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Electronic Supporting Information

Role of structure and metal ion in the fluorescence sensing of nitro compounds for a series of lanthanide(III) 9, 10-anthracene dicarboxylate coordination polymers

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Table S1: Elemental analysis of **1-28**. With the exception of compounds 9-14 which was synthesized with DMSO, the compounds made with DMF and DMA consistently returned with lower carbon contents despite repeated attempts. This could be the trapping of water molecules during hydrolysis of these solvents during the solvothermal synthesis. Since lanthanides are hygroscopic, it might hold onto these water molecules better. Hence the formulas are fixed with water molecules.

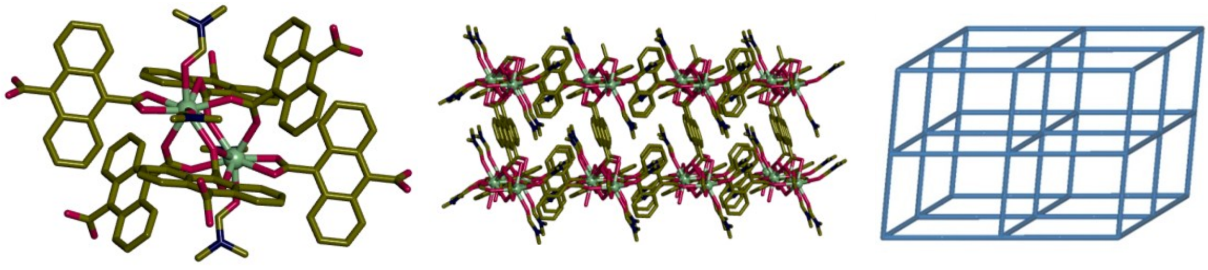
MOF	Experimental (%)			Theoretical (%)			Theoretical (after adjustment with water) (%)		
	C	H	N	C	H	N	C	H	N
1	51.04	3.99	5.14	53.6	2.5	4.96	Actual formula: $[La_2(ADC)_3(DMF)_4]\cdot DMF\cdot 3H_2O$		
							51.62	2.82	4.78
2	50.19	4.11	5.15	53.51	2.49	4.95	Actual formula: $[Ce_2(ADC)_3(DMF)_4]\cdot DMF\cdot 5H_2O$		
							50.3	3.02	4.66
3	50.04	4.10	5.03	53.45	2.49	4.95	Actual formula: $[Pr_2(ADC)_3(DMF)_4]\cdot DMF\cdot 5H_2O$		
							50.25	3.01	4.65
4	49.93	4.12	5.17	53.19	2.48	4.92	Actual formula: $[Nd_2(ADC)_3(DMF)_4]\cdot DMF\cdot 5H_2O$		
							50.03	3	4.63
5	46.38	4.03	4.80	52.74	2.46	4.88	Actual formula: $[Sm_2(ADC)_3(DMF)_4]\cdot DMF\cdot 10H_2O$		
							46.86	3.43	4.34
6	49.32	4.31	4.88	52.62	2.45	4.87	Actual formula: $[Eu_2(ADC)_3(DMF)_4]\cdot DMF\cdot 5H_2O$		
							49.52	2.97	4.58
7	49.8	4.06	4.98	52.24	2.44	4.83	Actual formula: $[Gd_2(ADC)_3(DMF)_4]\cdot DMF\cdot 5H_2O$		
							49.18	2.95	4.55
8	49.54	4.10	4.94	52.12	2.43	4.82	Actual formula: $[Tb_2(ADC)_3(DMF)_4]\cdot DMF\cdot 5H_2O$		

							49.07	**2.94**	**4.54**
9	**46.17**	**3.82**	**-**	**46.13**	**2.32**	**-**	**Actual formula: $[Dy_2(ADC)_3(DMSO)_6]$**		
							-	**-**	**-**
10	**45.88**	**4.23**	**-**	**45.98**	**2.32**	**-**	**Actual formula: $[Ho_2(ADC)_3(DMSO)_6]$**		
							-	**-**	**-**
11	**45.85**	**3.89**	**-**	**45.85**	**2.31**	**-**	**Actual formula: $[Er_2(ADC)_3(DMSO)_6]$**		
							-	**-**	**-**
12	**45.60**	**3.92**	**-**	**45.75**	**2.3**	**-**	**Actual formula: $[Tm_2(ADC)_3(DMSO)_6]$**		
							-	**-**	**-**
13	**44.93**	**4.00**	**-**	**45.51**	**2.29**	**-**	**Actual formula: $[Yb_2(ADC)_3(DMSO)_6]\cdot 2H_2O$**		
							44.5	**2.49**	**-**
14	**45.94**	**4.06**	**-**	**45.4**	**2.29**	**-**	**Actual formula: $[Lu_2(ADC)_3(DMSO)_6]$**		
							-	**-**	**-**
15	**53.27**	**4.84**	**5.46**	**55.11**	**3.47**	**5.36**	**Actual formula: $[La_2(ADC)_3(DMA)_6]\cdot 3H_2O$**		
							53.28	**3.73**	**5.18**
16	**50.62**	**4.83**	**5.08**	**55.03**	**3.46**	**5.35**	**Actual formula: $Ce_2(ADC)_3(DMA)_3\cdot 8H_2O$**		
							50.41	**4.11**	**4.9**
17	**52.55**	**5.16**	**5.09**	**54.97**	**3.46**	**5.34**	**Actual formula: $[Pr_2(ADC)_3(DMA)_6]\cdot 5H_2O$**		
							52	**3.88**	**5.05**
18	**49.65**	**4.79**	**4.96**	**54.74**	**3.45**	**5.32**	**Actual formula: $[Nd_2(ADC)_3(DMA)_6]\cdot 10H_2O$**		
							49.14	**4.24**	**4.78**
19	**49.44**	**4.64**	**5.00**	**54.32**	**3.42**	**5.28**	**Actual formula:**		

							$[Sm_2(ADC)_3(DMA)_6]\cdot 9H_2O$		
							49.3	4.14	4.79
20	**51.41**	**4.55**	**5.18**	**54.21**	**3.41**	**5.27**	**Actual formula:** $[Eu_2(ADC)_3(DMA)_6]$		
							51.31	3.83	4.99
21	**49.19**	**4.64**	**5.00**	**53.86**	**3.39**	**5.23**	**Actual formula:** $[Gd_2(ADC)_3(DMA)_6]\cdot 8H_2O$		
							49.42	4.03	4.8
22	**50.85**	**4.55**	**5.48**	**53.74**	**3.38**	**5.22**	**Actual formula:** $[Tb_2(ADC)_3(DMA)_6]\cdot 5H_2O$		
							50.89	3.8	4.95
23	**50.09**	**4.67**	**5.31**	**53.51**	**3.37**	**5.2**	**Actual formula:** $[Dy_2(ADC)_3(DMA)_6]\cdot 6H_2O$		
							50.15	3.86	4.87
24	**52.71**	**4.68**	**5.36**	**53.35**	**3.36**	**5.18**	**Actual formula:** $[Ho_2(ADC)_3(DMA)_6]\cdot H_2O$		
							52.76	3.44	5.13
25	**52.46**	**4.61**	**5.29**	**53.19**	**3.35**	**5.17**	**Actual formula:** $[Er_2(ADC)_3(DMA)_6]\cdot H_2O$		
							52.61	3.43	5.11
26	**52.11**	**4.35**	**5.12**	**53.08**	**3.34**	**5.16**	**Actual formula:** $[Tm_2(ADC)_3(DMA)_6]\cdot H_2O$		
							52.5	3.43	5.1
27	**52.25**	**4.43**	**5.08**	**52.82**	**3.32**	**5.13**	**Actual formula:** $[Yb_2(ADC)_3(DMA)_6]\cdot H_2O$		
							52.24	3.41	5.08
28	**50.36**	**4.40**	**4.60**	**52.69**	**3.32**	**5.12**	**Actual formula:** $[Lu_2(ADC)_3(DMA)_6]\cdot 4H_2O$		
							50.48	3.65	4.91

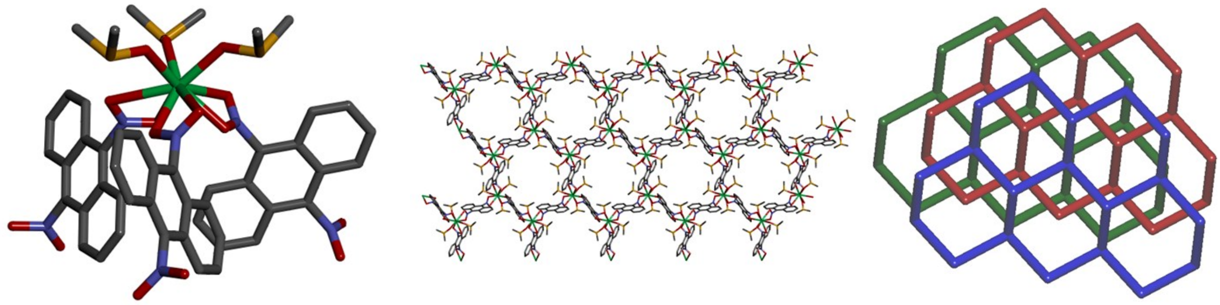
Table S2: Crystal parameters of 10-11.

	10	11
Empirical formula	$C_{10}H_{10}Er_{0.33}O_3S$	$C_{10}H_{10}Ho_{0.33}O_3S$
Formula weight (g/mol)	**265.99**	**265.22**
Temperature (K)	**100(2)**	**100(2)**
Crystal system	**Trigonal**	**Trigonal**
Space group	***R*-3**	***R*-3**
Unit cell dimensions		
a (Å)	**15.1961(18)**	**15.229(2)**
b (Å)	**15.1961(18)**	**15.229(2)**
c (Å)	**23.961(3)**	**23.906(4)**
α (°)	**90**	**90**
β (°)	**90**	**90**
γ (°)	**120**	**120**
Volume (Å^3)	**4791.8(13)**	**4801.3(16)**
Z	**18**	**18**
Calculated density (g/cm^3)	**1.659**	**1.651**
Goodness-of-fit on F^2	**1.098**	**1.097**
Final R indices [I > 2σ(I)]	R_1 = 0.0439, $_wR_2$ = 0.1186	R1 = 0.0574, wR2 = 0.1321



(a) (b) (c)

Figure S1: (a) Building unit, (b) packing, (c) topological representation of **1-8.**



(a) (b) (c)

Figure S2: (a) Building unit, (b) packing, (c) topological representation of **9-14.**

(a) (b) (c)

Figure S3: (a) Building unit, (b) packing, (c) topological representation of **15-28.**

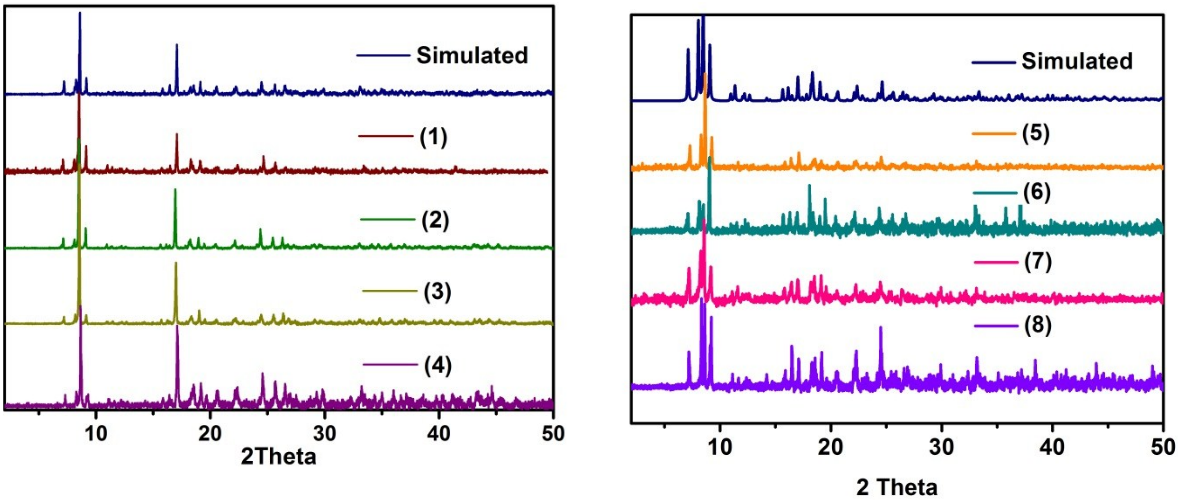


Figure S4: Powder XRD diffractograms of **1-8.** A representative simulated pattern from crystal data of **4**[1] (previous reported) was used to match the PXRD of the other compounds.

