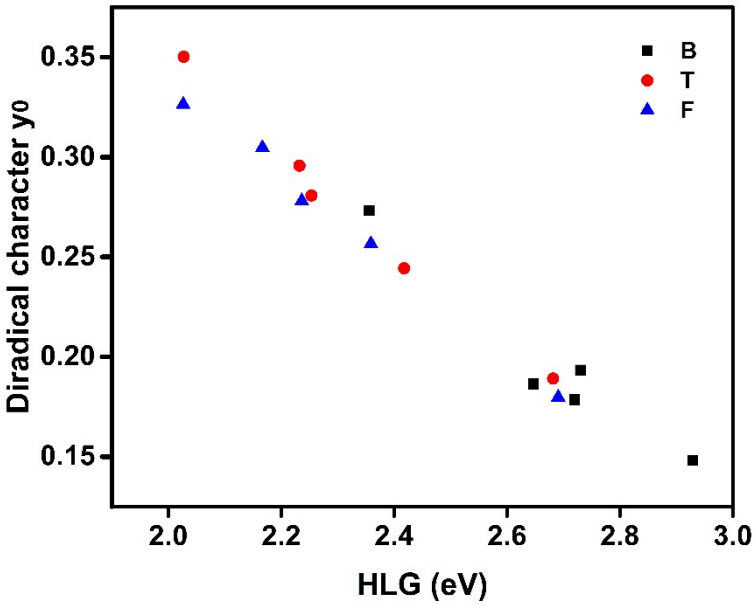


**Fig. S3** Diradical character $y_0$ as a function of HLG in DFF derivatives with different aromatic substituents.

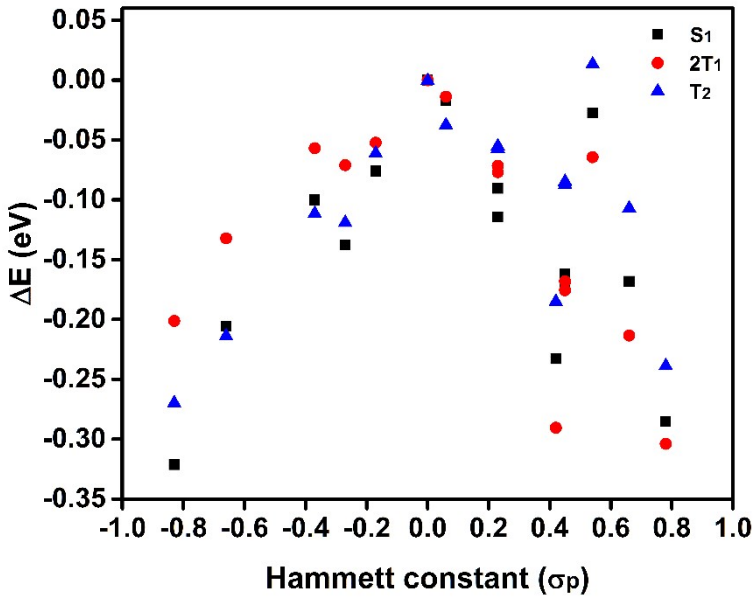


**Fig. S4** Energy differences between 1F-DFF derivatives and the pristine 1F-DFF in $E(S_1)$, $2E(T_1)$ and $E(T_2)$ with respect to the Hammett constant ($\sigma_p$) of the attached terminal substituents in toluene.

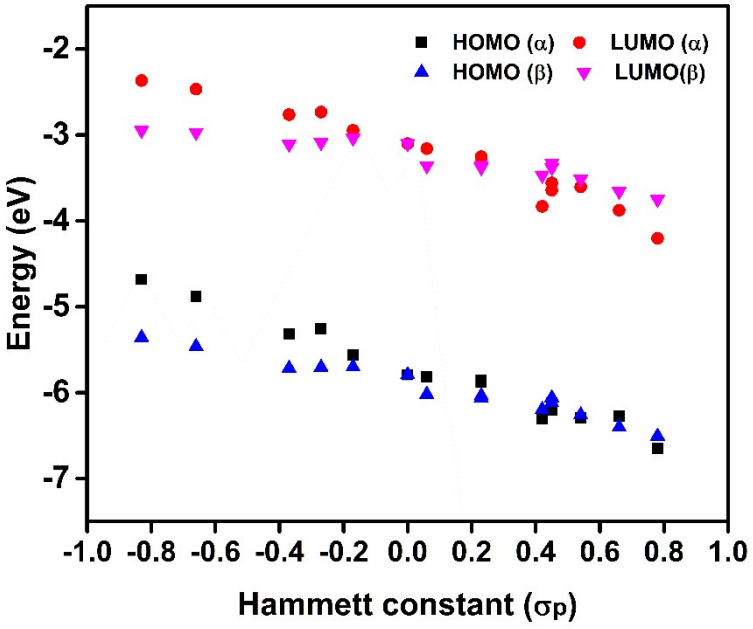


**Fig. S5** HOMO and LUMO energies for α- and β-substitutions in 1F-DFF derivatives with respect to the Hammett constant ($\sigma_p$) of the attached terminal substituents in toluene.

