Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences.

Supporting Information

Fluorescence Properties of Aurone Derivatives: An Experimental and Theoretical Study with Some Preliminary Biological Applications

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FLUORESCENCE LIFETIMES AT DIFFERENT EMISSION WAVELENGTHS

Table S1. Fluorescence lifetimes for aurone **4** at different emission wavelengths. The samples were excited at 405 nm.

λ_{em} / nm	τ_1 / ns (A_1)	τ_2 / ns (A_2)	χ^2
450	0.55 (0.24)	3.93 (0.76)	1.16
470	0.65 (0.21)	3.95 (0.79)	1.10
500	0.70 (0.21)	3.99 (0.79)	1.10
550	0.73 (0.39)	3.98 (0.61)	1.08

PHOTO-ISOMERIZATION STUDIES

Samples were irradiated using a custom-built PTI irradiation equipment working with a 150 W Xenon lamp, with temperature control and stirring capabilities. The irradiation wavelength was selected with a monochromator and the bandwidth used was 10 nm.

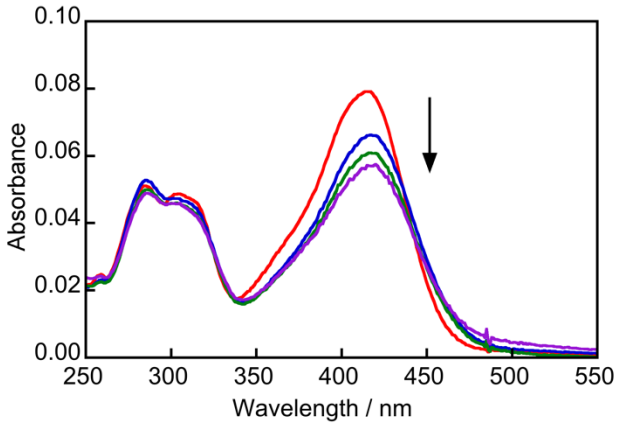

Figure S1. Absorption spectra for **aurone 1** in chloroform in the dark (red) and after 5 min (blue), 10 min (green) and 15 min (purple) of irradiation at the absorption maxima.

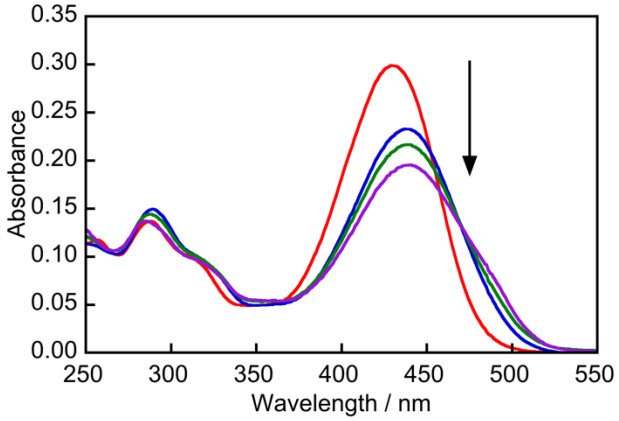

Figure S2. Absorption spectra for **aurone 2** in chloroform in the dark (red) and after 5 min (blue), 10 min (green) and 15 min (purple) of irradiation at the absorption maxima.

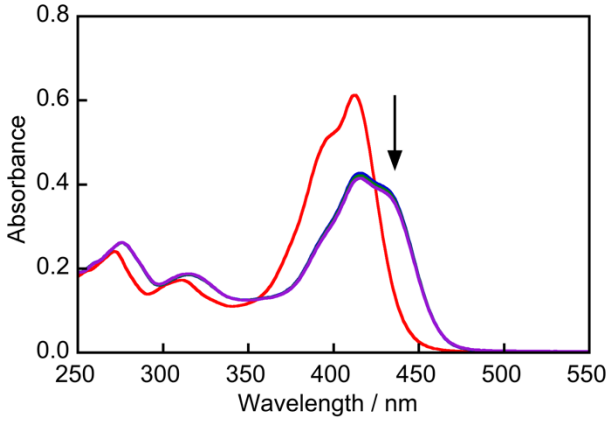

Figure S3. Absorption spectra for **aurone 3** in chloroform in the dark (red) and after 5 min (blue), 10 min (green) and 15 min (purple) of irradiation at the absorption maxima.