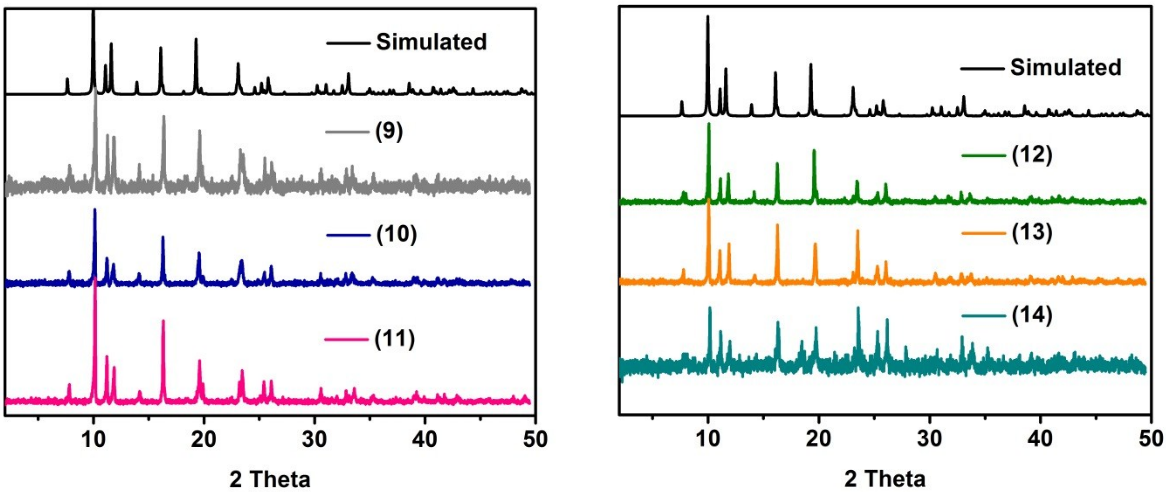


Figure S5: Powder XRD diffractograms of **9-14**. A representative simulated pattern from crystal data of **10** was used to match the PXRD of the other compounds.

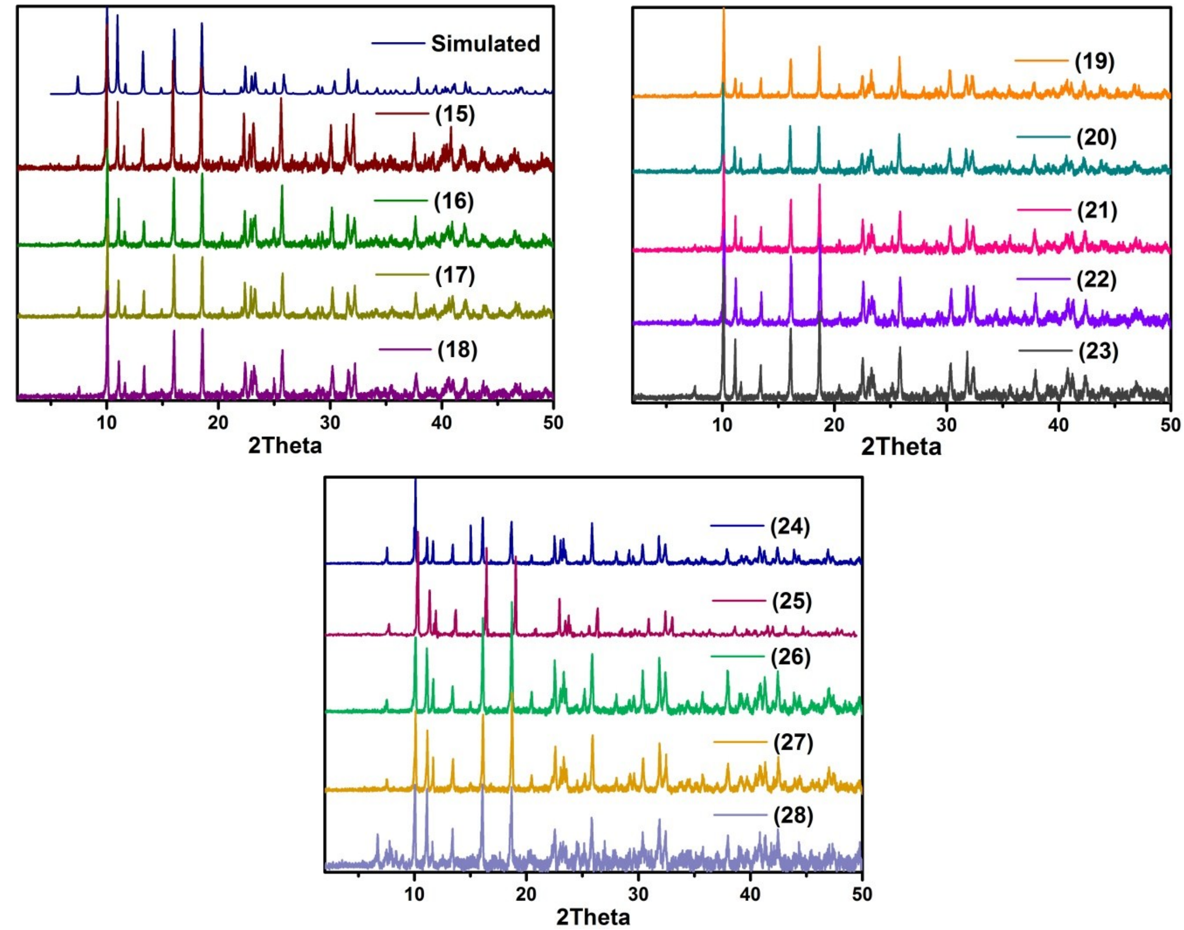
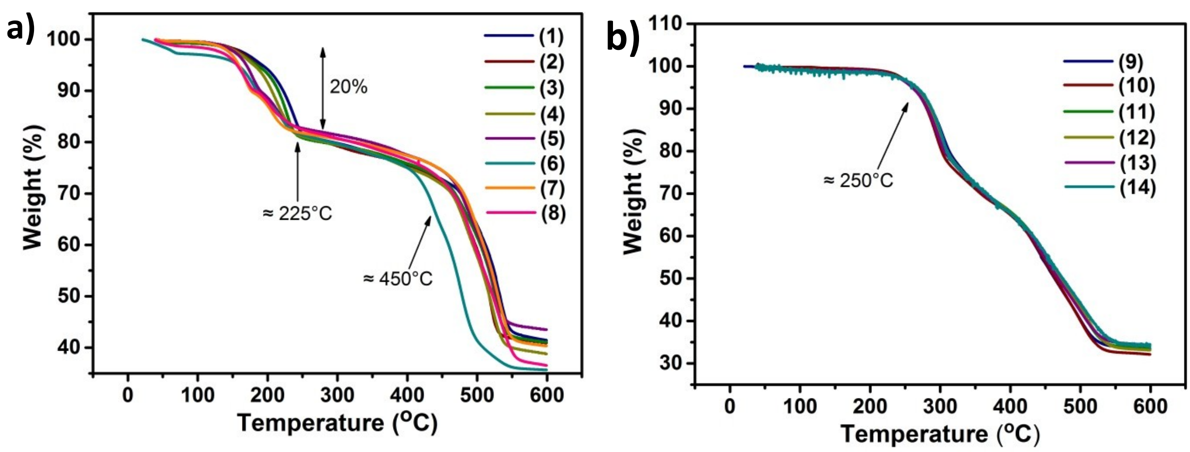


Figure S6: Powder XRD diffractograms of **15-28**. A representative simulated pattern from crystal data of **18**[1] (previous reported) was used to match the PXRD of the other compounds.



