

## Supporting Information

### **Zinc metal complex of *tert*-butyl substituted phthalocyanine: Assessment of photosensitizer potential with theoretical calculations**

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## 1. Photophysical and photochemical parameters

At room temperature, fluorescence excitation and emission spectra were recorded on a Shimadzu spectrofluorometer using a 1 cm path-length cuvette. Fluorescence quantum yield ( $\Phi_F$ ) is determined in DMSO by the comparative method using equation 1[1–3].

$$\Phi_F = \Phi_{F_{Std}} \frac{F * A_{Std} * \eta^2}{F_{Std} * A * \eta_{Std}^2} \quad (1)$$

where  $F$  and  $F_{Std}$  are the areas under the fluorescence emission curve of the sample and the standard, respectively.  $A$  and  $A_{Std}$  are the respective absorbances of the sample and standard at the excitation wavelengths, respectively.  $n^2$  and  $n_{Std}^2$  are the refractive indices of solvents used for the sample and standard, respectively. Reference (unsubstituted) ZnPc ( $\Phi_F = 0.20$ ) [4] was employed as the standard in DMSO. The solutions' absorbance at the excitation wavelength ranged between 0.04 and 0.05. Both the sample and standard were excited at the same wavelength. Singlet oxygen quantum yield ( $\Phi_\Delta$ ) determination was carried out using the experimental set-up described in the literature[5, 6]. Typically, a 3 mL portion of the respective unsubstituted zinc (II) phthalocyanine (ZnPc) and the studied phthalocyanine solutions ( $C = 1 \cdot 10^{-5}$  M) containing the singlet oxygen quencher was irradiated in the Q band region with the photo-irradiation set-up described in references [7–9]. Singlet oxygen quantum yield ( $\Phi_\Delta$ ) was determined in DMSO using the relative method with unsubstituted zinc (II) phthalocyanine (ZnPc) as a reference. DPBF was used as the chemical quencher for singlet oxygen in DMSO. Equation 2 was employed for the calculations:

$$\Phi_\Delta = \Phi_\Delta^{Std} \frac{R * I_{abs}^{Std}}{R^{Std} * I_{abs}} \quad (2)$$

where  $\Phi_\Delta^{std}$  is the singlet oxygen quantum yield for the standard unsubstituted zinc (II) phthalocyanine.  $R$  and  $R_{Std}$  are the DPBF photobleaching rates in the presence of studied phthalocyanine and standard, respectively.  $I_{abs}$  and  $I_{abs}^{Std}$  are the rates of light absorption by the studied phthalocyanine and standard, respectively. To avoid chain reactions induced by DPBF

in the presence of singlet oxygen, the concentration of quencher (DPBF) was lowered to  $\sim 5 \times 10^{-6}$  M. Solutions of sensitizer ( $C = 1 \cdot 10^{-6}$  M) containing DPBF were prepared in the dark and irradiated in the Q band region using the photoirradiation setup. DPBF degradation at 417 nm was monitored. The light intensity  $7.05 \cdot 10^{15}$  photons  $s^{-1} cm^{-2}$  was used for determinations. The absorption band of DPBF is reduced by light irradiation.

## 2. DFT optimization data

**Data S1.** The calculated optimized geometries of dt-ZnPc.

| Optimized geometry of dt-ZnPc (in gas-phase// B3LYP/6-31G(d)) |           |           |           | Optimized geometry of dt-ZnPc (in DMSO phase// B3LYP/6-31G(d)) |          |          |          |
|---------------------------------------------------------------|-----------|-----------|-----------|----------------------------------------------------------------|----------|----------|----------|
| C                                                             | 4.596524  | -4.741919 | -0.004085 | C                                                              | 4.597836 | -4.73984 | -0.00144 |
| C                                                             | 3.484805  | -5.614565 | 0.001372  | C                                                              | 3.486572 | -5.61263 | -0.00641 |
| C                                                             | 4.430644  | -3.354856 | -0.007927 | C                                                              | 4.431221 | -3.35379 | 0.072873 |
| C                                                             | 2.186979  | -5.119366 | 0.003087  | C                                                              | 2.189383 | -5.1186  | 0.064148 |
| C                                                             | 3.123072  | -2.871853 | -0.005852 | C                                                              | 3.12499  | -2.87196 | 0.141763 |
| C                                                             | 2.008289  | -3.733736 | -0.000536 | C                                                              | 2.010148 | -3.73468 | 0.140161 |
| C                                                             | 2.591787  | -1.509264 | -0.00756  | C                                                              | 2.590632 | -1.51001 | 0.206769 |
| C                                                             | 0.823509  | -2.886879 | 0.000681  | C                                                              | 0.826496 | -2.88535 | 0.207875 |
| N                                                             | 1.220545  | -1.571024 | -0.003415 | N                                                              | 1.223086 | -1.57304 | 0.24748  |
| N                                                             | -0.422057 | -3.355365 | 0.00527   | N                                                              | -0.42108 | -3.35413 | 0.200928 |
| N                                                             | 3.356223  | -0.421426 | -0.011944 | N                                                              | 3.355681 | -0.42023 | 0.192821 |
| C                                                             | -1.509895 | -2.59092  | 0.007579  | C                                                              | -1.51083 | -2.58902 | 0.214627 |
| C                                                             | 2.887733  | 0.824147  | -0.012282 | C                                                              | 2.886941 | 0.827356 | 0.202776 |
| N                                                             | -1.571658 | -1.219672 | 0.006076  | N                                                              | -1.57378 | -1.22137 | 0.250923 |
| C                                                             | -2.872477 | -3.122193 | 0.013123  | C                                                              | -2.87294 | -3.12363 | 0.155882 |
| C                                                             | -3.734357 | -2.007398 | 0.015446  | C                                                              | -3.73578 | -2.00888 | 0.154106 |
| C                                                             | -2.887507 | -0.822623 | 0.010561  | C                                                              | -2.88627 | -0.82496 | 0.21491  |
| C                                                             | -3.35548  | -4.429764 | 0.015991  | C                                                              | -3.35486 | -4.43015 | 0.09365  |
| C                                                             | -5.119979 | -2.18607  | 0.021597  | C                                                              | -5.12003 | -2.18863 | 0.085253 |
| C                                                             | -4.742539 | -4.595627 | 0.021809  | C                                                              | -4.7412  | -4.59727 | 0.026725 |
| C                                                             | -5.615178 | -3.483894 | 0.024972  | C                                                              | -5.61419 | -3.48616 | 0.021954 |
| N                                                             | -3.355996 | 0.42295   | 0.010302  | N                                                              | -3.35505 | 0.42261  | 0.205915 |
| C                                                             | -2.591562 | 1.510788  | 0.005615  | C                                                              | -2.58991 | 1.512406 | 0.215256 |
| N                                                             | -1.220321 | 1.572548  | 0.001261  | N                                                              | -1.22223 | 1.57551  | 0.250275 |
| C                                                             | -0.823285 | 2.888402  | -0.00295  | C                                                              | -0.82581 | 2.88783  | 0.208996 |
| C                                                             | -2.008066 | 3.735259  | -0.001558 | C                                                              | -2.00976 | 3.737092 | 0.145503 |
| C                                                             | -3.122846 | 2.873375  | 0.004011  | C                                                              | -3.12454 | 2.8743   | 0.151805 |
| N                                                             | 0.42228   | 3.356888  | -0.007449 | N                                                              | 0.421755 | 3.35657  | 0.197084 |
| C                                                             | 1.510119  | 2.592443  | -0.009631 | C                                                              | 1.511587 | 2.591512 | 0.207335 |
| N                                                             | 1.571882  | 1.221195  | -0.008442 | N                                                              | 1.57478  | 1.223936 | 0.246868 |
| C                                                             | 2.872704  | 3.123719  | -0.014283 | C                                                              | 2.873333 | 3.125916 | 0.138552 |
| C                                                             | 3.734586  | 2.008924  | -0.01634  | C                                                              | 3.736032 | 2.011062 | 0.133138 |
| C                                                             | 5.120213  | 2.187599  | -0.021407 | C                                                              | 5.119654 | 2.190305 | 0.051808 |

