

## Highly emissive supramolecular gold(I)-BTD materials

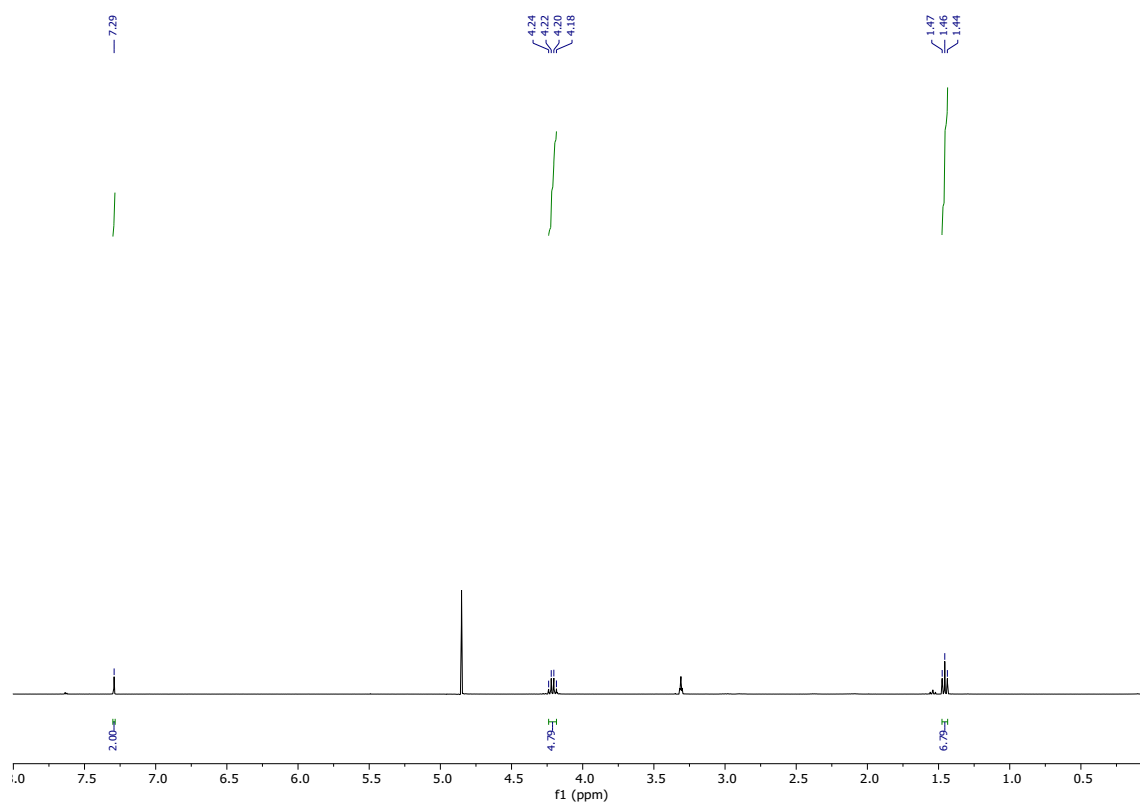
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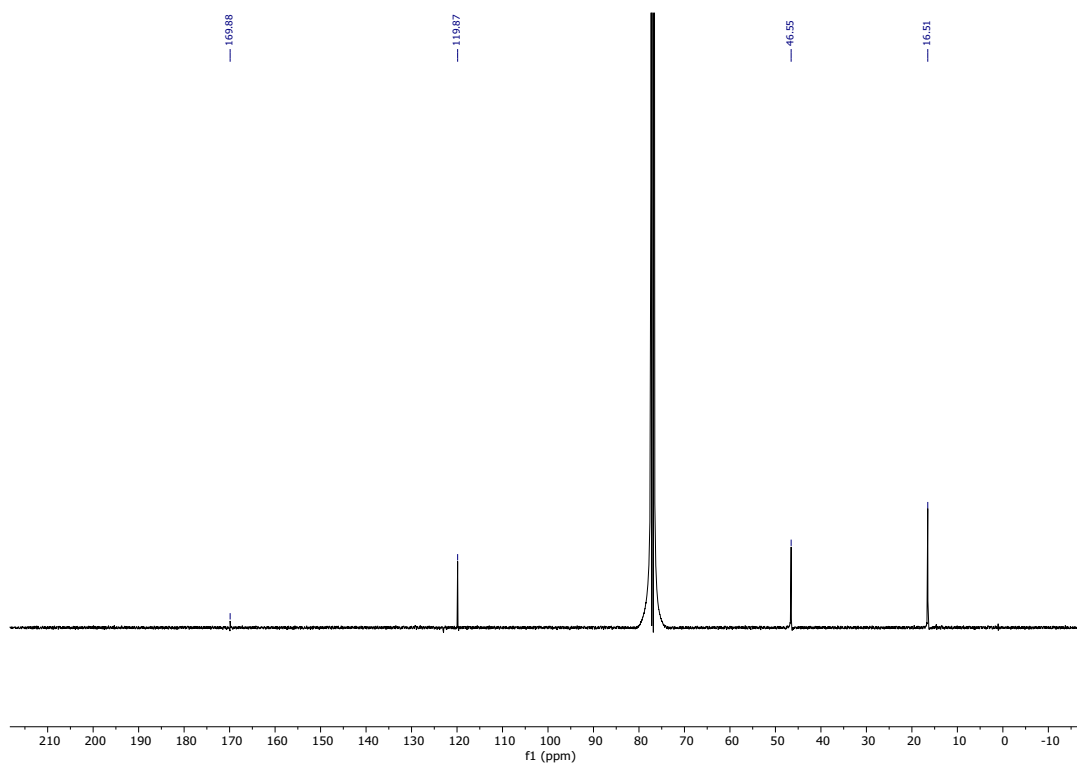
<sup>b</sup> *Institut de Nanociència i Nanotecnologia (IN<sup>2</sup>UB). Universitat de Barcelona, 08028  
Barcelona, Spain*