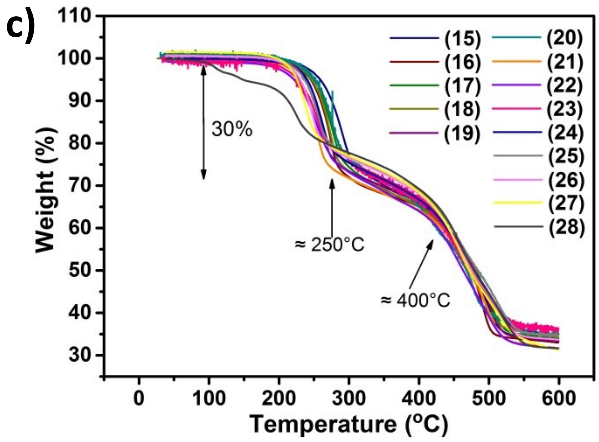
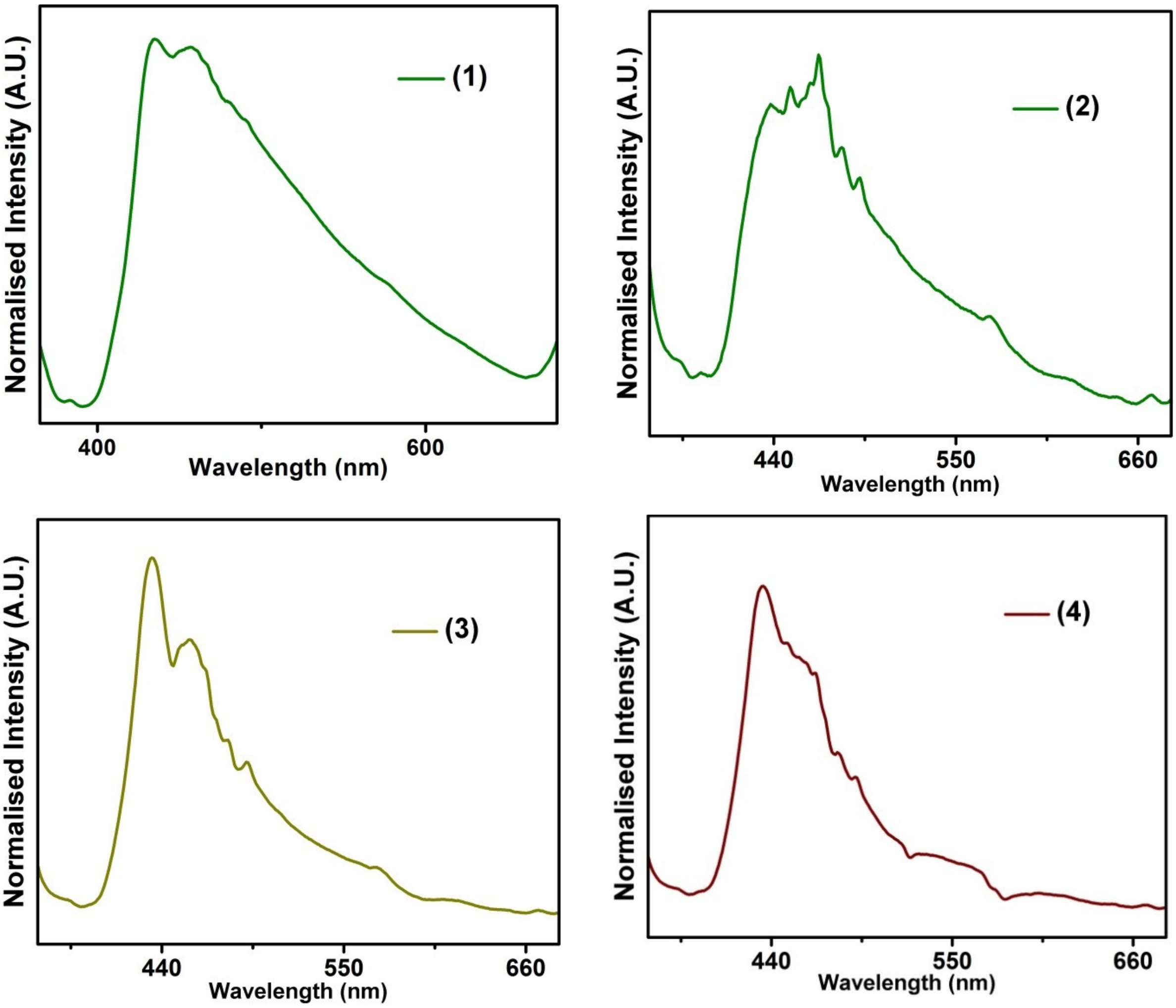
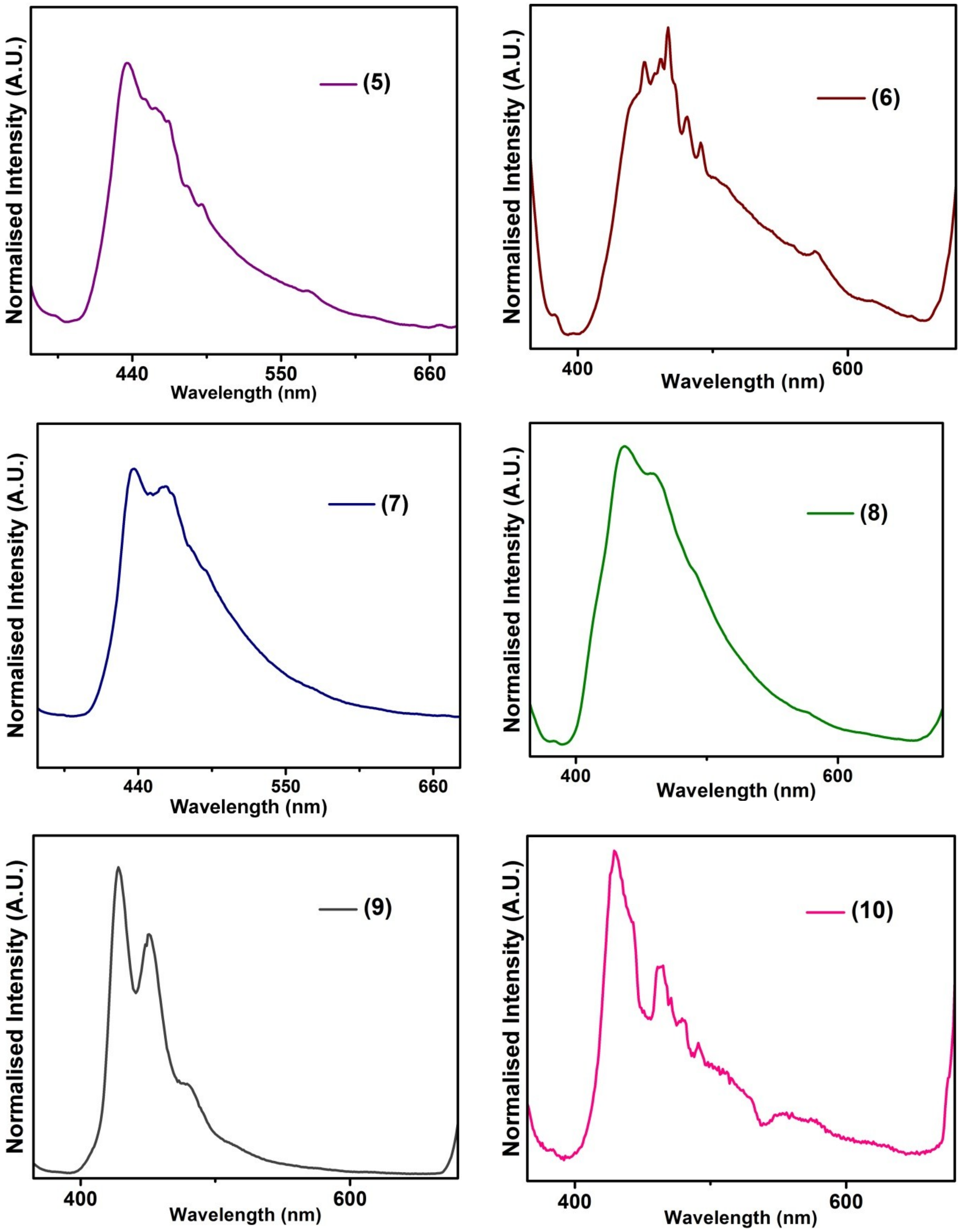


Figure S7: TGA overlay of compounds a) **1-8**, b) **9-14**, c) **15-28**.

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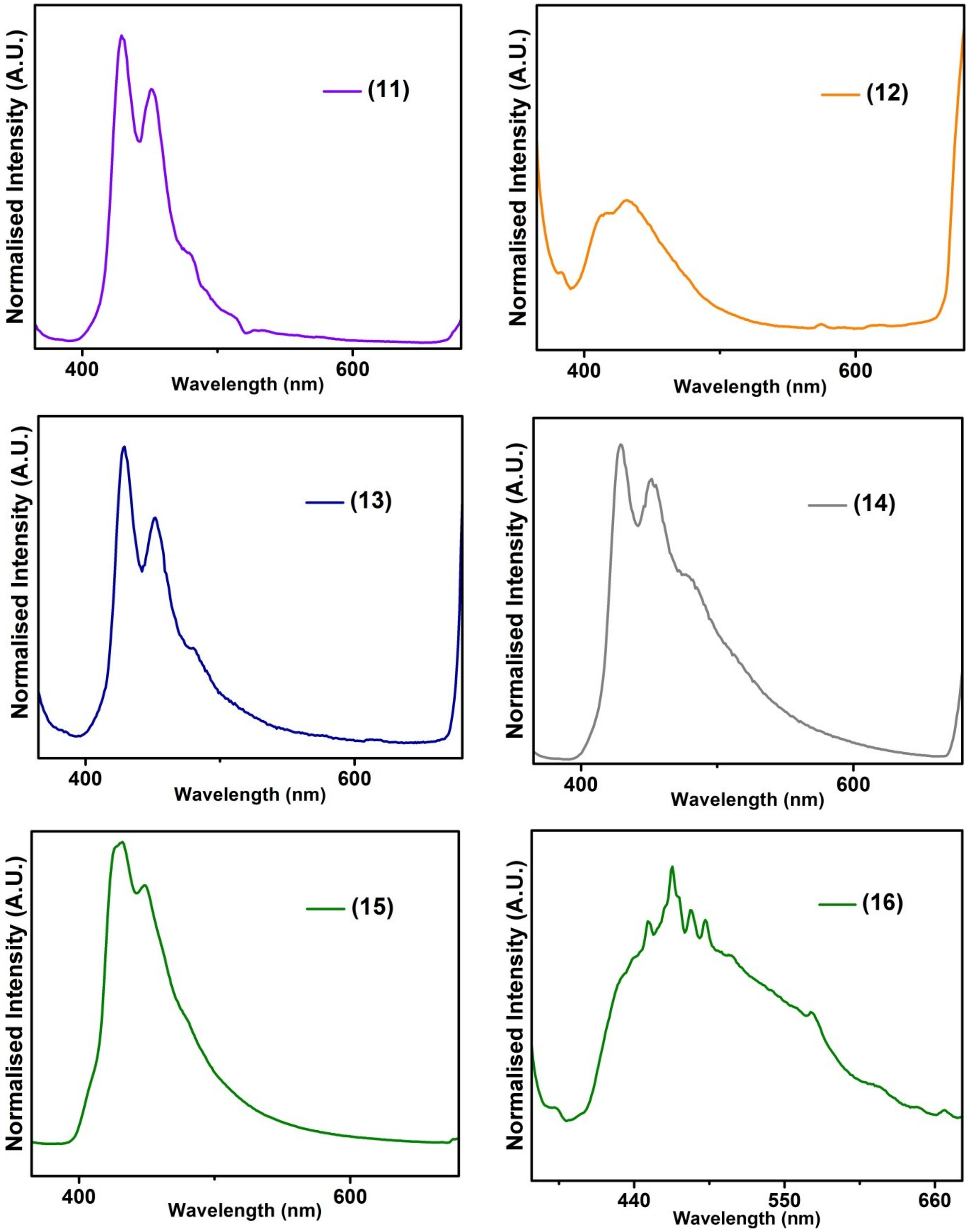
(5)
440
550
660
Wavelength (nm)
Normalised Intensity (A.U.)
(6)
400
600
Wavelength (nm)
Normalised Intensity (A.U.)
(7)
440
550
660
Wavelength (nm)
Normalised Intensity (A.U.)
(8)
400
600
Wavelength (nm)
Normalised Intensity (A.U.)
(9)
400
600
Wavelength (nm)
Normalised Intensity (A.U.)
(10)
400
600
Wavelength (nm)


