Electronic Supplementary Information to

Light Emission of a Polyfluorene Derivative Containing Complexed Europium Ions

Denis A. Turchetti[a], Mariela M. Nolasco[b], Daiane Szczerbowski[c], Luís D. Carlos[b*], Leni C. Akcelrud[a*].

[a] Paulo Scarpa Polymer Laboratory (LaPPS), Federal University of Parana, CP 19081, Curitiba/PR, 81531-990, Brazil.

[b] Physics Department and CICECO Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal.

[c] Semiochemicals Laboratory, Federal University of Parana, CP 19081, Curitiba/PR 81531-990, Brazil.

* Correspondence to: Dr. Leni C. Akcelrud, Chemistry Department, Federal University of Parana, P.O.BOX 19081, Zip Code 81.531-990 Curitiba, Parana, Brazil; Dr. Luis D. Carlos, Physics Department and CICECO Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal.

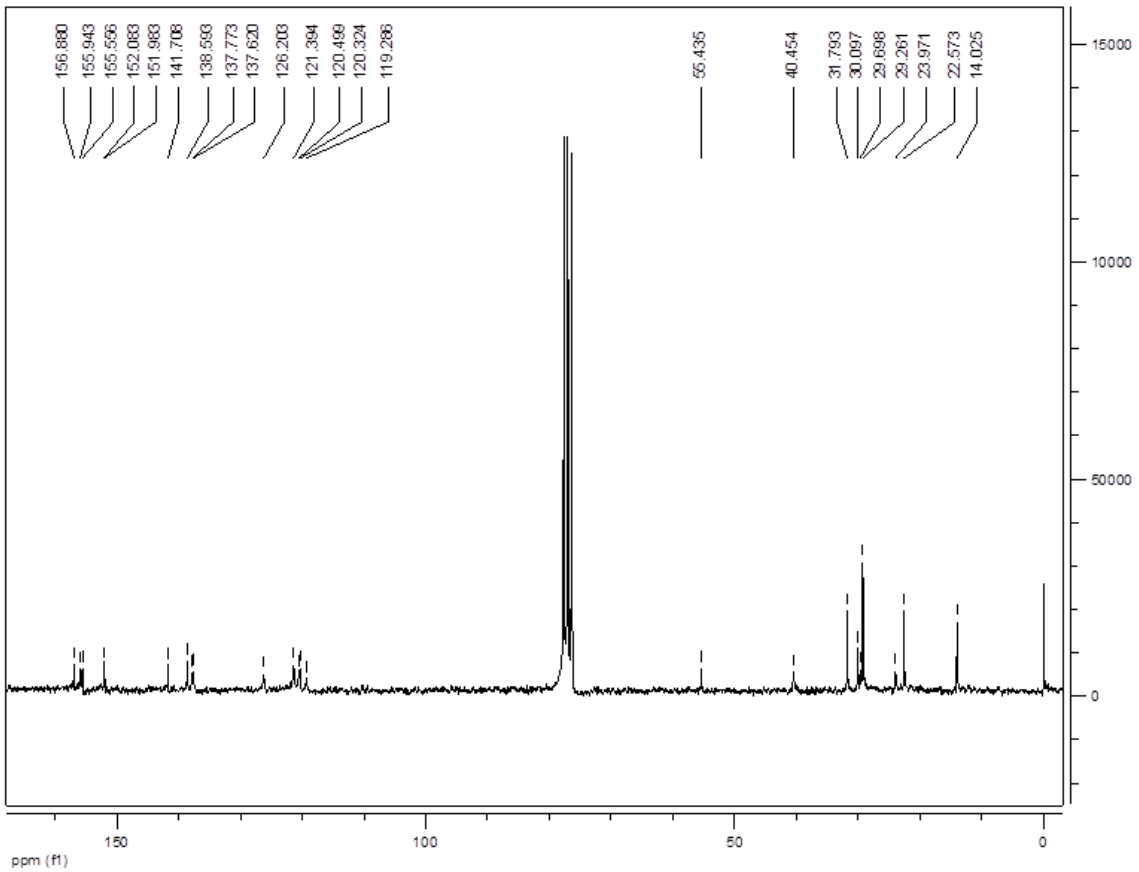
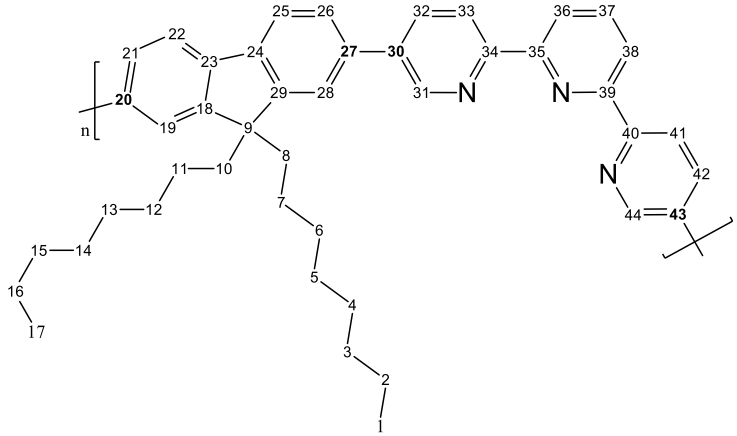


