Electronic Supplementary Information (ESI)

An aggregation-induced emission-active bis-heteroleptic ruthenium(II) complex of thiophenyl substituted phenanthroline for selective "turn-off" detection of picric acid

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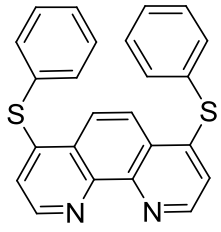
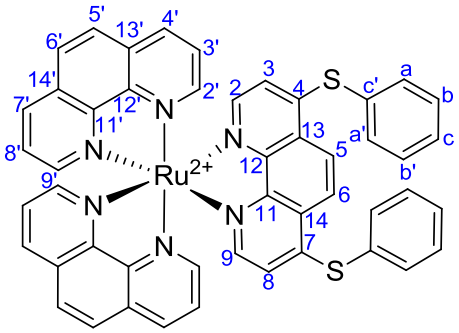
Chart S1: Compound used in this study



L1



Ru-1

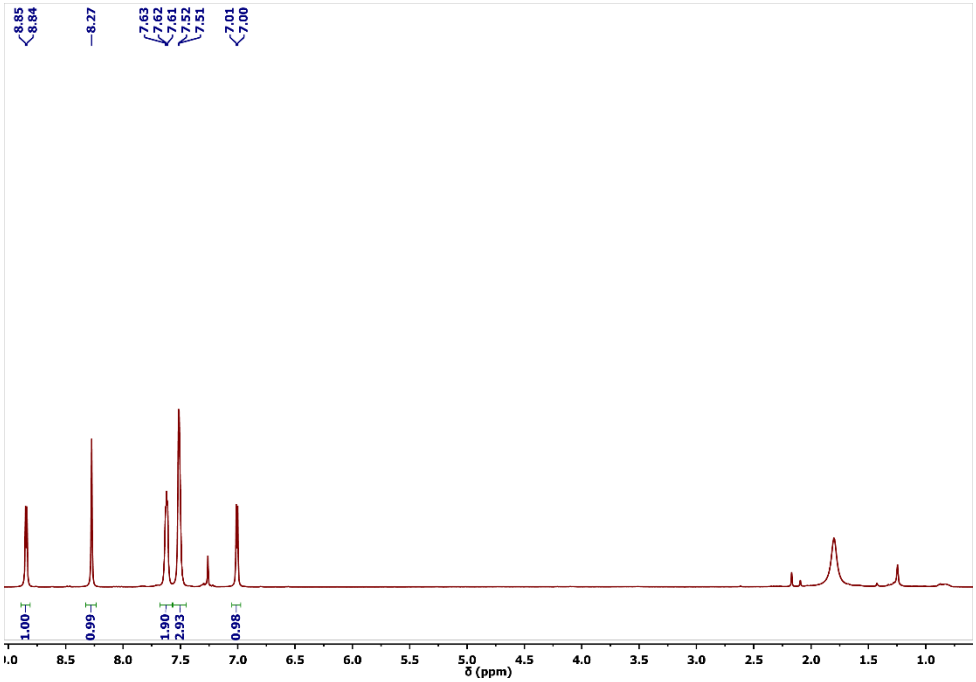


Figure S1. ^{1}H NMR spectrum of **L1** in $CDCl_3$.