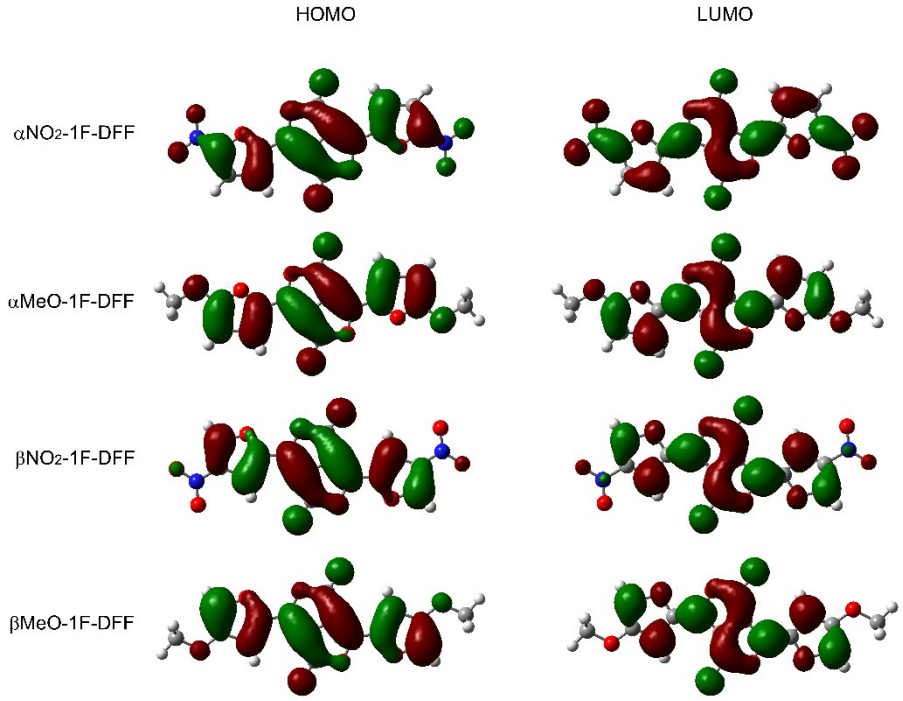


**Fig. S6** Electron density distributions of HOMO and LUMO in $\alpha NO_2$-1F-DFF, αMeO-1F-DFF, $\beta NO_2$-1F-DFF and βMeO-1F-DFF.

**Table S9** HOMO、LUMO energy levels and HOMO-LUMO gap (HLG) values in toluene (in eV), diradical character $y_0$ and tetraradical character $y_1$.

| Compound | HOMO | LUMO | HLG | $y_0$ | $y_1$ | $y_1/y_0$ |
|---|---|---|---|---|---|---|
| 1B-DFF | -6.087 | -3.157 | 2.929 | 0.148 | 0.015 | 0.101 |
| 2B-DFF | -5.886 | -3.167 | 2.720 | 0.179 | 0.031 | 0.172 |
| F2B-DFF | -5.920 | -3.189 | 2.730 | 0.193 | 0.052 | 0.271 |
| 3B-DFF | -5.822 | -3.175 | 2.647 | 0.186 | 0.044 | 0.237 |
| F3B-DFF | -5.605 | -3.249 | 2.356 | 0.273 | 0.141 | 0.515 |
| 1T-DFF | -5.848 | -3.166 | 2.682 | 0.189 | 0.020 | 0.104 |
| 2T-DFF | -5.466 | -3.234 | 2.232 | 0.296 | 0.063 | 0.214 |
| F2T-DFF | -5.634 | -3.216 | 2.418 | 0.244 | 0.035 | 0.143 |
| 3T-DFF | -5.293 | -3.266 | 2.027 | 0.350 | 0.114 | 0.326 |
| F3T-DFF | -5.492 | -3.238 | 2.254 | 0.281 | 0.052 | 0.186 |
| 1F-DFF | -5.792 | -3.101 | 2.691 | 0.180 | 0.015 | 0.086 |
| 2F-DFF | -5.342 | -3.106 | 2.236 | 0.278 | 0.050 | 0.179 |
| F2F-DFF | -5.501 | -3.142 | 2.359 | 0.257 | 0.032 | 0.125 |
| 3F-DFF | -5.141 | -3.115 | 2.026 | 0.326 | 0.093 | 0.285 |
| F3F-DFF | -5.307 | -3.141 | 2.167 | 0.305 | 0.050 | 0.163 |
| 1F-DPP | -5.188 | -2.679 | 2.509 | 0.208 | 0.014 | 0.068 |
| 1F-DTT | -5.819 | -3.179 | 2.640 | 0.206 | 0.018 | 0.088 |
| 1F-DSS | -5.798 | -3.083 | 2.715 | 0.194 | 0.019 | 0.097 |

