Electronic Supplementary Information (ESI)

Europium doped LaF_3 nanocrystals with organic 9-oxidophenalenone capping ligands that display visible light excitable steady-state blue and time delayed red emission

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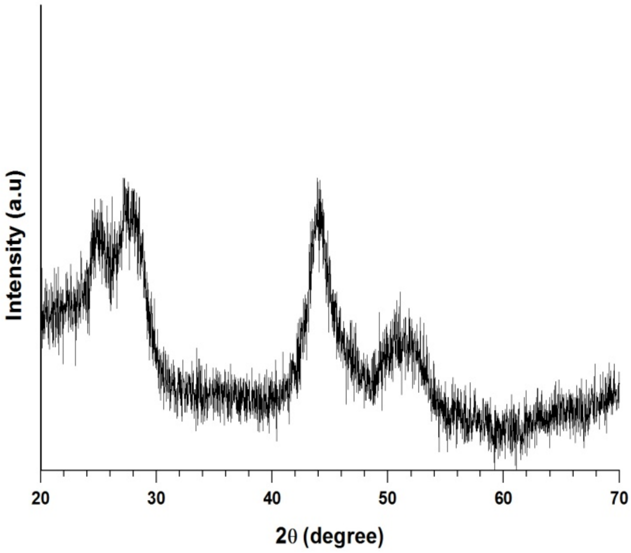

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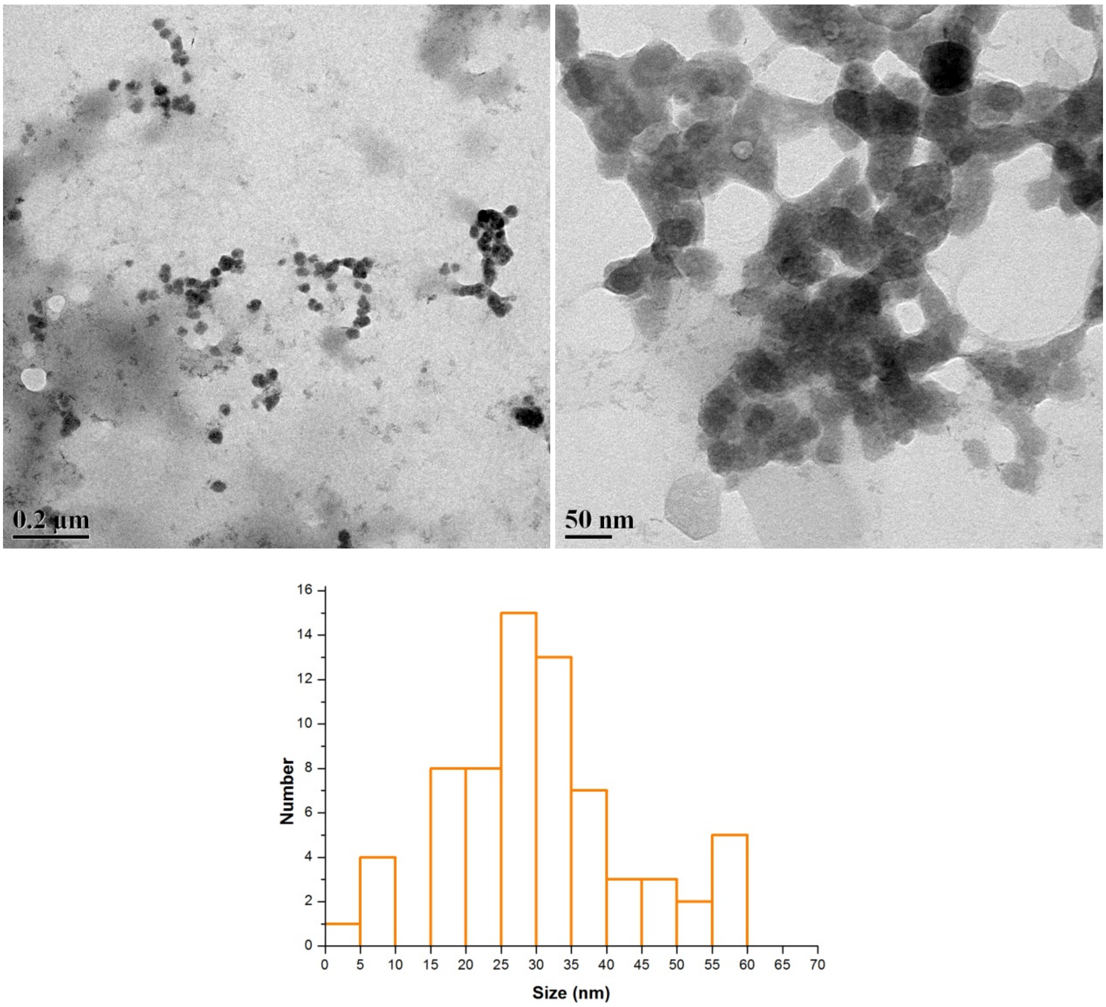

