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Organic light-emitting diodes comprising highly luminescent red-emitting dendrimers with carbazole-based dendrons

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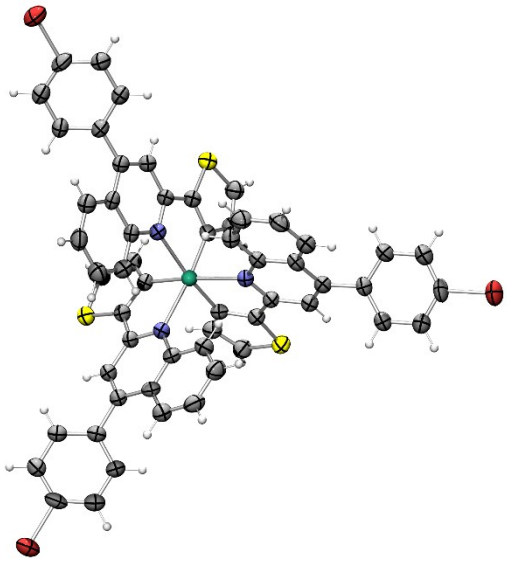


Figure S1 X-ray single crystal structure of the homoleptic 4-bromophenyl-functionalized iridium(III) complex **5**.

Table S1: Crystallography data summary for **5**.

Material	**5**
Empirical Formula	$C_{57}H_{33}Br_3IrN_3O_{0.17}S_3$
Formula Weight	1290.65
Temperature/K	100(2)
Crystal System	trigonal
Space Group	*P-3c1*
a/ Å	17.712(3)
b/ Å	17.712(3)
c/ Å	17.804(4)

α/ °	90
β/ °	90
γ/ °	120
Volume/ $Å^3$	4837.1(17)
Z	4
ρ_{calc} g/cm^3	1.772
μ/ mm^{-1}	5.411
F(000)	2509.0
Crystal Size/ mm^3	0.03 × 0.03 × 0.01
Radiation	synchrotron (λ = 0.7108)
2θ range for data collection/ °	2.656 to 52.744
Index ranges	$-21 \leq h \leq 22$, $-22 \leq k \leq 22$, $-22 \leq l \leq 22$
Reflections collected	67451
Independent reflections	3313 [R_{int} = 0.0797, R_{sigma} = 0.0213]
Data/restraints/parameters	3313/0/205
Goodness-of-fit on F^2	1.042
Final R indexes [I>2σ(I)]	R_1 = 0.0468, wR_2 = 0.1277
Final R indexes [all data]	R_1 = 0.0595, wR_2 = 0.1371
Largest diff. peak/hole / e $Å^{-3}$	1.67/-1.23

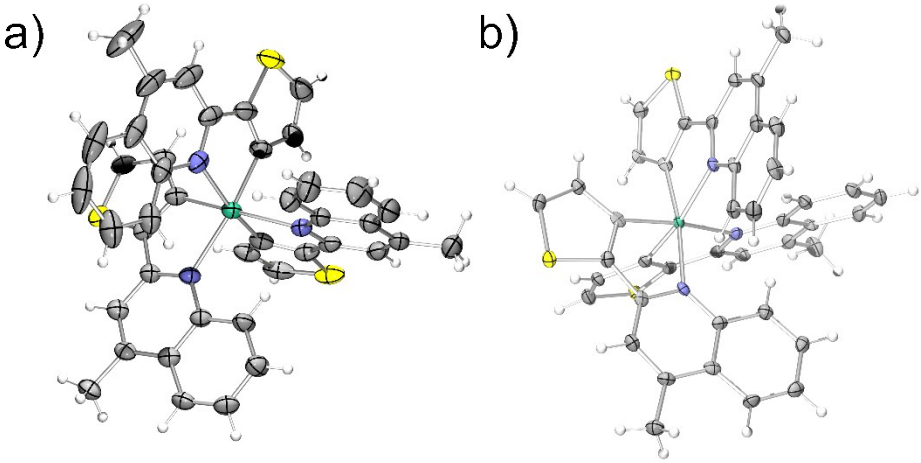


Figure S2 X-ray crystal structure of **1** of crystal grown from either a) solution by layer diffusion or b) sublimation. The structure in a) is solvated by a disordered dichloromethane molecule, which has not been included for clarity.

Table S2: Crystallography data summary for **1**.

