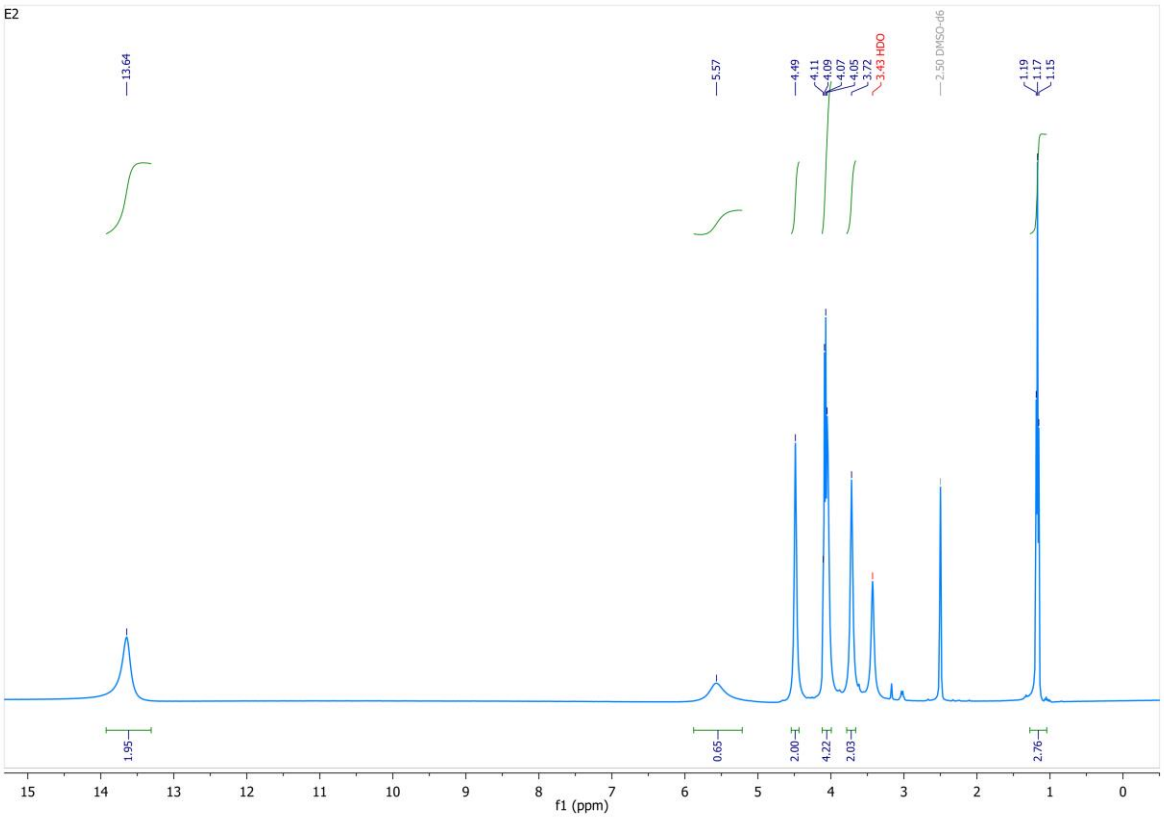
Novel hydroxyl-functionalized 1,2,4-triazole-based oligomers: synthetic approach, photoluminescence and coordination behaviour as uranyl chelators

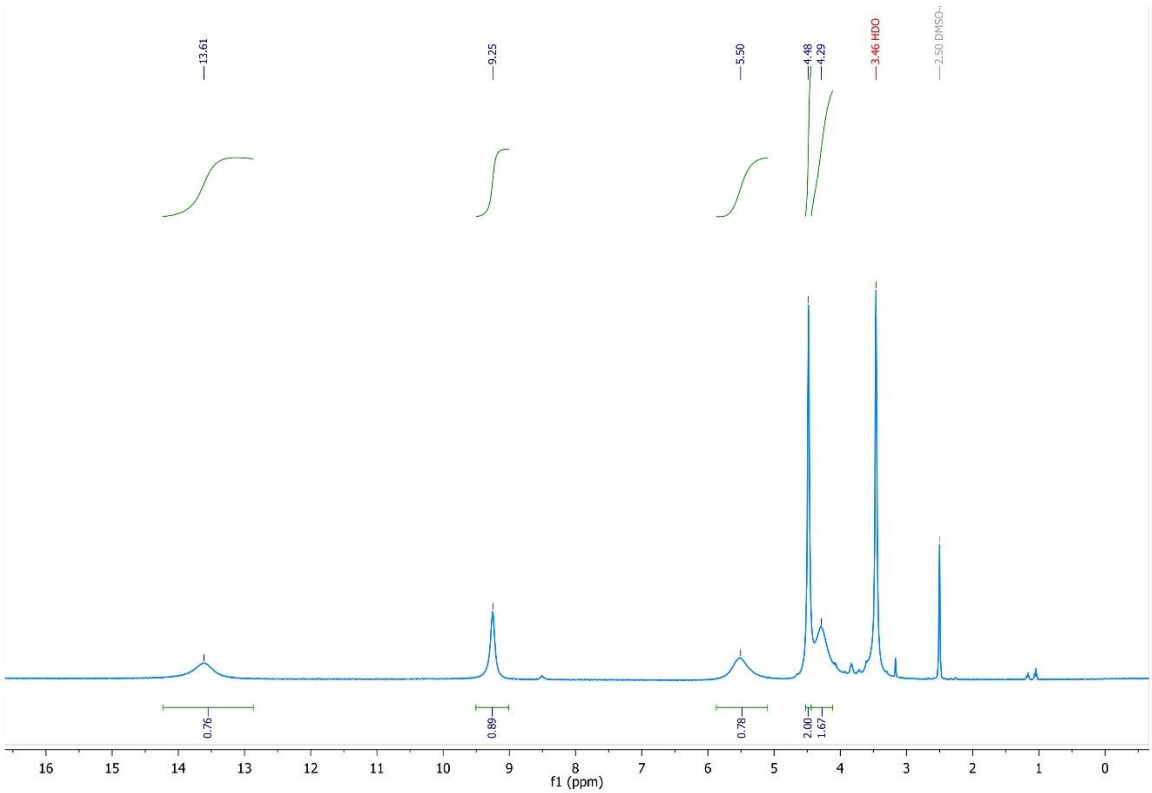
Dmytro M. Khomenko,[a,b] Oleksandr V. Vashchenko,[a] Roman O. Doroshchuk,[a,b] Viktoriia S. Starova,[a] Mariia Hreben,[a,c] Valerii Bukhanko,[a] Andrii V. Yatsymyrskyi,[a] Sergiu Shova,[d] Olga Yu. Vassilyeva[a*] and Rostyslav D. Lampeka[a]