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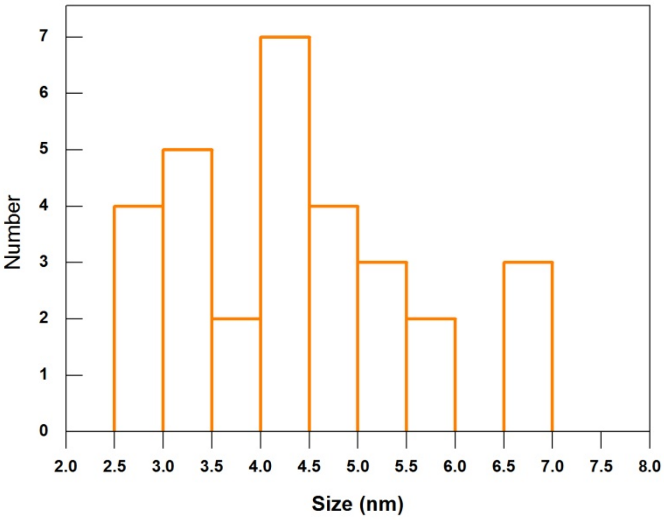
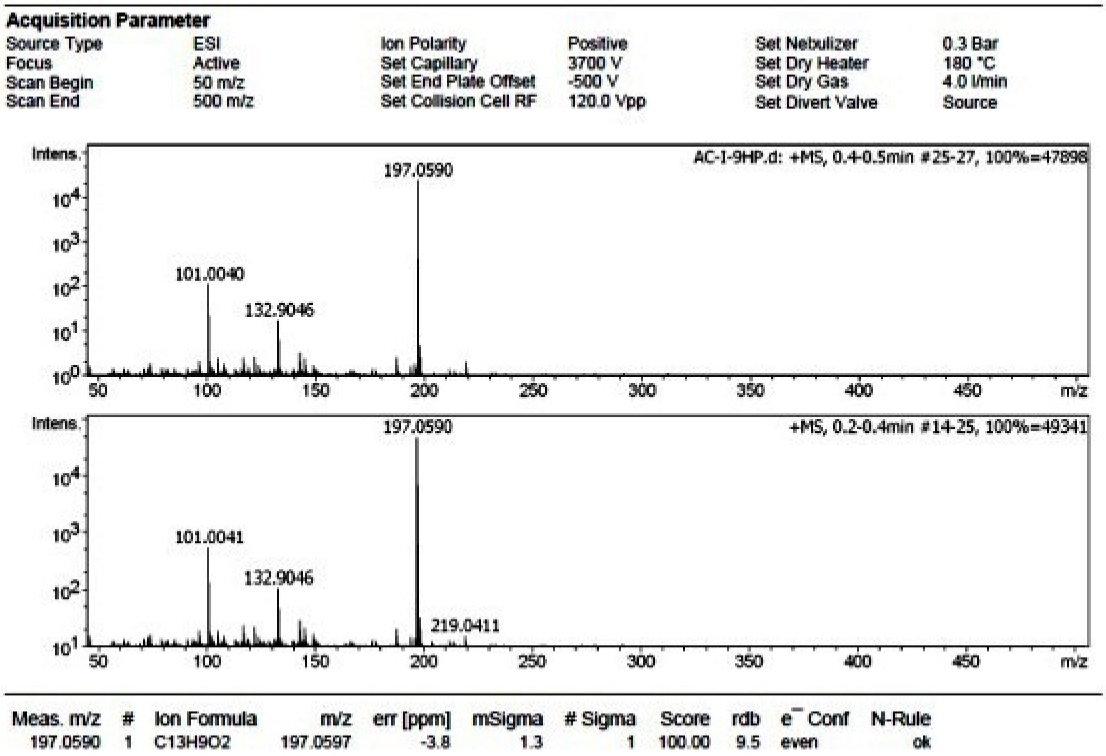