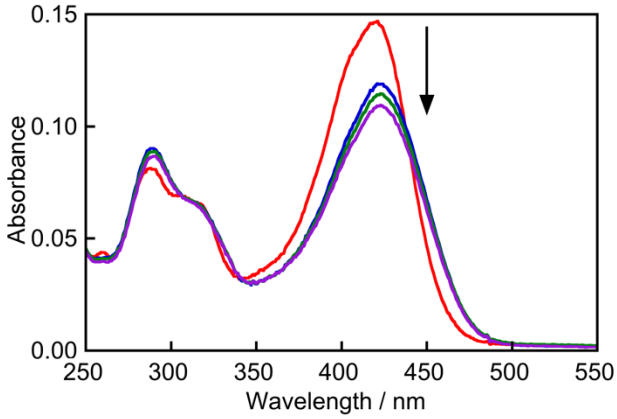

Figure S4. Absorption spectra for **aurone 4** in chloroform in the dark (red) and after 5 min (blue), 10 min (green) and 15 min (purple) of irradiation at the absorption maxima.

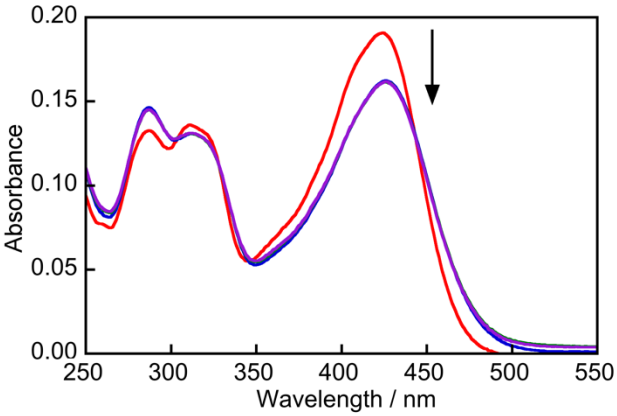

Figure S5. Absorption spectra for **aurone 5** in chloroform in the dark (red) and after 5 min (blue), 10 min (green) and 15 min (purple) of irradiation at the absorption maxima.

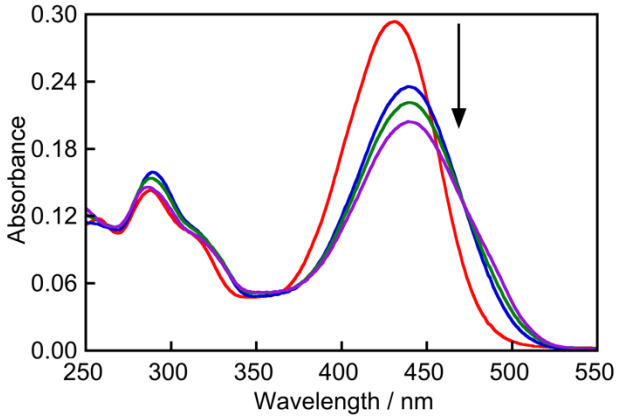

Figure S6. Absorption spectra for **aurone 6** in chloroform in the dark (red) and after 5 min (blue), 10 min (green) and 15 min (purple) of irradiation at the absorption maxima.

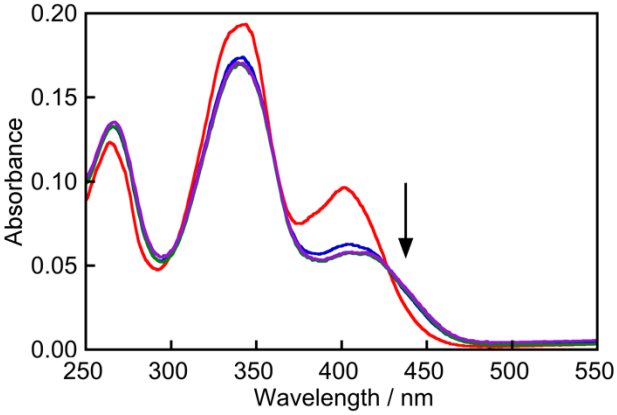

Figure S7. Absorption spectra for **aurone 7** in chloroform in the dark (red) and after 5 min (blue), 10 min (green) and 15 min (purple) of irradiation at the absorption maxima.

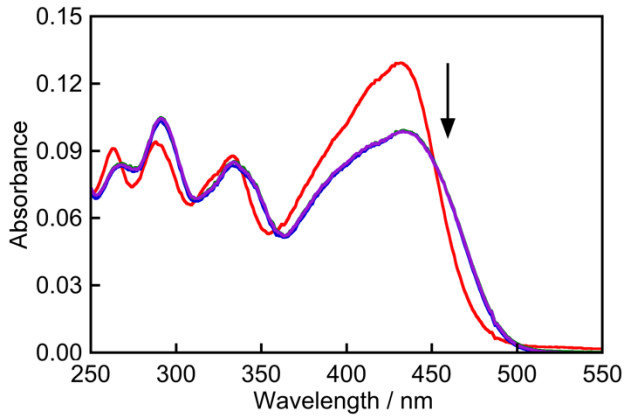

Figure S8. Absorption spectra for **aurone 8** in chloroform in the dark (red) and after 5 min (blue), 10 min (green) and 15 min (purple) of irradiation at the absorption maxima.

