Utilization of a Pt(II) di-yne Chromophore incorporating a 2,2'-bipyridine-5,5'-diyl spacer as a Chelate to Synthesize a Green and Red Emitting d-f-d Heterotrinuclear Complex

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Electronic Supporting Information

Table S1. Spherical atomic coordinates coordination polyhedron of the coordinated ligating atoms for the complex.

Ligand atom	Spherical coordinates		
	***R* (Å)**	***θ* (º)**	***ϕ* (º)**
N(bpy)	2.684	43.249	140.127
N(bpy)	2.647	53.235	54.811
O(β-diket.1)	2.416	121.819	108.611
O(β-diket.1)	2.428	109.439	186.236
O(β-diket.2)	2.399	142.021	279.170
O(β-diket.2)	2.415	122.055	17.380
O(β-diket.3)	2.407	61.180	246.040
O(β-diket.3)	2.422	62.825	326.377

Table S2. ZDO electronic densities (*q*) and electrophilic superdelocalizabilities (*SE*) for each atom directly coordinated to Eu(III) in complex **[Eu(btfa)$_3$1c]**, calculated with the Sparkle/PM6 model by considering the B3LYP geometry. Charge factors (*g*) and polarizabilities (α) were obtained from a fitting procedure, and the electric dipole intensity parameters (Ω_λ^{FED}) were calculated using such quantities.

Ligand atom	***QDC* parameters**			
	Q = 0.0658 au^{-1} D = 33.06 au^{-1}·Å^3 C = 21.20 Å^3 D/C = 1.56 au^{-1}			
	***q* (au)**	***SE* (au)**	***g***	**α (Å^3)**
N(bpy)	5.5415	-0.2127	0.3645	14.1654
N(bpy)	5.5451	-0.2636	0.3647	12.4798
O(β-diket.1)	6.8878	-0.5021	0.4530	4.5953
O(β-diket.1)	6.8491	-0.4979	0.4505	4.7339
O(β-diket.2)	6.9026	-0.5232	0.4540	3.8970
O(β-diket.2)	6.8582	-0.5287	0.4511	3.7159
O(β-diket.3)	6.8934	-0.4846	0.4534	5.1724
O(β-diket.3)	6.8588	-0.5045	0.4511	4.5153
	Ω_2^{FED} = 0.0115 ×10^{-20} cm^2 Ω_4^{FED} = 0.0347 ×10^{-20} cm^2 Ω_6^{FED} = 0.0862 ×10^{-20} cm^2			

Table S3. The HOMO and LUMO estimation by the computational studies (Sparkle/PM6, B3LYP and CAM-B3LYP).

Compound	**[Eu(btfa)$_3$1c]**		
	Sparkle/PM6[a]	**B3LYP**	**CAM-B3LYP[b]**
HOMO energy (eV)	-7.81	-5.40	-6.55
LUMO energy (eV)	-1.28	-2.18	-0.82
$\Delta E_{(HOMO-LUMO)}$ (eV)	6.53	3.19	5.73

[a]geometry optimized at the Sparkle/PM6 level.
[b]geometry optimized at the B3LYP/SVP/LANL68/MWB52 level

