Supplementary Information

Against the NEER Principle: The Third Type of Photochromism for GFP Chromophore Derivatives

*Jun-Wei Liao, Robert Sung and Kuangsen Sung**

Department of Chemistry, National Cheng Kung University, Tainan, Taiwan

Content Page

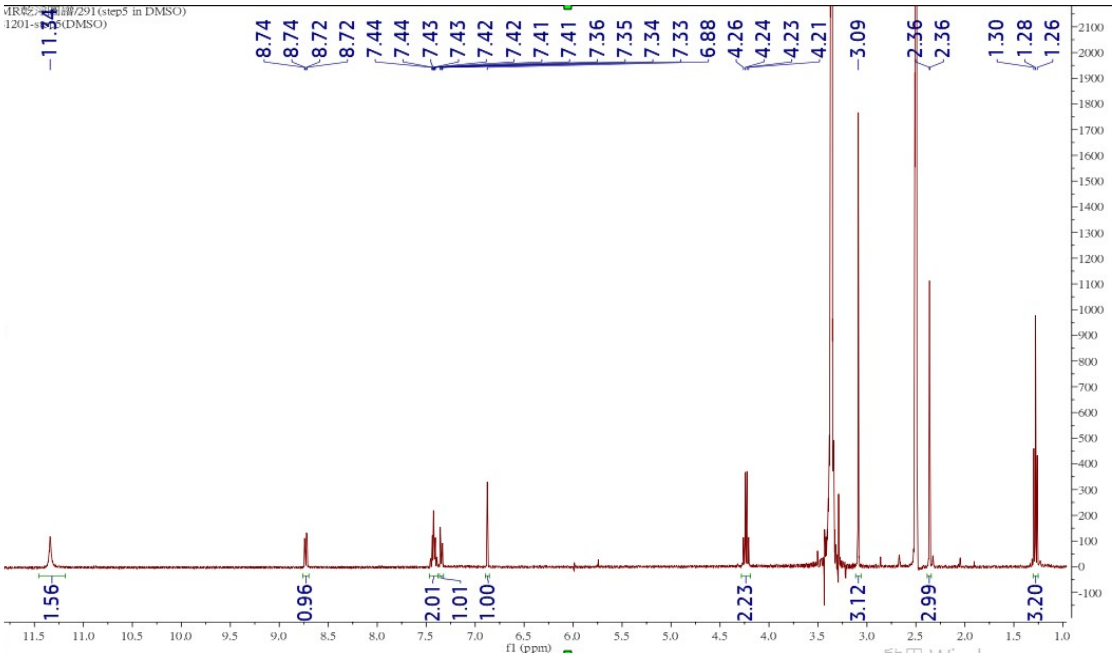

Figure S1. ^{1}H-NMR spectrum (400 MHz) of **1** in d_6-DMSO

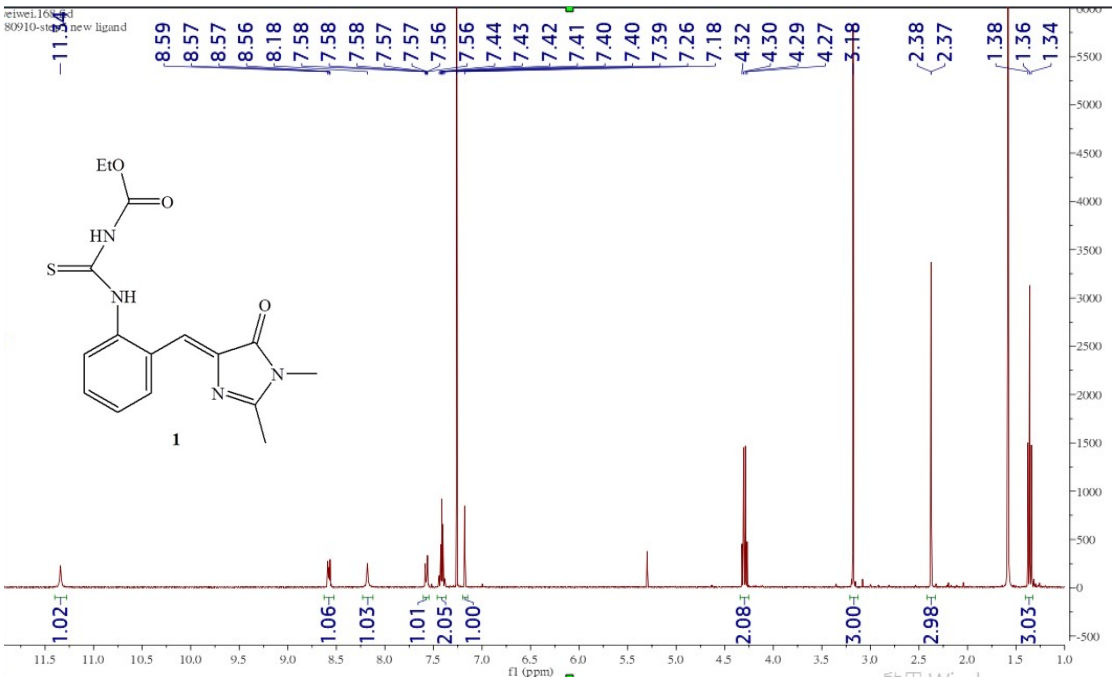

Figure S2. ^{1}H-NMR spectrum (400 MHz) of **1** in $CDCl_3$

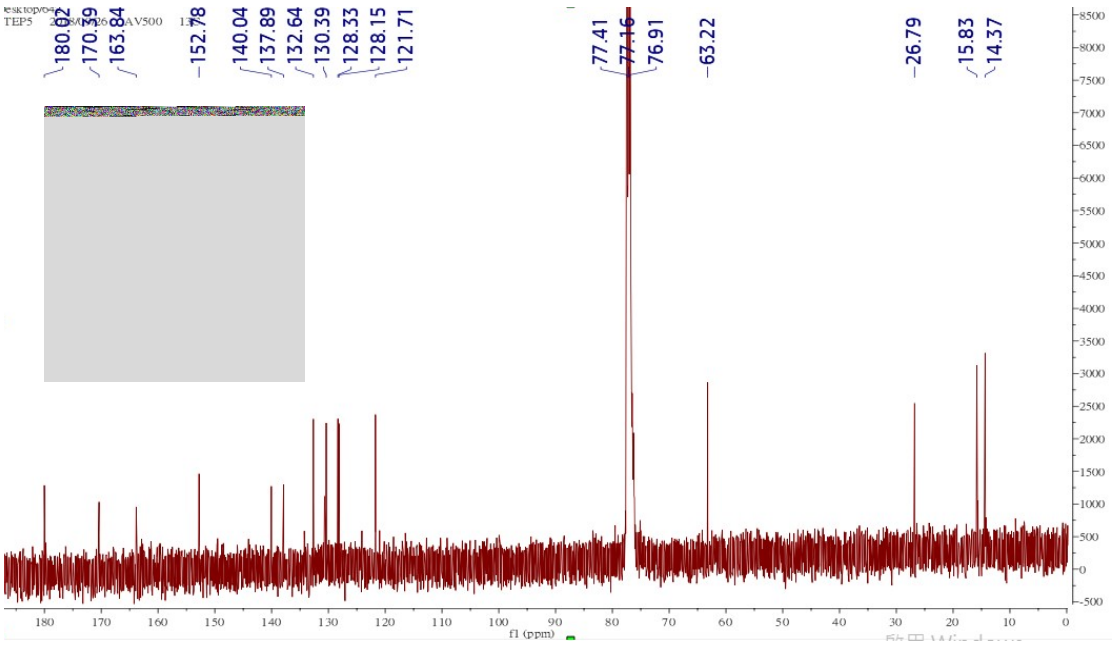

Figure S3. ^{13}C-NMR spectrum (125 MHz) of **1** in $CDCl_3$

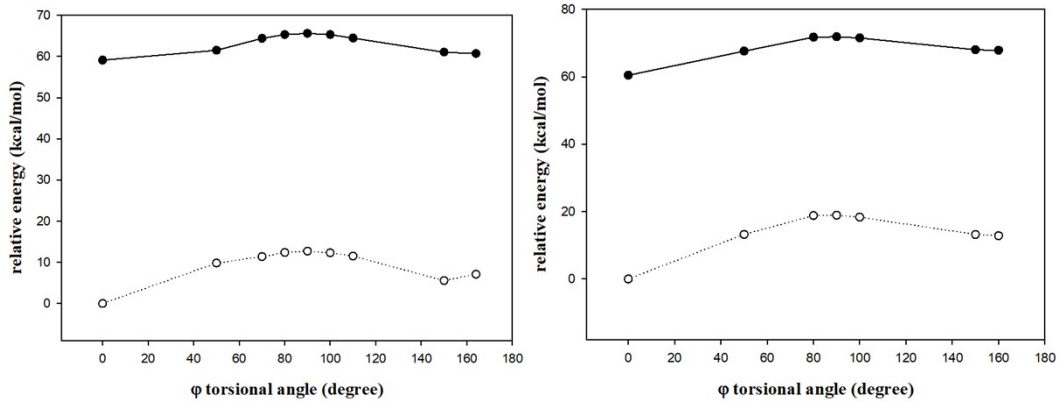

