Supporting Information

Activity-Based Photosensitizers with Optimized Triplet State Characteristics Toward Cancer Cell Selective and Image Guided Photodynamic Therapy

Eda Kilic, a,§ Zubeyir Elmazoglu, b,§ Toghrul Almammadov, a Dilay Kepil, b Thibaud Etienne, c Antoine Marion, b Gorkem Gunbas, b,* Safacan Kolemen a,d,e,f,g

a Department of Chemistry, Koç University, 34450 Istanbul, Turkey
b Department of Chemistry, Middle East Technical University (METU), 06800, Ankara, Turkey
c Université de Lorraine, CNRS, LPCT, F-54000 Nancy, France
d Surface Science and Technology Center (KUYTAM), Koç University, 34450 Istanbul, Turkey
e Boron and Advanced Materials Application and Research Center, Koç University, 34450 Istanbul, Turkey
f TUPRAS Energy Center (KUTEM), Koç University, 34450 Istanbul, Turkey
g E.K. and Z.E. contributed equally to this paper.

*Email: ggunbas@metu.edu.tr ; skolemen@ku.edu.tr
Materials and Methods

All reagents were commercially available and used without further purification unless otherwise noted. All dry solvents used in reactions were directly obtained from the Mbraun MBSPS5 solvent drying system. The inert atmosphere was obtained by Argon. The $^1$H and $^{13}$C-NMR spectra were recorded on a Varian (500 MHz) or Bruker Avance III Ultrashield (400 MHz) spectrometers using CDCl$_3$ or d$_6$-DMSO as the solvents. The chemical shifts are reported in parts per million (ppm) downfield from an internal TMS (trimethylsilane) reference. Coupling constants ($J$) are reported in hertz (Hz), and the spin multiplicities were specified by the following symbols: s (singlet), d (doublet), t (triplet), and m (multiplet). NMR spectra were processed with MestReNova program. Column chromatography was performed by using thick-walled glass columns and silica Gel 60 (Merck 230–400 mesh). Thin layer chromatography (TLC Merck Silica Gel 60 F254) was performed by using commercially prepared 0.25 mm silica gel plates and visualization was provided by UV lamp. The relative proportions of solvents in chromatography solvent mixtures refer to the volume: volume ratio. Electronic absorption spectra in solution were acquired using a Shimadzu Uv-3600 Uv-Vis-NIR spectrophotometer. Mass spectra were recorded on Waters Synapt G1 High-Definition mass spectrometer. HPLC analysis was performed on an Agilent 1260 series.

1. Photophysical Characterization

Unless otherwise stated, all the absorbance and fluorescence measurements were made according to the following procedure. In a 3-mL quartz cell of 1-cm optical length, 10 μM of the stock solution of DCM, DCM$_2$-I and I-DCM$_2$-Cl was dissolved in DMSO–PBS buffer (10 mM, pH 7.4, 1:1, v/v) at 37 °C. In all fluorescence measurements, both excitation and emission slit widths were set to 10 nm.

Figure S1 (a) Absorption and (b) fluorescence emission spectra of DCM$_2$-I in aqueous solutions with different pH values.

Figure S2 (a) Absorption and (b) fluorescence emission spectra of I-DCM$_2$-Cl in aqueous solutions with different pH values.
Table S1 Photophysical parameters and $^1\text{O}_2$ quantum yields of DCM derivatives.

|            | $\lambda_{\text{abs}}$ (nm) | $\lambda_{\text{em}}$ (nm) | $\epsilon$ (M$^{-1}$cm$^{-1}$) | $\phi_F$ (%) | $\phi_{\Delta}$ (%) |
|------------|-----------------------------|-----------------------------|---------------------------------|--------------|---------------------|
| DCM        | 560                         | 705                         | 20600                           | 58           | n.d.                |
| DCM$_{O}$-I| 555                         | 728                         | 22750                           | 24           | 5.2                 |
| I-DCM$_{O}$-Cl| 560             | 738                         | 11500                           | 6            | 0.6                 |

(a) The fluorescence quantum yield measurement was carried out using B-DCM-N in DCM (quantum yield was reported as 0.5958 in DCM$^2$). All experiments were done in DMSO (containing 1% PBS). For fluorescence measurement all spectra were collected with a slit width: (10/10).

Chemical Detection of Singlet Oxygen

Singlet oxygen generation of DCM, DCM$_{O}$-I and I-DCM$_{O}$-Cl was determined by using 1,4-diphenylbenzofuran (DPBF) in DMSO–PBS buffer (10 mM, pH 7.4, 1:1, v/v). Methylene blue ($\Phi_{\Delta} = 0.49$ in DMSO$^3$) was used as a reference compound for singlet oxygen quantum yield calculations. DCM, DCM$_{O}$-I or I-DCM$_{O}$-Cl were mixed in oxygen bubbled PBS and DMSO. The solutions were exposed to LED light source of 630 nm from 15 cm of distance and 20 second time interval for all the samples. The absorbance of DPBF was determined after each irradiation to evaluate producing $^1\text{O}_2$. Singlet oxygen quantum yields were calculated according to the equation given below:

$$\phi_{\Delta\text{sample}} = \phi_{\Delta\text{standard}} \left( \frac{1 - 10^{-\Delta A_{\text{std}}}}{1 - 10^{-\Delta A_{\text{sam}}}} \right) \left( \frac{m_{\text{sample}}}{m_{\text{standard}}} \right)$$

where sample and standard represent DCM, DCM$_{O}$-I or I-DCM$_{O}$-Cl and methylene blue respectively. $m$ is the slope of absorbance maxima of DPBF at 414 nm versus time graph. $A$ is the absorbance value of both sample and standard at irradiation wavelength, 630 nm.

Figure S3 (a) Absorption spectra of DPBF upon irradiating DCM$_{O}$-I (10 µM) containing DMSO solution (1% PBS, pH 7.4) with a 630 nm LED light. (b) change in the absorption signal of DPBF at 414 nm upon irradiation with 630 nm LED light.
Figure S4 Change in the absorption spectra of (a) DCM and (c) I-DCM<sub>0</sub>-Cl in 1% PBS/DMSO (1:99) solution containing DPBF trap molecule upon irradiation with a 630 nm LED light; (b), (d) change in the absorption signal of DPBF at 414 nm upon irradiation (b) DCM and (d) I-DCM<sub>0</sub>-Cl with 630 nm.