| Substituents | | HOMO | LUMO | HLG | $y_0$ | $y_1$ | $y_1/y_0$ |
|---|---|---|---|---|---|---|---|
| $-NMe_2$ | α | -4.683 | -2.366 | 2.317 | 0.137 | 0.009 | 0.062 |
| | β | -5.385 | -2.946 | 2.412 | 0.196 | 0.018 | 0.091 |
| $-NH_2$ | α | -4.882 | -2.467 | 2.415 | 0.146 | 0.010 | 0.066 |
| | β | -5.462 | -2.970 | 2.492 | 0.201 | 0.019 | 0.093 |
| -OMe | α | -5.258 | -2.733 | 2.525 | 0.151 | 0.010 | 0.068 |
| | β | -5.704 | -3.087 | 2.617 | 0.187 | 0.016 | 0.086 |
| -OH | α | -5.314 | -2.764 | 2.550 | 0.153 | 0.010 | 0.069 |
| | β | -5.715 | -3.108 | 2.607 | 0.193 | 0.017 | 0.089 |
| -Me | α | -5.558 | -2.946 | 2.612 | 0.180 | 0.015 | 0.084 |
| | β | -5.700 | -3.039 | 2.661 | 0.182 | 0.016 | 0.085 |
| -F | α | -5.815 | -3.158 | 2.656 | 0.167 | 0.013 | 0.076 |
| | β | -6.020 | -3.359 | 2.660 | 0.193 | 0.017 | 0.090 |
| -Cl | α | -5.876 | -3.262 | 2.614 | 0.189 | 0.017 | 0.088 |
| | β | -6.061 | -3.380 | 2.681 | 0.187 | 0.017 | 0.089 |
| -Br | α | -5.853 | -3.253 | 2.600 | 0.191 | 0.017 | 0.089 |
| | β | -6.037 | -3.357 | 2.680 | 0.186 | 0.016 | 0.088 |
| -COOMe | α | -6.118 | -3.558 | 2.559 | 0.209 | 0.021 | 0.100 |
| | β | -6.060 | -3.330 | 2.730 | 0.168 | 0.013 | 0.079 |
| -COOH | α | -6.205 | -3.643 | 2.562 | 0.211 | 0.021 | 0.101 |
| | β | -6.117 | -3.380 | 2.737 | 0.167 | 0.013 | 0.079 |
| $-CF_3$ | α | -6.293 | -3.604 | 2.688 | 0.194 | 0.018 | 0.091 |
| | β | -6.259 | -3.514 | 2.746 | 0.172 | 0.014 | 0.079 |
| -CHO | α | -6.309 | -3.832 | 2.476 | 0.243 | 0.033 | 0.134 |
| | β | -6.195 | -3.468 | 2.728 | 0.180 | 0.017 | 0.095 |
| -CN | α | -6.276 | -3.876 | 2.400 | 0.236 | 0.030 | 0.126 |
| | β | -6.403 | -3.656 | 2.747 | 0.182 | 0.017 | 0.092 |
| $-NO_2$ | α | -6.648 | -4.203 | 2.445 | 0.237 | 0.079 | 0.333 |
| | β | -6.507 | -3.752 | 2.755 | 0.175 | 0.058 | 0.333 |

**Table S10** Vertical excitation energies ($E(S_1)$v and $E(T_2)$v), adiabatic excitation energies ($E(S_1)$, $E(T_1)$ and $E(T_2)$) and the corresponding $\Delta E_{SF(v)}$, $\Delta E_{SF}$, $\Delta E_{TTA(v)}$, $\Delta E_{TTA}$ in toluene. (in eV).

