Luminescent Alkynyl-Gold(I) Coumarin Derivatives and Their Biological Activity

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Supplementary Material

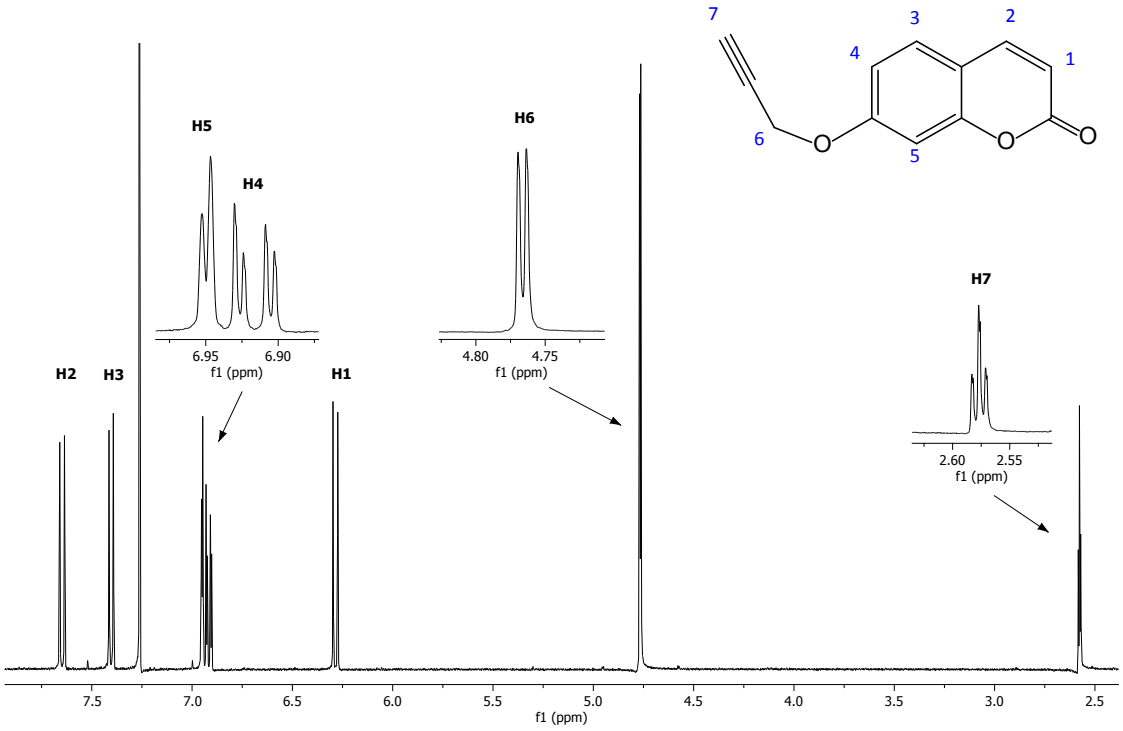

Figure S1. ^{1}H-NMR spectrum of compound **2** in $CDCl_3$.

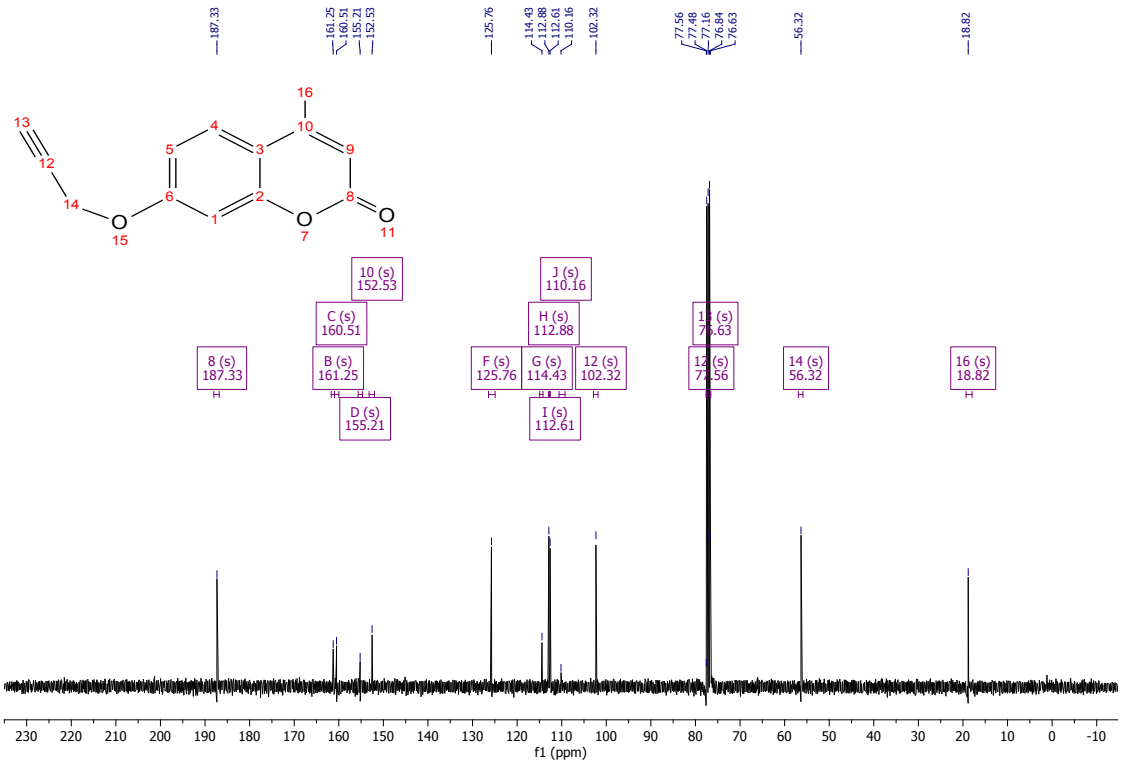

Figure S2. ^{13}C-NMR spectrum of compound **3** in $CDCl_3$.