Figure S5 (a) Absorption spectra of DPBF upon irradiating methylene blue containing DMSO solution (1% PBS, pH 7.4) with a 630 nm LED light. (b) change in the absorption signal of DPBF at 414 nm upon irradiation with 630 nm LED light.
Figure S6 (a) Absorption spectra of DPBF upon irradiating DCM₀-I-Cys containing DMSO solution (1% PBS, pH 7.4) with a 630 nm LED light. (b) change in the absorption signal of DPBF at 414 nm upon irradiation with 630 nm LED light.

Figure S7 (a) Absorption spectra of DPBF upon irradiating DCM₀-I-Cys + Cys containing DMSO solution (1% PBS, pH 7.4) with a 630 nm LED light. (b) change in the absorption signal of DPBF at 414 nm upon irradiation with 630 nm LED light.

Fluorescence Quantum Yield Calculation

The fluorescence quantum yield measurements of DCM₀-I and I-DCM₀-Cl were carried out using B-DCM-N (quantum yield was reported as 59.58% in DCM) as the reference. For both measurements, the samples were dissolved in DMSO (10 mM, containing 1% PBS) and absorbance values of samples at their excitation wavelengths were kept less than 0.1.

The fluorescence quantum yield ($\phi_F$) was calculated by using the following formula:

$$QY_{\text{sample}} = QY_{\text{standard}} \frac{F_{\text{sample}} A_{\text{standard}} n_{\text{sample}}^2}{F_{\text{standard}} A_{\text{sample}} n_{\text{standard}}^2}$$

where $QY_{\text{sample}}$ and $QY_{\text{standard}}$ are the fluorescence quantum yields of the sample and the standard (B-DCM-N), respectively. $F_{\text{sample}}$ and $F_{\text{standard}}$ are the integrated fluorescence emission of the sample, $A_{\text{sample}}$ and $A_{\text{standard}}$ represent the absorbance of the sample and standard at their respective excitation wavelengths. Measurements were carried out in 1 cm quartz cuvettes with a total sample volume of 3 mL.
2. HPLC Analysis:

HPLC analysis was performed using RP-HPLC System with UV-Vis detection and a reversed-phase C18 column (4 μm, 4.6 × 150 mm). The data collect and analysis was carried out using the Chemstation software. The oven temperature was maintained at 25 °C, the injection volume was 20 μL and the flow rate was 1.0 mL/min with detection wavelength at 480 nm. The separation program of gradient elution was as follows; where solvent A was water with 0.1% TFA and solvent B was acetonitrile.

Table S2 RP-HPLC Conditions

| Time/min | Phase A/% | Phase B/% |
|----------|-----------|-----------|
| 0        | 10.0      | 5.0       |
| 7.0      | 5.0       | 95.0      |
| 13.0     | 5.0       | 95.0      |
| 16.0     | 95.0      | 5.0       |

Figure S8 HPLC chromatograms of DCM$_2$-I-Cys before and after treatment with either 10 μM Cys or 100 μM Cys at 37 °C and DCM$_2$-I.
3. Activation Mechanism of DCM\textsubscript{O}-I-Cys in presence of Cysteine

Figure S9 Proposed activation mechanism of DCM\textsubscript{O}-I-Cys in the presence of Cys.

Figure S10 Absorbance (left) and fluorescence (right) spectra of DCM\textsubscript{O}-I-Cys (10 \textmu M) before and after addition of Cys (100 \textmu M) or GSH (100 \textmu M). Measurements were performed in DMSO–PBS buffer (10 mM, pH 7.4, 1:1, v/v) at 37 °C at 37 °C. Excitation 555 nm with slit width (10, 10).
4. Cell Culture and Treatments

Table S3 IC₅₀ values of DCM₁₀-I and DCM₁₀-I-Cys in HeLa and L929 cells.

|        | HeLa  | DCM₁₀-I | DCM₁₀-I-Cys | L929  | DCM₁₀-I | DCM₁₀-I-Cys |
|--------|-------|---------|-------------|-------|---------|-------------|
| 2 h    | 3.74 µM | 4.33 µM |             | 8.96 µM | 10 µM < |             |
| 1 h    | 6.32 µM | 6.11 µM |             | 9. 10 µM | 10 µM < |             |

Figure S11 Cell viability of HeLa cells treated with the IC₅₀ values of DCM₁₀-I (3.74 µM) or DCM₁₀-I-Cys (4.33 µM) for 2 h at dark, followed by 2 h LED light (595 nm 9.83 mW/cm²) illumination in the presence or absence of NaN₃ (1-10 mM) or NAC (1-10 mM) and then dark incubation up to 24 h. Ctrl(v): vehicle control, NAC: N-acetylcysteine, NaN₃: sodium azide. (n=5-6).

*p<0.05, †p<0.01, ‡p<0.001 vs IC₅₀.
Figure S12 Time dependent cellular internalization of DCM\textsubscript{O}-I in HeLa cells after 30 min (A1-3), 1 h (B1-3), 2 h (C1-3). Blue: Hoechst 33342; red: DCM\textsubscript{O}-I. Scale bar: 10 µm.

Figure S13 Time dependent cellular internalization of DCM\textsubscript{O}-I (A-C) and DCM\textsubscript{O}-I-Cys (D-F) in L929 cells after 30 min (A1-3, D1-3), 1 h (B1-3, E1-3), 2 h (C1-3, F1-3). Blue: Hoechst 33342; red: DCM\textsubscript{O}-I or DCM\textsubscript{O}-I-Cys. Scale bar: 10 µm.
5. Computational Studies:

TDDFT benchmark

A benchmark of density functionals and basis sets was conducted to determine the method of choice for the present study. The data is available Table S4-S5 and a summary is presented in Table S6. In the latter, we report the error made by the respective methods for the energy difference between bright singlet states of DCM\textsubscript{o-I} in DMSO compared to the experimental spectrum. We notice that the topology of the excited states does not change from one method to another (data not shown), and that only the energies and ordering of the states vary. Only the range-separated double-hybrid functionals with spin-component or spin-opposite scaling SCS/SOC-\ensuremath{\omega}PBEPP\ensuremath{\omega}6 reproduce accurately the energy difference between the ground state (S0) and the first excited singlet state (S1), with an error of 0.023 eV. The difference in energy between S1 and S2, as well as that between S2 and the third bright state (i.e., S3 or S4 depending on the method, further referred to as S3/4), are significantly over-estimated by the method with errors of 0.424 and 0.382 eV, respectively. The double-hybrid range separated functional with spin-component scaling B97X-2 significantly underestimates the S0-S1 energy difference and gives an unsatisfactory picture of the excited states. Other range-separated and double-hybrid range-separated functionals tested in this study were also found unsatisfactory. The hybrid functionals B3LYP, PBE0, and TPSSH, however, yield a fair prediction of the energy of S1 relative to the ground state, and offer the best energy difference between excited states over the methods tested in this benchmark. B3LYP slightly over-estimates the energy gap between S0 and S1 by 0.281 eV. The difference between S1-S2 and S2-S3/4 is, however, very well-reproduced by the method with errors compared to experiments of only 0.003 and -0.069 eV, respectively. Additionally, we find that B3LYP reproduces fairly well the solvent-induced red-shift on the absorption spectrum compared to other functional, while the choice of basis set only has a limited impact on the results (Table S4-S5).

