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Supporting Information

One-step Facile transformation from rofecoxib to reversible mechanofluorochromism materials with bright dual-state emission

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Characterization of NOR1

Synthesis of NOR1. (General procedure) Piperidine, 2 drops, was added to a mixture of 0.140 g (0.0004 mol) of intermediate (Rofecoxib) and 0.140 g of 2-Morpholinobezaldehyde in 10 ml of MeOH, and the mixture was stirred at room temperature for 12 h in dark atmosphere. The mixture was then cooled, and the precipitate was filtered off and washed with MeOH. The yellow powder (**NOR1**, 0.13 g) was obtained with the yield 92%.^{1}H NMR (600 MHz, DMSO-d_6) δ 9.01 , 8.10 (d, J = 7.5 Hz), 8.05 (d, J = 7.8 Hz), 7.75 – 7.60 (m), 7.35 (dd, J = 8.7, 5.2 Hz), 7.24 (d, J = 7.7 Hz), 6.12 , 3.30 , 1.50 , 1.28 . ^{13}C NMR (151 MHz, DMSO-d_6) δ 130.6, 116.6, 111.9, 110.1, 104.8, 100.3, 98.0, 93.3, 93.2, 92.6, 92.2, 92.1, 91.7, 91.5, 91.2, 90.5, 89.5, 88.8, 72.3, 42.0, 2.5, -8.9, -9.1. HRMS (ESI): calced for $C_{29}H_{27}NO_6S$: 518.1632 ([M+H]+), found:406.2795.

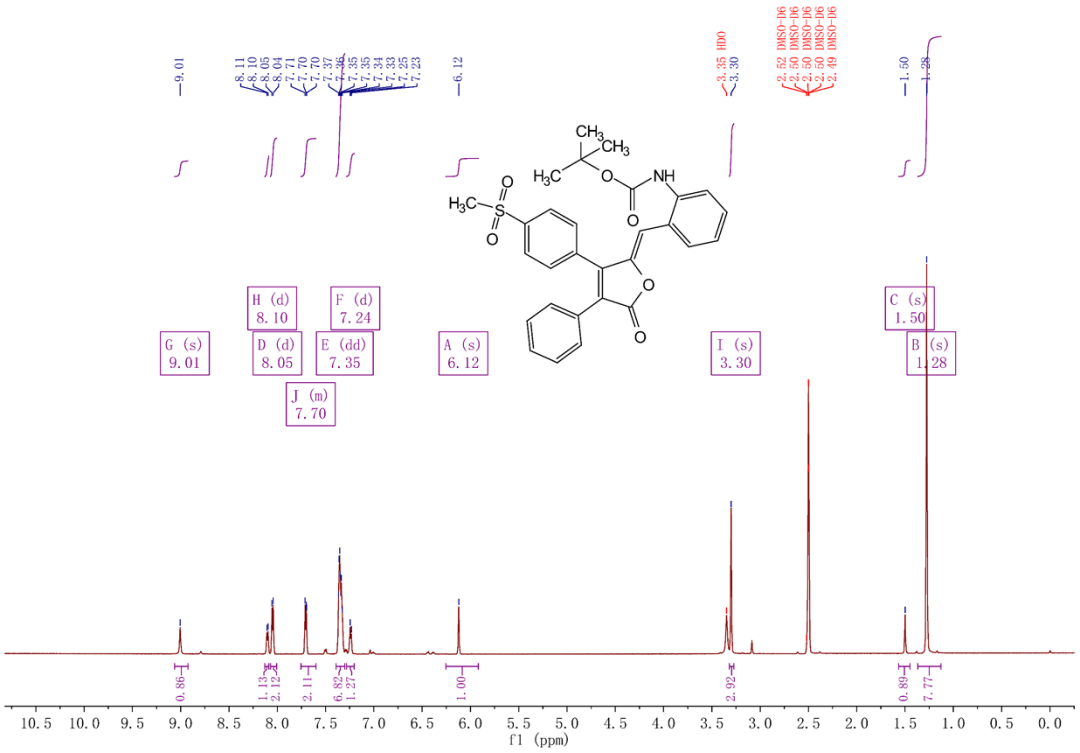

Figure S1. ^{1}H NMR spectrum of **NOR1** in DMSO-d_6 (600 MHz, 298K).

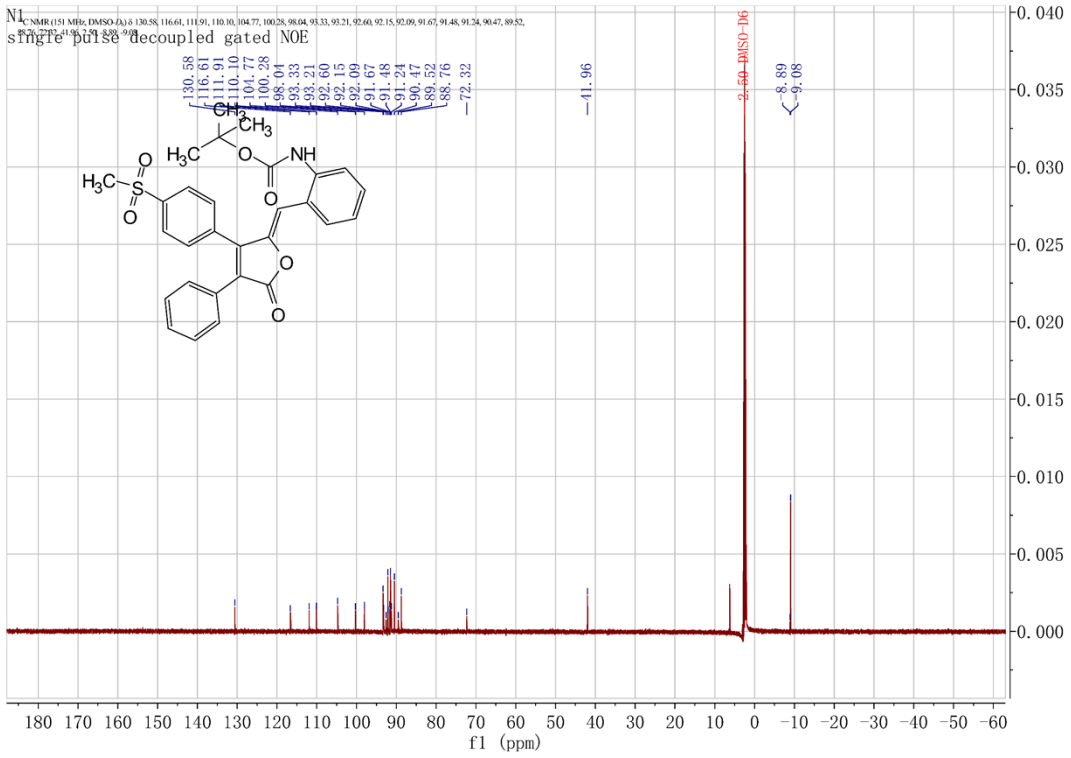

Figure S2. ^{13}C NMR spectrum of **NOR1** in DMSO-d_6 (151 MHz, 298K).