1 grown from:	**Solution**	**Sublimation**
Empirical Formula	$C_{43}H_{30}Cl_2IrN_3S_3$	$C_{42}H_{30}IrN_3S_3$
Formula Weight	953.98	865.07
Temperature/K	100(2)	100(2)
Crystal System	triclinic	triclinic
Space Group	*P-1*	*P-1*
a/ Å	11.047(2)	10.654(2)
b/ Å	15.964(3)	11.667(2)
c/ Å	21.775(4)	14.179(3)
α/ °	83.03(3)	91.75(3)
β/ °	81.84(3)	103.13(3)
γ/ °	77.02(3)	103.60(3)
Volume/ $Å^3$	3688.2(14)	1661.7(6)
Z	4	2
ρ_{calc} g/cm^3	1.718	1.729
μ/ mm^{-1}	3.975	4.243
F(000)	1844.0	856.0
Crystal Size/ mm^3	0.2 × 0.08 × 0.03	0.1 × 0.05 × 0.04
Radiation	synchrotron (λ = 0.7108)	synchrotron (λ = 0.7108)
2θ range for data collection/ °	1.898 to 52.75	2.962 to 49.43
Index ranges	$-13 \leq h \leq 13$, $-19 \leq k \leq 19$, $-27 \leq l \leq 27$	$-12 \leq h \leq 12$, $-13 \leq k \leq 13$, $-16 \leq l \leq 16$
Reflections collected	51255	17557
Independent reflections	13663 [R_{int} = 0.0339, R_{sigma} = 0.0320]	5123 [R_{int} = 0.0263, R_{sigma} = 0.0257]
Data/restraints/parameters	13663/0/1000	5123/0/446
Goodness-of-fit on F^2	1.056	1.135
Final R indexes [I>2σ(I)]	R_1 = 0.0365, wR_2 = 0.0885	R_1 = 0.0273, wR_2 = 0.0810
Final R indexes [all data]	R_1 = 0.0409, wR_2 =	R_1 = 0.0280, wR_2 =