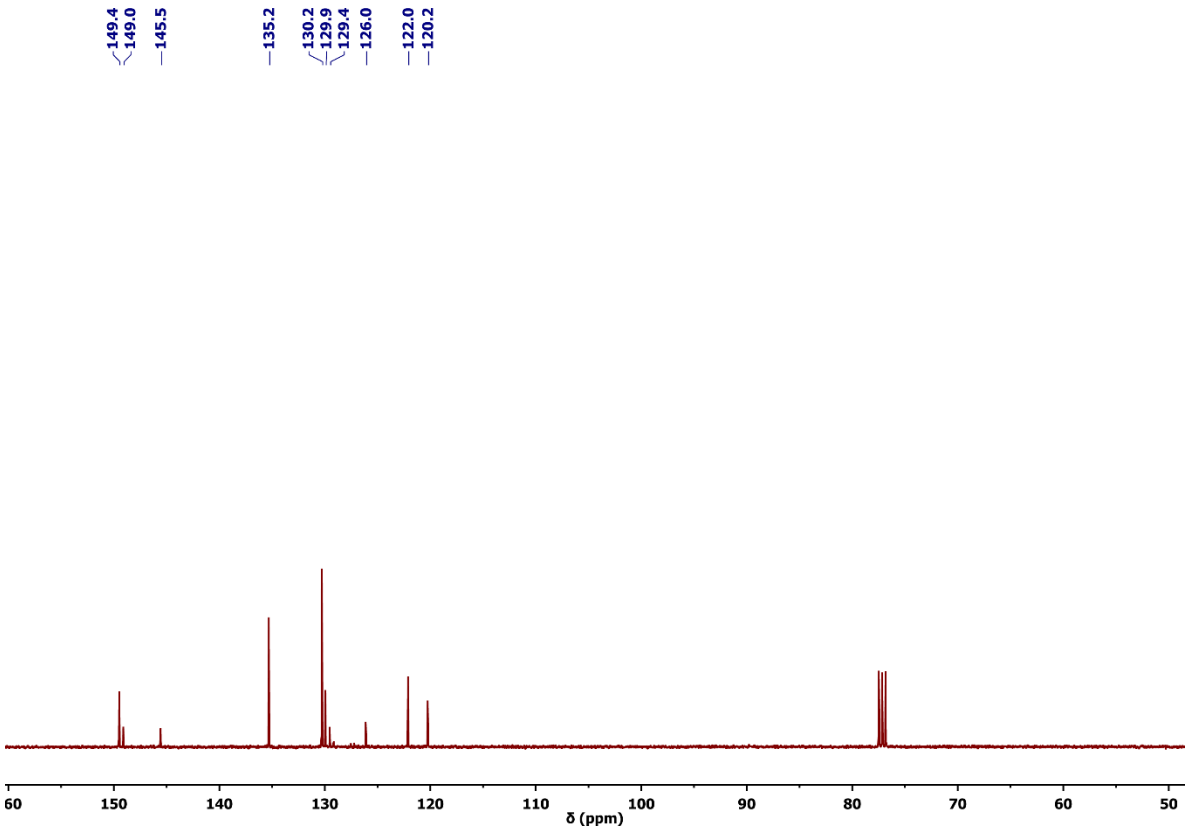


Figure S2. ^{13}C NMR spectrum of **L1** in $CDCl_3$.

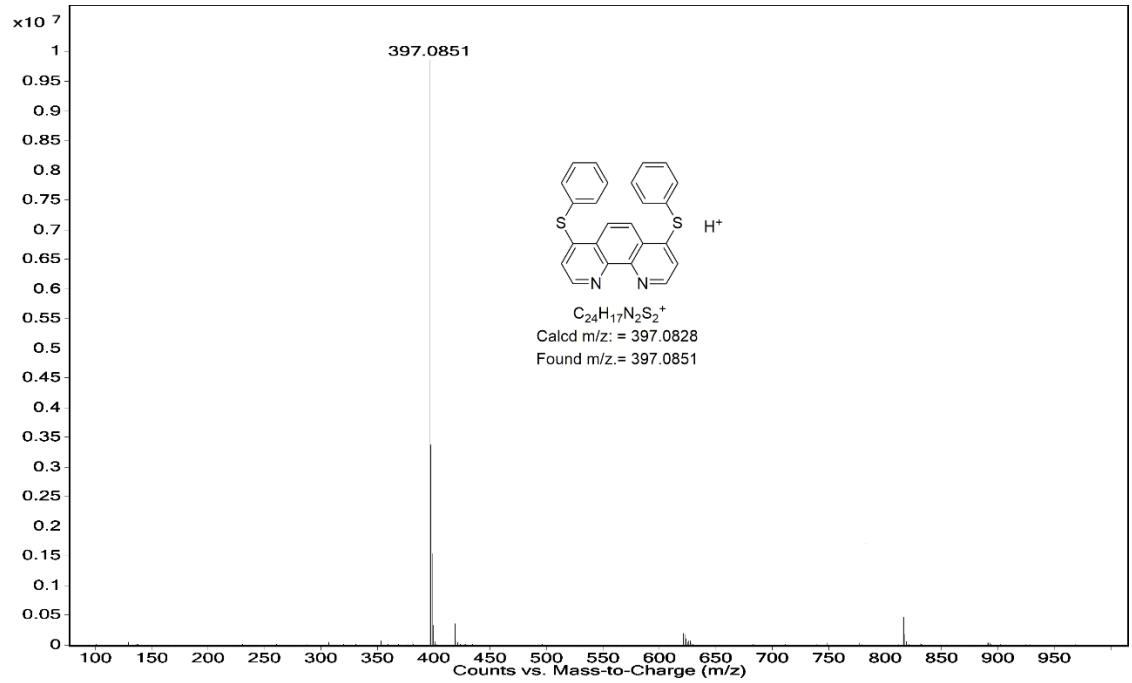


Figure S3. ESI-MS spectrum of **L1** in CH_3OH.