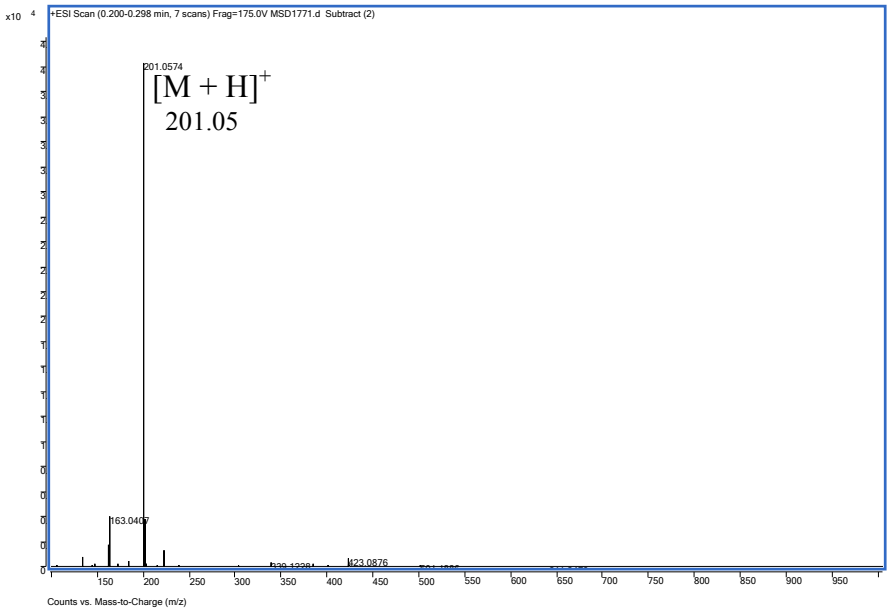

Figure S3. ESI-MS(+) spectrum of compound **2**.

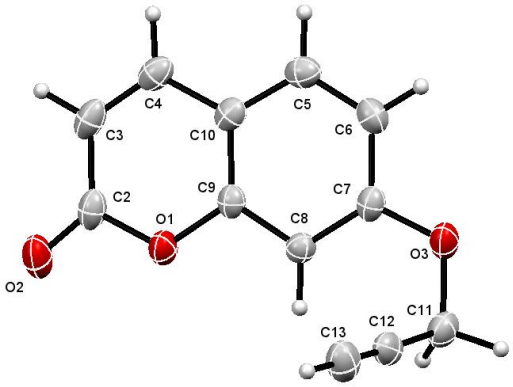

Figure S4. Molecular structure for **2**.

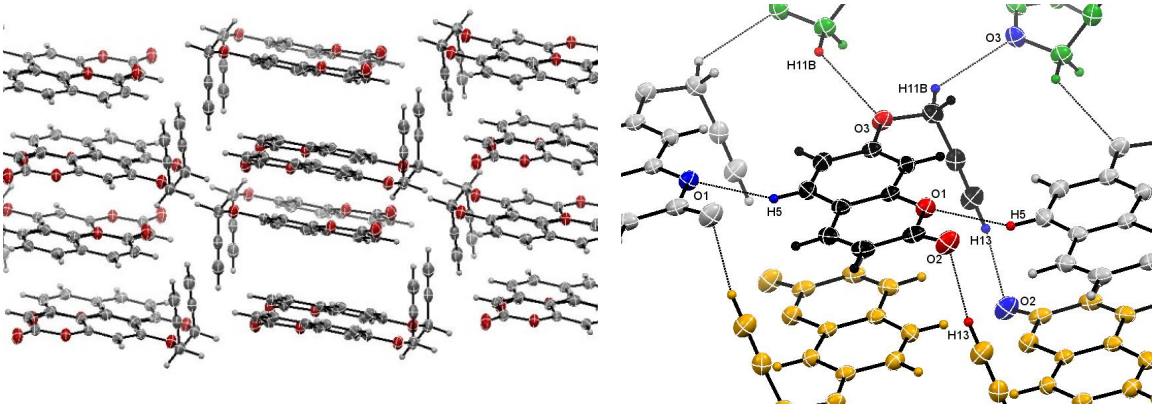

Figure S5. Crystal packing along the *b* axis (left) and view of the six hydrogen bonds that connect the molecules of **2** in the crystal (right). Reference molecule is shown in black color.

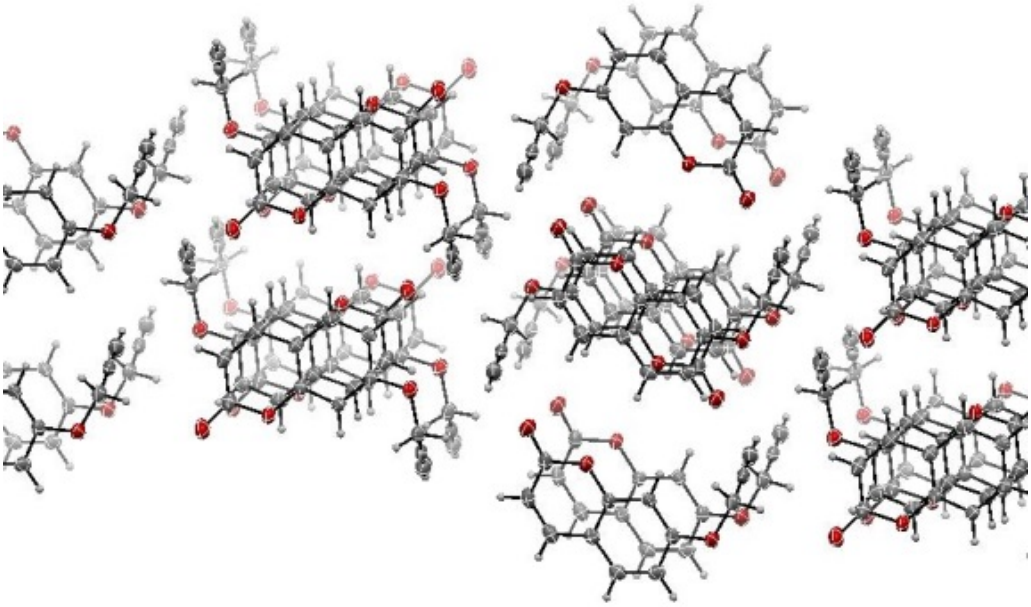

Figure S6. Crystal packing of **2** along *a* axis.