(11)
Normalised Intensity (A.U.)
Wavelength (nm)
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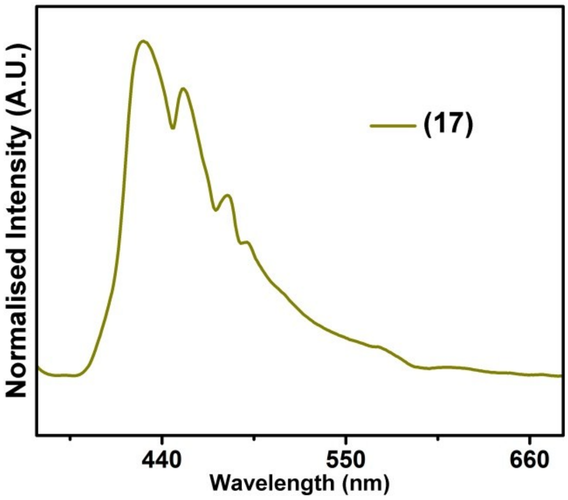
600
(12)
Normalised Intensity (A.U.)
Wavelength (nm)
400
600
(13)
Normalised Intensity (A.U.)
Wavelength (nm)
400
600
(14)
Normalised Intensity (A.U.)
Wavelength (nm)
400
600
(15)
Normalised Intensity (A.U.)
Wavelength (nm)
400
600
(16)
Normalised Intensity (A.U.)
Wavelength (nm)
440
550
660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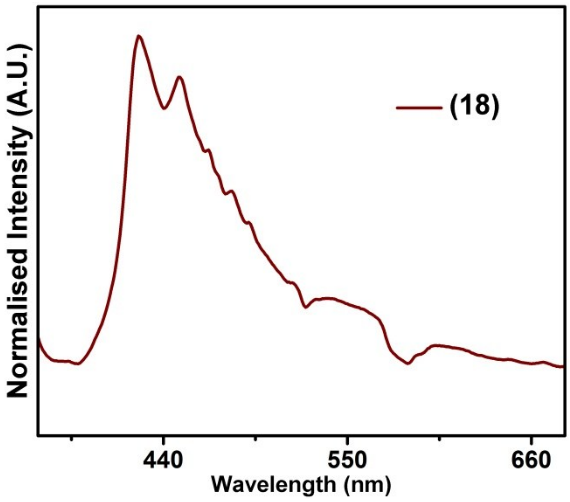
Wavelength (nm)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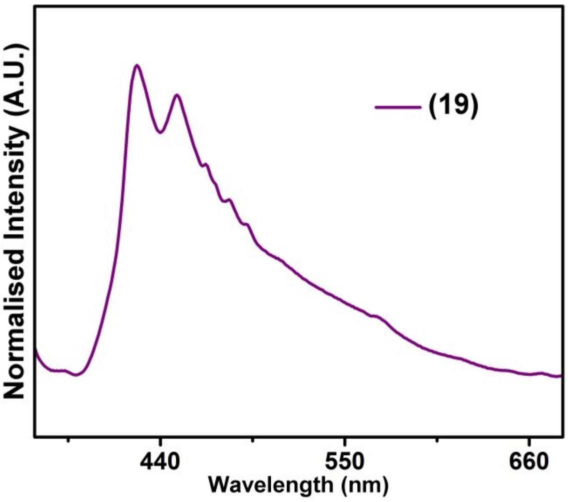
Wavelength (nm)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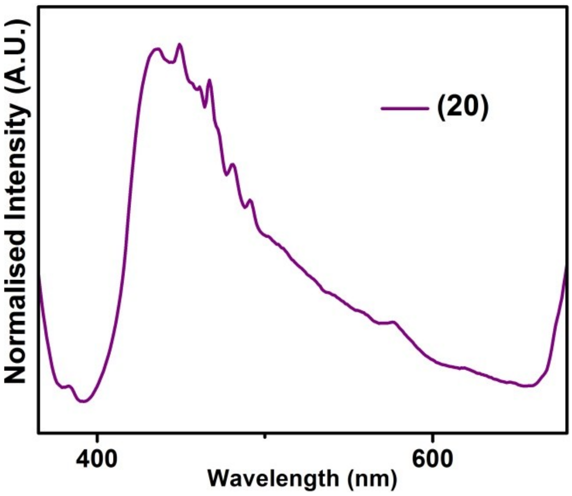
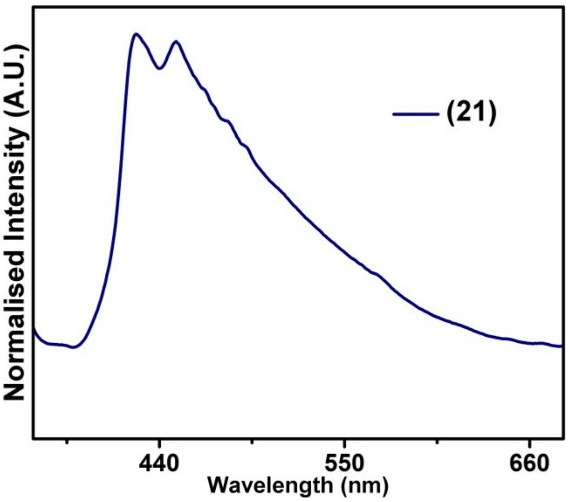
550
660
Wavelength (nm)


Normalised Intensity (A.U.)
(20)
400
600
Wavelength (nm)


Normalised Intensity (A.U.)
(21)
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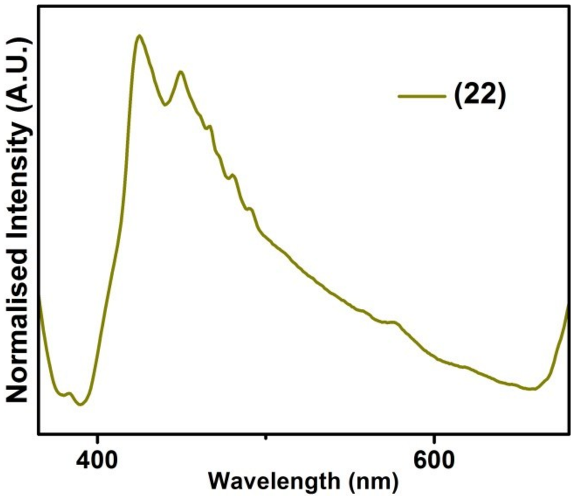
550
660
Wavelength (nm)


Normalised Intensity (A.U.)
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600
Wavelength (nm)

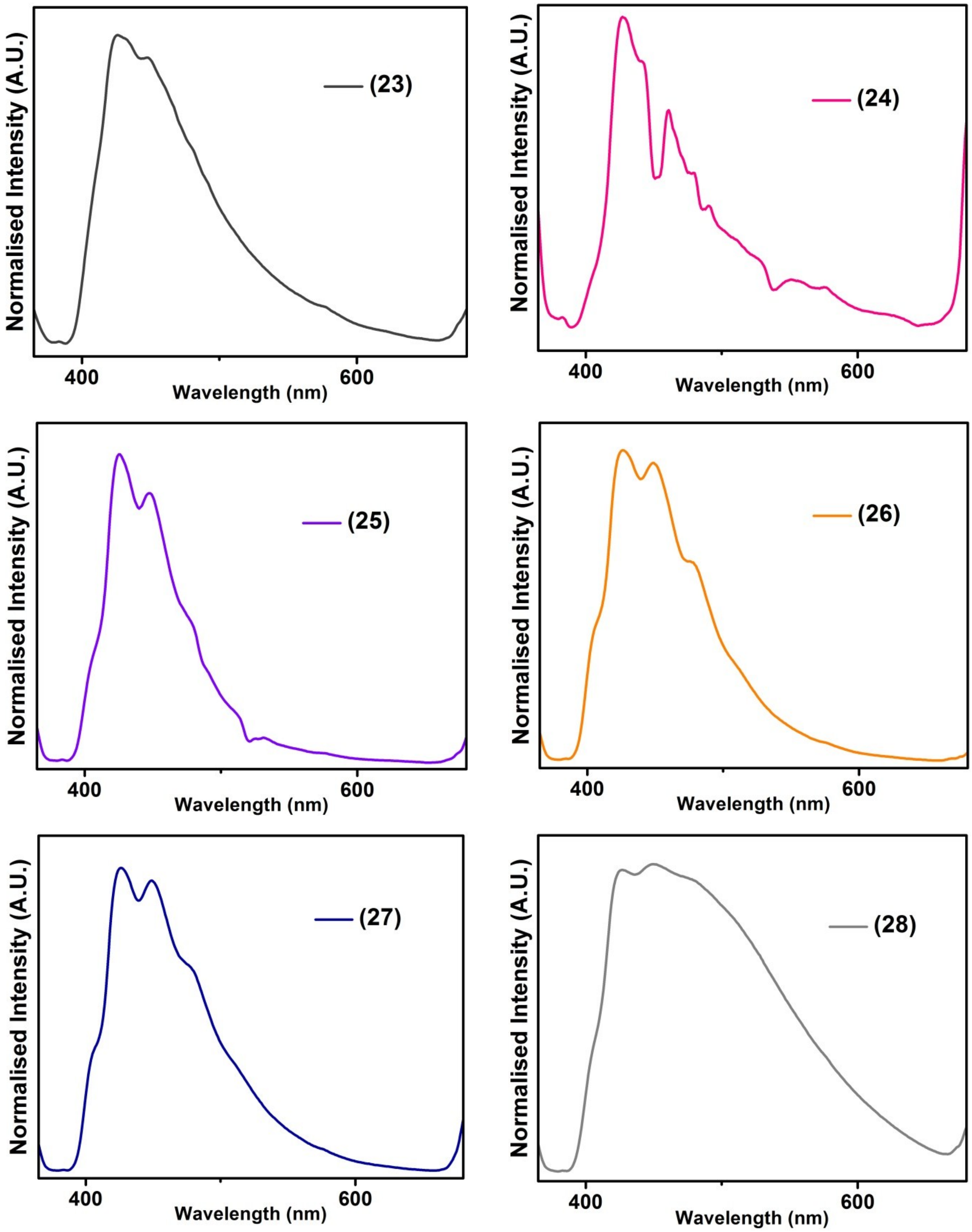
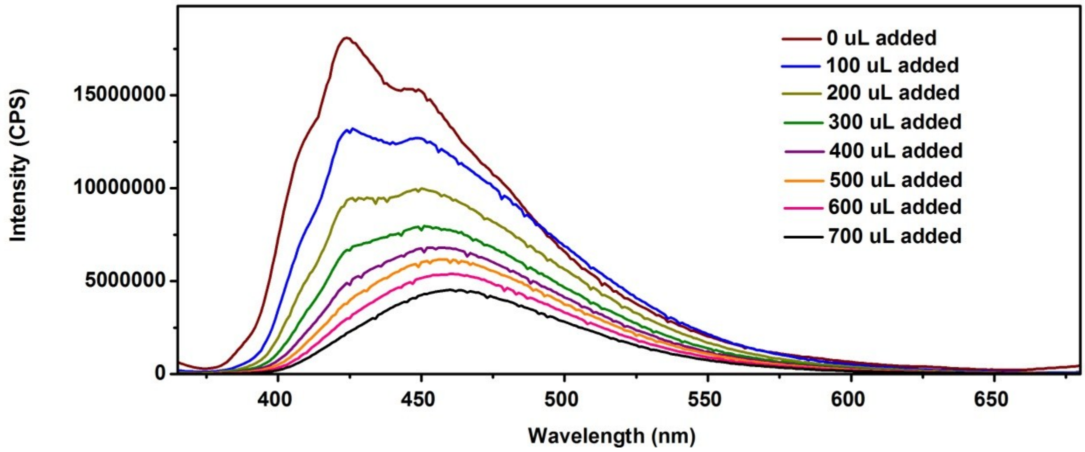
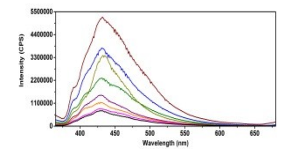
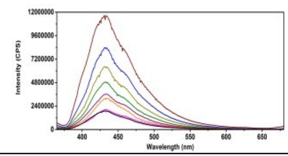
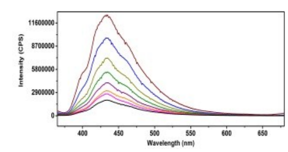
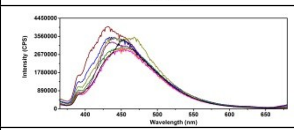
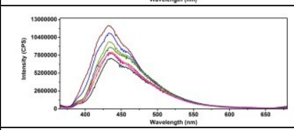
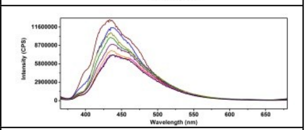
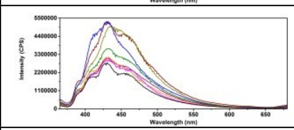
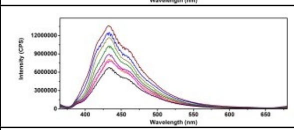
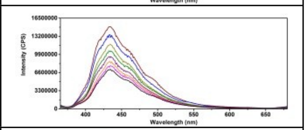
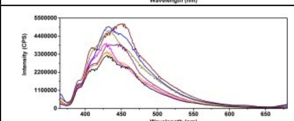
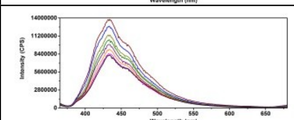
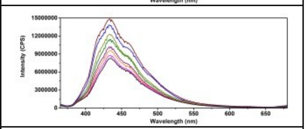
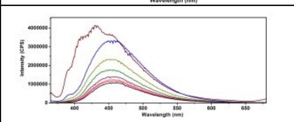
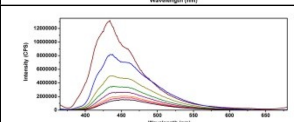
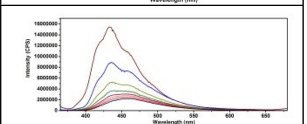
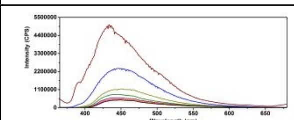
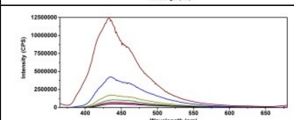
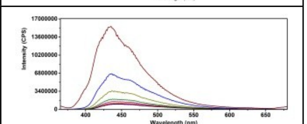
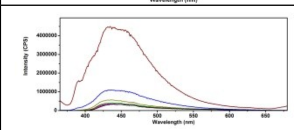
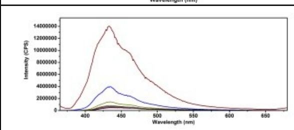
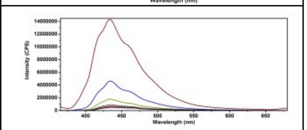
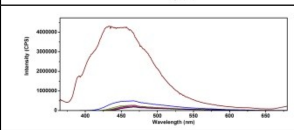
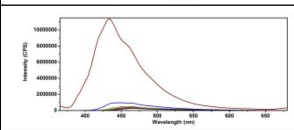
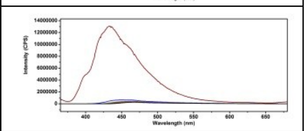


Figure S8: Solid State photoluminescence of **1-28**.