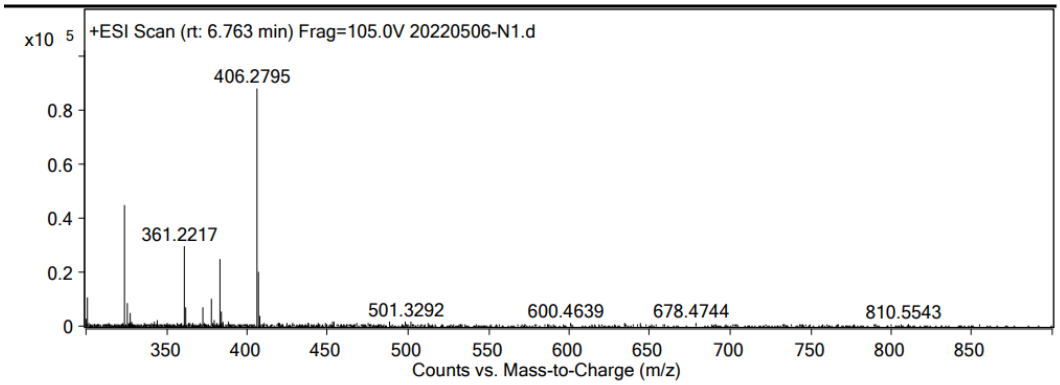

Figure S3. HRMS spectrum of **NOR1**

Characterization of NOR2

Synthesis of NOR2. The orange-red powder (**NOR2**, 0.12 g) was synthesized following the the general procedure with the yield 83%. ^{1}H NMR (600 MHz, DMSO-d_6) δ 9.67 (s, 1H), 8.06 (d, J = 6.7 Hz, 2H), 7.71 (dd, J = 25.9, 6.8 Hz, 4H), 7.55 (s, 1H), 7.33 (p, J = 4.9, 4.1 Hz, 5H), 6.00 (s, 1H), 3.31 (s, 4H), 1.67 – 1.30 (m, 9H). ^{13}C NMR (151 MHz, DMSO-d_6) δ 168.2, 153.1, 149.5, 146.7, 142.2, 141.3, 135.7, 132.0, 130.9, 130.0, 129.6, 129.5, 129.0, 128.8, 128.1, 127.3, 125.1, 118.6, 113.7, 80.1, 40.1, 28.6, 28.6. HRMS (ESI): calced for $C_{29}H_{27}NO_6S$: 518.1632 ([M+H]+), found:406.2798.

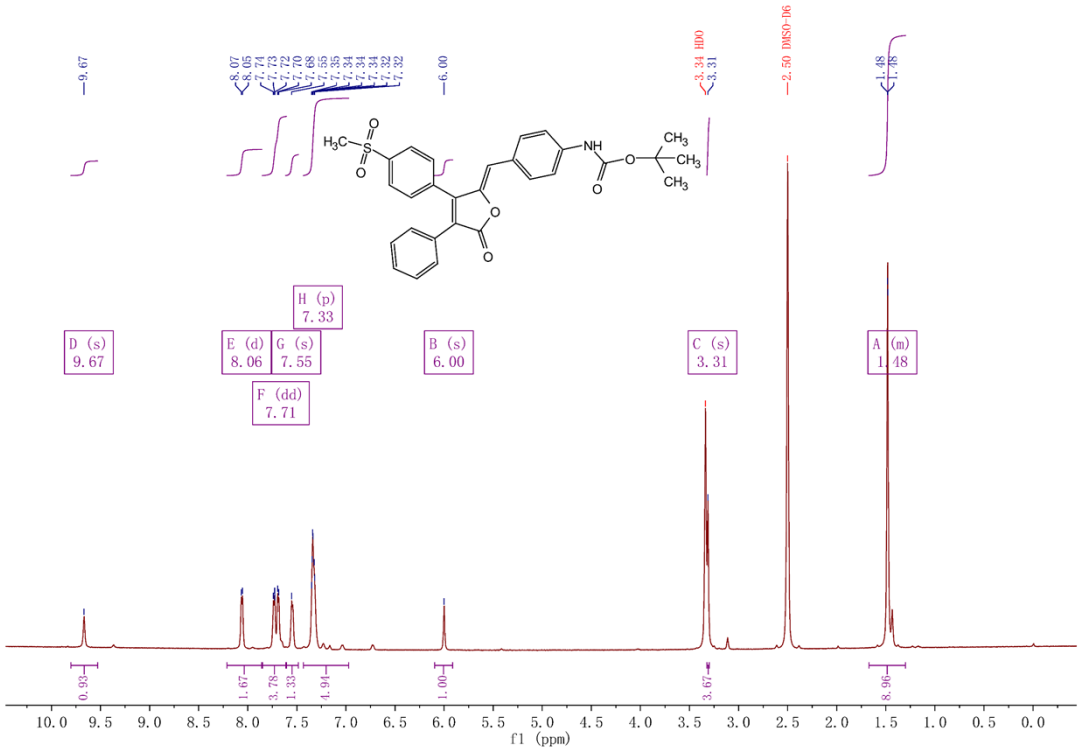

Figure S4. ^{1}H NMR spectrum of **NOR2** in DMSO-d_6 (600 MHz, 298K).

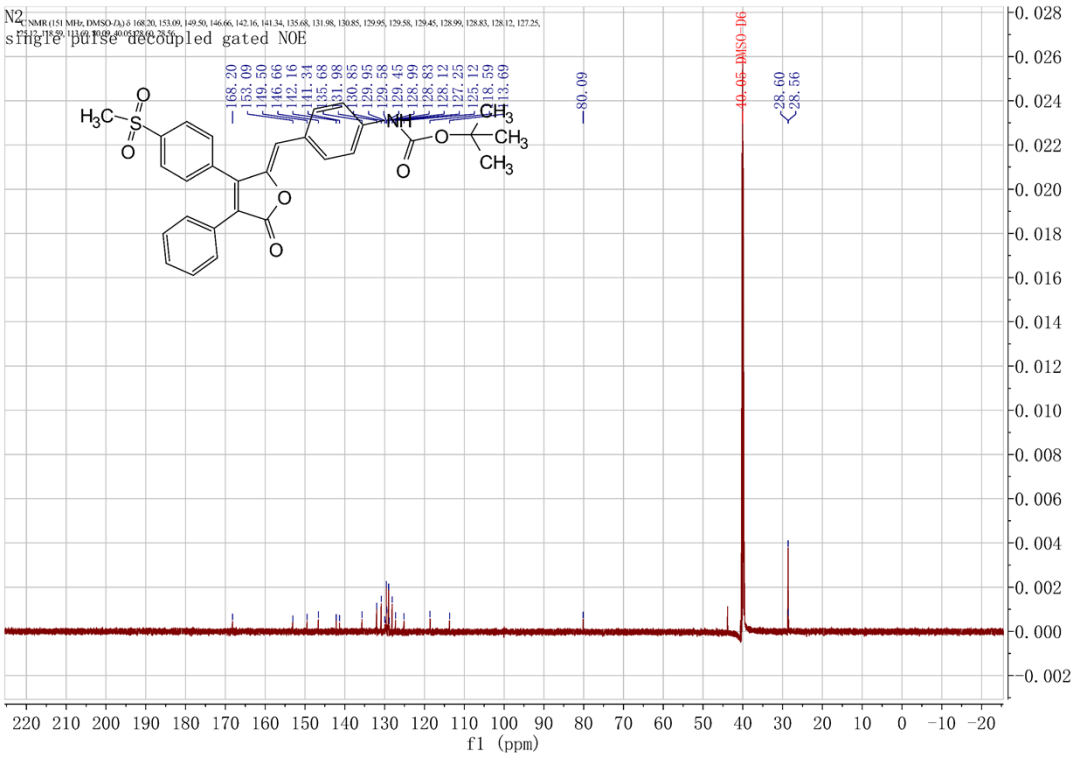

Figure S5. ^{13}C NMR spectrum of **NOR2** in DMSO-d_6 (151 MHz, 298K).

