

Supporting Information

Visualization of Cellular Membranes in 2D and 3D Conditions Using a New Fluorescent Dithienothiophene *S,S*-Dioxide Derivative

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1. Atomic coordinates of compound 2 optimized at the m062x-D3/6-311(d,p) level of theory in dichloromethane (SMD solvation model)

| | 0,1 | C,0,-2.37219832,0.07350747,-2.69044705 | C,0,-2.34595732,0.06656501,-1.2820429 | C,0,-1.10017705,-0.04254907,-0.72544291 | S,0,0.10529631,-0.15045617,-1.94271188 | C,0,-1.1015934,-0.03002768,-3.2117402 | C,0,-2.3459568,0.06656117,1.28204337 | C,0,-1.10017673,-0.0425512,0.72544258 | C,0,-2.37219713,0.07350081,2.69044754 | C,0,-1.10159202,-0.03003606,3.21173987 | S,0,0.10529715,-0.15046136,1.94271077 | C,0,-0.75370488,-0.04097559,-4.61707822 | H,0,-3.25908081,0.15535194,3.30387828 | C,0,-0.75370298,-0.04098616,4.61707776 | C,0,0.49627544,-0.02593215,5.11268044 | C,0,0.8771948,-0.03724322,6.51996616 | C,0,0.49627354,-0.02592748,-5.11268104 | C,0,0.8771932,-0.03723864,-6.51996669 | C,0,2.22933598,0.08749449,-6.86814653 | C,0,-0.042207,-0.16663138,-7.57389081 | C,0,0.35864423,-0.15924427,-8.89469796 | C,0,1.7253284,-0.01720896,-9.24378767 | C,0,2.6543681,0.09944323,-8.1847072 | C,0,-0.04220497,-0.16664407,7.57388965 | C,0,0.35864542,-0.15925399,8.89469706 | C,0,1.7253283,-0.01720841,9.24378762 | C,0,2.65436777,0.09945101,8.18470773 | C,0,2.22933638,0.08750031,6.8681468 | H,0,-1.61337513,-0.04868452,-5.28090782 | H,0,-1.61337304,-0.04870115,5.28090756 | H,0,1.33531802,0.01163402,4.41863712 | H,0,1.33531632,0.01163264,-4.41863761 | H,0,2.96927716,0.17972105,-6.07882162 | H,0,-1.09922299,-0.28208035,-7.36050972 | H,0,-0.39077595,-0.2658506,-9.66729532 | N,0,2.12556565,0.00381621,-10.54862256 | H,0,3.71073747,0.19809505,-8.393411 | H,0,-1.09921977,-0.28210243,7.36050786 | H,0,-0.39077426,-0.26586706,9.66729394 | N,0,2.12556488,0.00381906,10.54862267 | H,0,3.71073623,0.19811118,8.39341216 | H,0,2.96927714,0.17973349,6.07882226 | C,0,1.15177045,-0.1639648,11.61177691 | C,0,3.53588598,0.12008636,10.86987485 | C,0,3.53588741,0.12007698,-10.86987416 | C,0,1.15177108,-0.16396457,-11.61177712 | H,0,1.66293645,-0.11424246,12.57045495 | H,0,0.3940528,0.62618283,11.5884721 | H,0,0.64053717,-1.13082017,11.54355898 | H,0,3.65363099,0.133244,11.95089137 | H,0,4.11255362,-0.72200728,10.47080244 | H,0,3.96099286,1.04602052,10.46867425 | H,0,3.65363292,0.13323539,-11.95089062 | H,0,3.96099853,1.0460086,-10.46867224 | H,0,4.11255087,-0.72201983,-10.47080239 | H,0,1.66293803,-0.11424638,-12.57045484 | H,0,0.64053327,-1.13081747,-11.54355787 | H,0,0.39405701,0.62618652,-11.58847433 | H,0,-3.25908227,0.15536003,-3.3038772 | S,0,-3.58501656,0.1804147,0.00000065 | O,0,-4.21321423,1.49337253,0.00000286 | O,0,-4.44387803,-0.99467967,-0.0000011 | | Version=EM64W-G09RevD.01 | State=1-A | HF=-2536.9020247 | RMSD=6.944e-009 | PG=C01 [X(C28H26N2O2S3)] | | @