PL quenching experiments



An example of the quenching graph. The same colours representing the amount of analyte added are used for all the quenching curves. The legends are hence not shown for clarity.

Analyte	Eu (6)	Gd (7)	Tb (8)
4-Nitrophenyl phenyl ether			
4 Nitrobenzyl chloride			
1-Chloro-4-nitrobenzene			
1-Iodo-3-nitrobenzene			
2,4 Dinitrophenol			
2,5 Dinitrophenol			
2-nitrophenol			
2,4 Dinitroaniline			

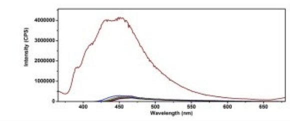
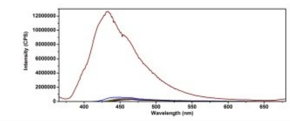
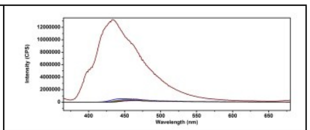
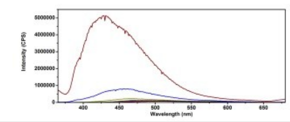
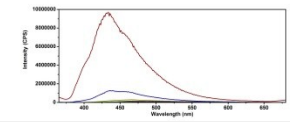
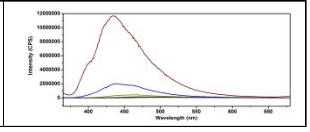
4-Nitroaniline			
2,4-Dinitrophenylhydrazine			

Figure S9: PL quenching of **6-8** with various analytes.

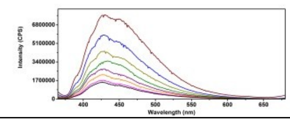
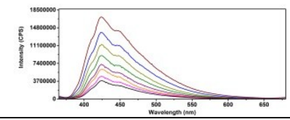
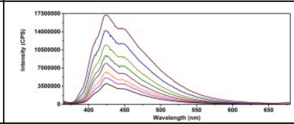
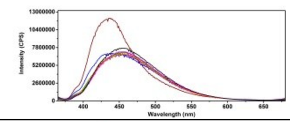
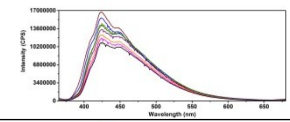
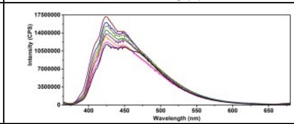
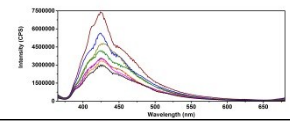
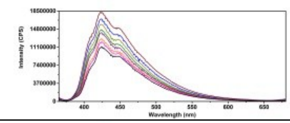
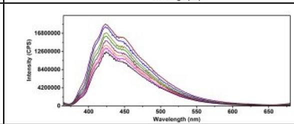
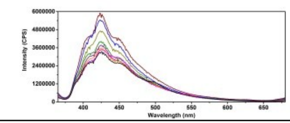
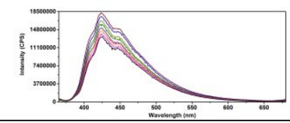
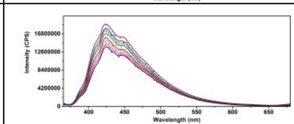
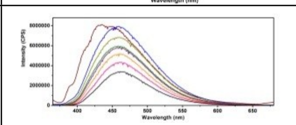
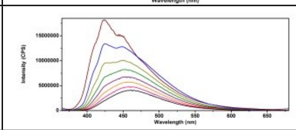
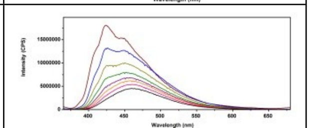
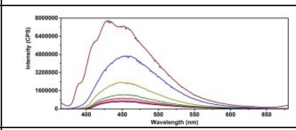
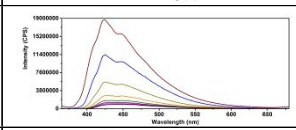
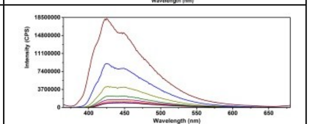
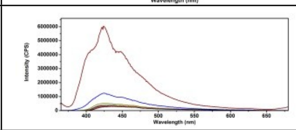
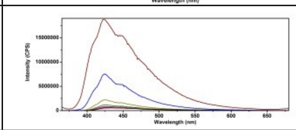
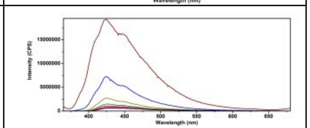
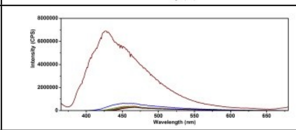
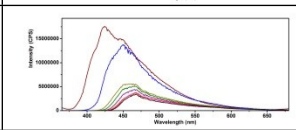
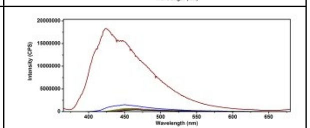
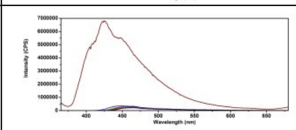
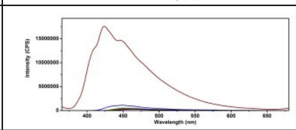
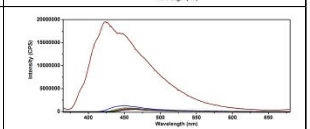
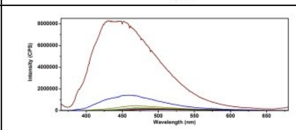
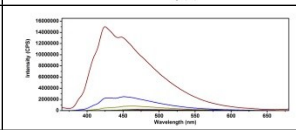
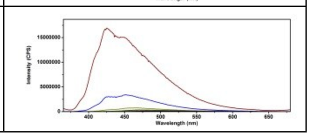
Analyte	Eu (20)	Gd (21)	Tb (22)
4-Nitrophenyl phenyl ether			
4 Nitrobenzyl chloride			
1-Chloro-4-nitrobenzene			
1-Iodo-3-nitrobenzene			
2,4 Dinitrophenol			
2,5 Dinitrophenol			
2-nitrophenol			
2,4 Dinitroaniline			
4-Nitroaniline			
2,4-Dinitrophenylhydrazine			

Figure S10: PL quenching of **20-22** with various analytes.

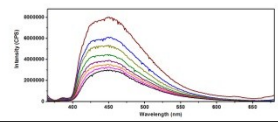
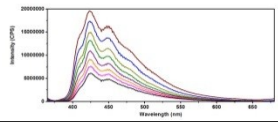
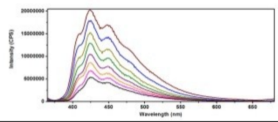
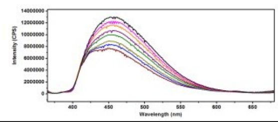
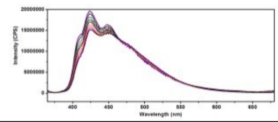
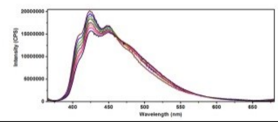
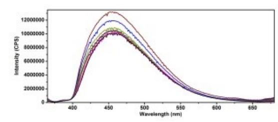
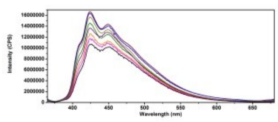
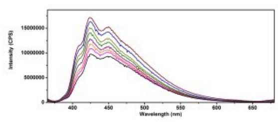
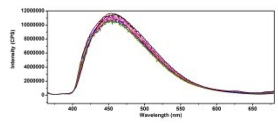
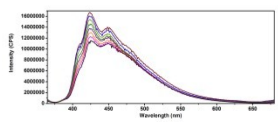
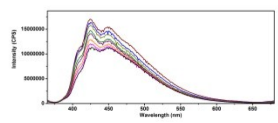
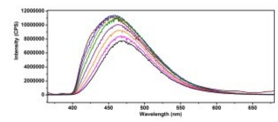
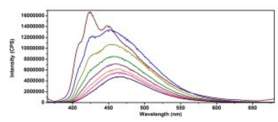
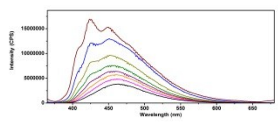
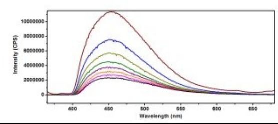
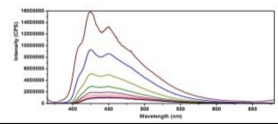
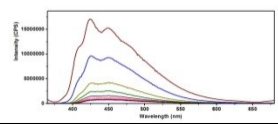
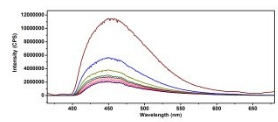
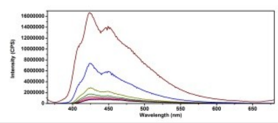
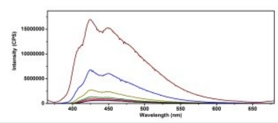
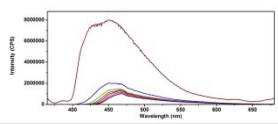
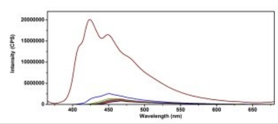
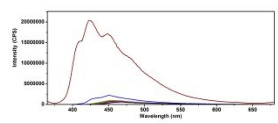
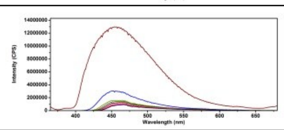
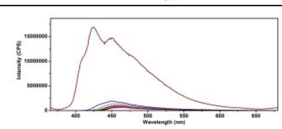
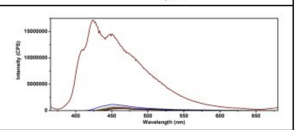
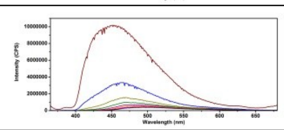
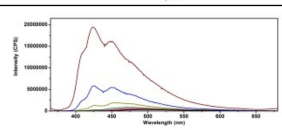
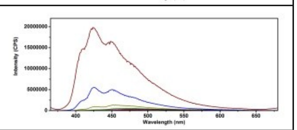
Analyte	Eu exfoliated (6)	Gd exfoliated (7)	Tb exfoliated (8)
4-Nitrophenyl phenyl ether			
4 Nitrobenzyl chloride			
1-Chloro-4-nitrobenzene			
1-Iodo-3-nitrobenzene			
2,4 Dinitrophenol			
2,5 Dinitrophenol			
2-nitrophenol			
2,4 Dinitroaniline			
4-Nitroaniline			
2,4-Dinitrophenylhydrazine			

Figure S11: PL quenching of exfoliated **6-8** with various analytes.

