

Supporting Information

Highly emissive dibenzofuran fluorophores with aggregation-induced emission for bioimaging in HeLa cell lines

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1. Characterization data of compounds

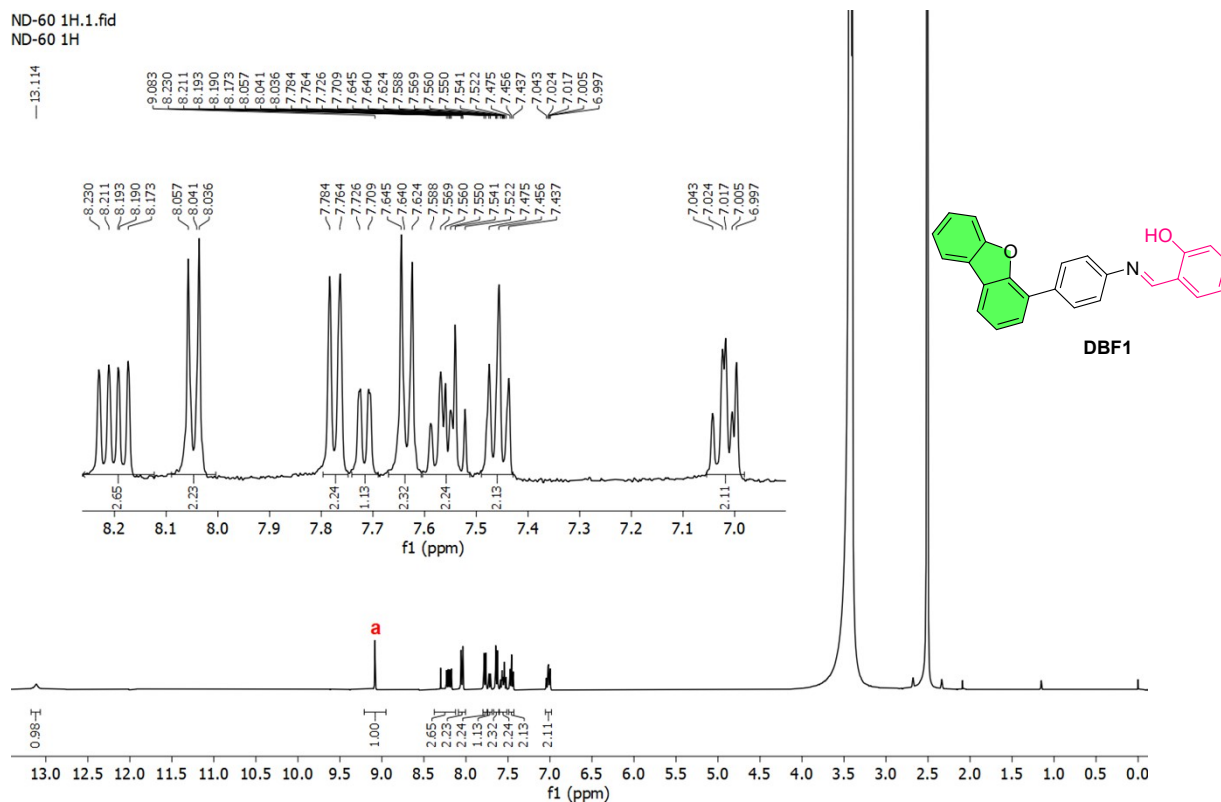


Figure S1. ^1H NMR spectra of (*E*)-2-(((4-(dibenzo[b,d]furan-4-yl)phenyl)imino)methyl)phenol (DBF1). [recorded on 400 MHz FT-NMR Spectrometer. Probe: 5mm BBO probe at 25°C]