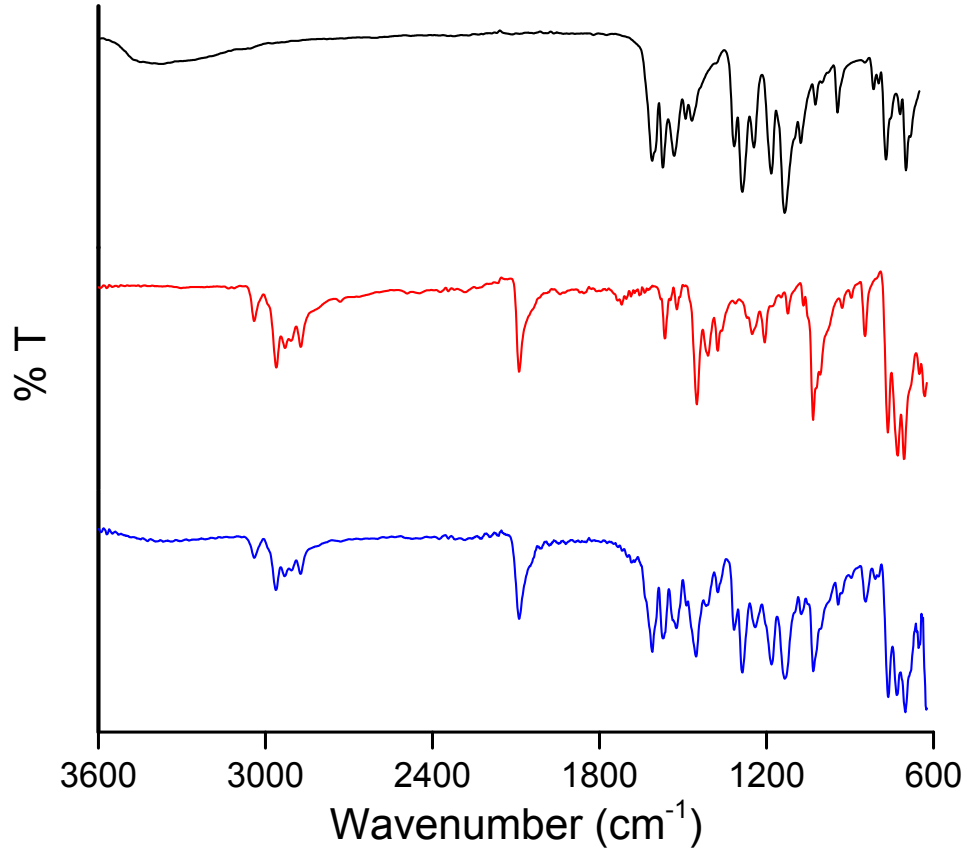

Fig. S1. FT–IR spectra of [Eu(btfa)$_3$(H_2O)$_2$] (black), (1c) (red) and heterotrinuclear **[Eu(btfa)$_3$1c]** complex (blue).