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Spain*

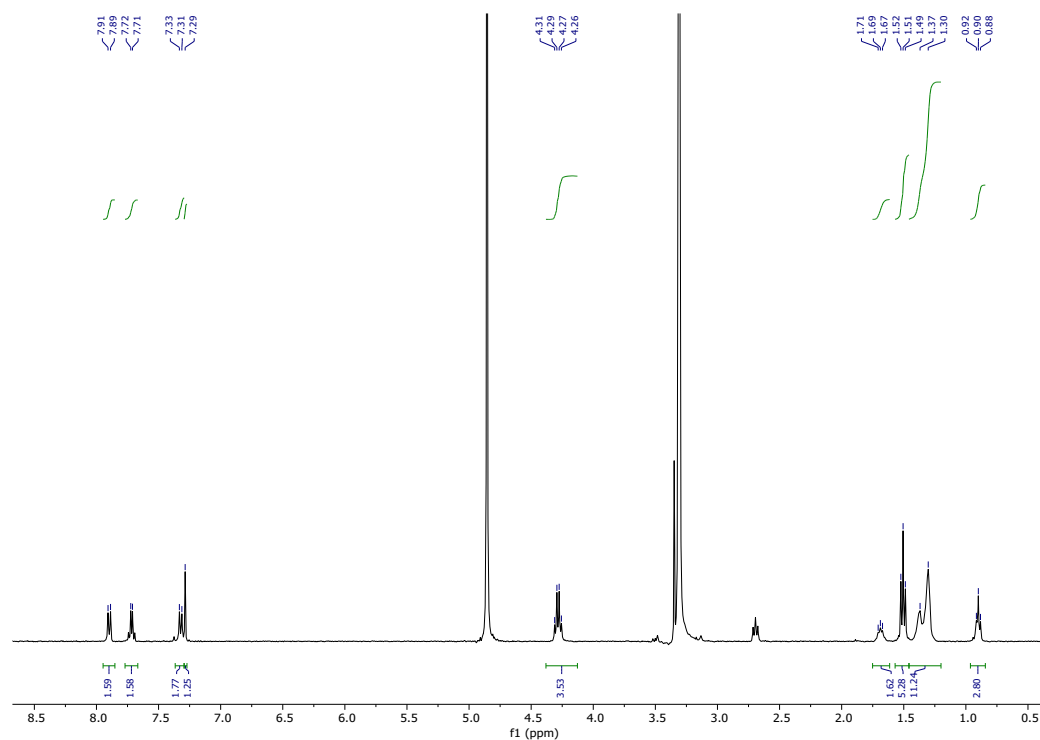
## Supporting information



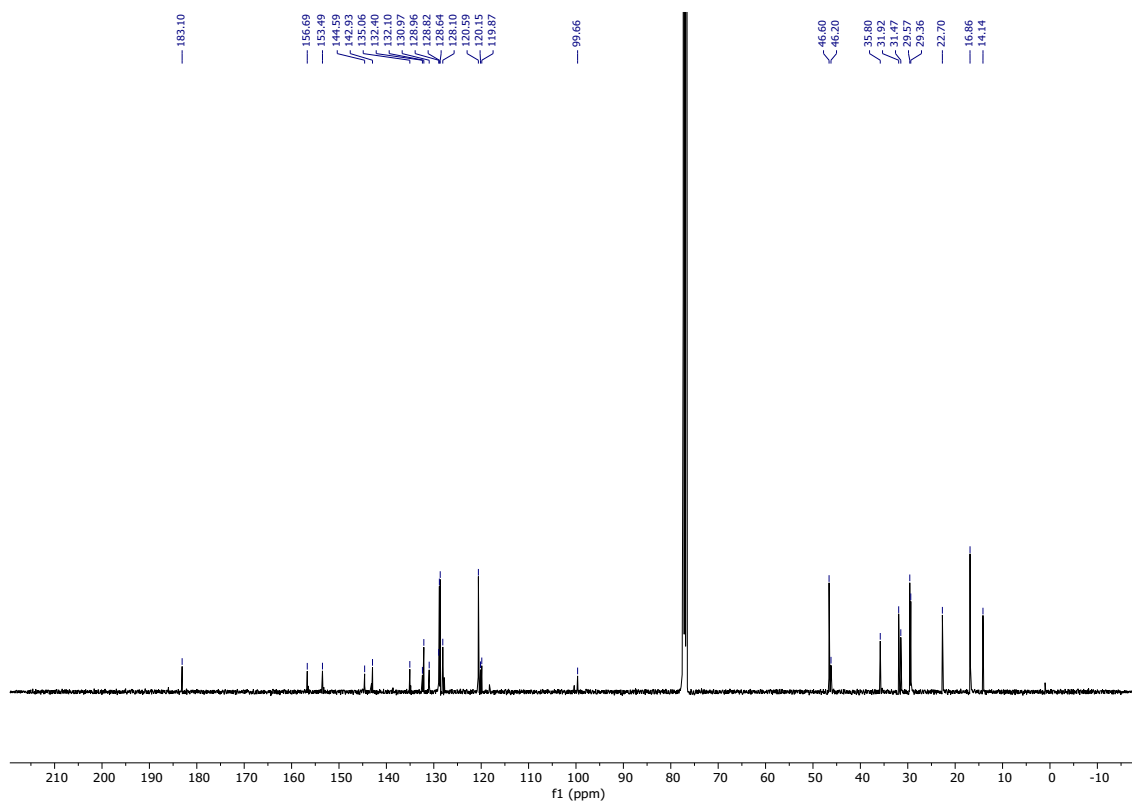
**Figure S1.**  $^1\text{H}$  NMR spectra of  $[\text{AuCl}(\text{Im}1)]$  in  $\text{CD}_3\text{OD}$ .



**Figure S2.**  $^{13}\text{C}$  NMR spectra of  $[\text{AuCl}(\text{Im}1)]$  in  $\text{CDCl}_3$ .



**Figure S3.**  $^1\text{H}$  NMR spectra of **1** in  $\text{CD}_3\text{OD}$ .



**Figure S4.**  $^{13}\text{C}$  NMR spectra of **1** in  $\text{CDCl}_3$ .

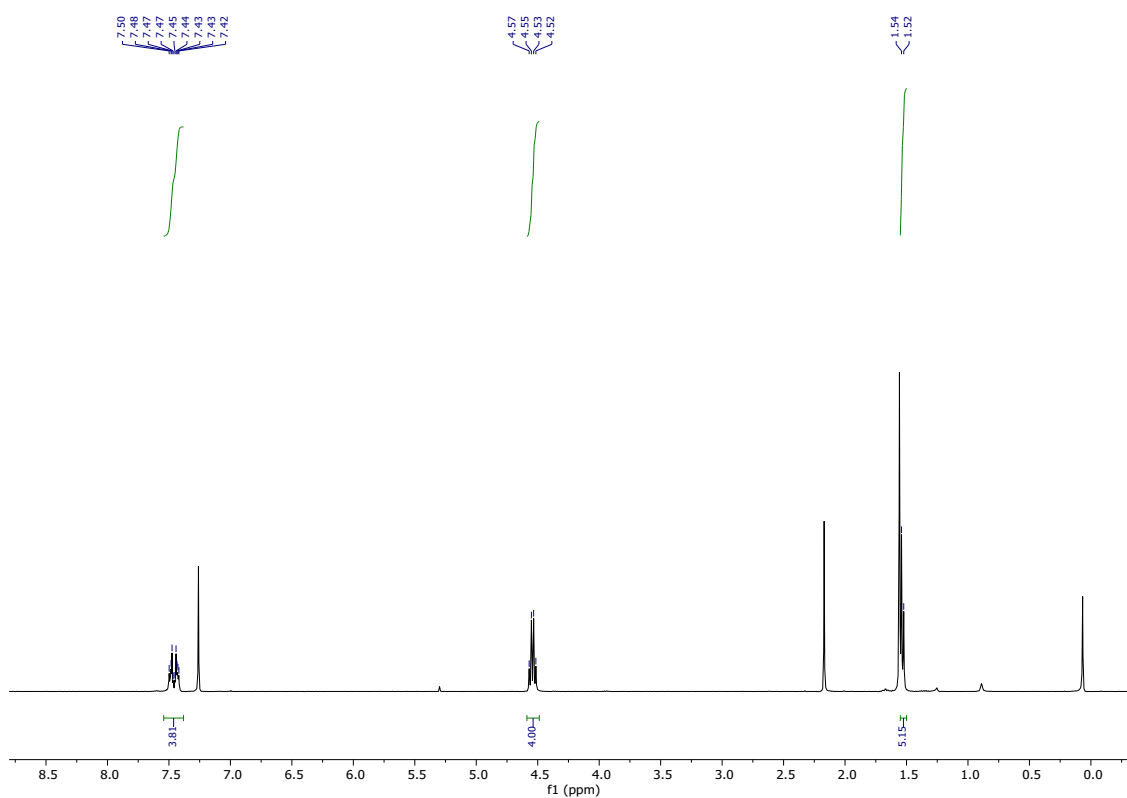


Figure S5.  $^1\text{H-NMR}$  spectra of  $[\text{AuCl}(\text{Im}2)]$  in  $\text{CDCl}_3$ .

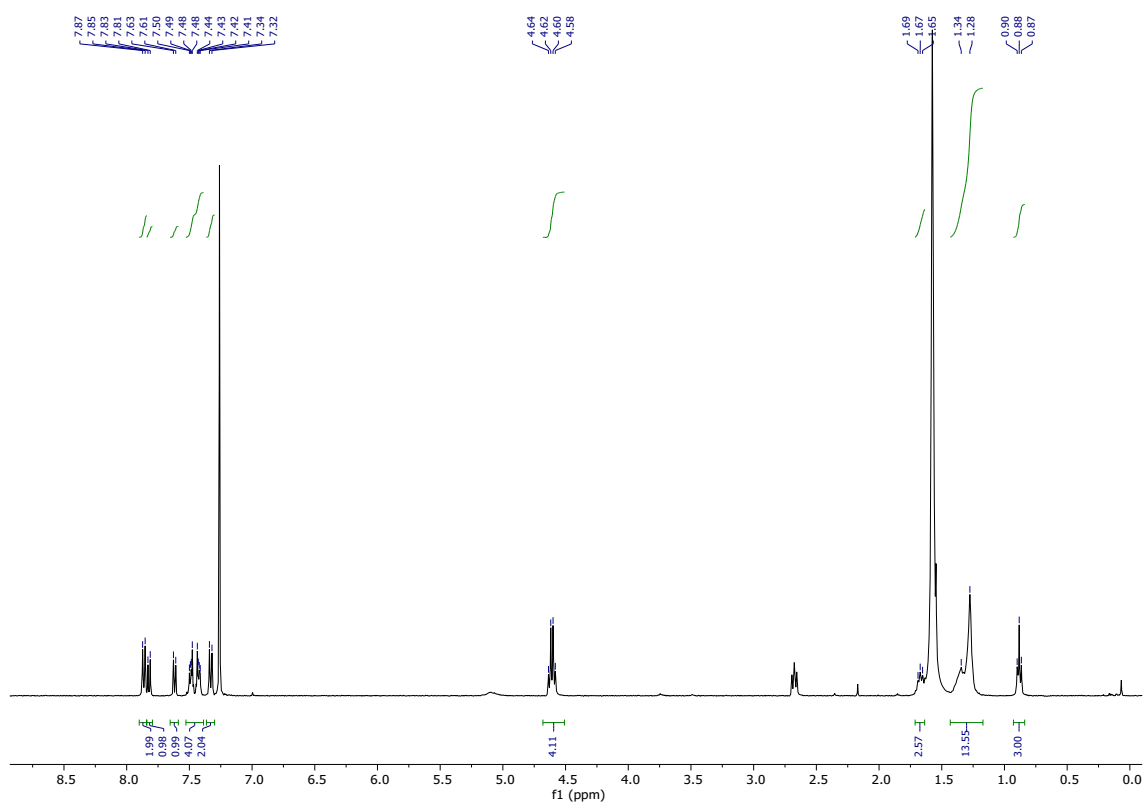


Figure S6.  $^1\text{H-NMR}$  spectra of **2** in  $\text{CDCl}_3$ .

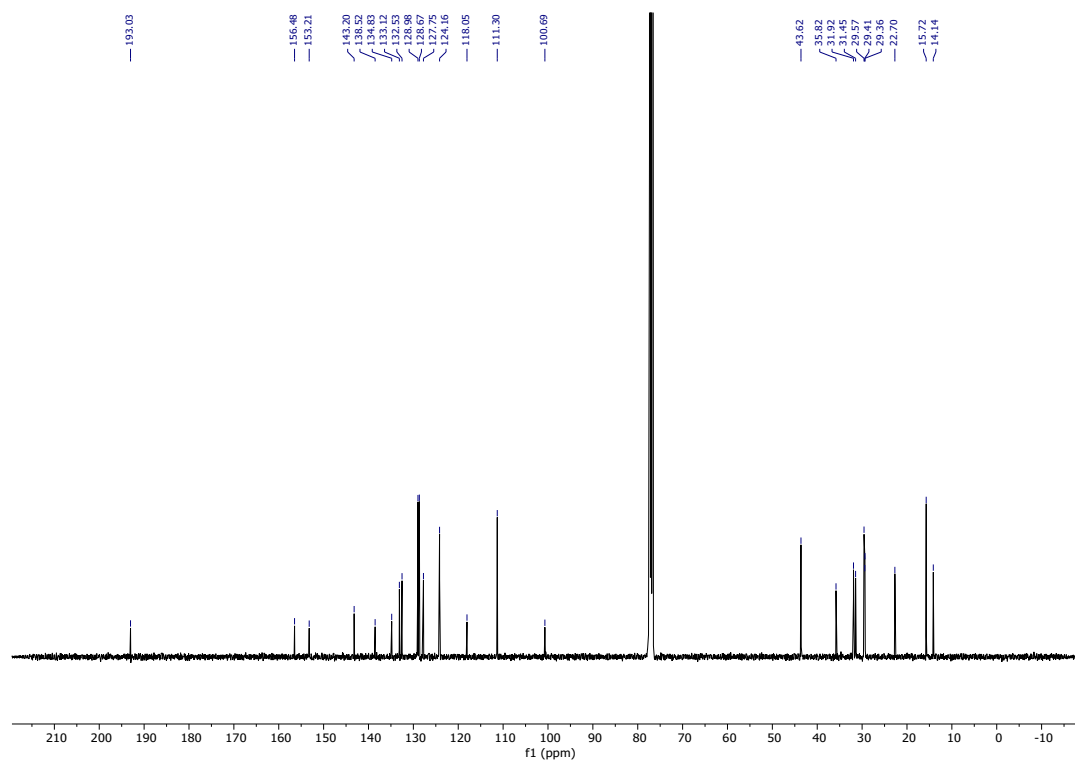


Figure S7.  $^{13}\text{C}$  NMR spectra of **2** in  $\text{CDCl}_3$ .