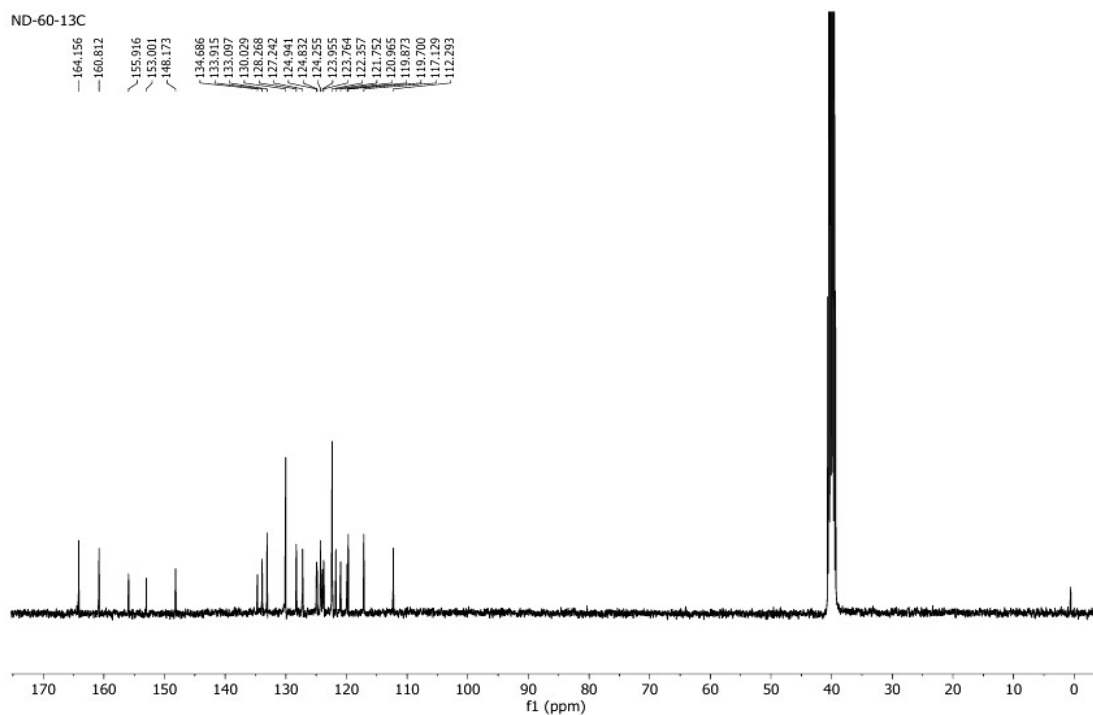


Figure S2. ^{13}C NMR spectra of (*E*)-2-(((4-(dibenzo[b,d]furan-4-yl)phenyl)imino)methyl)phenol (DBF1). [recorded on 100 MHz FT-NMR Spectrometer. Probe: 5mm BBO probe at 25°C]



Figure S3. LCMS of (*E*)-2-(((4-(dibenzo[b,d]furan-4-yl)phenyl)imino)methyl)phenol (**DBF1**). [recorded on LCMS-8060NX with heated ESI probe from Shimadzu].