Fig. S4. The S_1 (solid line) and Franck-Condon S_0 (dashed line) relaxed PESs of *s*-*E*-**1** along φ-torsion relaxation in gas phase (left) and DMSO (right) at the TD-CAM-B3LYP/6-31+G* level

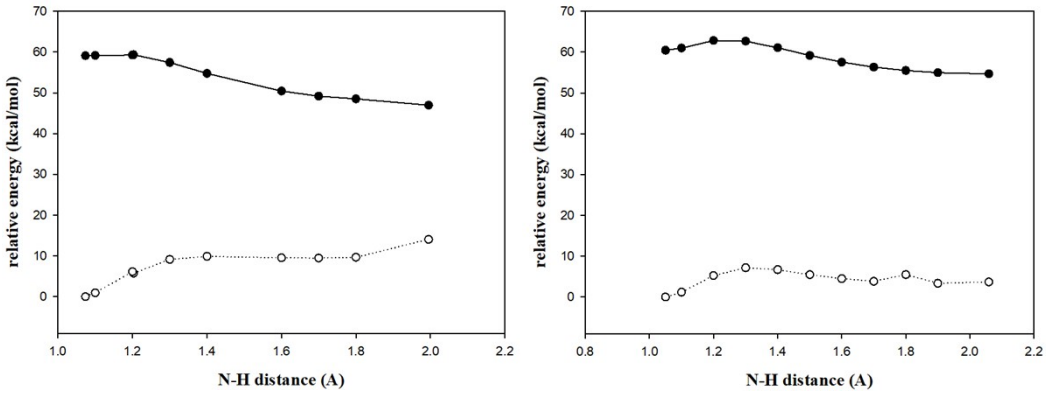

Fig. S5. The S_1 (solid line) and Franck-Condon S_0 (dashed line) relaxed PESs for ESIPT of *s*-*Z*-**1** in gas phase (left) and DMSO (right) at the TD-CAM-B3LYP/6-31+G* level

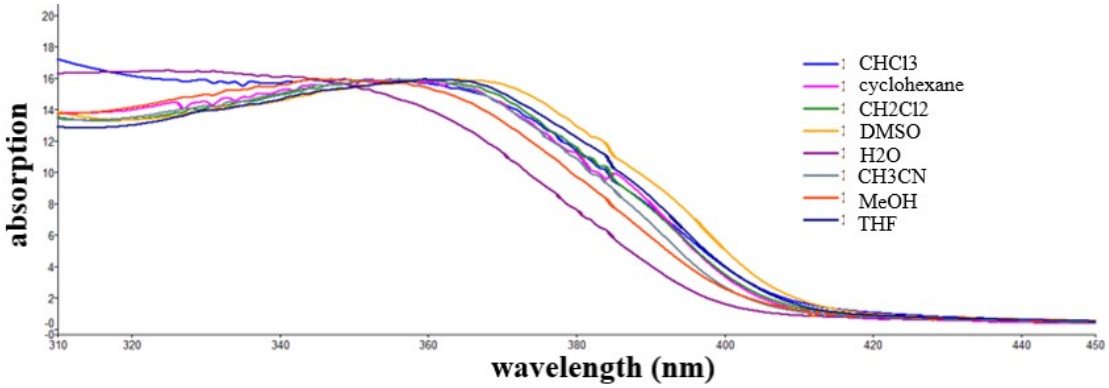

Figure S6. Normalized electronic absorption (λ_{abs}) of *s*-*E*-**1** in solvents of $CHCl_3$ (blue), cyclohexane (pink), CH_2Cl_2 (green), DMSO (yellow), H_2O (violet), CH_3CN (pale green), MeOH (orange) and THF (dark blue).