COMPUTATIONAL STUDIES

E- and *Z*-isomers

In the DFT calculations, *E*- and *Z*-isomers of aurones were considered. However, the Z-isomers were always more stable than their *E*-isomers. Specifically, the ground states of the *Z* forms of compounds **1**, **4**, **5** and **8** are 3.80, 3.71, 3.54 and 3.35 kcal/mol above the ground states of the *E*-isomers. Consequently, the Z-isomers are presented for results in the main article.

Frontier molecular orbitals

Table S2. Energy of frontier molecular orbitals (HOMO and LUMO) and HOMO-LUMO energy gap (ΔHL) in the ground state S_0.

E-isomers	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔHL (eV)
1	-5.91	-2.63	3.28
4	-6.01	-2.72	3.30
5	-5.88	-2.65	3.22
8	-5.97	-2.74	3.23
Z-isomers			
1	-5.94	-2.56	3.37
4	-6.04	-2.65	3.39
5	-5.92	-2.59	3.33
8	-6.02	-2.68	3.34

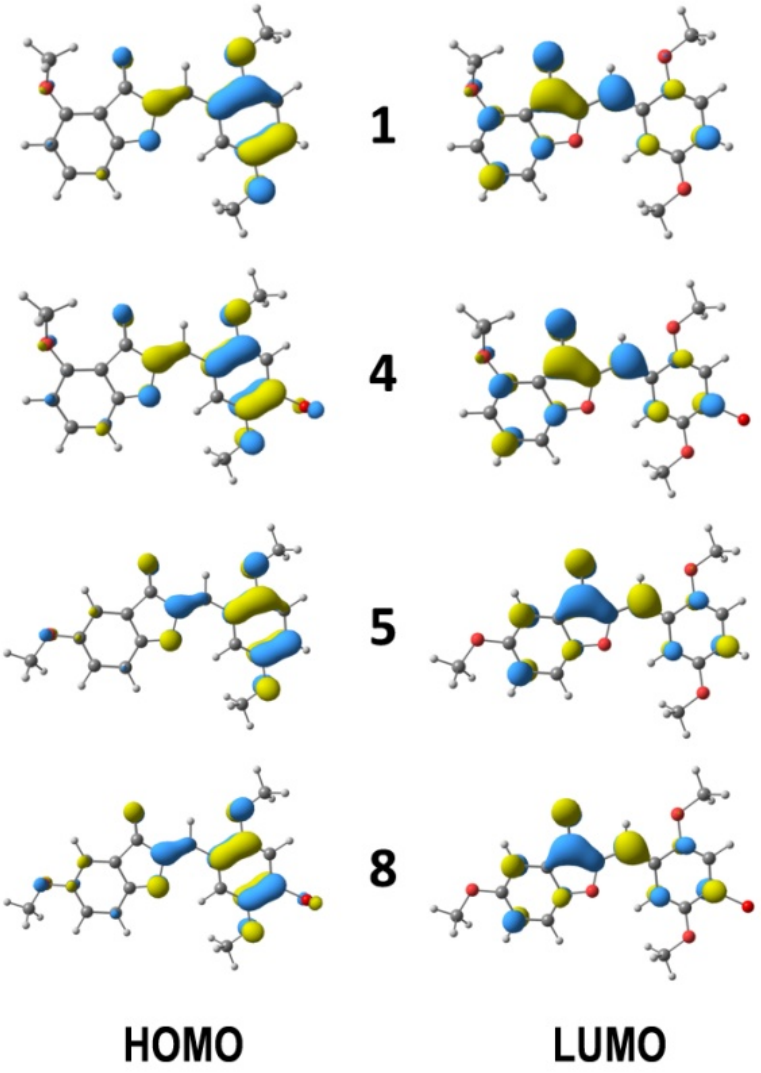

Figure S9. Surfaces of the frontier molecular orbitals (HOMO and LUMO) of systems **1**, **4**, **5** and **8** in the ground state S_0. Isosurface value of 0.05 a.u.