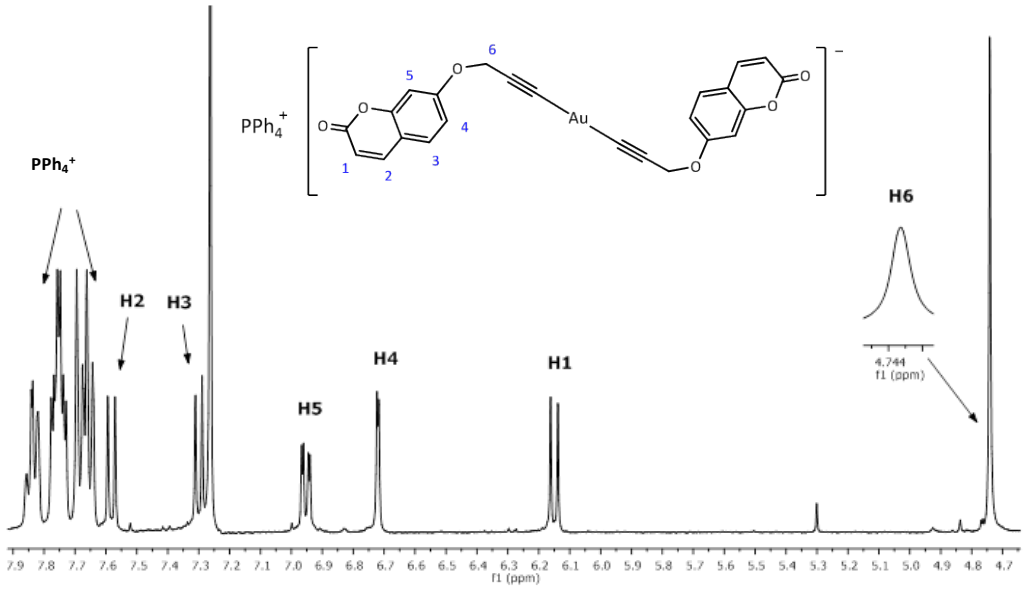

Figure S7. ^{1}H-NMR spectrum of **2a** in $CDCl_3$.

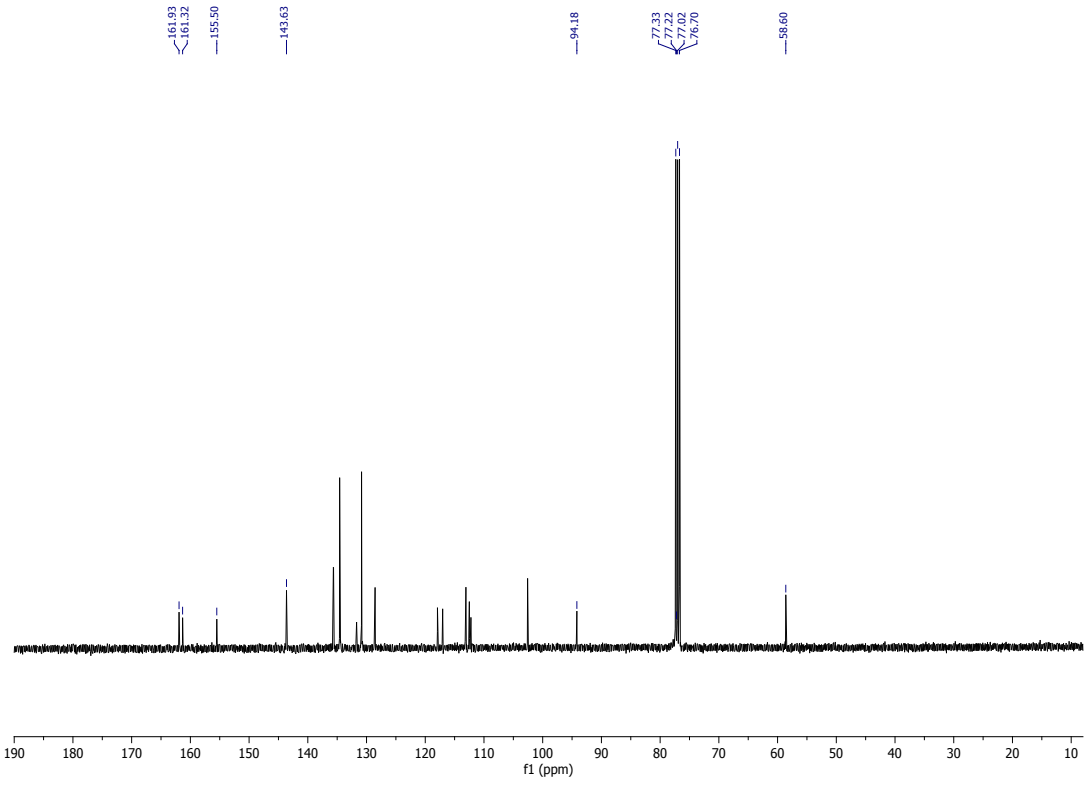

Figure S8. ^{13}C-NMR spectrum of **2a** in $CDCl_3$.

