# SUPPLEMENTARY INFORMATION

**«Halogen-free α,α-bis(BODIPY) bichromofore photosensitizer: synthesis, spectral properties and water-soluble forms with Pluronic® F127 micelles» by**

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# Content

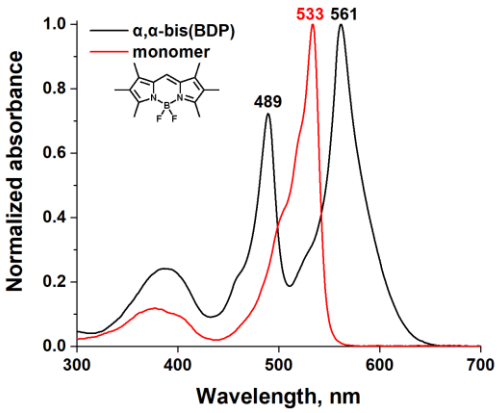



**Figure S1.** Normalized absorption spectra of α,α-bis(BODIPY) and monomer analogue BODIPY in chloroform

**Table S1.** The xyz coordinates for optimized structure of the α,α-bis(BDP) in the $S_0$ state

| | | | |
|---|---|---|---|
| F | 1.006081000000 | -0.873767000000 | -1.299390000000 |
| B | 2.025835000000 | 0.004637000000 | -0.991116000000 |
| F | 2.302178000000 | 0.834007000000 | -2.079113000000 |
| N | 3.328179000000 | -0.780159000000 | -0.620849000000 |
| C | 3.933770000000 | -1.715616000000 | -1.347833000000 |
| C | 3.374601000000 | -2.228440000000 | -2.625359000000 |
| C | 5.134186000000 | -2.118361000000 | -0.714714000000 |
| C | 6.075679000000 | -3.158400000000 | -1.228219000000 |
| C | 5.248406000000 | -1.374906000000 | 0.443461000000 |
| C | 6.343101000000 | -1.444183000000 | 1.453598000000 |
| C | 4.108240000000 | -0.533729000000 | 0.498479000000 |
| C | 3.706825000000 | 0.383082000000 | 1.440699000000 |
| C | 2.509477000000 | 1.075736000000 | 1.335988000000 |
| C | 1.892436000000 | 1.976934000000 | 2.226153000000 |
| C | 2.430827000000 | 2.473683000000 | 3.523000000000 |
| C | 0.659816000000 | 2.302704000000 | 1.675583000000 |
| C | -0.362840000000 | 3.225115000000 | 2.247634000000 |
| C | 0.562145000000 | 1.589825000000 | 0.472101000000 |
| C | -0.562434000000 | 1.590486000000 | -0.470016000000 |
| C | -0.660327000000 | 2.305209000000 | -1.672421000000 |
| C | 0.362316000000 | 3.228435000000 | -2.243213000000 |
| C | -1.893099000000 | 1.980374000000 | -2.223176000000 |
| C | -2.431678000000 | 2.478846000000 | -3.519281000000 |
| C | -2.510010000000 | 1.077864000000 | -1.334226000000 |
| N | -1.671007000000 | 0.868266000000 | -0.257480000000 |
| B | -2.025864000000 | 0.003133000000 | 0.991100000000 |
| F | -1.005837000000 | -0.875295000000 | 1.298246000000 |
| F | -2.302609000000 | 0.830925000000 | 2.080240000000 |
| N | -3.327872000000 | -0.781499000000 | 0.619585000000 |
| C | -3.932749000000 | -1.718768000000 | 1.344852000000 |
| C | -3.372427000000 | -2.233879000000 | 2.620955000000 |
| C | -5.133426000000 | -2.120416000000 | 0.711558000000 |
| C | -6.074451000000 | -3.161873000000 | 1.223025000000 |
| C | -5.248429000000 | -1.374499000000 | -0.444992000000 |
| C | -6.344045000000 | -1.441403000000 | -1.454275000000 |
| C | -4.108558000000 | -0.532879000000 | -0.498790000000 |
| C | -3.707478000000 | 0.385536000000 | -1.439629000000 |
| N | 1.670728000000 | 0.867841000000 | 0.258707000000 |
| H | 2.526114000000 | -2.886758000000 | -2.428405000000 |
| H | 3.008155000000 | -1.408561000000 | -3.242609000000 |
| H | 4.129943000000 | -2.786653000000 | -3.176217000000 |
| H | 6.477372000000 | -2.889284000000 | -2.208214000000 |
| H | 6.919894000000 | -3.287844000000 | -0.551094000000 |
| H | 5.585020000000 | -4.128830000000 | -1.333006000000 |
| H | 6.384012000000 | -2.431208000000 | 1.919607000000 |
| H | 7.314761000000 | -1.261826000000 | 0.990043000000 |
| H | 6.211385000000 | -0.708699000000 | 2.246362000000 |
| H | 4.332761000000 | 0.554572000000 | 2.306704000000 |
| H | 2.449806000000 | 3.565878000000 | 3.541489000000 |