Figure S1: ^{13}C NMR of LaPPS66

Table S1: Chemical shifts of ^{13}C NMR of LaPPS66

n°	δ(ppm)
1, 17	14.02
2, 16	22.57
3, 15	23.97
4, 14	29.26
5, 13	29.69
6, 12	30.09
7, 11	31.79
8, 10	40.45
9	55.43
36, 38	119.28
33, 41	120.32
21, 26	120.49
19, 28	121.39
22, 25	126.20
30, 43	**137.62**
32, 42	137.77
20, 27	**138.59**
23, 24	141.70
37	151.98
18, 29	152.08
31, 44	155.55
34, 40	155.94
35, 39	156.88



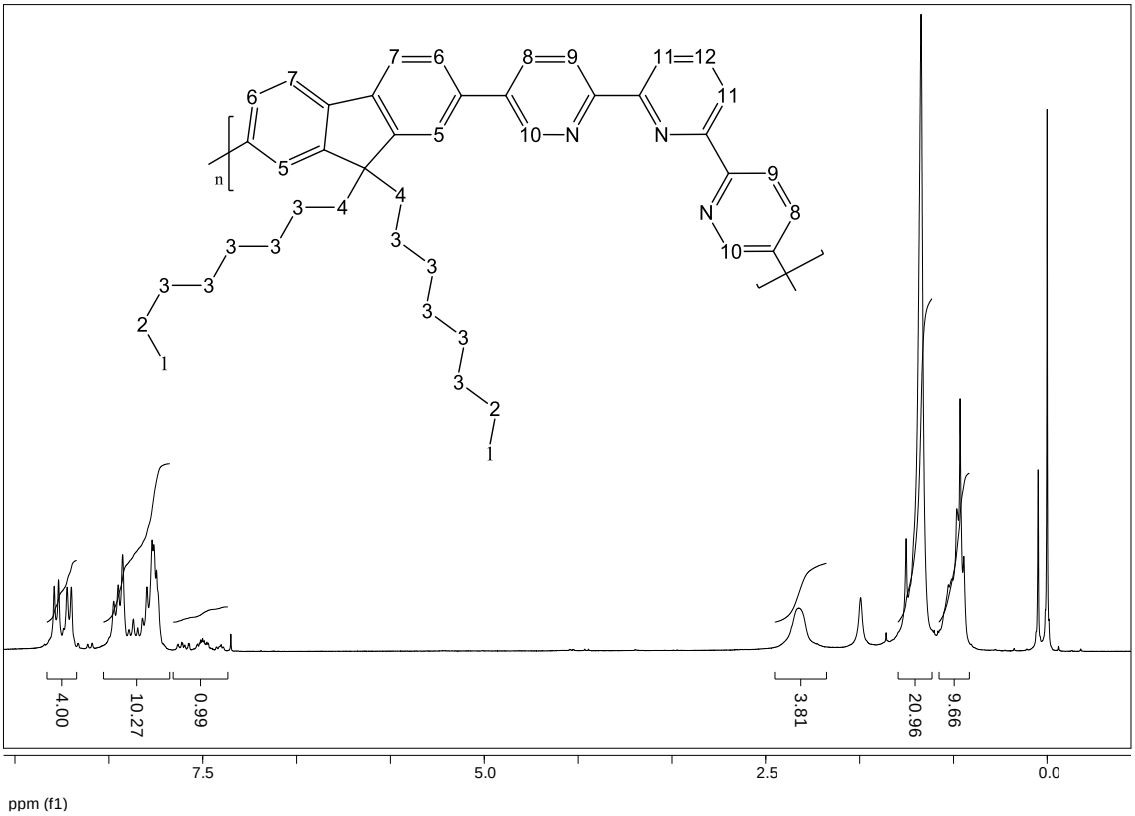
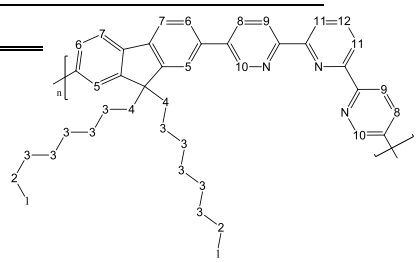