|    |           |           |           |    |          |          |          |
|----|-----------|-----------|-----------|----|----------|----------|----------|
| C  | 3.355709  | 4.431291  | -0.016436 | C  | 3.354943 | 4.43217  | 0.068568 |
| C  | 5.615413  | 3.485423  | -0.024021 | C  | 5.613429 | 3.487509 | -0.02024 |
| C  | 4.742771  | 4.597155  | -0.021201 | C  | 4.740684 | 4.598791 | -0.01129 |
| C  | -4.430419 | 3.356377  | 0.006393  | C  | -4.43107 | 3.355987 | 0.087925 |
| C  | -2.186758 | 5.120888  | -0.005195 | C  | -2.18947 | 5.12099  | 0.069855 |
| C  | -3.484585 | 5.616086  | -0.003242 | C  | -3.48699 | 5.614876 | 0.004272 |
| C  | -4.596301 | 4.743439  | 0.002531  | C  | -4.59815 | 4.741979 | 0.01386  |
| H  | -6.683684 | -3.67518  | 0.029723  | H  | -6.68191 | -3.67339 | -0.03229 |
| H  | -5.789472 | -1.331589 | 0.023646  | H  | -5.79565 | -1.33891 | 0.080009 |
| H  | -2.680758 | -5.276931 | 0.013618  | H  | -2.68258 | -5.27941 | 0.094547 |
| H  | -5.277572 | 2.681649  | 0.010875  | H  | -5.28038 | 2.68377  | 0.092365 |
| H  | -1.332289 | 5.790386  | -0.009576 | H  | -1.33972 | 5.796524 | 0.060898 |
| H  | -3.675886 | 6.684597  | -0.006083 | H  | -3.67417 | 6.68231  | -0.05549 |
| H  | 2.680985  | 5.278457  | -0.014299 | H  | 2.682888 | 5.281621 | 0.072214 |
| H  | 6.683923  | 3.676711  | -0.027915 | H  | 6.680647 | 3.674369 | -0.0847  |
| H  | 5.789708  | 1.333118  | -0.023193 | H  | 5.79503  | 1.340425 | 0.043253 |
| H  | 1.332509  | -5.788863 | 0.007276  | H  | 1.339519 | -5.79403 | 0.058702 |
| H  | 5.2778    | -2.680129 | -0.012158 | H  | 5.280649 | -2.6817  | 0.073587 |
| H  | 3.676105  | -6.683076 | 0.004194  | H  | 3.673439 | -6.6801  | -0.06658 |
| O  | 5.373361  | 5.819498  | -0.023656 | O  | 5.365845 | 5.819791 | -0.09086 |
| O  | 5.818872  | -5.372504 | -0.005011 | O  | 5.818844 | -5.36531 | -0.07853 |
| O  | -5.373126 | -5.817969 | 0.025094  | O  | -5.36677 | -5.81876 | -0.04223 |
| O  | -5.81865  | 5.374022  | 0.003669  | O  | -5.81958 | 5.367225 | -0.05862 |
| Zn | 0.000108  | 0.000761  | -0.002336 | Zn | 0.000812 | 0.00135  | 0.499729 |
| C  | -4.613656 | -6.99765  | 0.017944  | C  | -4.60968 | -7.00134 | -0.01698 |
| C  | -4.284932 | -7.594549 | 1.258519  | C  | -4.36467 | -7.61815 | 1.233822 |
| C  | -4.299226 | -7.589072 | -1.228982 | C  | -4.21681 | -7.57524 | -1.25045 |
| C  | -3.443085 | -8.714311 | 1.204138  | C  | -3.52644 | -8.74275 | 1.216371 |
| C  | -3.4565   | -8.708777 | -1.189034 | C  | -3.3855  | -8.70228 | -1.17361 |
| C  | -2.985239 | -9.255989 | 0.003693  | C  | -2.99567 | -9.2709  | 0.039324 |
| H  | -3.136075 | -9.195422 | 2.124544  | H  | -3.28116 | -9.23957 | 2.14677  |
| H  | -3.159579 | -9.185607 | -2.114961 | H  | -3.03285 | -9.16803 | -2.08544 |
| C  | 6.998531  | -4.612993 | -0.011437 | C  | 7.002301 | -4.60977 | -0.04964 |
| C  | 7.596618  | -4.286955 | 1.229279  | C  | 7.622008 | -4.37573 | 1.201869 |
| C  | 7.588744  | -4.295837 | -1.258242 | C  | 7.574358 | -4.20791 | -1.2811  |
| C  | 8.716277  | -3.444907 | 1.175576  | C  | 8.74842  | -3.53984 | 1.188751 |
| C  | 8.708498  | -3.453228 | -1.217614 | C  | 8.703382 | -3.37972 | -1.19993 |
| C  | 9.256816  | -2.984493 | -0.024388 | C  | 9.275526 | -3.00109 | 0.01489  |
| H  | 9.198247  | -3.139812 | 2.096164  | H  | 9.247601 | -3.30288 | 2.120056 |
| H  | 9.184448  | -3.154357 | -2.14337  | H  | 9.167939 | -3.02067 | -2.10987 |
| C  | 4.613877  | 6.999175  | -0.01726  | C  | 4.610922 | 7.003476 | -0.05617 |
| C  | 4.286329  | 7.59606   | -1.258153 | C  | 4.202332 | 7.577319 | -1.28459 |
| C  | 4.29826   | 7.590606  | 1.229361  | C  | 4.384219 | 7.621665 | 1.197452 |
| C  | 3.444403  | 8.715802  | -1.204571 | C  | 3.375289 | 8.706731 | -1.19729 |
| C  | 3.455586  | 8.710321  | 1.188612  | C  | 3.54889  | 8.748551 | 1.190487 |
| C  | 2.985435  | 9.257503  | -0.004566 | C  | 3.003917 | 9.277559 | 0.020369 |
| H  | 3.138231  | 9.19689   | -2.125268 | H  | 3.011384 | 9.172632 | -2.10462 |
| H  | 3.157816  | 9.187172  | 2.114256  | H  | 3.317387 | 9.246631 | 2.123767 |