2. Partial output data of the TDDFT m062x/6-311+G(2d,p)//m062x-D3/6-311G(d,p) calculations in dichloromethane (SMD solvation model)

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.4766 eV 500.62 nm f=1.6745 <S**2>=0.000
134 -> 137 -0.17875
135 -> 138 -0.14008
136 -> 137 0.66210

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -2536.82807020

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.2038 eV 386.99 nm f=0.2357 <S**2>=0.000
133 -> 137 -0.12118
135 -> 137 0.63684
136 -> 138 -0.25539

Excited State 3: Singlet-A 3.8045 eV 325.89 nm f=0.7521 <S**2>=0.000
128 -> 137 0.10237
134 -> 137 -0.38471
135 -> 138 0.31999
136 -> 139 0.45137

Excited State 4: Singlet-A 3.8992 eV 317.98 nm f=0.1018 <S**2>=0.000

134 -> 138	-0.10844	
135 -> 137	0.25582	
135 -> 139	0.22060	
136 -> 138	0.58711	
Excited State 5:	Singlet-A	4.2446 eV 292.10 nm f=0.0793 <S**2>=0.000
134 -> 137	0.48579	
135 -> 138	0.13603	
135 -> 145	0.21116	
136 -> 137	0.16567	
136 -> 139	0.29004	
136 -> 144	0.22112	
Excited State 6:	Singlet-A	4.3165 eV 287.23 nm f=0.1944 <S**2>=0.000
131 -> 137	0.10066	
132 -> 138	0.10209	
134 -> 145	0.12454	
135 -> 144	0.41611	
136 -> 138	-0.10944	
136 -> 145	0.48627	
Excited State 7:	Singlet-A	4.3254 eV 286.64 nm f=0.1636 <S**2>=0.000
134 -> 137	-0.20915	
134 -> 139	0.10324	
135 -> 145	0.36396	
136 -> 139	-0.23336	
136 -> 144	0.43811	
Excited State 8:	Singlet-A	4.4437 eV 279.01 nm f=0.0089 <S**2>=0.000
134 -> 140	-0.10666	
134 -> 142	-0.21700	
136 -> 140	0.32450	
136 -> 142	0.48212	
136 -> 143	0.12887	
136 -> 146	0.17595	
Excited State 9:	Singlet-A	4.5985 eV 269.62 nm f=0.0000 <S**2>=0.000
134 -> 143	0.11272	
135 -> 141	-0.23277	
136 -> 140	0.52633	
136 -> 142	-0.30171	
Excited State 10:	Singlet-A	4.6937 eV 264.15 nm f=0.0595 <S**2>=0.000
130 -> 137	0.21447	
134 -> 139	0.22890	
135 -> 138	0.50811	
136 -> 137	0.15448	
136 -> 139	-0.22903	
136 -> 149	0.14996	
Excited State 11:	Singlet-A	4.6983 eV 263.89 nm f=0.0298 <S**2>=0.000
134 -> 141	0.10462	
135 -> 140	-0.23880	
135 -> 142	0.16037	
135 -> 143	-0.28926	
135 -> 160	-0.11191	
136 -> 141	0.51021	

136 -> 159 0.12042

Excited State 12: Singlet-A 4.7865 eV 259.03 nm f=0.0005 <S**2>=0.000

134 -> 140 0.13395

135 -> 141 -0.34045

135 -> 159 -0.10499

136 -> 140 -0.17294

136 -> 143 0.49033

136 -> 160 0.12129

3. NMR spectra