Geometry of ground (S_0) and first excited states (S_1)

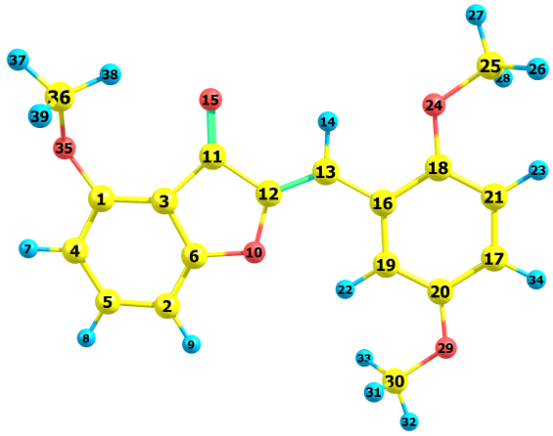

Figure S10. Atoms labels used in Table S3. Molecule was taken as representative.

Table S3. Selected bond distances (*d*) and angles (∠) of systems **1**, **4**, **5** and **8** in their ground state (S_0) and first singlet excites state (S_1). Calculations were performed at the PBE0/6-31+G(d) level of theory in chloroform as solvent. RMSD is the root mean square deviation in the atomic coordinates. Distances are in angstroms (Å), and angles are in degrees (°).

	ground state (S_0)				*first singlet excited state (S_1)*			
parameter	**1**	**4**	**5**	**8**	**1**	**4**	**5**	**8**
*d*C12-C13	1.35	1.35	1.35	1.35	1.37	1.38	1.37	1.38
*d*C12-C11	1.48	1.48	1.49	1.49	1.47	1.47	1.47	1.47
*d*C11-O15	1.23	1.23	1.23	1.23	1.25	1.25	1.25	1.25
*d*C12-O10	1.38	1.37	1.38	1.38	1.37	1.36	1.37	1.36
*d*C13-C16	1.45	1.45	1.45	1.45	1.44	1.43	1.44	1.43
*d*C16-C18	1.42	1.42	1.42	1.42	1.45	1.45	1.45	1.45
*d*C16-C19	1.41	1.41	1.41	1.41	1.39	1.40	1.39	1.40
*d*C17-Br1	-	1.88	-	1.88	-	1.87	-	1.87
∠O10-O12-O13	125.09	125.02	124.96	124.90	123.63	123.64	123.55	123.51
∠C12-C13-C16	130.41	130.09	130.45	130.11	128.29	128.42	128.37	128.58

∠C13-C16-C19	122.87	122.99	122.82	122.91	124.66	124.74	124.57	124.67
∠C13-C12-C11	125.12	125.16	125.14	125.18	126.14	126.02	126.25	126.28
∠O15-O11-O12	125.03	124.94	126.84	126.72	124.27	124.10	125.66	125.69
∠C13-C16-C18	118.29	118.51	118.34	118.57	118.68	118.65	118.72	118.64
RMSD					0.072	0.048	0.055	0.041

Oscillator strength

As noted in Table 3, the oscillator strength for the $S_0 \rightarrow S_1$ transition is higher in the **4** system compared with those of **1**, **5** and **8**. In this regard, we analyze the relation between oscillator strength *f* and the transition dipole moment *D*, which is given by:

$$f = \frac{2}{3} \Delta E \cdot (D_x^2 + D_y^2 + D_z^2) \quad (1)$$

where ΔE is the transition energy associated to the $S_0 \rightarrow S_1$ excitation, and D_x, D_y and D_z are the *x*, *y* and *z* components of the transition dipole moment *D*; note that D_x, D_y and D_z are related to molecular polarization during the electronic excitation.

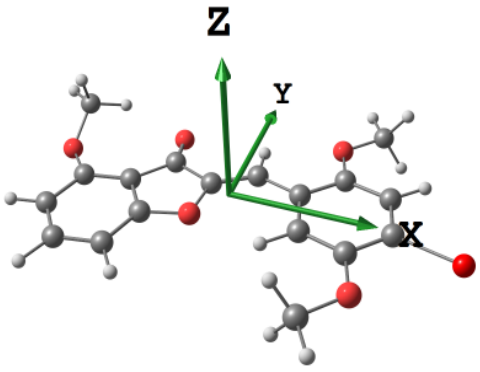

Figure S11. Cartesian axis for the **4** compound as representative.