Based on a Wigner distribution around the ground state minimum geometry of DCM\textsubscript{o-I} at 300 K, we calculated the absorption spectrum of the molecule at the B3LYP/aug-cc-pVDZ/cc-pVTZ-DK (iodine)/CPCM(DMSO) level and present it in Figure S14. The experimental and theoretical spectra are normalized to the intensity of the brightest peak, corresponding to the S0-S1 absorption. The sticks corresponding to the absorption in the minimum geometry are also shown in the figure, and a decomposition of the spectrum is given in terms of the different singlet states. Because S3 and S4 are very close in energy, their order is often inverted with distortion of the geometry through the Wigner distribution. One of them, nevertheless, is always dark while this other one is bright. The contribution of the third bright state is therefore referred to as S3/4. Considering vibrational distortion at 300 K broadens and red shifts all peaks, resulting in a predicted spectrum in fairly good agreement with the experimental one.
Table S4 Benchmark of the energy (in eV) of the first 6 singlet states of DCM$_{\text{r}}$-I. The basis set is given for H, C, N, O, and that of iodine was (aug-cc-pVTZ-DK in all cases, with diffuse functions added consistently with the main basis set. For aug-cc-pVDZ*, diffuse functions on iodine were omitted. The time is the user time on 4 cores on Intel(R) Xeon(R) Gold 6258R CPU@2.70GHz. The oscillator strength for each state is given in parenthesis. For comparison, the first three bright states of DCM$_{\text{r}}$-I in DMSO are found experimentally at 1.9 eV, 2.9 eV, and 3.1 eV. “g.p.” stands for gas phase.