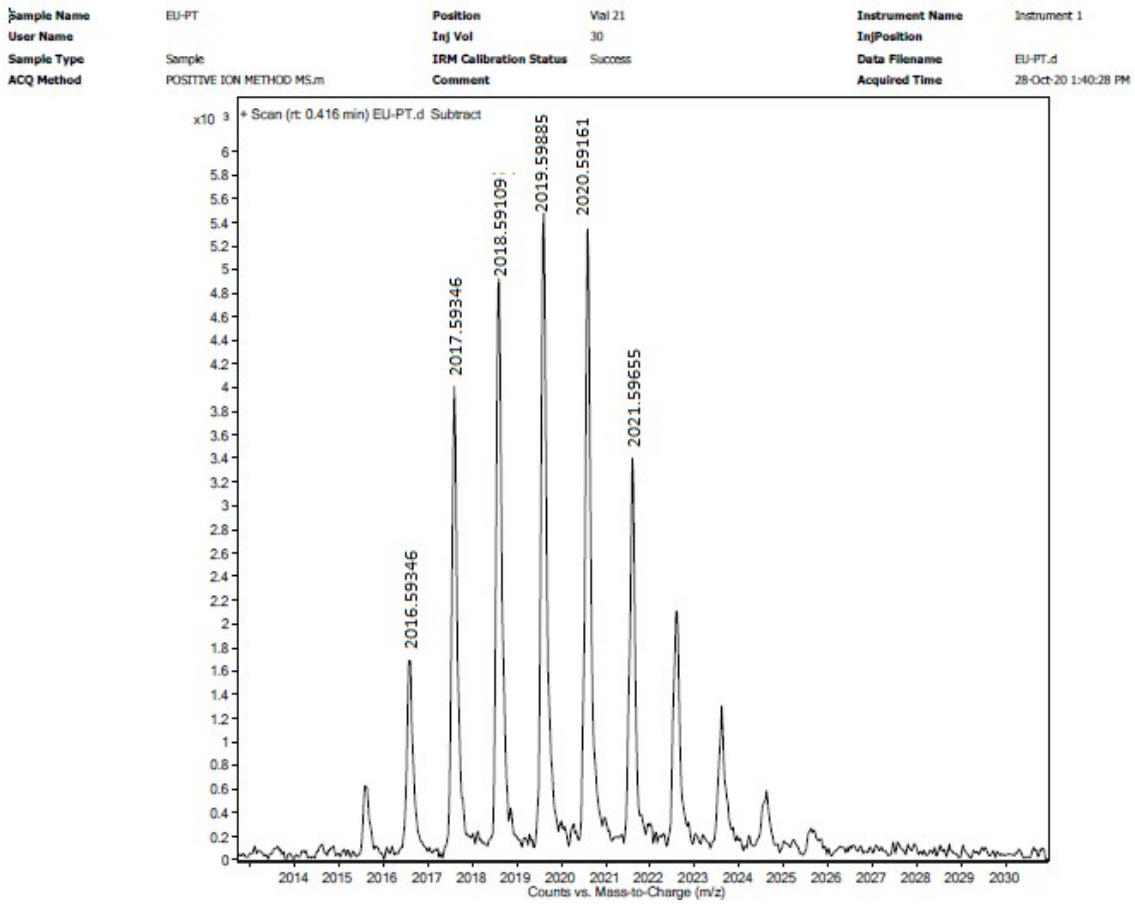

Fig. S2. (Q-TOF) LC/MS spectrum of heterotrinuclear **[Eu(btfa)$_3$(1c)]** in positive mode. 2016.59346 m/z.

