Table S1 Energy and % contribution of atomic orbitals to each molecular orbital in the frontier region for (a) $[Ru(bipy)_2(L1)]^+$ and (b) $[Ru(bipy)_2(HL1)]^{2+}$. The contribution of both **HL1** and **L1**$^-$, the protonated and the deprotonated pyridyltriazole ligands, is divided into a pyridinetriazole component , *pytrz* and a contribution from the dimethoxyphenyl moiety, *ph*.

(a) Deprotonated

MO	eV	Ru	bipy1	bipy2	pytrz	ph
L+4	-2.95	4	60	19	17	0
L+3	-3.06	3	35	56	6	0
L+2	-3.30	5	8	22	65	0
L+1	-3.58	9	50	37	4	0
LUMO	-3.93	2	38	50	10	0
HOMO	-8.76	37	6	16	30	11
H-1	-9.15	57	20	10	13	0
H-2	-9.63	20	9	7	17	48
H-3	-10.00	72	7	6	5	9
H-4	-10.33	4	8	2	33	53

(b) Protonated

MO	eV	Ru	bipy1	bipy2	pytrz	ph
L+4	-5.26	2	23	8	66	1
L+3	-5.30	1	79	2	18	1
L+2	-5.97	8	9	74	9	0
L+1	-6.06	9	57	1	32	1
LUMO	-6.33	1	29	20	50	1
HOMO	-11.99	38	2	6	25	29
H-1	-12.22	69	15	13	3	0
H-2	-12.27	69	12	4	13	1
H-3	-12.43	29	2	5	5	60
H-4	-13.15	3	0	1	7	88