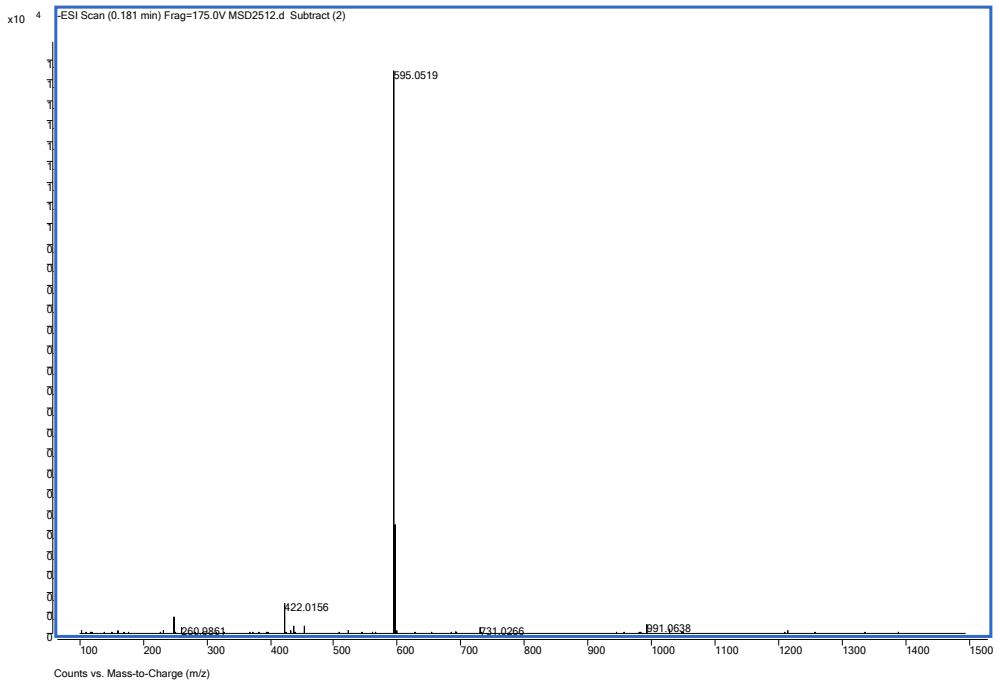

Figure S9. ESI-MS(+) spectrum of compound **2a**.

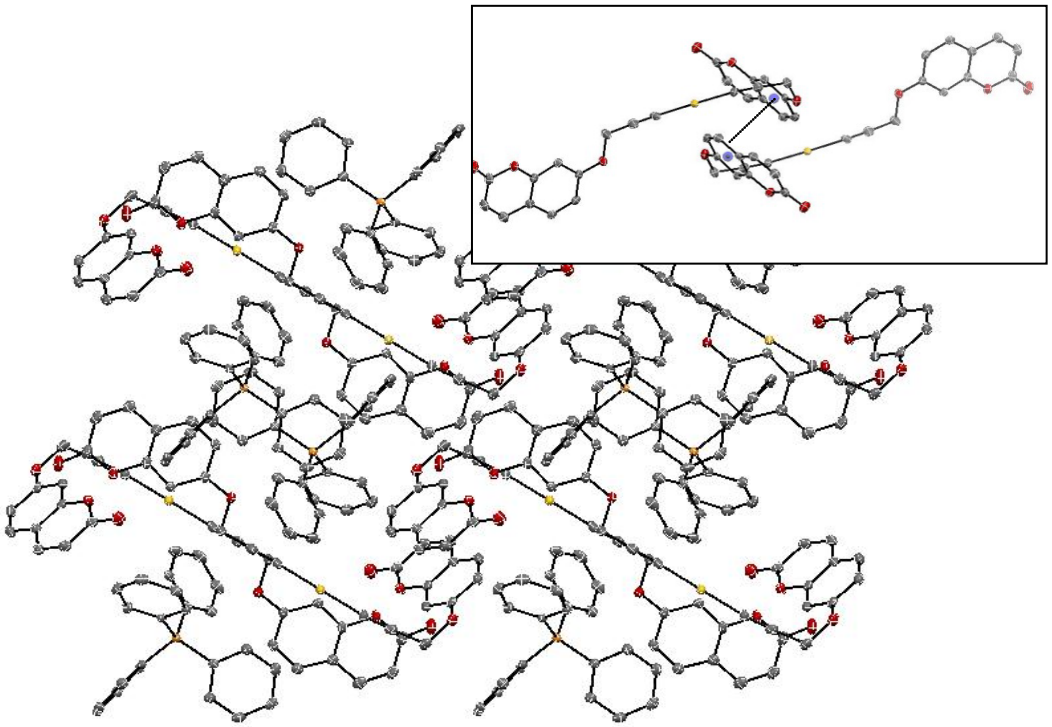

Figure S10. Crystal packing of **2a** along the *b* axis. Insert: π···π interaction between two anionic units of **2a**.