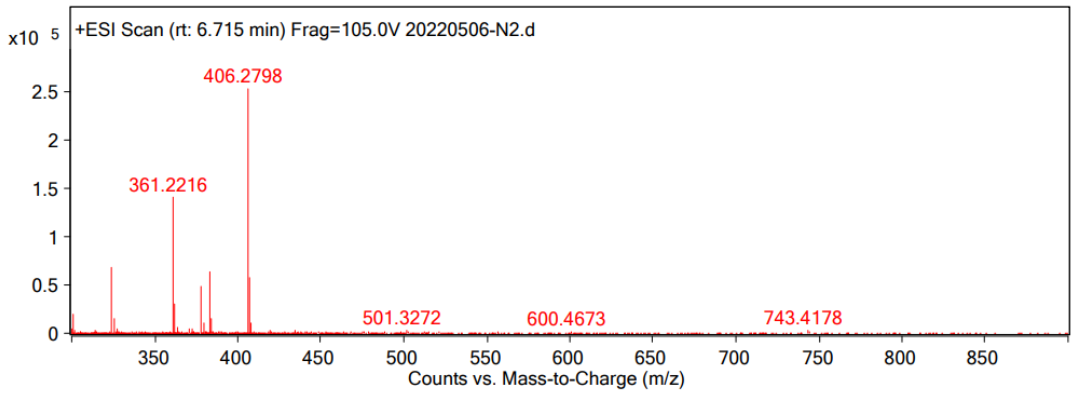

Figure S6. HRMS spectrum of **NOR2**

Beer-Lambert's plot and linear fitting of NOR1 and NOR2

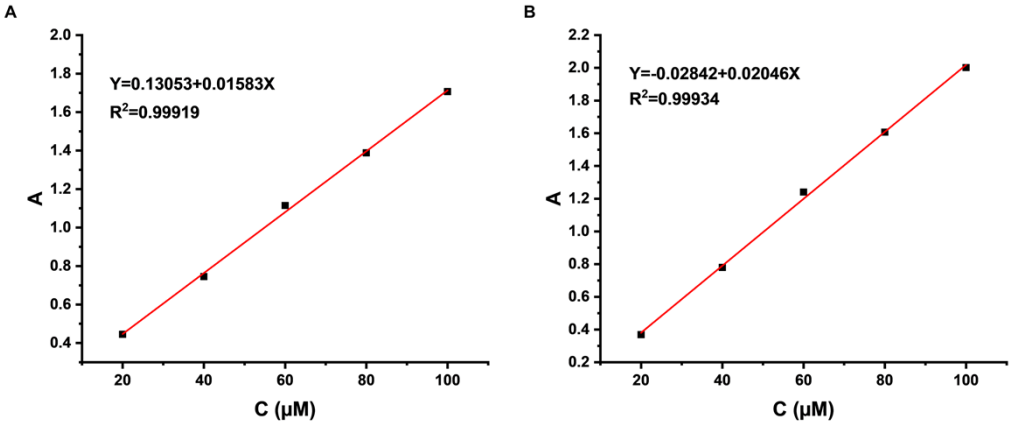

Figure S7. Beer-Lambert's plot and linear fitting of **NOR1** (A) and **NOR2** (B). (Y=0.13053+0.01583X, R^2=0.99919; Y=-0.02842+0.02046X, R^2=0.99934).

Solvatochromism of NOR1 and NOR2

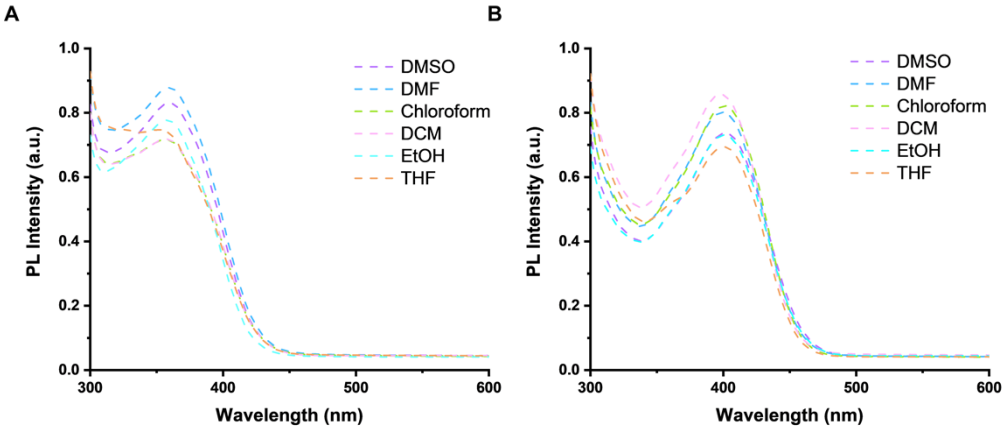

Figure S8. Normalized absorption of compounds (A) **NOR1**, (B) **NOR2** in various solvents at the concentration of 50 μM, such as DMSO, DMF, chloroform, DCM, EtOH, THF, respectively.

Table S1. Photophysical data of **NOR1** and **NOR2** in various solvents.

Compd.	Solvents	ε [a]	n [b]	Δf [c]	λ_{abs} [d] (nm)	λ_{em} [e] (nm)	Δv [f] (cm^{-1})
NOR1	Chloroform	4.81	1.4459	0.148	356	496	7929
	DCM	9.08	1.4244	0.217	356	496	7929
	THF	7.58	1.4070	0.210	352	490	8001
	EtOH	24.5	1.3611	0.2886	358	522	8776
	DMF	37.6	1.3330	0.2742	360	524	8694
	DMSO	48.9	1.4795	0.265	364	526	8461
NOR2	Chloroform	4.81	1.4459	0.148	400	510	5392
	DCM	9.08	1.4244	0.217	398	518	5821
	THF	7.58	1.4070	0.210	400	526	5989
	EtOH	24.5	1.3611	0.2886	400	534	6273
	DMF	37.6	1.3330	0.2742	400	534	6273
	DMSO	48.9	1.4795	0.265	402	546	6561

[a] Static dielectric constant; [b] index of refraction; [c] orientation polarizability; [d] the maximum absorption wavelength; [e] the maximum emission wavelength;[f] Δν were calculated using the equation $(1/\lambda_{abs}-1/\lambda_{em})\times10^7$.

The solvatochromic Lippert-Mataga equation:

$$\Delta v = \frac{1}{4\pi\varepsilon_0} \frac{2\Delta\mu^2}{hca^3}\Delta f + Const. \quad (1)$$

Where

$$\Delta f = \frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2n^2 - 1} \quad (2)$$

$$a = \left(\frac{3M}{4\pi d N_a}\right)^{1/3}$$

（3）

In the above equations, Δν is the Stokes shift, ε_0 is the vacuum permittivity, h is Planck's constant, *c* is the velocity of light, a is the Onsager radius of compound, $\Delta\mu = \mu_e - \mu_g$ is the difference in the dipole moment of compound between the excited (μ_e) and the ground (μ_g) states, ε and n are the static dielectronic constant and the refractive index of the solvent, respectively, Δf is the orientation polarizability, *M* is the molecular weight, *d* is the density of molecule, and N_a is Avogadro's number

Table S2. DFT calculation data of NOR1 and NOR2

Calculation method: opt freq b3lyp/6-311g(d,p) scrf=(solvent=dmso) em=gd3 with Gaussian 09

Cartesian coordinates of optimized structure of **NOR1**

Total energy: -2026,151524 Hartrees

Atom	X	Y	Z
C	-4.526651	-0.952741	0.50385
C	-3.437461	-1.254897	1.315814
C	-2.183615	-0.764359	0.967243
C	-2.026623	0.026848	-0.178362
C	-3.140368	0.321088	-0.976822
C	-4.394645	-0.171347	-0.642305
C	-0.705105	0.568874	-0.545434
C	-0.3723	1.873892	-0.774401
C	1.049032	1.904498	-1.156842
O	1.505604	0.582902	-1.149672
C	0.469227	-0.254208	-0.77632
C	-1.172403	3.096094	-0.635077
O	1.794593	2.804865	-1.432808
C	-0.976475	4.173277	-1.514481
C	-1.74098	5.330228	-1.394794
C	-2.704484	5.435934	-0.392546