Figure S2: ^{1}H NMR of LaPPS66

Table S2: Chemical shifts of ^{1}H NMR of LaPPS66

n°	δ(ppm)	n° of protons
1, 2	0.70 – 0.95	9.66
3	1.03 - 1.32	20.96
4	**1.96 – 2.42**	**3.81**
5,6,7,8,11	7.79 – 8.38	10.36
9,10	8.62 – 8.90	4.00
12	7.28 – 7.76	0.99



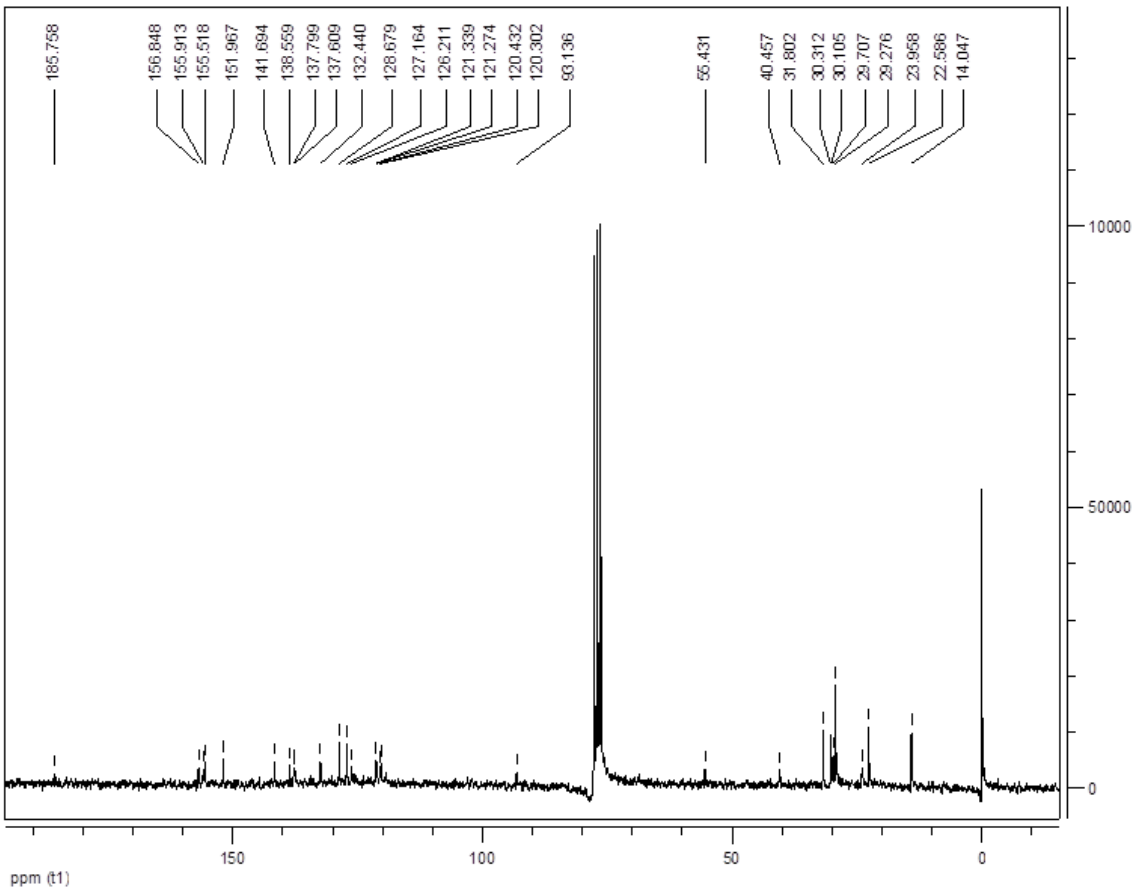
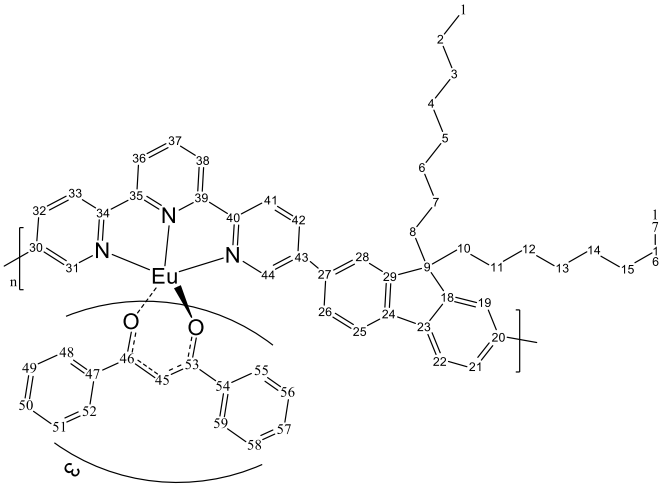