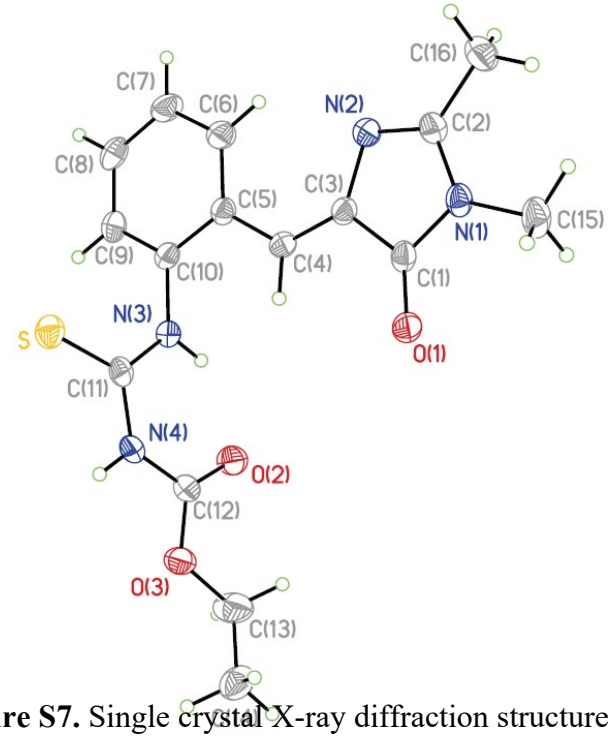

Figure S7. Single crystal X-ray diffraction structure of *s*-*E*-**1** with thermal ellipsoids at the 50% probability level

Table S1. Crystal data and structure refinement for *s*-*E*-**1**

Identification code	c16h18	
Empirical formula	C16 H18 N4 O3 S	
Formula weight	346.40	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 10.7329(4) Å	α= 90°.
	b = 15.3130(6) Å	β= 111.0676(16)°.
	c = 10.9752(4) Å	γ = 90°.
Volume	1683.23(11) $Å^3$	
Z	4	
Density (calculated)	1.367 Mg/m^3	
Absorption coefficient	0.215 mm^{-1}	
F(000)	728	
Crystal size	0.540 x 0.460 x 0.310 mm^3	
Theta range for data collection	3.322 to 27.155°.	
Index ranges	-13<=h<=13, -19<=k<=19, -14<=l<=14	
Reflections collected	28452	
Independent reflections	3718 [R(int) = 0.0455]	
Completeness to theta = 25.242°	99.8 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9281 and 0.8340
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3718 / 0 / 231
Goodness-of-fit on F^2	1.170
Final R indices [I>2sigma(I)]	R1 = 0.0501, wR2 = 0.1201
R indices (all data)	R1 = 0.0720, wR2 = 0.1375
Extinction coefficient	n/a
Largest diff. peak and hole	0.535 and -0.349 e.$Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for *s-E*-**1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S	5594(1)	812(1)	7938(1)	31(1)
O(1)	1518(2)	563(1)	2291(2)	32(1)
O(2)	4082(2)	-1708(1)	5646(2)	36(1)
O(3)	6178(2)	-1725(1)	5619(2)	35(1)
N(1)	-342(2)	1430(1)	1932(2)	26(1)
N(2)	-425(2)	1529(1)	3953(2)	27(1)
N(3)	3637(2)	-348(1)	6934(2)	24(1)
N(4)	5625(2)	-639(1)	6649(2)	24(1)
C(1)	732(2)	943(2)	2684(2)	25(1)
C(2)	-977(2)	1752(2)	2735(2)	27(1)
C(3)	672(2)	1004(2)	4014(2)	24(1)
C(4)	1569(2)	602(2)	5047(2)	24(1)
C(5)	1675(2)	596(1)	6408(2)	24(1)
C(6)	768(2)	1037(2)	6844(2)	30(1)
C(7)	892(3)	1009(2)	8138(2)	34(1)
C(8)	1923(2)	546(2)	9041(2)	32(1)
C(9)	2842(2)	111(2)	8641(2)	27(1)
C(10)	2717(2)	138(1)	7339(2)	23(1)
C(11)	4893(2)	-94(1)	7147(2)	23(1)
C(12)	5193(2)	-1399(2)	5941(2)	27(1)
C(13)	5880(3)	-2528(2)	4845(3)	50(1)
C(14)	6858(3)	-2615(2)	4178(3)	42(1)
C(15)	-746(3)	1530(2)	516(2)	37(1)
C(16)	-2193(3)	2305(2)	2197(3)	39(1)

Table S3. Bond lengths [Å] and angles [°] for *s*-*E*-**1**.

S-C(11)	1.666(2)
O(1)-C(1)	1.224(3)
O(2)-C(12)	1.213(3)
O(3)-C(12)	1.327(3)
O(3)-C(13)	1.463(3)
N(1)-C(1)	1.372(3)
N(1)-C(2)	1.385(3)
N(1)-C(15)	1.463(3)
N(2)-C(2)	1.298(3)
N(2)-C(3)	1.406(3)
N(3)-C(11)	1.340(3)
N(3)-C(10)	1.429(3)
N(3)-H(3A)	0.84(3)
N(4)-C(12)	1.384(3)
N(4)-C(11)	1.385(3)
N(4)-H(4A)	0.80(3)
C(1)-C(3)	1.488(3)
C(2)-C(16)	1.488(3)
C(3)-C(4)	1.344(3)
C(4)-C(5)	1.457(3)
C(4)-H(4B)	0.9500
C(5)-C(10)	1.402(3)
C(5)-C(6)	1.402(3)
C(6)-C(7)	1.379(3)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.386(4)
C(7)-H(7A)	0.9500
C(8)-C(9)	1.386(3)
C(8)-H(8A)	0.9500
C(9)-C(10)	1.387(3)
C(9)-H(9A)	0.9500
C(13)-C(14)	1.485(4)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800

C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800

C(12)-O(3)-C(13)	116.25(18)
C(1)-N(1)-C(2)	108.06(17)
C(1)-N(1)-C(15)	124.05(19)
C(2)-N(1)-C(15)	127.8(2)
C(2)-N(2)-C(3)	105.37(18)
C(11)-N(3)-C(10)	123.97(19)
C(11)-N(3)-H(3A)	115.0(18)
C(10)-N(3)-H(3A)	120.6(19)
C(12)-N(4)-C(11)	127.24(19)
C(12)-N(4)-H(4A)	116.9(18)
C(11)-N(4)-H(4A)	115.6(18)
O(1)-C(1)-N(1)	125.6(2)
O(1)-C(1)-C(3)	130.9(2)
N(1)-C(1)-C(3)	103.47(18)
N(2)-C(2)-N(1)	114.46(19)
N(2)-C(2)-C(16)	124.8(2)
N(1)-C(2)-C(16)	120.8(2)
C(4)-C(3)-N(2)	129.50(19)
C(4)-C(3)-C(1)	121.87(19)
N(2)-C(3)-C(1)	108.63(18)
C(3)-C(4)-C(5)	129.5(2)
C(3)-C(4)-H(4B)	115.3
C(5)-C(4)-H(4B)	115.3
C(10)-C(5)-C(6)	117.52(19)
C(10)-C(5)-C(4)	119.89(19)
C(6)-C(5)-C(4)	122.6(2)
C(7)-C(6)-C(5)	121.0(2)
C(7)-C(6)-H(6A)	119.5
C(5)-C(6)-H(6A)	119.5
C(6)-C(7)-C(8)	120.6(2)