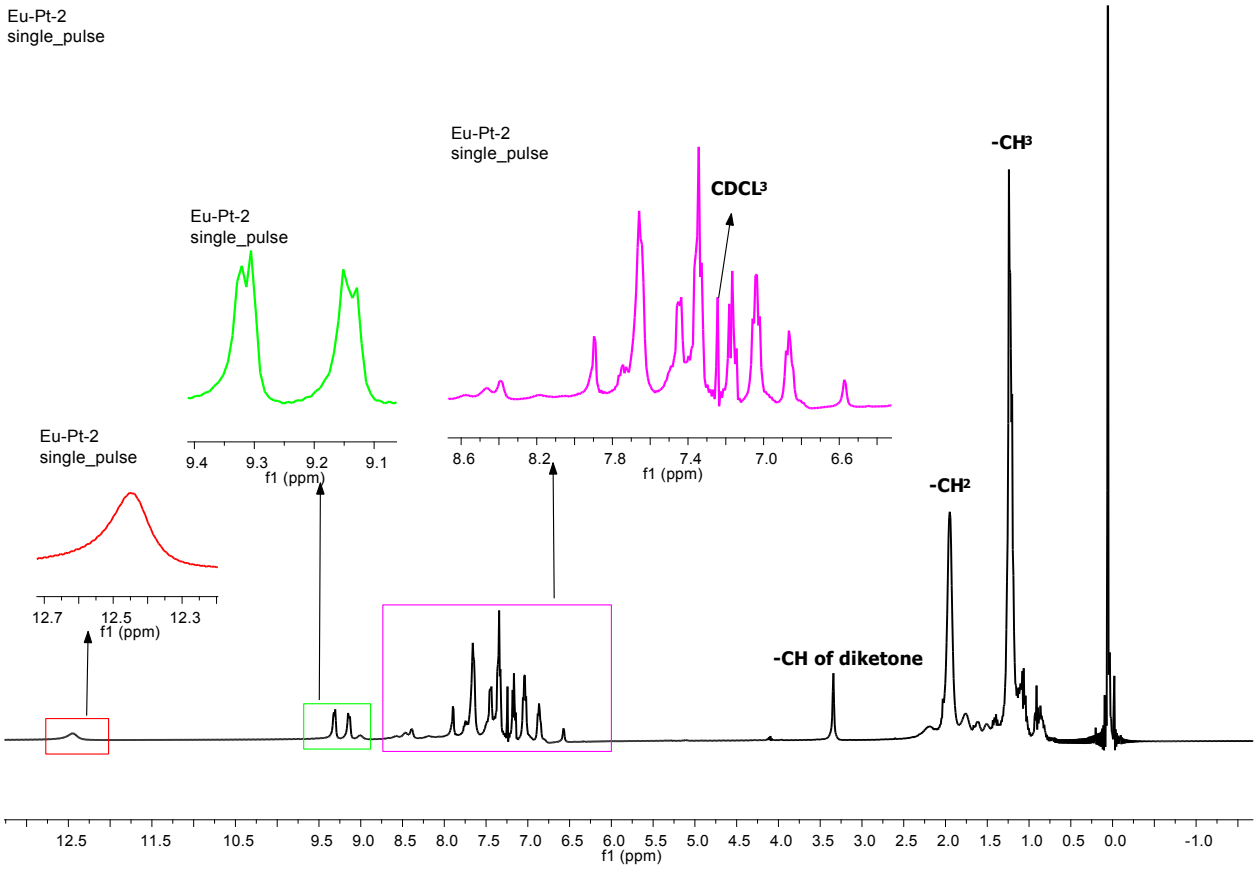

Fig. S3. 400 MHz ^{1}H NMR spectrum of the **[Eu(btfa)$_3$1c]** in $CDCl_3$.