| | $E(S_1)$v | $E(S_1)$ | $E(T_2)$v | $E(T_2)$ | $E(T_1)$ | $\Delta E_{SF(v)}$ | $\Delta E_{SF}$ | $\Delta E_{TTA(v)}$ | $\Delta E_{TTA.}$ |
|---|---|---|---|---|---|---|---|---|---|
| *1*B-DFF | 2.720 | 2.548 | 2.739 | 2.529 | 1.385 | -0.050 | -0.223 | -0.031 | -0.241 |
| *2*B-DFF | 2.457 | 2.291 | 2.542 | 2.368 | 1.330 | -0.203 | -0.369 | -0.117 | -0.292 |
| F*2*B-DFF | 2.507 | 2.369 | 2.306 | 2.190 | 1.337 | -0.168 | -0.305 | -0.368 | -0.484 |
| *3*B-DFF | 2.357 | 2.191 | 2.445 | 2.276 | 1.319 | -0.280 | -0.446 | -0.192 | -0.362 |
| F*3*B-DFF | 2.098 | 2.018 | 1.633 | 1.520 | 1.194 | -0.290 | -0.369 | -0.755 | -0.867 |
| *1*T-DFF | 2.519 | 2.370 | 2.392 | 2.191 | 1.216 | 0.087 | -0.062 | -0.040 | -0.241 |
| *2*T-DFF | 2.027 | 1.880 | 1.906 | 1.706 | 1.000 | 0.026 | -0.120 | -0.095 | -0.294 |
| F*2*T-DFF | 2.229 | 2.103 | 2.150 | 1.994 | 1.109 | 0.011 | -0.115 | -0.068 | -0.225 |
| *3*T-DFF | 1.785 | 1.648 | 1.650 | 1.452 | 0.937 | -0.090 | -0.227 | -0.225 | -0.423 |
| F*3*T-DFF | 2.045 | 1.931 | 2.005 | 1.868 | 1.057 | -0.068 | -0.182 | -0.108 | -0.245 |
| *1*F-DFF | 2.565 | 2.435 | 2.476 | 2.284 | 1.210 | 0.144 | 0.014 | 0.056 | -0.137 |
| *2*F-DFF | 2.064 | 1.967 | 2.004 | 1.881 | 1.023 | 0.018 | -0.080 | -0.042 | -0.165 |
| F*2*F-DFF | 2.245 | 2.138 | 2.155 | 2.004 | 1.050 | 0.145 | 0.039 | 0.056 | -0.096 |
| *3*F-DFF | 1.807 | 1.725 | 1.736 | 1.634 | 0.961 | -0.116 | -0.197 | -0.187 | -0.288 |
| F*3*F-DFF | 2.043 | 1.952 | 1.980 | 1.862 | 0.983 | 0.077 | -0.014 | 0.014 | -0.104 |
| *1*F-DPP | 2.362 | 2.236 | 2.636 | 2.487 | 1.053 | 0.256 | 0.129 | 0.529 | 0.380 |
| *1*F-DTT | 2.470 | 2.346 | 2.354 | 2.180 | 1.202 | 0.066 | -0.058 | -0.050 | -0.224 |
| *1*F-DSS | 2.503 | 2.372 | 2.336 | 2.163 | 1.273 | -0.043 | -0.174 | -0.210 | -0.383 |

| | | $E(S_1)$v | $E(S_1)$ | $E(T_2)$v | $E(T_2)$ | $E(T_1)$ | $\Delta E_{SF(v)}$ | $\Delta E_{SF}$ | $\Delta E_{TTA(v)}$ | $\Delta E_{TTA.}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| -$NMe_2$ | α | 2.184 | 2.114 | 2.146 | 2.014 | 1.110 | -0.036 | -0.106 | -0.073 | -0.206 |
| | β | 2.230 | 2.127 | 1.934 | 1.765 | 1.014 | 0.022 | -0.081 | -0.274 | -0.444 |
| -$NH_2$ | α | 2.310 | 2.229 | 2.223 | 2.070 | 1.144 | 0.021 | -0.060 | -0.066 | -0.219 |
| | β | 2.374 | 2.291 | 2.138 | 1.979 | 1.121 | 0.132 | 0.049 | -0.105 | -0.263 |
| -OMe | α | 2.397 | 2.297 | 2.339 | 2.165 | 1.175 | 0.047 | -0.053 | -0.011 | -0.185 |
| | β | 2.490 | 2.379 | 2.386 | 2.241 | 1.180 | 0.130 | 0.019 | 0.026 | -0.119 |
| -OH | α | 2.438 | 2.335 | 2.351 | 2.172 | 1.182 | 0.073 | -0.029 | -0.013 | -0.192 |
| | β | 2.495 | 2.383 | 2.372 | 2.221 | 1.167 | 0.161 | 0.049 | 0.037 | -0.113 |
| -Me | α | 2.478 | 2.359 | 2.405 | 2.223 | 1.184 | 0.109 | -0.010 | 0.036 | -0.146 |
| | β | 2.527 | 2.404 | 2.456 | 2.271 | 1.201 | 0.124 | 0.001 | 0.053 | -0.132 |
| -F | α | 2.541 | 2.418 | 2.445 | 2.246 | 1.204 | 0.134 | 0.011 | 0.038 | -0.161 |
| | β | 2.548 | 2.418 | 2.453 | 2.267 | 1.182 | 0.184 | 0.055 | 0.089 | -0.096 |
| -Cl | α | 2.471 | 2.344 | 2.417 | 2.229 | 1.175 | 0.121 | -0.005 | 0.067 | -0.121 |
| | β | 2.540 | 2.408 | 2.475 | 2.287 | 1.196 | 0.149 | 0.017 | 0.083 | -0.105 |
| -Br | α | 2.445 | 2.321 | 2.411 | 2.227 | 1.172 | 0.101 | -0.023 | 0.067 | -0.117 |
| | β | 2.532 | 2.401 | 2.474 | 2.287 | 1.197 | 0.137 | 0.006 | 0.079 | -0.108 |
| -COOMe | α | 2.410 | 2.265 | 2.372 | 2.197 | 1.126 | 0.157 | 0.013 | 0.119 | -0.056 |
| | β | 2.575 | 2.436 | 2.529 | 2.328 | 1.228 | 0.118 | -0.021 | 0.072 | -0.129 |
| -COOH | α | 2.419 | 2.273 | 2.374 | 2.199 | 1.123 | 0.174 | 0.027 | 0.129 | -0.046 |
| | β | 2.583 | 2.443 | 2.538 | 2.335 | 1.229 | 0.124 | -0.016 | 0.079 | -0.124 |
| -$CF_3$ | α | 2.555 | 2.408 | 2.494 | 2.297 | 1.178 | 0.198 | 0.051 | 0.137 | -0.059 |
| | β | 2.604 | 2.460 | 2.555 | 2.348 | 1.224 | 0.156 | 0.012 | 0.107 | -0.099 |
| -CHO | α | 2.346 | 2.202 | 2.258 | 2.099 | 1.065 | 0.215 | 0.072 | 0.127 | -0.032 |
| | β | 2.572 | 2.432 | 2.508 | 2.314 | 1.225 | 0.123 | -0.018 | 0.059 | -0.135 |
| -CN | α | 2.414 | 2.267 | 2.348 | 2.177 | 1.104 | 0.206 | 0.059 | 0.140 | -0.031 |
| | β | 2.588 | 2.440 | 2.553 | 2.350 | 1.223 | 0.142 | -0.006 | 0.107 | -0.096 |
| -$NO_2$ | α | 2.299 | 2.150 | 2.214 | 2.045 | 1.059 | 0.182 | 0.033 | 0.097 | -0.072 |
| | β | 2.590 | 2.435 | 2.562 | 2.360 | 1.222 | 0.146 | -0.009 | 0.118 | -0.084 |