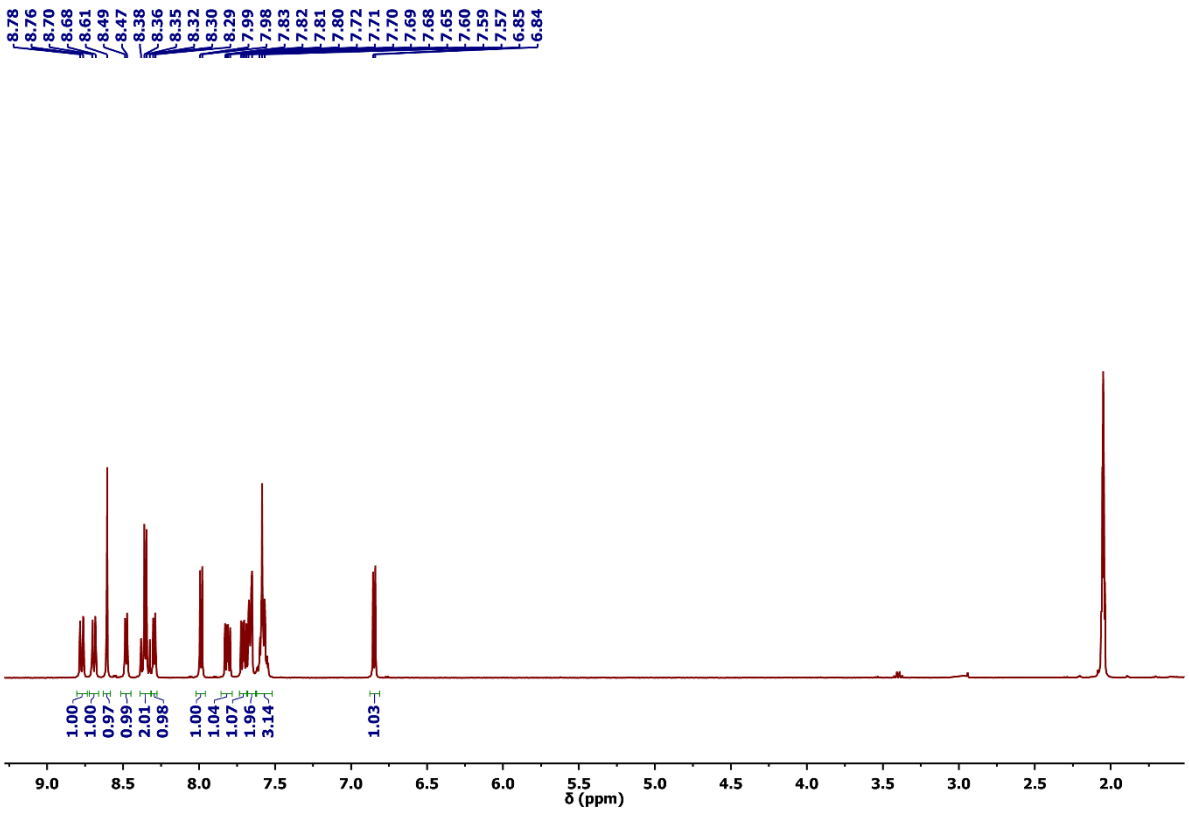


Figure S4. ^{1}H NMR spectrum of **Ru-1** in Acetone-d_6.