|   |           |           |           |   |          |          |          |
|---|-----------|-----------|-----------|---|----------|----------|----------|
| C | -6.998304 | 4.614509  | 0.010973  | C | -7.00252 | 4.611016 | -0.02547 |
| C | -7.597083 | 4.288164  | -1.229329 | C | -7.57883 | 4.209002 | -1.25486 |
| C | -7.587818 | 4.297655  | 1.258184  | C | -7.6173  | 4.37605  | 1.228271 |
| C | -8.716722 | 3.446146  | -1.174806 | C | -8.70651 | 3.379374 | -1.16969 |
| C | -8.707573 | 3.455006  | 1.218376  | C | -8.74264 | 3.538671 | 1.219193 |
| C | -9.256571 | 2.985998  | 0.025572  | C | -9.27343 | 2.999481 | 0.04718  |
| H | -9.199219 | 3.140856  | -2.095054 | H | -9.1741  | 3.020135 | -2.078   |
| H | -9.182989 | 3.156326  | 2.144469  | H | -9.23799 | 3.300824 | 2.152323 |
| C | 7.14406   | -4.885347 | 2.590359  | C | 7.183831 | -5.05676 | 2.529109 |
| C | 8.146933  | -4.541852 | 3.715864  | C | 8.216102 | -4.81082 | 3.653954 |
| H | 8.17863   | -3.468172 | 3.933192  | H | 8.275087 | -3.75591 | 3.943864 |
| H | 7.833906  | -5.048828 | 4.634969  | H | 7.90989  | -5.37508 | 4.541335 |
| H | 9.16302   | -4.878467 | 3.482793  | H | 9.219957 | -5.14975 | 3.375528 |
| C | 5.767252  | -4.351983 | 3.053093  | C | 5.828908 | -4.52586 | 3.055241 |
| H | 5.748604  | -3.256139 | 3.057274  | H | 5.837927 | -3.43264 | 3.134988 |
| H | 4.944784  | -4.701944 | 2.429196  | H | 4.986491 | -4.81371 | 2.425704 |
| H | 5.570363  | -4.693896 | 4.076623  | H | 5.644184 | -4.93312 | 4.056769 |
| C | 7.101055  | -6.43062  | 2.490556  | C | 7.104768 | -6.59142 | 2.332152 |
| H | 6.388157  | -6.770898 | 1.738166  | H | 6.369725 | -6.87053 | 1.575713 |
| H | 8.088787  | -6.829991 | 2.231863  | H | 8.079325 | -6.99327 | 2.030075 |
| H | 6.809404  | -6.856886 | 3.458329  | H | 6.823546 | -7.07046 | 3.277851 |
| C | 7.12805   | -4.904424 | -2.612033 | C | 7.084358 | -4.70999 | -2.66833 |
| C | 8.123582  | -4.568587 | -3.746327 | C | 8.059853 | -4.29434 | -3.79367 |
| H | 7.805199  | -5.082707 | -4.659592 | H | 7.717239 | -4.73388 | -4.73668 |
| H | 8.153047  | -3.496536 | -3.971908 | H | 8.094817 | -3.20828 | -3.93447 |
| H | 9.141405  | -4.902628 | -3.517157 | H | 9.078809 | -4.65288 | -3.61197 |
| C | 7.086943  | -6.448976 | -2.500544 | C | 7.032543 | -6.25837 | -2.67447 |
| H | 8.076647  | -6.845686 | -2.245304 | H | 8.022423 | -6.67986 | -2.46256 |
| H | 6.379184  | -6.784227 | -1.741065 | H | 6.329802 | -6.64689 | -1.93552 |
| H | 6.789391  | -6.882593 | -3.463248 | H | 6.721843 | -6.61404 | -3.66434 |
| C | 5.747925  | -4.375738 | -3.070368 | C | 5.700121 | -4.1387  | -3.05637 |
| H | 4.929344  | -4.722659 | -2.439679 | H | 4.893981 | -4.52191 | -2.43039 |
| H | 5.727793  | -3.279979 | -3.081667 | H | 5.693345 | -3.04449 | -2.99078 |
| H | 5.545802  | -4.724639 | -4.090507 | H | 5.471086 | -4.41354 | -4.09321 |
| C | 10.425443 | -2.02601  | -0.031605 | C | 10.45372 | -2.05508 | 0.056187 |
| H | 11.057177 | -2.155928 | 0.853721  | H | 11.08731 | -2.24214 | 0.929526 |
| H | 11.053194 | -2.164484 | -0.918473 | H | 11.07355 | -2.14674 | -0.84204 |
| H | 10.084261 | -0.981867 | -0.035895 | H | 10.12079 | -1.01006 | 0.114509 |
| C | 4.883266  | 7.142126  | -2.619389 | C | 4.695749 | 7.088606 | -2.67537 |
| C | 4.350499  | 5.764224  | -3.079527 | C | 4.120715 | 5.705465 | -3.06166 |
| H | 4.701979  | 4.942948  | -2.454916 | H | 4.506361 | 4.898295 | -2.43852 |
| H | 3.254667  | 5.744619  | -3.082287 | H | 3.026873 | 5.699944 | -2.99003 |
| H | 4.691277  | 5.566206  | -4.103216 | H | 4.389556 | 5.477096 | -4.10023 |
| C | 4.537492  | 8.143138  | -3.745833 | C | 4.274365 | 8.065954 | -3.79698 |
| H | 4.873818  | 9.159774  | -3.51476  | H | 4.63481  | 9.084357 | -3.61596 |
| H | 5.043292  | 7.829103  | -4.665244 | H | 4.708157 | 7.724245 | -4.74298 |
| H | 3.463457  | 8.173842  | -3.961566 | H | 3.187538 | 8.102006 | -3.93143 |
| C | 6.428694  | 7.100499  | -2.521353 | C | 6.244036 | 7.035294 | -2.69106 |

|   |           |            |           |   |          |          |          |
|---|-----------|------------|-----------|---|----------|----------|----------|
| H | 6.827578  | 8.088863   | -2.264325 | H | 6.667777 | 8.024476 | -2.48039 |
| H | 6.770381  | 6.388787   | -1.768468 | H | 6.636513 | 6.331121 | -1.95557 |
| H | 6.854097  | 6.807988   | -3.489248 | H | 6.593229 | 6.725668 | -3.68355 |
| C | 4.908267  | 7.131255   | 2.582992  | C | 5.072025 | 7.181256 | 2.520444 |
| C | 4.574765  | 8.12868    | 3.716332  | C | 4.833246 | 8.212505 | 3.647768 |
| H | 3.503088  | 8.159194   | 3.943521  | H | 3.780056 | 8.271995 | 3.943758 |
| H | 5.090052  | 7.811285   | 4.629281  | H | 5.402346 | 7.904921 | 4.531582 |
| H | 4.909132  | 9.145943   | 3.485148  | H | 5.171334 | 9.216385 | 3.36842  |
| C | 6.452648  | 7.088678   | 2.469749  | C | 6.60555  | 7.10093  | 2.31531  |
| H | 6.786463  | 6.379704   | 1.710784  | H | 6.880049 | 6.366787 | 1.556323 |
| H | 6.849894  | 8.077734   | 2.212834  | H | 7.006774 | 8.07557  | 2.012656 |
| H | 6.887092  | 6.791973   | 3.432339  | H | 7.089207 | 6.817821 | 3.258091 |
| C | 4.378908  | 5.752249   | 3.043935  | C | 4.542438 | 5.826305 | 3.047838 |
| H | 3.283146  | 5.733147   | 3.056657  | H | 3.449641 | 5.836332 | 3.133061 |
| H | 4.724258  | 4.932447   | 2.41397   | H | 4.826253 | 4.984224 | 2.416019 |
| H | 4.728924  | 5.551234   | 4.063913  | H | 4.954504 | 5.640133 | 4.047132 |
| C | 2.026983  | 10.426155  | 0.002676  | C | 2.058826 | 10.45622 | 0.068548 |
| H | 2.165721  | 11.054072  | 0.889381  | H | 2.250934 | 11.08837 | 0.941835 |
| H | 2.156669  | 11.057717  | -0.882811 | H | 2.145962 | 11.07739 | -0.82921 |
| H | 0.982833  | 10.085     | 0.007308  | H | 1.013941 | 10.12378 | 0.131987 |
| C | -4.910487 | -7.12972   | -2.58205  | C | -4.73214 | -7.08981 | -2.6344  |
| C | -4.578242 | -8.127281  | -3.715642 | C | -4.32383 | -8.06701 | -3.76094 |
| H | -5.094433 | -7.809907  | -4.628088 | H | -4.77237 | -7.72783 | -4.70094 |
| H | -3.506804 | -8.157935  | -3.943934 | H | -3.23894 | -8.09961 | -3.91108 |
| H | -4.912481 | -9.144488  | -3.484024 | H | -4.67819 | -9.08642 | -3.57371 |
| C | -6.454756 | -7.08692   | -2.467349 | C | -6.28062 | -7.04202 | -2.62682 |
| H | -6.851898 | -8.07592   | -2.210058 | H | -6.69761 | -8.03251 | -2.40891 |
| H | -6.787769 | -6.377894  | -1.708082 | H | -6.66419 | -6.33865 | -1.88588 |
| H | -6.890053 | -6.790166  | -3.429539 | H | -6.64607 | -6.73442 | -3.61409 |
| C | -4.381376 | -5.750827  | -3.043622 | C | -4.16802 | -5.70499 | -3.03102 |
| H | -4.726021 | -4.930905  | -2.413424 | H | -4.54866 | -4.89805 | -2.40445 |
| H | -3.285625 | -5.731868  | -3.057383 | H | -3.07334 | -5.69478 | -2.97429 |
| H | -4.732331 | -5.549871  | -4.06329  | H | -4.45189 | -5.47991 | -4.06627 |
| C | -4.880585 | -7.140601  | 2.62031   | C | -5.0372  | -7.17933 | 2.565162 |
| C | -6.426109 | -7.099143  | 2.523746  | C | -6.57341 | -7.10489 | 2.378813 |
| H | -6.768582 | -6.387473  | 1.771176  | H | -6.85968 | -6.37151 | 1.623423 |
| H | -6.825132 | -8.08755   | 2.267101  | H | -6.97464 | -8.0809  | 2.080649 |
| H | -6.850631 | -6.806668  | 3.492039  | H | -7.04673 | -6.8238  | 3.327432 |
| C | -4.347515 | -5.762609  | 3.079815  | C | -4.50668 | -5.82186 | 3.08507  |
| H | -3.251682 | -5.74291   | 3.08154   | H | -3.41292 | -5.8275  | 3.157391 |
| H | -4.699656 | -4.941441  | 2.455437  | H | -4.80137 | -4.98154 | 2.455889 |
| H | -4.687345 | -5.564511  | 4.103803  | H | -4.90768 | -5.63646 | 4.088987 |
| C | -4.533593 | -8.141496  | 3.74648   | C | -4.78016 | -8.20881 | 3.690066 |
| H | -4.870073 | -9.158176  | 3.515828  | H | -5.11839 | -9.21412 | 3.416088 |
| H | -3.459336 | -8.172091  | 3.961116  | H | -3.72296 | -8.26438 | 3.972208 |
| H | -5.038482 | -7.827433  | 4.666383  | H | -5.33862 | -7.90249 | 4.581068 |
| C | -2.0268   | -10.424644 | -0.004476 | C | -2.04659 | -10.4468 | 0.075478 |
| H | -2.155758 | -11.056316 | 0.881041  | H | -2.2262  | -11.0799 | 0.950754 |