Figure S3: Histogram showing size TEM size distribution 30 discernible 9-oxidophenalenone capped ~5% Eu^{3+}-doped LaF_3 NCs.

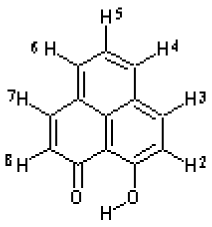


Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	500 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
197.0590	1	C13H9O2	197.0597	-3.8	1.3	1	100.00	9.5	even	ok

Figure S4: Electrospray ionisation mass spectrum in positive ion mode ($ESI-MS^+$) of 9-hydroxyphenalenone ligand recorded on Bruker Maxis Impact mass spectrometer.



9-hydroxyphenalenone

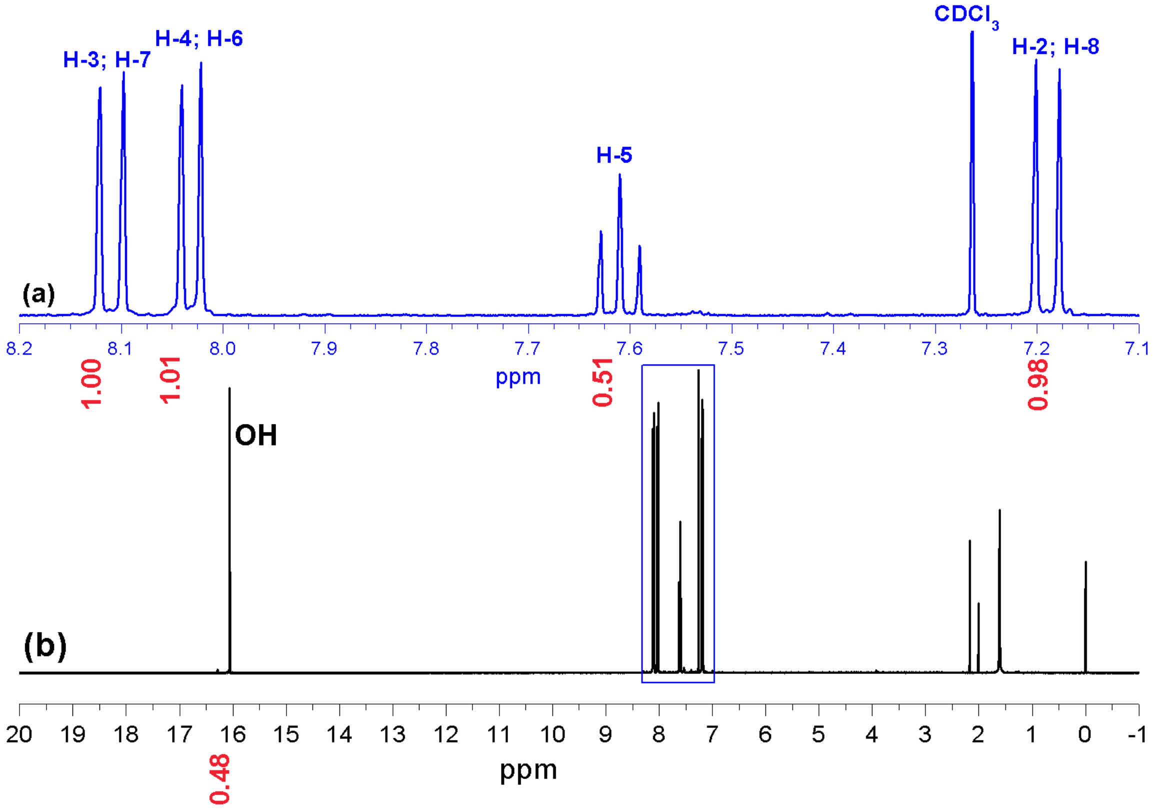


Figure S5: The ^{1}H NMR spectrum of 9-hydroxyphenalenone in $CDCl_3$, (a) full spectrum and (b) expansion of 7.1-8.2 ppm region. The spectrum was recorded on 400 MHz Bruker Avance III spectrometer. The proton resonances are assignments according to the literature (*J. Chem. Edu.,* 2008, **85**, 413).

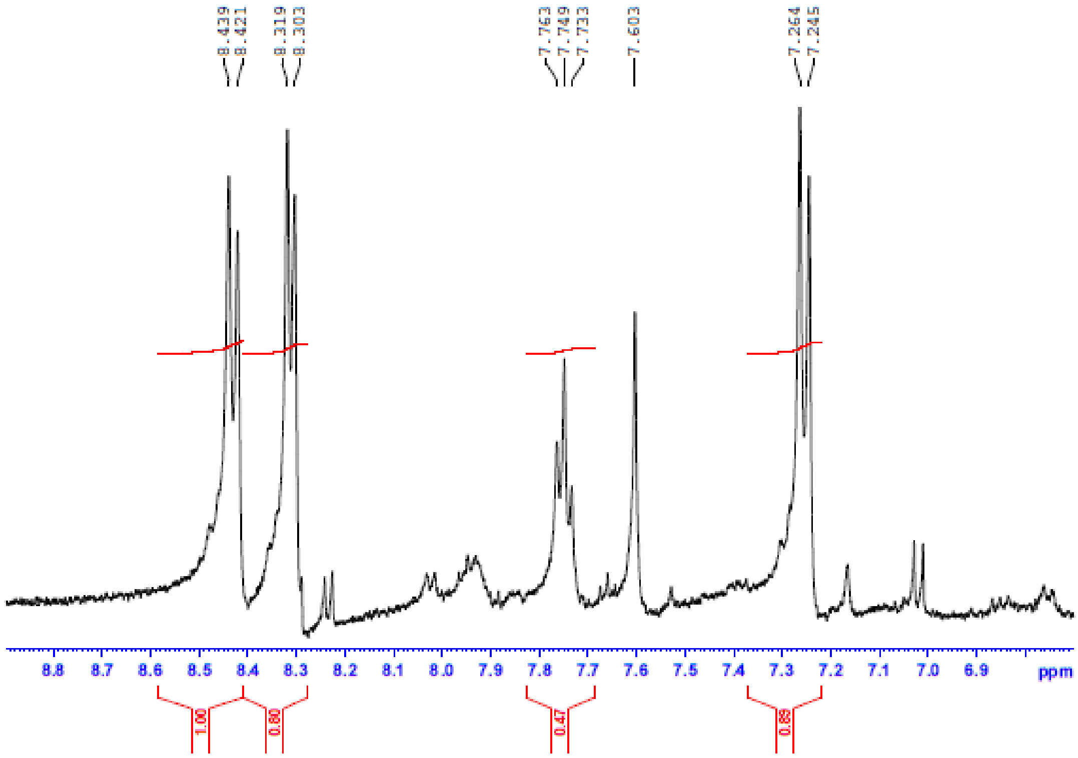
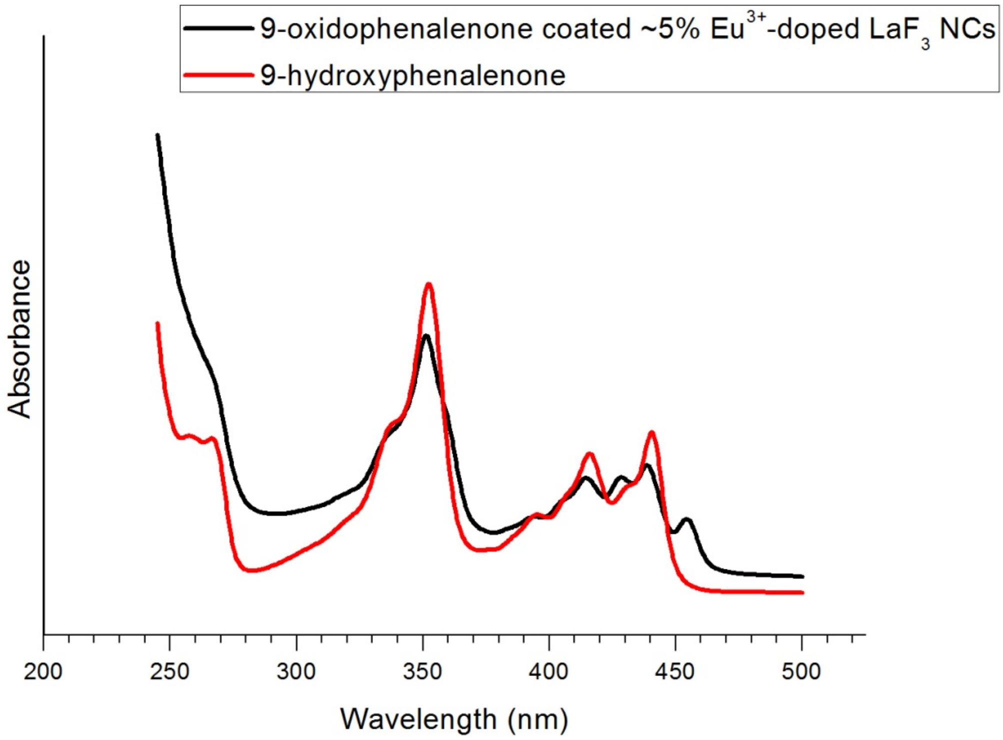