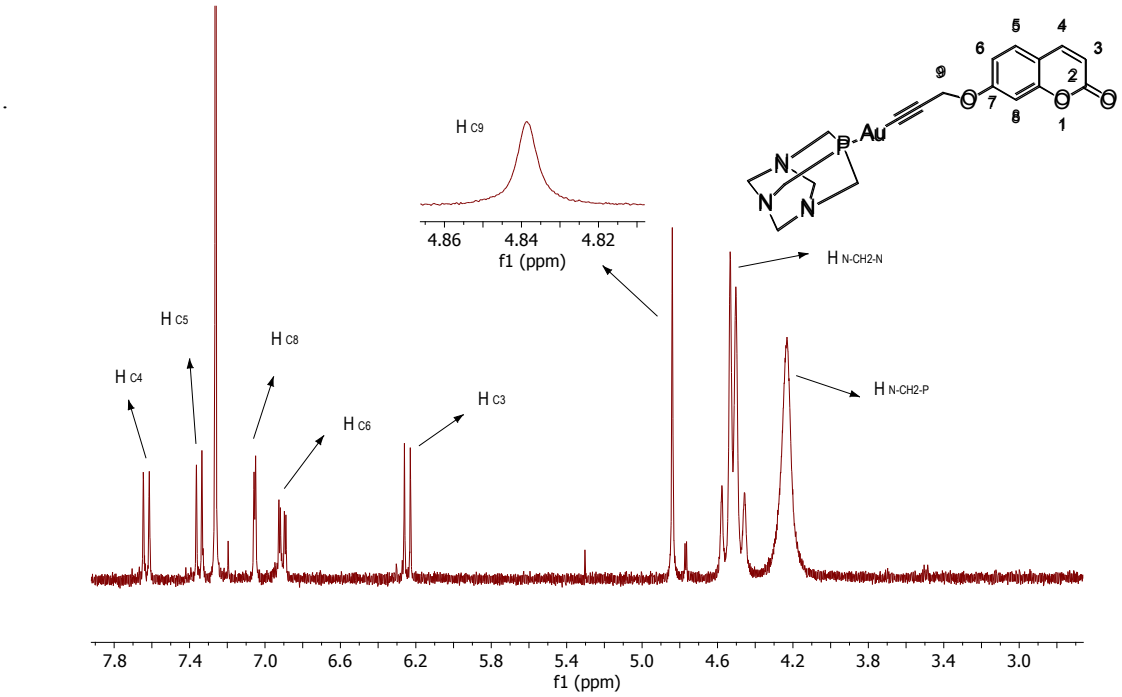

Figure S11. ^{1}H-NMR spectrum of **2b** in $CDCl_3$.

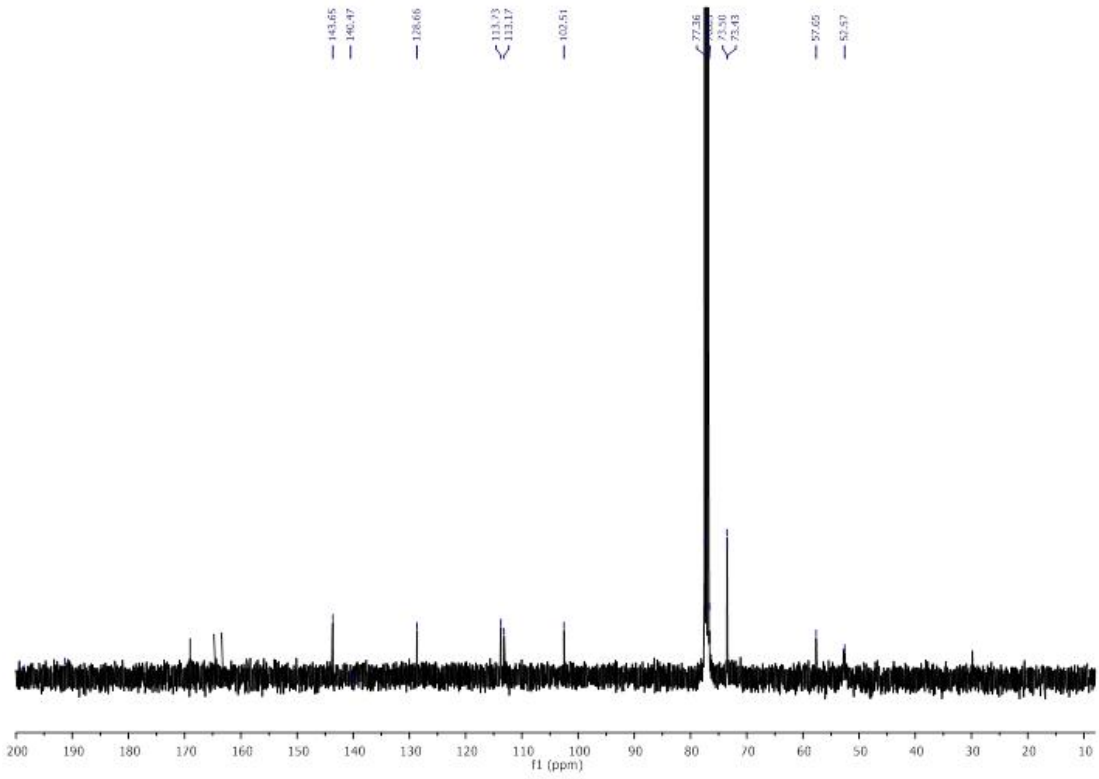

Figure S12. ^{13}C-NMR spectrum of **2b** in $CDCl_3$.