C(6)-C(7)-H(7A)	119.7
C(8)-C(7)-H(7A)	119.7
C(9)-C(8)-C(7)	119.7(2)
C(9)-C(8)-H(8A)	120.2
C(7)-C(8)-H(8A)	120.2
C(10)-C(9)-C(8)	119.7(2)
C(10)-C(9)-H(9A)	120.1
C(8)-C(9)-H(9A)	120.1
C(9)-C(10)-C(5)	121.5(2)
C(9)-C(10)-N(3)	118.9(2)
C(5)-C(10)-N(3)	119.57(18)
N(3)-C(11)-N(4)	115.7(2)
N(3)-C(11)-S	124.74(17)
N(4)-C(11)-S	119.58(16)
O(2)-C(12)-O(3)	125.7(2)
O(2)-C(12)-N(4)	125.2(2)
O(3)-C(12)-N(4)	109.15(18)
O(3)-C(13)-C(14)	108.4(2)
O(3)-C(13)-H(13A)	110.0
C(14)-C(13)-H(13A)	110.0
O(3)-C(13)-H(13B)	110.0
C(14)-C(13)-H(13B)	110.0
H(13A)-C(13)-H(13B)	108.4
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
N(1)-C(15)-H(15A)	109.5
N(1)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
N(1)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(2)-C(16)-H(16A)	109.5
C(2)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5

C(2)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for *s*-***E*-1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S	30(1)	29(1)	32(1)	-3(1)	9(1)	-5(1)
O(1)	24(1)	51(1)	24(1)	-4(1)	12(1)	1(1)
O(2)	26(1)	37(1)	45(1)	-12(1)	13(1)	-6(1)
O(3)	25(1)	32(1)	47(1)	-12(1)	12(1)	-1(1)
N(1)	24(1)	37(1)	18(1)	2(1)	7(1)	-2(1)
N(2)	27(1)	30(1)	23(1)	0(1)	9(1)	3(1)
N(3)	23(1)	25(1)	22(1)	-2(1)	6(1)	0(1)
N(4)	18(1)	28(1)	25(1)	0(1)	5(1)	0(1)
C(1)	20(1)	34(1)	20(1)	-2(1)	6(1)	-5(1)
C(2)	23(1)	29(1)	26(1)	1(1)	7(1)	-1(1)
C(3)	22(1)	29(1)	20(1)	-3(1)	8(1)	-2(1)
C(4)	24(1)	30(1)	21(1)	-2(1)	10(1)	2(1)
C(5)	24(1)	26(1)	20(1)	-1(1)	8(1)	-2(1)
C(6)	32(1)	35(1)	25(1)	0(1)	12(1)	5(1)
C(7)	40(1)	39(1)	28(1)	-3(1)	20(1)	4(1)
C(8)	42(1)	34(1)	21(1)	-3(1)	14(1)	-6(1)
C(9)	31(1)	27(1)	20(1)	1(1)	7(1)	-4(1)
C(10)	25(1)	24(1)	21(1)	-3(1)	9(1)	-3(1)
C(11)	24(1)	26(1)	15(1)	6(1)	3(1)	2(1)
C(12)	24(1)	28(1)	26(1)	1(1)	6(1)	4(1)
C(13)	36(1)	35(2)	80(2)	-25(1)	24(2)	-7(1)
C(14)	55(2)	32(1)	36(1)	-4(1)	15(1)	6(1)
C(15)	35(1)	57(2)	19(1)	8(1)	9(1)	-2(1)
C(16)	34(1)	44(2)	36(1)	8(1)	7(1)	12(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for *s*-*E*-**1**.

	x	y	z	U(eq)
H(3A)	3380(30)	-795(19)	6460(30)	36(8)
H(4A)	6400(30)	-523(16)	6860(20)	23(6)
H(4B)	2231	273	4862	29
H(6A)	58	1359	6238	36
H(7A)	265	1310	8413	40
H(8A)	1999	526	9930	38
H(9A)	3555	-204	9256	32
H(13A)	4962	-2504	4190	60
H(13B)	5945	-3038	5419	60
H(14A)	6672	-3151	3654	62
H(14B)	6784	-2110	3608	62
H(14C)	7764	-2643	4833	62
H(15A)	-1537	1905	193	190(30)
H(15B)	-15	1796	309	140(20)
H(15C)	-956	955	99	140(20)
H(16A)	-2415	2382	1256	220(30)
H(16B)	-2940	2020	2353	250(40)
H(16C)	-2025	2877	2627	280(40)

Compound: *s*-*E*-**1** in gas phase

Method/basis set: CAM-B3LYP/6-31+G*

Energy of the optimized structure: -1384.3866644 Hartree

# of imaginary frequencies: 0

Cartesian coordinate of the optimized structure:

6	2.021208	3.674006	-0.922981
6	0.782805	3.079645	-0.723798
6	0.700844	1.724161	-0.429895
6	1.861016	0.932229	-0.331385
6	3.103088	1.551490	-0.554143
6	3.180838	2.905062	-0.841124
1	2.080343	4.734558	-1.147513
1	-0.130731	3.660400	-0.786470
1	4.001099	0.949948	-0.490457
1	4.151260	3.364636	-1.002071
7	-0.583810	1.119083	-0.289260
6	1.736615	-0.476521	0.019401
1	0.744089	-0.818468	0.299873
6	2.678839	-1.437621	0.063106
7	4.052335	-1.350569	-0.234579
6	2.353681	-2.837805	0.464500
7	3.594804	-3.467809	0.367344
6	4.523118	-2.533078	-0.043506
8	1.306288	-3.354948	0.796226
1	3.756299	-4.443220	0.571473
1	5.562687	-2.806015	-0.186592
6	-1.435450	1.349663	0.724070
1	-0.899599	0.467217	-1.008899
7	-2.650199	0.664610	0.639831
6	-3.076510	-0.213803	-0.327849
8	-2.447939	-0.530287	-1.323318
8	-4.289867	-0.673853	-0.021022
6	-4.863013	-1.627928	-0.943864
1	-4.929090	-1.156976	-1.927748
1	-4.186264	-2.482695	-1.017185
6	-6.218901	-2.015714	-0.402199
1	-6.874692	-1.143861	-0.324912
1	-6.687085	-2.740402	-1.075479

1	-6.129432	-2.473013	0.587162
1	-3.273132	0.829984	1.420621
16	-1.169662	2.333167	2.036735

Compound: *s*-*E*-**1** in DMSO

Method/basis set: CAM-B3LYP/6-31+G*; SCRF(PCM, solvent=DMSO)

Energy of the optimized structure: -1384.4110014 Hartree

# of imaginary frequencies: 0

Cartesian coordinate of the optimized structure:

6	1.842600	3.777257	-0.812711
6	0.635739	3.112769	-0.625210
6	0.623834	1.742452	-0.401189
6	1.818287	0.996869	-0.371191
6	3.025346	1.689370	-0.564591
6	3.036886	3.060484	-0.779804
1	1.848573	4.848634	-0.985944
1	-0.305834	3.651497	-0.648050
1	3.953230	1.132224	-0.544041
1	3.982834	3.572289	-0.926592
7	-0.641810	1.089260	-0.259529
6	1.757561	-0.441425	-0.141120
1	0.765812	-0.859393	0.005082
6	2.752937	-1.346726	-0.081861
7	4.140804	-1.160960	-0.227025
6	2.485181	-2.794234	0.167247
7	3.753797	-3.343125	0.148037
6	4.661819	-2.333201	-0.086086
8	1.433408	-3.389731	0.347515
1	3.969617	-4.322241	0.282542
1	5.722415	-2.547162	-0.141008
6	-1.310323	0.975600	0.890161
1	-1.104641	0.728491	-1.096281
7	-2.550518	0.363201	0.818785
6	-3.195258	-0.134448	-0.296320
8	-2.746784	-0.107522	-1.431396
8	-4.368059	-0.643514	0.049760
6	-5.174649	-1.213352	-1.015013
1	-5.372999	-0.427366	-1.746669