|   |            |            |           |   |          |          |          |
|---|------------|------------|-----------|---|----------|----------|----------|
| H | -2.166273  | -11.052452 | -0.891142 | H | -2.14287 | -11.0678 | -0.82144 |
| H | -0.982653  | -10.083494 | -0.009922 | H | -1.00199 | -10.1113 | 0.126371 |
| C | -7.126432  | 4.906607   | 2.611575  | C | -7.17529 | 5.05774  | 2.553874 |
| C | -8.121402  | 4.571105   | 3.746463  | C | -8.20339 | 4.810677 | 3.682281 |
| H | -8.150737  | 3.499124   | 3.972399  | H | -8.25985 | 3.755781 | 3.97276  |
| H | -7.802575  | 5.085517   | 4.659408  | H | -7.89504 | 5.375715 | 4.568425 |
| H | -9.139345  | 4.905053   | 3.517691  | H | -9.20868 | 5.147993 | 3.4071   |
| C | -7.085369  | 6.451129   | 2.499641  | C | -7.09882 | 6.592466 | 2.356395 |
| H | -6.377999  | 6.786171   | 1.739708  | H | -6.36664 | 6.872336 | 1.597453 |
| H | -8.0752    | 6.847777   | 2.244799  | H | -8.07488 | 6.993066 | 2.057516 |
| H | -6.787323  | 6.885006   | 3.462075  | H | -6.81502 | 7.072016 | 3.301069 |
| C | -5.746085  | 4.37804    | 3.069389  | C | -5.81787 | 4.528697 | 3.075433 |
| H | -5.725923  | 3.282284   | 3.080907  | H | -5.82512 | 3.435472 | 3.155278 |
| H | -4.927791  | 4.724847   | 2.438264  | H | -4.97797 | 4.81768  | 2.443032 |
| H | -5.543513  | 4.727158   | 4.089364  | H | -5.63035 | 4.936277 | 4.076306 |
| C | -7.145231  | 4.886191   | -2.590804 | C | -7.0949  | 4.712464 | -2.64369 |
| C | -8.148672  | 4.542373   | -3.7157   | C | -8.07437 | 4.296278 | -3.76538 |
| H | -7.836102  | 5.049063   | -4.63512  | H | -7.73616 | 4.736895 | -4.70948 |
| H | -8.1805    | 3.468628   | -3.93268  | H | -8.10849 | 3.210263 | -3.90677 |
| H | -9.164634  | 4.879082   | -3.48222  | H | -9.09305 | 4.653358 | -3.57933 |
| C | -5.768654  | 4.3527     | -3.054066 | C | -5.71148 | 4.143167 | -3.03759 |
| H | -4.9459    | 4.702757   | -2.430603 | H | -4.90334 | 4.527067 | -2.41461 |
| H | -5.750044  | 3.256854   | -3.058041 | H | -5.70305 | 3.048924 | -2.97269 |
| H | -5.572215  | 4.694407   | -4.077752 | H | -5.48696 | 4.418931 | -4.07517 |
| C | -7.102178  | 6.43149    | -2.491442 | C | -7.04505 | 6.260912 | -2.64908 |
| H | -8.089779  | 6.830929   | -2.232352 | H | -8.03461 | 6.681024 | -2.433   |
| H | -6.388893  | 6.771971   | -1.739512 | H | -6.33986 | 6.649857 | -1.91268 |
| H | -6.811024  | 6.857495   | -3.45948  | H | -6.73872 | 6.617587 | -3.63995 |
| C | -10.425184 | 2.027506   | 0.033674  | C | -10.4501 | 2.051746 | 0.092718 |
| H | -11.0576   | 2.157423   | -0.851168 | H | -11.0729 | 2.141918 | -0.80361 |
| H | -10.08399  | 0.983366   | 0.03769   | H | -10.1154 | 1.007258 | 0.150629 |
| H | -11.052256 | 2.165969   | 0.921022  | H | -11.0812 | 2.238352 | 0.967939 |

**Data S2.** The calculated optimized geometries of dt-ZnPc.

| Optimized geometry of dt-ZnPc (in gas-phase//6-311++G(2d,2p)//Zn/gen/6-31G(d,p) |          |          |          | Optimized geometry of relaxed excited state of dt-ZnPc (in DMSO phase// B3LYP/6-31G(d)) |          |          |          |
|---------------------------------------------------------------------------------|----------|----------|----------|-----------------------------------------------------------------------------------------|----------|----------|----------|
| C                                                                               | 4.58268  | -4.73781 | -0.00768 | C                                                                                       | 1.675195 | -6.40178 | 0.125933 |
| C                                                                               | 3.474095 | -5.60634 | -0.00348 | C                                                                                       | 0.285226 | -6.61665 | 0.126855 |
| C                                                                               | 4.417714 | -3.35663 | -0.00903 | C                                                                                       | 2.208035 | -5.10023 | 0.147681 |
| C                                                                               | 2.18133  | -5.11226 | -0.00055 | C                                                                                       | -0.60488 | -5.54148 | 0.148293 |
| C                                                                               | 3.11476  | -2.87279 | -0.00601 | C                                                                                       | 1.305096 | -4.04893 | 0.172347 |
| C                                                                               | 2.002675 | -3.73072 | -0.00184 | C                                                                                       | -0.08146 | -4.25211 | 0.172724 |
| C                                                                               | 2.58669  | -1.51115 | -0.00613 | C                                                                                       | 1.518237 | -2.58151 | 0.191939 |
| C                                                                               | 0.819915 | -2.88462 | 0.000488 | C                                                                                       | -0.70707 | -2.91886 | 0.191669 |
| N                                                                               | 1.219423 | -1.57354 | -0.00221 | N                                                                                       | 0.290166 | -1.95848 | 0.204858 |
| N                                                                               | -0.42484 | -3.34542 | 0.004549 | N                                                                                       | -2.00828 | -2.73936 | 0.173626 |
| N                                                                               | 3.346282 | -0.4242  | -0.00947 | N                                                                                       | 2.714925 | -2.04307 | 0.175    |