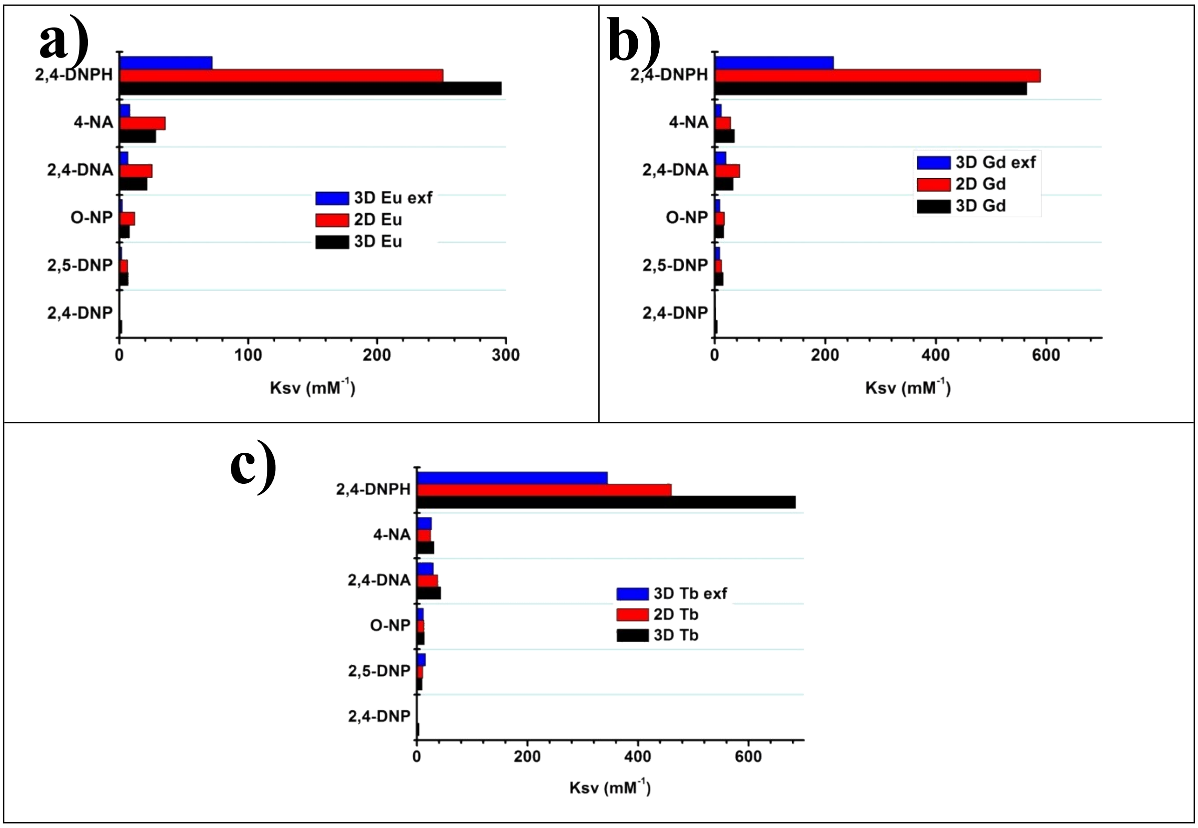
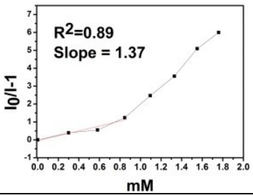
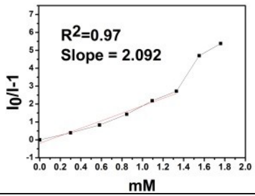
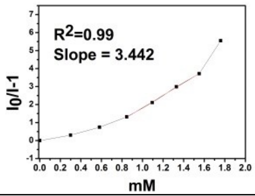
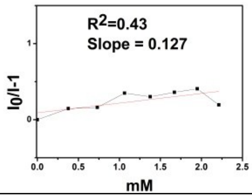
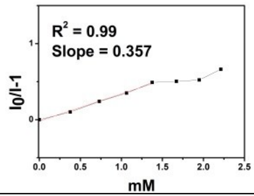
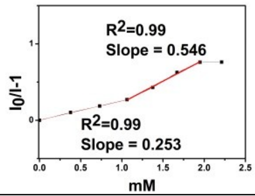
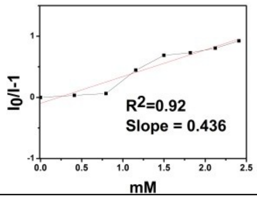
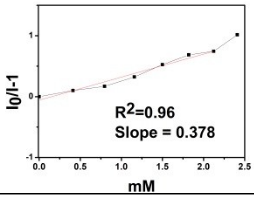
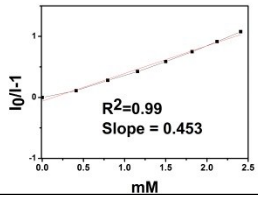
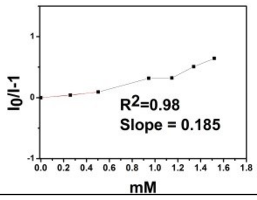
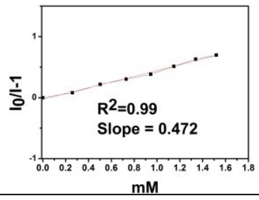
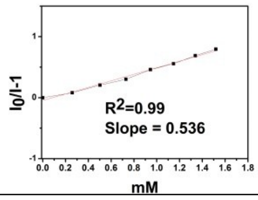
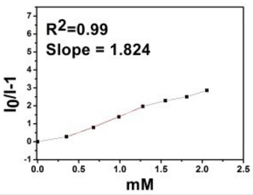
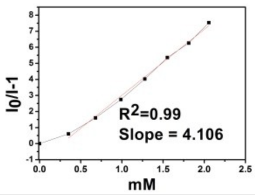
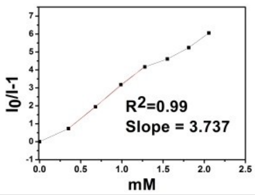
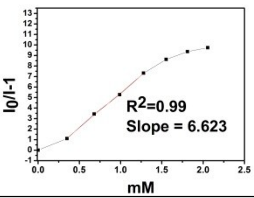
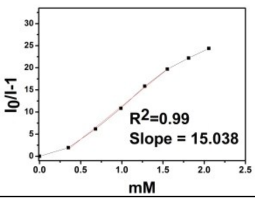
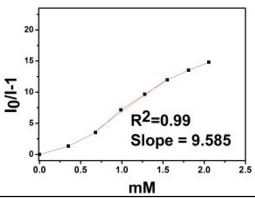
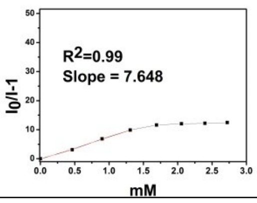
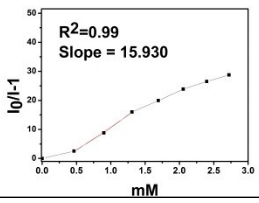
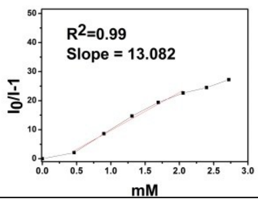


Figure S12: K_{sv} values of the CP when 2,4-dinitrophenylhydrazine, 4-nitroaniline, 2,4-dinitroaniline, 2-nitrophenol, 2,5-dinitrophenol and 2,4-dinitrophenol used for the sensing. (a) K_{sv} values of CP **6**, **20** and exfoliated **6**; (b) K_{sv} values of CP **7**, **21** and exfoliated **7**; (c) K_{sv} values of CP **8**, **22** and exfoliated **8**.

Stern-Volmer plot

Analyte	Eu (6)	Gd (7)	Tb (8)
4-Nitrophenyl phenyl ether			
4 Nitrobenzyl chloride			
1-Chloro-4-nitrobenzene			
1-Iodo-3-nitrobenzene			
2,4 Dinitrophenol			
2,5 Dinitrophenol			
2-nitrophenol			

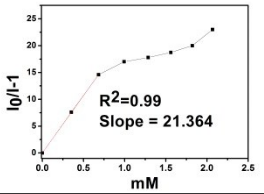
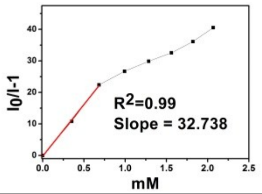
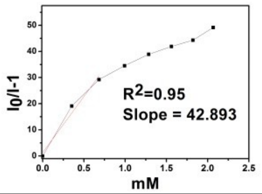
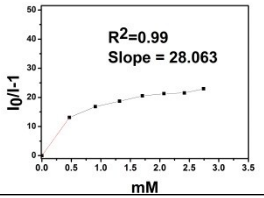
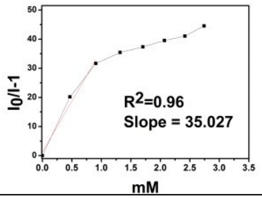
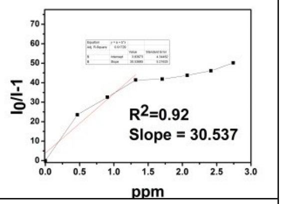
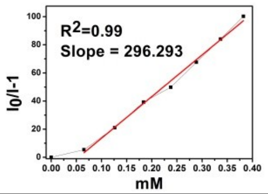
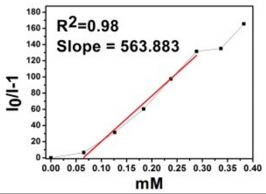
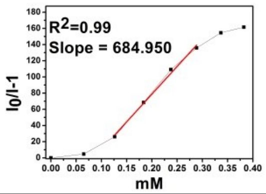
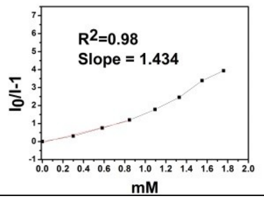
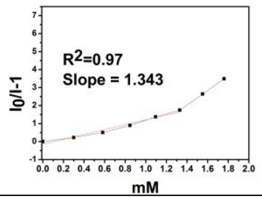
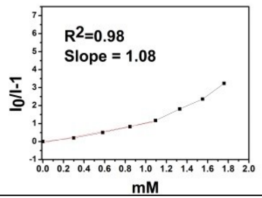
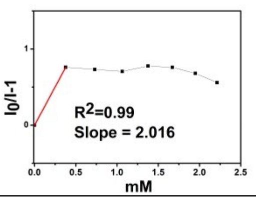
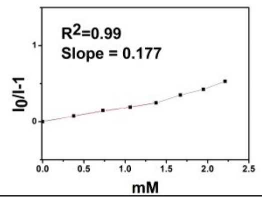
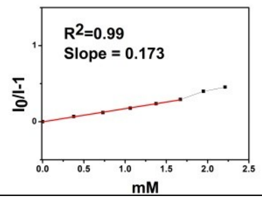
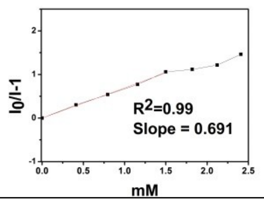
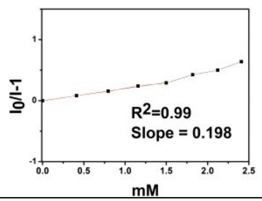
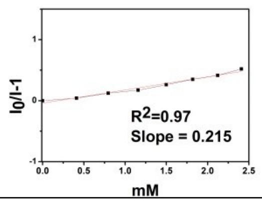
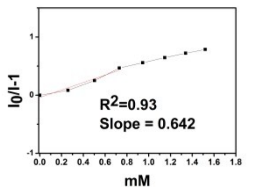
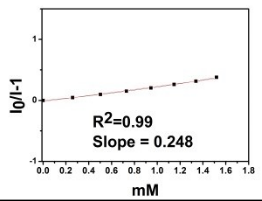
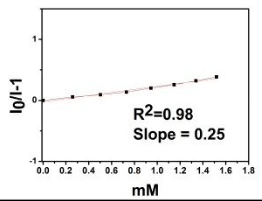
2,4 Dinitroaniline			
4-Nitroaniline			
2,4-Dinitrophenylhydrazine			

Figure S13: Stern-Volmer plot of **6-8** with various analytes.