[a] *Department of Chemistry, Taras Shevchenko National University of Kyiv, 12 Hetman Pavlo Skoropadskyi St., Kyiv 01601, Ukraine.*
[b] *Enamine Ltd, 78 Winston Churchill St., Kyiv 02094, Ukraine.*
[c] *L.I. Medved's Research Center of Preventive Toxicology, Food and Chemical Safety, Ministry of Health, Ukraine (State Enterprise), 6 Heroiv Oborony St., Kyiv 03127, Ukraine*
[d] *"PetruPoni" Institute of Macromolecular Chemistry, Aleea Gr. GhicaVoda 41 A, Iasi 700487, Romania.*

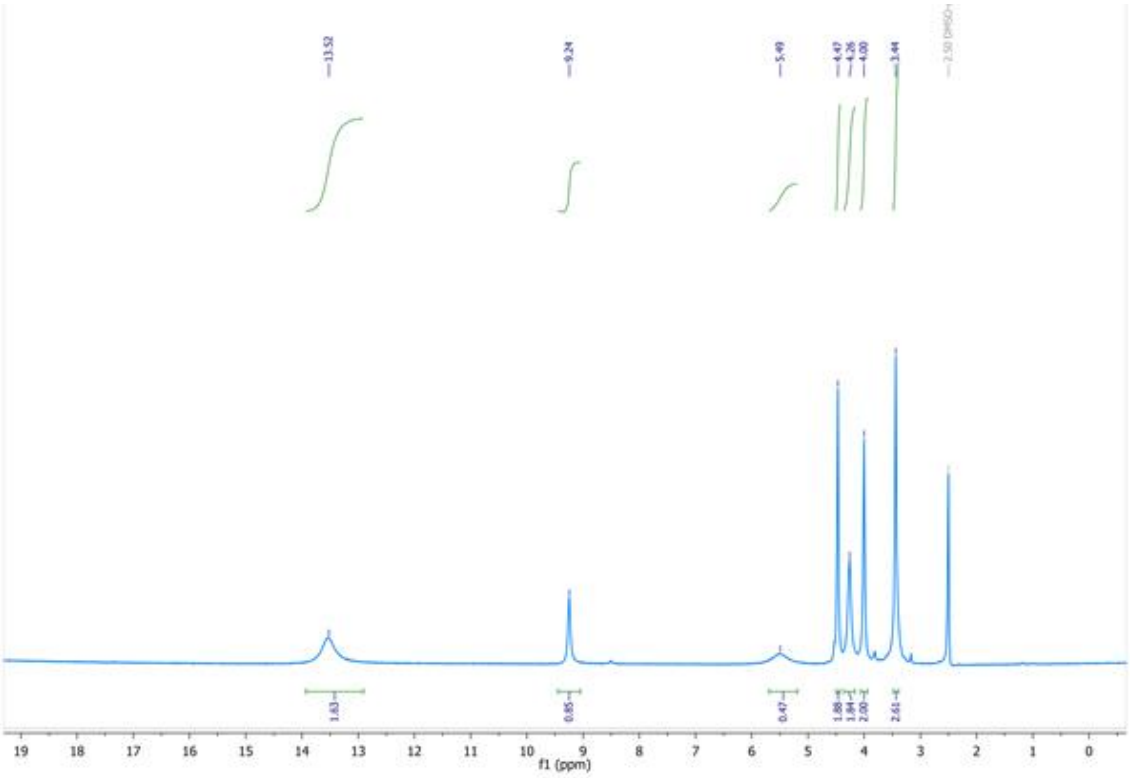
Supplementary information


E2
13.64
5.57
4.49
4.11
4.09
4.07
4.05
3.72
3.43 HDO
2.50 DMSO-d6
1.19
1.17
1.15
1.95
0.65
2.00
4.22
2.03
2.76
f1 (ppm)

(a)