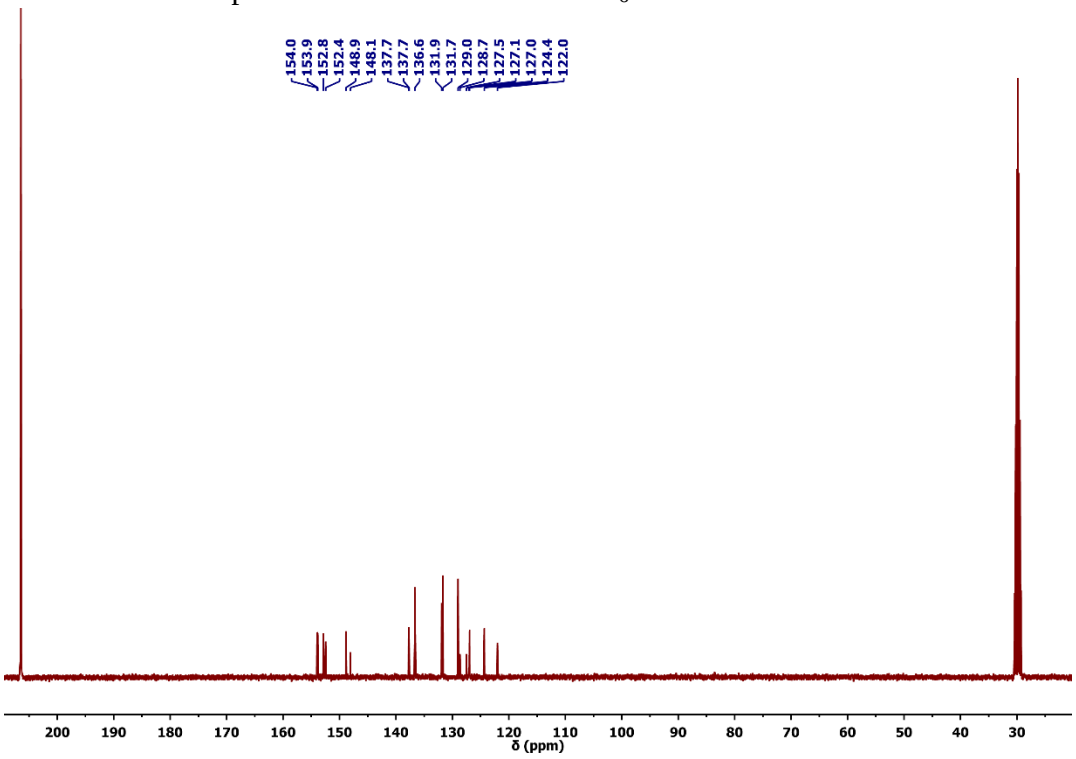


Figure S5. ^{13}C NMR spectrum of **Ru-1** in Acetone-d_6.

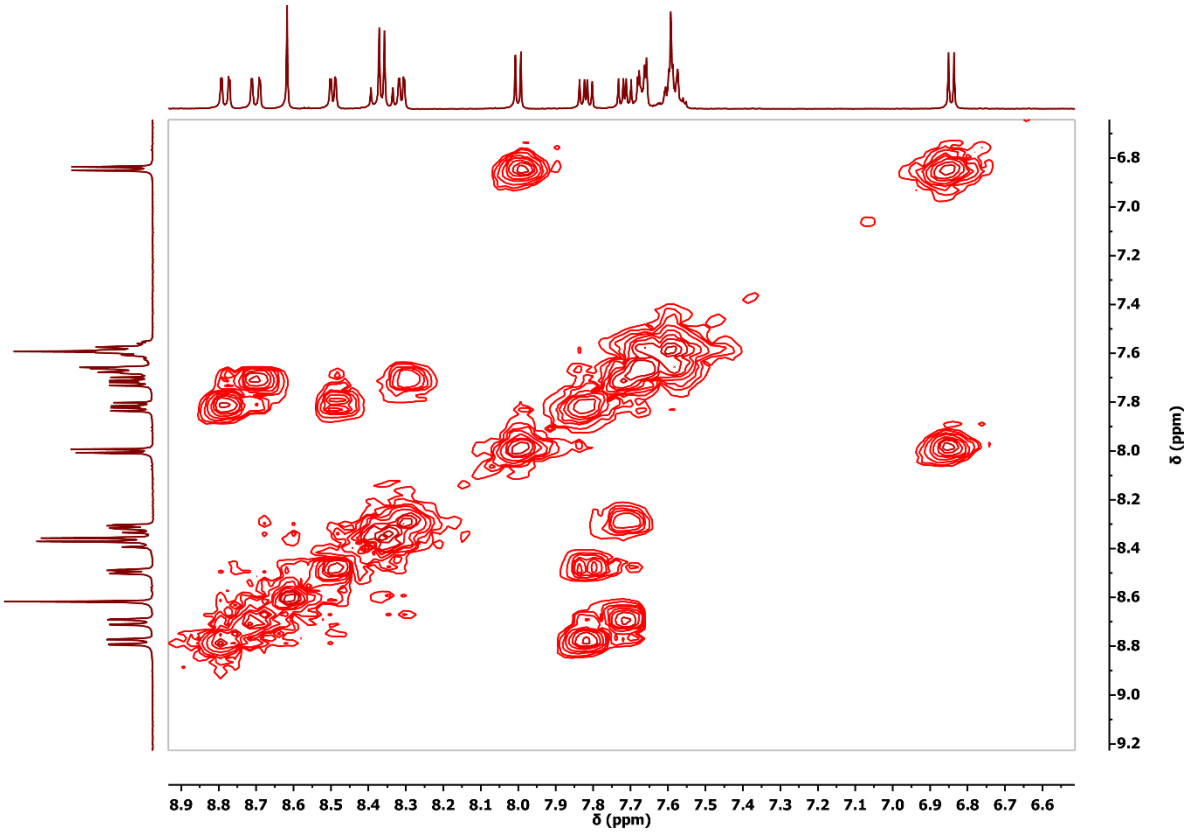


Figure S6. ^{1}H-^{1}H COSY NMR spectrum of **Ru-1** in Acetone-d_6.