| | | | |
|---|---|---|---|
| H | 3.443897000000 | 2.119591000000 | 3.712418000000 |
| H | 1.799643000000 | 2.149055000000 | 4.353647000000 |
| H | 0.080154000000 | 4.192037000000 | 2.498830000000 |
| H | -1.176004000000 | 3.392713000000 | 1.542625000000 |
| H | -0.805014000000 | 2.808440000000 | 3.153975000000 |
| H | -0.080835000000 | 4.195536000000 | -2.493475000000 |
| H | 1.175204000000 | 3.395463000000 | -1.537761000000 |
| H | 0.804776000000 | 2.812851000000 | -3.149904000000 |
| H | -3.446790000000 | 2.129441000000 | -3.706494000000 |
| H | -2.445521000000 | 3.571090000000 | -3.538392000000 |
| H | -1.803690000000 | 2.150747000000 | -4.351005000000 |
| H | -4.125170000000 | -2.798852000000 | 3.168420000000 |
| H | -2.519586000000 | -2.886011000000 | 2.422372000000 |
| H | -3.011696000000 | -1.414374000000 | 3.242118000000 |
| H | -5.585159000000 | -4.133833000000 | 1.319830000000 |
| H | -6.471347000000 | -2.897896000000 | 2.206349000000 |
| H | -6.921967000000 | -3.285612000000 | 0.548952000000 |
| H | -6.208841000000 | -0.709456000000 | -2.249713000000 |
| H | -6.390713000000 | -2.429808000000 | -1.916750000000 |
| H | -7.314437000000 | -1.252113000000 | -0.990751000000 |
| H | -4.333743000000 | 0.558515000000 | -2.305100000000 |

**Table S2.** The xyz coordinates for optimized structure of the α,α-bis(BDP) in the $S_1$ state

| | | | |
|---|---|---|---|
| F | 1.117402000000 | -0.596424000000 | -1.455125000000 |
| B | 2.140336000000 | 0.219257000000 | -1.004994000000 |
| F | 2.453663000000 | 1.177693000000 | -1.970952000000 |
| N | 3.427235000000 | -0.613690000000 | -0.723769000000 |
| C | 4.041097000000 | -1.443904000000 | -1.570347000000 |
| C | 3.488292000000 | -1.780327000000 | -2.904949000000 |
| C | 5.248262000000 | -1.916235000000 | -0.989864000000 |
| C | 6.184338000000 | -2.875581000000 | -1.647212000000 |
| C | 5.358157000000 | -1.327417000000 | 0.255919000000 |
| C | 6.422561000000 | -1.501606000000 | 1.284440000000 |
| C | 4.206568000000 | -0.510486000000 | 0.417835000000 |
| C | 3.783426000000 | 0.244135000000 | 1.495053000000 |
| C | 2.550812000000 | 0.893963000000 | 1.474225000000 |
| C | 1.845690000000 | 1.486913000000 | 2.549018000000 |
| C | 2.382957000000 | 1.711003000000 | 3.920824000000 |
| C | 0.577803000000 | 1.771701000000 | 2.088058000000 |
| C | -0.494878000000 | 2.484163000000 | 2.838141000000 |
| C | 0.545121000000 | 1.391704000000 | 0.714265000000 |
| C | -0.544636000000 | 1.550337000000 | -0.204005000000 |
| C | -0.576798000000 | 2.369660000000 | -1.370350000000 |
| C | 0.495837000000 | 3.292374000000 | -1.838186000000 |
| C | -1.844768000000 | 2.256623000000 | -1.900285000000 |
| C | -2.381097000000 | 2.928594000000 | -3.117439000000 |
| C | -2.550110000000 | 1.336924000000 | -1.087362000000 |
| N | -1.749723000000 | 0.958023000000 | -0.026941000000 |
| B | -2.137185000000 | -0.136856000000 | 1.017353000000 |
| F | -1.115763000000 | -1.059799000000 | 1.156971000000 |
| F | -2.442744000000 | 0.434562000000 | 2.254036000000 |
| N | -3.428208000000 | -0.821505000000 | 0.475192000000 |
| C | -4.043270000000 | -1.887338000000 | 0.993554000000 |
| C | -3.489258000000 | -2.654076000000 | 2.135923000000 |
| C | -5.252067000000 | -2.133959000000 | 0.289892000000 |
| C | -6.190507000000 | -3.256376000000 | 0.586790000000 |
| C | -5.361405000000 | -1.159837000000 | -0.684698000000 |
| C | -6.427123000000 | -0.977442000000 | -1.710513000000 |
| C | -4.208003000000 | -0.338637000000 | -0.563989000000 |
| C | -3.783522000000 | 0.733580000000 | -1.324816000000 |
| N | 1.750319000000 | 0.893819000000 | 0.348225000000 |
| H | 2.591952000000 | -2.397161000000 | -2.802672000000 |
| H | 3.188350000000 | -0.875568000000 | -3.436312000000 |
| H | 4.221698000000 | -2.322379000000 | -3.499466000000 |
| H | 6.534194000000 | -2.496791000000 | -2.610648000000 |
| H | 7.061308000000 | -3.060813000000 | -1.028038000000 |
| H | 5.703634000000 | -3.839375000000 | -1.832446000000 |
| H | 6.085881000000 | -2.149339000000 | 2.098976000000 |