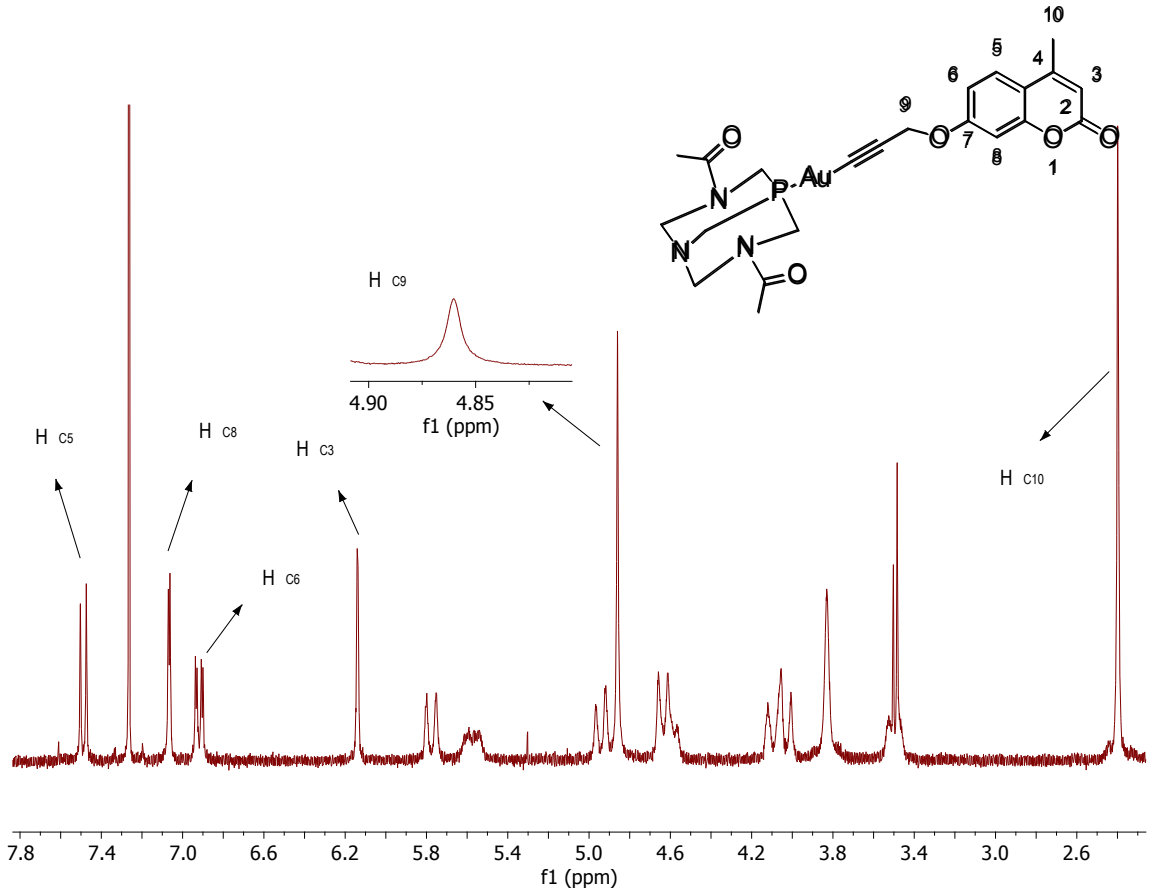

Figure S13. ^{1}H-NMR spectrum of **2c** in $CDCl_3$.

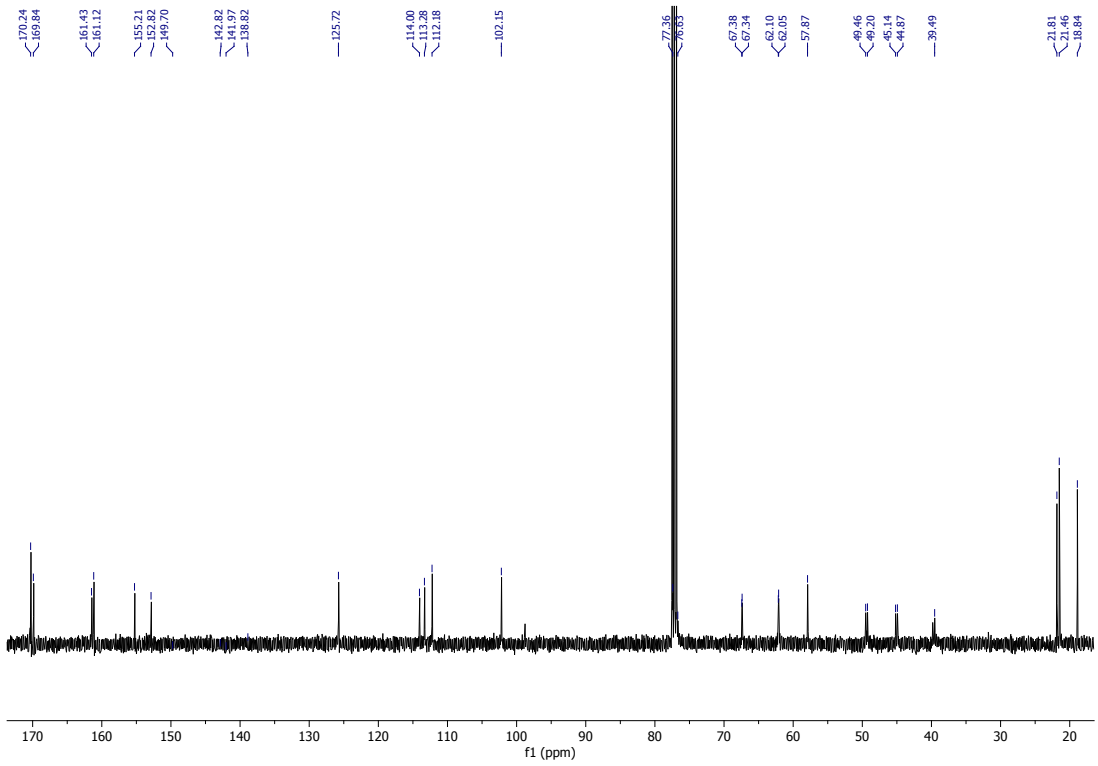

Figure S14. ^{13}C-NMR spectrum of **3c** in $CDCl_3$.