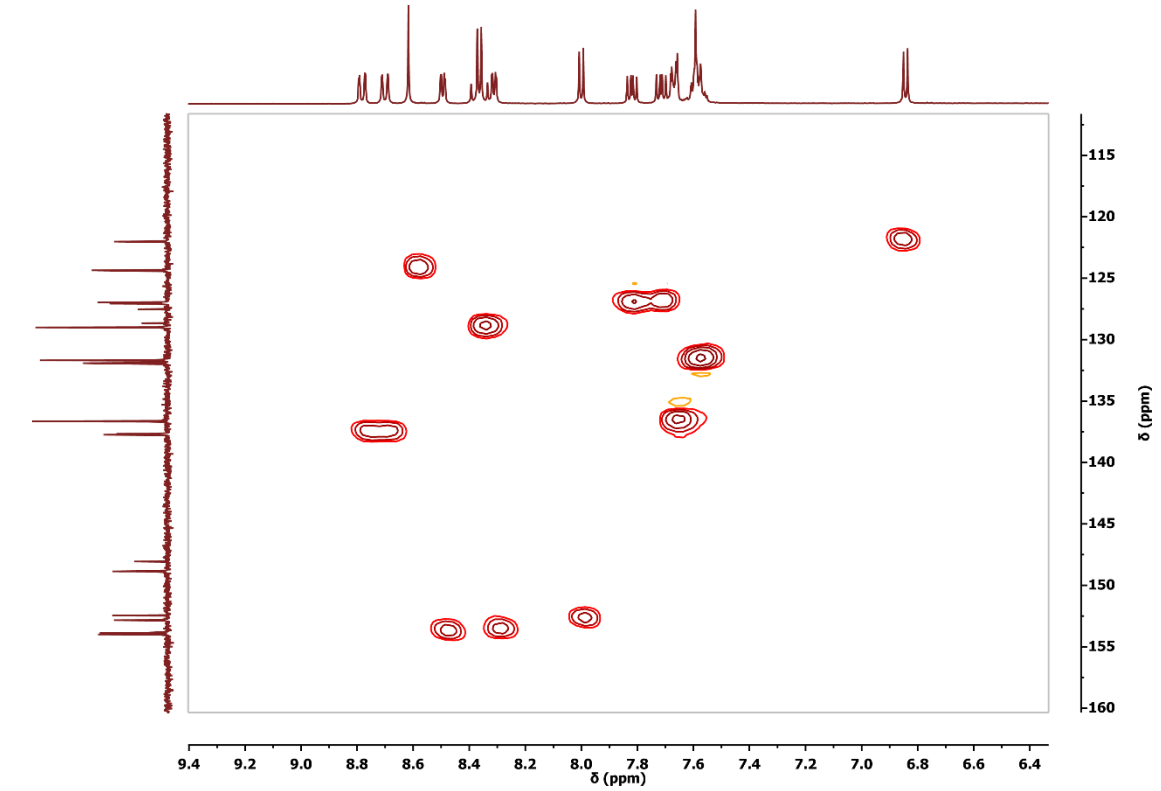


Figure S7. ^{1}H-^{13}C HSQC NMR spectrum of **Ru-1** in Acetone-d_6.