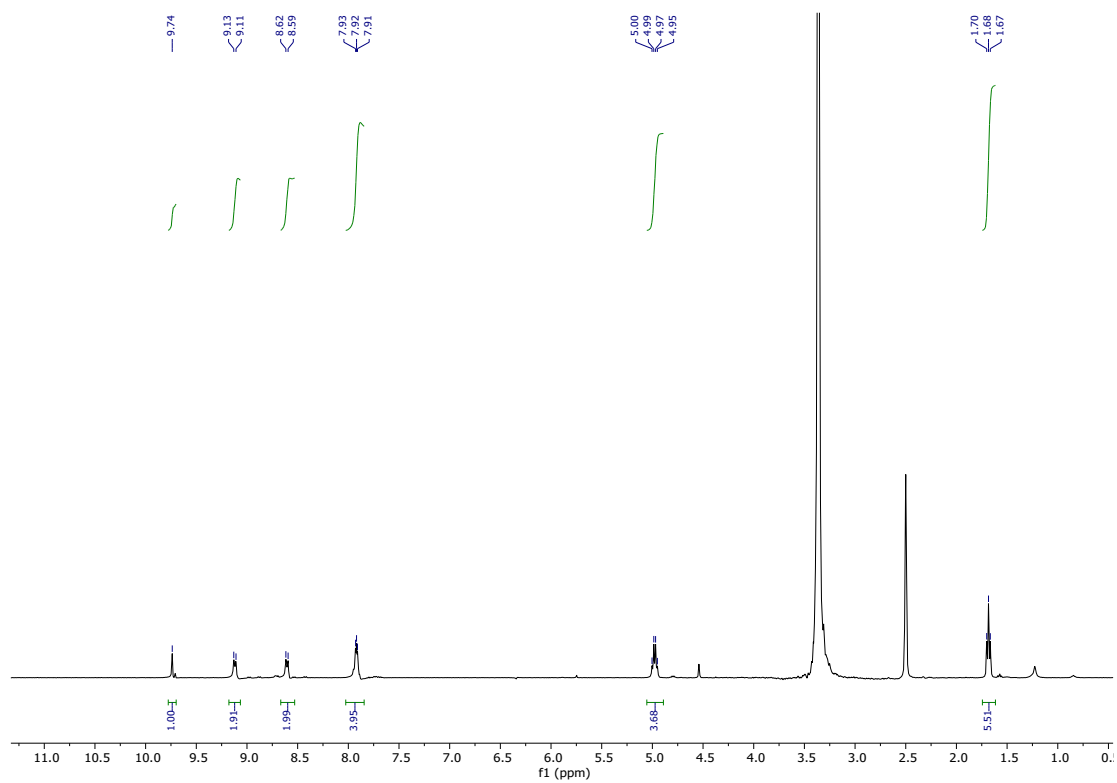


Figure S8.  $^1\text{H}$ -NMR spectra of **Im3** in  $\text{DMSO-d}_6$ .

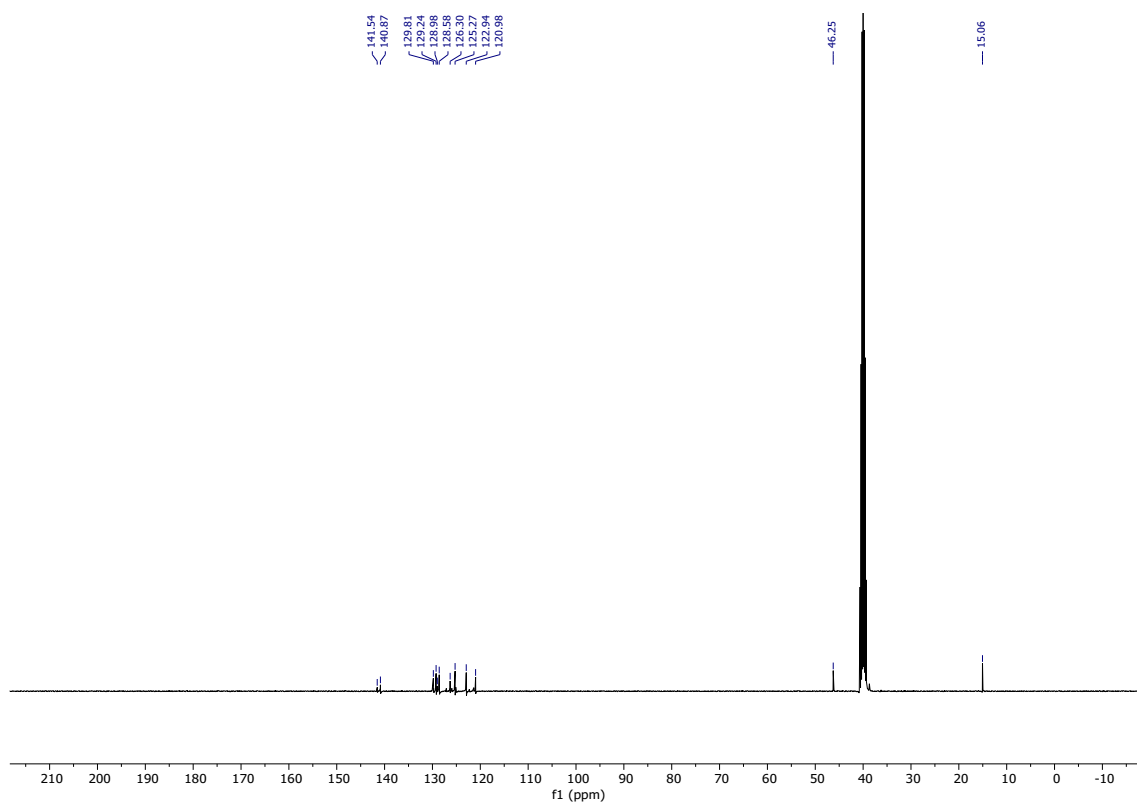


Figure S9.  $^{13}\text{C}$  NMR spectra of **Im3** in  $\text{DMSO-d}_6$ .

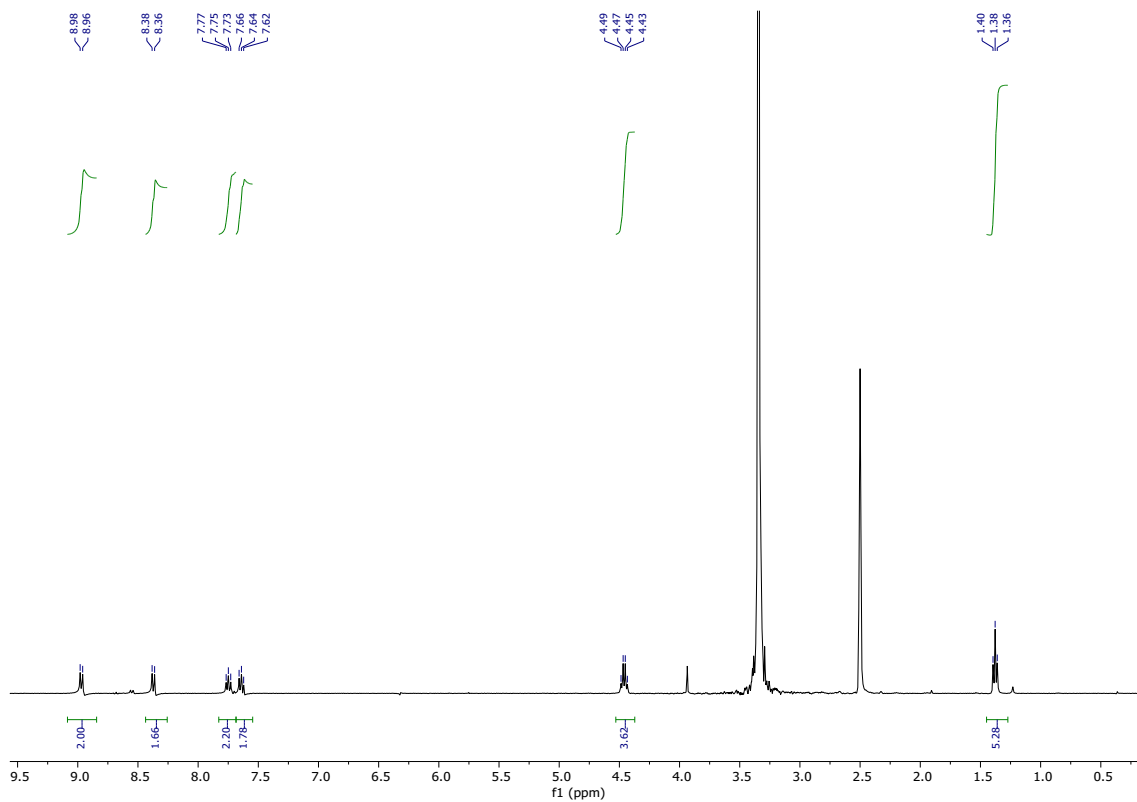


Figure S10.  $^1\text{H}$ -NMR spectra of  $[\text{AuCl}(\text{Im}3)]$  in  $\text{DMSO-d}_6$ .