Figure S3: ^{13}C NMR of LaPPS66Eu

Table S3: Chemical shifts of ^{13}C NMR of LaPPS66Eu

n°	δ(ppm)
1, 17	14.04
2, 16	22.58
3, 15	23.95
4, 14	29.27
5, 13	29.70
6, 12	30.10
7, 11	31.80
8, 10	40.45
9	55.43
45	**93.13**
36, 38	120.30
33, 41	120.43
21, 26	121.27
19, 28	121.33
22, 25	126.21
51, 56, 58, 49	127.16
48, 52, 55, 59	128.67
50,57	132.44
30, 43	**137.62**
32, 42	137.79
20, 27	**138.55**
23, 24	141.69
37	151.96
31, 44	155.51
34, 40	155.91
35, 39	156.84
46, 53	185.75



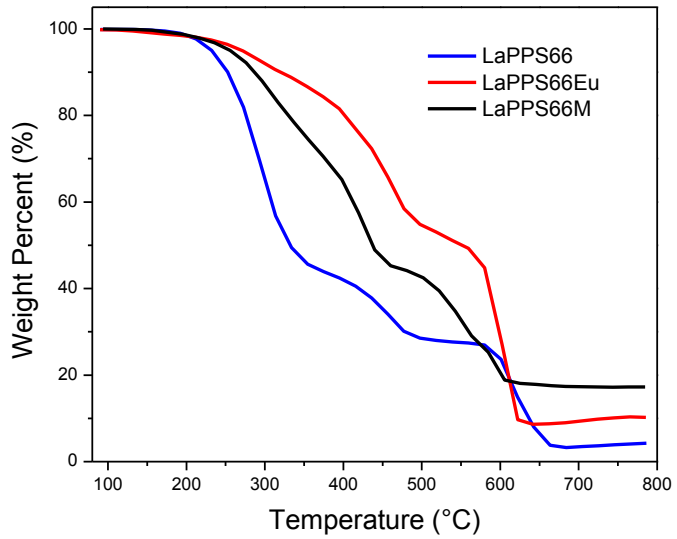


Figure S4: TGA of LaPPS66 (blue line), LaPPS66Eu (red line) and LaPPS66M (black line).

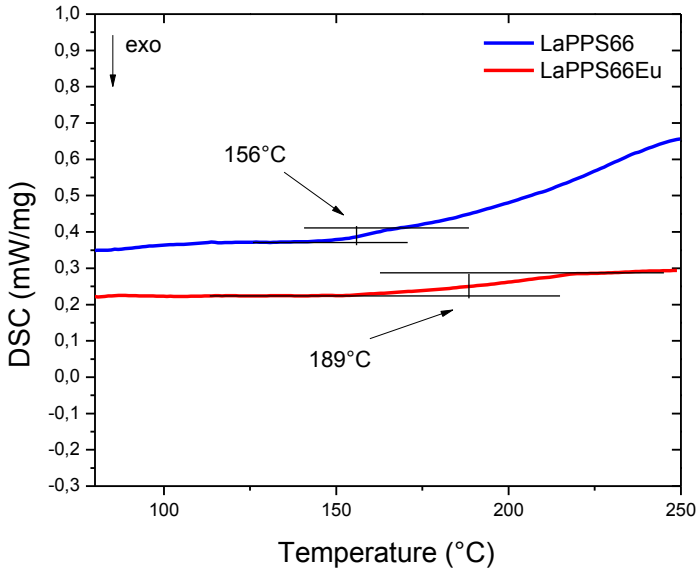


Figure S5: DSC analysis of LaPPS66 (black line) and LaPPS66Eu (red line).