C	-2.896983	4.376655	0.495394
C	-2.139011	3.217172	0.377039
S	-6.149009	-1.596757	0.943768
O	-6.178343	-1.798275	2.402138
O	-7.166365	-0.735893	0.317868
C	0.57576	-1.59842	-0.719045
C	-6.205468	-3.211533	0.150064
C	1.673251	-2.536342	-0.941173
C	1.277314	-3.828238	-1.353691
C	2.186047	-4.847476	-1.579032
C	3.54441	-4.600128	-1.376271
C	3.97314	-3.349508	-0.954308
C	3.062086	-2.308149	-0.72277
N	3.513418	-1.062825	-0.269299
C	4.62604	-0.804093	0.494795
O	4.688053	0.530553	0.6794
O	5.40695	-1.625779	0.932021
C	5.767794	1.164808	1.464717
C	5.39886	2.644508	1.380003
C	5.719305	0.6703	2.910769
C	7.1178	0.897364	0.798618
H	-3.569147	-1.848677	2.211021
H	-1.329979	-0.975826	1.598583
H	-3.019514	0.938298	-1.857853
H	-5.260321	0.056282	-1.250578
H	-0.226258	4.099735	-2.290657
H	-1.583247	6.150017	-2.086116
H	-3.29739	6.338484	-0.29963
H	-3.635257	4.455798	1.284979

H	-2.287375	2.406454	1.078885
H	-0.370935	-2.083903	-0.510464
H	-6.10545	-3.073502	-0.925103
H	-5.396567	-3.82101	0.54929
H	-7.175487	-3.642075	0.398292
H	0.219635	-4.016197	-1.500934
H	1.842626	-5.822627	-1.901985
H	4.275071	-5.382175	-1.547304
H	5.023086	-3.166723	-0.784153
H	2.971542	-0.244672	-0.516736
H	6.135375	3.244002	1.91895
H	5.373942	2.970864	0.338133
H	4.414827	2.817558	1.821161
H	6.42963	1.242835	3.512153
H	5.975943	-0.385865	2.972703
H	4.719251	0.818751	3.325226
H	7.089133	1.212131	-0.247312
H	7.893628	1.471875	1.310338
H	7.374536	-0.159542	0.844546

Cartesian coordinates of optimized structure of **NOR2**

Total energy: -2026,154392 Hartrees

Atom	X	Y	Z
C	-3.739045	2.694784	-0.029331
C	-2.893836	2.327708	-1.072322
C	-2.362783	1.042242	-1.085672
C	-2.679797	0.133658	-0.067435
C	-3.538071	0.526676	0.968918
C	-4.068734	1.809288	0.995063
C	-2.133403	-1.236396	-0.081374

C	-2.82361	-2.415551	-0.018242
C	-1.826744	-3.499726	-0.002023
O	-0.568228	-2.912944	-0.068712
C	-0.717307	-1.539934	-0.102184
C	-4.268741	-2.668264	-0.01941
O	-1.944145	-4.697839	0.046603
C	-4.802746	-3.741225	0.713186
C	-6.174789	-3.975981	0.725352
C	-7.036591	-3.152231	0.002269
C	-6.515439	-2.092019	-0.74063
C	-5.145941	-1.852172	-0.753526
S	-4.415802	4.361789	0.002655
O	-4.443129	4.869743	-1.379337
O	-5.665634	4.332326	0.78075
C	0.333365	-0.687509	-0.101541
C	-3.195445	5.30838	0.927449
C	1.754883	-0.961098	-0.097222
C	2.643719	0.131508	-0.098181
C	4.020631	-0.028627	-0.092535
C	4.572118	-1.31986	-0.0833
C	3.695301	-2.423001	-0.085366
C	2.324636	-2.252994	-0.09255
N	5.941947	-1.610517	-0.080806
C	7.081712	-0.82935	-0.017738
O	6.808566	0.473676	0.054653
O	8.186228	-1.339702	-0.028722
C	7.884944	1.496861	0.12315
C	7.087061	2.7969	0.18507
C	8.704454	1.293966	1.396501

C	8.735472	1.433423	-1.144149
H	-2.668575	3.027909	-1.866248
H	-1.717893	0.736073	-1.899616
H	-3.789421	-0.178019	1.7513
H	-4.738366	2.115712	1.78814
H	-4.13896	-4.387642	1.27167
H	-6.57085	-4.804113	1.301941
H	-8.104494	-3.33752	0.012103
H	-7.176353	-1.453933	-1.315943
H	-4.751729	-1.035942	-1.345448
H	0.058169	0.361009	-0.101505
H	-2.246301	5.260022	0.39645
H	-3.566446	6.332449	0.968539
H	-3.113685	4.884723	1.926836
H	2.241759	1.139006	-0.105082
H	4.663525	0.835286	-0.095434
H	4.104834	-3.427516	-0.079705
H	1.686735	-3.124312	-0.092683
H	6.178542	-2.592361	-0.115278
H	7.770078	3.646683	0.242359
H	6.466134	2.907646	-0.706521
H	6.441177	2.807447	1.065617
H	9.400519	2.128143	1.511712
H	9.270369	0.365196	1.355067
H	8.045454	1.272362	2.267654
H	8.10019	1.521169	-2.028671
H	9.441705	2.267036	-1.14303
H	9.292193	0.499666	-1.196306

Table S3. TDDFT calculations of NOR1 and NOR2

NOR1 absorbance prediction

TD(nstates=20) 6-311g(d,p) scrf=(solvent=dmso) pbe1pbe

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.9675 eV 417.81 nm f=0.5566 <S**2>=0.000

135 ->137 -0.13533

136 ->137 0.69077

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

Total Energy, E(TD-HF/TD-KS) = -2023.94364915

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

Excited State 2: Singlet-A 3.4758 eV 356.71 nm f=0.3877 <S**2>=0.000

135 ->137 0.68412

136 ->137 0.13315

Excited State 3: Singlet-A 3.8775 eV 319.75 nm f=0.0730 <S**2>=0.000

134 ->137 0.69007

Excited State 4: Singlet-A 4.0110 eV 309.11 nm f=0.0164 <S**2>=0.000

133 ->137 0.68830

Excited State 5: Singlet-A 4.1382 eV 299.61 nm f=0.1623 <S**2>=0.000

136 ->138 0.69025

Excited State 6: Singlet-A 4.3252 eV 286.66 nm f=0.0469 <S**2>=0.000

126 ->137 0.20013

127 ->137 0.20586

130 ->137 0.34144

131 ->137 0.36008

132 ->137 0.36659

Excited State 7: Singlet-A 4.5122 eV 274.78 nm f=0.0071 <S**2>=0.000

130 ->137 -0.44455

131 ->137 0.51162

Excited State 8: Singlet-A 4.6189 eV 268.43 nm f=0.0062 <S**2>=0.000

130 ->137 -0.25969

131 ->137	-0.26906					
132 ->137	0.57837					
Excited State 9:	Singlet-A	4.6480 eV	266.75 nm	f=0.0144	<S**2>=0.000	
130 ->137	0.11832					
135 ->138	-0.12898					
135 ->139	0.10998					
136 ->139	0.66108					
Excited State 10:	Singlet-A	4.7110 eV	263.18 nm	f=0.0052	<S**2>=0.000	
126 ->137	0.18633					
127 ->137	0.11052					
129 ->137	0.14137					
135 ->138	0.56653					
136 ->139	0.14859					
136 ->141	0.19616					
Excited State 11:	Singlet-A	4.7735 eV	259.73 nm	f=0.0467	<S**2>=0.000	
126 ->137	0.38080					
127 ->137	0.30553					
128 ->137	0.12177					
129 ->137	0.17227					
130 ->137	-0.27103					
131 ->137	-0.10964					
132 ->137	-0.11083					
135 ->138	-0.27352					
136 ->140	0.10490					
Excited State 12:	Singlet-A	5.0011 eV	247.91 nm	f=0.0757	<S**2>=0.000	
129 ->137	0.15712					
134 ->138	0.25519					
135 ->138	-0.22277					
135 ->143	0.11619					
136 ->140	0.10172					