	0.0915	0.0817
Largest diff. peak/hole / e Å^{-3}	1.83/-1.83	0.89/-1.83

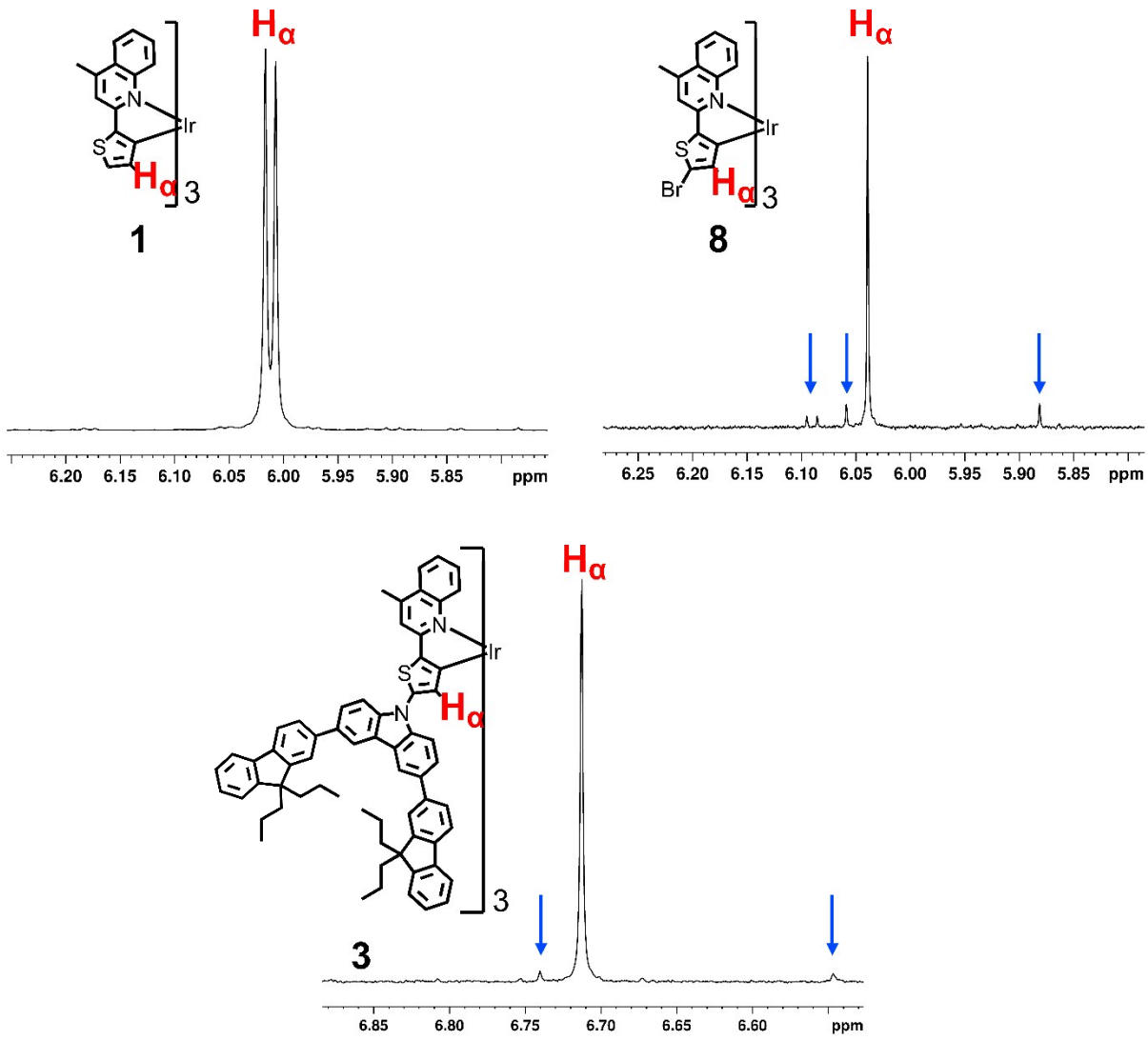


Figure S3 ^{1}H NMR investigation of the regioisomers formed during the bromination of **1** and carry through to dendrimer **3**. The thiophenyl proton alpha to the Ir-C bond (H_α) was used as the diagnostic peak. The signals corresponding to the H_α of the major isomer are labelled in red. The small signals corresponding to the minor regioisomer(s) are indicated by blue arrows.

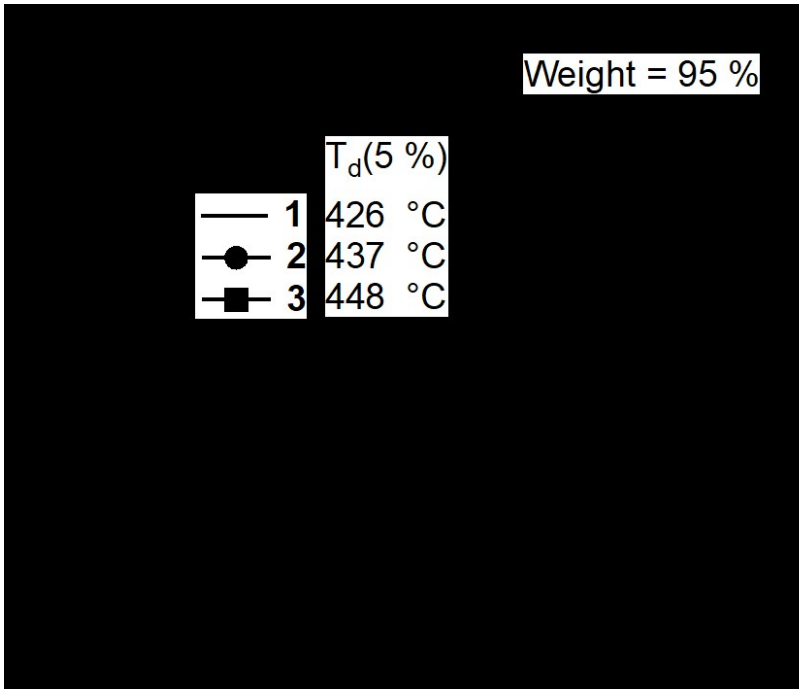


Figure S4 Thermal gravimetric analysis of the three materials.