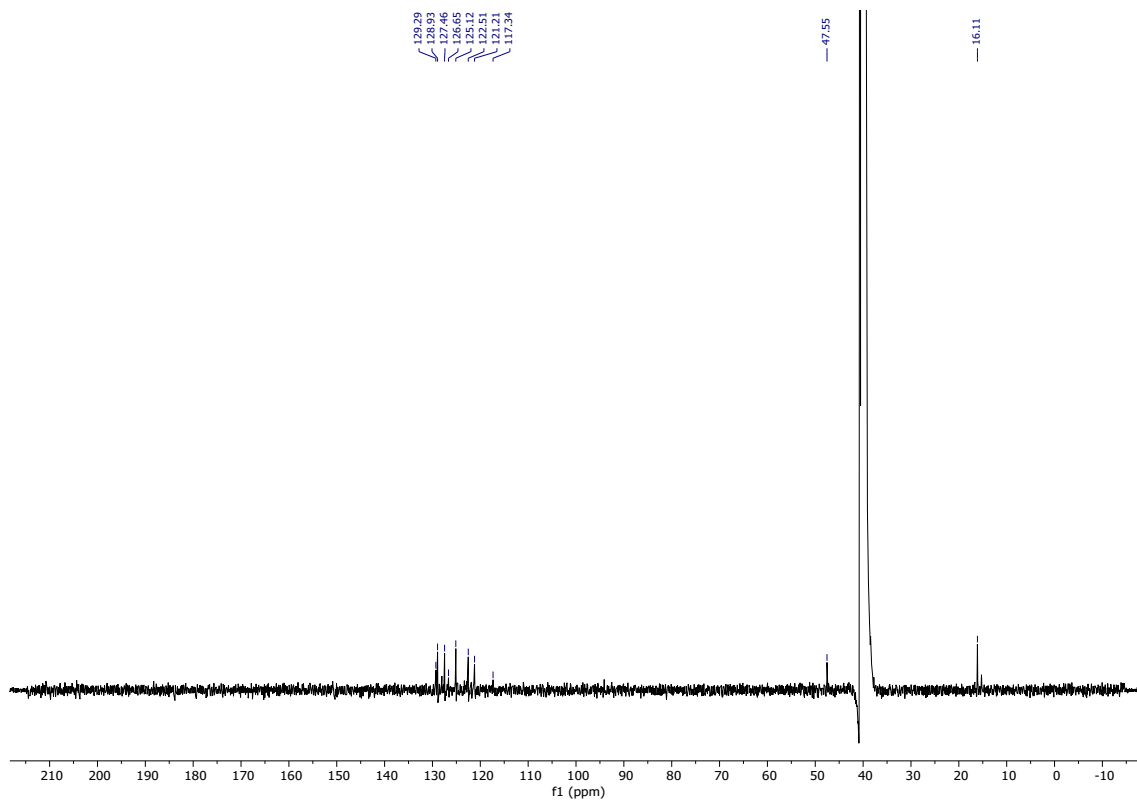


Figure S11.  $^{13}\text{C}$  NMR spectra of  $[\text{AuCl}(\text{Im}3)]$  in  $\text{DMSO-d}_6$ .

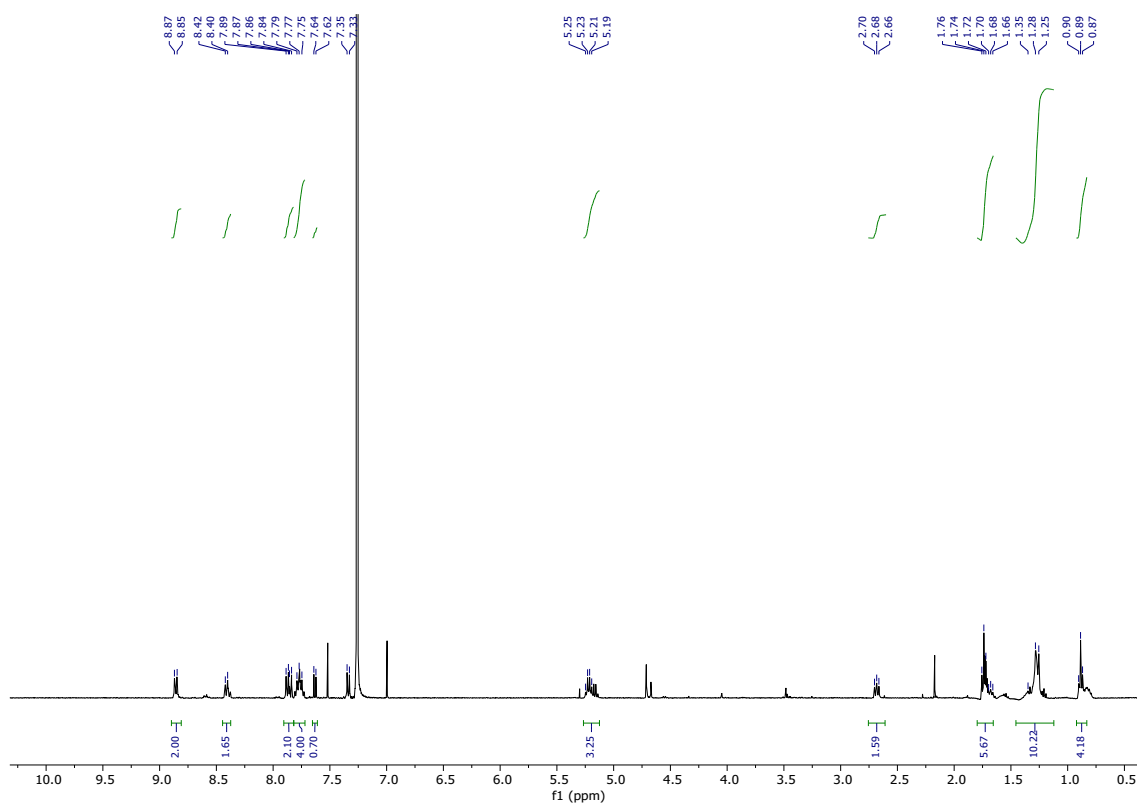


Figure S12.  $^1\text{H}$ -NMR spectra of **3** in  $\text{CDCl}_3$ .

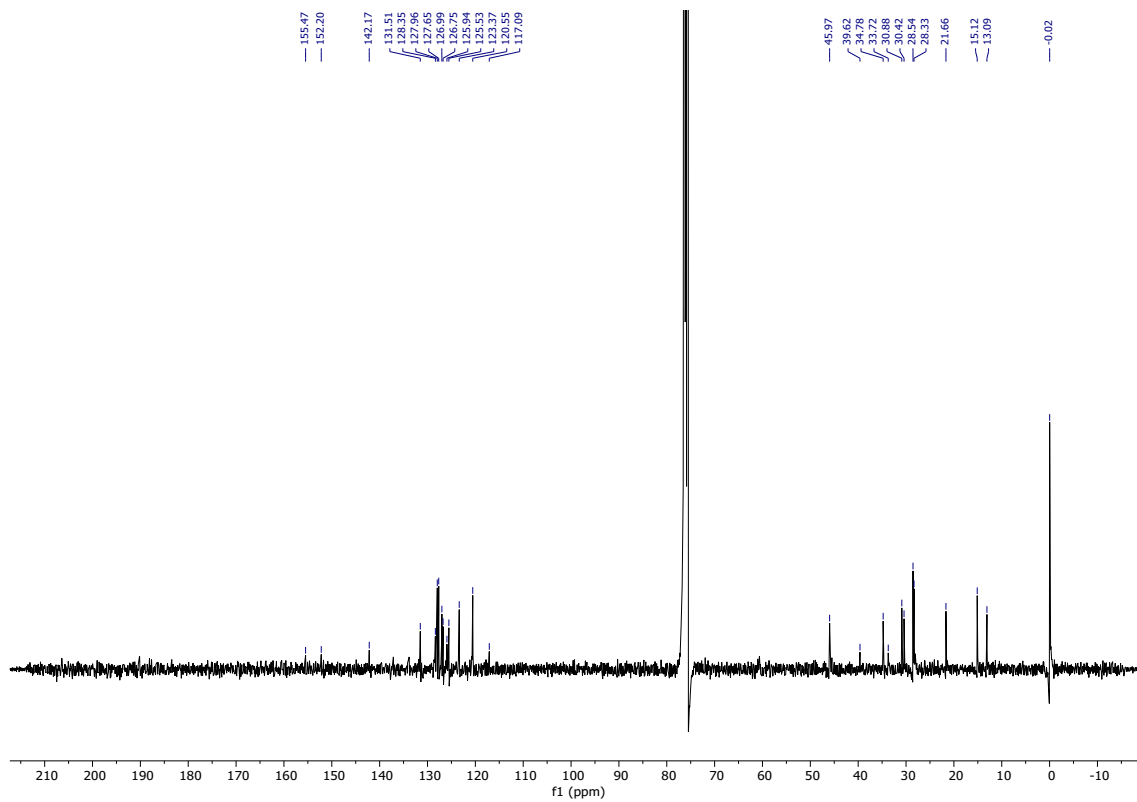


Figure S13.  $^{13}\text{C}$  NMR spectra of **3** in  $\text{CDCl}_3$ .