136 ->141 0.50109

136 ->143 -0.16963

Excited State 13: Singlet-A 5.0972 eV 243.24 nm f=0.1502 <S**2>=0.000

134 ->138 0.14313

136 ->140 0.64352

136 ->141 -0.13413

Excited State 14: Singlet-A 5.1472 eV 240.87 nm f=0.0176 <S**2>=0.000

127 ->137 -0.24251

129 ->137 0.48984

134 ->138 -0.14714

136 ->141 -0.19981

136 ->142 0.11824

136 ->143 -0.30388

Excited State 15: Singlet-A 5.2238 eV 237.35 nm f=0.0654 <S**2>=0.000

129 ->137 -0.10524

131 ->138 -0.13981

133 ->140 -0.18728

134 ->138 -0.14065

134 ->139 0.20005

135 ->139 -0.36677

135 ->142 0.11210

136 ->139 0.10490

136 ->141 0.13759

136 ->142 0.37363

Excited State 16: Singlet-A 5.2385 eV 236.68 nm f=0.0398 <S**2>=0.000

131 ->138 0.14921

133 ->138 -0.18375

133 ->140 -0.14107

134 ->138 0.39484

135 ->139 0.10495

135 ->142 0.13621

136 ->140 -0.12669

136 ->141 -0.15038

136 ->142 0.35714

Excited State 17: Singlet-A 5.2706 eV 235.24 nm f=0.0008 <S**2>=0.000

127 ->137 -0.18447

128 ->137 0.65151

129 ->137 -0.12255

Excited State 18: Singlet-A 5.2906 eV 234.35 nm f=0.0088 <S**2>=0.000

126 ->137 0.15255

127 ->137 -0.10357

128 ->137 -0.17626

129 ->137 -0.11541

134 ->138 -0.36926

135 ->139 0.39359

136 ->142 0.20379

Excited State 19: Singlet-A 5.3369 eV 232.32 nm f=0.0186 <S**2>=0.000

126 ->137 0.45535

127 ->137 -0.38974

129 ->137 -0.16126

134 ->138 0.18381

135 ->139 -0.13305

Excited State 20: Singlet-A 5.3902 eV 230.02 nm f=0.0136 <S**2>=0.000

133 ->138 0.62954

135 ->139 0.19100

136 ->142 0.16209

NOR2 absorbance prediction

TD(nstates=20) 6-311g(d,p) scrf=(solvent=dmso) pbe1pbe

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.9201 eV 424.58 nm f=1.3016 <S**2>=0.000

136 ->137 0.70494

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

Total Energy, E(TD-HF/TD-KS) = -2023.94986945

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

Excited State 2: Singlet-A 3.7568 eV 330.03 nm f=0.1082 <S**2>=0.000

132 ->137 0.10799

135 ->137 0.68964

Excited State 3: Singlet-A 3.9270 eV 315.72 nm f=0.2333 <S**2>=0.000

136 ->138 0.69903

Excited State 4: Singlet-A 4.0650 eV 305.01 nm f=0.0140 <S**2>=0.000

134 ->137 0.68530

Excited State 5: Singlet-A 4.2184 eV 293.91 nm f=0.0033 <S**2>=0.000

133 ->137 0.64970

136 ->141 -0.23530

Excited State 6: Singlet-A 4.3123 eV 287.51 nm f=0.0213 <S**2>=0.000

128 ->137 0.32148

130 ->137 0.20693

131 ->137 0.55889

Excited State 7: Singlet-A 4.4203 eV 280.49 nm f=0.0172 <S**2>=0.000

136 ->139 0.69639

Excited State 8: Singlet-A 4.5714 eV 271.22 nm f=0.0221 <S**2>=0.000

130 ->137 0.45771

131 ->137 -0.22023

132 ->137 0.46100

Excited State 9: Singlet-A 4.6589 eV 266.12 nm f=0.0357 <S**2>=0.000

128 ->137 -0.27870

130 ->137 -0.31846

131 ->137 0.25822

132 ->137	0.44161				
136 ->143	0.12155				
Excited State 10:	Singlet-A	4.7910 eV	258.78 nm	f=0.0674	<S**2>=0.000
127 ->137	0.11505				
128 ->137	0.39310				
130 ->137	-0.29357				
131 ->137	-0.13088				
132 ->137	0.19120				
133 ->137	-0.10948				
136 ->140	0.36348				
136 ->141	-0.10299				
136 ->143	0.10870				
Excited State 11:	Singlet-A	4.8226 eV	257.09 nm	f=0.0223	<S**2>=0.000
128 ->137	0.24601				
130 ->137	-0.15715				
131 ->137	-0.10853				
133 ->137	0.22718				
136 ->140	-0.31588				
136 ->141	0.44929				
Excited State 12:	Singlet-A	4.9043 eV	252.81 nm	f=0.0209	<S**2>=0.000
135 ->138	0.46837				
136 ->140	-0.34739				
136 ->141	-0.35055				
Excited State 13:	Singlet-A	5.0128 eV	247.34 nm	f=0.0855	<S**2>=0.000
128 ->137	-0.17190				
131 ->137	0.13889				
135 ->138	0.49263				
136 ->140	0.32727				
136 ->141	0.25493				
Excited State 14:	Singlet-A	5.0290 eV	246.54 nm	f=0.0002	<S**2>=0.000

129 ->137	0.69355				
Excited State 15:	Singlet-A	5.0715 eV	244.47 nm	f=0.0202	<S**2>=0.000
134 ->140	-0.16486				
135 ->142	0.15785				
136 ->142	0.64708				
Excited State 16:	Singlet-A	5.2666 eV	235.42 nm	f=0.0149	<S**2>=0.000
130 ->137	0.11633				
130 ->138	-0.27772				
131 ->138	0.14896				
131 ->139	0.17812				
132 ->138	-0.15050				
134 ->138	-0.25796				
135 ->139	0.45757				
136 ->143	0.16037				
Excited State 17:	Singlet-A	5.2735 eV	235.11 nm	f=0.1910	<S**2>=0.000
124 ->137	-0.10768				
132 ->137	-0.14600				
135 ->139	-0.12856				
136 ->143	0.63072				
Excited State 18:	Singlet-A	5.3924 eV	229.92 nm	f=0.0015	<S**2>=0.000
127 ->137	0.12934				
134 ->138	0.62293				
135 ->139	0.24602				
136 ->142	0.10684				
Excited State 19:	Singlet-A	5.4086 eV	229.24 nm	f=0.0070	<S**2>=0.000
127 ->137	0.63381				
127 ->138	0.15578				
128 ->137	-0.17581				
134 ->138	-0.13010				
Excited State 20:	Singlet-A	5.6105 eV	220.98 nm	f=0.0324	<S**2>=0.000