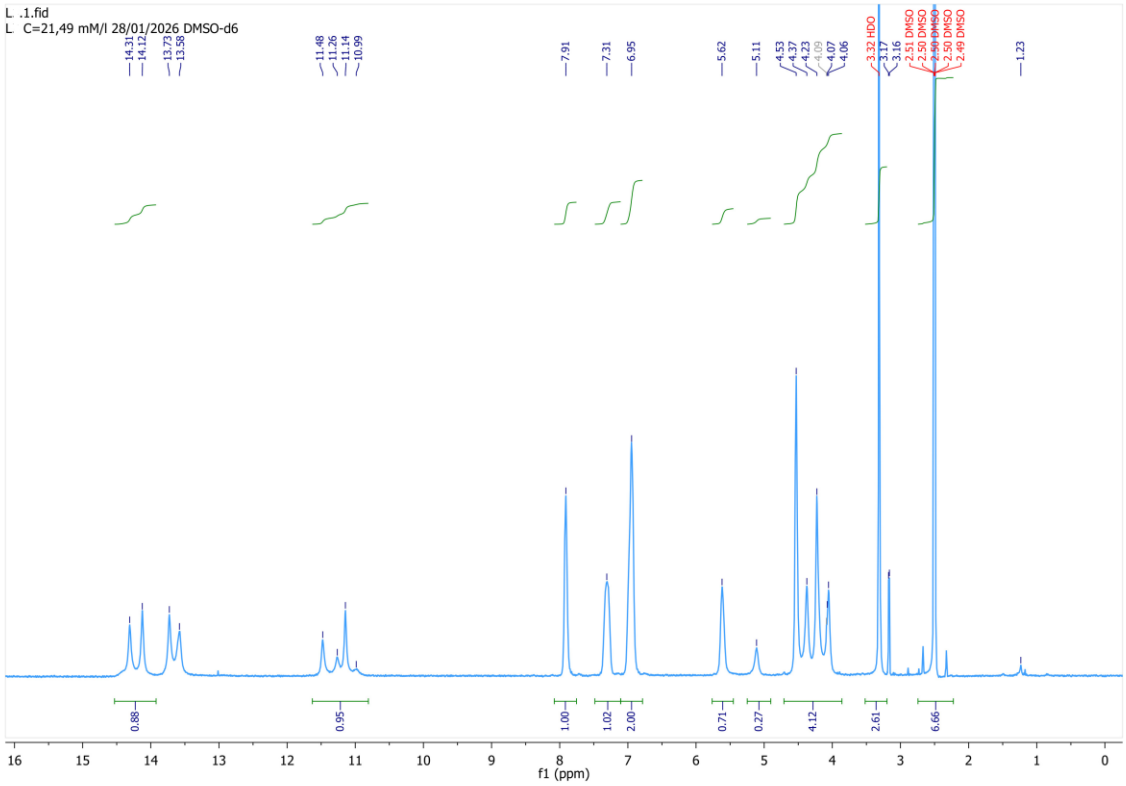

13.61
9.25
5.50
4.48
4.29
3.46 HDO
2.50 DMSO-
0.76
0.89
0.78
2.00
1.67
f1 (ppm)

(b)

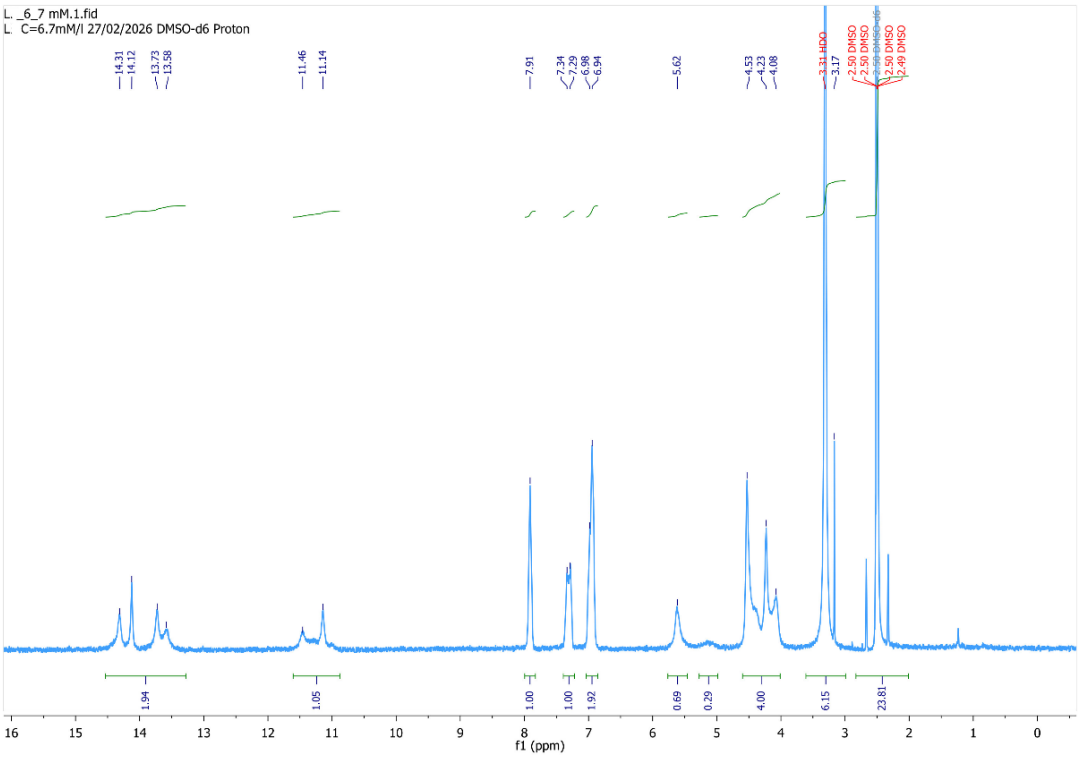


(c)

Fig. S1. ^{1}H NMR spectra of initial 1,2,4-triazole containing acetic acid ethyl ester and hydrazides **E2** (a), **H2** (b) and **H3** (c) in DMSO-d_6.



(a)



(b)

Fig. S2. ^{1}H NMR spectra of $\mathbf{H_2L^2}$ in DMSO-d_6: (a) C = 21.5 mM, (b) C = 6.7 mM.