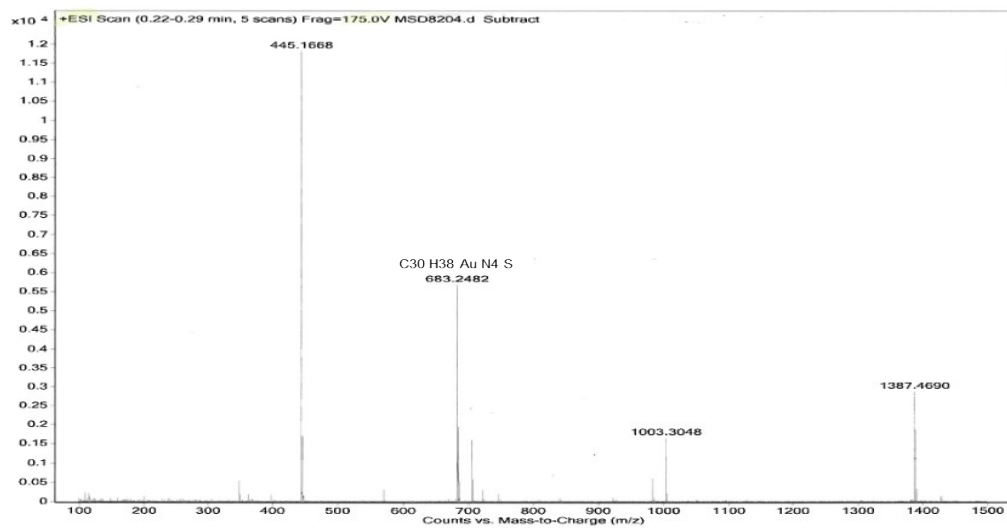
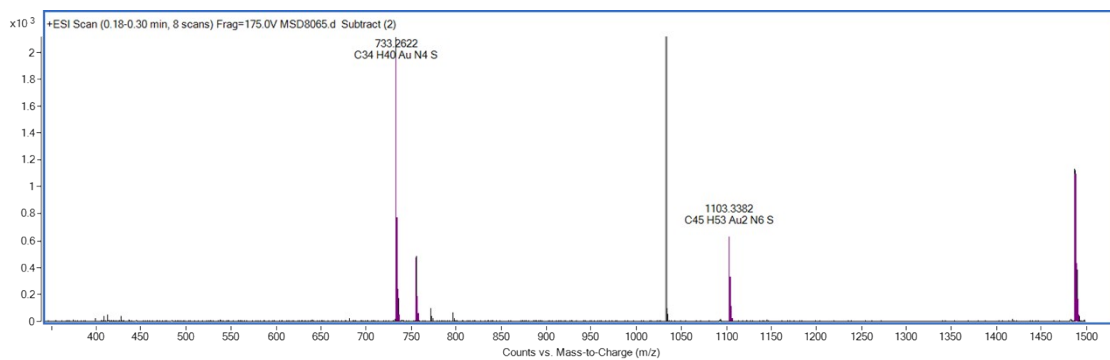


Figure S14. Mass spectra of **1**.





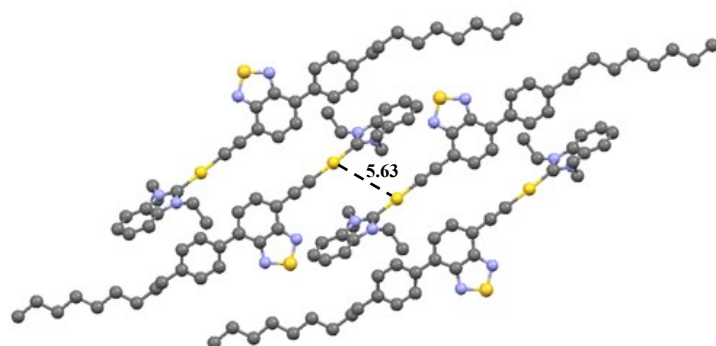
**Figure S15.** Mass spectra of **2**.



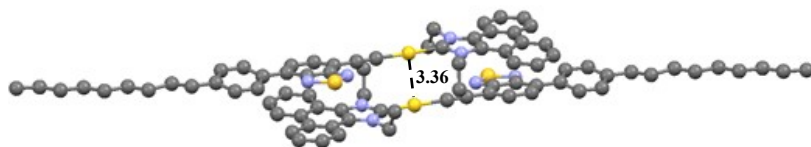
**Figure S16.** Mass spectra of **3**.

**Table S1.** Crystal data and structure for **2** and **3**.

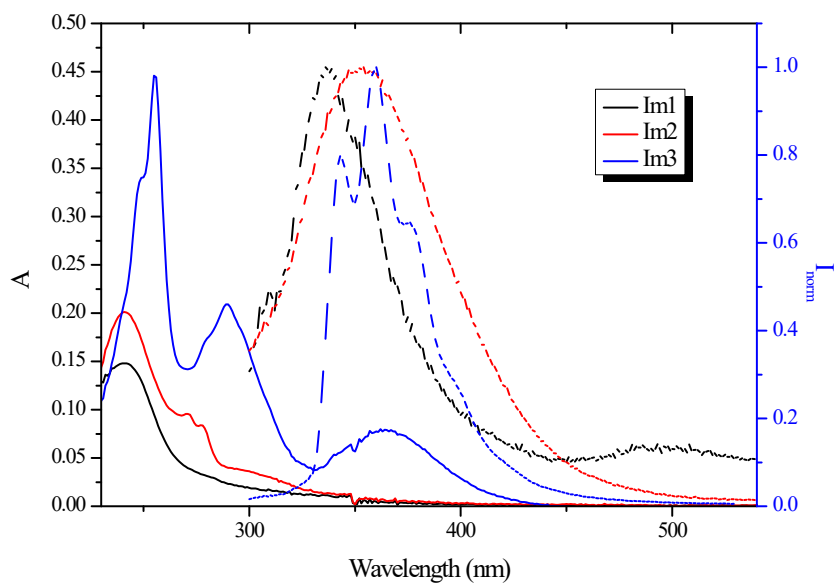
Compound	<b>2</b>	<b>3</b>
Formula	C <sub>34</sub> H <sub>39</sub> AuN <sub>4</sub> S	C <sub>42</sub> H <sub>43</sub> AuN <sub>4</sub> S
Crystal size, nm	0.253 x 0.217 x 0.067	0.265 x 0.215 x 0.108
Fw	732.72	848.83
Temp., K	200(2)	200(2)
Wavelength, Å	0.71073	0.71073
Crystal system	Triclinic	Triclinic
Space group	P-1	P-1
a, Å	9.4798(3)	11.1580(4)
b, Å	12.6101(3)	12.2292(5)
c, Å	14.3603(4)	14.6217(7)
α, °	97.6410(10)	86.513(3)
β, °	100.288(2)	68.107(2)
γ, °	109.9550(10)	84.983(2)
Volume, Å <sup>3</sup>	1552.35(8)	1843.34(14)
Z	2	2
D <sub>calc</sub> , mg m <sup>-3</sup>	1.568	1.529
Abs. coef., mm <sup>-1</sup>	4.835	4.085
F(000)	732	852
θ range for data coll, °	1.76 to 25.35	3.00 to 25.35
Reflns coll./independent	82971/5673	62560/6749
Data/restraint/parameters	5673/0/364	6749/0/452
GOF on F <sup>2</sup>	1.107	1.066
Final R index (I > 2σ(I))	R1 = 0.0138,wR2 = 0.0350	R1 = 0.0195,wR2 = 0.0578
R index (all data)	R1 = 0.0157,wR2 = 0.0356	R1 = 0.0216,wR2 = 0.0590
Peak and hole, e Å <sup>-3</sup>	0.323 and -0.328	1.133 and -0.299
CCDC	2160186	2160187



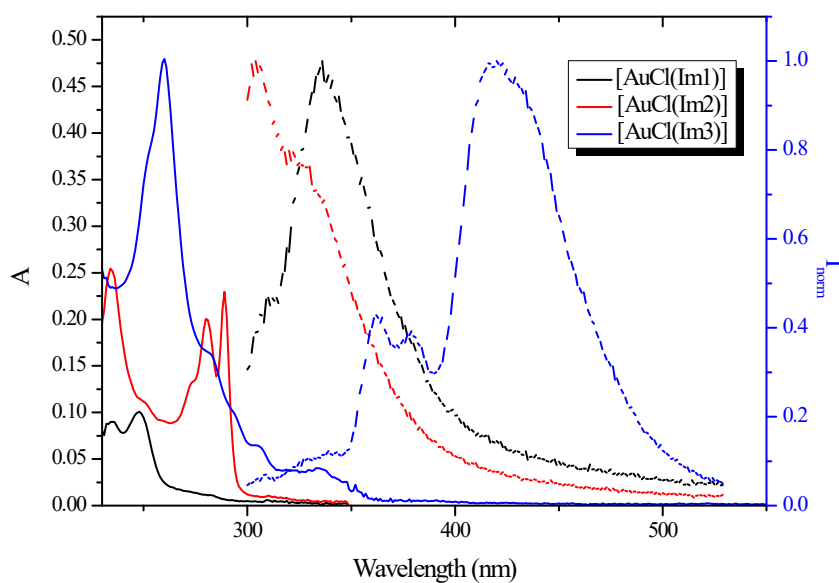
**Figure S17.** Representation of the X-ray crystal structure of **2**.