| | | | |
|---|---|---|---|
| H | 7.319652000000 | -1.949004000000 | 0.858031000000 |
| H | 6.707927000000 | -0.544148000000 | 1.725110000000 |
| H | 4.378301000000 | 0.271752000000 | 2.397419000000 |
| H | 1.816966000000 | 2.486303000000 | 4.437405000000 |
| H | 3.430079000000 | 2.018040000000 | 3.898031000000 |
| H | 2.316127000000 | 0.801630000000 | 4.524428000000 |
| H | -0.101698000000 | 3.405626000000 | 3.275061000000 |
| H | -1.332297000000 | 2.737550000000 | 2.192587000000 |
| H | -0.887588000000 | 1.865662000000 | 3.645161000000 |
| H | 0.102102000000 | 4.306553000000 | -1.942827000000 |
| H | 1.332705000000 | 3.316274000000 | -1.144503000000 |
| H | 0.889895000000 | 2.979006000000 | -2.804908000000 |
| H | -3.431402000000 | 3.200204000000 | -2.998048000000 |
| H | -1.822049000000 | 3.838434000000 | -3.336660000000 |
| H | -2.302945000000 | 2.279035000000 | -3.993630000000 |
| H | -4.216510000000 | -3.375691000000 | 2.503930000000 |
| H | -2.583717000000 | -3.186534000000 | 1.834784000000 |
| H | -3.203161000000 | -1.982099000000 | 2.946939000000 |
| H | -5.714490000000 | -4.227463000000 | 0.429482000000 |
| H | -6.533960000000 | -3.227266000000 | 1.623708000000 |
| H | -7.071077000000 | -3.216161000000 | -0.053342000000 |
| H | -6.687052000000 | 0.076353000000 | -1.828712000000 |
| H | -6.105153000000 | -1.347028000000 | -2.688368000000 |
| H | -7.336494000000 | -1.513073000000 | -1.440026000000 |
| H | -4.378185000000 | 1.063907000000 | -2.165114000000 |