| DFT | Basis set | Solvent | S1 | S2 | S3 | S4 | S5 | S6 | Time (min) |
|-----|-----------|---------|----|----|----|----|----|----|------------|
| bp86 | cc-pVDZ   | g.p.    | 1.809(0.00) | 1.910(0.43) | 2.551(0.62) | 2.666(0.00) | 2.674(0.05) | 2.817(0.22) | 4.5 |
| bp86 | cc-pVTZ   | g.p.    | 1.851(0.00) | 1.901(0.46) | 2.539(0.53) | 2.615(0.16) | 2.719(0.00) | 2.796(0.20) | 9.2 |
| bp86 | aug-cc-pVDZ | g.p.    | 1.872(0.00) | 1.895(0.49) | 2.525(0.54) | 2.604(0.16) | 2.740(0.00) | 2.762(0.22) | 12.8 |
| bp86 | aug-cc-pVDZ* | g.p.    | 1.868(0.00) | 1.892(0.49) | 2.522(0.51) | 2.596(0.18) | 2.735(0.00) | 2.757(0.22) | 10.4 |
| bp86 | aug-cc-pVTZ | g.p.    | 1.880(0.00) | 1.894(0.50) | 2.525(0.51) | 2.597(0.19) | 2.750(0.00) | 2.763(0.21) | 30.6 |
| bp86 | cc-pVDZ   | DMSO    | 1.968(1.02) | 2.153(0.00) | 2.673(0.60) | 2.831(0.02) | 2.948(0.19) | 3.163(0.00) | 5.2  |
| bp86 | cc-pVTZ   | DMSO    | 1.951(1.06) | 2.245(0.00) | 2.674(0.58) | 2.770(0.01) | 2.914(0.21) | 3.114(0.00) | 10.4 |
| bp86 | aug-cc-pVDZ | DMSO    | 1.941(1.11) | 2.297(0.00) | 2.669(0.55) | 2.762(0.01) | 2.899(0.22) | 3.109(0.00) | 11.1 |
| bp86 | aug-cc-pVDZ* | DMSO    | 1.940(1.10) | 2.294(0.00) | 2.667(0.55) | 2.754(0.02) | 2.898(0.22) | 3.102(0.00) | 12.6 |
| bp86 | aug-cc-pVTZ | DMSO    | 1.940(1.11) | 2.305(0.00) | 2.668(0.55) | 2.755(0.02) | 2.897(0.22) | 3.095(0.00) | 31.5 |
| pbe  | cc-pVDZ   | g.p.    | 1.782(0.00) | 1.907(0.43) | 2.549(0.61) | 2.638(0.00) | 2.668(0.06) | 2.818(0.22) | 4.6  |
| pbe  | cc-pVTZ   | g.p.    | 1.823(0.00) | 1.899(0.46) | 2.536(0.50) | 2.610(0.19) | 2.691(0.00) | 2.798(0.21) | 9.5  |
| pbe  | aug-cc-pVDZ | g.p.    | 1.847(0.00) | 1.892(0.49) | 2.522(0.52) | 2.599(0.17) | 2.713(0.00) | 2.757(0.23) | 14.1 |
| pbe  | aug-cc-pVDZ* | g.p.    | 1.844(0.00) | 1.889(0.48) | 2.517(0.48) | 2.590(0.21) | 2.708(0.00) | 2.751(0.23) | 11.6 |
| pbe  | aug-cc-pVTZ | g.p.    | 1.854(0.00) | 1.890(0.49) | 2.520(0.48) | 2.591(0.22) | 2.722(0.00) | 2.756(0.22) | 33.4 |
| pbe  | cc-pVDZ   | DMSO    | 1.966(1.01) | 2.123(0.00) | 2.670(0.61) | 2.823(0.02) | 2.947(0.20) | 3.131(0.00) | 5.0  |
| pbe  | cc-pVTZ   | DMSO    | 1.949(1.05) | 2.211(0.00) | 2.673(0.58) | 2.762(0.01) | 2.915(0.21) | 3.096(0.00) | 10.2 |
| pbe  | aug-cc-pVDZ | DMSO    | 1.939(1.10) | 2.268(0.00) | 2.666(0.56) | 2.754(0.02) | 2.898(0.22) | 3.093(0.00) | 12.3 |
| pbe  | aug-cc-pVDZ* | DMSO    | 1.938(1.09) | 2.265(0.00) | 2.664(0.56) | 2.745(0.02) | 2.897(0.22) | 3.083(0.00) | 11.3 |
| pbe  | aug-cc-pVTZ | DMSO    | 1.937(1.10) | 2.274(0.00) | 2.665(0.55) | 2.745(0.02) | 2.896(0.22) | 3.074(0.00) | 46.3 |
| tpss | cc-pVDZ   | g.p.    | 1.940(0.00) | 1.975(0.49) | 2.645(0.72) | 2.788(0.04) | 2.842(0.00) | 2.921(0.16) | 4.9  |
| tpss | cc-pVTZ   | g.p.    | 1.969(0.52) | 1.983(0.00) | 2.638(0.68) | 2.731(0.08) | 2.898(0.00) | 2.904(0.15) | 11.5 |
| tpss | aug-cc-pVDZ | g.p.    | 1.960(0.55) | 2.000(0.00) | 2.620(0.69) | 2.720(0.08) | 2.862(0.16) | 2.912(0.00) | 14.8 |
| Method  | Basis Set  | Temperature (K) | Pressure (bar) |
|---------|------------|-----------------|----------------|
|          | tpss       | 1958(0.54)      | 997(0.00)      |
|          | aug-cc-pVDZ | 2.617(0.67)     | 2.711(0.09)    |
|          | aug-cc-pVTZ | 2.857(0.17)     | 2.907(0.00)    |
|          | cc-pVDZ    | 2.026(1.10)     | 2.293(0.00)    |
|          | cc-pVTZ    | 2.760(0.60)     | 2.950(0.06)    |
|          | aug-cc-pVDZ | 2.433(0.00)     | 2.755(0.54)    |
|          | aug-cc-pVTZ | 2.431(0.00)     | 2.754(0.55)    |
|          | aug-cc-pVDZ* | 1.999(1.17)    | 2.011(1.14)    |
|          | aug-cc-pVTZ | 2.011(1.14)     | 2.386(0.00)    |
| m06L    | cc-pVDZ    | 2.056(0.54)     | 2.141(0.00)    |
| m06L    | cc-pVTZ    | 2.045(0.57)     | 2.186(0.00)    |
| m06L    | aug-cc-pVDZ | 2.034(0.59)     | 2.188(0.00)    |
| m06L    | aug-cc-pVTZ | 2.033(0.58)     | 2.186(0.00)    |
| m06L    | aug-cc-pVDZ* | 2.033(0.60)    | 2.210(0.00)    |
| m06L    | cc-pVDZ    | 2.103(1.14)     | 2.488(0.00)    |
| m06L    | cc-pVTZ    | 2.087(1.19)     | 2.598(0.00)    |
| m06L    | aug-cc-pVDZ | 2.071(1.20)     | 2.595(0.00)    |
| m06L    | aug-cc-pVTZ | 2.072(1.20)     | 2.595(0.00)    |
| m06L    | aug-cc-pVDZ* | 2.073(1.23)    | 2.646(0.00)    |
| b3lyp   | cc-pVDZ    | 2.268(0.95)     | 2.817(0.00)    |
| b3lyp   | cc-pVTZ    | 2.248(0.97)     | 2.853(0.00)    |
| b3lyp   | aug-cc-pVDZ | 2.229(1.02)     | 2.867(0.00)    |
| b3lyp   | aug-cc-pVDZ* | 2.227(1.00)    | 2.862(0.00)    |
| b3lyp   | aug-cc-pVTZ | 2.227(1.01)     | 2.875(0.00)    |
| b3lyp   | cc-pVDZ    | 2.225(1.50)     | 3.189(0.00)    |
| b3lyp   | cc-pVTZ    | 2.200(1.51)     | 3.196(0.40)    |
| b3lyp   | aug-cc-pVDZ | 2.181(1.55)     | 3.185(0.38)    |
| b3lyp   | aug-cc-pVDZ* | 2.181(1.54)    | 3.184(0.39)    |
| b3lyp   | aug-cc-pVTZ | 2.181(1.55)     | 3.185(0.38)    |
| b3lyp   | cc-pVDZ    | 2.351(1.08)     | 3.000(0.00)    |
| pbe0    | cc-pVDZ    | 3.000(0.00)     | 3.139(0.63)    |

S12
| DFT       | Basis set | solvent | S1         | S2         | S3         | S4         | S5         | S6         | time (min) |
|-----------|-----------|---------|------------|------------|------------|------------|------------|------------|------------|
| m062x     | cc-pVDZ   | g.p.    | 2.503(1.53)| 3.605(0.28)| 3.678(0.00)| 3.870(0.20)| 4.076(0.00)| 4.316(0.01)| 12.6       |
| m062x     | cc-pVTZ   | g.p.    | 2.478(1.54)| 3.603(0.26)| 3.735(0.00)| 3.845(0.20)| 4.150(0.00)| 4.252(0.04)| 39.8       |
| m062x     | aug-cc-pVDZ| g.p.    | 2.445(1.54)| 3.543(0.24)| 3.671(0.00)| 3.711(0.00)| 3.809(0.21)| 3.917(0.00)| 59.1       |
| m062x     | aug-cc-pVDZ*| g.p.    | 2.446(1.53)| 3.539(0.24)| 3.666(0.00)| 3.707(0.00)| 3.810(0.21)| 3.922(0.00)| 56.1       |
| m062x     | aug-cc-pVTZ| g.p.    | 2.450(1.55)| 3.569(0.23)| 3.722(0.00)| 3.750(0.00)| 3.819(0.21)| 3.964(0.00)| 431.4      |

