Supporting Information for How Well Does a Solvated Octa-Acid Capsule Shield the Embedded Chromophore? A Computational Analysis Based on an Anisotropic Dielectric Continuum Model

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SI Table S1: TDDFT calculated excitation energies (free solvated coumarins) at 6-31+G and CC-pVTZ basis sets, to complement the values in Table 1 (eV).

ε	Coumarin	TDDFT		
		IEF-PCM		PEqS
		ptSS	equilibrium	
		CC-PVTZ		
3	C-1	3.35	3.39	3.43
	C-153	2.99	3.01	3.04
	C-480	3.18	3.20	3.22
78	C-1	3.16	3.20	3.23
	C-153	2.84	2.86	2.87
	C-480	3.05	3.07	3.08
		6-31+G*		
3	C-1	3.31	3.35	3.38
	C-153	2.94	2.97	3.00
	C-480	3.15	3.17	3.18
78	C-1	3.11	3.15	3.18
	C-153	2.79	2.81	2.82
	C-480	3.02	3.04	3.04

SI Table S2: TDDFT excitation energies using anisotropic solvation models (eV). PEqS values are compared to those obtained using IEF* and PEqS* (based on increasing the vdW atomic radii). The ptSS* non equilibrium correction is smaller than 0.001 eV in absolute value in all cases.

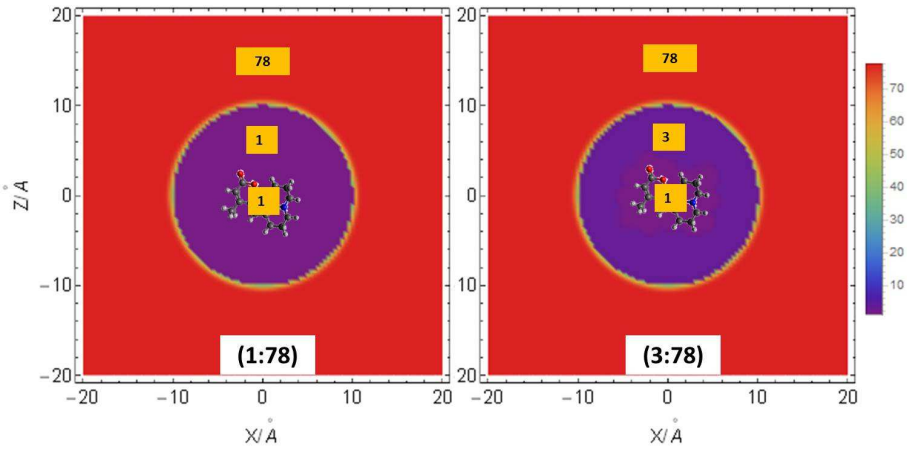
Coumarin	PEqS (1:78)	PEqS* (1:78)	IEF* (1:78)	PEqS* (1:3)	IEF* (1:3)
		6-31G*			
C-1	3.43	3.47	3.47	3.57	3.57
C-153	3.08	3.13	3.13	3.21	3.21
C-480	3.26	3.27	3.27	3.35	3.34
		6-31+G*			
C-1	3.39	3.38	3.38	NA	NA
C-153	3.04	3.03	3.03	NA	NA
C-480	3.21	3.19	3.19	NA	NA

SI Table S3: Absorption state energies (eV) of reoriented molecules within the capsule. PEqS obtained upon rotating the coumarin within the capsule cavity (see illustrated in SI Figure S2). PEqS* values are obtained using a surrounding spherical surface of 10Å radius for the dielectric interface.

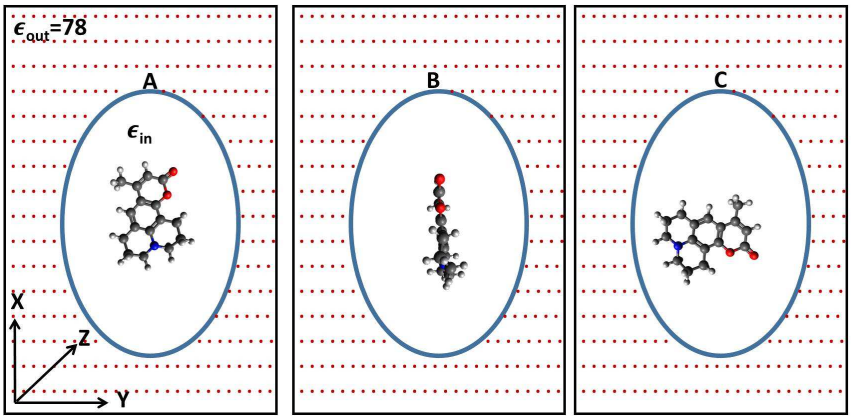
Coumarin system	Exp.	PEqS* (1:78)	PEqS (1:78)
C-1	3.43	3.46	A→ 3.43
			B→ 3.44
			C→ 3.46
C-153	2.93	3.13	A→ 3.08
			B→ 3.10
			C→ 3.12
C-480	3.28	3.27	A→ 3.26
			B→ 3.26
			C→ 3.27

SI Table S4: TDDFT excitation energies using anisotropic solvation models and based on an effective constant are compared to experiment (eV). The PEqS* (1:78) and (3:78) are due to dielectric interface set to a spherical surface surrounding the coumarin of the noted radius in the parenthesis.