Analyte	Eu (20)	Gd (21)	Tb (22)
4-Nitrophenyl phenyl ether			
4 Nitrobenzyl chloride			
1-Chloro-4-nitrobenzene			
1-Iodo-3-nitrobenzene			

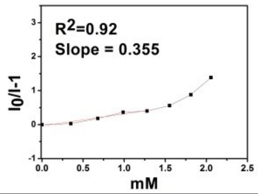
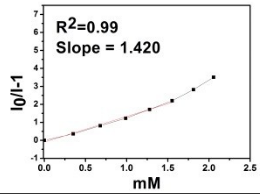
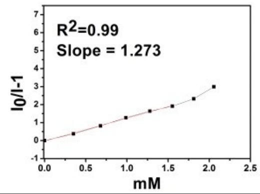
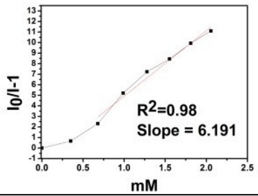
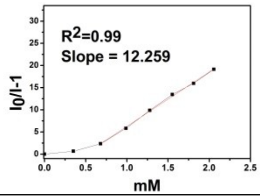
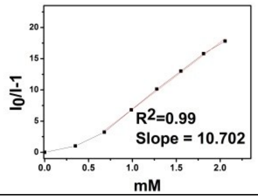
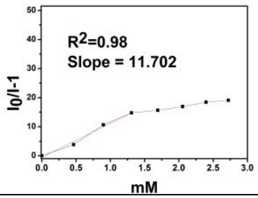
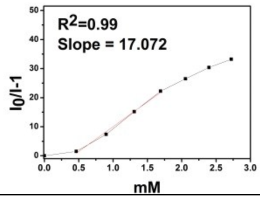
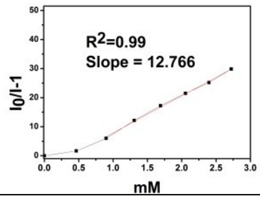
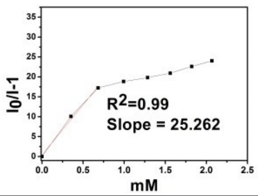
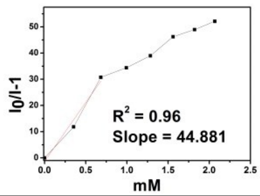
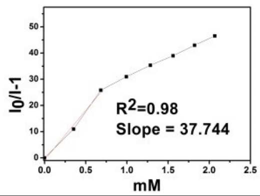
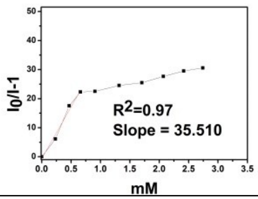
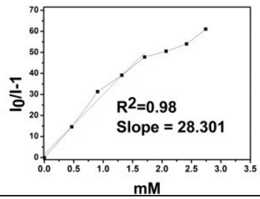
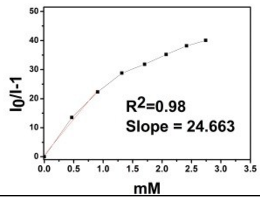
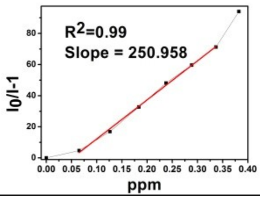
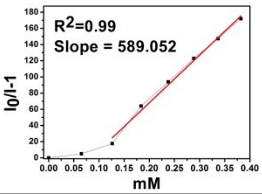
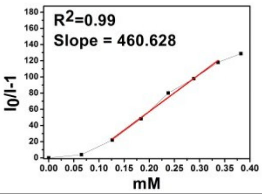
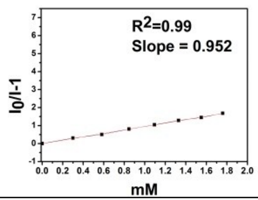
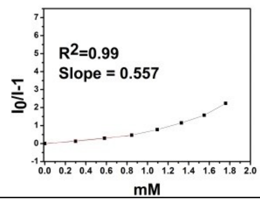
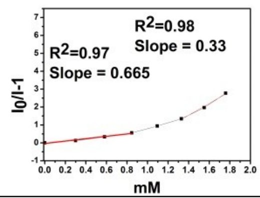
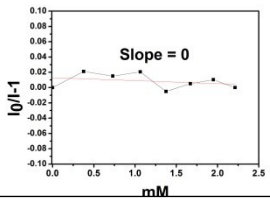
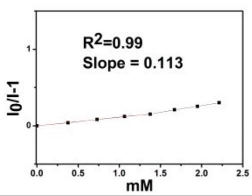
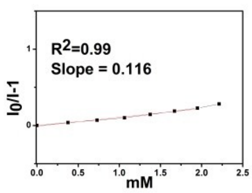
2,4 Dinitrophenol			
2,5 Dinitrophenol			
2-nitrophenol			
2,4 Dinitroaniline			
4-Nitroaniline			
2,4-Dinitrophenylhydrazine			

Figure S14: Stern-Volmer plot of **20-22** with various analytes.

Analyte	Eu exfoliated (6)	Gd exfoliated (7)	Tb exfoliated (8)
4-Nitrophenyl phenyl ether			
4 Nitrobenzyl chloride			

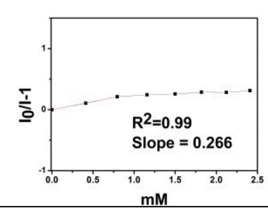
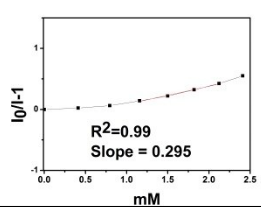
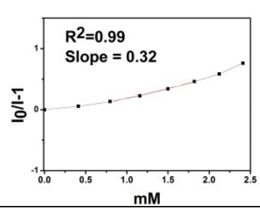
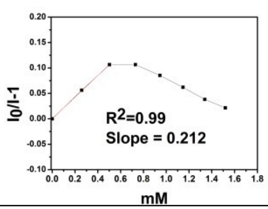
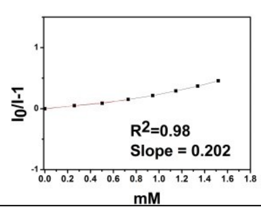
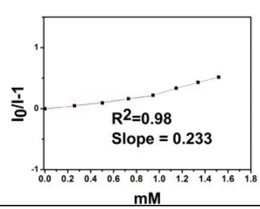
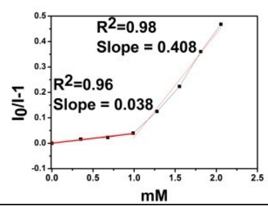
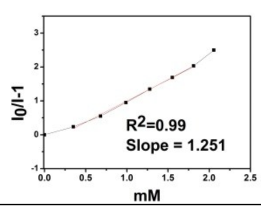
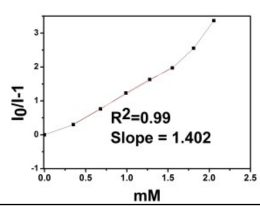
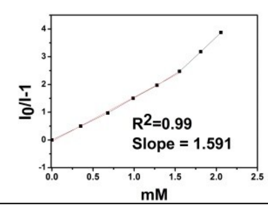
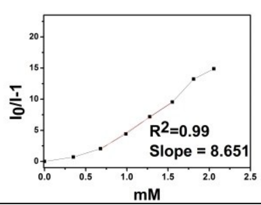
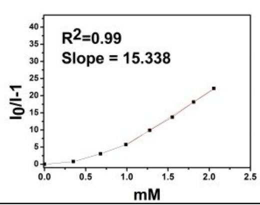
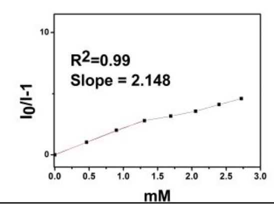
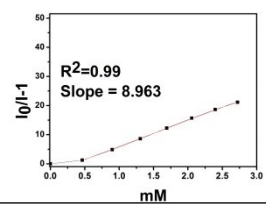
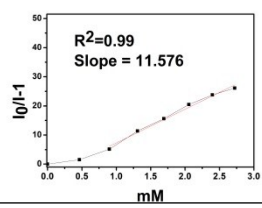
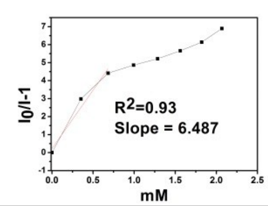
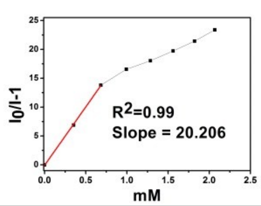
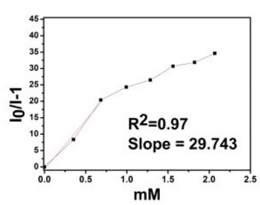
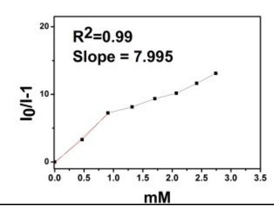
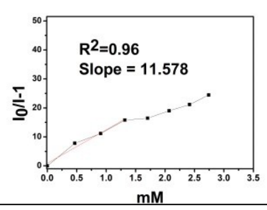
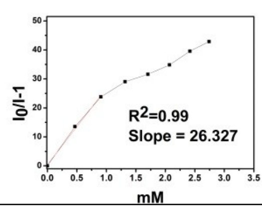
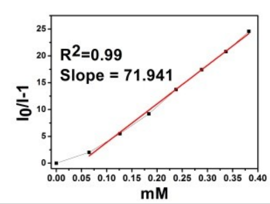
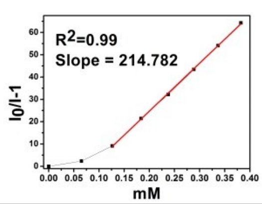
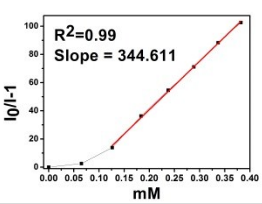
1-Chloro-4-nitrobenzene			
1-Iodo-3-nitrobenzene			
2,4 Dinitrophenol			
2,5 Dinitrophenol			
2-nitrophenol			
2,4 Dinitroaniline			
4-Nitroaniline			
2,4-Dinitrophenylhydrazine			

Figure S15: Stern-Volmer plot of exfoliated **6-8** with various analytes.