1	-4.593253	-2.003840	-1.493968
6	-6.441435	-1.739008	-0.384575
1	-7.001570	-0.935221	0.101331
1	-7.073381	-2.177319	-1.162545
1	-6.219750	-2.513195	0.355280
1	-3.038138	0.276379	1.702542
16	-0.756781	1.496830	2.388937

Compound: *s-Z*-**1** in gas phase

Method/basis set: CAM-B3LYP/6-31+G*

Energy of the optimized structure: -1384.38403475 Hartree

# of imaginary frequencies: 0

Cartesian coordinate of the optimized structure:

6	3.445654	-2.580829	-1.178198
6	2.099007	-2.303881	-0.996924
6	1.684817	-1.097004	-0.439454
6	2.636059	-0.130686	-0.070034
6	3.994767	-0.446145	-0.229469
6	4.401995	-1.648476	-0.784055
1	3.747679	-3.528616	-1.612689
1	1.345398	-3.034814	-1.267678
1	4.736886	0.284826	0.079146
1	5.459818	-1.859460	-0.905786
7	0.288771	-0.891510	-0.235782
6	2.329173	1.190965	0.483335
1	3.006081	1.565204	1.249160
6	1.364831	2.040997	0.099210
7	0.421737	1.846637	-0.925947
6	1.176275	3.401065	0.684639
7	0.105284	3.894379	-0.064299
6	-0.272615	2.927810	-0.974455
8	1.766943	3.982575	1.569861
1	-0.297740	4.812316	0.055904
1	-1.098284	3.088563	-1.658041
6	-0.436452	-1.615063	0.630132
1	-0.151988	-0.118041	-0.744197
7	-1.809300	-1.358583	0.652551
6	-2.571689	-0.576168	-0.180898

8	-2.156628	0.138587	-1.070903
8	-3.864930	-0.716418	0.143091
6	-4.803219	0.046145	-0.642014
1	-4.569446	1.107917	-0.525370
1	-4.670963	-0.218613	-1.694113
6	-6.188093	-0.289298	-0.138617
1	-6.295391	-0.027554	0.917836
1	-6.932733	0.272911	-0.710730
1	-6.398419	-1.356196	-0.254755
1	-2.308843	-1.911170	1.338184
16	0.141022	-2.766767	1.689493

Compound: *s*-*Z*-**1** in DMSO

Method/basis set: CAM-B3LYP/6-31+G*; SCRF(PCM, solvent=DMSO)

Energy of the optimized structure: -1384.4084241 Hartree

# of imaginary frequencies: 0

Cartesian coordinate of the optimized structure:

6	3.443210	-2.580234	-1.219369
6	2.094568	-2.312906	-1.024356
6	1.684685	-1.107820	-0.460870
6	2.629326	-0.132981	-0.101604
6	3.988625	-0.437472	-0.274037
6	4.396059	-1.639584	-0.833800
1	3.748695	-3.523503	-1.660684
1	1.341389	-3.045165	-1.295272
1	4.730210	0.297155	0.025764
1	5.453627	-1.842676	-0.968532
7	0.287891	-0.902946	-0.246269
6	2.300110	1.181856	0.458769
1	2.961975	1.552581	1.238726
6	1.329227	2.021006	0.067066
7	0.409809	1.841059	-0.983953
6	1.109341	3.367822	0.673913
7	0.064640	3.868698	-0.081820
6	-0.287142	2.925583	-1.023380
8	1.680303	3.926682	1.596281
1	-0.361315	4.778286	0.040106

1	-1.091284	3.116251	-1.723679
6	-0.411560	-1.514395	0.709554
1	-0.180042	-0.198089	-0.823777
7	-1.776346	-1.280720	0.733073
6	-2.563876	-0.656126	-0.215707
8	-2.152681	-0.125806	-1.230305
8	-3.838633	-0.724494	0.154369
6	-4.807948	-0.107505	-0.730221
1	-4.548650	0.948164	-0.835843
1	-4.731485	-0.588634	-1.707685
6	-6.169566	-0.299514	-0.106644
1	-6.221890	0.177129	0.876269
1	-6.927489	0.155958	-0.750778
1	-6.404777	-1.361918	0.002989
1	-2.265436	-1.715498	1.506149
16	0.229516	-2.518132	1.903149

Compound: *s*-*E*-**1** dimer in gas phase
Method/basis set: CAM-B3LYP/6-31+G*
Energy of the optimized structure: -2768.7942539 Hartree
# of imaginary frequencies: 0
Cartesian coordinate of the optimized structure:

6	5.565331	3.497377	-0.214938
6	4.208723	3.329491	-0.453828
6	3.675375	2.049953	-0.562189
6	4.498519	0.913970	-0.427685
6	5.874359	1.107860	-0.211566
6	6.399185	2.384879	-0.101073
1	5.975440	4.499051	-0.128922
1	3.550816	4.184425	-0.557008
1	6.514758	0.238688	-0.125398
1	7.462445	2.516755	0.074459
7	2.306838	1.874174	-0.902087
6	3.888011	-0.406504	-0.461069
1	2.804211	-0.430518	-0.396891
6	4.463196	-1.622942	-0.529817
7	5.826772	-1.953690	-0.650891
6	3.660759	-2.874335	-0.498968

7	4.633087	-3.857270	-0.623053
6	5.867002	-3.238084	-0.704239
8	2.461661	-3.066732	-0.388649
1	4.439795	-4.848168	-0.649418
1	6.776109	-3.819730	-0.805989
6	1.245259	2.267890	-0.170592
1	2.085656	1.402290	-1.782560
7	0.005219	1.979081	-0.732512
6	-0.239107	1.312060	-1.913467
8	0.615998	0.904751	-2.686213
8	-1.546285	1.162012	-2.106729
6	-1.926129	0.428124	-3.298217
1	-1.460468	0.912631	-4.159663
1	-1.532344	-0.586589	-3.207294
6	-3.433986	0.444891	-3.378619
1	-3.815741	1.469063	-3.430657
1	-3.751917	-0.088832	-4.279840
1	-3.879366	-0.054073	-2.514405
1	-0.811142	2.313316	-0.211115
16	1.316341	3.016503	1.316466
8	-2.461721	3.066785	0.388325
6	-3.660800	2.874394	0.498858
6	-4.463226	1.622998	0.529868
7	-4.633116	3.857325	0.623064
6	-3.888038	0.406566	0.461080
7	-5.826785	1.953736	0.651145
6	-5.867015	3.238131	0.704452
1	-4.439831	4.848225	0.649366
6	-4.498542	-0.913909	0.427790
1	-2.804247	0.430589	0.396731
1	-6.776110	3.819772	0.806330
6	-3.675380	-2.049888	0.562218
6	-5.874399	-1.107801	0.211782
6	-4.208733	-3.329428	0.453885
7	-2.306825	-1.874102	0.902033
6	-6.399230	-2.384819	0.101323
1	-6.514806	-0.238629	0.125667
6	-5.565361	-3.497315	0.215107