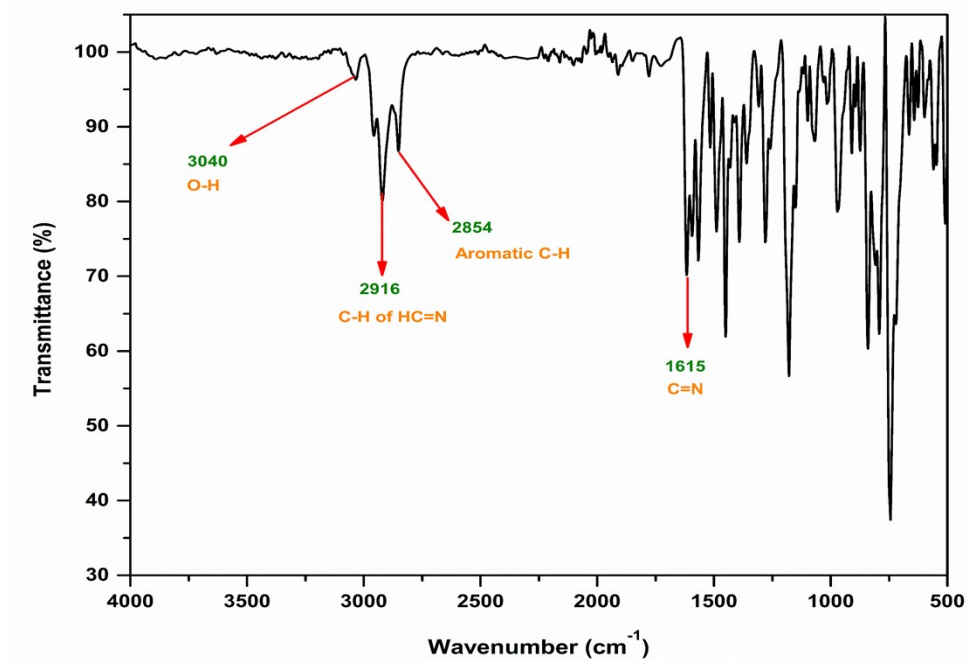


Figure S4. Infrared spectrum of (*E*)-2-(((4-(dibenzo[b,d]furan-4-yl)phenyl)imino)methyl)phenol (**DBF1**).

ND-84 1H.1.fid
ND-84 1H

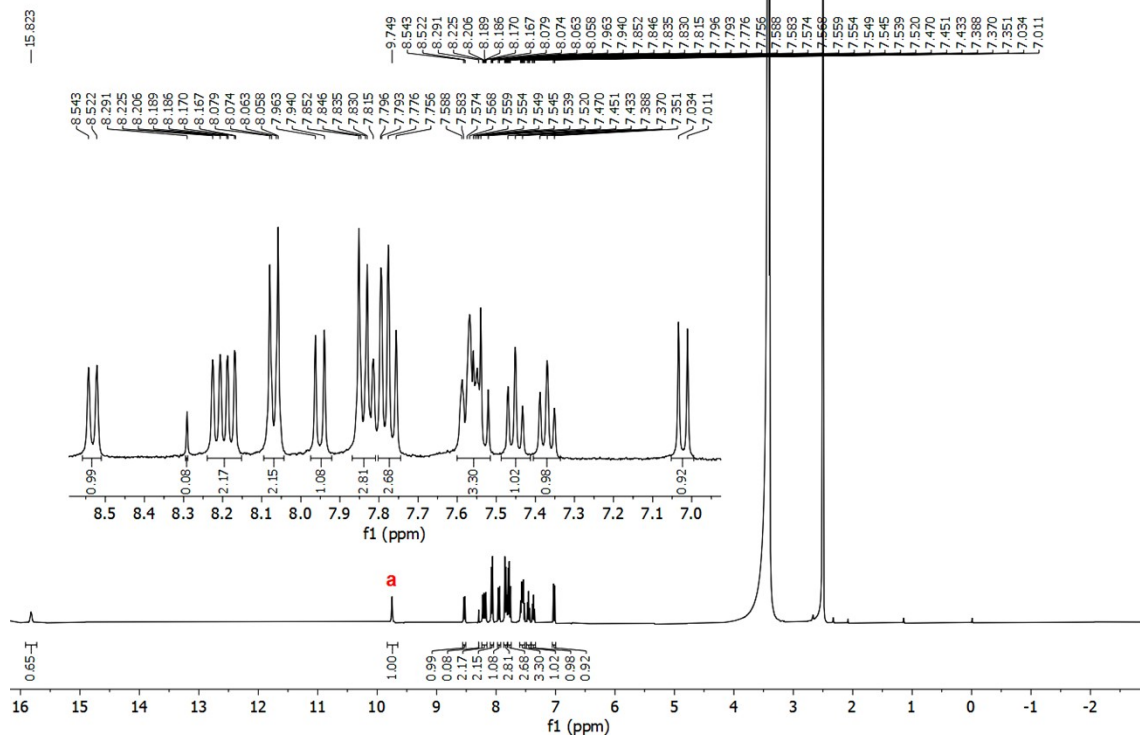


Figure S5. ^1H NMR spectra of (*E*)-1-(((4-(dibenzo[b,d]furan-4-yl)phenyl)imino)methyl)naphthalen-2-ol (DBF2). [recorded on 400 MHz FT-NMR Spectrometer. Probe: 5mm BBO probe at 25°C]