|    |          |          |          |    |          |          |          |
|----|----------|----------|----------|----|----------|----------|----------|
| C  | -1.51178 | -2.58582 | 0.006929 | C  | -2.59389 | -1.5127  | 0.164959 |
| C  | 2.885477 | 0.820557 | -0.0094  | C  | 2.923566 | -0.6958  | 0.164749 |
| N  | -1.57418 | -1.21855 | 0.005906 | N  | -1.9753  | -0.28999 | 0.224525 |
| C  | -2.87342 | -3.11389 | 0.011232 | C  | -4.02878 | -1.31092 | 0.063814 |
| C  | -3.73135 | -2.0018  | 0.012713 | C  | -4.23309 | 0.090585 | 0.06508  |
| C  | -2.88525 | -0.81904 | 0.009246 | C  | -2.92355 | 0.695581 | 0.166254 |
| C  | -3.35725 | -4.41685 | 0.013599 | C  | -5.093   | -2.20841 | -0.03122 |
| C  | -5.11288 | -2.18045 | 0.016765 | C  | -5.52769 | 0.613137 | -0.02955 |
| C  | -4.73843 | -4.58181 | 0.01754  | C  | -6.3807  | -1.66947 | -0.12345 |
| C  | -5.60696 | -3.47322 | 0.019174 | C  | -6.5951  | -0.27182 | -0.12169 |
| N  | -3.34606 | 0.42572  | 0.009307 | N  | -2.7149  | 2.042844 | 0.177233 |
| C  | -2.58647 | 1.512668 | 0.005975 | C  | -1.5182  | 2.581259 | 0.193883 |
| N  | -1.2192  | 1.575061 | 0.002048 | N  | -0.29012 | 1.958205 | 0.205516 |
| C  | -0.81969 | 2.886139 | -0.00065 | C  | 0.707106 | 2.918617 | 0.192787 |
| C  | -2.00245 | 3.73224  | 0.001676 | C  | 0.081478 | 4.25188  | 0.175309 |
| C  | -3.11454 | 2.874305 | 0.005855 | C  | -1.30507 | 4.048693 | 0.175551 |
| N  | 0.425061 | 3.346941 | -0.00471 | N  | 2.008306 | 2.739133 | 0.174188 |
| C  | 1.512007 | 2.587343 | -0.00709 | C  | 2.593906 | 1.512481 | 0.164621 |
| N  | 1.574403 | 1.22007  | -0.00606 | N  | 1.975343 | 0.289742 | 0.224022 |
| C  | 2.873638 | 3.11541  | -0.0114  | C  | 4.028738 | 1.31074  | 0.062617 |
| C  | 3.731573 | 2.003319 | -0.01288 | C  | 4.23305  | -0.09076 | 0.063147 |
| C  | 5.113104 | 2.181973 | -0.01694 | C  | 5.527597 | -0.61327 | -0.03246 |
| C  | 3.357474 | 4.418367 | -0.01377 | C  | 5.092913 | 2.208279 | -0.03261 |
| C  | 5.607181 | 3.474742 | -0.01936 | C  | 6.594952 | 0.271726 | -0.12482 |
| C  | 4.738652 | 4.583333 | -0.01772 | C  | 6.380559 | 1.669369 | -0.12581 |
| C  | -4.41749 | 3.358146 | 0.008874 | C  | -2.20803 | 5.100028 | 0.152621 |
| C  | -2.18111 | 5.113776 | 0.000388 | C  | 0.604894 | 5.541273 | 0.151866 |
| C  | -3.47388 | 5.607858 | 0.003312 | C  | -0.28523 | 6.616465 | 0.132143 |
| C  | -4.58246 | 4.739327 | 0.007515 | C  | -1.6752  | 6.401599 | 0.132007 |
| H  | -6.67113 | -3.6611  | 0.022291 | H  | -7.61542 | 0.090485 | -0.1958  |
| H  | -5.78086 | -1.33121 | 0.017953 | H  | -5.69891 | 1.685244 | -0.03106 |
| H  | -2.68539 | -5.26046 | 0.012336 | H  | -4.92838 | -3.27906 | -0.03394 |
| H  | -5.26109 | 2.686287 | 0.01208  | H  | -3.27724 | 4.926725 | 0.150312 |
| H  | -1.33187 | 5.78176  | -0.00283 | H  | 1.676751 | 5.712668 | 0.149266 |
| H  | -3.66175 | 6.672035 | 0.002415 | H  | 0.078071 | 7.638918 | 0.115268 |
| H  | 2.685616 | 5.261977 | -0.01251 | H  | 4.928293 | 3.278927 | -0.03476 |
| H  | 6.671355 | 3.662614 | -0.02249 | H  | 7.615227 | -0.09055 | -0.19967 |
| H  | 5.781088 | 1.332728 | -0.01814 | H  | 5.698811 | -1.68538 | -0.03457 |
| H  | 1.332089 | -5.78024 | 0.002663 | H  | -1.67674 | -5.71288 | 0.146178 |
| H  | 5.26132  | -2.68477 | -0.01224 | H  | 3.277246 | -4.92693 | 0.144814 |
| H  | 3.661971 | -6.67052 | -0.00258 | H  | -0.07808 | -7.63909 | 0.109096 |
| O  | 5.367987 | 5.803555 | -0.02033 | O  | 7.523586 | 2.4248   | -0.22504 |
| O  | 5.8029   | -5.36715 | -0.01011 | O  | 2.441071 | -7.53868 | 0.101615 |
| O  | -5.36776 | -5.80204 | 0.020132 | O  | -7.52378 | -2.42486 | -0.22236 |
| O  | -5.80268 | 5.368667 | 0.009953 | O  | -2.44108 | 7.538538 | 0.10962  |
| Zn | 0.000112 | 0.00076  | -2.4E-05 | Zn | 0.00007  | -0.0002  | 0.528602 |
| C  | -4.6088  | -6.97996 | 0.018098 | C  | -7.44367 | -3.82692 | -0.24057 |
| C  | -4.28233 | -7.57233 | 1.255759 | C  | -7.55409 | -4.52342 | 0.987337 |