**Table S3.** The xyz coordinates for optimized structure of the α,α-bis(BDP) in the $T_1$ state

| | | | |
|---|---|---|---|
| F | 1.025888000000 | -0.770304000000 | -1.371374000000 |
| B | 2.051834000000 | 0.076324000000 | -1.000759000000 |
| F | 2.357324000000 | 0.956453000000 | -2.040357000000 |
| N | 3.339764000000 | -0.739328000000 | -0.650451000000 |
| C | 3.946228000000 | -1.646350000000 | -1.411166000000 |
| C | 3.394260000000 | -2.101745000000 | -2.713161000000 |
| C | 5.140746000000 | -2.081067000000 | -0.786413000000 |
| C | 6.080529000000 | -3.104146000000 | -1.335607000000 |
| C | 5.250152000000 | -1.386938000000 | 0.401752000000 |
| C | 6.337171000000 | -1.502940000000 | 1.415738000000 |
| C | 4.112919000000 | -0.542586000000 | 0.483876000000 |
| C | 3.706479000000 | 0.331780000000 | 1.462226000000 |
| C | 2.509228000000 | 1.030336000000 | 1.379789000000 |
| C | 1.874335000000 | 1.869248000000 | 2.316027000000 |
| C | 2.398313000000 | 2.299967000000 | 3.642056000000 |
| C | 0.638645000000 | 2.206973000000 | 1.778780000000 |
| C | -0.393962000000 | 3.088080000000 | 2.396126000000 |
| C | 0.559288000000 | 1.566596000000 | 0.533233000000 |
| C | -0.555686000000 | 1.603553000000 | -0.410927000000 |
| C | -0.651386000000 | 2.351953000000 | -1.610386000000 |
| C | 0.385864000000 | 3.288259000000 | -2.130528000000 |
| C | -1.871252000000 | 2.055070000000 | -2.166385000000 |
| C | -2.462985000000 | 2.554639000000 | -3.435502000000 |
| C | -2.512349000000 | 1.109616000000 | -1.290786000000 |
| N | -1.693808000000 | 0.878071000000 | -0.219313000000 |
| B | -2.035475000000 | -0.041406000000 | 0.984041000000 |
| F | -1.009393000000 | -0.936903000000 | 1.239535000000 |
| F | -2.290766000000 | 0.723456000000 | 2.127654000000 |
| N | -3.333686000000 | -0.792508000000 | 0.578172000000 |
| C | -3.951779000000 | -1.777444000000 | 1.288437000000 |
| C | -3.386424000000 | -2.320180000000 | 2.542678000000 |
| C | -5.153470000000 | -2.148703000000 | 0.630652000000 |
| C | -6.086915000000 | -3.205685000000 | 1.118990000000 |
| C | -5.261097000000 | -1.364231000000 | -0.494382000000 |
| C | -6.315017000000 | -1.333968000000 | -1.543652000000 |
| C | -4.101924000000 | -0.510204000000 | -0.511180000000 |
| C | -3.732060000000 | 0.459029000000 | -1.448352000000 |
| N | 1.682965000000 | 0.876217000000 | 0.285360000000 |
| H | 2.525860000000 | -2.743208000000 | -2.550931000000 |
| H | 3.058166000000 | -1.252084000000 | -3.307247000000 |
| H | 4.143451000000 | -2.660068000000 | -3.271984000000 |

| | | | |
|---|---|---|---|
| H | 6.487312000000 | -2.798874000000 | -2.302753000000 |
| H | 6.921330000000 | -3.262674000000 | -0.660482000000 |
| H | 5.586659000000 | -4.067862000000 | -1.479670000000 |
| H | 6.378669000000 | -2.512104000000 | 1.831391000000 |
| H | 7.311491000000 | -1.293656000000 | 0.969421000000 |
| H | 6.196335000000 | -0.808926000000 | 2.243493000000 |
| H | 4.323657000000 | 0.460128000000 | 2.341861000000 |
| H | 2.395340000000 | 3.389382000000 | 3.723975000000 |
| H | 3.417761000000 | 1.955786000000 | 3.814801000000 |
| H | 1.770979000000 | 1.915167000000 | 4.449572000000 |
| H | 0.035810000000 | 4.052284000000 | 2.679173000000 |
| H | -1.218602000000 | 3.268503000000 | 1.708112000000 |
| H | -0.817965000000 | 2.629102000000 | 3.290324000000 |
| H | -0.056459000000 | 4.253385000000 | -2.385605000000 |
| H | 1.169786000000 | 3.451926000000 | -1.392612000000 |
| H | 0.864257000000 | 2.882909000000 | -3.022586000000 |
| H | -3.438711000000 | 3.018284000000 | -3.265705000000 |
| H | -1.814272000000 | 3.292457000000 | -3.906241000000 |
| H | -2.612963000000 | 1.738090000000 | -4.147874000000 |
| H | -4.078301000000 | -3.020374000000 | 3.007159000000 |
| H | -2.439759000000 | -2.828823000000 | 2.345260000000 |
| H | -3.164284000000 | -1.511794000000 | 3.242518000000 |
| H | -5.586548000000 | -4.173962000000 | 1.191380000000 |
| H | -6.474717000000 | -2.964471000000 | 2.111426000000 |
| H | -6.938711000000 | -3.322168000000 | 0.450617000000 |
| H | -6.775817000000 | -0.344427000000 | -1.610780000000 |
| H | -5.896734000000 | -1.560818000000 | -2.528405000000 |
| H | -7.104661000000 | -2.056432000000 | -1.342196000000 |
| H | -4.351389000000 | 0.655788000000 | -2.308921000000 |