ND-84 13C.1.fid
ND-84 13C

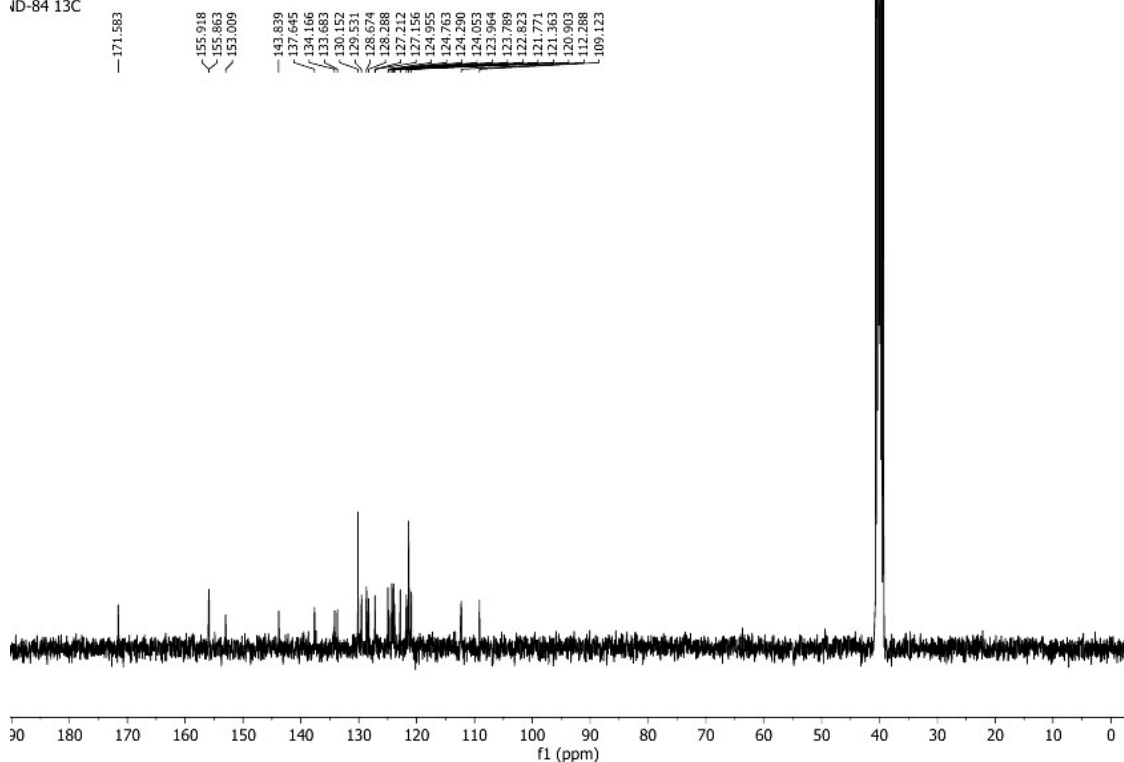


Figure S6. ^{13}C NMR spectra of (*E*)-1-(((4-(dibenzo[b,d]furan-4-yl)phenyl)imino)methyl)naphthalen-2-ol (DBF2). [recorded on 100 MHz FT-NMR Spectrometer. Probe: 5mm BBO probe at 25°C]