Hole-electron distributions

The hole-electron distributions were obtained as:

$$\Delta\rho(r) = \rho^{electron}(r) - \rho^{hole}(r) \quad (1)$$

$$\rho^{hole}(r) = \sum_{i\to l}\left(w_i^l\right)^2 \varphi_i(r)\varphi_i(r) + \sum_{i\to l}\sum_{j\neq i\to l} w_i^l w_j^l \varphi_i(r)\varphi_j(r) \quad (2)$$

$$\rho^{electron}(r) = \sum_{i\to l}(w_i^l)^2 \varphi_i(r)\varphi_i(r) + \sum_{i\to l}\sum_{i\to m\neq l} w_i^l w_i^m \varphi_l(r)\varphi_m(r) \quad (3)$$

where ρ^{hole} and $\rho^{electron}$ are the electron density distributions of hole and electron in a given excited state wavefunction, respectively; w is the weighting coefficient of each monoexcitations due to the single electron promotion from the occupied orbital i to the virtual orbital j; φ stands for the occupied (or virtual) molecular orbital (T. Lu and F. Chen, *J. Comput. Chem.*, 2012, **33**, 580-592.)

S6. XYZ coordinates of the optimized molecular structures of systems 1, 4, 5 and 8 in their ground states, and in chloroform as solvent

System 1

C	4.19877900	-0.00461300	-0.10594300
C	2.63380000	2.38542000	-0.07795500
C	2.78820400	-0.07499700	-0.06796100
C	4.79560400	1.25880100	-0.15977200
C	4.02689700	2.42242100	-0.14710800
C	2.06248400	1.12781700	-0.04565500
H	5.87939400	1.31098500	-0.19247400
H	4.53065200	3.38484800	-0.17894300
H	2.02809700	3.28516000	-0.06282400
O	0.71017700	0.93016900	-0.02590300
C	1.78522800	-1.14439400	-0.14721400

C	0.48902800	-0.42659700	-0.08438500
C	-0.72383600	-1.01454900	-0.08653300
H	-0.67021700	-2.09842000	-0.14480300
O	1.91277600	-2.35925400	-0.27130700
C	-2.04710300	-0.43433400	-0.02509100
C	-4.65166800	0.59578600	0.08311400
C	-3.16277600	-1.30616300	-0.02376300
C	-2.27105700	0.95658300	0.02988500
C	-3.56075100	1.47142100	0.08360600
C	-4.45540900	-0.77741200	0.03013500
H	-1.41259400	1.61489200	0.02782800
H	-5.32106400	-1.43036500	0.03135400
O	-2.89770900	-2.63387200	-0.07514900
C	-3.98413000	-3.54108100	-0.08365600
H	-4.58207400	-3.45295100	0.83141700
H	-3.53877500	-4.53545300	-0.13112500
H	-4.62370900	-3.38599200	-0.96084000
O	-3.86021100	2.79772500	0.13741300
C	-2.78611400	3.71732900	0.13737600
H	-2.13807700	3.57324600	1.01115600
H	-3.24011700	4.70817300	0.18335700
H	-2.18911100	3.63291100	-0.77951700
H	-5.65691100	1.00571700	0.12474100
O	5.03467100	-1.06112000	-0.13465200
C	4.78107900	-2.16071100	0.74340200
H	5.64670600	-2.81693400	0.64202700
H	3.86671500	-2.68778700	0.46351100
H	4.71391800	-1.80157300	1.77702600

System 4

C	-5.29115000	-0.29234900	-0.08505700
C	-3.49155600	-2.51179600	-0.09013900
C	-3.89461400	-0.08000600	-0.05823000
C	-5.75724300	-1.60951900	-0.14585200
C	-4.87466800	-2.68902600	-0.14904800
C	-3.05102500	-1.20336400	-0.05169000
H	-6.83040100	-1.77113200	-0.17035800
H	-5.27854600	-3.69727400	-0.18512900
H	-2.79789800	-3.34574900	-0.08728100
O	-1.72466800	-0.86906400	-0.04115000
C	-3.00646400	1.08604500	-0.13716900
C	-1.64294800	0.50229500	-0.09103600
C	-0.49560000	1.20872800	-0.10158800
H	-0.65415100	2.28254100	-0.15100000
O	-3.25541100	2.28242500	-0.25134000
C	0.87665400	0.75640300	-0.05787700