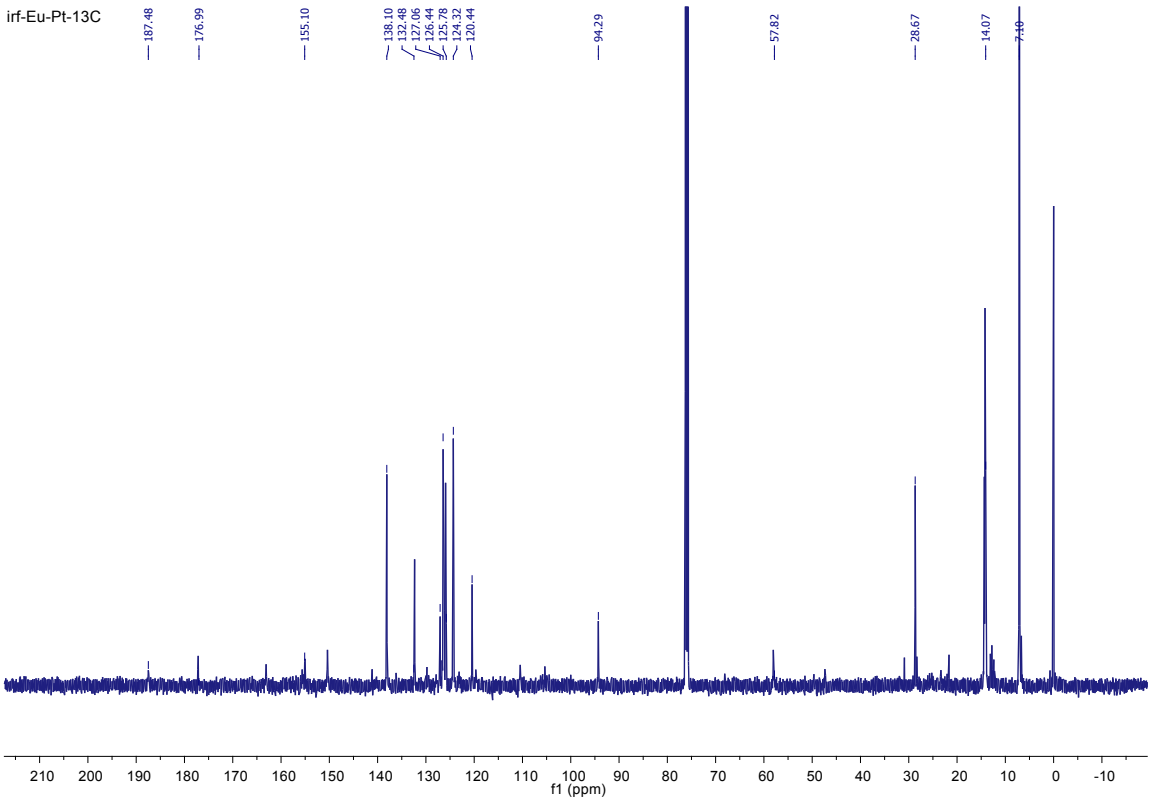

Fig. S4. 100.6 MHz ^{13}C NMR spectrum of the **[Eu(btfa)$_3$1c]** in $CDCl_3$.

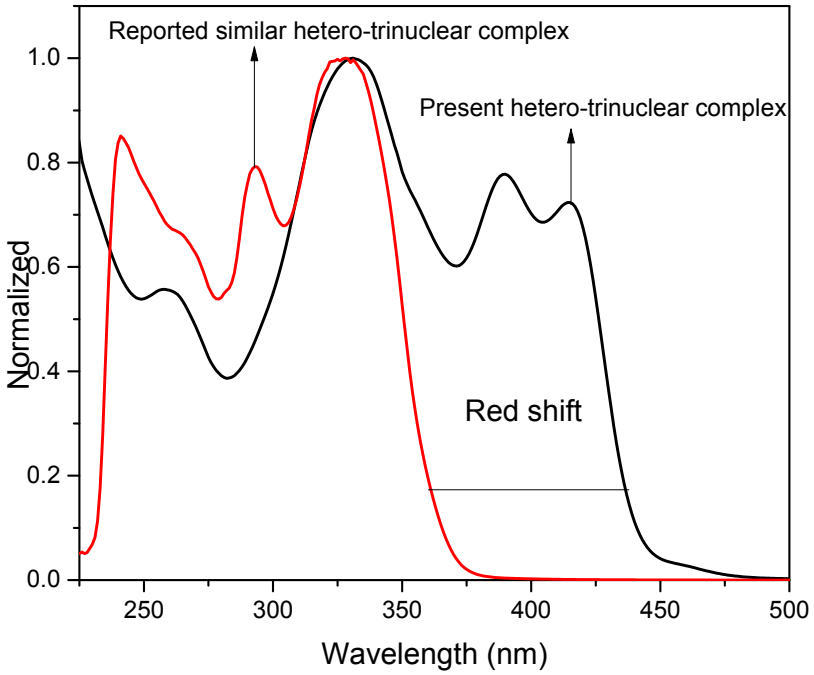

Fig. S5. Room temperature optical absorption spectra of **[Eu(btfa)$_3$1c]** (red) and its reported kinked analogue **[Eu(btfa)$_3$1d]**[1] displaying the red shift.