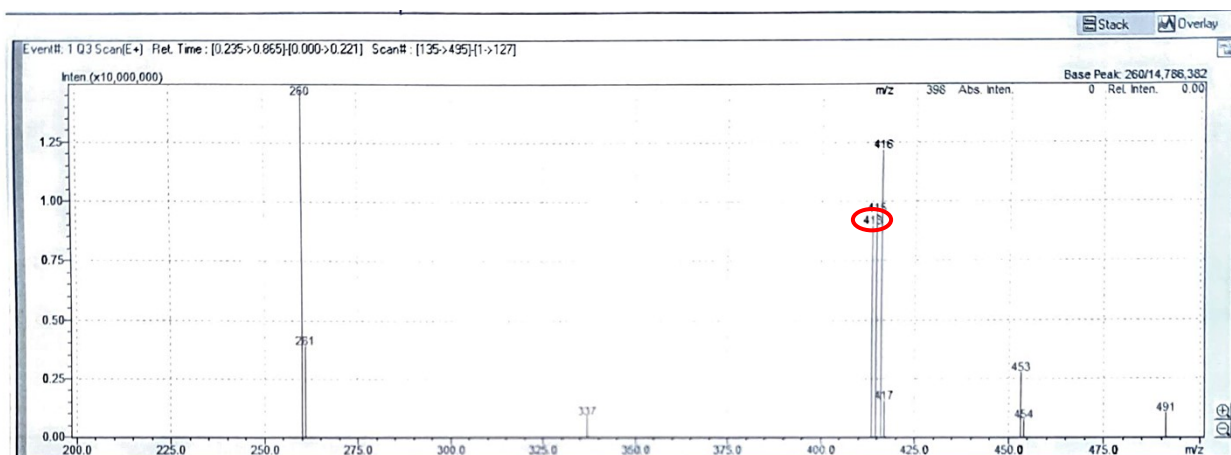


Figure S7. LCMS spectrum of (*E*)-1-(((4-(dibenzo[b,d]furan-4-yl)phenyl)imino)methyl)naphthalen-2-ol (**DBF2**). [recorded on LCMS-8060NX with heated ESI probe from Shimadzu].

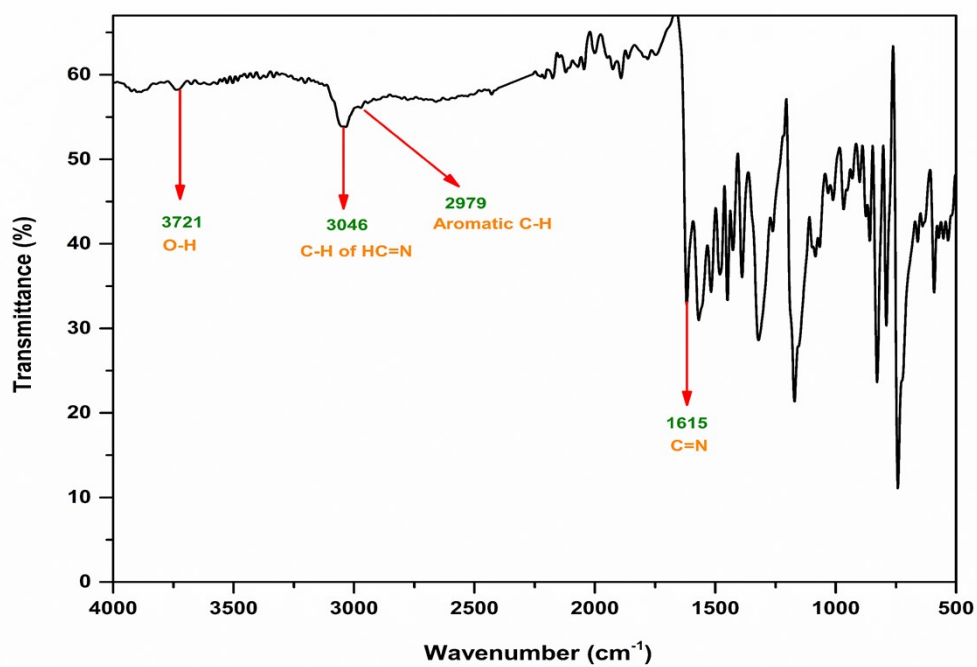


Figure S8. Infrared spectra of (*E*)-1-(((4-(dibenzo[b,d]furan-4-yl)phenyl)imino)methyl)naphthalen-2-ol (**DBF2**).