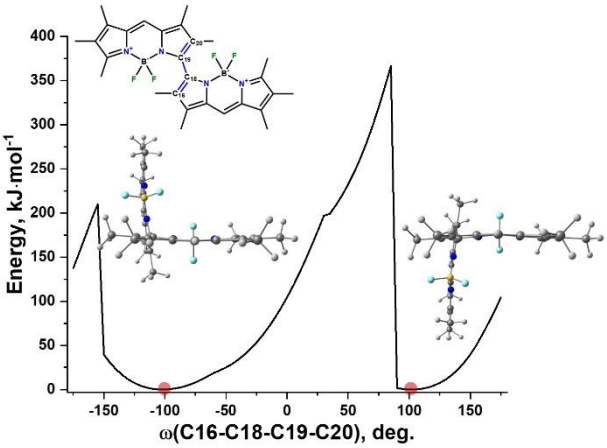
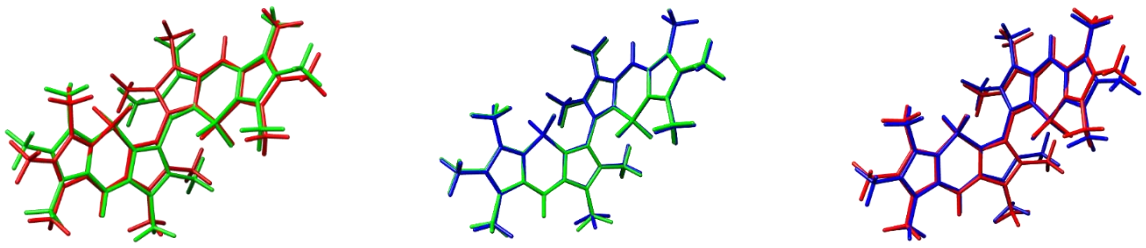



**Figure S2**. Potential energy surface scan for energies vs. the C16−C18−C19−C20 torsion angle of α,α-bis(BDP)



$S_0$ vs. $S_1$ $S_0$ vs. $T_1$ $S_1$ vs. $T_1$

**Figure S3.** α,α-bis(BDP) geometry in $S_0$, $S_1$, and $T_1$ states

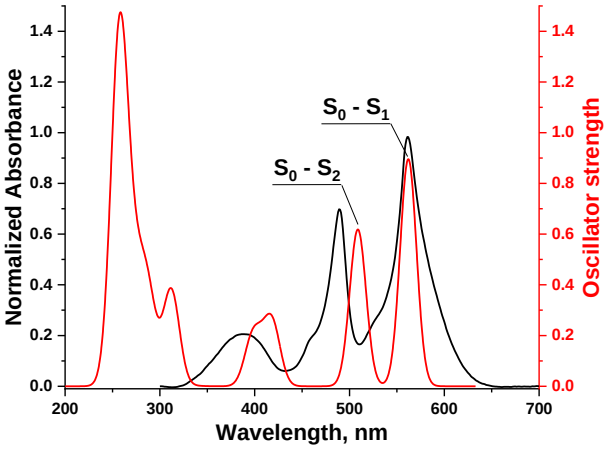
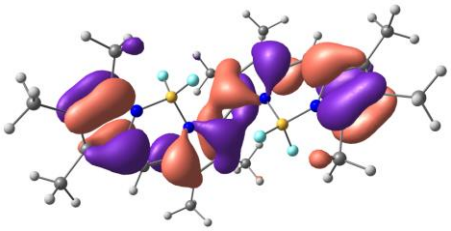
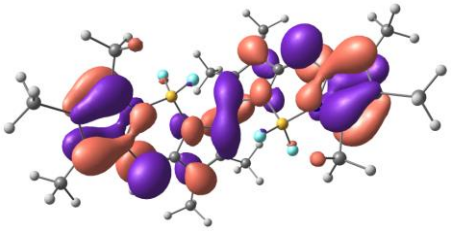
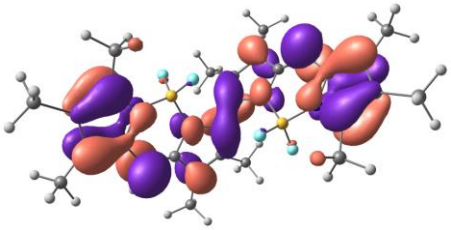
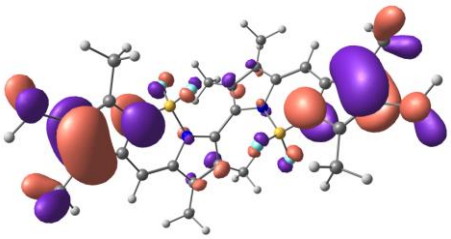