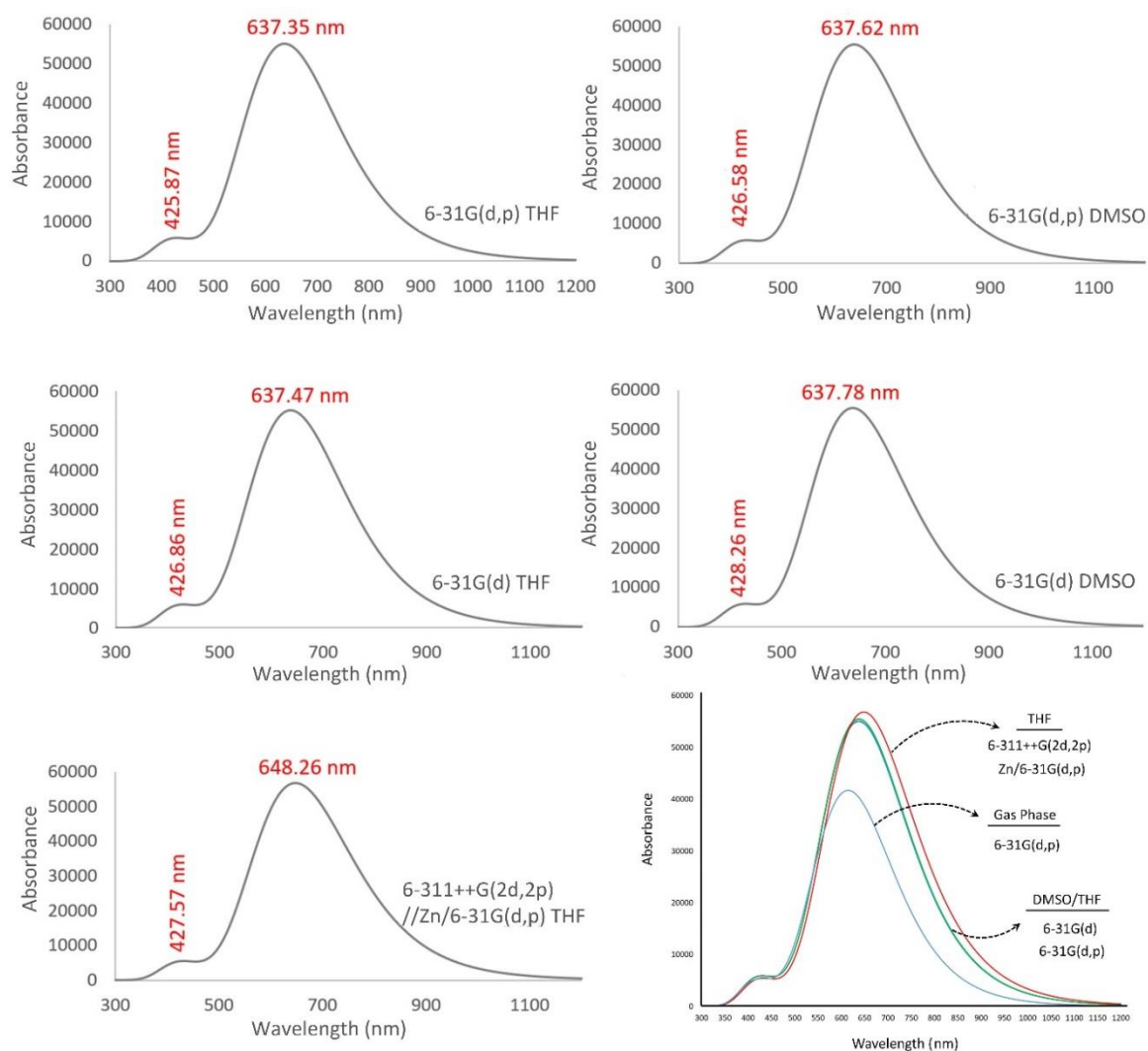
|   |          |          |          |   |          |          |          |
|---|----------|----------|----------|---|----------|----------|----------|
| C | -4.28991 | -7.57304 | -1.22119 | C | -7.35991 | -4.48094 | -1.49375 |
| C | -3.4382  | -8.68465 | 1.207072 | C | -7.37446 | -5.91334 | 0.930274 |
| C | -3.44548 | -8.68535 | -1.17698 | C | -7.18746 | -5.87246 | -1.45643 |
| C | -2.97566 | -9.22506 | 0.013773 | C | -7.14847 | -6.59676 | -0.26476 |
| H | -3.13571 | -9.16108 | 2.125523 | H | -7.42132 | -6.49497 | 1.842542 |
| H | -3.14859 | -9.16231 | -2.09699 | H | -7.08999 | -6.42276 | -2.38398 |
| C | 6.980815 | -4.60819 | -0.01487 | C | 3.843918 | -7.44894 | 0.094066 |
| C | 7.57721  | -4.28349 | 1.221323 | C | 4.526374 | -7.48192 | 1.334099 |
| C | 7.569859 | -4.28752 | -1.25562 | C | 4.510524 | -7.4349  | -1.15495 |
| C | 8.68938  | -3.43929 | 1.17022  | C | 5.915803 | -7.29753 | 1.28128  |
| C | 8.682306 | -3.44315 | -1.21383 | C | 5.900556 | -7.25217 | -1.11272 |
| C | 9.225899 | -2.97504 | -0.02417 | C | 6.61125  | -7.13898 | 0.082371 |
| H | 9.168799 | -3.13813 | 2.087548 | H | 6.487497 | -7.28647 | 2.200874 |
| H | 9.156269 | -3.14495 | -2.13496 | H | 6.460586 | -7.20616 | -2.03838 |
| C | 4.609035 | 6.981488 | -0.01828 | C | 7.44348  | 3.826873 | -0.24248 |
| C | 4.282566 | 7.573862 | -1.25594 | C | 7.358986 | 4.481542 | -1.49527 |
| C | 4.290143 | 7.574564 | 1.221012 | C | 7.554622 | 4.522745 | 0.985716 |
| C | 3.438424 | 8.686184 | -1.20724 | C | 7.186564 | 5.873042 | -1.45714 |
| C | 3.445715 | 8.686866 | 1.176818 | C | 7.374971 | 5.912689 | 0.929472 |
| C | 2.975891 | 9.226584 | -0.01394 | C | 7.148287 | 6.596728 | -0.26508 |
| H | 3.135923 | 9.162611 | -2.12568 | H | 7.08855  | 6.423817 | -2.38435 |
| H | 3.148833 | 9.163823 | 2.096823 | H | 7.422367 | 6.493853 | 1.84201  |
| C | -6.98061 | 4.609721 | 0.014719 | C | -3.84394 | 7.448851 | 0.103874 |
| C | -7.57705 | 4.285073 | -1.22146 | C | -4.5122  | 7.436228 | -1.14427 |
| C | -7.56962 | 4.289017 | 1.255485 | C | -4.52476 | 7.480462 | 1.344847 |
| C | -8.68922 | 3.440869 | -1.17035 | C | -5.90217 | 7.253483 | -1.10042 |
| C | -8.68206 | 3.444657 | 1.213707 | C | -5.91426 | 7.296147 | 1.293643 |
| C | -9.2257  | 2.976588 | 0.024042 | C | -6.61129 | 7.138962 | 0.095478 |
| H | -9.16867 | 3.139723 | -2.08766 | H | -6.46342 | 7.208514 | -2.0254  |
| H | -9.156   | 3.14642  | 2.134836 | H | -6.48475 | 7.284072 | 2.213974 |
| C | 7.129215 | -4.88311 | 2.581624 | C | 3.841949 | -7.7992  | 2.693466 |
| C | 8.126856 | -4.53068 | 3.70507  | C | 4.887601 | -8.01333 | 3.812265 |
| H | 8.154891 | -3.46103 | 3.914504 | H | 5.448454 | -7.10005 | 4.039947 |
| H | 7.812252 | -5.03118 | 4.620771 | H | 4.366521 | -8.31169 | 4.728325 |
| H | 9.139025 | -4.86531 | 3.477569 | H | 5.602278 | -8.80558 | 3.564323 |
| C | 5.750998 | -4.36029 | 3.04028  | C | 2.912993 | -6.65936 | 3.174465 |
| H | 5.729249 | -3.27008 | 3.054738 | H | 3.442316 | -5.69963 | 3.190905 |
| H | 4.938965 | -4.70505 | 2.409709 | H | 2.023553 | -6.547   | 2.553808 |
| H | 5.550359 | -4.71143 | 4.0541   | H | 2.574683 | -6.87272 | 4.195703 |
| C | 7.099484 | -6.42657 | 2.485603 | C | 3.038068 | -9.11876 | 2.580573 |
| H | 6.383587 | -6.77619 | 1.748065 | H | 2.242602 | -9.05221 | 1.836602 |
| H | 8.083218 | -6.81458 | 2.217431 | H | 3.697191 | -9.95099 | 2.306145 |
| H | 6.825952 | -6.84932 | 3.453944 | H | 2.582445 | -9.35754 | 3.549195 |
| C | 7.113804 | -4.89143 | -2.61134 | C | 3.809059 | -7.70057 | -2.51676 |
| C | 8.10512  | -4.54307 | -3.74164 | C | 4.84069  | -7.87339 | -3.65557 |
| H | 7.785206 | -5.04661 | -4.65383 | H | 4.308033 | -8.13725 | -4.57556 |
| H | 8.132224 | -3.47415 | -3.95489 | H | 5.399372 | -6.95244 | -3.85603 |
| H | 9.118479 | -4.87718 | -3.51872 | H | 5.557679 | -8.67461 | -3.4461  |