**Coordinates of the four dimers.**

Dimer 1

| | | | |
|---|---|---|---|
| O | 0.51230000 | 6.25870000 | 8.25060000 |
| O | 1.59510000 | 8.12320000 | 8.93380000 |
| C | 0.65150000 | 7.66590000 | 8.33940000 |
| C | -0.48810000 | 8.20270000 | 7.63320000 |
| C | -0.63420000 | 5.93140000 | 7.54440000 |
| C | -0.94050000 | 4.53500000 | 7.39260000 |
| C | -2.11810000 | 4.12810000 | 6.80340000 |
| C | -2.42590000 | 2.81280000 | 6.65980000 |
| C | -1.51650000 | 1.87360000 | 7.11210000 |
| C | -0.34470000 | 2.23610000 | 7.67690000 |
| C | -0.04500000 | 3.57290000 | 7.82570000 |
| H | -2.71930000 | 4.71090000 | 6.53620000 |
| H | -3.24290000 | 2.64600000 | 6.32150000 |
| H | -1.70490000 | 1.28480000 | 6.95070000 |
| H | 0.22870000 | 1.72830000 | 7.95000000 |
| H | 0.74050000 | 3.79320000 | 8.21650000 |
| C | -1.24840000 | 7.09230000 | 7.17130000 |
| C | -1.10230000 | 9.36360000 | 7.26010000 |
| C | -2.38800000 | 7.62910000 | 6.46510000 |
| O | -2.24880000 | 9.03630000 | 6.55400000 |
| C | -0.79600000 | 10.76000000 | 7.41190000 |
| O | -3.33160000 | 7.17180000 | 5.87070000 |
| C | 0.38150000 | 11.16690000 | 8.00110000 |
| C | -1.69150000 | 11.72210000 | 6.97880000 |
| C | 0.68940000 | 12.48220000 | 8.14470000 |
| H | 0.98280000 | 10.58410000 | 8.26830000 |
| C | -1.39180000 | 13.05890000 | 7.12760000 |
| H | -2.47700000 | 11.50180000 | 6.58800000 |
| C | -0.22000000 | 13.42140000 | 7.69240000 |
| H | 1.50640000 | 12.64900000 | 8.48300000 |
| H | -1.96520000 | 13.56670000 | 6.85450000 |
| H | -0.03160000 | 14.01020000 | 7.85380000 |
| O | -1.81470000 | -1.38880000 | 2.85280000 |
| O | -2.89750000 | 0.47570000 | 2.16960000 |
| C | -1.95390000 | 0.01840000 | 2.76400000 |
| C | -0.81430000 | 0.55520000 | 3.47020000 |
| C | -0.66820000 | -1.71610000 | 3.55900000 |
| C | -0.36190000 | -3.11250000 | 3.71070000 |
| C | 0.81570000 | -3.51940000 | 4.30000000 |
| C | 1.12350000 | -4.83470000 | 4.44360000 |