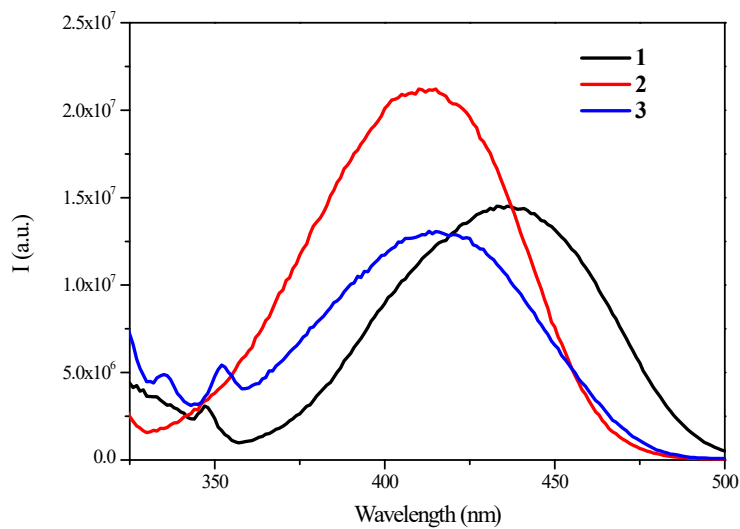
**Figure S18.** Representation of the X-ray crystal structure of **3**.



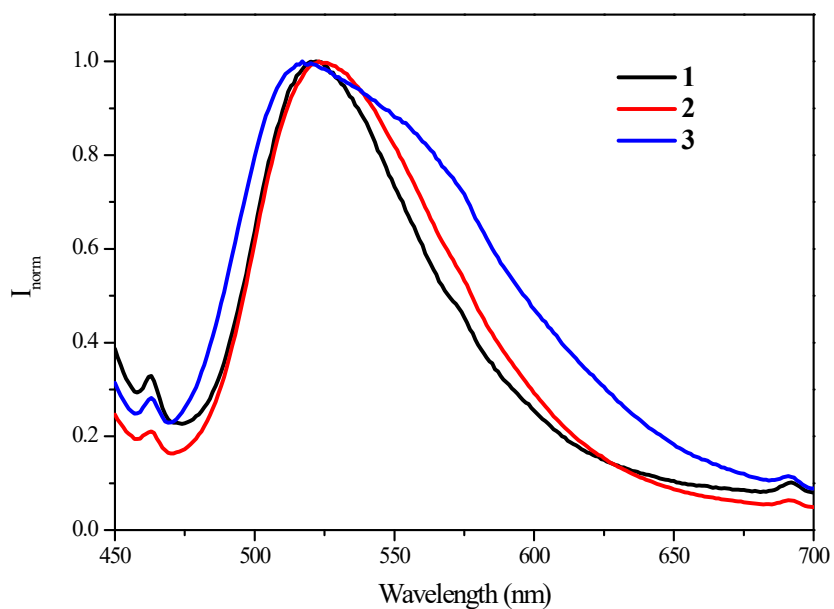
**Figure S19.** Absorption (solid lines) and emission (dash lines) spectra of **Im1-3** in dichloromethane.



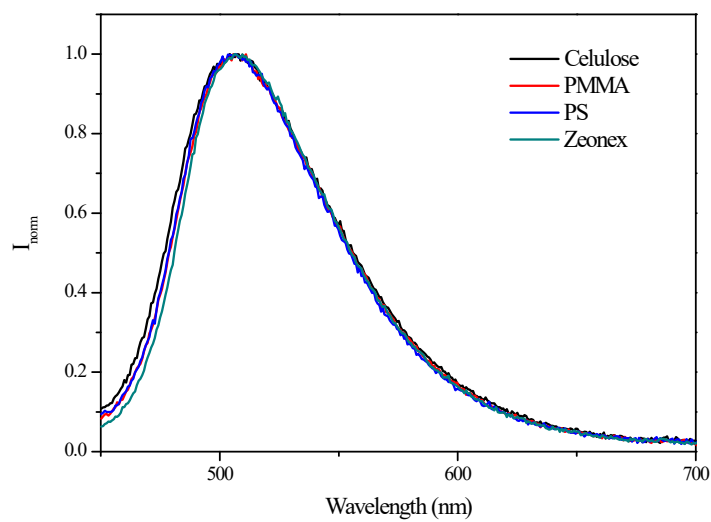
**Figure S20.** Absorption (solid lines) and emission (dash lines) spectra of **[AuCl(Im1-3)]** in dichloromethane.



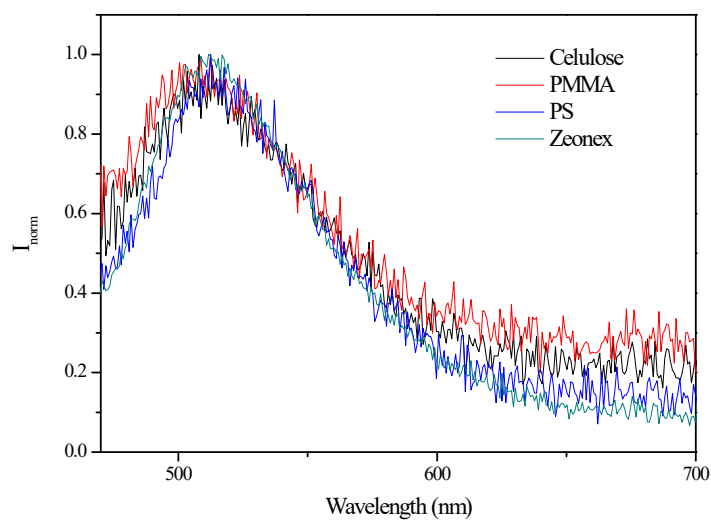
**Figure S21.** Excitation spectra of gold(I) complexes **1-3** in dichloromethane.



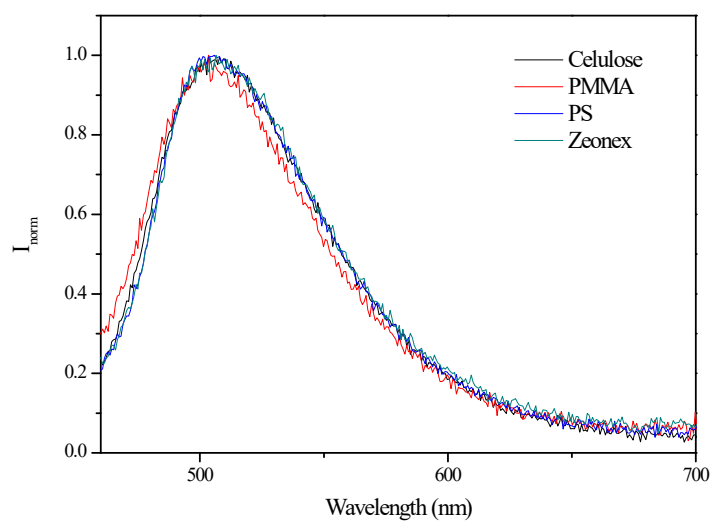
**Figure S22.** Emission spectra of gold(I) complexes **1-3** in solid state. **Emission of 3** corresponds to the as-obtained polymorph.



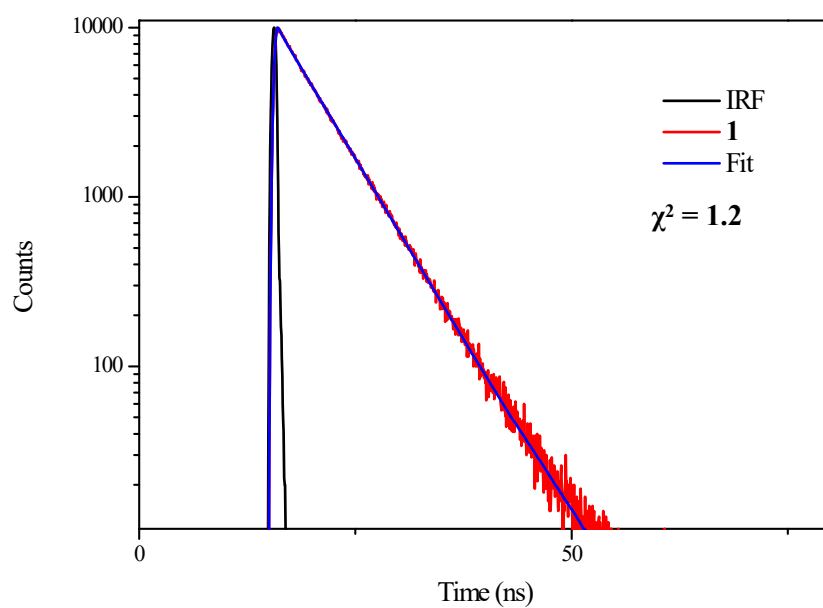
**Figure S23.** Normalized emission spectra of **2** in different matrices.



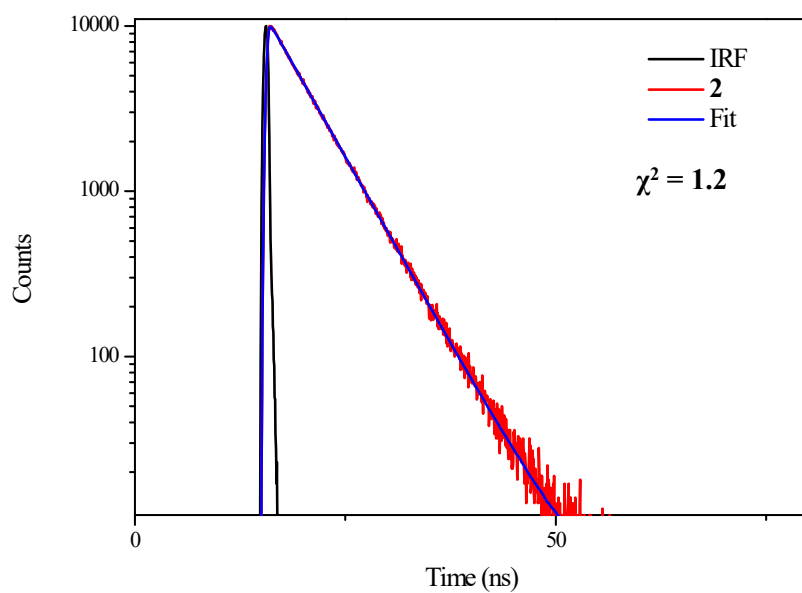
**Figure S24.** Normalized emission spectra of **1** in different matrices.