|   |          |          |          |   |          |          |          |
|---|----------|----------|----------|---|----------|----------|----------|
| C | 7.084    | -6.43455 | -2.51023 | C | 3.005094 | -9.02286 | -2.44347 |
| H | 8.069074 | -6.82211 | -2.24635 | H | 3.66669  | -9.86533 | -2.20914 |
| H | 6.372118 | -6.78157 | -1.7676  | H | 2.21934  | -8.98395 | -1.68732 |
| H | 6.804895 | -6.86025 | -3.47569 | H | 2.53685  | -9.2246  | -3.41449 |
| C | 5.733189 | -4.36945 | -3.0637  | C | 2.87586  | -6.54267 | -2.94324 |
| H | 4.924708 | -4.71151 | -2.42712 | H | 1.994359 | -6.45285 | -2.30783 |
| H | 5.711973 | -3.27928 | -3.08184 | H | 3.406324 | -5.58352 | -2.93014 |
| H | 5.52637  | -4.72402 | -4.07508 | H | 2.524763 | -6.71724 | -3.96752 |
| C | 10.38637 | -2.01093 | -0.02915 | C | 8.100228 | -6.87945 | 0.077788 |
| H | 11.01581 | -2.14009 | 0.851054 | H | 8.587267 | -7.32226 | 0.953    |
| H | 11.01015 | -2.14238 | -0.91304 | H | 8.575591 | -7.28674 | -0.82078 |
| H | 10.0359  | -0.97585 | -0.02937 | H | 8.314378 | -5.80242 | 0.097962 |
| C | 4.880265 | 7.121446 | -2.61562 | C | 7.541595 | 3.764923 | -2.86291 |
| C | 4.356923 | 5.741665 | -3.06896 | C | 6.358337 | 2.831185 | -3.21145 |
| H | 4.702566 | 4.931774 | -2.43612 | H | 6.301133 | 1.95899  | -2.55983 |
| H | 3.266692 | 5.71981  | -3.08189 | H | 5.403345 | 3.365925 | -3.15108 |
| H | 4.706722 | 5.537648 | -4.08256 | H | 6.473785 | 2.466707 | -4.23948 |
| C | 4.526118 | 8.115337 | -3.74185 | C | 7.650669 | 4.783674 | -4.02099 |
| H | 4.860966 | 9.128285 | -3.51816 | H | 8.465481 | 5.499468 | -3.86715 |
| H | 5.025338 | 7.797772 | -4.65722 | H | 7.857667 | 4.24019  | -4.94919 |
| H | 3.456168 | 8.142571 | -3.94984 | H | 6.721478 | 5.34414  | -4.17256 |
| C | 6.423856 | 7.092167 | -2.52173 | C | 8.863415 | 2.956848 | -2.85803 |
| H | 6.812157 | 8.076787 | -2.25724 | H | 9.720355 | 3.617807 | -2.68129 |
| H | 6.77461  | 6.378654 | -1.78242 | H | 8.865939 | 2.180342 | -2.09138 |
| H | 6.845245 | 6.815594 | -3.4898  | H | 9.006401 | 2.47653  | -3.83361 |
| C | 4.895956 | 7.122889 | 2.57736  | C | 7.950693 | 3.850637 | 2.330475 |
| C | 4.549226 | 8.117861 | 3.70495  | C | 8.236931 | 4.906275 | 3.423403 |
| H | 3.480619 | 8.145671 | 3.919642 | H | 7.341665 | 5.474261 | 3.699798 |
| H | 5.054065 | 7.80088  | 4.617443 | H | 8.587531 | 4.392953 | 4.325258 |
| H | 4.883037 | 9.130491 | 3.47829  | H | 9.016101 | 5.614289 | 3.120795 |
| C | 6.438934 | 7.092711 | 2.474185 | C | 9.257503 | 3.039214 | 2.145696 |
| H | 6.784901 | 6.378504 | 1.7333   | H | 9.141831 | 2.237077 | 1.415013 |
| H | 6.826154 | 8.076943 | 2.206686 | H | 10.07445 | 3.691438 | 1.814581 |
| H | 6.865972 | 6.816612 | 3.439912 | H | 9.552863 | 2.591772 | 3.102496 |
| C | 4.374569 | 5.743767 | 3.034931 | C | 6.838797 | 2.931698 | 2.889698 |
| H | 3.284423 | 5.722615 | 3.054561 | H | 5.884811 | 3.466707 | 2.962376 |
| H | 4.715797 | 4.933195 | 2.400572 | H | 6.682478 | 2.039096 | 2.283451 |
| H | 4.730458 | 5.540268 | 4.046523 | H | 7.114509 | 2.600116 | 3.89821  |
| C | 2.011789 | 10.38707 | -0.01132 | C | 6.896327 | 8.087052 | -0.27    |
| H | 2.144728 | 11.01389 | 0.870186 | H | 7.394763 | 8.581    | 0.570784 |
| H | 2.139447 | 11.01347 | -0.89391 | H | 7.249739 | 8.550545 | -1.19715 |
| H | 0.976704 | 10.03661 | -0.00814 | H | 5.823695 | 8.307695 | -0.18577 |
| C | -4.89572 | -7.12139 | -2.57754 | C | -7.54333 | -3.76362 | -2.8609  |
| C | -4.549   | -8.1164  | -3.7051  | C | -7.65305 | -4.78177 | -4.01945 |
| H | -5.05383 | -7.79943 | -4.6176  | H | -7.86065 | -4.23781 | -4.94724 |
| H | -3.4804  | -8.14423 | -3.91979 | H | -6.72391 | -5.34209 | -4.17188 |
| H | -4.88283 | -9.12901 | -3.47842 | H | -8.46771 | -5.4977  | -3.86548 |
| C | -6.4387  | -7.09119 | -2.47435 | C | -8.86518 | -2.95559 | -2.85484 |

|   |          |          |          |   |          |          |          |
|---|----------|----------|----------|---|----------|----------|----------|
| H | -6.82593 | -8.07542 | -2.20683 | H | -9.722   | -3.61667 | -2.67798 |
| H | -6.78465 | -6.37697 | -1.73348 | H | -8.86729 | -2.17949 | -2.08777 |
| H | -6.86574 | -6.81511 | -3.44008 | H | -9.00873 | -2.47475 | -3.83008 |
| C | -4.37432 | -5.74228 | -3.03515 | C | -6.3603  | -2.82967 | -3.20963 |
| H | -4.71555 | -4.93169 | -2.40081 | H | -6.30275 | -1.95781 | -2.5576  |
| H | -3.28418 | -5.72114 | -3.05478 | H | -5.40526 | -3.36441 | -3.15008 |
| H | -4.73021 | -5.53881 | -4.04674 | H | -6.47634 | -2.46466 | -4.23741 |
| C | -4.88005 | -7.11991 | 2.615434 | C | -7.94939 | -3.852   | 2.332667 |
| C | -6.42364 | -7.09058 | 2.521501 | C | -9.25626 | -3.04041 | 2.14901  |
| H | -6.77434 | -6.37704 | 1.782193 | H | -9.14093 | -2.2379  | 1.418681 |
| H | -6.81197 | -8.07518 | 2.25699  | H | -10.0734 | -3.69242 | 1.817992 |
| H | -6.84504 | -6.81401 | 3.489566 | H | -9.55108 | -2.59345 | 3.106199 |
| C | -4.35667 | -5.74016 | 3.068814 | C | -6.83715 | -2.93342 | 2.891778 |
| H | -3.26644 | -5.71834 | 3.081767 | H | -5.88315 | -3.4685  | 2.963647 |
| H | -4.70228 | -4.93024 | 2.435988 | H | -6.68113 | -2.04049 | 2.285931 |
| H | -4.70648 | -5.53616 | 4.082419 | H | -7.1123  | -2.60237 | 3.90062  |
| C | -4.52596 | -8.11384 | 3.741643 | C | -8.2351  | -4.9082  | 3.425192 |
| H | -4.86085 | -9.12677 | 3.517933 | H | -9.01449 | -5.616   | 3.122644 |
| H | -3.45601 | -8.14113 | 3.949644 | H | -7.33972 | -5.4764  | 3.700784 |
| H | -5.02517 | -7.79627 | 4.65702  | H | -8.58516 | -4.39533 | 4.327515 |
| C | -2.01155 | -10.3855 | 0.011196 | C | -6.89651 | -8.08708 | -0.2706  |
| H | -2.13981 | -11.0124 | 0.893362 | H | -7.3945  | -8.58147 | 0.570185 |
| H | -2.14389 | -11.0119 | -0.87074 | H | -7.25039 | -8.55009 | -1.19781 |
| H | -0.97647 | -10.0351 | 0.008922 | H | -5.82383 | -8.30776 | -0.18704 |
| C | -7.11349 | 4.892867 | 2.611212 | C | -3.83857 | 7.796162 | 2.703701 |
| C | -8.10475 | 4.544518 | 3.741565 | C | -4.8828  | 8.009117 | 3.824054 |
| H | -8.13188 | 3.4756   | 3.954794 | H | -5.44338 | 7.09561  | 4.051483 |
| H | -7.78476 | 5.048028 | 4.653743 | H | -4.36055 | 8.306495 | 4.739768 |
| H | -9.11811 | 4.878672 | 3.518717 | H | -5.59778 | 8.801647 | 3.577854 |
| C | -7.08362 | 6.435991 | 2.510152 | C | -3.03472 | 9.115789 | 2.591331 |
| H | -6.37177 | 6.783008 | 1.767495 | H | -2.24017 | 9.050043 | 1.84631  |
| H | -8.0687  | 6.823598 | 2.246334 | H | -3.69412 | 9.948386 | 2.31867  |
| H | -6.80445 | 6.861644 | 3.475606 | H | -2.5779  | 9.353418 | 3.559669 |
| C | -5.73286 | 4.370821 | 3.063482 | C | -2.90914 | 6.655673 | 3.18223  |
| H | -5.7117  | 3.280648 | 3.081596 | H | -3.43857 | 5.695999 | 3.198277 |
| H | -4.9244  | 4.712857 | 2.426864 | H | -2.02052 | 6.543896 | 2.560295 |
| H | -5.52597 | 4.72536  | 4.074859 | H | -2.56949 | 6.86785  | 4.203268 |
| C | -7.12908 | 4.884724 | -2.58176 | C | -3.8125  | 7.703428 | -2.50669 |
| C | -8.12665 | 4.532183 | -3.70525 | C | -4.84559 | 7.877267 | -3.64401 |
| H | -7.81208 | 5.032739 | -4.62093 | H | -4.31414 | 8.142132 | -4.56441 |
| H | -8.15453 | 3.462536 | -3.91471 | H | -5.40441 | 6.956451 | -3.8447  |
| H | -9.13887 | 4.866681 | -3.47778 | H | -5.56242 | 8.678174 | -3.43283 |
| C | -5.7508  | 4.362031 | -3.04037 | C | -2.87962 | 6.546144 | -2.93554 |
| H | -4.93882 | 4.706864 | -2.40977 | H | -1.99732 | 6.455815 | -2.30131 |
| H | -5.72895 | 3.27182  | -3.05482 | H | -3.4099  | 5.58689  | -2.92281 |
| H | -5.55016 | 4.713179 | -4.05418 | H | -2.52982 | 6.721855 | -3.96006 |
| C | -7.09951 | 6.42818  | -2.48578 | C | -3.00866 | 9.025776 | -2.43301 |
| H | -8.08329 | 6.816098 | -2.21763 | H | -3.67009 | 9.86788  | -2.19691 |