130 ->138	0.30590
131 ->138	-0.17187
131 ->139	-0.25299
132 ->138	0.20914
134 ->138	-0.13021
134 ->140	0.18104
135 ->139	0.35041
135 ->142	-0.17711
136 ->142	0.13112

NOR1 emission prediction

Calculation method: TD opt 6-311g(d,p) scrf=(solvent=dmso) pbe1pbe with Gaussian 09

Cartesian coordinates of optimized structure of **NOR1**

Atom	X	Y	Z
C	-4.73084184	-0.83046697	0.20368912
C	-3.75562278	-1.33691406	1.05815162
C	-2.45740198	-0.86629754	0.95512737
C	-2.11395558	0.10806126	0.00250742
C	-3.12470168	0.60748023	-0.8392046
C	-4.42318065	0.14177357	-0.74554111
C	-0.7482587	0.59901019	-0.12404938
C	-0.30911751	1.930333	-0.32632571
C	1.11784055	1.8841076	-0.5319212
O	1.49873174	0.52413975	-0.44194981
C	0.39586181	-0.24047272	-0.22603237
C	-1.02212445	3.1778685	-0.2041852
O	1.97653073	2.71116987	-0.70943535
C	-0.54790465	4.34638257	-0.84294952
C	-1.21820267	5.54938666	-0.71253353
C	-2.37520963	5.63593069	0.06149933

C	-2.85164944	4.49729988	0.70990245
C	-2.19324579	3.2874979	0.57982118
S	-6.3932751	-1.43920457	0.32174806
O	-6.59781311	-1.94909514	1.67924075
O	-7.29587315	-0.40494185	-0.18825194
C	0.44519316	-1.6291614	-0.23534945
C	-6.45036094	-2.82170059	-0.79883217
C	1.453532	-2.63371929	-0.32249865
C	0.94622199	-3.9531752	-0.47160832
C	1.74830025	-5.06385737	-0.54937009
C	3.14429881	-4.91920567	-0.47476865
C	3.7020816	-3.67065309	-0.31891991
C	2.90313885	-2.51505367	-0.2360034
N	3.46727052	-1.28267478	-0.06411732
C	4.79564805	-0.96072611	0.19262395
O	4.87396473	0.36564427	0.22328335
O	5.69554023	-1.74725402	0.36183267
C	6.14850162	1.05765245	0.48047075
C	5.74578329	2.52044448	0.41008232
C	6.65504156	0.69930205	1.86899441
C	7.14805892	0.71746219	-0.61416068
H	-4.01879021	-2.07057685	1.81136461
H	-1.70498323	-1.23141813	1.64526882
H	-2.87855771	1.3582317	-1.58121266
H	-5.19728631	0.53048537	-1.39723497
H	0.34946673	4.29063652	-1.44573747
H	-0.83989661	6.42967233	-1.22182166
H	-2.89778135	6.58120716	0.16144009
H	-3.74124995	4.55746273	1.32821644

H	-2.56548753	2.42078454	1.1119106
H	-0.55168125	-2.05422462	-0.19773415
H	-6.23003169	-2.46985111	-1.80612276
H	-5.72556051	-3.56756148	-0.47461622
H	-7.46374833	-3.22231828	-0.74525082
H	-0.13037115	-4.07024066	-0.528934
H	1.30448391	-6.04562438	-0.66869178
H	3.78887729	-5.78834845	-0.54144612
H	4.77296781	-3.55434351	-0.25076911
H	2.86614302	-0.46414568	-0.15772225
H	6.6190165	3.15104572	0.5915669
H	5.34001377	2.75957246	-0.57551018
H	4.98810364	2.74723286	1.16386568
H	7.52882295	1.31447321	2.09878502
H	6.94252848	-0.35016282	1.93044267
H	5.88622672	0.90595919	2.61828461
H	6.72403982	0.93858238	-1.59727894
H	8.0418921	1.33260931	-0.48251231
H	7.43935633	-0.33198324	-0.57715081

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.3052 eV 537.85 nm f=0.9614 <S**2>=0.000

136 ->137 -0.70355

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

Total Energy, E(TD-HF/TD-KS) = -2023.95917681

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

Excited State 2: Singlet-A 2.9899 eV 414.68 nm f=0.3565 <S**2>=0.000

135 ->137 -0.69850

Excited State 3: Singlet-A 3.4265 eV 361.84 nm f=0.1352 <S**2>=0.000

134 ->137 -0.69823

NOR2 emission prediction

Calculation method: TD opt 6-311g(d,p) scrf=(solvent=dmso) pbe1pbe with Gaussian 09

Cartesian coordinates of optimized structure of **NOR2**

Atom	X	Y	Z
C	3.7603324	2.74900689	0.04863332
C	2.75434277	2.43787234	0.9611619
C	2.23040819	1.15737244	0.97903446
C	2.69575633	0.16834616	0.0927408
C	3.72188679	0.51216012	-0.80937439
C	4.24710453	1.79002422	-0.83830733
C	2.1408932	-1.17505471	0.09654682
C	2.80951576	-2.41210545	-0.07465776
C	1.7880555	-3.43653323	-0.14652198
O	0.54552079	-2.8029021	-0.00332085
C	0.74587819	-1.46526354	0.10299075
C	4.21212081	-2.7307987	-0.0179306
O	1.81555392	-4.63838607	-0.25446809
C	4.71164649	-3.91333994	-0.61207948
C	6.05626206	-4.22989643	-0.54372094
C	6.94968322	-3.39146288	0.12363078
C	6.47463906	-2.22853148	0.72886987
C	5.13345041	-1.89731121	0.65859133
S	4.42491303	4.3902347	0.0073964
O	4.23740606	4.99500022	1.32833622
O	5.77672476	4.32291023	-0.5530465
C	-0.33751532	-0.59139034	0.10248397
C	3.39660285	5.27085669	-1.14935482
C	-1.71956995	-0.88890495	0.10266028
C	-2.63906881	0.19896824	0.04272746
C	-3.99794128	0.02275139	0.04110496

C	-4.53510405	-1.28298939	0.1039744
C	-3.64040627	-2.37819545	0.1709789
C	-2.28400063	-2.19751116	0.17079071
N	-5.87400701	-1.58682354	0.11029355
C	-7.03610464	-0.82554922	0.04596731
O	-6.79460836	0.46786299	-0.04732106
O	-8.11291425	-1.37616193	0.07697943
C	-7.89831076	1.4493131	-0.12572423
C	-7.15510089	2.7708586	-0.21491896
C	-8.71403944	1.19915773	-1.38366675
C	-8.73403636	1.38027893	1.14182518
H	2.40833837	3.18523897	1.66595666
H	1.47654251	0.90574855	1.71659737
H	4.09372887	-0.23269924	-1.50327933
H	5.03436739	2.04697863	-1.53785453
H	4.02618111	-4.57137357	-1.13046559
H	6.41621832	-5.13712583	-1.01798254
H	8.00345351	-3.64373438	0.17488227
H	7.15791606	-1.57851997	1.26559712
H	4.7803764	-1.00242032	1.15606607
H	-0.07390414	0.4597324	0.0863652
H	2.37104188	5.2692579	-0.78184898
H	3.78563555	6.28899627	-1.19857588
H	3.46682115	4.78581095	-2.12230765
H	-2.24324406	1.20828258	-0.00540293
H	-4.65713787	0.87528154	-0.00722506
H	-4.04553358	-3.38401372	0.22441368
H	-1.63366142	-3.05884881	0.22368117
H	-6.09939439	-2.57103629	0.1713875

H	-7.87432172	3.59043053	-0.27814334
H	-6.53218211	2.92451997	0.6697115
H	-6.52020371	2.79796806	-1.10393926
H	-9.43901735	2.00838101	-1.50287857
H	-9.25244697	0.2534087	-1.32798379
H	-8.06405145	1.1920332	-2.26264056
H	-8.10064586	1.51236208	2.02300476
H	-9.46862276	2.18949323	1.12593452
H	-9.26255754	0.43049808	1.21852415