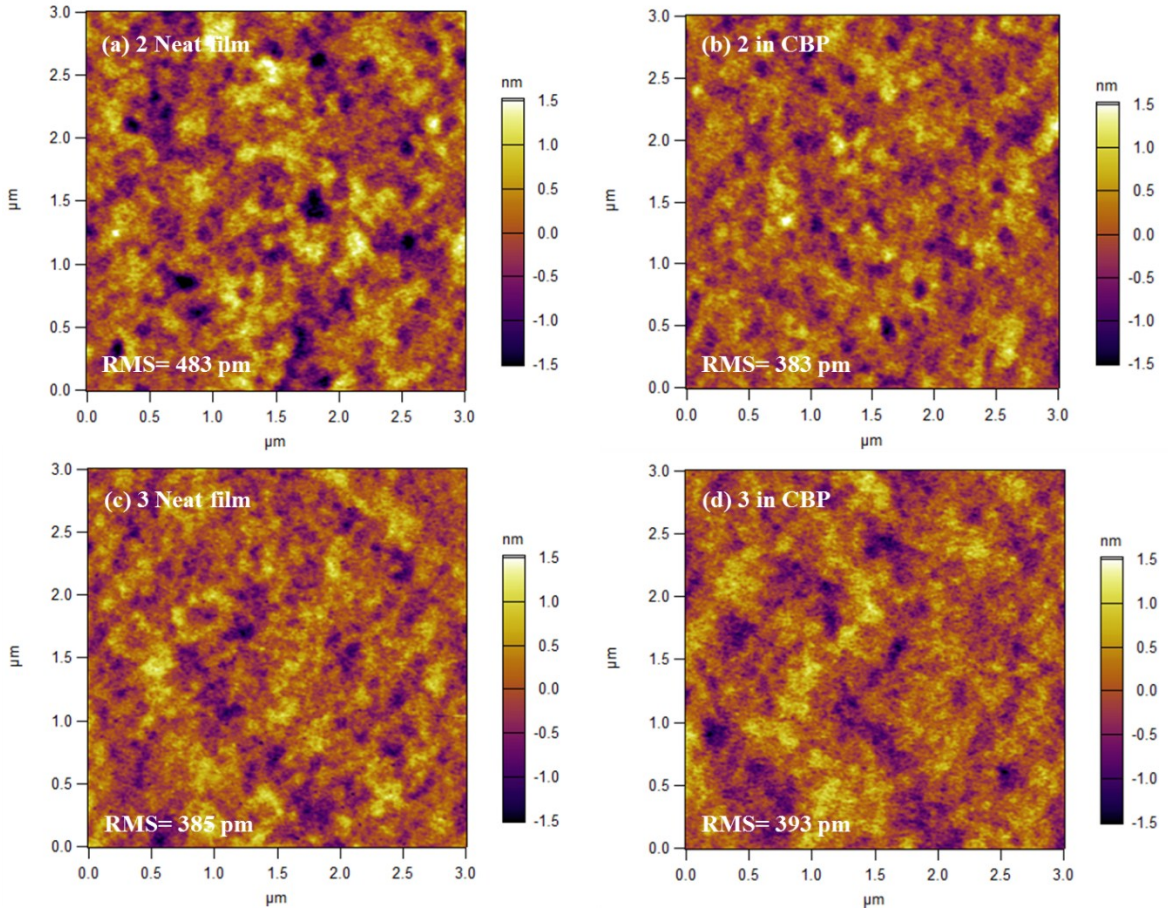


Figure S5 AFM images showing the surface topology of the films. Neat and blend film of **2** [(a) and (b), respectively] and neat and blend of **3** [(a) and (b), respectively].