**Figure S4.** Experimental absorption (black) and TDDFT (red) spectrum of the α,α-bis(BDP). The TDDFT spectrum is red-shifted at 87 nm (0.4 eV) for better comparison

**Table S4**. Results of TDDFT analysis for α,α-bis(BDP)

| Transition (%) | Energy, eV (nm) | Oscillator strength | FMO type |
|---|---|---|---|
| HOMO – LUMO (33) | 2.61 (475) | 0.90 |  HOMO  LUMO |
| HOMO – LUMO+1 (25) | 2.94 (422) | 0.62 |  LUMO+1 |
| HOMO-4 – LUMO (18) | 3.99 (311) | 0.18 |  HOMO-4 |

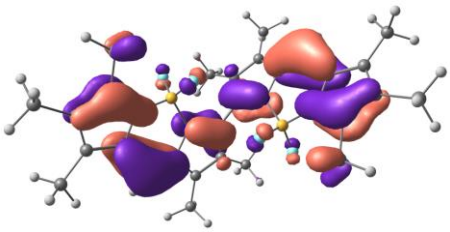
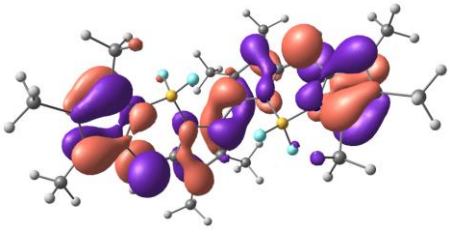
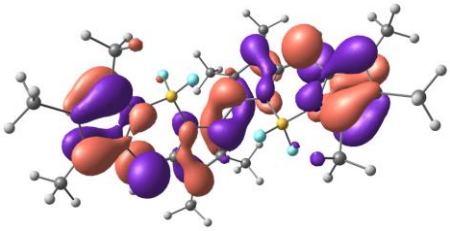
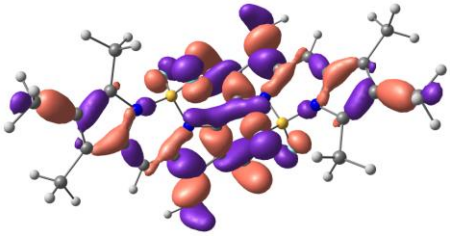
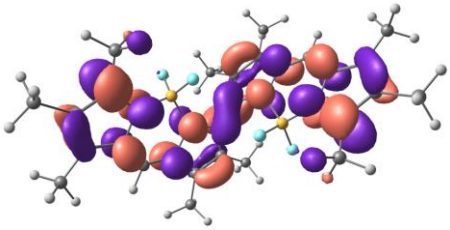
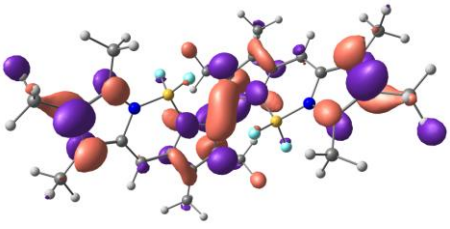
| | | | |
|---|---|---|---|
| HOMO-6 – LUMO (30) | 5.51 (225) | 0.36 |  HOMO-6 |
| HOMO – LUMO+2 (33) | 6.19 (200) | 0.34 |  LUMO+2 |
| HOMO-2 – LUMO+2 (7) | 7.1686 | 0.24 |  HOMO-2 |
| HOMO-18 – LUMO (5) | 7.27 | 0.20 |  HOMO+18 |
| HOMO-4 – LUMO+4 (8) | 7.28 | 0.32 |  LUMO+4 |
| HOMO-1 – LUMO+8 (5) | 7.31 | 0.20 |  LUMO+8 |