|   |          |          |          |   |          |          |          |
|---|----------|----------|----------|---|----------|----------|----------|
| H | -6.38366 | 6.777901 | -1.74823 | H | -2.22192 | 8.986169 | -1.67792 |
| H | -6.82601 | 6.850941 | -3.45412 | H | -2.54171 | 9.228646 | -3.40442 |
| C | -10.3862 | 2.012493 | 0.02906  | C | -8.10028 | 6.879467 | 0.092576 |
| H | -11.0152 | 2.141063 | -0.85157 | H | -8.57686 | 7.287965 | -0.8048  |
| H | -10.0357 | 0.977403 | 0.030167 | H | -8.31443 | 5.802416 | 0.111605 |
| H | -11.0104 | 2.144533 | 0.912532 | H | -8.58612 | 7.32113  | 0.969038 |

### 3. TDDFT calculation



**Figure S1.** The calculated UV-vis spectra of dt-ZnPc.

**Table S1.** Vertical Excitation TDDFT calculation on Pcs (eV//nm) by B3lyp/6-31G(d)

| Comp.                | Solvent | S1<br>(eV//nm) | S2<br>(eV//nm) | T1<br>(eV//nm) | T2<br>(eV//nm) | S1-T1<br>(eV//nm) | S1-T2<br>(eV//nm) |
|----------------------|---------|----------------|----------------|----------------|----------------|-------------------|-------------------|
| Pc                   | -       | 2.065//600.39  | 2.089//593.52  | 1.023//1212.39 | 1.190//1041.60 | 1.043//1188.73    | 0.875//1416.96    |
|                      | THF     | 1.982//625.49  | 1.984//625.03  | 1.003//1235.81 | 1.182//1048.56 | 0.979//1266.44    | 0.800//1549.80    |
|                      | DMSO    | 1.977//627.17  | 1.982//625.69  | 1.000//1240.29 | 1.181//1049.74 | 0.977//1269.03    | 0.796//1557.59    |
| dt-H <sub>2</sub> Pc | -       | 1.905//651.02  | 1.931//642.00  | 1.006//1232.93 | 1.168//1061.21 | 0.899//1379.13    | 0.736//1684.57    |
|                      | THF     | 1.903//651.52  | 1.929//642.60  | 0.985//1258.41 | 1.154//1074.14 | 0.918//1350.59    | 0.749//1655.33    |
|                      | DMSO    | 1.898//653.18  | 1.925//644.03  | 0.982//1263.22 | 1.152//1076.39 | 0.917//1352.06    | 0.746//1661.98    |
| dt-ZnPc              | THF     | 1.945//637.47  | 2.905//426.86  | 1.115//1111.80 | 2.591//478.57  | 0.830//1493.79    | -0.646//1919      |
|                      | DMSO    | 1.944//637.78  | 2.895//428.26  | 1.116//1110.93 | 2.588//479.11  | 0.828//1497.39    | -0.644//1925      |

**Table S2.** Vertical Excitation TDDFT calculation on Pcs (eV//nm) by B3lyp/6-311++G(2d,2p)//Zn/6-31G(d,p)

| Comp.   | Solvent | S1<br>(eV//nm) | S2<br>(eV//nm) | T1<br>(eV//nm) | T2<br>(eV//nm) | S1-T1<br>(eV//nm) | S1-T2<br>(eV//nm) |
|---------|---------|----------------|----------------|----------------|----------------|-------------------|-------------------|
| dt-ZnPc | THF     | 1.913//648.26  | 2.900//427.57  | 1.095//1132.57 | 2.584//479.85  | 0.818//1515.70    | -0.671//1847      |

**Table S3.** Adiabatic Excitation TDDFT calculation on Pcs (eV//nm) by B3lyp/6-31G(d)

| Comp.   | Solvent | S1<br>(eV//nm) | S2<br>(eV//nm) | T1<br>(eV//nm) | T2<br>(eV//nm) | S1-T1<br>(eV//nm) | S1-T2<br>(eV//nm) |
|---------|---------|----------------|----------------|----------------|----------------|-------------------|-------------------|
| dt-ZnPc | THF     | 1.699//729.87  | 2.699//459.36  | 0.839//1478.54 | 1.318//940.44  | 0.860//1441.68    | 0.380//3262.74    |
|         | DMSO    | 1.663//745.43  | 2.693//460.39  | 0.839//1477.91 | 1.319//939.89  | 0.824//1504.66    | 0.344//3604.19    |

**Table S4.** Spin-orbit coupling (SOC)-TDDFT calculation on Pcs (eV//nm) by B3lyp/6-31G(d)

| Comp.                | Solvent | S1<br>(eV//nm) | S2<br>(eV//nm) | T1<br>(eV//nm) | T2<br>(eV//nm) | S1-T1<br>(eV//nm) | S1-T2<br>(eV//nm) |
|----------------------|---------|----------------|----------------|----------------|----------------|-------------------|-------------------|
| dt-H <sub>2</sub> Pc | THF     | 1.895//654.27  | 2.669//464.53  | 0.976//1270.33 | 1.146//1.146   | 0.919//1349.12    | 0.749//1655       |
| dt-ZnPc              | THF     | 1.931//642.07  | 2.886//429.61  | 1.101//1126.10 | 2.565//483.37  | 0.830//1493.78    | -0.634//1956      |

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