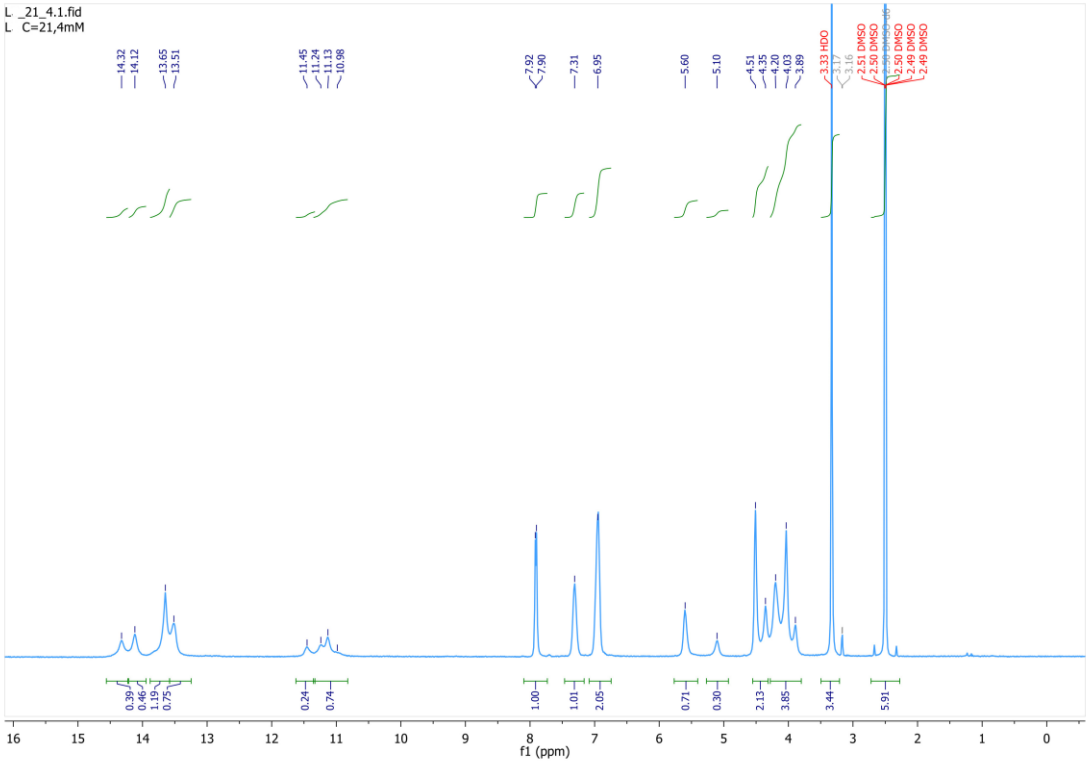


Fig. S3. ^{1}H NMR spectrum of $\mathbf{H_2L^3}$ in DMSO-d_6, C = 21.4 mM.

***Comment**: Due to the presence of fast exchange/tautomeric processes in solution, the nuclei of labile protons exhibit significantly shorter relaxation times. Consequently, they undergo stronger signal attenuation during the pulse sequence, resulting in DOSY signal intensities that are substantially lower (or absent altogether) than those of non-labile protons.*

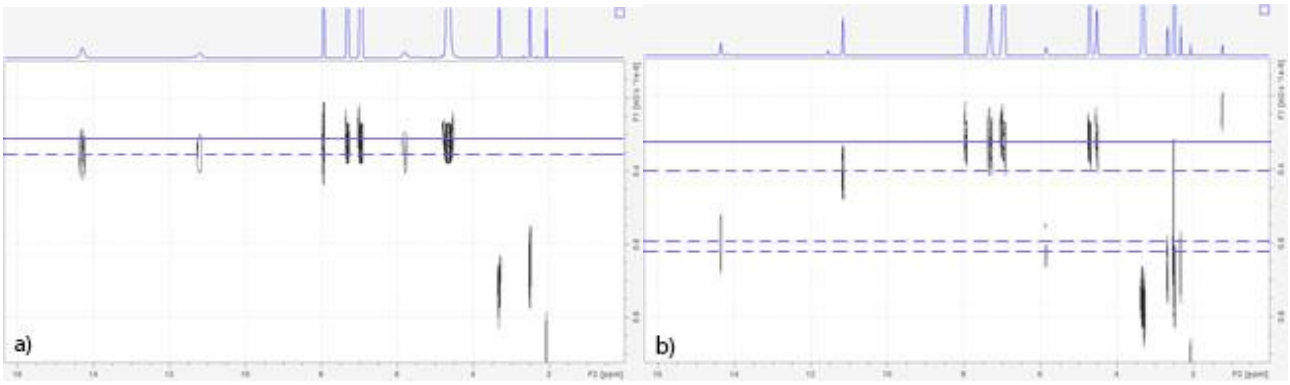


Fig. S4. ^{1}H DOSY NMR spectra of **H_2L^1** in DMSO-d_6: (a) C = 33.02 mM; (b) C = 11.3 mM.

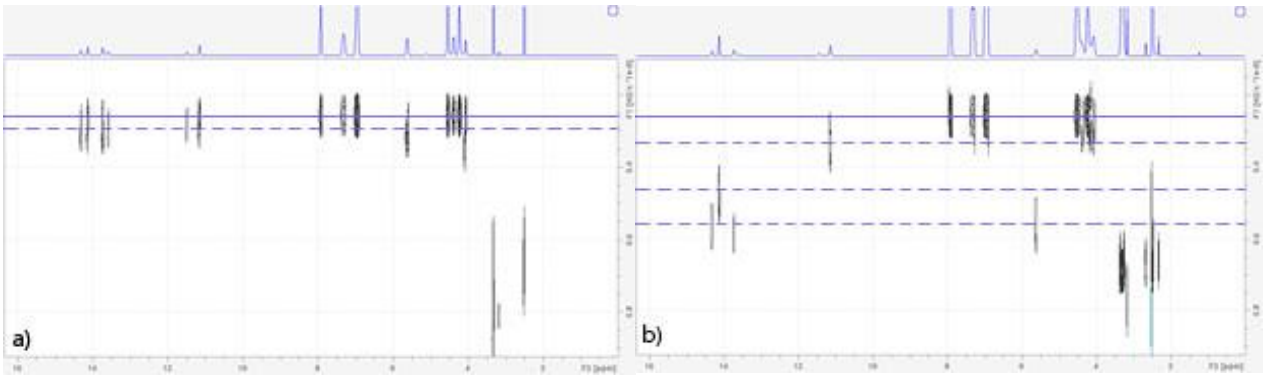


Fig. S5. ^{1}H DOSY NMR spectra of **H_2L^2** in DMSO-d_6: (a) C = 23.2 mM; (b) C = 6.8 mM.