**Table S5** Table S4 Continued
| m062x | cc-pVDZ | DMSO | 2.378(1.81) | 3.750(0.26) | 3.929(0.21) | 4.053(0.00) | 4.140(0.00) | 4.386(0.11) | 16.7 |
|------|--------|------|-------------|-------------|-------------|-------------|-------------|-------------|-----|
| m062x | cc-pVTZ | DMSO | 2.354(1.81) | 3.717(0.27) | 3.934(0.19) | 4.163(0.00) | 4.236(0.00) | 4.309(0.09) | 39.2 |
| m062x | aug-cc-pVDZ | DMSO | 2.329(1.82) | 3.675(0.27) | 3.892(0.18) | 4.066(0.00) | 4.161(0.00) | 4.213(0.13) | 60.4 |
| m062x | aug-cc-pVDZ* | DMSO | 2.329(1.82) | 3.675(0.27) | 3.890(0.18) | 4.122(0.00) | 4.160(0.00) | 4.233(0.12) | 52.3 |
| cam-b3lyp | cc-pVDZ | g.p. | 2.551(1.57) | 3.699(0.24) | 3.734(0.00) | 3.895(0.21) | 4.147(0.00) | 4.354(0.04) | 17.5 |
| cam-b3lyp | cc-pVTZ | g.p. | 2.519(1.57) | 3.679(0.23) | 3.772(0.00) | 3.866(0.22) | 4.200(0.00) | 4.266(0.05) | 43.2 |
| cam-b3lyp | aug-cc-pVDZ | g.p. | 2.488(1.60) | 3.645(0.20) | 3.783(0.00) | 3.840(0.23) | 3.940(0.00) | 4.096(0.00) | 49.6 |
| cam-b3lyp | aug-cc-pVDZ* | g.p. | 2.488(1.58) | 3.640(0.20) | 3.777(0.00) | 3.840(0.23) | 3.977(0.00) | 4.191(0.00) | 37.9 |
| cam-b3lyp | aug-cc-pVTZ | g.p. | 2.488(1.59) | 3.646(0.20) | 3.791(0.00) | 3.840(0.23) | 3.940(0.00) | 4.082(0.00) | 275.4 |
| cam-b3lyp | cc-pVDZ | DMSO | 2.433(1.84) | 3.780(0.26) | 4.028(0.19) | 4.143(0.00) | 4.202(0.00) | 4.389(0.10) | 14.9 |
| cam-b3lyp | cc-pVTZ | DMSO | 2.404(1.84) | 3.742(0.27) | 4.012(0.18) | 4.237(0.00) | 4.279(0.00) | 4.310(0.10) | 45.3 |
| cam-b3lyp | aug-cc-pVDZ | DMSO | 2.380(1.85) | 3.709(0.27) | 3.995(0.16) | 4.160(0.00) | 4.236(0.12) | 4.282(0.00) | 66.0 |
| cam-b3lyp | aug-cc-pVDZ* | DMSO | 2.380(1.85) | 3.710(0.28) | 3.992(0.16) | 4.234(0.00) | 4.252(0.10) | 4.278(0.00) | 68.2 |
| cam-b3lyp | aug-cc-pVTZ | DMSO | 2.381(1.85) | 3.709(0.27) | 3.994(0.16) | 4.179(0.00) | 4.231(0.12) | 4.289(0.00) | 250.3 |
| wb97x-d3bj | cc-pVDZ | g.p. | 2.621(1.75) | 4.002(0.13) | 4.120(0.00) | 4.279(0.25) | 4.501(0.00) | 4.561(0.10) | 17.3 |
| wb97x-d3bj | cc-pVTZ | g.p. | 2.590(1.74) | 3.969(0.13) | 4.156(0.00) | 4.253(0.23) | 4.483(0.11) | 4.532(0.00) | 36.7 |
| wb97x-d3bj | aug-cc-pVDZ | g.p. | 2.555(1.75) | 3.932(0.12) | 4.168(0.00) | 4.223(0.20) | 4.280(0.00) | 4.368(0.15) | 48.4 |
| wb97x-d3bj | aug-cc-pVDZ* | g.p. | 2.556(1.74) | 3.931(0.12) | 4.163(0.00) | 4.221(0.21) | 4.306(0.00) | 4.392(0.13) | 49.8 |
| wb97x-d3bj | aug-cc-pVTZ | g.p. | 2.558(1.75) | 3.932(0.12) | 4.171(0.00) | 4.224(0.19) | 4.261(0.00) | 4.364(0.15) | 483.5 |
| wb97x-d3bj | cc-pVDZ | DMSO | 2.506(1.94) | 3.937(0.26) | 4.443(0.09) | 4.536(0.24) | 4.536(0.00) | 4.561(0.00) | 19.2 |
| wb97x-d3bj | cc-pVTZ | DMSO | 2.479(1.93) | 3.896(0.27) | 4.389(0.04) | 4.480(0.26) | 4.609(0.00) | 4.630(0.00) | 42.4 |
| wb97x-d3bj | aug-cc-pVDZ | DMSO | 2.455(1.94) | 3.860(0.28) | 4.332(0.00) | 4.430(0.29) | 4.503(0.00) | 4.671(0.00) | 72.5 |
| wb97x-d3bj | aug-cc-pVDZ* | DMSO | 2.455(1.94) | 3.860(0.28) | 4.341(0.01) | 4.439(0.27) | 4.562(0.00) | 4.668(0.00) | 67.3 |
| wb97x-d3bj | aug-cc-pVTZ | DMSO | 2.458(1.94) | 3.861(0.28) | 4.328(0.00) | 4.426(0.29) | 4.517(0.00) | 4.676(0.00) | 249.5 |
| RSX-ODH | cc-pVDZ | g.p. | 2.688(1.80) | 4.175(0.13) | 4.371(0.00) | 4.459(0.23) | 4.746(0.13) | 4.879(0.00) | 28.2 |
| RSX-ODH | cc-pVTZ | g.p. | 2.653(1.79) | 4.130(0.13) | 4.426(0.19) | 4.388(0.00) | 4.649(0.17) | 4.900(0.00) | 92.3 |
| RSX-ODH | aug-cc-pVDZ | g.p. | 2.624(1.79) | 4.095(0.12) | 4.439(0.04) | 4.495(0.01) | 4.508(0.31) | 4.724(0.00) | 90.4 |
| Method          | Model    | g.p. | 2.625(1.79) | 4.093(0.12) | 4.405(0.10) | 4.525(0.00) | 4.541(0.25) | 4.400(0.01) | 82.2   |
|-----------------|----------|------|-------------|-------------|-------------|-------------|-------------|-------------|--------|
| RSX-0DH         | aug-cc-pVDZ* | g.p. | 2.623(1.79) | 4.093(0.12) | 4.513(0.00) | 4.419(0.04) | 4.501(0.32) | 4.395(0.00) | 346.4  |
| RSX-0DH         | aug-cc-pVTZ | g.p. | 2.576(1.96) | 4.100(0.24) | 4.629(0.03) | 4.708(0.33) | 4.955(0.00) | 4.821(0.00) | 30.5   |
| RSX-0DH         | cc-pVDZ   | DMSO | 2.546(1.95) | 4.051(0.25) | 4.559(0.01) | 4.637(0.34) | 4.992(0.00) | 4.891(0.00) | 95.9   |
| RSX-0DH         | cc-pVTZ   | DMSO | 2.525(1.95) | 4.018(0.26) | 4.495(0.01) | 4.593(0.33) | 4.840(0.00) | 5.106(0.00) | 102.7  |
| RSX-0DH         | aug-cc-pVDZ | DMSO | 2.525(1.95) | 4.018(0.26) | 4.507(0.00) | 4.600(0.32) | 4.893(0.00) | 5.133(0.00) | 95.5   |
| RSX-0DH         | aug-cc-pVTZ* | DMSO | 2.525(1.95) | 4.017(0.26) | 4.491(0.01) | 4.586(0.32) | 4.861(0.00) | 5.109(0.00) | 336.4  |
| wPBEPP86        | cc-pVDZ   | g.p. | 2.326(1.56) | 3.677(0.11) | 3.742(0.22) | 3.586(0.00) | 4.351(0.10) | 4.573(0.00) | 23.0   |
| wPBEPP86        | cc-pVTZ   | g.p. | 2.280(1.53) | 3.616(0.11) | 3.705(0.19) | 4.221(0.13) | 3.569(0.00) | 4.618(0.00) | 87.7   |
| wPBEPP86        | aug-cc-pVDZ | g.p. | 2.261(1.54) | 3.586(0.10) | 4.111(0.00) | 3.771(0.09) | 4.031(0.25) | 4.367(0.00) | 72.6   |
| wPBEPP86        | aug-cc-pVDZ* | g.p. | 2.261(1.53) | 3.583(0.10) | 4.115(0.00) | 3.733(0.13) | 4.087(0.20) | 4.370(0.00) | 88.6   |