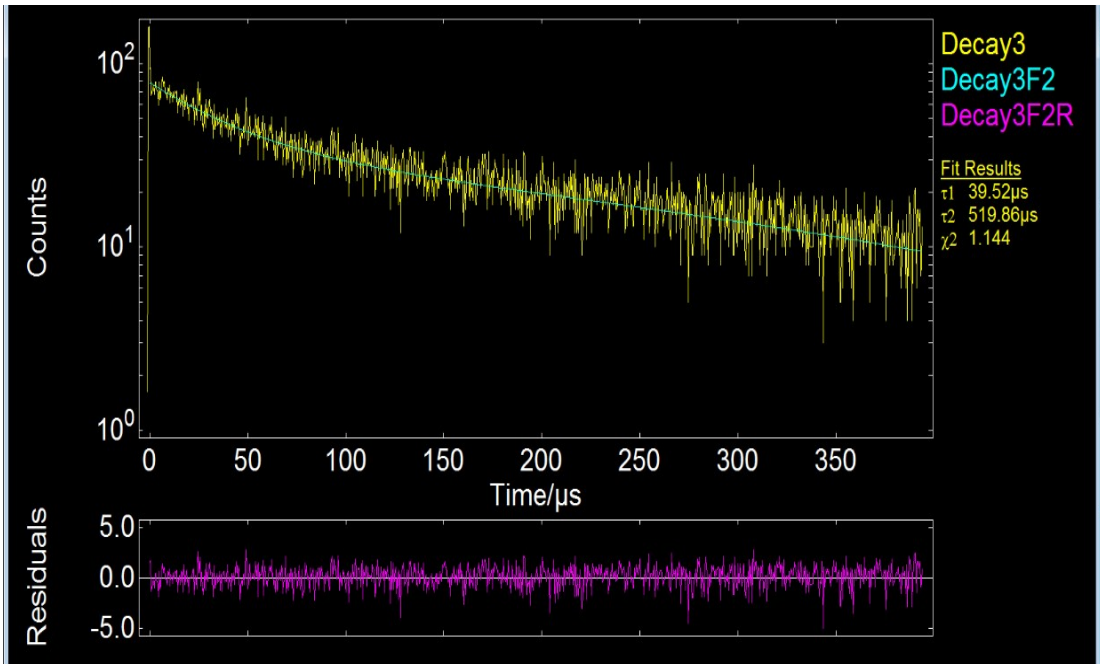

Fig. S6. Decay curve of **[Eu(btfa)$_3$1c]** with fitted curve and observed luminescence lifetime in DCM at room temperature.

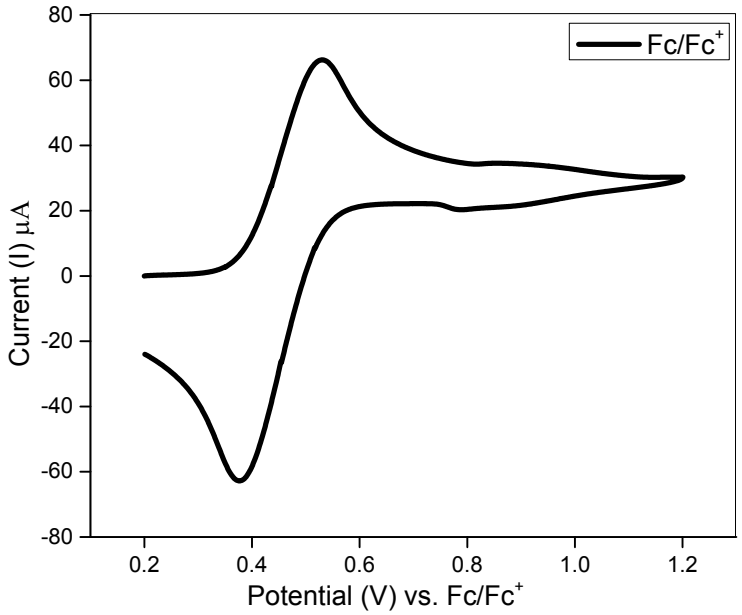

Fig. S7. CV of ferrocene/ferrocenium in the 0.0 to 1.4 V region on glassy carbon electrode in 0.1 M Bu_4NPF_6 solution in DCM at a scan rate of 100 mV/s.

References

1. R. Ilmi, A. Haque, I. J. Al-Busaidi, N. K. Al Rasbi and M. S. Khan, *Dyes Pigm.*, 2019, **162**, 59-66.