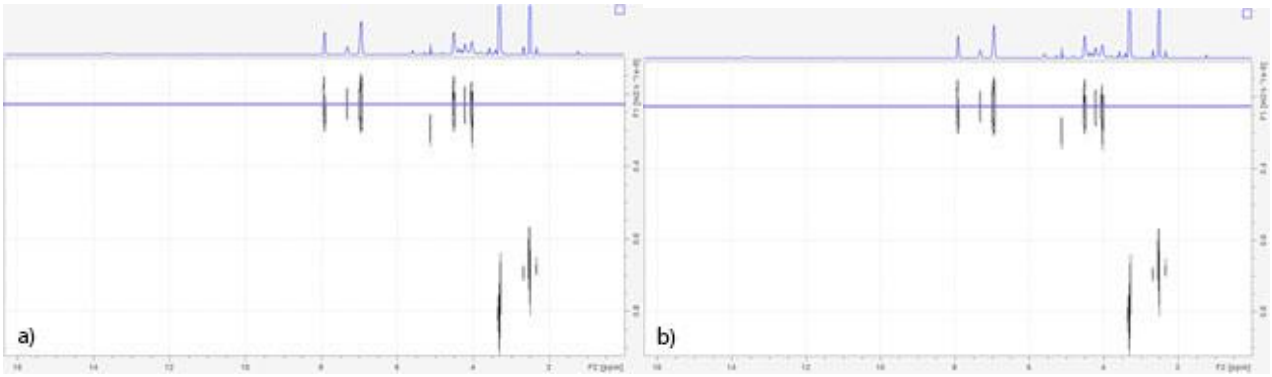


Fig. S6. ^{1}H DOSY NMR spectra **H_2L^3** in DMSO-d_6: (a) C = 21.4 mM; (b) C = 7.0 mM.

Table S1. Self-diffusion coefficients of **$H_2L^{1–3}$** and complexes **1–3** calculated using the DOSY signals of the molecular framework

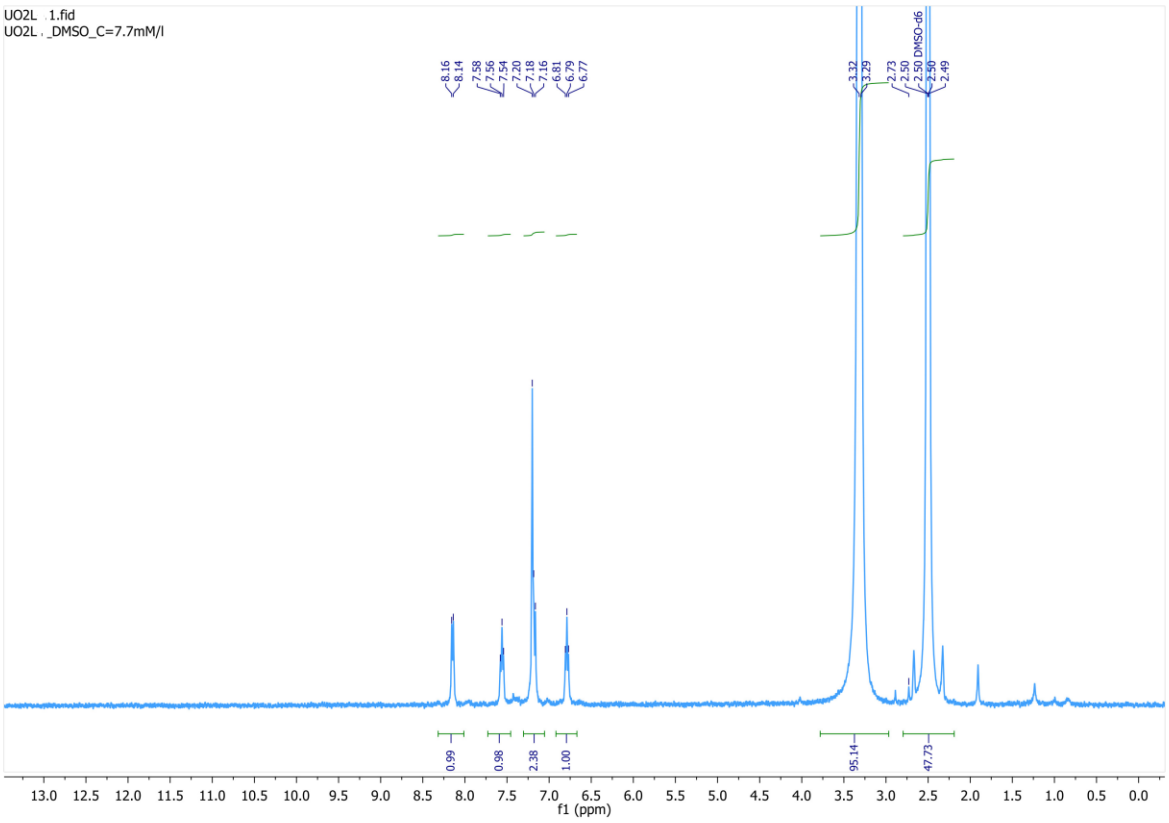
Compound	Concentration, mM	$D \times 10^{-10}$ m^2s^{-1}
H_2L^1	33.02 11.3	3.22 3.22
H_2L^2	23.2 6.8	2.56 2.59
H_2L^3	21.4 7.0	1.97 2.19
1	7.2	2.03
[**2**–4DMF]	6.1	1.99
3	2.1	2.20
DMSO-d_6		6.63*
H_2O		7.78*