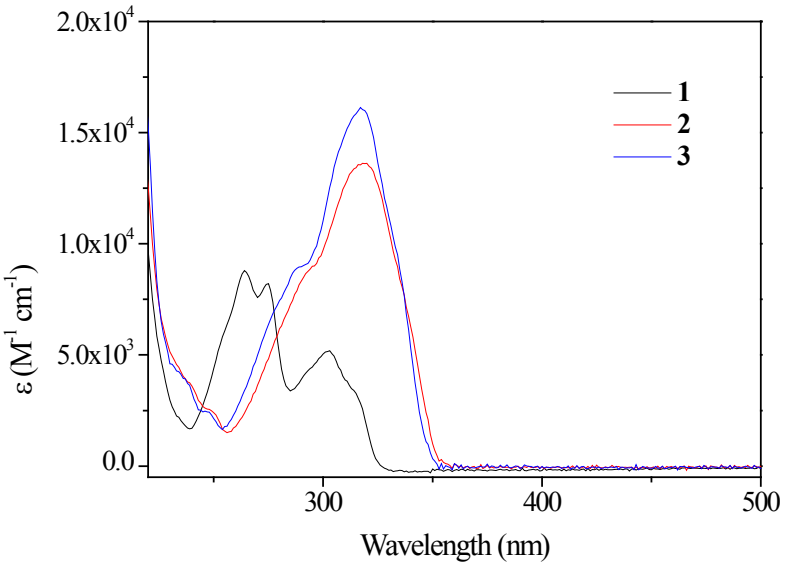

Figure S15. Absorption spectra of **1-3** in methanol at *ca*. 1x10^{-5} M concentration.

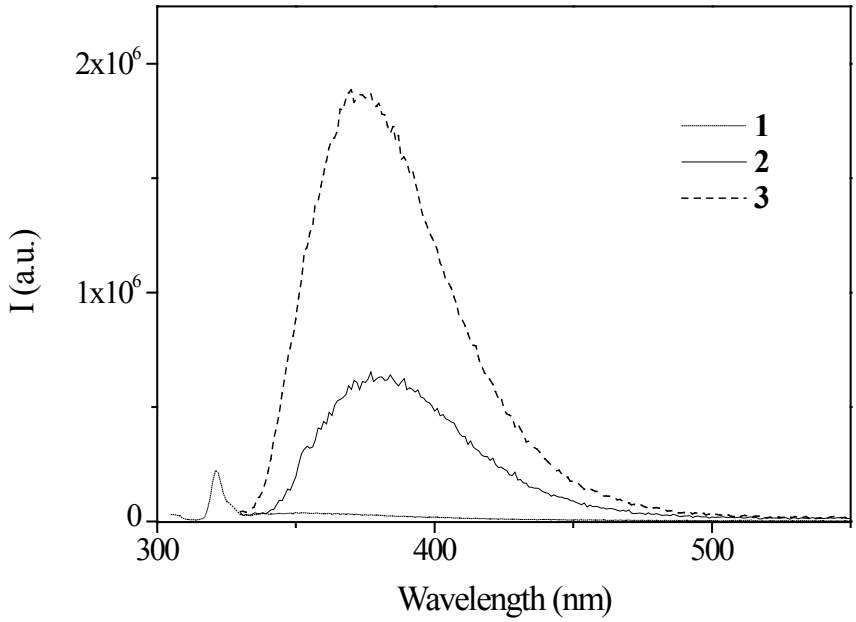

Figure S16. Emission spectra of **1-3**. λ_{exc} = 294 nm for **1** and 320 nm for **2** and **3**.

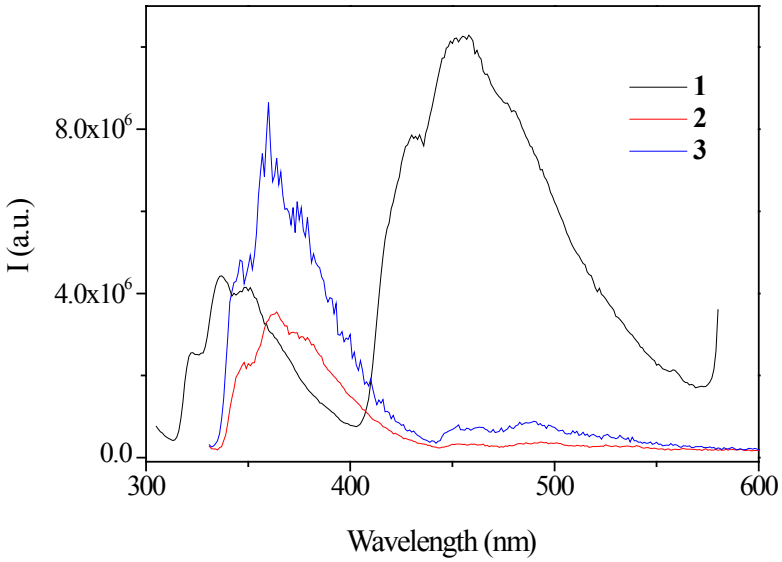

Figure S17. Emission spectra of **1-3** recorded at 77K. λ_{exc} = 294 nm for **1** and 320 nm for **2** and **3**.

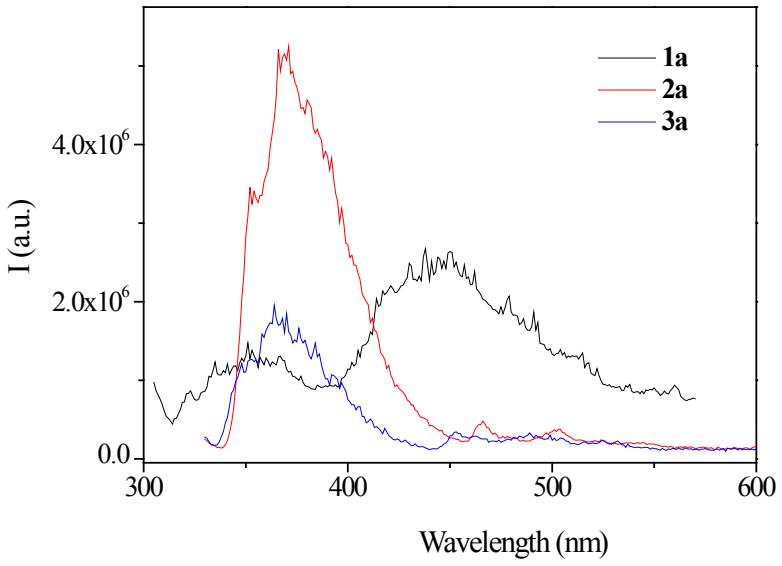

Figure S18. Emission spectra of **1-3a** recorded at 77K. λ_{exc} = 294 nm for **1a** and 320 nm for **2a** and **3a**.