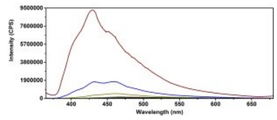
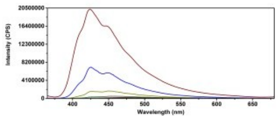
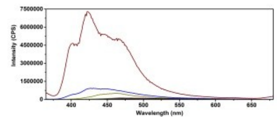
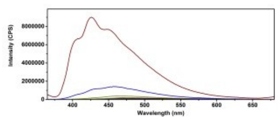
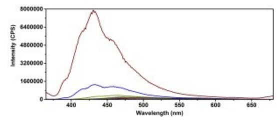
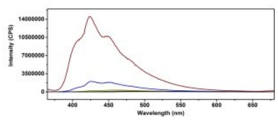
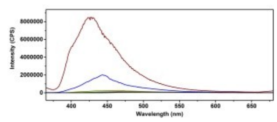
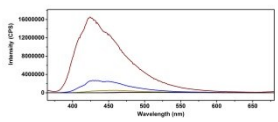
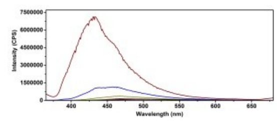
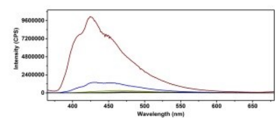
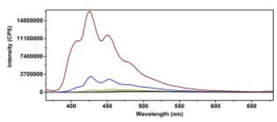
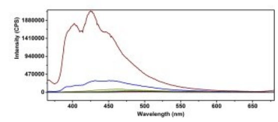
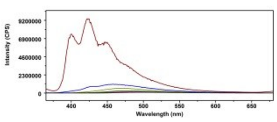
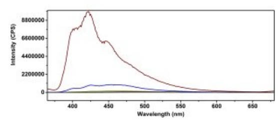
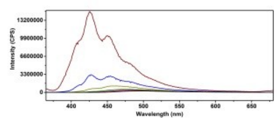
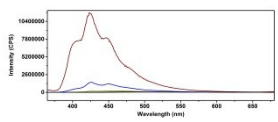
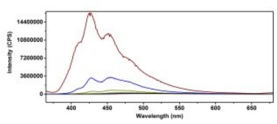
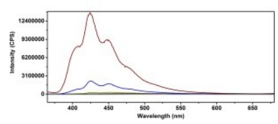
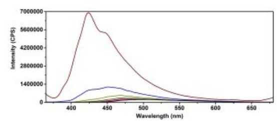
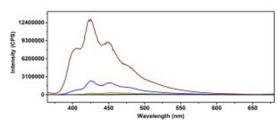
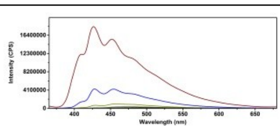
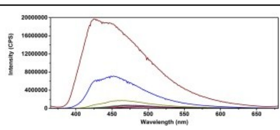
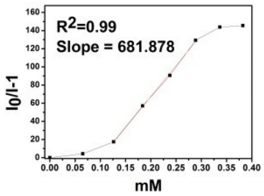
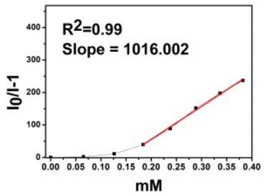
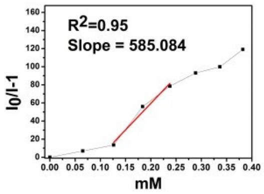
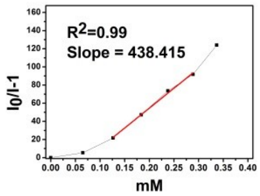
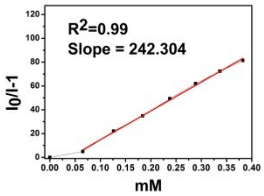
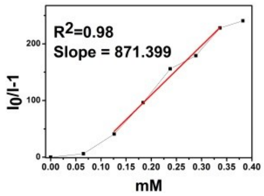
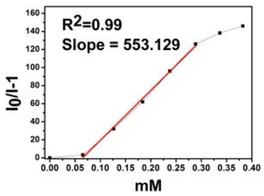
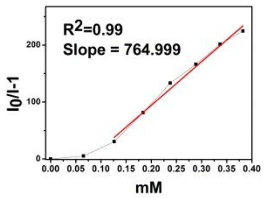
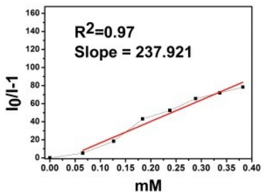
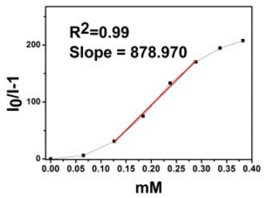
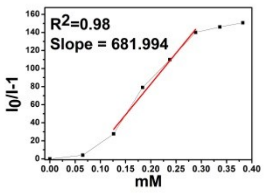
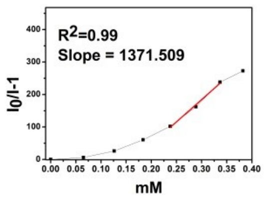
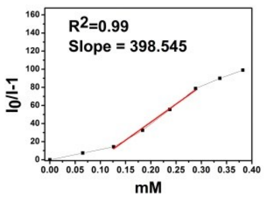
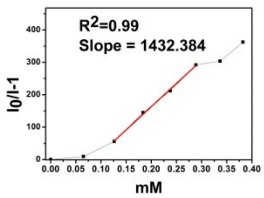
Metal ion	Compound 1-14	Compound 15-28
La		
Ce		
Pr		
Nd		
Sm		
Dy		
Ho		
Er		
Tm		
Yb		
Lu		

Figure S16: PL quenching of **1-28** with various Brady's reagent.

Metal ion	1-14	15-28
La		
Ce		
Pr		
Nd		
Sm		
Dy		
Ho		

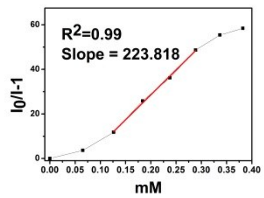
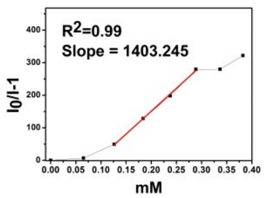
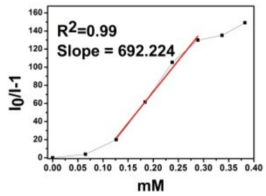
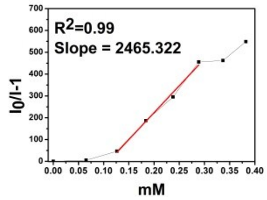
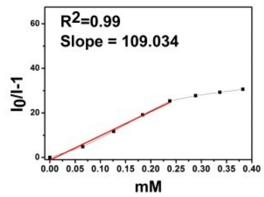
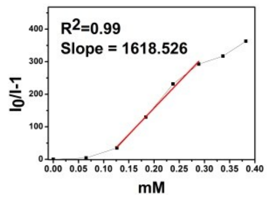
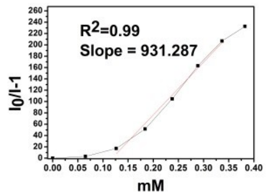
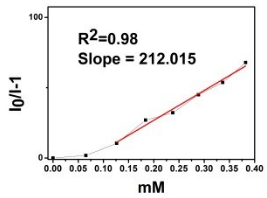
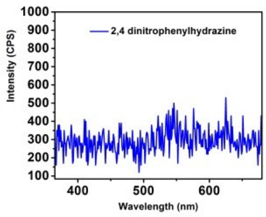
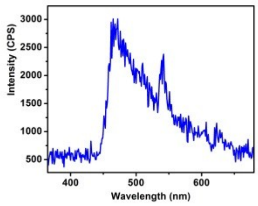
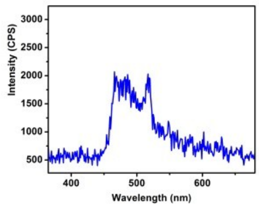
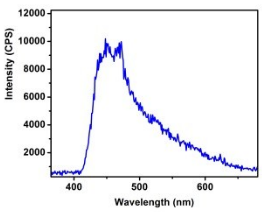
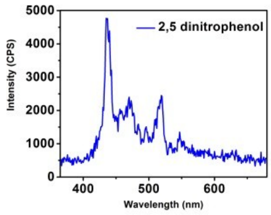
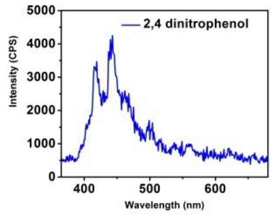
Er		
Tm		
Yb		
Lu		

Figure S17: Stern-Volmer plot of **1-28** with various Brady's reagent.

2,4-Dinitrophenylhydrazine	**4-Nitroaniline**	**2,4-Dinitroaniline**
		
2-nitrophenol	**2,5-Dinitrophenol**	**2,4-Dinitrophenol**
		
1-Iodo-3-nitrobenzene	**1-Chloro-4-nitrobenzene**	**4-Nitrobenzyl chloride**

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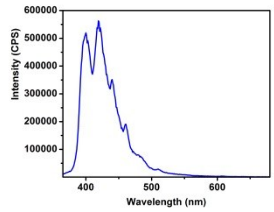
<td>
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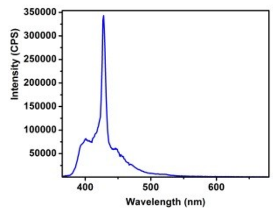
<td>
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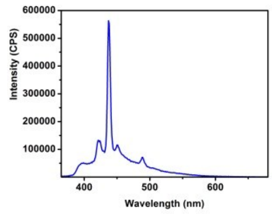
<td>
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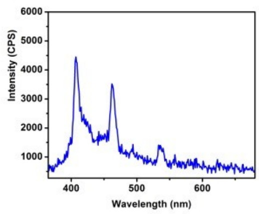
<td>
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Figure S18: PL emission of the analytes.

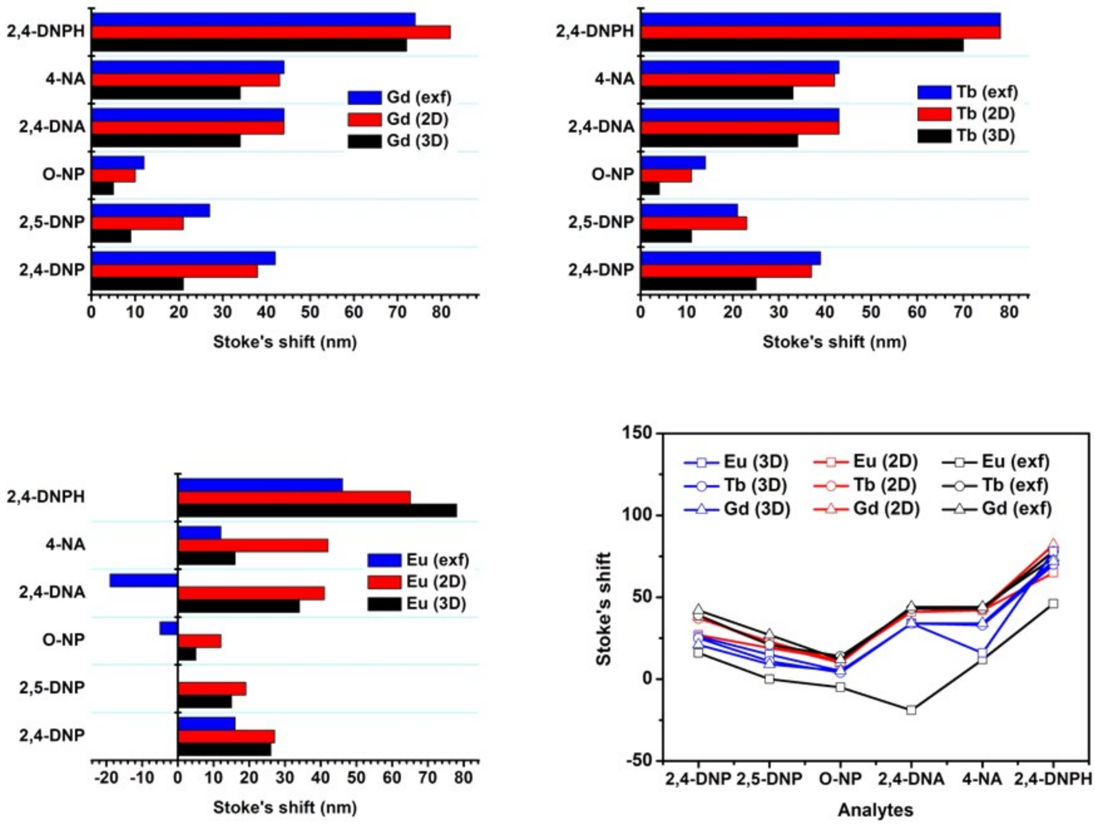

Figure S19: Stoke's shift of the CPs with various analytes added. Values of the CP when 2,4-dinitrophenylhydrazine, 4-nitroaniline, 2,4-dinitroaniline, 2-nitrophenol, 2,5-dinitrophenol and 2,4-dinitrophenol used for the sensing.