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.2524 eV 550.45 nm f=1.4546 <S**2>=0.000

136 ->137 0.70642

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

Total Energy, E(TD-HF/TD-KS) = -2023.96594272

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

Excited State 2: Singlet-A 3.1971 eV 387.81 nm f=0.2295 <S**2>=0.000

135 ->137 0.69766

Excited State 3: Singlet-A 3.6028 eV 344.13 nm f=0.3203 <S**2>=0.000

136 ->138 0.70123

Absorption spectra of NOR1 and NOR2 in DMSO/water mixtures

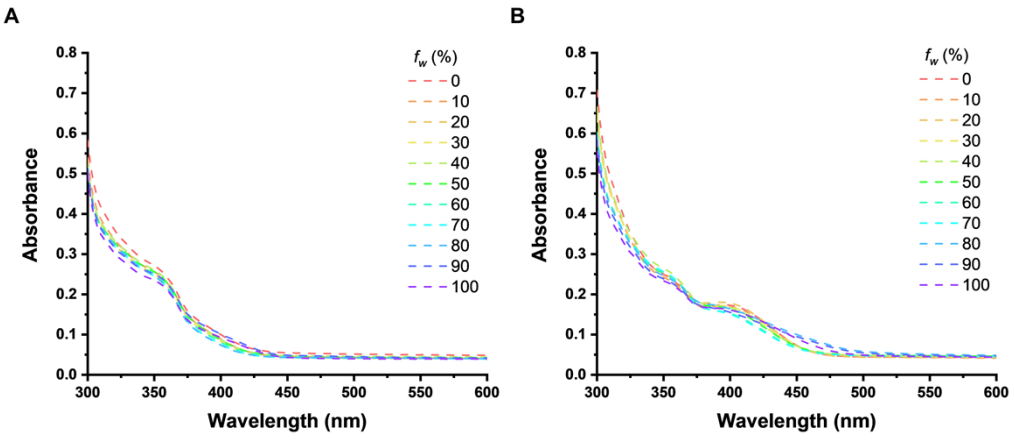

Figure S9. Absorption spectra of (A) **NOR1**, (B) **NOR2** in DMSO/water mixtures with varied f_w.

SEM images of NOR1

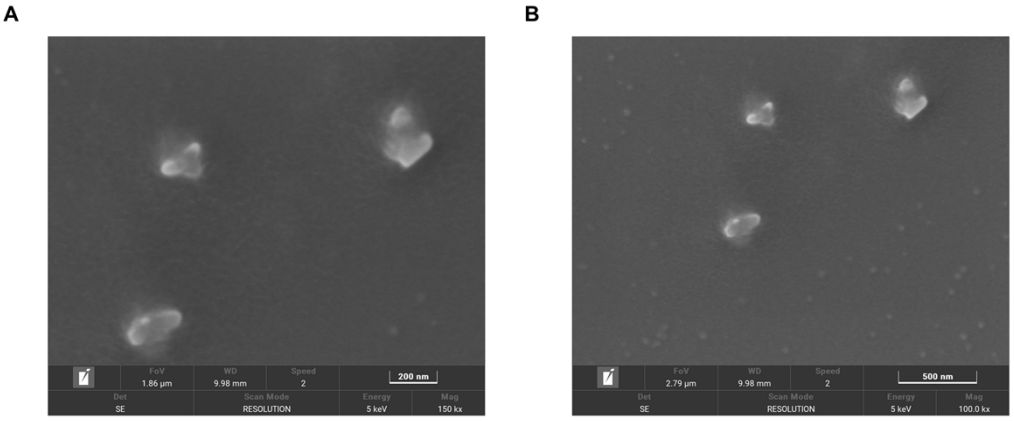

Figure S10 (A) SEM images of **NOR1** at 90 vol % of water in DMSO/water mixture, scale bare 200 nm. (B) SEM images of **NOR1** at 90 vol % of water in DMSO/water mixture, scale bare 500 nm.

Molecular conformation of NOR2

Table S4. Crystal data and structure refinement for **NOR2**

Identification code	**NOR2**
Empirical formula	$C_{29}H_{27}NO_6S$
Formula weight	517.57
Temperature/K	301.2(3)
Crystal system	monoclinic
Space group	C2/c
a/Å	17.5736(14)
b/Å	13.0560(9)
c/Å	24.5284(18)
α/°	90
β/°	103.023(8)
γ/°	90
Volume/Å^3	5483.1(7)

Z	8
ρ_{calc}g/cm^3	1.254
μ/mm^{-1}	0.160
F(000)	2176.0
Crystal size/mm^3	0.3 × 0.26 × 0.25
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.058 to 50
Index ranges	-17 ≤ h ≤ 20, -15 ≤ k ≤ 15, -29 ≤ l ≤ 29
Reflections collected	17466
Independent reflections	4714 [Rint = 0.0730, Rsigma = 0.0604]
Data/restraints/parameters	4714/60/342
Goodness-of-fit on F^2	1.037
Final R indexes [I>=2σ (I)]	R1 = 0.0667, wR2 = 0.1539
Final R indexes [all data]	R1 = 0.1086, wR2 = 0.1767
Largest diff. peak/hole / e Å^{-3}	0.46/-0.19

Directions a, b, and c of **NOR2** crystal

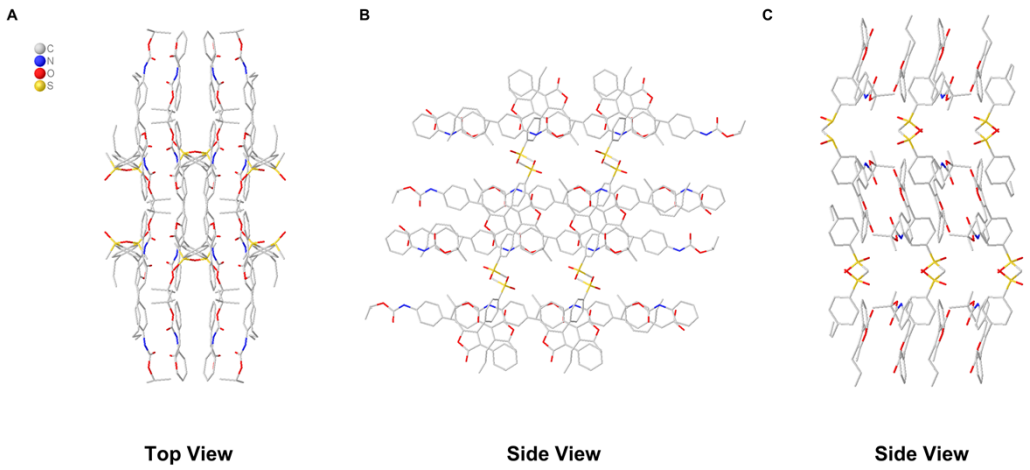

Figure S11. (A) Top view and (B-C) side view of packing structure of **NOR2** crystal.