C	3.55723200	-0.02991500	0.02254400
C	1.90841800	1.72627200	-0.06346100
C	1.23373900	-0.60335600	-0.01132800
C	2.56090700	-1.01539500	0.02900100
C	3.24222500	1.32130700	-0.02304700
H	0.44249100	-1.34123700	-0.00835000
H	4.04727800	2.04591400	-0.02582900
O	1.52826800	3.02267400	-0.10796700
C	2.53035100	4.02402700	-0.12186200
H	3.13947800	3.98661600	0.78908300
H	1.99731400	4.97427300	-0.16327200
H	3.17362500	3.92747100	-1.00448800
O	2.96609500	-2.30443200	0.07463800
C	1.97396300	-3.31403300	0.08152200
H	1.32548500	-3.22698200	0.96180900
H	2.51560600	-4.25965900	0.12160500
H	1.36654400	-3.27955200	-0.83109500
O	-6.22961000	0.67385300	-0.09626500
C	-6.07901100	1.78751300	0.78789000
H	-7.00665700	2.35461200	0.69872800
H	-5.22451900	2.40515100	0.50423100
H	-5.96686100	1.42978200	1.81804300
Br	5.36224500	-0.55175400	0.07738600

System 5

C	3.84390200	-1.16135200	0.00003000
C	2.85704900	1.50215000	-0.00001400
C	2.47956300	-0.89520100	-0.00002500
C	4.72552700	-0.07885900	0.00006000
C	4.22870900	1.23805500	0.00003900
C	2.00374300	0.41487000	-0.00004400
H	4.91384400	2.07881000	0.00006900
H	2.48503400	2.52200300	-0.00002700
O	0.63224300	0.48529200	-0.00008500
C	1.29884300	-1.76492800	-0.00008900
C	0.15958800	-0.81107200	-0.00009200
C	-1.14330400	-1.15835800	-0.00010500
H	-1.29626100	-2.23443800	-0.00011600
O	1.23261900	-2.98877400	-0.00005300
C	-2.33316000	-0.33690400	-0.00009900
C	-4.69517000	1.17181600	-0.00006000
C	-3.59435000	-0.98070800	-0.00009500
C	-2.28884600	1.07239400	-0.00009500
C	-3.45760300	1.82406700	-0.00006600
C	-4.76333100	-0.21468000	-0.00008300
H	-1.32024900	1.55426000	-0.00011100

H	-5.73731300	-0.69118900	-0.00010200
O	-3.58630800	-2.33536300	-0.00015200
C	-4.82545900	-3.01946700	0.00041200
H	-5.40959900	-2.78149900	0.89750300
H	-4.57707200	-4.08136200	0.00065800
H	-5.41011900	-2.78205400	-0.89648900
O	-3.49996500	3.18424900	-0.00006900
C	-2.27045300	3.88244100	0.00024400
H	-1.68097100	3.65102600	0.89645500
H	-2.52789600	4.94250800	0.00041400
H	-1.68071200	3.65138600	-0.89589100
H	-5.60452200	1.76625800	-0.00004600
H	4.22347300	-2.17903000	0.00004200
O	6.04822100	-0.38770800	0.00012000
C	6.98641500	0.67138300	0.00001500
H	6.88443400	1.29489600	-0.89692500
H	7.96893800	0.19795500	-0.00000600
H	6.88452500	1.29499600	0.89689500

System 8

C	-5.08521200	0.83540300	0.00007900
C	-3.72577800	-1.65885700	-0.00028100
C	-3.69674300	0.76808500	-0.00008700
C	-5.80208200	-0.36276100	0.00004200
C	-5.12125000	-1.59462300	-0.00014400
C	-3.03836000	-0.46030100	-0.00023900
H	-5.67808200	-2.52536500	-0.00017500
H	-3.21087200	-2.61453800	-0.00039500
O	-1.66992500	-0.33320600	-0.00028200
C	-2.65270700	1.79790000	-0.00016400
C	-1.38797300	1.01608600	-0.00014100
C	-0.14806800	1.54496200	-0.00002900
H	-0.14532000	2.63175000	0.00003300
O	-2.75942200	3.01825300	0.00014900
C	1.14208500	0.89349700	-0.00000300
C	3.67517600	-0.28594400	-0.00013700
C	2.30719100	1.69856200	-0.00001200
C	1.29196200	-0.50513700	0.00002300
C	2.54280200	-1.11154700	-0.00001200
C	3.56588400	1.09801900	-0.00006000
H	0.39854300	-1.11535800	0.00006600
H	4.47071500	1.69344100	-0.00004500
O	2.12378800	3.03753600	-0.00001300
C	3.26306700	3.87950600	0.00004600
H	3.87237500	3.72006000	0.89750800
H	2.87642100	4.89897200	0.00011200