* - *independent on compound concentration*

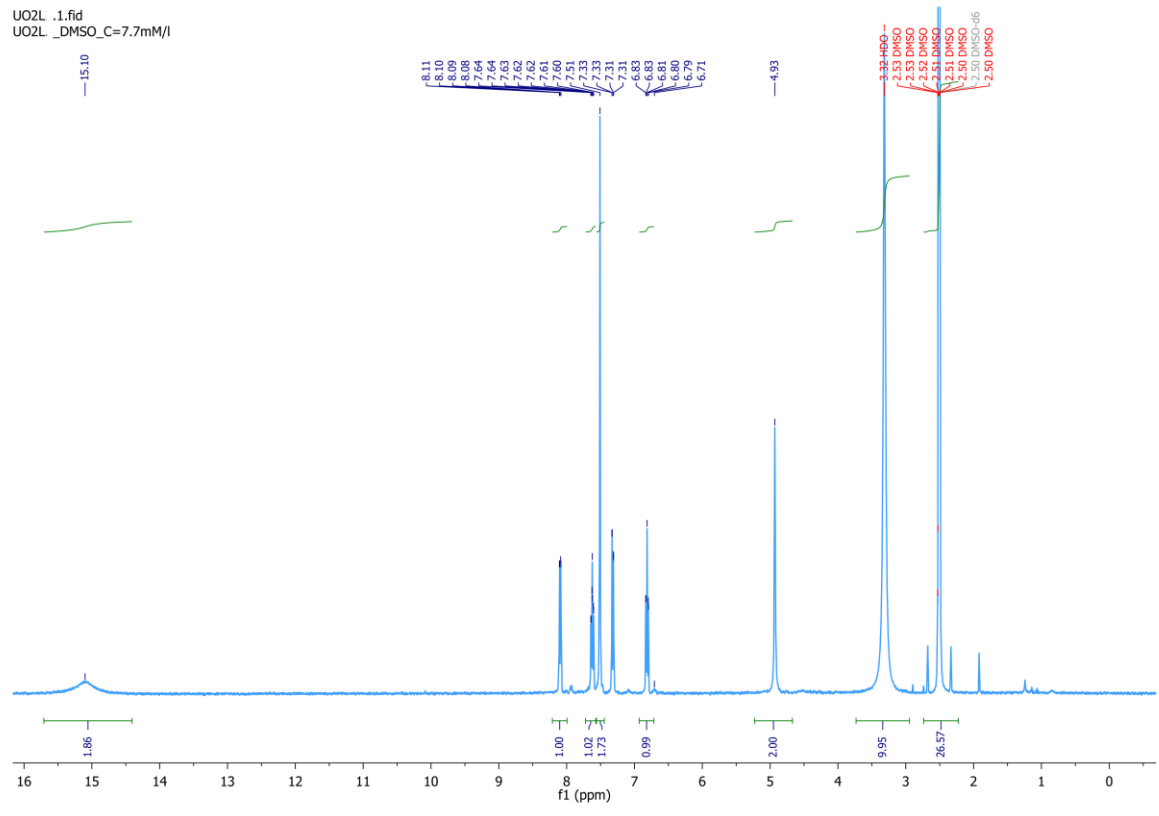
Table S2. Self-diffusion coefficients of labile protons in **$H_2L^{1–3}$**

Compound	Concentration, mM	Group	$D \times 10^{-10}$ m^2s^{-1}
H_2L^1	33.02	N*H* Ph-O*H* CH_2-O*H*	3.78
	11.3	N*H* Ph-O*H* CH_2-O*H*	6.02 4.07 6.09
H_2L^2	23.2	N*H* Ph-O*H* CH_2-O*H*	2.91 2.59 3.15
	6.8	N*H* Ph-O*H* CH_2-O*H*	4.80 3.48 5.36
H_2L^3	21.4	N*H* Ph-O*H* CH_2-O*H*	2.28 2.07 2.42
	7.0	N*H* Ph-O*H* CH_2-O*H*	3.24 2.78 3.01
DMSO-d_6			6.63*
H_2O			7.78*

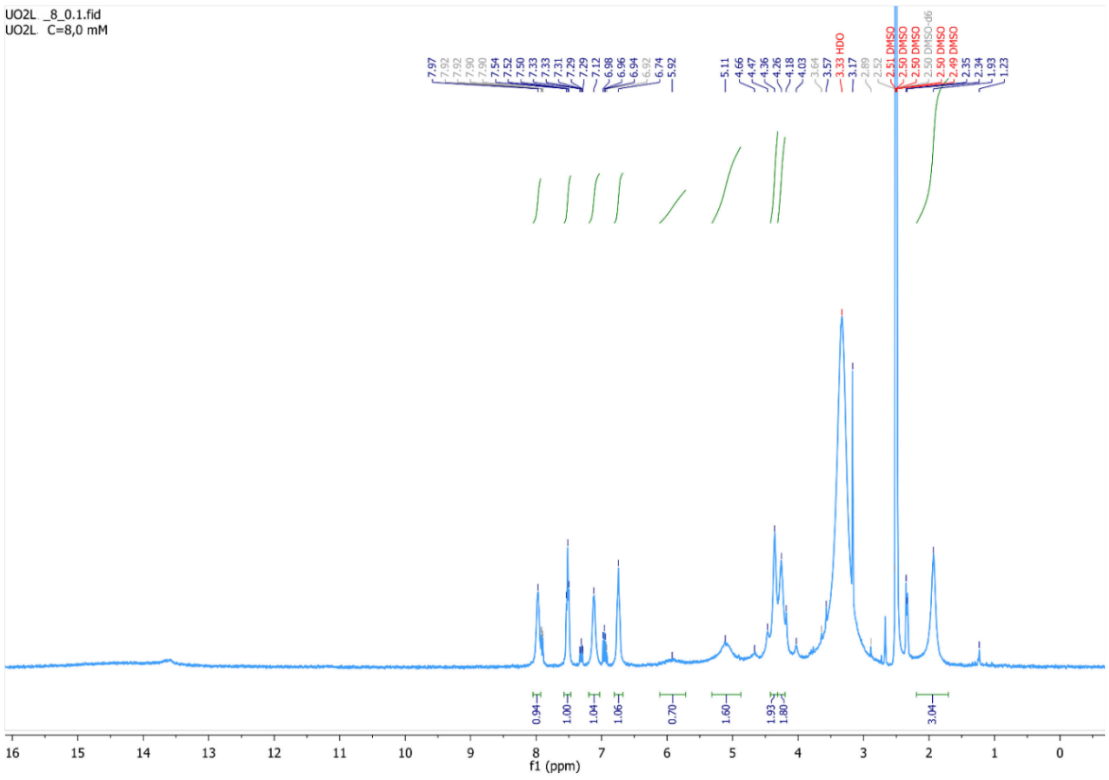
* - *independent on compound concentration*