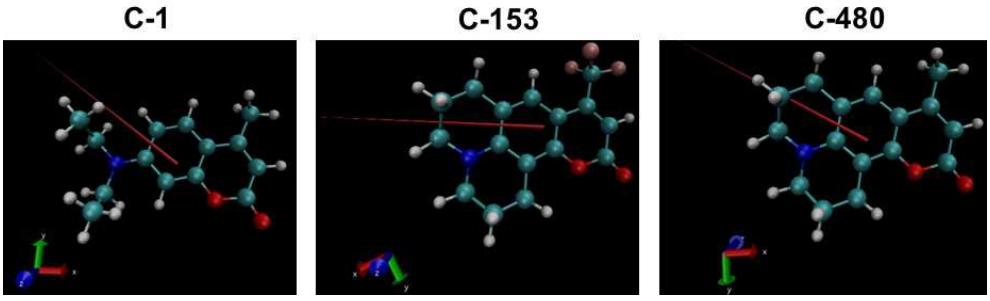
Coumarin	Exp.	PEqS $\varepsilon_{\text{eff}} = 3$	PEqS* (3:78)	PEqS* (1:78)	PEqS (1:78)
C-1	3.43	3.48	3.28 (7.5Å) 3.30 (10Å) 3.30 (15Å)	3.46 (7.5Å) 3.46 (10Å) 3.47 (15Å)	3.43
C-153	2.93	3.11	2.94 (7.5Å) 2.96 (10Å) 2.97 (15Å)	3.13 (7.5Å) 3.13 (10Å) 3.13 (15Å)	3.08
C-480	3.28	3.27	3.14 (7.5Å) 3.14 (10Å) 3.16 (15Å)	3.27 (7.5Å) 3.27 (10Å) 3.27 (15Å)	3.26



SI Figure S1: 2D contour plotting of the dielectric distribution of PEqS* (1:78) and (3:7) setups based on spherical surfaces as the dielectric interface. Radii of the sphere is set at 10Å.



SI Figure S2: Illustrating of the coumarins in a 1:78 setup. The different orientations of the coumarins used in the calculations reported in SI Table S3 are illustrated, where orientations B and C are obtained by rotating the coumarin within the capsule. Here for demonstration we represent the capsule as an ellipsoid.



SI Figure S3: Ground state dipole moment of each coumarin. The C-153 dipole is skewed compared to C-1 and C-480 dipoles.

SI Table S5: C-1 atomic coordinates (Å) at B3LYP/6-31G(d) IEF-PCM level.

C	1.443890000000000	0.839910000000000	-0.041840000000000
C	0.986810000000000	-0.491480000000000	-0.121280000000000
C	3.704810000000000	0.003820000000000	0.134060000000000
H	4.777280000000000	0.130110000000000	0.232020000000000
C	3.238960000000000	-1.359260000000000	0.053410000000000
C	3.392610000000000	2.481380000000000	0.180260000000000
H	2.973940000000000	3.005830000000000	1.047460000000000
H	3.119110000000000	3.062410000000000	-0.708480000000000
H	4.481500000000000	2.483370000000000	0.270410000000000
C	2.860140000000000	1.076600000000000	0.091310000000000
O	1.865970000000000	-1.543380000000000	-0.073200000000000
O	3.925620000000000	-2.367610000000000	0.084720000000000
C	-0.354590000000000	-0.824430000000000	-0.246280000000000
C	-1.342480000000000	0.186490000000000	-0.312820000000000
C	-0.890940000000000	1.538490000000000	-0.217580000000000
N	-2.673430000000000	-0.117440000000000	-0.479400000000000
C	-3.696030000000000	0.934510000000000	-0.513420000000000
H	-4.561520000000000	0.521200000000000	-1.038810000000000
C	0.449960000000000	1.840510000000000	-0.093060000000000
H	0.742450000000000	2.883800000000000	-0.028530000000000
C	-3.126660000000000	-1.511040000000000	-0.544140000000000
H	-4.093310000000000	-1.510490000000000	-1.055400000000000
H	-0.603930000000000	-1.875910000000000	-0.287590000000000
H	-1.600060000000000	2.355180000000000	-0.239510000000000
C	-3.268420000000000	-2.206330000000000	0.816550000000000
H	-4.021180000000000	-1.709170000000000	1.436430000000000
H	-3.580290000000000	-3.246900000000000	0.670970000000000
H	-2.322450000000000	-2.209190000000000	1.367260000000000
C	-4.132300000000000	1.452560000000000	0.863150000000000
H	-4.581460000000000	0.653490000000000	1.461450000000000
H	-3.286200000000000	1.862340000000000	1.424180000000000
H	-4.877390000000000	2.247280000000000	0.742300000000000
H	-2.444290000000000	-2.076580000000000	-1.188300000000000
H	-3.335430000000000	1.762940000000000	-1.132320000000000

SI Table S6: C-153 atomic coordinates (Å) at B3LYP/6-31G(d) IEF-PCM level.