Figure S6: The ^{1}H NMR spectrum 9-oxidophenalenone coated ~5% Eu^{3+}-doped LaF$_3$ NCs in DMSO-d$_6$. The spectrum was recorded on 400 MHz Bruker Avance III spectrometer.

The proton resonances observed in the spectrum are weak due to poor dispersibility of the NCs. However, the proton resonances at 8.4 and 8.3 ppm, both doublets and integrating for two protons each, can be easily related to the similar resonances observed in the ^{1}H NMR spectrum of free 9-hydroxyphenalenone ligand at 8.10 ppm and 8.03 ppm and assigned to H-3, H-7 and H-4, H-6 protons, respectively (Figure S5, ESI†). The triplet observed at 7.74 ppm, which integrates for one proton can be related to the triplet observed at 7.61 ppm and assigned to H-5 proton in the free 9-hydroxyphenalenone ligand. Finally a doublet observed at 7.25 ppm and integrating for two protons can be easily related to a doublet at 7.18 ppm in the free 9-hydroxyphenalenone and assigned to H-2 and H-8 protons. No resonance around 16 ppm due to OH protons is observed in the 9-oxidophenalenone capped NCs. The resonances observed in the free ligand are clearly very sharp as compared to the resonances observed in the NCs (Figure S5, ESI†). A sharp resonance at 7.6 ppm, integrating for less than one proton with respect to resonances identified for capping ligands, could most probably be due to some solvent impurity in the NMR tube and is visible only due to weak intensity (because of poor dispersibility of NCs in DMSO-d6) of the proton resonances of the NCs.