UO2L .1.fid
UO2L _DMSO_C=7.7mM/l
8.16
8.14
7.58
7.56
7.54
7.20
7.18
7.16
6.81
6.79
6.77
3.32
3.29
2.73
2.50 DMSO-d6
2.50
2.49
0.99
0.98
2.38
1.00
95.14
47.73
f1 (ppm)

(a)


UO2L .1.fid
UO2L _DMSO_C=7.7mM/l
15.10
8.11
8.10
8.09
8.08
7.64
7.64
7.63
7.62
7.62
7.61
7.60
7.51
7.33
7.33
7.31
7.31
6.83
6.81
6.80
6.79
6.71
4.93
3.32 HDO
2.53 DMSO
2.53 DMSO
2.52 DMSO
2.51 DMSO
2.51 DMSO
2.50 DMSO
2.50 DMSO-d6
2.50 DMSO
1.86
1.00
1.02
1.73
0.99
2.00
9.95
26.57
f1 (ppm)

(b)



(c)

Fig. S7. ^{1}H NMR spectra of complexes **1** (a), [**2**–4DMF] (b) and **3** (c) in DMSO-d_6.

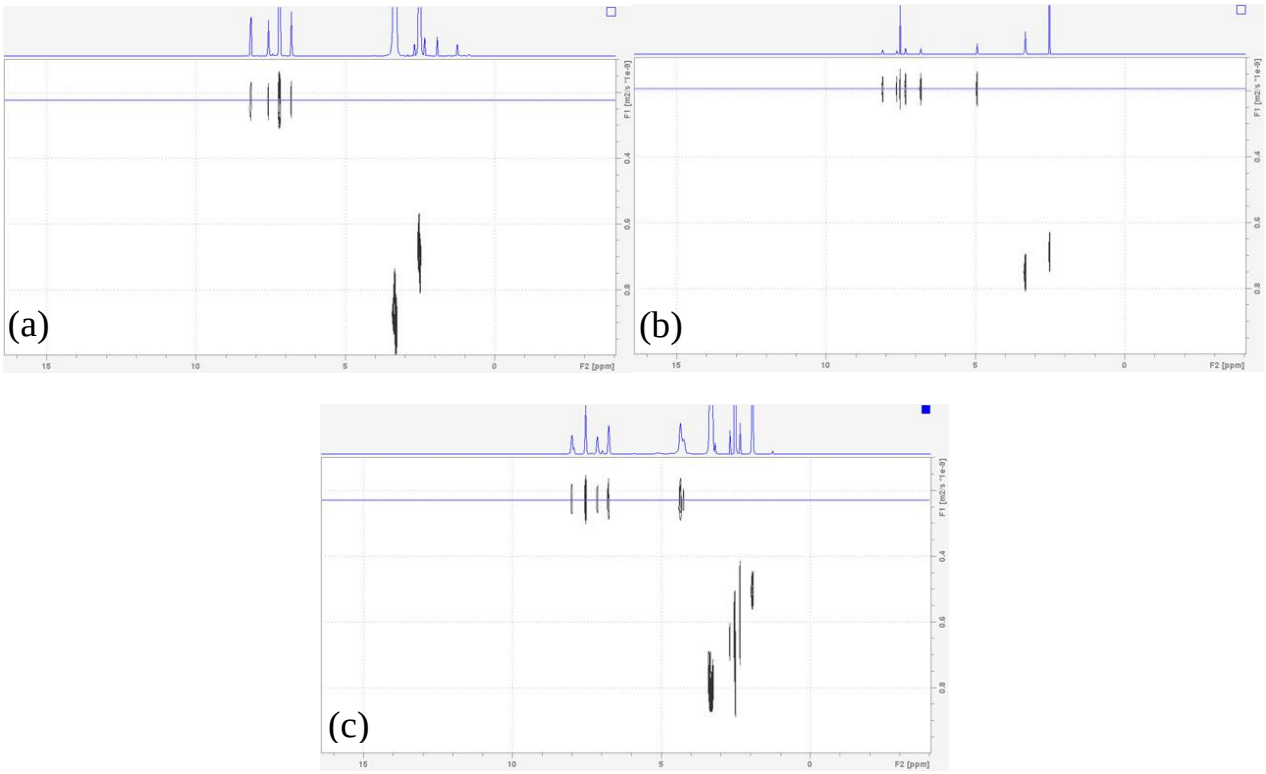
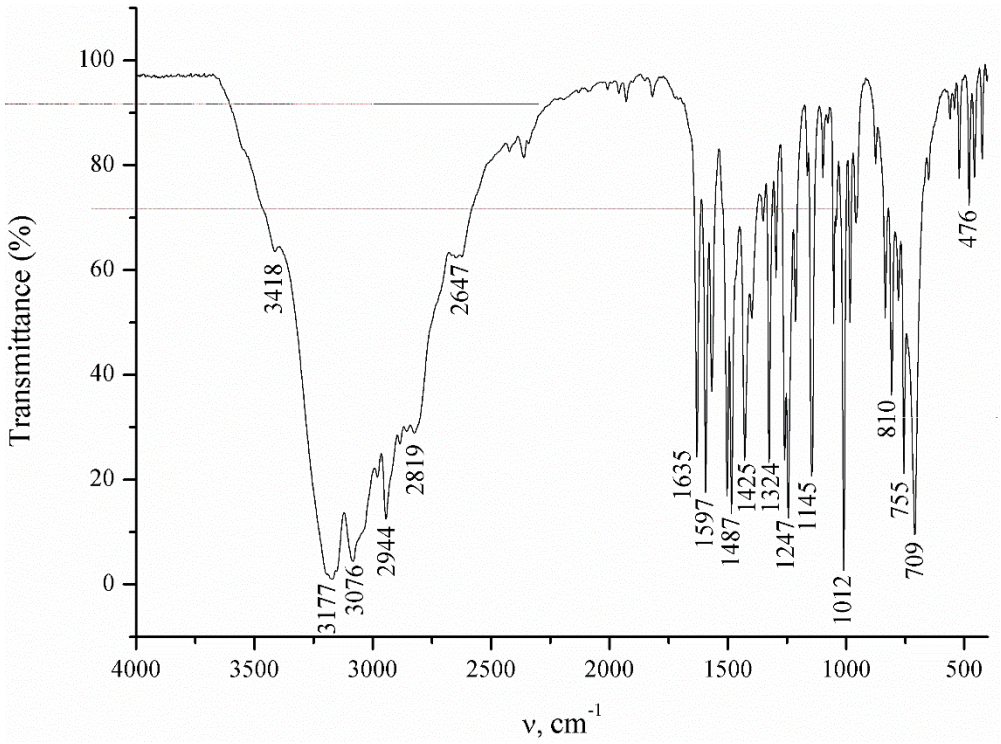
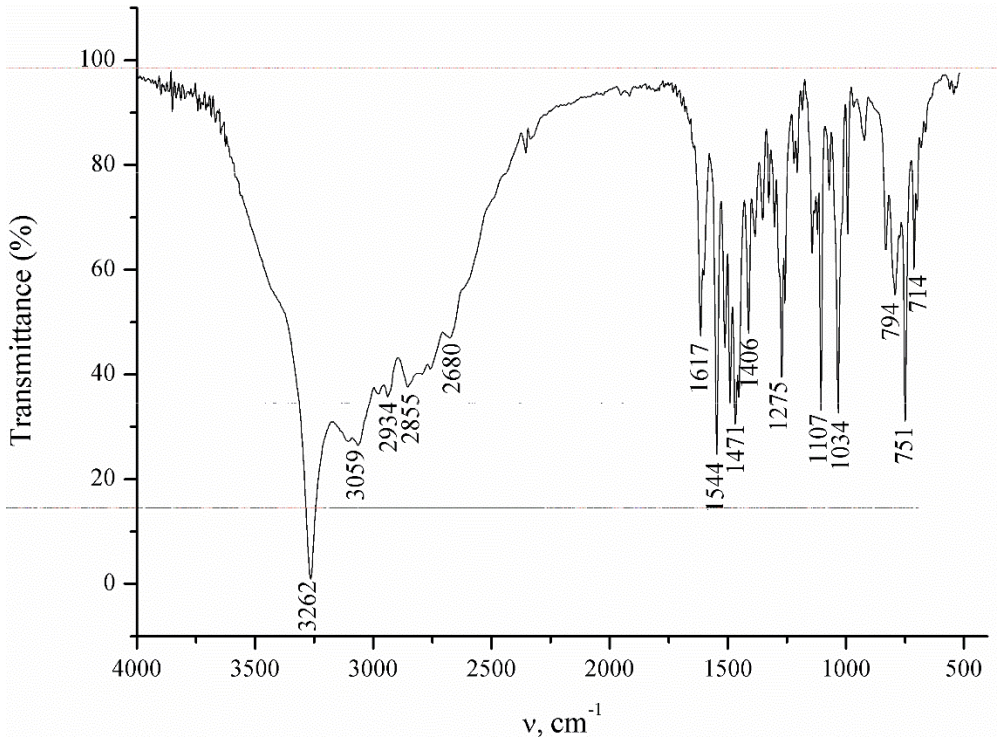