2. Solvatochromic properties: Absorbance spectra

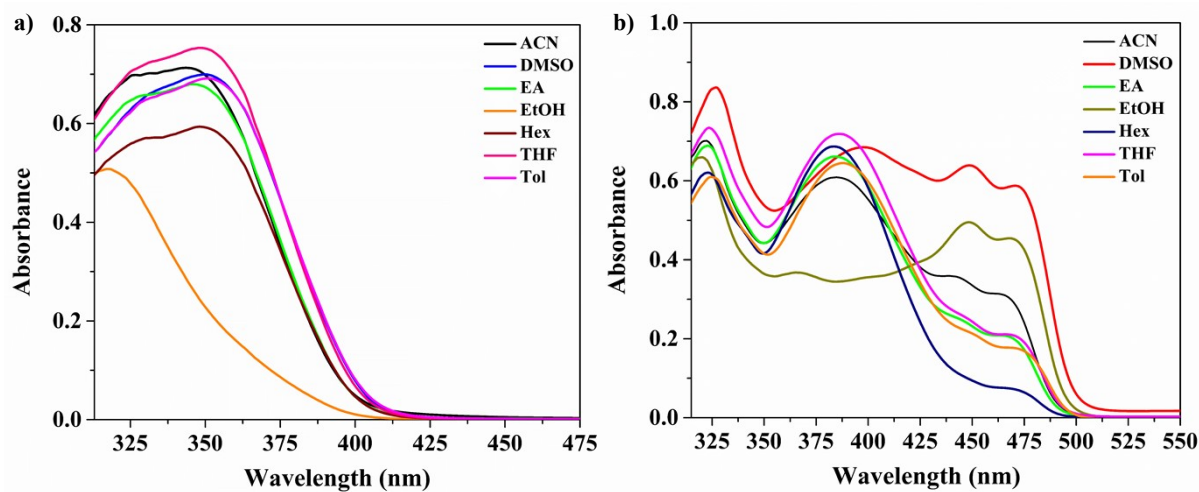


Figure S9. Solvent-dependent absorbance spectra of a) DBF1, b) DBF2. Concentration: 30 μ M.

3. AIE/AIEE properties: Absorbance spectra

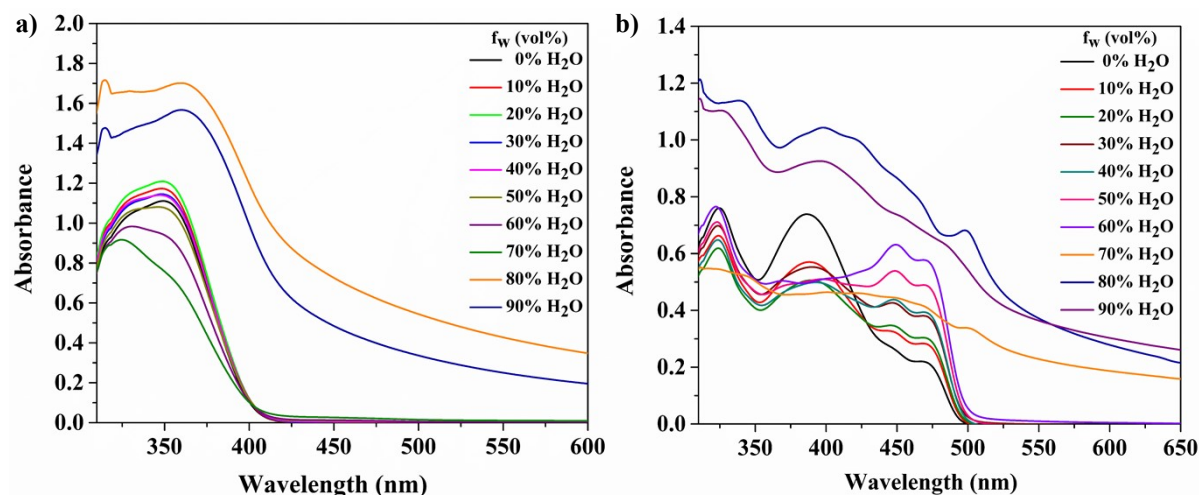


Figure S10. Absorbance spectra of a) DBF1 with varying water fractions; b) DBF2 with varying water fractions (concentration – 30 μ M).

4. Photophysical properties of DBF1 and DBF2

Table S1. Photophysical properties of **DBF1** in the solution state.

Solvent	$\lambda_{\text{max.abs}}$ (nm)	λ_{em} (nm)	Stokes shift (nm) with respect to the λ_{em} max
Hexane	349	398 (max), 423	49
Toluene	351	406 (max), 431	55
THF	349	407	58
Ethyl acetate	345	401 (max), 424	56
DMSO	350	439	89
Acetonitrile	344	402, 422 (max)	78
Ethanol	315	426	111

Table S2. Photophysical properties of **DBF2** in the solution state.

Solvent	$\lambda_{\text{max.abs}}$ (nm)	λ_{em} (nm)	Stokes shift (nm) with respect to the λ_{em} max
Hexane	323	366	43
Toluene	325	374	49
THF	324	418	94
Ethyl acetate	322	417	95
DMSO	327	439, 496 (max)	169
Acetonitrile	322	426	114

Ethanol	320	421 (max), 495	101
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5. %Cell viability and IC₅₀ values of HeLa cells treated with DBF1 and DBF2

Table S3. %Cell viability and IC₅₀ values of HeLa cells treated with **DBF1** for 24 hours.