H	3.87238000	3.72018400	-0.89743400
O	2.75131600	-2.44733000	0.00002300
C	1.61964900	-3.29758200	0.00000700
H	1.00776000	-3.14347700	0.89709300
H	2.01451300	-4.31411100	-0.00007000
H	1.00770100	-3.14336000	-0.89701800
H	-5.60810800	1.78742400	0.00020500
O	-7.15496300	-0.24688400	0.00016600
C	-7.93169900	-1.42961900	0.00032500
H	-7.74147400	-2.03188400	-0.89670600
H	-8.97190800	-1.10194800	0.00054500
H	-7.74109000	-2.03189000	0.89727000
Br	5.38121300	-1.07459300	0.00009700

S7. XYZ coordinates of the optimized molecular structures of systems 1, 4, 5 and 8 in their first singlet excited states, and in chloroform as solvent

System 1

C	4.19104600	0.00046100	-0.13054500
C	2.60178300	2.36557000	-0.07848400
C	2.77914900	-0.10346700	-0.08059400
C	4.77352700	1.27096600	-0.17462300
C	4.00034600	2.43364500	-0.15303500
C	2.05348300	1.10337700	-0.04574000
H	5.85746200	1.32990500	-0.21571400
H	4.49054400	3.40257900	-0.18213000
H	1.97963800	3.25493200	-0.05811900
O	0.69741000	0.87119800	-0.01754500
C	1.79725900	-1.17504900	-0.12829600
C	0.50518700	-0.48032200	-0.06402600
C	-0.73314300	-1.07251500	-0.06101000
H	-0.69887500	-2.15485400	-0.10544900
O	1.92626100	-2.41795200	-0.22216600
C	-2.02462800	-0.43881400	-0.01518100
C	-4.67108700	0.64812700	0.06813500
C	-3.20723300	-1.27160700	-0.02567800
C	-2.23027300	0.93875800	0.03811800
C	-3.52965200	1.48087100	0.07958600
C	-4.49913900	-0.72094700	0.01559600
H	-1.36945200	1.59259400	0.04709400
H	-5.36927900	-1.36762100	0.00572400
O	-2.96617000	-2.57830500	-0.07738700
C	-4.04512000	-3.50696600	-0.09723200

H	-4.64524900	-3.41729800	0.81383500
H	-3.58002500	-4.49076600	-0.14086100
H	-4.66934300	-3.34906400	-0.98239500
O	-3.78152200	2.78975300	0.13163400
C	-2.70308000	3.72040500	0.14761500
H	-2.07435900	3.56628100	1.03004800
H	-3.16955600	4.70369800	0.19181000
H	-2.10448300	3.63264500	-0.76440100
H	-5.65781200	1.09799900	0.10058600
O	5.03649200	-1.05800900	-0.18727800
C	4.82754300	-2.11224200	0.75382300
H	5.62673400	-2.83300400	0.57011700
H	3.85072600	-2.58214300	0.60608200
H	4.91775200	-1.72087200	1.77514000

System 4

C	-5.28319100	-0.31942300	-0.09711500
C	-3.45066000	-2.50341100	-0.07400400
C	-3.88986200	-0.06495100	-0.06548500
C	-5.72653800	-1.64776800	-0.14275300
C	-4.83506700	-2.72032600	-0.13452200
C	-3.04169700	-1.18936200	-0.04259900
H	-6.79853200	-1.82108600	-0.17013900
H	-5.21941800	-3.73584600	-0.16182600
H	-2.73596900	-3.32033800	-0.06341500
O	-1.71775100	-0.81637200	-0.03074300
C	-3.02288200	1.10285600	-0.12973700
C	-1.66725300	0.54375300	-0.07680000
C	-0.49303400	1.26414000	-0.08236200
H	-0.64392400	2.33691200	-0.12079800
O	-3.27450200	2.32493900	-0.23350700
C	0.84902400	0.77482900	-0.04706400
C	3.58014200	-0.02750100	0.02044700
C	1.93741200	1.73110600	-0.05427100
C	1.20386800	-0.57889900	-0.00628100
C	2.54072300	-0.99402800	0.02782200
C	3.27194700	1.32216100	-0.02004900
H	0.41710500	-1.32021000	-0.00162500
H	4.07461300	2.04959100	-0.02455900
O	1.56388000	3.00728200	-0.09626800
C	2.54716600	4.03618900	-0.10996600
H	3.15218900	4.00080300	0.80188500
H	1.98935800	4.97076200	-0.14970600
H	3.18601800	3.94445300	-0.99436700
O	2.92422600	-2.26827800	0.06826000
C	1.94229800	-3.29844600	0.07718500