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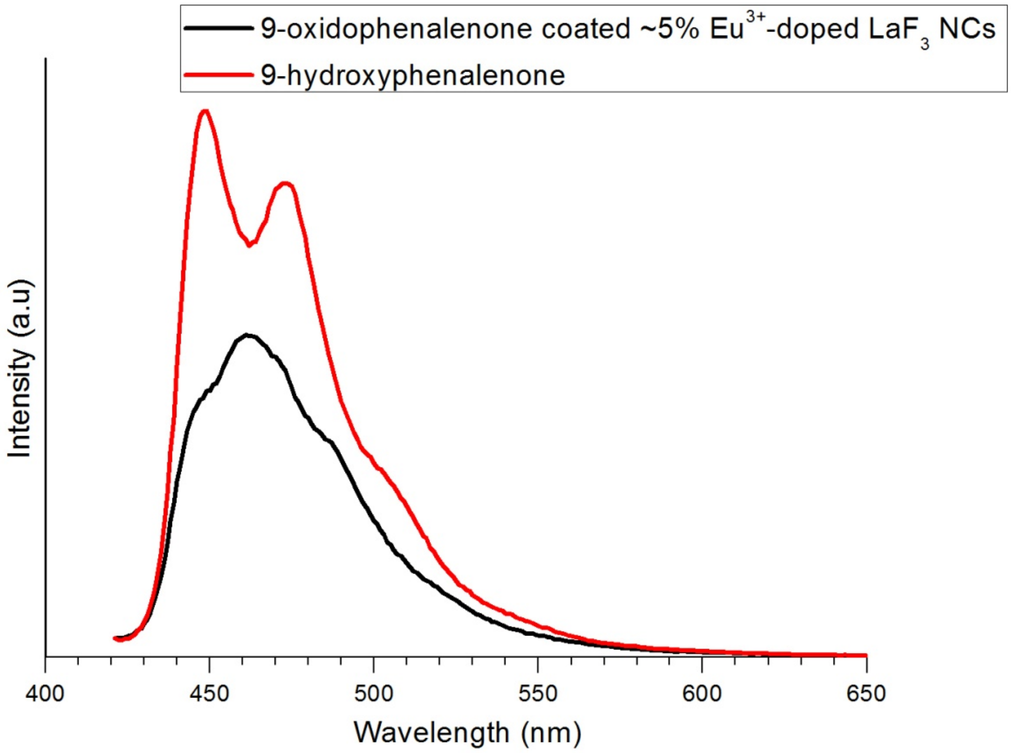

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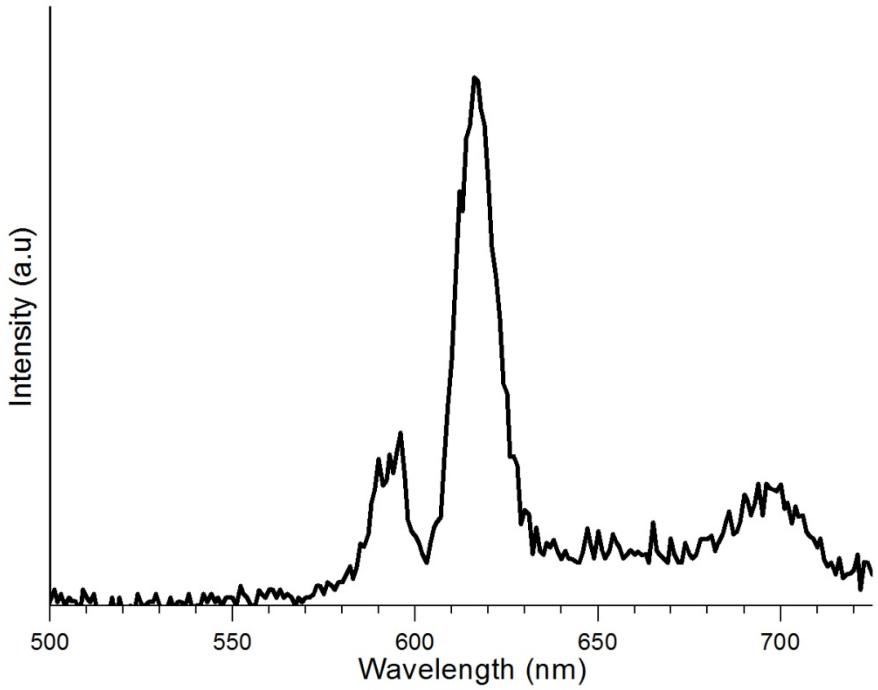

Figure S9: Emission spectrum of a dried (solid) sample of 9-oxidophenalenone coated ~5% Eu^{3+}-doped LaF_3 NCs collected upon excitation of the organic capping ligands at 457 nm, with 0.1 ms delay time (phosphorescence mode).