C	1.907590000000000	-0.145060000000000	-0.065290000000000
C	1.174290000000000	-1.378620000000000	-0.069640000000000
C	1.200130000000000	1.087360000000000	-0.046600000000000
C	-0.938520000000000	-0.148080000000000	-0.023810000000000
C	-0.190430000000000	1.050220000000000	-0.033970000000000
C	-2.975330000000000	1.191720000000000	0.008500000000000
H	-4.050990000000000	1.299940000000000	0.027020000000000
C	-2.202940000000000	2.413180000000000	-0.007420000000000
C	-3.227340000000000	-1.271780000000000	0.016410000000000
C	-2.367360000000000	-0.027250000000000	0.000090000000000
O	-0.825310000000000	2.270070000000000	-0.031070000000000
O	-2.646660000000000	3.547770000000000	-0.003320000000000
N	3.282510000000000	-0.155320000000000	-0.059540000000000
C	1.912230000000000	-2.700690000000000	-0.126840000000000
H	1.338580000000000	-3.469130000000000	0.403110000000000
H	1.987610000000000	-3.035810000000000	-1.171770000000000
C	3.319860000000000	-2.570090000000000	0.454640000000000
H	3.894800000000000	-3.487700000000000	0.293090000000000
H	3.269420000000000	-2.396880000000000	1.536640000000000
C	4.036650000000000	-1.401130000000000	-0.211960000000000
H	4.203660000000000	-1.619070000000000	-1.279450000000000
H	5.020790000000000	-1.246130000000000	0.241920000000000
C	-0.203740000000000	-1.354730000000000	-0.037030000000000
H	-0.731770000000000	-2.301740000000000	-0.031740000000000
C	4.033300000000000	1.083360000000000	-0.268960000000000
H	5.045880000000000	0.924390000000000	0.114180000000000
H	4.123500000000000	1.297970000000000	-1.346320000000000
C	3.367810000000000	2.252640000000000	0.448250000000000
H	3.940660000000000	3.167760000000000	0.266170000000000
H	3.382270000000000	2.064560000000000	1.528720000000000
C	1.927330000000000	2.416160000000000	-0.038630000000000
H	1.925610000000000	2.845790000000000	-1.050830000000000
H	1.388910000000000	3.130370000000000	0.591990000000000
F	-4.543780000000000	-0.990010000000000	0.045200000000000

SI Table S7: C-480 atomic coordinates (Å) at B3LYP/6-31G(d) IEF-PCM level.

C	1.323454246800000	-0.947715324400000	0.015106945400000
C	0.999619325800000	0.464710116200000	0.028681008600000
C	3.661745005900000	-0.327909524700000	-0.060442904600000
H	4.720855427900000	-0.576425106400000	-0.101553734500000
C	3.361861030400000	1.059710250500000	-0.040795716700000
C	3.061998679700000	-2.791907575100000	-0.043374835900000
H	2.646371670200000	-3.311820520000000	-0.922373848200000
H	2.687881159000000	-3.321391890500000	0.848250831500000
H	4.151891506600000	-2.911259309900000	-0.069834940200000
C	2.686897129000000	-1.340193554600000	-0.026456472200000
O	1.964649042200000	1.405493827800000	0.027280218400000
O	4.116012619200000	2.015950749900000	-0.069166164000000
C	-1.372823360000000	-0.015176295600000	0.083564498800000
C	-1.090204017100000	-1.419481963200000	0.073856728900000
C	-0.300536144900000	0.929527245200000	0.042956449900000
N	-2.673615755600000	0.430915471400000	0.118981322600000
C	-2.216998815300000	-2.419360757000000	0.128982824700000
H	-1.939807089300000	-3.318191368600000	-0.439297592800000
H	-2.367219727400000	-2.745030600400000	1.172743171200000
C	-3.512130932700000	-1.815806608500000	-0.402009284800000
H	-4.360081210100000	-2.494804162300000	-0.240155797200000
H	-3.431706074600000	-1.633426777300000	-1.483716993400000
C	-3.776538646700000	-0.497506527500000	0.309125391600000
H	-3.938933233300000	-0.679211555600000	1.389462490100000
H	-4.685753593400000	-0.019119272100000	-0.080464519200000
C	0.223495106700000	-1.853179867000000	0.032928202400000
H	0.423696537600000	-2.924050874400000	0.017574704600000
C	-2.962600880000000	1.841232056100000	0.329156799500000
H	-3.993393447400000	2.021950372600000	-0.005483240900000
H	-2.919596017500000	2.081904268700000	1.409399940300000
C	-1.978023003500000	2.716474071000000	-0.432501954300000
H	-2.227652628900000	3.773862054900000	-0.270464376800000
H	-2.076102332300000	2.512120077100000	-1.508837318000000
C	-0.559749960100000	2.415354348700000	0.037235907200000