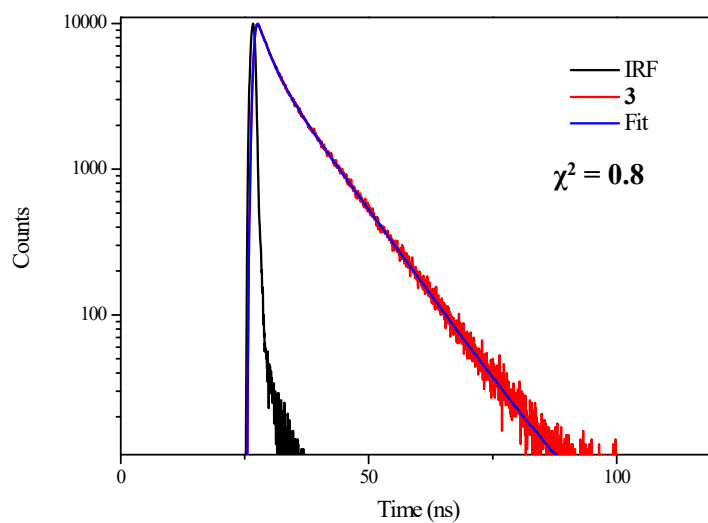
**Figure S25.** Normalized emission spectra of **3** in different matrices.



**Figure S26.** Fluorescent lifetime of **1** in dichloromethane solution.

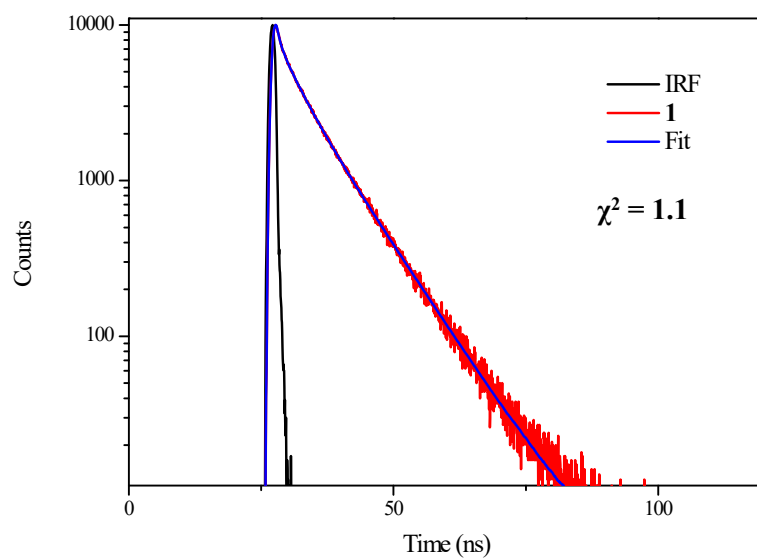


**Figure S27.** Fluorescent lifetime of **2** in dichloromethane solution.

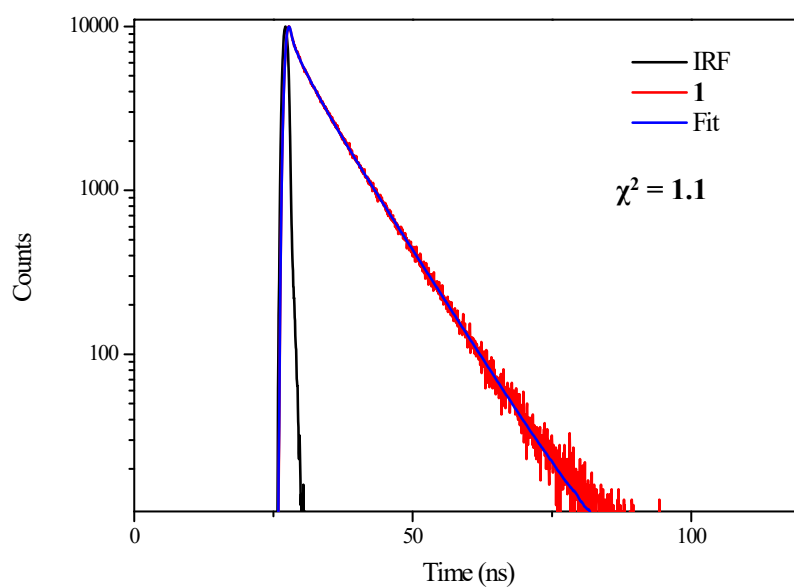


**Figure S28.** Fluorescent lifetime of **3** in dichloromethane solution.

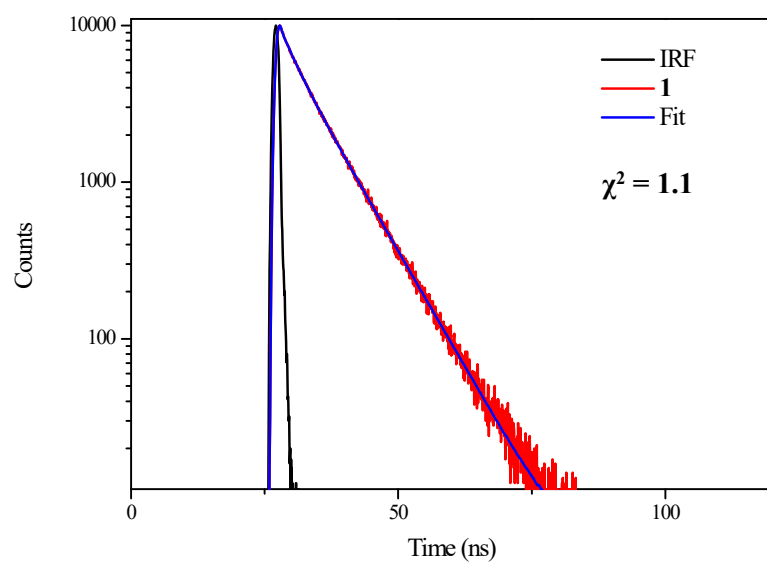




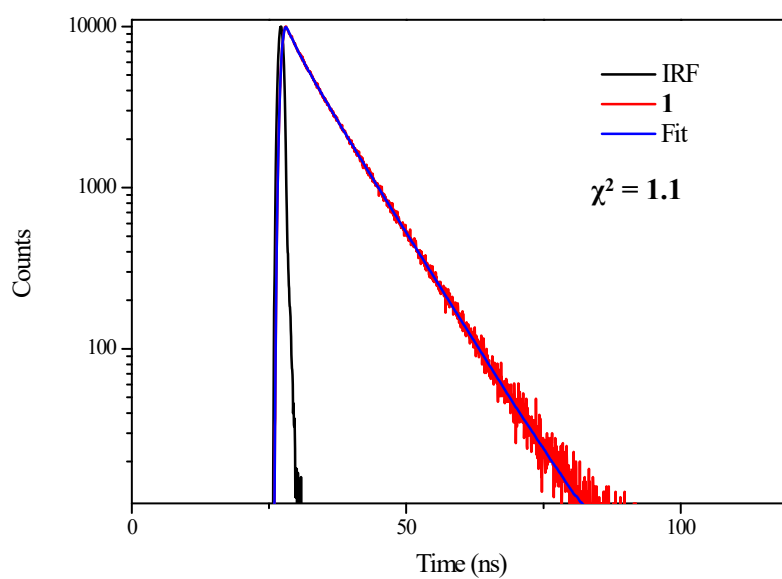
**Figure S29.** Fluorescent lifetime of **1** in cellulose.



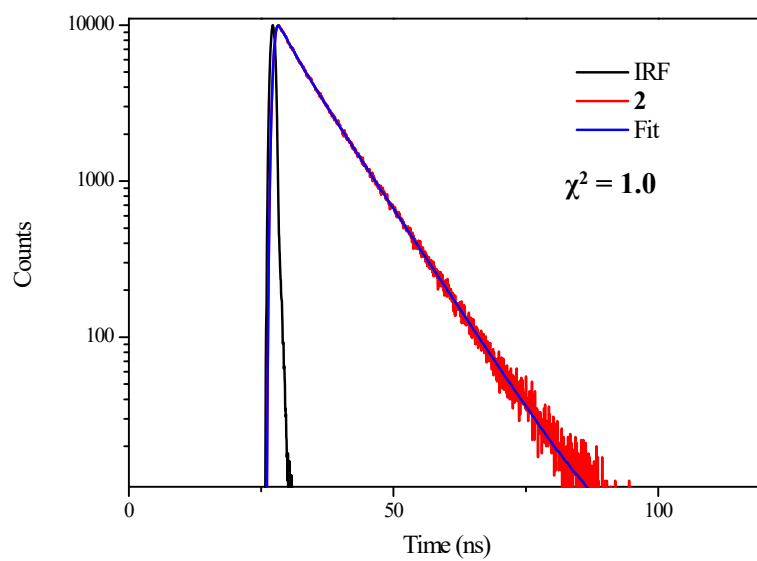
**Figure S30.** Fluorescent lifetime of **1** in PMMA.