MTT assay summary-DBF1 vs HeLa		
Culture condition	% Cell viability	IC ₅₀ conc (µg/ml)
Untreated	100	42.08
Std control	35.73	
DBF1-10 µg	72.68	
DBF1-50 µg	49.54	
DBF1-100 µg	36.41	
DBF1-150 µg	33.75	
DBF1-200 µg	16.06	

Table S4. %Cell viability and IC₅₀ values of HeLa cells treated with **DBF2** for 24 hours.

MTT assay summary-DBF2 vs HeLa		
Culture condition	% Cell viability	IC ₅₀ conc (µg/ml)
Untreated	100	39.74
Std control	35.73	
DBF2-10 µg	63.63	
DBF2-50 µg	49.09	
DBF2-100 µg	39.71	
DBF2-150 µg	38.72	
DBF2-200 µg	30.58	

6. Chart of comparative IC₅₀ values of DBF1 and DBF2

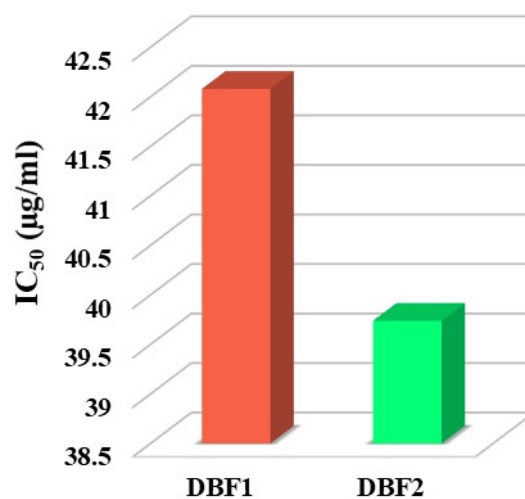


Figure S11. IC₅₀ values of **DBF1** and **DBF2** against the HeLa cells after the incubation period of 24 hours by MTT assay.

7. Photostability study

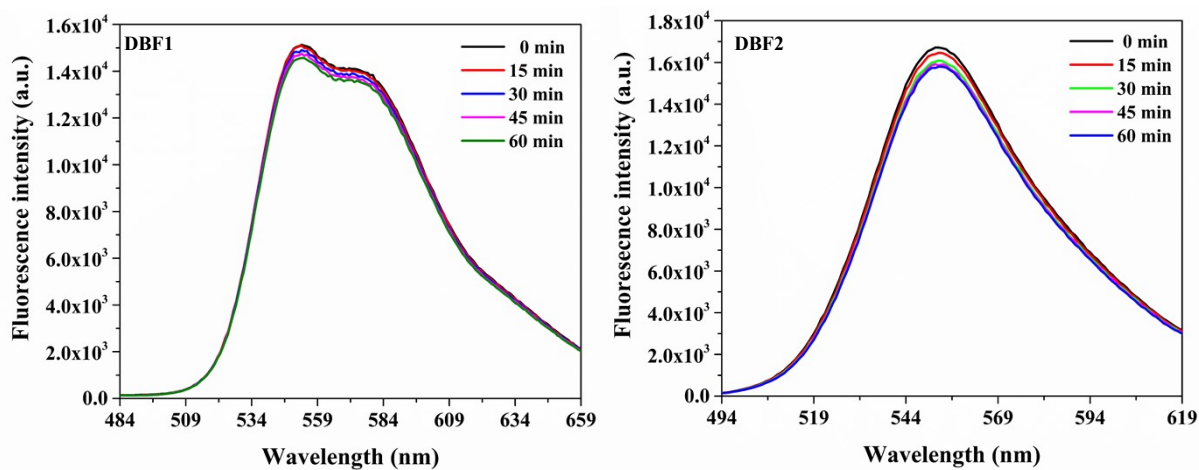


Figure S11. Photostability study using emission spectra for **DBF1** and **DBF2** recorded for 0 minutes to 60 minutes after every 15 minutes in solid-state.