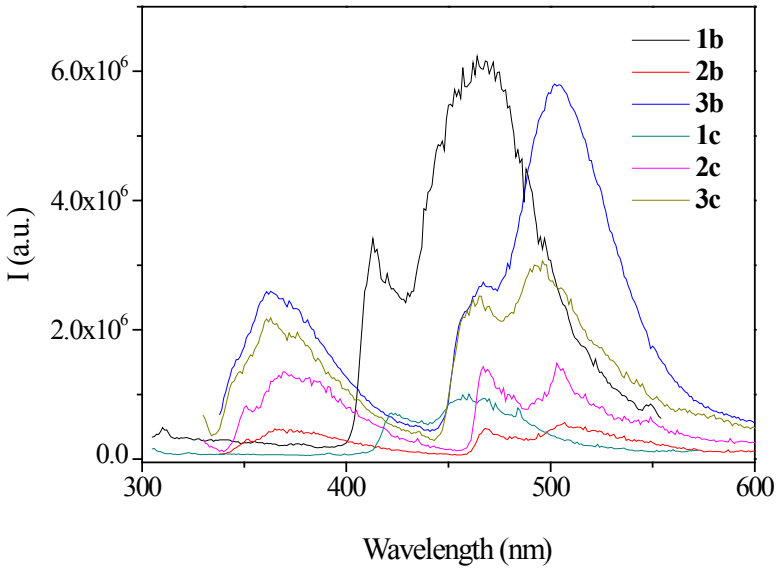

Figure S19. Emission spectra of **1-3b/c** recorded at 77K. λ_{exc} = 294 nm for **1b/c** and 320 nm for **2b/c** and **3b/c**.

Table S1. X-ray crystallographic data for **2** and **2a**.

	2	**2a**
Empirical Formula	$C_{12}H_8O_3$	$C_{48}H_{34}AuO_6P$
Molecular Weight (g/mol)	200.18	934.69
Temperature (K)	170	123
Wavelength (Å)	0.71073	1.54184 Å
Crystal System, space group	Monoclínic, $P\,2_1/c$ (No. 14)	triclinic, $P\,\bar{1}$ (No. 2)
a (Å)	7.0432(2)	10.4254(3)
b (Å)	6.4967(3)	12.8050(3)
c (Å)	20.6568(6)	14.7713(4)
α (º)	90	98.028(2)
β (º)	91.044(3)	103.649(2)
γ (º)	90	95.056(2)
V (Å^3)	945.05(6)	1882.38(9)
Z, D_{calcld} (g cm^{-3})	4, 1.407	2, 1.649
Absorption coefficient (mm^{-1})	0.102	8.175
F(000)	416	928
Crystal size (mm)	0.39 x 0.19 x 0.06	0.26 x 0.23 x 0.13
θ range for data collection [°]	2.9 to 25.5	3.1 to 67.0
Index ranges	$-6 \le h \le 8$	$-12 \le h \le 11$
	$-7 \le k \le 4$	$-15 \le k \le 14$
	$-17 \le l \le 25$	$-16 \le l \le 17$
Collected reflections No.	2947	12816
Independent reflections No. / $R_{Int.}$	1753 / 0.0117	6652 / 0.0242
Reflections No. $I \ge 2\sigma(I)$	1432	6573
Refinement method	full-matrix least-squares on F^2	full-matrix least-squares on F^2
Data/restraints/parameters	1753 / 0 / 136	6652 / 0 / 505
Goodness-of-fit on F^2	1.041	1.027
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0415, wR2 = 0.1252	R1 = 0.0233, wR2 = 0.0602
R indices (all data)	R1 = 0.0524, wR2 = 0.1347	R1 = 0.0236, wR2 = 0.0604
Largest diff. peak and hole (eÅ^{-3})	0.169<Δρ<– 0.237	1.076<Δρ<– 1.399

Table S2. Selected bond lengths [Å] and angles [°] of **2**.

Distance	(Å)	Angle	(°)
O1-C2	1.384(2)	O1-C2-C3	117.06(18)
O1-C9	1.378(2)	O1-C2-O2	116.02(19)
O2-C2	1.213(2)	O2-C2-C3	126.93(18)
C2-C3	1.441(3)	C2-O1-C9	121.70(16)
C3-C4	1.337(3)	C3-C4-C10	120.70(19)
C4-C10	1.435(3)	C7-O3-C11	117.77(15)
O3-C7	1.374(2)	C11-C12-C13	177.6(2)
C11-C12	1.466(3)		
C12-C13	1.180(3)		

Table S3. Selected bond lengths [Å] and angles [°] for **2a**.

Distance	(Å)	Distance	(Å)	Angle	(°)	Angle	(°)
Au1-C13	2.004(3)	Au1-C14	2.007(3)	C13-Au1-C14	178.71(11)	C14-C15-C16	177.5(4)
O1-C2	1.390(3)	O4-C16	1.433(4)	C11-C12-C13	176.9(3)	C15-C16-O4	108.5(2)
O2-C2	1.209(4)	O5-C17	1.383(4)	O3-C11-C12	113.4(2)	C16-O4-C22	116.9(2)
O3-C11	1.444(4)	O6-C17	1.205(4)	C7-O3-C11	118.0(2)		
C3-C4	1.344(4)	C14-C15	1.178(5)				
C11-C12	1.470(4)	C15-C16	1.464(4)				
C12-C13	1.188(4)	C18-C19	1.338(5)				