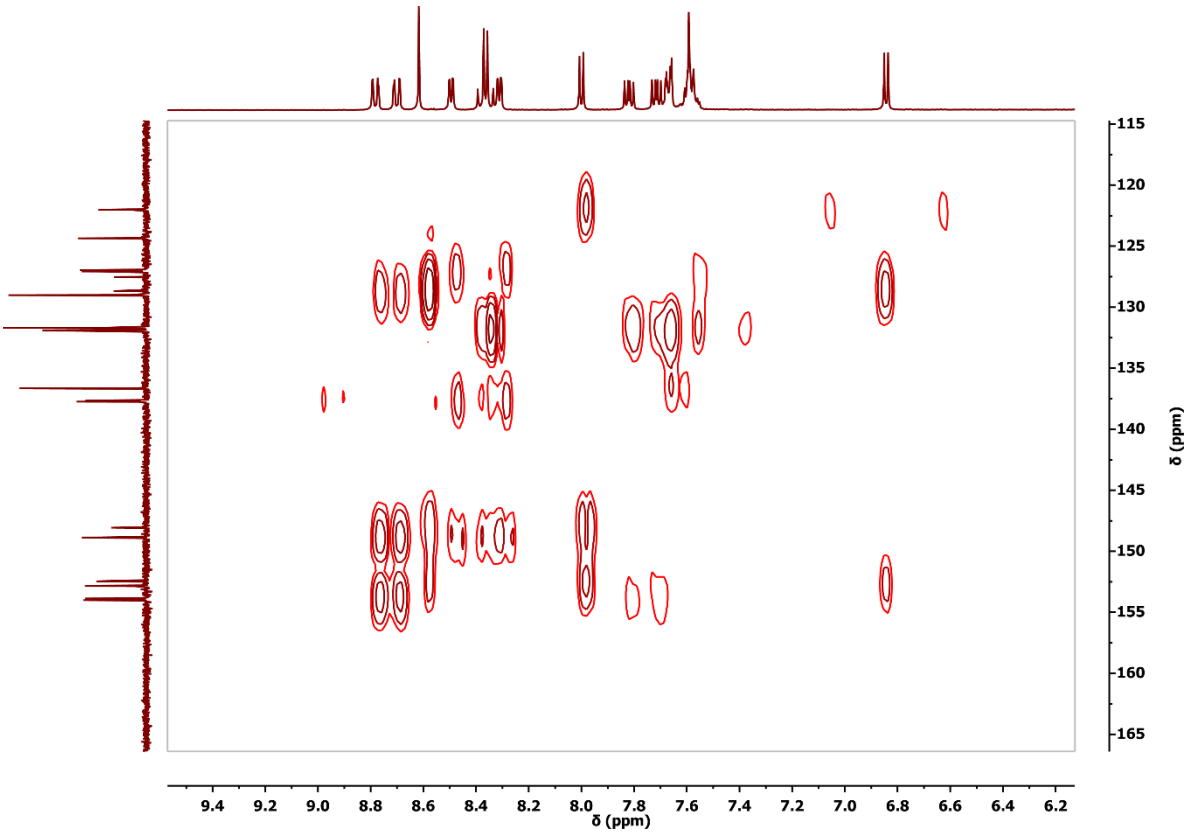


Figure S8. Partial ^{1}H-^{13}C HMBC NMR spectrum of **Ru-1** in Acetone-d_6.