**Table S5.** The fit parameters of the time resolved fluorescence decays of α,α-bis(BDP) ($C_{\alpha,\alpha\text{-bis(BDP)}}$ = 6.5 μM) in different solvents

| Solvent | $\lambda_{fl}$ | fit | $\chi^2$ | $\tau_1$, ns | $A_1$ | $\tau_2$, ns | $A_2$ | $\tau_3$, ns | $A_3$ | $\tau$, ns |
|---|---|---|---|---|---|---|---|---|---|---|
| Cyclohexane | 648 | mono | 1.31 | 3.437 ± 0.002 | 11.44 | - | - | - | - | 3.44 |
| Benzene | 653 | mono | 1.23 | 3.321 ± 0.006 | 11.59 | - | - | - | - | 3.32 |
| Toluene | 651 | mono | 1.21 | 3.322 ± 0.004 | 11.39 | - | - | - | - | 3.32 |
| Chloroform | 650 | mono | 1.20 | 3.414 ± 0.004 | 11.49 | - | - | - | - | 3.41 |
| THF | 650 | mono | 1.26 | 3.216 ± 0.006 | 11.53 | - | - | - | - | 3.22 |
| Ethanol | 648 | bi | 1.26 | 0.979 ± 0.003 | 13.53 | 3.65±0.34 | 0.095 | - | - | 1.05 |
| DMF | 653 | bi | 1.24 | 0.783 ± 0.004 | 14.43 | 2.67±0.46 | 0.088 | - | - | 0.82 |
| ACN | 649 | three | 1.44 | 0.150 ± 0.056 | 4.60 | 4.39±0.38 | 0.027 | 0.338±0.009 | 16.4 | 0.39 |
| DMSO | 656 | bi | 1.35 | 0.509 ± 0.002 | 16.42 | 4.57±0.33 | 0.034 | - | - | 0.58 |

**Table S6.** Spectral and photophysical parameters of α,α-$CH_2$-bis(BDP) in organic solvents (T = 298 K)[1]

| Solvent | $\lambda_{abs}$, nm (lgε) | $\Delta\nu_{es}$, $cm^{-1}$ | $\lambda_{fl}$, nm | $\Delta\nu_{SS}$, $cm^{-1}$ | $\Phi_{fl}$ | $K_{rad}\cdot10^{-8}$, $s^{-1}$ | $K_{nrad}\cdot10^{-8}$, $s^{-1}$ | $\tau_{fl}$, ns |
|---|---|---|---|---|---|---|---|---|
| heptane | 562; 500; 378 | 2207 | 578 | 493 | 0.80 | 2.22 | 0.30 | 3.97 |
| cyclohexane | 564; 501; 385 | 2230 | 580 | 490 | 0.99 | 2.94 | 0.03 | 3.37 |
| benzene | 566 (5.01); 500; 380 | 2332 | 583 | 515 | 0.87 | 2.40 | 0.36 | 3.63 |
| chloroform | 564 (5.11); 500;381 | 2270 | 581 | 519 | 0.95 | 2.75 | 0.15 | 3.46 |
| THF | 559; 495; 376 | 2312 | 580 | 647 | 0.58 | 1.89 | 1.37 | 3.06 |
| ethanol | 557 (5.08); 496; 377 | 2208 | 573 | 501 | 0.10 | 1.27 | 11.39 | 0.79 |
| DMF | 556 (5.04); 495; 382 | 2216 | 583 | 833 | 0.05 | 0.65 | 12.3 | 0.77 |
| DMSO | 556; 496; 381 | 2176 | 581 | 774 | 0.08 | 0.85 | 9.79 | 0.94 |

*Note:* absorption maxima ($\lambda_{abs}$, nm), molar absorption coefficients (lgε), exciton splitting ($\Delta\nu_{es}$, $cm^{-1}$), emission maxima ($\lambda_{fl}$, nm), Stokes shift ($\Delta\nu_{SS}$, $cm^{-1}$), fluorescence quantum yield ($\Phi_{fl}$), fluorescence lifetime ($\tau_{fl}$, ns), radiative constants $K_{rad}$, $s^{-1}$) and non-radiative ($K_{nrad}$, $s^{-1}$). *The intensity of singlet oxygen generation is close to zero, regardless of the solvent.*