Normalized solid-state PL spectra of NOR2 in the pristine state, ground state

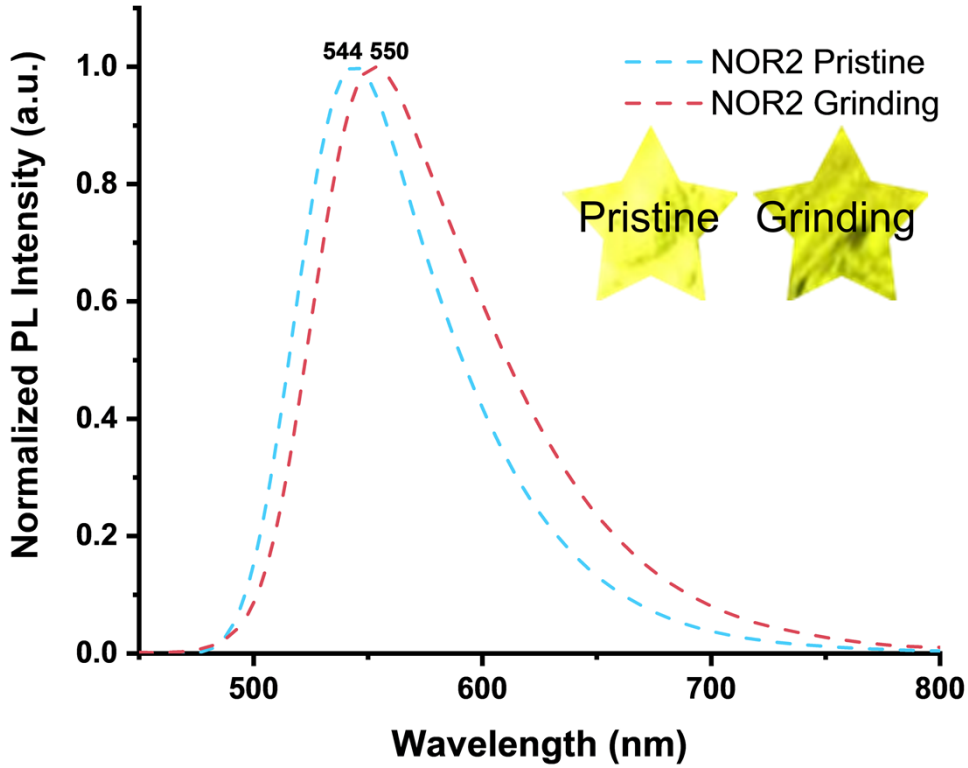

Figure S12. PL spectra of pristine and grinding powders of **NOR2**

Differential scanning calorimetry and powder X-ray diffraction of NOR2

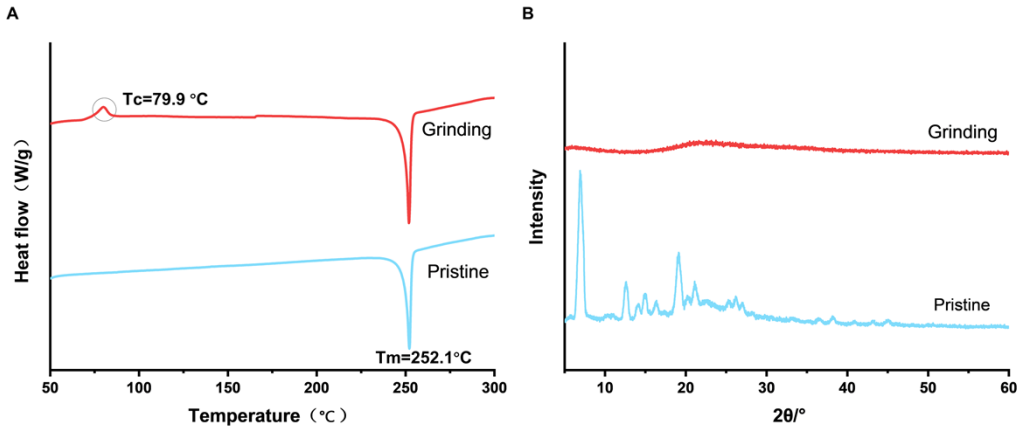

Figure S13. (A) DSC of **NOR2** in different states: pristine (black line), grinding (red line), immersing with acetone (blue line) and heating (green line). (B) PXRD of **NOR2** in different states: pristine (black line), grinding (red line).

Viscochromism of NOR1

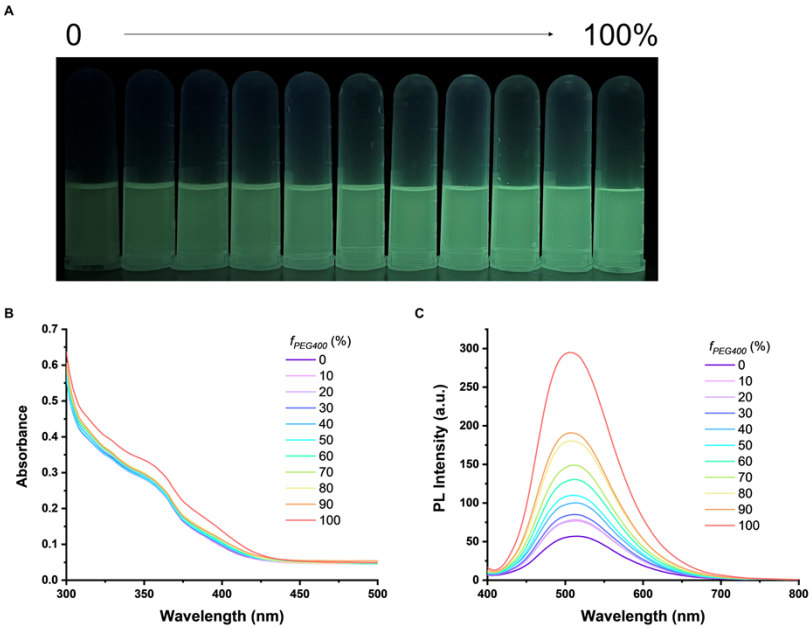

Figure S14. (A) Naked eye visualization of **NOR1** under UV light with increasing volume fractions of PEG400 at the concentration of 10 μM. (B) Absorbance and (C) PL spectra of **NOR1** at the concentration of 10 μM in ethanol–PEG400 mixtures with different volume fractions of PEG400.

Cell viability assay of NOR1

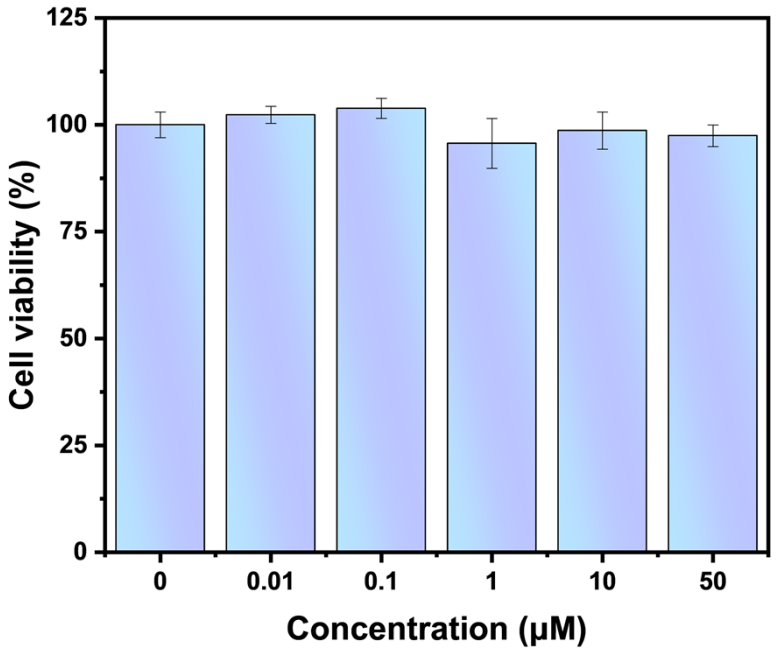

Figure S15. Cell viability values (%) estimated by CCK8 assays using Hela cells, cultured in the presence of 0-50.0 μM of **NOR1** for 24 h at 37 °C