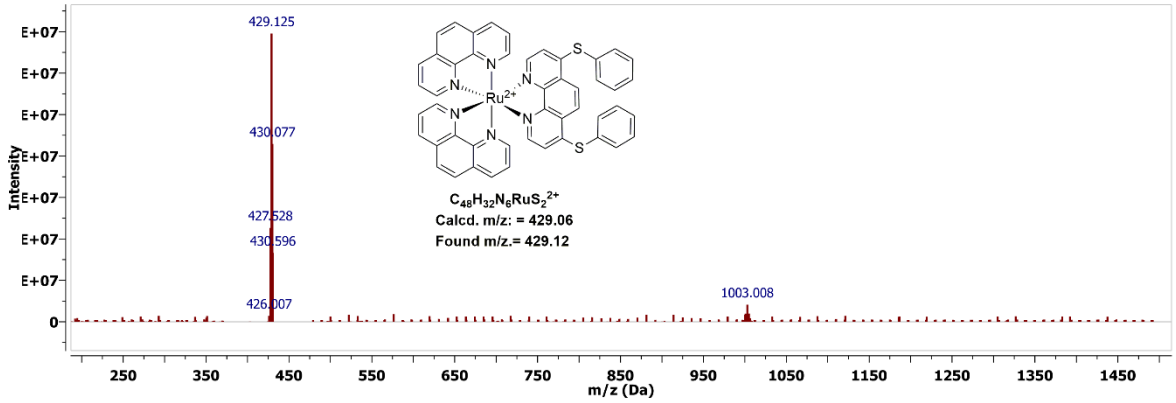


Figure S9. ESI-MS spectrum of **Ru-1** in CH_3CN

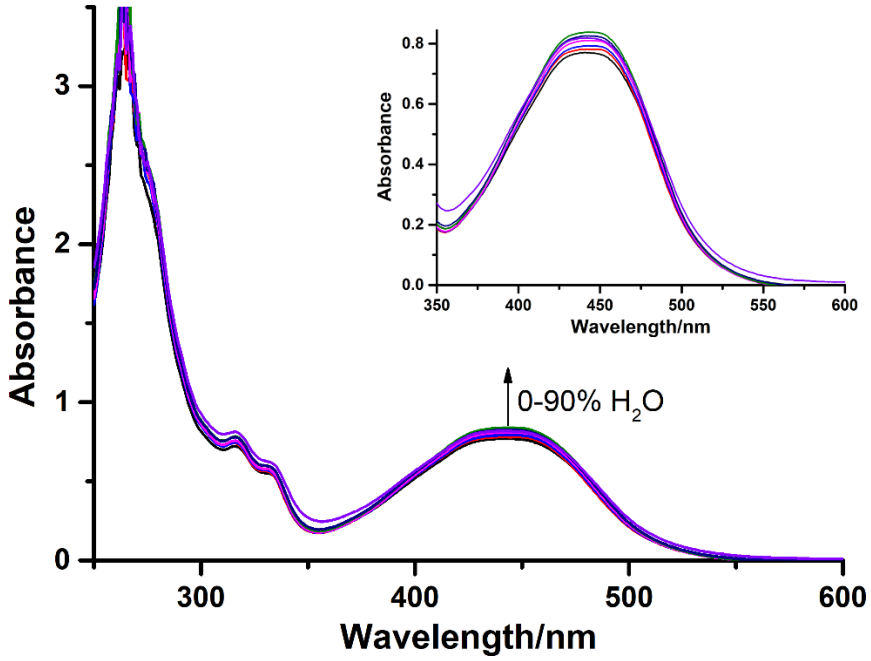


Figure S10. UV-vis spectra of **Ru-1** (25 μM) in CH_3CN with increasing water fractions (0-90%).

Table S1. List of reported picric acid selective probes and their Limit of Detection (LOD)

SL No	Probe	Limit of Detection (LOD)	Medium	References
1	Anthracene-bridged poly(N-vinyl pyrrolidone)	6.0 μM	Water	*Analyst*, 2019, **144**, 3620–3634
2	Pyrene based polymer	56 μM	Water	*ACS Appl. Mater.Interfaces* 2018, **10**, 41717−41723.
3.	Bispyrene-Based	1.0 μM	Water	*Langmuir*, 2014, **30**, 7645−7653
4.	Zn(II)-based MOF	1.0 μM	Water	*CrystEngComm*, 2015, **17**, 9404–9412
5.	Anthracene Derivatives	0.5 ppm	THF	*Chem. Eur. J.* 2016, **22**, 2012 – 2019
6.	a-cyanostilbene Derivatives	1.9 μM	H_2O/THF (7:3 v/v)	*Chem. Eur. J.* 2014, **20**, 12215 – 12222
7.	Triphenylamine	20 μM	H_2O: THF (9:1)	*Chemistry Select*, 2019, **4**, 2868 –2873
8.	Lanthanide based coordination polymer	49 μM	Chloroform	*Cryst. Growth Des*. 2017, **17**, 3907-3916.
9.	Triazole trindane based probe	5.48 μM	H_2O/DMSO (1:1)	*Chemistry Select*, 2019, **4**, 10895-10901
10.	Benzimidazole-acrylonitriles derivative	41, 34, 11 μM	Water	*J. Photochem. Photobiol., A: Chemistry*, 2021, **404**, 112874
11.	Triphenylbenzene	1.5 ppm	Acetonitrile	*New J. Chem.*, 2015, **39**, 886-892
12.	Zn(II) MOF	1.12 ppm	DMF	*Dalton Trans.*, 2018, **47**, 9627–9633
13.	Pyrene derivative	19 μM	DMSO	*Chem. – Eur. J.*, 2008, **14**, 1822–1827
14.	Polymer	40.7 μM	Water	*Anal. Chem.*,2010, **82**, 4015–4019
15.	Ru(II) complex	4.7 μM or 1.08 ppm	H_2O: CH_3CN (7:3 v/v)	***This Work***

Table S2. Selected bond lengths and angles in the optimized structure of **Ru-1**

Bond lengths (Å)			
N(32)- Ru(47)	2.1135	N(39)- Ru(47)	2.1135
N(25)- Ru(47)	2.1275	N(18)- Ru(47)	2.1223
N(11)-Ru(47)	2.1275	N(4)-Ru(47)	2.1223
Bond angles (°)			
N(4)- Ru(47)- N(11)	78.52	N(4)- Ru(47)- N(18)	173.25
N(4)- Ru(47)- N(25)	96.60	N(4)- Ru(47)- N(32)	89.09
N(4)- Ru(47)- N(39)	96.17	N(11)- Ru(47)- N(18)	96.60
N(11)- Ru(47)- N(25)	88.80	N(11)- Ru(47)- N(32)	96.87
N(11)- Ru(47)- N(39)	172.68	N(18)- Ru(47)- N(25)	78.52
N(18)- Ru(47)- N(32)	96.17	N(18)- Ru(47)- N(39)	89.09
N(25)- Ru(47)- N(32)	172.68	N(25)- Ru(47)- N(39)	96.87
N(32)- Ru(47)- N(39)	77.87		

Table S3: The x,y,z Cartesian coordinates of the complex **Ru-1** calculated using Gaussian 09 at B3LYP/6-31G(d) level and LANL2DZ for ruthenium and silver.