| | | | |
|---|---|---|---|
| C | 0.21410000 | -5.77390000 | 3.99130000 |
| C | -0.95770000 | -5.41140000 | 3.42650000 |
| C | -1.25740000 | -4.07460000 | 3.27770000 |
| H | 1.41690000 | -2.93660000 | 4.56720000 |
| H | 1.94050000 | -5.00150000 | 4.78190000 |
| H | 0.40260000 | -6.36270000 | 4.15270000 |
| H | -1.53110000 | -5.91920000 | 3.15340000 |
| H | -2.04280000 | -3.85430000 | 2.88690000 |
| C | -0.05390000 | -0.55520000 | 3.93210000 |
| C | -0.20010000 | 1.71610000 | 3.84320000 |
| C | 1.08560000 | -0.01840000 | 4.63830000 |
| O | 0.94640000 | 1.38880000 | 4.54940000 |
| C | -0.50640000 | 3.11250000 | 3.69150000 |
| O | 2.02920000 | -0.47570000 | 5.23270000 |
| C | -1.68390000 | 3.51940000 | 3.10230000 |
| C | 0.38910000 | 4.07460000 | 4.12450000 |
| C | -1.99180000 | 4.83470000 | 2.95870000 |
| H | -2.28520000 | 2.93660000 | 2.83510000 |
| C | 0.08940000 | 5.41140000 | 3.97570000 |
| H | 1.17460000 | 3.85430000 | 4.51540000 |
| C | -1.08240000 | 5.77390000 | 3.41100000 |
| H | -2.80880000 | 5.00150000 | 2.62040000 |
| H | 0.66280000 | 5.91920000 | 4.24890000 |
| H | -1.27080000 | 6.36270000 | 3.24960000 |

Dimer 2

| | | | |
|---|---|---|---|
| O | 0.51230000 | 6.25870000 | 8.25060000 |
| O | 1.59510000 | 8.12320000 | 8.93380000 |
| C | 0.65150000 | 7.66590000 | 8.33940000 |
| C | -0.48810000 | 8.20270000 | 7.63320000 |
| C | -0.63420000 | 5.93140000 | 7.54440000 |
| C | -0.94050000 | 4.53500000 | 7.39260000 |
| C | -2.11810000 | 4.12810000 | 6.80340000 |
| C | -2.42590000 | 2.81280000 | 6.65980000 |
| C | -1.51650000 | 1.87360000 | 7.11210000 |
| C | -0.34470000 | 2.23610000 | 7.67690000 |
| C | -0.04500000 | 3.57290000 | 7.82570000 |
| H | -2.71930000 | 4.71090000 | 6.53620000 |
| H | -3.24290000 | 2.64600000 | 6.32150000 |
| H | -1.70490000 | 1.28480000 | 6.95070000 |
| H | 0.22870000 | 1.72830000 | 7.95000000 |
| H | 0.74050000 | 3.79320000 | 8.21650000 |

| | | | |
|---|---|---|---|
| C | -1.24840000 | 7.09230000 | 7.17130000 |
| C | -1.10230000 | 9.36360000 | 7.26010000 |
| C | -2.38800000 | 7.62910000 | 6.46510000 |
| O | -2.24880000 | 9.03630000 | 6.55400000 |
| C | -0.79600000 | 10.76000000 | 7.41190000 |
| O | -3.33160000 | 7.17180000 | 5.87070000 |
| C | 0.38150000 | 11.16690000 | 8.00110000 |
| C | -1.69150000 | 11.72210000 | 6.97880000 |
| C | 0.68940000 | 12.48220000 | 8.14470000 |
| H | 0.98280000 | 10.58410000 | 8.26830000 |
| C | -1.39180000 | 13.05890000 | 7.12760000 |
| H | -2.47700000 | 11.50180000 | 6.58800000 |
| C | -0.22000000 | 13.42140000 | 7.69240000 |
| H | 1.50640000 | 12.64900000 | 8.48300000 |
| H | -1.96520000 | 13.56670000 | 6.85450000 |
| H | -0.03160000 | 14.01020000 | 7.85380000 |
| O | 6.28930000 | 6.25870000 | 8.25060000 |
| O | 7.37210000 | 8.12320000 | 8.93380000 |
| C | 6.42850000 | 7.66590000 | 8.33940000 |
| C | 5.28890000 | 8.20270000 | 7.63320000 |
| C | 5.14280000 | 5.93140000 | 7.54440000 |
| C | 4.83650000 | 4.53500000 | 7.39260000 |
| C | 3.65890000 | 4.12810000 | 6.80340000 |
| C | 3.35110000 | 2.81280000 | 6.65980000 |
| C | 4.26050000 | 1.87360000 | 7.11210000 |
| C | 5.43230000 | 2.23610000 | 7.67690000 |
| C | 5.73200000 | 3.57290000 | 7.82570000 |
| H | 3.05770000 | 4.71090000 | 6.53620000 |
| H | 2.53410000 | 2.64600000 | 6.32150000 |
| H | 4.07210000 | 1.28480000 | 6.95070000 |
| H | 6.00570000 | 1.72830000 | 7.95000000 |
| H | 6.51750000 | 3.79320000 | 8.21650000 |
| C | 4.52860000 | 7.09230000 | 7.17130000 |
| C | 4.67470000 | 9.36360000 | 7.26010000 |
| C | 3.38900000 | 7.62910000 | 6.46510000 |
| O | 3.52820000 | 9.03630000 | 6.55400000 |
| C | 4.98100000 | 10.76000000 | 7.41190000 |
| O | 2.44540000 | 7.17180000 | 5.87070000 |
| C | 6.15850000 | 11.16690000 | 8.00110000 |
| C | 4.08550000 | 11.72210000 | 6.97880000 |
| C | 6.46640000 | 12.48220000 | 8.14470000 |
| H | 6.75980000 | 10.58410000 | 8.26830000 |
| C | 4.38520000 | 13.05890000 | 7.12760000 |
| H | 3.30000000 | 11.50180000 | 6.58800000 |