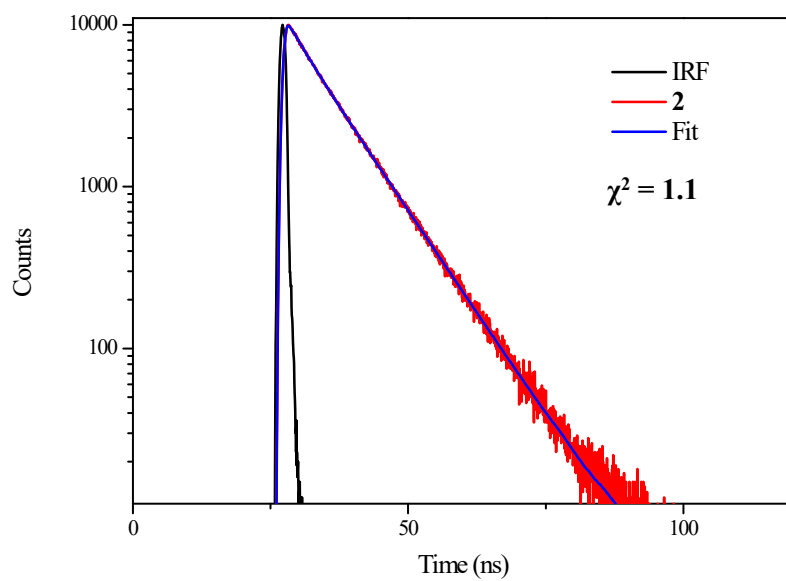
**Figure S31.** Fluorescent lifetime of **1** in PS.



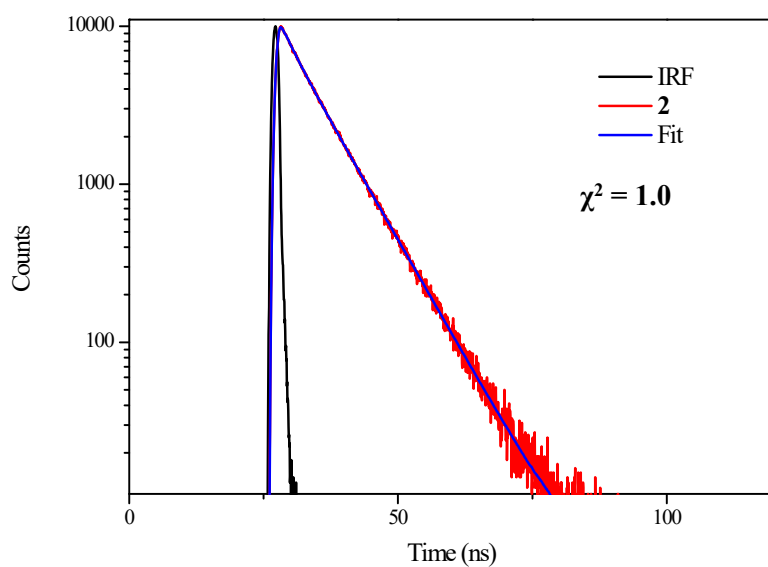
**Figure S32.** Fluorescent lifetime of **1** in Zeonex.



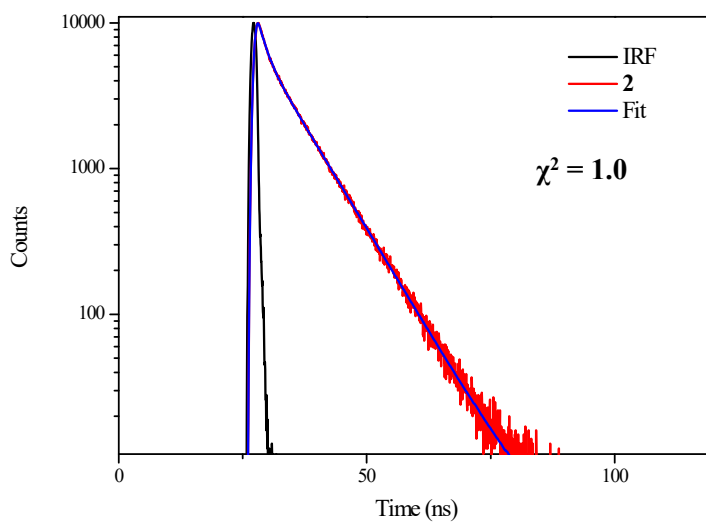
**Figure S33.** Fluorescent lifetime of **2** in cellulose.



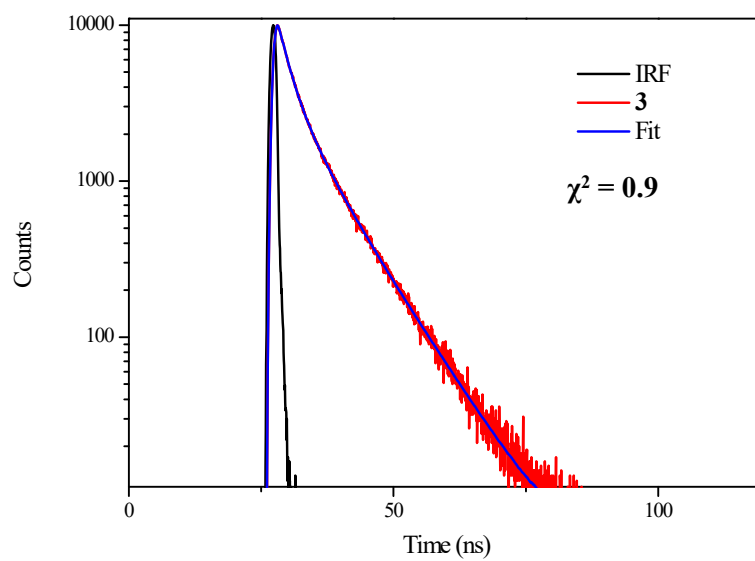
**Figure S34.** Fluorescent lifetime of **2** in PMMA.



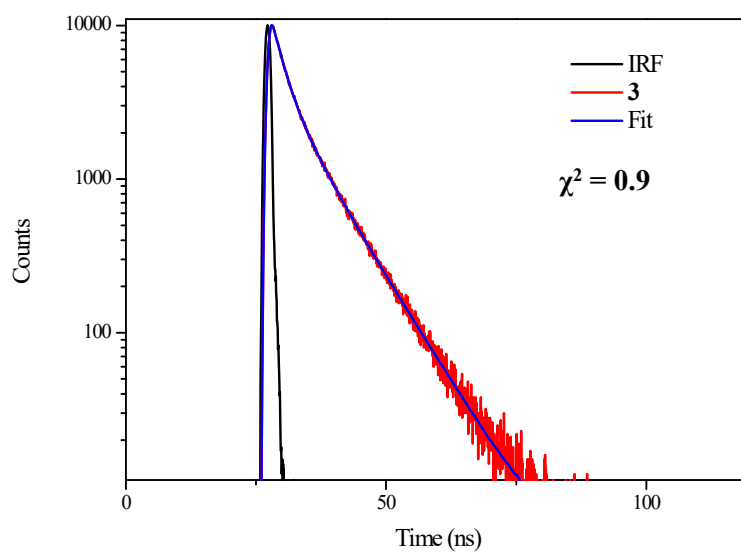
**Figure S35.** Fluorescent lifetime of 2 in PS.



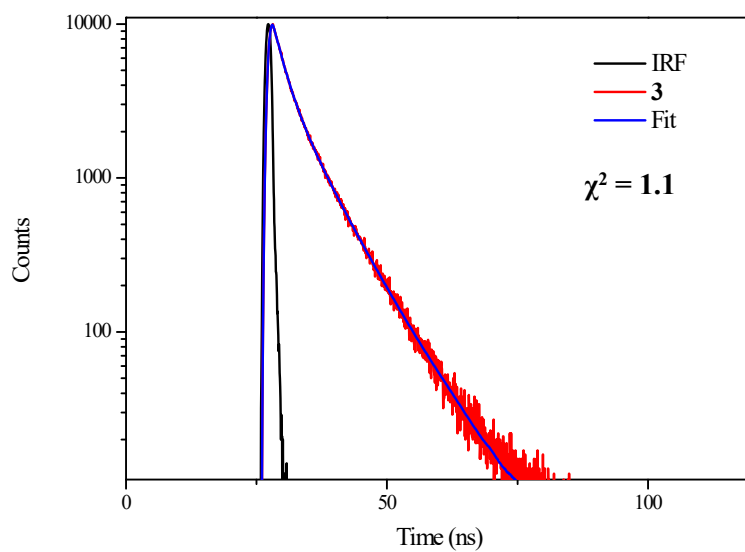
**Figure S36.** Fluorescent lifetime of 2 in Zeonex.



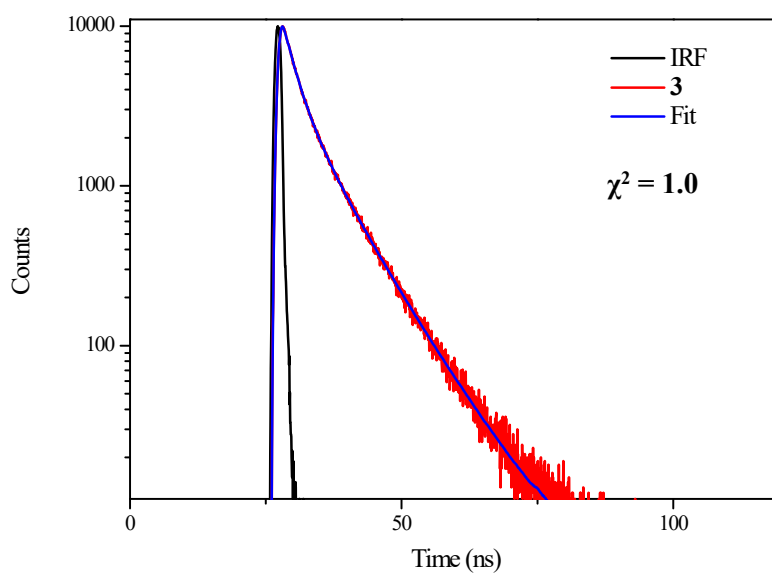
**Figure S37.** Fluorescent lifetime of **3** in cellulose.



**Figure S38.** Fluorescent lifetime of **3** in PMMA.



**Figure S39.** Fluorescent lifetime of **3** in PS.



**Figure S40.** Fluorescent lifetime of **3** in Zeonex.