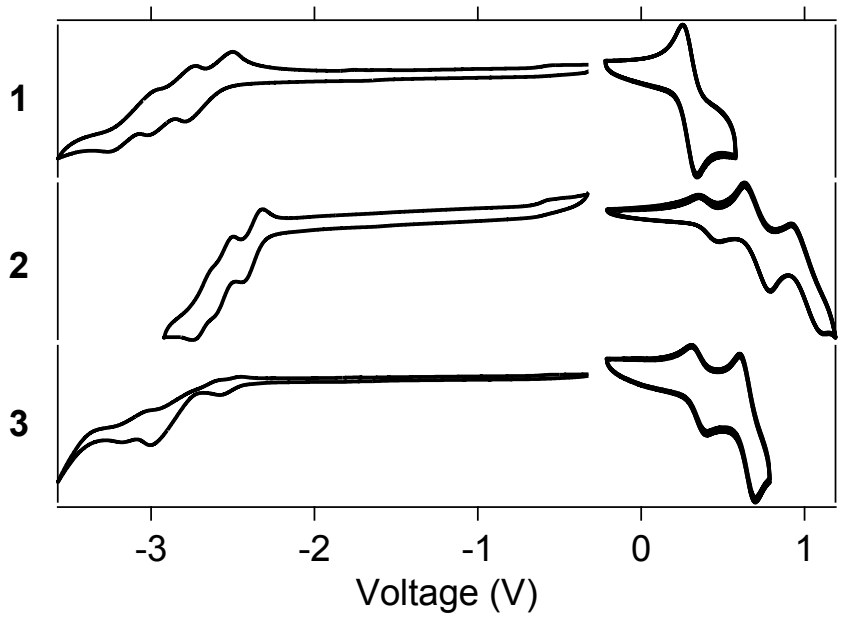
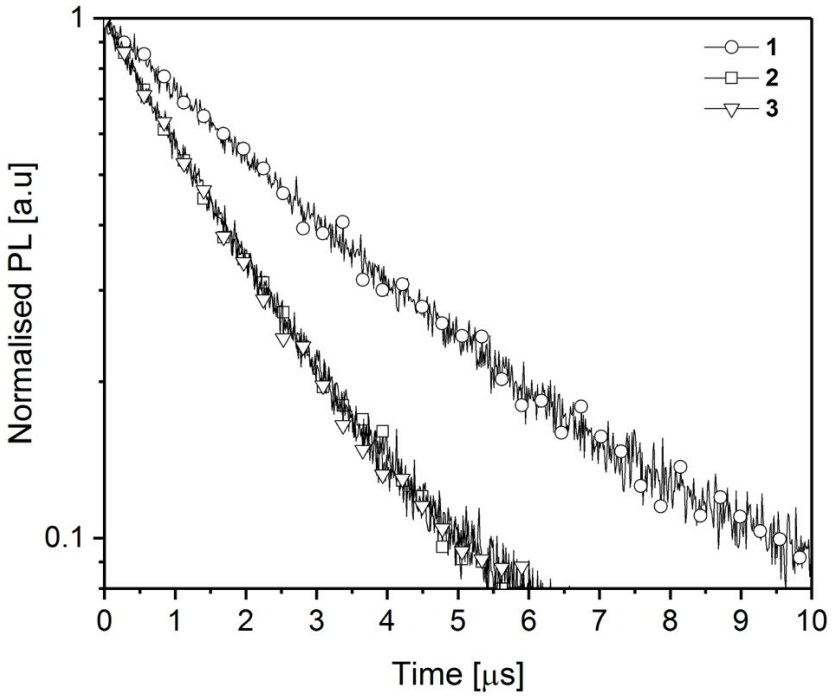


Figure S6 Cyclic voltammograms of red-emitting iridium(III) complexes versus Fc/Fc^{+} redox couple. Oxidations were performed in anhydrous dichloromethane while reductions were in anhydrous tetrahydrofuran. Tetrabutylammonium perchlorate was utilized as the electrolyte with a glassy carbon working electrode, platinum counter electrode and silver/silver(I) nitrate in acetonitrile reference electrode.

a)



b)