| | | | |
|---|---|---|---|
| C | 5.55700000 | 13.42140000 | 7.69240000 |
| H | 7.28340000 | 12.64900000 | 8.48300000 |
| H | 3.81180000 | 13.56670000 | 6.85450000 |
| H | 5.74540000 | 14.01020000 | 7.85380000 |

Dimer3

| | | | |
|---|---|---|---|
| O | -1.81470000 | -1.38880000 | 2.85280000 |
| O | -2.89750000 | 0.47570000 | 2.16960000 |
| C | -1.95390000 | 0.01840000 | 2.76400000 |
| C | -0.81430000 | 0.55520000 | 3.47020000 |
| C | -0.66820000 | -1.71610000 | 3.55900000 |
| C | -0.36190000 | -3.11250000 | 3.71070000 |
| C | 0.81570000 | -3.51940000 | 4.30000000 |
| C | 1.12350000 | -4.83470000 | 4.44360000 |
| C | 0.21410000 | -5.77390000 | 3.99130000 |
| C | -0.95770000 | -5.41140000 | 3.42650000 |
| C | -1.25740000 | -4.07460000 | 3.27770000 |
| H | 1.41690000 | -2.93660000 | 4.56720000 |
| H | 1.94050000 | -5.00150000 | 4.78190000 |
| H | 0.40260000 | -6.36270000 | 4.15270000 |
| H | -1.53110000 | -5.91920000 | 3.15340000 |
| H | -2.04280000 | -3.85430000 | 2.88690000 |
| C | -0.05390000 | -0.55520000 | 3.93210000 |
| C | -0.20010000 | 1.71610000 | 3.84320000 |
| C | 1.08560000 | -0.01840000 | 4.63830000 |
| O | 0.94640000 | 1.38880000 | 4.54940000 |
| C | -0.50640000 | 3.11250000 | 3.69150000 |
| O | 2.02920000 | -0.47570000 | 5.23270000 |
| C | -1.68390000 | 3.51940000 | 3.10230000 |
| C | 0.38910000 | 4.07460000 | 4.12450000 |
| C | -1.99180000 | 4.83470000 | 2.95870000 |
| H | -2.28520000 | 2.93660000 | 2.83510000 |
| C | 0.08940000 | 5.41140000 | 3.97570000 |
| H | 1.17460000 | 3.85430000 | 4.51540000 |
| C | -1.08240000 | 5.77390000 | 3.41100000 |
| H | -2.80880000 | 5.00150000 | 2.62040000 |
| H | 0.66280000 | 5.91920000 | 4.24890000 |
| H | -1.27080000 | 6.36270000 | 3.24960000 |
| O | -1.81470000 | 13.90620000 | 2.85280000 |
| O | -2.89750000 | 15.77070000 | 2.16960000 |
| C | -1.95390000 | 15.31340000 | 2.76400000 |

| | | | |
|---|---|---|---|
| C | -0.81430000 | 15.85020000 | 3.47020000 |
| C | -0.66820000 | 13.57890000 | 3.55900000 |
| C | -0.36190000 | 12.18250000 | 3.71070000 |
| C | 0.81570000 | 11.77560000 | 4.30000000 |
| C | 1.12350000 | 10.46030000 | 4.44360000 |
| C | 0.21410000 | 9.52110000 | 3.99130000 |
| C | -0.95770000 | 9.88360000 | 3.42650000 |
| C | -1.25740000 | 11.22040000 | 3.27770000 |
| H | 1.41690000 | 12.35840000 | 4.56720000 |
| H | 1.94050000 | 10.29350000 | 4.78190000 |
| H | 0.40260000 | 8.93230000 | 4.15270000 |
| H | -1.53110000 | 9.37580000 | 3.15340000 |
| H | -2.04280000 | 11.44070000 | 2.88690000 |
| C | -0.05390000 | 14.73980000 | 3.93210000 |
| C | -0.20010000 | 17.01110000 | 3.84320000 |
| C | 1.08560000 | 15.27660000 | 4.63830000 |
| O | 0.94640000 | 16.68380000 | 4.54940000 |
| C | -0.50640000 | 18.40750000 | 3.69150000 |
| O | 2.02920000 | 14.81930000 | 5.23270000 |
| C | -1.68390000 | 18.81440000 | 3.10230000 |
| C | 0.38910000 | 19.36960000 | 4.12450000 |
| C | -1.99180000 | 20.12970000 | 2.95870000 |
| H | -2.28520000 | 18.23160000 | 2.83510000 |
| C | 0.08940000 | 20.70640000 | 3.97570000 |
| H | 1.17460000 | 19.14930000 | 4.51540000 |
| C | -1.08240000 | 21.06890000 | 3.41100000 |
| H | -2.80880000 | 20.29650000 | 2.62040000 |
| H | 0.66280000 | 21.21420000 | 4.24890000 |
| H | -1.27080000 | 21.65770000 | 3.24960000 |