H	1.30133600	-3.21291300	0.96047200
H	2.50341100	-4.23136000	0.11459000
H	1.33785200	-3.26309600	-0.83483100
O	-6.24391100	0.63119800	-0.12949000
C	-6.11033800	1.74734600	0.75293400
H	-7.00374300	2.35379400	0.59377400
H	-5.20910300	2.32401800	0.52554500
H	-6.08864300	1.39512100	1.79187100
Br	5.36027300	-0.58772400	0.06670900

System 5

C	3.84751800	-1.16807900	0.00001800
C	2.82335700	1.48045900	-0.00011400
C	2.46972000	-0.93540900	-0.00012800
C	4.71122100	-0.06684900	0.00007800
C	4.21084900	1.24563100	0.00001000
C	1.99646200	0.38435700	-0.00016900
H	4.88273500	2.09617200	0.00006400
H	2.43108400	2.49337200	-0.00014200
O	0.61500900	0.42423700	-0.00021400
C	1.30867400	-1.80232800	-0.00028000
C	0.16771300	-0.86910700	-0.00017900
C	-1.15987400	-1.21181700	-0.00009800
H	-1.33465700	-2.28157000	-0.00009700
O	1.22967200	-3.05002500	-0.00005000
C	-2.30807700	-0.34181500	-0.00002600
C	-4.69635900	1.23405700	0.00009200
C	-3.62701900	-0.93268200	0.00004900
C	-2.24524700	1.05001800	-0.00002900
C	-3.41675400	1.83275000	0.00003000
C	-4.78978200	-0.14323900	0.00010100
H	-1.27459800	1.52596800	-0.00008400
H	-5.76761400	-0.61151400	0.00014600
O	-3.64169900	-2.26248300	0.00005700
C	-4.87928200	-2.96630000	0.00017700
H	-5.45625300	-2.72668200	0.89895900
H	-4.61231600	-4.02214100	0.00022500
H	-5.45636200	-2.72679500	-0.89856600
O	-3.41246500	3.16646200	0.00002800
C	-2.17495400	3.87222600	-0.00001100
H	-1.59604700	3.63476600	0.89788800
H	-2.44338800	4.92785000	0.00003000
H	-1.59613200	3.63481400	-0.89797700
H	-5.57879200	1.86515700	0.00013100
H	4.25293800	-2.17573700	0.00005600
O	6.04050700	-0.36572900	0.00020100

C	6.96673400	0.70099900	0.00022600
H	6.85838000	1.32513200	-0.89597200
H	7.95516800	0.23907500	0.00030700
H	6.85826200	1.32519300	0.89636700

System 8

C	-5.09420300	0.83569200	0.00005600
C	-3.70011100	-1.63937700	-0.00000400
C	-3.69916500	0.80432900	0.00000600
C	-5.79028300	-0.38098500	0.00006700
C	-5.10556100	-1.60781200	0.00003600
C	-3.04134600	-0.43346800	-0.00001600
H	-5.64771000	-2.54631400	0.00004500
H	-3.16426900	-2.58409900	-0.00002100
O	-1.67079800	-0.27256500	-0.00003800
C	-2.67217700	1.82962700	-0.00003100
C	-1.41168700	1.06754400	-0.00002300
C	-0.14075500	1.59565000	-0.00002300
H	-0.12179800	2.67981600	-0.00001400
O	-2.77078200	3.07426100	0.00002600
C	1.11185700	0.90527600	-0.00003100
C	3.68552300	-0.30889100	0.00001900
C	2.33254200	1.68281000	-0.00001500
C	1.25343300	-0.48714000	-0.00005000
C	2.51064900	-1.10431900	-0.00003800
C	3.58877900	1.07246900	0.00000400
H	0.36120600	-1.09759000	-0.00007500
H	4.49467000	1.66643000	0.00000700
O	2.15944200	3.00240500	-0.00001000
C	3.28897300	3.86787800	0.00002700
H	3.89378800	3.70937900	0.89875900
H	2.88136900	4.87786800	0.00003200
H	3.89382600	3.70940400	-0.89868500
O	2.69360400	-2.42328500	-0.00005400
C	1.56464600	-3.28957900	-0.00010200
H	0.95857900	-3.13359000	0.89804600
H	1.97526800	-4.29854400	-0.00011100
H	0.95862700	-3.13355400	-0.89827700
H	-5.64323600	1.77295700	0.00007800
O	-7.14556900	-0.27551600	0.00010600
C	-7.91246300	-1.46325100	0.00015500
H	-7.71605400	-2.06460200	-0.89629600
H	-8.95578600	-1.14492200	0.00020600
H	-7.71596000	-2.06458800	0.89659600
Br	5.35936500	-1.13654900	-0.00004700