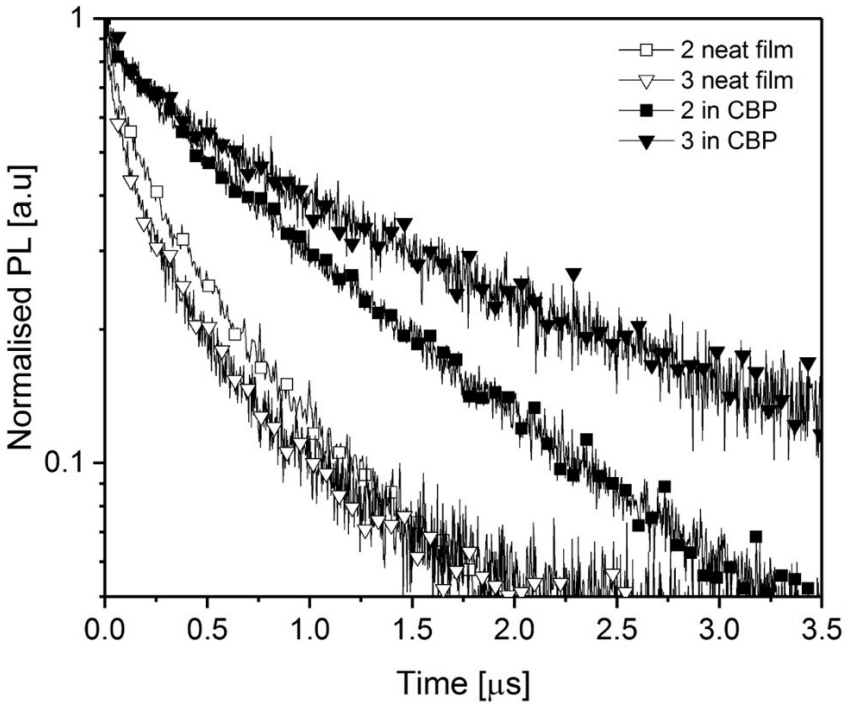


Figure S7 TCSPC decays of a) **1** (at 589 nm), **2** and **3** (both at 609 nm) in toluene and as neat films, and b) at 610 nm for the neat **2** and **3**, and 10 wt% dendrimer:CBP blend films. Excitation wavelength = 372 nm.

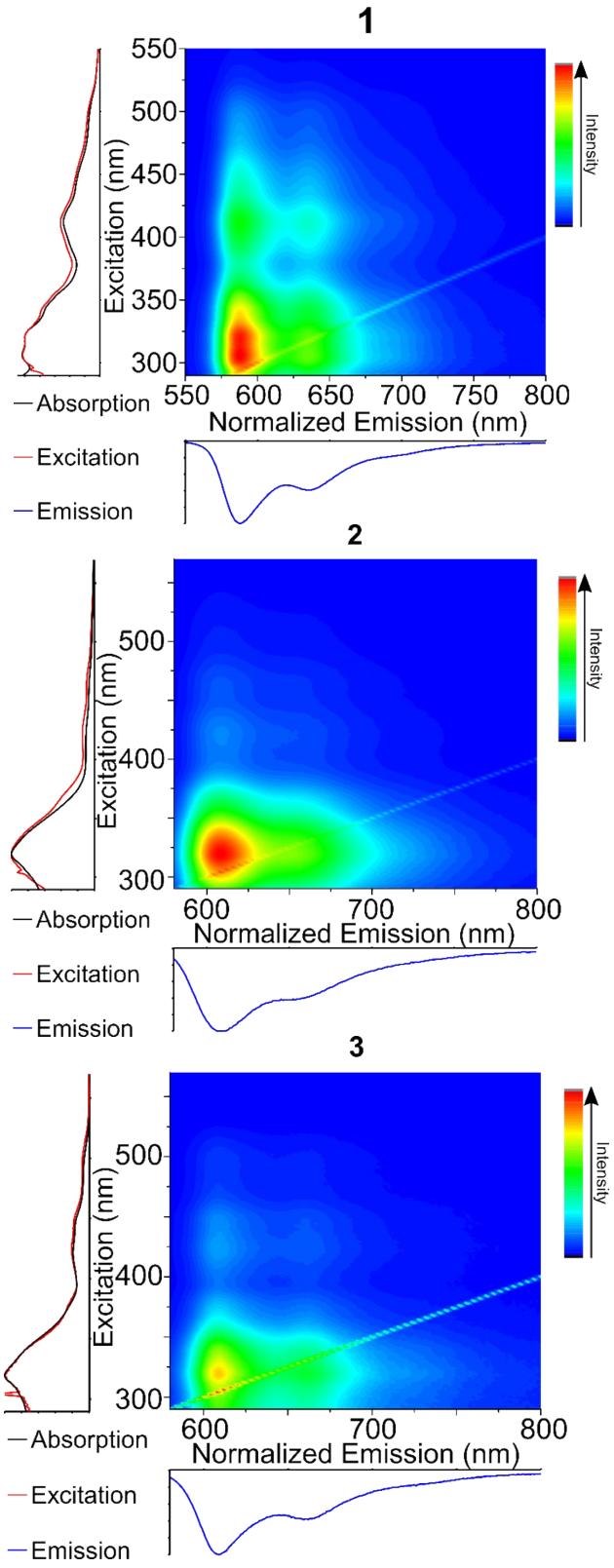


Figure S8 Emission versus excitation contour plots of **1**, **2**, and **3** in solution (toluene). One-dimensional emission, excitation and adsorption spectra are shown as axis projections for comparison.