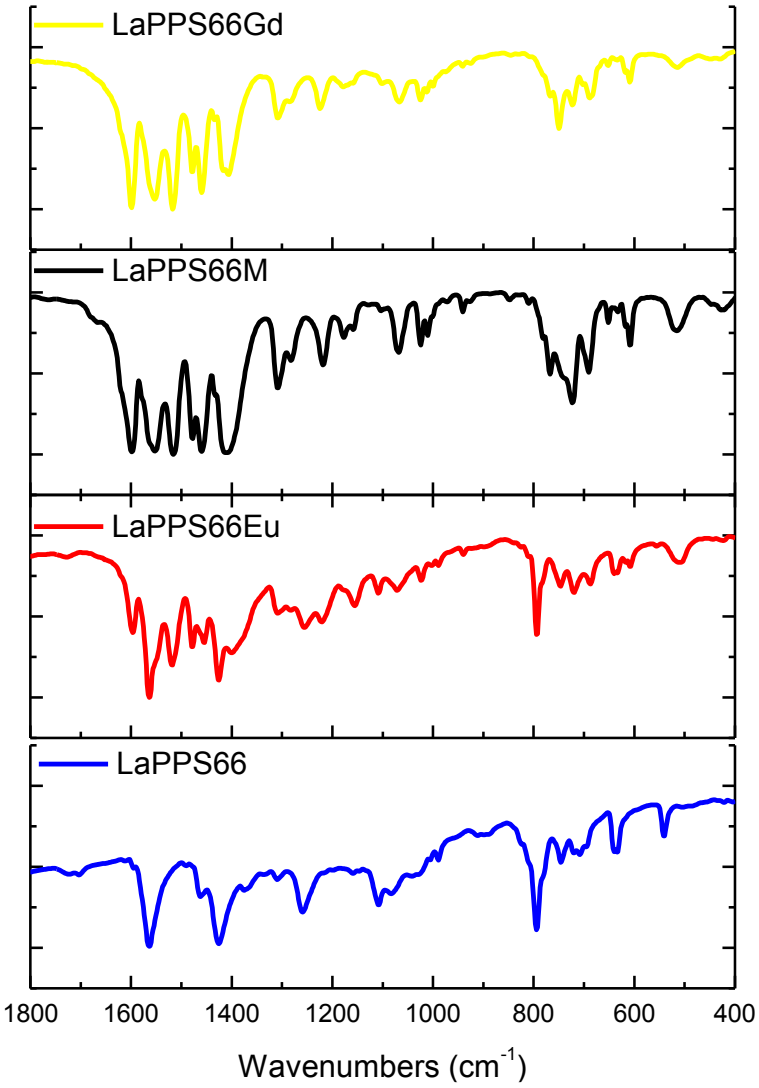
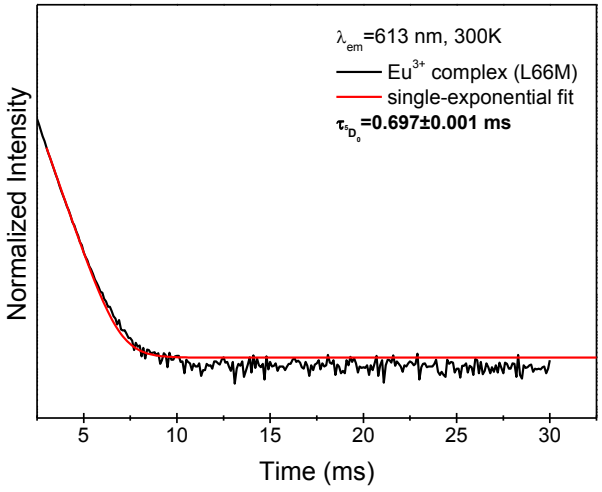
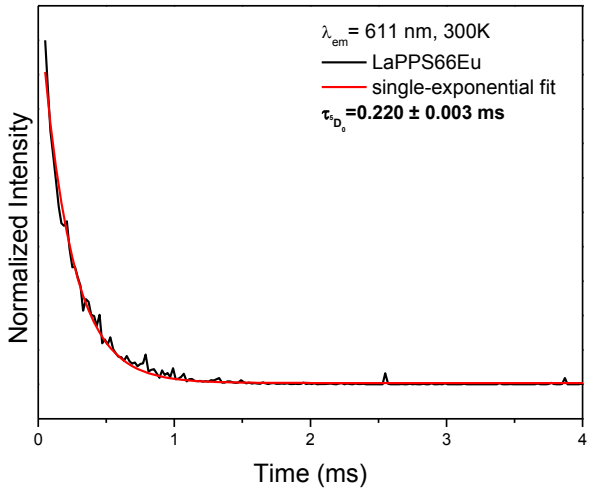