1	-3.550817	-4.184361	0.557006
6	-1.245276	-2.267842	0.170506
1	-2.085597	-1.402244	1.782508
1	-7.462504	-2.516696	-0.074122
1	-5.975471	-4.498990	0.129115
7	-0.005217	-1.979069	0.732403
16	-1.316406	-3.016414	-1.316570
6	0.239150	-1.312093	1.913373
1	0.811128	-2.313303	0.210981
8	-0.615931	-0.904712	2.686107
8	1.546343	-1.162145	2.106630
6	1.926269	-0.428264	3.298099
1	1.532807	0.586561	3.207019
1	1.460355	-0.912534	4.159539
6	3.434111	-0.445488	3.378679
1	3.879754	0.053212	2.514448
1	3.752104	0.088258	4.279865
1	3.815538	-1.469774	3.430904

Compound: *s*-*E*-**1** dimer in DMSO

Method/basis set: CAM-B3LYP/6-31+G*; SCRF(PCM, solvent=DMSO)

Energy of the optimized structure: -1384.4084241 Hartree

# of imaginary frequencies: 0

Cartesian coordinate of the optimized structure:

6	-5.371111	3.771089	-0.429229
6	-4.022044	3.618374	-0.133579
6	-3.523543	2.371465	0.222953
6	-4.368829	1.248054	0.306145
6	-5.731335	1.427553	0.009472
6	-6.224176	2.670780	-0.357981
1	-5.755581	4.746817	-0.708780
1	-3.344133	4.464154	-0.177056
1	-6.394029	0.573988	0.071894
1	-7.279402	2.784440	-0.585410
7	-2.143071	2.259728	0.575056
6	-3.804548	-0.041392	0.681502
1	-2.724307	-0.072727	0.789622
6	-4.422619	-1.214528	0.921581

7	-5.796410	-1.521182	0.892224
6	-3.668119	-2.440334	1.299288
7	-4.665309	-3.373399	1.471248
6	-5.878713	-2.766984	1.214821
8	-2.464493	-2.629744	1.443298
1	-4.521968	-4.339597	1.735344
1	-6.802445	-3.327479	1.291155
6	-1.128977	2.254260	-0.297102
1	-1.889022	2.240893	1.565327
7	0.144209	2.230461	0.240743
6	0.488296	2.210609	1.576620
8	-0.303318	2.189090	2.508580
8	1.807131	2.216667	1.708427
6	2.327891	2.183914	3.061944
1	1.914430	3.034815	3.607419
1	1.984454	1.261106	3.534592
6	3.833290	2.247971	2.965481
1	4.156227	3.172158	2.477643
1	4.258615	2.224110	3.973207
1	4.228119	1.396752	2.404299
1	0.921038	2.265609	-0.427677
16	-1.307264	2.253962	-1.971006
8	2.464578	2.629486	-1.443423
6	3.668161	2.440280	-1.298757
6	4.422633	1.214501	-0.920947
7	4.665289	3.373552	-1.469905
6	3.804572	0.041256	-0.681377
7	5.796367	1.521336	-0.890821
6	5.878654	2.767242	-1.213020
1	4.521937	4.339807	-1.733785
6	4.368815	-1.248229	-0.306097
1	2.724376	0.072501	-0.789966
1	6.802342	3.327894	-1.288730
6	3.523565	-2.371705	-0.223346
6	5.731266	-1.427730	-0.009187
6	4.022069	-3.618691	0.132897
7	2.143101	-2.259941	-0.575526
6	6.224105	-2.671040	0.357997

1	6.393928	-0.574114	-0.071246
6	5.371097	-3.771421	0.428735
1	3.344186	-4.464511	0.176040
6	1.129018	-2.254205	0.296641
1	1.889063	-2.241544	-1.565808
1	7.279292	-2.784708	0.585604
1	5.755574	-4.747210	0.708065
7	-0.144184	-2.230346	-0.241161
16	1.307353	-2.253650	1.970542
6	-0.488319	-2.210724	-1.577034
1	-0.920980	-2.265474	0.427292
8	0.303273	-2.189546	-2.509023
8	-1.807153	-2.216496	-1.708799
6	-2.327927	-2.183852	-3.062314
1	-1.984001	-1.261376	-3.535252
1	-1.914928	-3.035143	-3.607538
6	-3.833356	-2.247096	-2.965809
1	-4.227730	-1.395540	-2.404819
1	-4.258685	-2.223244	-3.973533
1	-4.156776	-3.170997	-2.477750

Compound: S_1 excited state of *s*-*E*-**1** in gas phase
Method/basis set: CAM-B3LYP-TD/6-31+G*
Energy of the optimized structure: -1384.2642547 Hartree
# of imaginary frequencies: 0
Cartesian coordinate of the optimized structure:

6	1.820970	3.750168	-0.708375
6	0.623377	3.066004	-0.573774
6	0.618583	1.688236	-0.315064
6	1.845477	0.988785	-0.186509
6	3.039615	1.708690	-0.364798
6	3.035888	3.071823	-0.611574
1	1.804062	4.816609	-0.913323
1	-0.319850	3.582968	-0.712594
1	3.976083	1.170753	-0.286798
1	3.974136	3.604661	-0.727678
7	-0.593317	1.013637	-0.212412
6	1.852037	-0.417001	0.184372

1	0.950328	-0.819951	0.642492
6	2.850240	-1.320017	0.082482
7	4.134315	-1.154004	-0.470830
6	2.705844	-2.719671	0.572314
7	3.947002	-3.273451	0.251312
6	4.714639	-2.296606	-0.348566
8	1.783238	-3.291460	1.117984
1	4.210064	-4.228893	0.443215
1	5.724211	-2.507277	-0.683247
6	-1.772261	1.604680	0.153080
1	-0.628058	0.004691	-0.346568
7	-2.946208	0.859430	-0.014347
6	-3.036204	-0.502646	-0.134918
8	-2.090277	-1.271407	-0.110962
8	-4.312202	-0.868784	-0.320486
6	-4.543993	-2.284165	-0.485994
1	-3.978081	-2.627421	-1.355784
1	-4.159739	-2.802752	0.395814
6	-6.032367	-2.478495	-0.660027
1	-6.397834	-1.943706	-1.541465
1	-6.249788	-3.543365	-0.788828
1	-6.579579	-2.119427	0.216317
1	-3.818584	1.368363	-0.082188
16	-1.854816	2.763748	1.484774