Ru-1			
C	2.33107 -0.84047 4.82271	C	-1.06127 -0.72036 -0.02556
C	1.39254 0.09224 4.42262	C	-2.28394 -1.4397 -0.05901
C	1.22252 0.36056 3.05375	C	-1.06243 0.71699 0.02437
N	1.93546 -0.25057 2.10372	C	-2.28634 1.43435 0.05755
C	2.86392 -1.18019 2.488	C	-3.50187 0.67857 0.02433
C	3.10155 -1.50903 3.8449	C	-3.50075 -0.68602 -0.02597
C	3.61389 -1.82788 1.45319	N	0.16531 1.32745 0.02571
C	4.59669 -2.79079 1.78903	C	0.19803 2.66253 0.03201
C	4.81951 -3.10383 3.1729	C	-0.95397 3.45138 0.07289
C	4.10186 -2.49099 4.15781	C	-2.21891 2.86532 0.10039
N	3.3326 -1.47747 0.16029	S	-3.58389 3.99855 0.03679
C	4.02472 -2.06723 -0.81832	C	-4.8235 3.38133 1.1847
C	5.0188 -3.02998 -0.57396	S	-3.57872 -4.00437 -0.03836

C	5.30706	-3.39553	0.72767	C	-4.81715	-3.38601	-1.18701
C	2.33249	0.84236	-4.82246	Ru	1.81079	0.00053	-0.00003
C	1.3952	-0.09183	-4.4229	C	-6.13369	-3.26033	-0.72565
C	1.22481	-0.36039	-3.05412	C	-7.14388	-2.8976	-1.61966
N	1.93624	0.25186	-2.10368	C	-6.84028	-2.64705	-2.95891
C	2.86346	1.18293	-2.48744	C	-5.52428	-2.77465	-3.4129
C	3.10135	1.51214	-3.84421	C	-4.51074	-3.15862	-2.53503
C	3.61182	1.83179	-1.45222	C	-6.14529	3.28304	0.73164
C	4.59329	2.79626	-1.78749	C	-7.1543	2.92242	1.62784
C	4.81641	3.10966	-3.17123	C	-6.84458	2.64713	2.96083
C	4.10029	2.49567	-4.15656	C	-5.52343	2.74768	3.40662
N	3.33036	1.48092	-0.15948	C	-4.51062	3.1291	2.5268
C	4.02099	2.07177	0.81953	H	2.48146	-1.06418	5.87491
C	5.01368	3.03609	0.57575	H	0.78364	0.62267	5.14683
C	5.3021	3.40211	-0.72572	H	0.49459	1.08866	2.71394
C	-2.21425	-2.87053	-0.10182	H	5.57443	-3.84373	3.42172
C	-0.94853	-3.45472	-0.07401	H	4.27783	-2.73719	5.20073
C	0.20226	-2.66399	-0.03283	H	3.77808	-1.76648	-1.83047
N	0.16742	-1.32897	-0.02654	H	5.54539	-3.47357	-1.41215
H	0.49783	-1.08963	-2.71473	H	6.06977	-4.13857	0.94206
H	5.57029	3.85075	-3.41962	H	2.48313	1.06629	-5.87457
H	4.27647	2.74215	-5.19937	H	0.78756	-0.62322	-5.14746
H	3.77424	1.77061	1.83154	H	-4.44384	-1.21501	-0.04748
H	5.53909	3.48051	1.41424	H	1.18004	3.12233	0.02916
H	6.06375	4.14636	-0.93967	H	-0.85188	4.53082	0.1063
H	-0.84481	-4.534	-0.10734	H	-6.36683	-3.45104	0.31777
H	1.18503	-3.12217	-0.02966	H	-8.16683	-2.81033	-1.2656
H	-4.44587	1.20594	0.04569	H	-7.62797	-2.36403	-3.65062
H	-8.18113	2.85639	1.28048	H	-5.2901	-2.597	-4.45861
H	-7.63139	2.36595	3.65429	H	-3.49573	-3.295	-2.89628
H	-5.28426	2.55079	4.44774	H	-6.38318	3.4933	-0.30692