| wPBEPP86        | cc-pVDZ   | DMSO | 2.208(1.67) | 3.608(0.23) | 4.078(0.11) | 4.289(0.22) | 4.648(0.00) | 4.691(0.06) | 22.3   |
| wPBEPP86        | cc-pVTZ   | DMSO | 2.171(1.65) | 3.539(0.23) | 4.037(0.05) | 4.172(0.26) | 4.707(0.00) | 4.982(0.00) | 105.5  |
| wPBEPP86        | aug-cc-pVDZ | DMSO | 2.161(1.67) | 3.515(0.24) | 4.029(0.00) | 4.087(0.30) | 4.501(0.00) | 4.928(0.00) | 122.2  |
| wPBEPP86        | aug-cc-pVTZ | DMSO | 2.149(1.65) | 3.505(0.24) | 4.026(0.00) | 4.071(0.30) | 4.554(0.00) | 4.794(0.00) | 590.7  |
| wb97x-2         | cc-pVDZ   | g.p. | 1.746(1.20) | 2.970(0.10) | 2.821(0.16) | 4.059(0.00) | 2.394(0.00) | 3.805(0.10) | 23.4   |
| wb97x-2         | cc-pVTZ   | g.p. | 1.686(1.17) | 2.883(0.10) | 2.797(0.14) | 4.107(0.01) | 3.680(0.11) | 2.324(0.00) | 92.0   |
| wb97x-2         | aug-cc-pVDZ | g.p. | 1.674(1.18) | 2.862(0.09) | 3.529(0.00) | 3.800(0.00) | 3.178(0.02) | 3.739(0.01) | 91.7   |
| wb97x-2         | aug-cc-pVDZ* | g.p. | 1.674(1.17) | 2.857(0.09) | 3.531(0.00) | 3.207(0.04) | 3.558(0.03) | 3.335(0.21) | 87.6   |
| wb97x-2         | aug-cc-pVTZ | g.p. | 1.648(1.16) | 3.711(0.00) | 2.847(0.09) | 3.907(0.00) | 3.285(0.02) | 3.828(0.01) | 819.5  |
| wb97x-2         | cc-pVDZ   | DMSO | 1.599(1.24) | 2.842(0.18) | 3.425(0.07) | 4.072(0.01) | 3.660(0.20) | 5.135(0.00) | 29.3   |
| wb97x-2         | cc-pVTZ   | DMSO | 1.548(1.21) | 2.743(0.18) | 3.366(0.03) | 3.517(0.23) | 4.207(0.00) | 4.937(0.00) | 101.1  |
| wb97x-2         | aug-cc-pVDZ | DMSO | 1.554(1.23) | 2.726(0.19) | 3.402(0.00) | 3.952(0.00) | 3.400(0.25) | 4.205(0.00) | 87.9   |
| wb97x-2         | aug-cc-pVDZ* | DMSO | 1.551(1.22) | 2.727(0.19) | 3.384(0.00) | 3.866(0.07) | 3.597(0.19) | 4.283(0.00) | 87.2   |
| wb97x-2         | aug-cc-pVTZ | DMSO | 1.526(1.21) | 2.705(0.19) | 3.401(0.00) | 4.065(0.00) | 3.378(0.25) | 4.324(0.00) | 316.0  |
| SCS-wPBEPP86    | cc-pVDZ   | g.p. | 2.119(1.42) | 3.530(0.11) | 3.589(0.21) | 3.512(0.00) | 4.188(0.10) | 4.477(0.00) | 25.2   |
| Method          | Basis Set        | Model  | 1,2  | 3,4  | 4,5  | 5,6  | 6,7  | 7,8  | 8,9  | 9,10 |
|----------------|-----------------|--------|------|------|------|------|------|------|------|------|
| SCS-wPBEPP86   | cc-pVTZ         | g.p.   | 2.060(1.38) | 3.457(0.11) | 3.540(0.19) | 4.044(0.13) | 3.492(0.00) | 4.514(0.00) | 95.9 |
| SCS-wPBEPP86   | aug-cc-pVDZ     | g.p.   | 2.045(1.39) | 3.433(0.10) | 4.008(0.00) | 3.611(0.09) | 3.869(0.24) | 4.271(0.00) | 77.2 |
| SCS-wPBEPP86   | aug-cc-pVDZ*    | g.p.   | 2.046(1.39) | 3.430(0.10) | 4.011(0.00) | 3.574(0.13) | 3.922(0.19) | 4.273(0.00) | 90.6 |
| SCS-wPBEPP86   | aug-cc-pVTZ     | g.p.   | 2.026(1.38) | 3.419(0.10) | 4.063(0.00) | 3.621(0.07) | 3.841(0.25) | 4.303(0.01) | 569.8 |
| SCS-wPBEPP86   | cc-pVTZ         | DMSO   | 1.980(1.50) | 3.447(0.22) | 3.909(0.10) | 4.106(0.21) | 4.552(0.00) | 4.500(0.06) | 22.7 |
| SCS-wPBEPP86   | aug-cc-pVDZ     | DMSO   | 1.924(1.48) | 3.346(0.23) | 3.849(0.00) | 3.908(0.29) | 4.399(0.00) | 4.825(0.00) | 129.3 |
| SCS-wPBEPP86   | aug-cc-pVDZ*    | DMSO   | 1.923(1.48) | 3.347(0.23) | 3.842(0.01) | 3.930(0.27) | 4.456(0.00) | 4.824(0.00) | 107.4 |
| SCS-wPBEPP86   | aug-cc-pVTZ     | DMSO   | 1.906(1.47) | 3.331(0.22) | 3.838(0.00) | 3.885(0.29) | 4.445(0.00) | 4.683(0.00) | 601.9 |
| SOS-wPBEPP86   | cc-pVDZ         | g.p.   | 2.123(1.42) | 3.581(0.11) | 3.683(0.22) | 3.579(0.00) | 4.202(0.10) | 4.542(0.00) | 23.9 |
| SOS-wPBEPP86   | cc-pVTZ         | g.p.   | 2.066(1.39) | 3.509(0.11) | 3.631(0.19) | 4.060(0.13) | 3.559(0.00) | 4.576(0.00) | 101.2 |
| SOS-wPBEPP86   | aug-cc-pVDZ     | g.p.   | 2.056(1.40) | 3.491(0.10) | 4.112(0.00) | 3.690(0.09) | 3.918(0.24) | 4.361(0.00) | 80.2 |
| SOS-wPBEPP86   | aug-cc-pVDZ*    | g.p.   | 2.057(1.39) | 3.489(0.10) | 4.117(0.00) | 3.660(0.13) | 3.963(0.20) | 4.387(0.00) | 90.4 |
| SOS-wPBEPP86   | aug-cc-pVTZ     | g.p.   | 2.032(1.38) | 3.472(0.10) | 4.168(0.00) | 3.691(0.08) | 3.890(0.25) | 4.409(0.01) | 563.0 |
| SOS-wPBEPP86   | cc-pVDZ         | DMSO   | 1.983(1.50) | 3.486(0.22) | 3.960(0.11) | 4.107(0.21) | 4.618(0.00) | 4.522(0.06) | 23.7 |
| SOS-wPBEPP86   | cc-pVTZ         | DMSO   | 1.933(1.47) | 3.405(0.22) | 3.888(0.05) | 3.991(0.25) | 4.661(0.00) | 4.915(0.00) | 103.6 |
| SOS-wPBEPP86   | aug-cc-pVDZ     | DMSO   | 1.935(1.49) | 3.389(0.23) | 3.878(0.00) | 3.947(0.29) | 4.479(0.00) | 4.882(0.00) | 121.2 |
| SOS-wPBEPP86   | aug-cc-pVDZ*    | DMSO   | 1.934(1.49) | 3.390(0.23) | 3.877(0.01) | 3.962(0.27) | 4.540(0.00) | 4.881(0.00) | 97.6 |
| SOS-wPBEPP86   | aug-cc-pVTZ     | DMSO   | 1.911(1.47) | 3.368(0.23) | 3.861(0.00) | 3.919(0.29) | 4.525(0.00) | 4.767(0.00) | 574.6 |
Table S6 Error (eV) with respect to experimental observations for the prediction of energy differences between bright states of DCM$_2$-I as summary of the benchmark of density functionals for DCM$_2$-I. All calculations presented in the table were performed with the Douglas-Kroll-Hess Hamiltonian, aug-cc-pVDZ/cc-pVTZ-DK(iodine) basis set, in implicit DMSO on structures optimized with the same functional without diffuse basis function in the gas phase.