Compound: S_1 excited state of *s*-*E*-**1** in DMSO

Method/basis set: CAM-B3LYP-TD/6-31+G*; SCRF(PCM, solvent=DMSO)

Energy of the optimized structure: -1384.28244198 Hartree

# of imaginary frequencies: 0

Cartesian coordinate of the optimized structure:

6	1.913231	3.761844	-0.506583
6	0.704327	3.080406	-0.549738
6	0.664207	1.689034	-0.359837
6	1.869035	0.973274	-0.134766
6	3.075536	1.691649	-0.131676
6	3.105433	3.069012	-0.301384
1	1.923576	4.836545	-0.660260
1	-0.207827	3.609878	-0.802870

1	3.996215	1.146545	0.035833
1	4.052045	3.598636	-0.275224
7	-0.555986	1.034739	-0.408977
6	1.827887	-0.450140	0.158591
1	0.893118	-0.850883	0.546338
6	2.808815	-1.370771	0.052462
7	4.118885	-1.212841	-0.438518
6	2.612300	-2.790077	0.455638
7	3.839573	-3.358246	0.166963
6	4.662012	-2.380230	-0.350777
8	1.636856	-3.358918	0.927625
1	4.080995	-4.330203	0.308878
1	5.675914	-2.613916	-0.652386
6	-1.734257	1.638558	-0.043051
1	-0.585350	0.023091	-0.501501
7	-2.918807	0.910819	-0.206883
6	-3.039079	-0.450629	-0.098753
8	-2.104539	-1.210900	0.115183
8	-4.302343	-0.828179	-0.296601
6	-4.569376	-2.250948	-0.262112
1	-3.960486	-2.732601	-1.030566
1	-4.266770	-2.633197	0.715347
6	-6.047339	-2.437031	-0.510540
1	-6.334444	-2.037952	-1.487580
1	-6.284622	-3.504910	-0.491907
1	-6.640842	-1.939440	0.261761
1	-3.768957	1.425805	-0.407023
16	-1.807151	2.807598	1.261160

Compound: S_1 excited state of *s*-*Z*-**1** in gas phase
Method/basis set: CAM-B3LYP-TD/6-31+G*
Energy of the optimized structure: -1384.26685387 Hartree
# of imaginary frequencies: 0
Cartesian coordinate of the optimized structure:

6	3.113815	-2.968351	-0.825348
6	1.832993	-2.435769	-0.823141
6	1.582038	-1.109518	-0.394851
6	2.665750	-0.221303	-0.088037

6	3.940578	-0.828968	-0.077251
6	4.173230	-2.153913	-0.421803
1	3.283619	-3.981731	-1.172825
1	1.021398	-2.997440	-1.273335
1	4.782973	-0.208618	0.215640
1	5.188150	-2.538608	-0.408591
7	0.244356	-0.752585	-0.185570
6	2.606566	1.169097	0.238205
1	3.530487	1.601426	0.612019
6	1.583537	2.080869	0.090303
7	0.321993	1.845403	-0.451736
6	1.703936	3.501369	0.412144
7	0.452864	4.006813	0.014484
6	-0.309508	2.983039	-0.478722
8	2.617210	4.165685	0.892222
1	0.197339	4.980607	0.083637
1	-1.318845	3.115004	-0.843917
6	-0.579632	-1.591001	0.412063
1	-0.021006	0.264837	-0.406696
7	-1.925210	-1.313275	0.539086
6	-2.681214	-0.396583	-0.174881
8	-2.256575	0.381544	-0.994743
8	-3.962175	-0.522409	0.195918
6	-4.898220	0.363732	-0.456138
1	-4.604116	1.393639	-0.237994
1	-4.824863	0.207968	-1.535299
6	-6.273692	0.038579	0.077398
1	-6.320995	0.189794	1.159512
1	-7.012569	0.693755	-0.394169
1	-6.544515	-0.998135	-0.141731
1	-2.454686	-1.945704	1.125725
16	-0.031821	-3.066720	1.132334

Compound: S_1 excited state of *s*-*Z*-**1** in DMSO

Method/basis set: CAM-B3LYP-TD/6-31+G*; SCRF(PCM, solvent=DMSO)

Energy of the optimized structure: -1384.29423559 Hartree

# of imaginary frequencies: 0

Cartesian coordinate of the optimized structure:

6	3.122198	-2.941570	-0.950107
6	1.866248	-2.562298	-0.547023
6	1.563355	-1.221333	-0.235844
6	2.589589	-0.188012	-0.389353
6	3.888341	-0.661733	-0.779862
6	4.155110	-1.973722	-1.046454
1	3.317842	-3.976853	-1.208634
1	1.076101	-3.298127	-0.486317
1	4.677045	0.077393	-0.877453
1	5.151882	-2.274413	-1.352248
7	0.303347	-0.878405	0.182474
6	2.491454	1.197322	-0.176240
1	3.433419	1.728916	-0.280612
6	1.426338	2.076663	0.124914
7	0.095301	1.796030	0.231522
6	1.629613	3.503905	0.347380
7	0.330410	3.970460	0.588142
6	-0.529036	2.932335	0.506548
8	2.655431	4.196030	0.347385
1	0.089621	4.933744	0.786331
1	-1.596556	3.035398	0.643725
6	-0.607958	-1.636311	0.852696
1	0.019889	0.126371	0.069746
7	-1.905547	-1.158629	0.758172
6	-2.494423	-0.561113	-0.349032
8	-1.928609	-0.285910	-1.385772
8	-3.783848	-0.350942	-0.090783
6	-4.567577	0.247619	-1.152998
1	-4.130296	1.219599	-1.392148
1	-4.496723	-0.395223	-2.033110
6	-5.986257	0.370329	-0.650939
1	-6.035131	1.006968	0.237033
1	-6.606384	0.820774	-1.431583
1	-6.401933	-0.610928	-0.405014
1	-2.546976	-1.514341	1.457686
16	-0.283884	-2.934460	1.853854

Compound: S_1 excited state of the *s*-*Z*-**1** tautomer in gas phase

Method/basis set: CAM-B3LYP-TD/6-31+G*

Energy of the optimized structure: -1384.28616952 Hartree

# of imaginary frequencies: 0

Cartesian coordinate of the optimized structure:

6	3.557560	-2.680646	-1.134581
6	2.196744	-2.401068	-1.095990
6	1.726392	-1.212637	-0.546358
6	2.620822	-0.207140	-0.115946
6	3.992990	-0.536939	-0.137276
6	4.458717	-1.744176	-0.629378
1	3.907497	-3.623921	-1.541921
1	1.472460	-3.125300	-1.456363
1	4.700260	0.204239	0.224889
1	5.525017	-1.949426	-0.634844
7	0.313264	-1.039416	-0.467658
6	2.261261	1.131798	0.304898
1	3.019068	1.669409	0.866763
6	1.180612	1.935118	-0.010676
7	0.074638	1.682679	-0.820102
6	1.060589	3.324973	0.398656
7	-0.132954	3.755058	-0.225400
6	-0.700570	2.757450	-0.932396
8	1.773571	4.037460	1.099837
1	-0.481084	4.699181	-0.140970
1	-1.631659	2.795141	-1.471683
6	-0.277459	-1.253069	0.633754
1	-0.189906	0.759727	-1.166392
7	-1.661531	-1.105634	0.755083
6	-2.550556	-0.653161	-0.201168
8	-2.279038	-0.109489	-1.247032
8	-3.797832	-0.887201	0.235460
6	-4.867194	-0.424573	-0.615149
1	-4.772920	0.658553	-0.731155
1	-4.748712	-0.884428	-1.599260
6	-6.169283	-0.814321	0.045300
1	-6.263130	-0.352375	1.032249
1	-7.008107	-0.479473	-0.572676

1	-6.239603	-1.899515	0.161283
1	-2.080268	-1.384293	1.631920
16	0.507488	-1.737009	2.138527

Compound: S_1 excited state of the *s-Z*-**1** tautomer in DMSO
Method/basis set: CAM-B3LYP-TD/6-31+G*; SCRF(PCM, solvent=DMSO)
Energy of the optimized structure: -1384.3034491 Hartree
# of imaginary frequencies: 0
Cartesian coordinate of the optimized structure:

6	2.446436	-2.891331	-1.259463
6	1.410383	-2.330373	-0.546793
6	1.474949	-0.998824	-0.057029
6	2.621895	-0.171375	-0.397040
6	3.689115	-0.820137	-1.055299
6	3.612036	-2.133755	-1.485223
1	2.366976	-3.904667	-1.638191
1	0.510365	-2.901302	-0.353450
1	4.588130	-0.246967	-1.260681
1	4.449261	-2.571462	-2.019497
7	0.490441	-0.471331	0.703091
6	2.805354	1.210113	-0.092166
1	3.825397	1.565781	-0.210631
6	1.936287	2.248422	0.224282
7	0.551171	2.279881	0.288717
6	2.371155	3.613384	0.455801
7	1.175793	4.323487	0.650011
6	0.117167	3.504100	0.543241
8	3.503746	4.110057	0.488055
1	1.128480	5.317171	0.838621
1	-0.917616	3.789111	0.649961
6	-0.241866	-1.165463	1.564659
1	-0.058724	1.456268	0.232452
7	-1.519342	-0.687181	1.847486
6	-2.269054	0.225383	1.143968
8	-1.881578	0.906017	0.208163
8	-3.502679	0.266329	1.643462
6	-4.424474	1.203927	1.034235
1	-3.999720	2.206469	1.121773

1	-4.516976	0.952669	-0.024572
6	-5.739959	1.078315	1.764921
1	-5.624941	1.321001	2.825107
1	-6.461831	1.775102	1.328700
1	-6.143072	0.065475	1.676420
1	-2.004295	-1.174477	2.591384
16	0.283653	-2.487883	2.498807

Compound: S_1/S_0 conical intersection (CI) of *s*-*E*-**1** along τ-torsion relaxation in gas phase

Method/basis set: CASSCF(6,6)/4-31G

Energy of the optimized structure: -1376.2376534321 Hartree

# of imaginary frequencies: 0

Cartesian coordinate of the optimized structure:

6	0.959780	1.715652	3.355341
6	0.291589	2.096304	2.135441
6	0.653049	1.562899	0.966818
6	1.710567	0.537030	0.903741
6	2.443553	0.272838	2.146378
6	2.012509	0.880145	3.354452
1	0.620524	2.159418	4.269111
1	-0.498098	2.810534	2.183778
1	3.442716	-0.091961	2.086278
1	2.540838	0.655414	4.257330
7	0.103029	1.929996	-0.281412
6	1.821927	-0.310578	-0.173415
1	1.119588	-0.253810	-0.978700
6	2.690187	-1.494634	-0.057751
7	3.727096	-1.892036	-0.856249
6	2.694433	-2.196012	1.112316
7	3.790234	-3.045707	1.019587
6	4.340457	-2.850311	-0.203718
8	2.036707	-1.870652	2.178396
1	4.058952	-3.717023	1.694710
1	5.145739	-3.431318	-0.582529
6	-1.150740	2.239141	-0.590533
1	0.761847	1.957556	-1.035314
7	-1.386569	2.572637	-1.907678

6	-0.520137	2.601107	-2.958832
8	0.668002	2.329837	-2.900465
8	-1.142819	2.965775	-4.069147
6	-0.409132	3.057052	-5.332912
1	0.385353	3.773502	-5.203389
1	0.021701	2.090499	-5.536295
6	-1.413212	3.480526	-6.376267
1	-1.846049	4.437811	-6.123541
1	-0.926249	3.565999	-7.339458
1	-2.209379	2.754451	-6.456771
1	-2.332123	2.805555	-2.108223
16	-2.543533	2.230268	0.450255

Compound: S_1/S_0 conical intersection (CI) of *s*-*Z*-**1** along τ-torsion relaxation in gas phase

Method/basis set: CASSCF(6,6)/4-31G

Energy of the optimized structure: -1376.2477234233 Hartree

# of imaginary frequencies: 0

Cartesian coordinate of the optimized structure:

6	4.437997	-3.438204	-0.941259
6	3.104236	-3.694870	-0.971818
6	2.170520	-2.646537	-0.830084
6	2.684657	-1.292160	-0.695408
6	4.113804	-1.102658	-0.636389
6	4.966636	-2.132690	-0.754477
1	5.119551	-4.255882	-1.064432
1	2.750891	-4.690835	-1.093835
1	4.471206	-0.100240	-0.514584
1	6.025660	-1.988013	-0.722752
7	0.836087	-2.811876	-0.844955
6	1.862648	-0.196926	-0.609749
1	2.343382	0.751956	-0.420071
6	0.417109	-0.234454	-0.821084
7	-0.440959	0.108901	0.284409
6	-0.134901	0.395340	-2.013634
7	-1.372235	0.872624	-1.576238
6	-1.466159	0.686743	-0.210749
8	0.321109	0.526608	-3.148542

1	-2.036372	1.304473	-2.166910
1	-2.315221	1.008960	0.345984
6	0.124953	-3.906448	-0.512329
1	0.341291	-1.771065	-0.965223
7	-1.179273	-3.929425	-0.911637
6	-1.837382	-3.192030	-1.864221
8	-1.371029	-2.332800	-2.570922
8	-3.107933	-3.599864	-1.919368
6	-4.023426	-2.987070	-2.874716
1	-4.051114	-1.927438	-2.678466
1	-3.628886	-3.144207	-3.865559
6	-5.362940	-3.651877	-2.670210
1	-5.715087	-3.497414	-1.660213
1	-6.089557	-3.235336	-3.356540
1	-5.291822	-4.715352	-2.848793
1	-1.720066	-4.656230	-0.501518
16	0.647893	-5.219316	0.460421