Dimer4

| | | | |
|---|---|---|---|
| O | 6.28930000 | 6.25870000 | 8.25060000 |
| O | 7.37210000 | 8.12320000 | 8.93380000 |
| C | 6.42850000 | 7.66590000 | 8.33940000 |
| C | 5.28890000 | 8.20270000 | 7.63320000 |
| C | 5.14280000 | 5.93140000 | 7.54440000 |
| C | 4.83650000 | 4.53500000 | 7.39260000 |
| C | 3.65890000 | 4.12810000 | 6.80340000 |
| C | 3.35110000 | 2.81280000 | 6.65980000 |
| C | 4.26050000 | 1.87360000 | 7.11210000 |
| C | 5.43230000 | 2.23610000 | 7.67690000 |
| C | 5.73200000 | 3.57290000 | 7.82570000 |

| | | | |
|---|---|---|---|
| H | 3.05770000 | 4.71090000 | 6.53620000 |
| H | 2.53410000 | 2.64600000 | 6.32150000 |
| H | 4.07210000 | 1.28480000 | 6.95070000 |
| H | 6.00570000 | 1.72830000 | 7.95000000 |
| H | 6.51750000 | 3.79320000 | 8.21650000 |
| C | 4.52860000 | 7.09230000 | 7.17130000 |
| C | 4.67470000 | 9.36360000 | 7.26010000 |
| C | 3.38900000 | 7.62910000 | 6.46510000 |
| O | 3.52820000 | 9.03630000 | 6.55400000 |
| C | 4.98100000 | 10.76000000 | 7.41190000 |
| O | 2.44540000 | 7.17180000 | 5.87070000 |
| C | 6.15850000 | 11.16690000 | 8.00110000 |
| C | 4.08550000 | 11.72210000 | 6.97880000 |
| C | 6.46640000 | 12.48220000 | 8.14470000 |
| H | 6.75980000 | 10.58410000 | 8.26830000 |
| C | 4.38520000 | 13.05890000 | 7.12760000 |
| H | 3.30000000 | 11.50180000 | 6.58800000 |
| C | 5.55700000 | 13.42140000 | 7.69240000 |
| H | 7.28340000 | 12.64900000 | 8.48300000 |
| H | 3.81180000 | 13.56670000 | 6.85450000 |
| H | 5.74540000 | 14.01020000 | 7.85380000 |
| O | -1.81470000 | -1.38880000 | 2.85280000 |
| O | -2.89750000 | 0.47570000 | 2.16960000 |
| C | -1.95390000 | 0.01840000 | 2.76400000 |
| C | -0.81430000 | 0.55520000 | 3.47020000 |
| C | -0.66820000 | -1.71610000 | 3.55900000 |
| C | -0.36190000 | -3.11250000 | 3.71070000 |
| C | 0.81570000 | -3.51940000 | 4.30000000 |
| C | 1.12350000 | -4.83470000 | 4.44360000 |
| C | 0.21410000 | -5.77390000 | 3.99130000 |
| C | -0.95770000 | -5.41140000 | 3.42650000 |
| C | -1.25740000 | -4.07460000 | 3.27770000 |
| H | 1.41690000 | -2.93660000 | 4.56720000 |
| H | 1.94050000 | -5.00150000 | 4.78190000 |
| H | 0.40260000 | -6.36270000 | 4.15270000 |
| H | -1.53110000 | -5.91920000 | 3.15340000 |
| H | -2.04280000 | -3.85430000 | 2.88690000 |
| C | -0.05390000 | -0.55520000 | 3.93210000 |
| C | -0.20010000 | 1.71610000 | 3.84320000 |
| C | 1.08560000 | -0.01840000 | 4.63830000 |
| O | 0.94640000 | 1.38880000 | 4.54940000 |
| C | -0.50640000 | 3.11250000 | 3.69150000 |
| O | 2.02920000 | -0.47570000 | 5.23270000 |
| C | -1.68390000 | 3.51940000 | 3.10230000 |

| | | | |
|---|---|---|---|
| C | 0.38910000 | 4.07460000 | 4.12450000 |
| C | -1.99180000 | 4.83470000 | 2.95870000 |
| H | -2.28520000 | 2.93660000 | 2.83510000 |
| C | 0.08940000 | 5.41140000 | 3.97570000 |
| H | 1.17460000 | 3.85430000 | 4.51540000 |
| C | -1.08240000 | 5.77390000 | 3.41100000 |
| H | -2.80880000 | 5.00150000 | 2.62040000 |
| H | 0.66280000 | 5.91920000 | 4.24890000 |
| H | -1.27080000 | 6.36270000 | 3.24960000 |

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