| DFT           | Error on $\Delta E_{S0-S1}$ | Error on $\Delta E_{S1-S2}$ | Error on $\Delta E_{S2-S3/4}$* |
|---------------|-----------------------------|-----------------------------|-------------------------------|
| B3LYP         | 0.281                       | 0.003                       | -0.069                        |
| PBE0          | 0.349                       | 0.079                       | -0.082                        |
| TPSSH         | 0.228                       | -0.117                      | -0.032                        |
| M06-2X        | 0.429                       | 0.346                       | 0.014                         |
| CAM-B3LYP     | 0.480                       | 0.330                       | 0.082                         |
| wB97X-D3BJ    | 0.555                       | 0.405                       | 0.378                         |
| RSX-0DH       | 0.625                       | 0.494                       | 0.382                         |
| wPBEPP86      | 0.260                       | 0.356                       | 0.395                         |
| wB97X-2       | -0.349                      | 0.176                       | 0.670                         |
| SCS-wPBEPP86  | 0.023                       | 0.424                       | 0.382                         |

* S3/4 refers to the third bright state. There is a dark singlet state in the same range of energy and the energy ordering varies from one method to another.

Figure S14 Experimental and calculated absorption spectrum of DCM$_2$-I in DMSO. The theoretical spectrum was calculated from a Wigner distribution at 300 K with B3LYP/aug-cc-pVDZ/cc-pVTZ-DK(iodine)/CPCM(DMSO). A decomposition of the spectrum into contributions of the different singlet state is given as filled curved. S3 (dark state) and S4 (bright state) are very close in energy and their order can be inverted from one geometry to another. Yet, one of them is always bright while the other is dark and the bright state is correspondingly labeled as S3/4. The line spectrum in the ground state optimized geometry is given as sticks.
Computational Studies – Additional Figures & Tables:

**Figure S15** Natural transition orbitals for the first 10 singlet states of DCM$_0$-I.

**Figure S16** Natural transition orbitals for the first 10 triplet states of DCM$_0$-I.

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**Figure S17** Natural transition orbitals for the first 10 singlet states of DCM\(_0\).