**Table S7.** The fit parameters of the time resolved fluorescence decays of α,α-bis(BDP) ($C_{\alpha,\alpha\text{-bis(BDP)}}$ = 6.5 μM) in THF-water mixture with different $f_w$

| $f_w$ %, ($\lambda_{fl}$) | fit | $\chi^2$ | $\tau_1$, ns | $A_1$ | $\tau_2$, ns | $A_2$ | $\tau_3$, ns | $A_3$ | $\tau$, ns |
|---|---|---|---|---|---|---|---|---|---|
| 0 (649) | mono | 1.30 | 3.219±0.003 | 11.6 | - | - | - | - | 3.219±0.003 |
| 70 (665) | three | 1.39 | 0.798±0.034 | 6.4 | 4.50±0.33 | 0.05 | 0.377±0.029 | 10.37 | 0.711±0.009 |
| 93 (661) | three | 1.53 | 0.545±0.043 | 5.9 | 3.97±0.94 | 0.02 | 0.277±0.021 | 12.90 | 0.449±0.009 |
| 95 (660) | three | 1.59 | 0.523±0.018 | 4.6 | 5.53±0.52 | 0.01 | 0.244±0.008 | 15.83 | 0.415±0.008 |

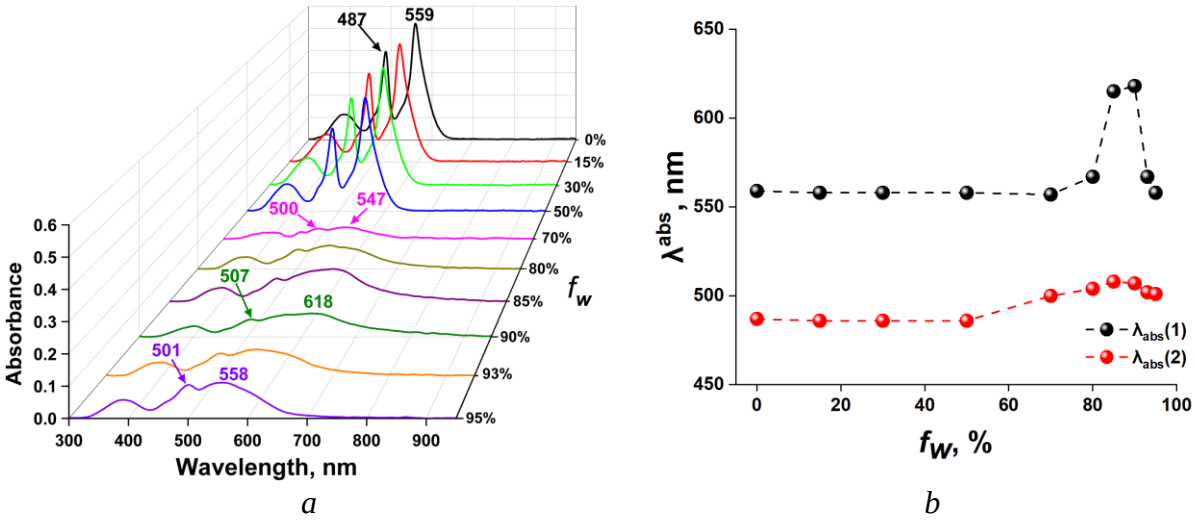



**Figure S5.** Absorption (*a*) spectra of α,α-bis(BDP) at $C_{\alpha,\alpha\text{-bis(BDP)}}$ = 6.5 μM and various volumetric water content ($f_w$) in the THF-water mixtures after 24 hours; dependences of maximum absorption wavelengths (*b*) of α,α-bis(BDP) on $f_w$ in THF-water mixtures.

## References

1. a) A. Kalyagin, L. Antina, A. Ksenofontov, E. Antina, M. Berezin, *IJMS* **2022**, *23*, 14402; b) L. A. Antina, V. A. Kalinkina, A. S. Sherudillo, A. A. Kalyagin, M. M. Lukanov, A. A. Ksenofontov, M. B. Berezin, E. V. Antina, *Journal of Luminescence* **2024**, *269*, 120411.