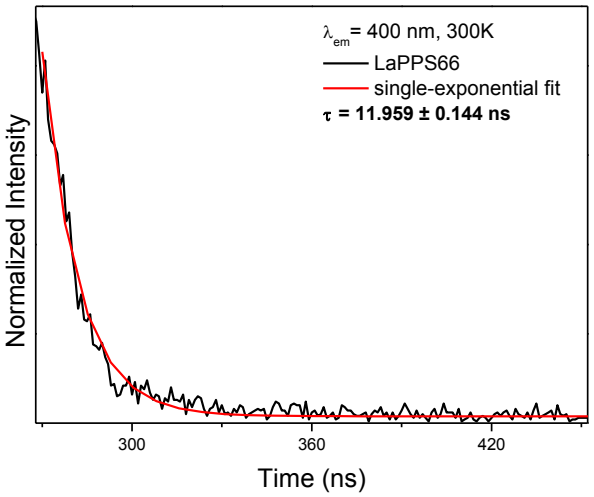
Figure S6: FT-IR analysis



(a)



(b)



(c)

Figure S7: Decay curves. a) LaPPS66M λ_{exc} = 355 nm; b) LaPPS66Eu λ_{exc} = 365 nm; c) LaPPS66 λ_{exc} = 330 nm

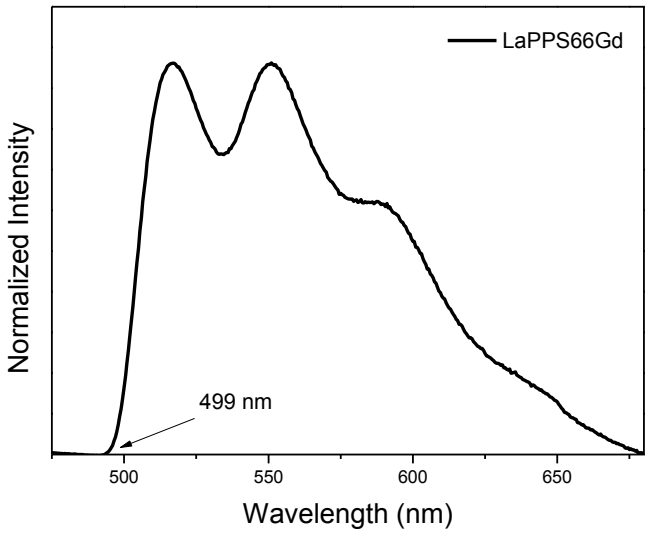


Figure S8: Normalized emission spectra of LaPPS66Gd in solid state at 11 K.

λ_{exc} = 416nm

Table S4: Absolute quantum yield

	λ_{max}1 (nm)	Φ1	λ_{max}2 (nm)	Φ2	λ_{max}3 (nm)	Φ3
LaPPS66	270	0.16	379	0.10	---	---
LaPPS66Eu	276	<0.01	365	<0.01	390	<0.01
LaPPS66M	355	0.53	412	0.31	420	0.28

Table S5: Partial molecular orbital compositions, in the ground-state singlet (S_0), for the LaPPS66M and LaPPS66Eu compounds. H stands for HOMO and L stands for LUMO.

	LaPPS66M		**LaPPS66Eu**	
Orbital	**DBM (%)**	**Terpy (%)**	**DBM (%)**	**Terpy (%)**
H-1	98.62	1.38	98.36	1.64
H	98.91	1.09	98.61	1.39
L+3	94.13	5.87	95.15	4.85
L+4	97.01	2.99	94.80	5.20

Table S6: Calculated TD-B3LYP vertical electronic excitation energies related with the triplet states, in the ground-state singlet (S_0), for the LaPPS66M and LaPPS66Eu compounds.

LaPPS66M	**Composição[a]**	**CI[b]**	**LaPPS66Eu**	**Composição[a]**	**CI[b]**
	H-1→L+3	0.48244		H-1→L+3	0.38075
T_1	H-1→L+4	0.23150	T_1	H-1→L+4	0.26388
	H→L+3	0.29603		H→L+3	0.36461

[a] Only the three primary transitions are reported; H stands for HOMO and L stands for LUMO.
[b] The CI coefficients are in absolute values.