**Triplet states of DCM\(_0\)**

| T1  | T6  | T6  |
|------|------|------|
| (1.01) | (0.56) | (0.30) |
| ![Image](image1) | ![Image](image2) | ![Image](image3) |
| T2  | T7  | T7  |
| (0.85) | (0.62) | (0.28) |
| ![Image](image4) | ![Image](image5) | ![Image](image6) |
| T3  | T8  | T8  |
| (0.85) | (0.62) | (0.34) |
| ![Image](image7) | ![Image](image8) | ![Image](image9) |
| T4  | T9  | T9  |
| (1.00) | (0.70) | (0.24) |
| ![Image](image10) | ![Image](image11) | ![Image](image12) |
| T5  | T10 | T10 |
| (0.42) | (0.15) | (0.06) |
| ![Image](image13) | ![Image](image14) | ![Image](image15) |

**Figure S18** Natural transition orbitals for the first 10 triplet states of DCM\(_0\).
**Figure S19** Natural transition orbitals for the first 10 singlet states of DCM$_2$-Cl.

**Figure S20** Natural transition orbitals for the first 10 triplet states of DCM$_2$-Cl.
Figure S21 Natural transition orbitals for the first 10 singlet states of I-DCM$_O$.

Figure S22 Natural transition orbitals for the first 10 triplet states of I-DCM$_O$. 

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Natural transition orbitals for the first 10 singlet states of I-DCM₂-Cl.

Table S7 Square modulus of spin-orbit coupling matrix elements (in cm⁻¹; bold font) between singlet and triplet states of DCM₂-I. The energy of each state is also given in eV and the oscillator strength of the singlet states in indicated as “f”.

| Singlet | 0   | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   | 9   | 10  |
|---------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| energy  | 0.00| 2.17| 3.18| 3.26| 3.31| 3.46| 3.63| 3.88| 3.93| 3.97| 4.00|
| f       | 0.00| 1.46| 0.44| 0.00| 0.16| 0.06| 0.00| 0.01| 0.00| 0.00| 0.03|

| Triplet | energy |
|---------|--------|
| 1       | 1.42   |
| 2       | 2.35   |
| 3       | 2.67   |
| 4       | 3.10   |
| 5       | 3.11   |
| 6       | 3.21   |
| 7       | 3.30   |
| 8       | 3.41   |
| 9       | 3.44   |
| 10      | 3.67   |

Table S8. Square modulus of spin-orbit coupling matrix elements (in cm⁻¹; bold font) between singlet and triplet states of DCM₂. The energy of each state is also given in eV and the oscillator strength of the singlet states in indicated as “f”.

| Singlet | 0   | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   | 9   | 10  |
|---------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| energy  | 0.00| 2.18| 3.16| 3.16| 3.31| 3.82| 3.89| 3.95| 4.05| 4.10|
| f       | 0.00| 1.47| 0.40| 0.00| 0.21| 0.00| 0.00| 0.00| 0.08| 0.10|

| Triplet | energy |
|---------|--------|
| 1       | 1.35   |
| 2       | 2.38   |
| 3       | 2.63   |
| 4       | 2.98   |
Table S9 Square modulus of spin-orbit coupling matrix elements (in cm⁻¹; bold font) between singlet and triplet states of DCM₁₀-Cl. The energy of each state is also given in eV and the oscillator strength of the singlet states in indicated as "f".

| Triplet | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---------|---|---|---|---|---|---|---|---|---|----|
| energy  | 1.41 | 0.50 | 0.02 | 0.04 | 0.07 | 17.17 | 0.05 | 0.21 | 0.09 | 4.87 |
| f       | 0.00 | 1.45 | 0.41 | 0.21 | 0.00 | 0.01 | 0.01 | 0.00 | 0.00 | 0.17 |

Table S10. Square modulus of spin-orbit coupling matrix elements (in cm⁻¹; bold font) between singlet and triplet states of I-DCM₁₀. The energy of each state is also given in eV and the oscillator strength of the singlet states in indicated as "f".

| Triplet | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---------|---|---|---|---|---|---|---|---|---|----|
| energy  | 1.32 | 1.25 | 0.10 | 0.64 | 19.72 | 0.71 | 63.36 | 0.80 | 0.51 | 0.08 |
| f       | 0.00 | 1.49 | 0.43 | 0.00 | 0.22 | 0.00 | 0.01 | 0.02 | 0.00 | 0.04 |

Table S11 Square modulus of spin-orbit coupling matrix elements (in cm⁻¹; bold font) between singlet and triplet states of I-DCM₁₀-Cl. The energy of each state is also given in eV and the oscillator strength of the singlet states in indicated as "f".

| Triplet | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---------|---|---|---|---|---|---|---|---|---|----|
| energy  | 1.37 | 0.99 | 0.11 | 0.45 | 0.80 | 17.09 | 2.46 | 66.82 | 0.93 | 0.19 |
| f       | 0.00 | 1.47 | 0.40 | 0.26 | 0.00 | 0.00 | 0.00 | 0.01 | 0.01 | 0.04 |
6. NMR Spectra

Figure S24 $^1$H NMR spectrum of DCM$_0$- I in d$_6$-DMSO.
Figure S25 $^{13}$C NMR spectrum of DCM$_{O}$-I in $d_6$-DMSO.

Figure S26 $^1$H NMR spectrum of DCM$_{O}$-I-Cys in CDCl$_3$. 

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Figure S27 $^{13}$C NMR spectrum of DCM$_{10}$-I-Cys in CDCl$_3$.

Figure S28 $^1$H NMR spectrum of 3 in CDCl$_3$. 
Figure S29 $^{13}$C NMR spectrum of 3 in CDCl$_3$.

Figure S30 $^1$H NMR spectrum of 4 in CDCl$_3$. 
Figure S31 $^{13}$C NMR spectrum of 4 in CDCl$_3$.

Figure S32 $^1$H NMR spectrum of 5 in CDCl$_3$. 

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**Figure S33** $^{13}$C NMR spectrum of 5 in CDCl$_3$. 
Figure S34 $^1$H NMR spectrum of I-DCM$_2$-Cl in d$_6$-DMSO.

Figure S35 $^{13}$C NMR spectrum of I-DCM$_2$-Cl in d$_6$-DMSO.
7. HR-MS Spectra:

**Figure S36** HRMS spectrum of DCM$_2$I.

**Figure S37** HRMS spectrum of Compound 5.
Figure S38 HRMS spectrum of I-DCM$_2$-Cl.

Figure S39 HRMS spectrum of DCM$_2$-I-Cys.
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