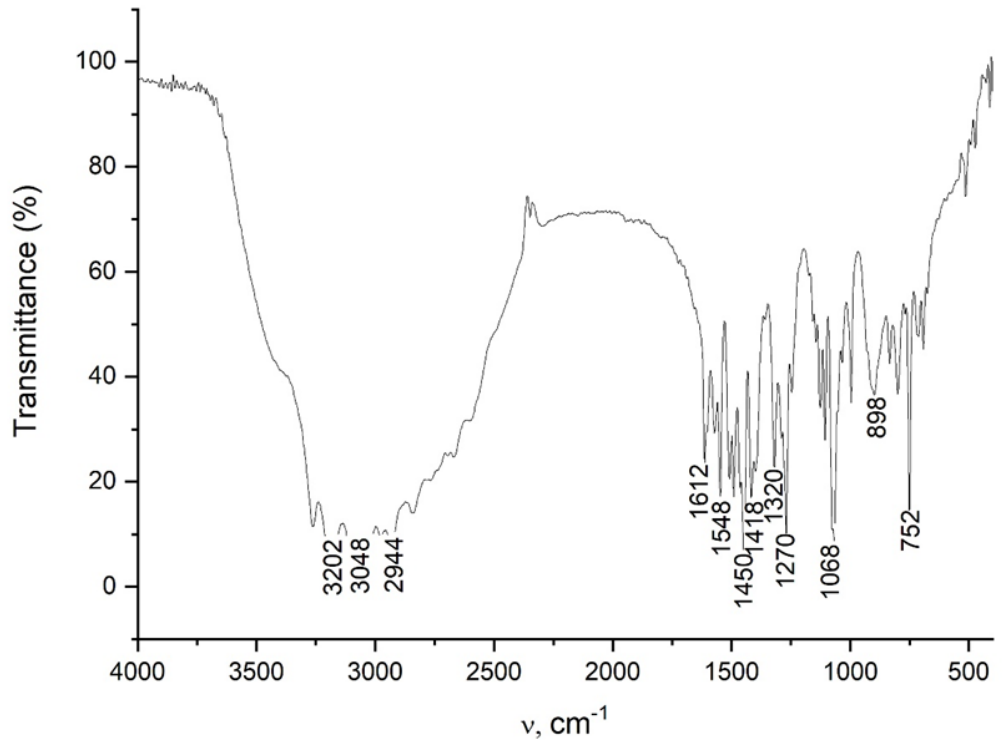
Fig. S8. ^{1}H DOSY NMR spectra of complexes in DMSO-d_6: (a) **1**, C = 7.2 mM; (b) [**2**–4DMF], C = 6.1 mM and (c) **3**, C = 2.1 mM.


Transmittance (%)
ν, cm-1
3418
3177
3076
2944
2819
2647
1635
1597
1487
1425
1324
1247
1145
1012
810
755
709
476

(a)

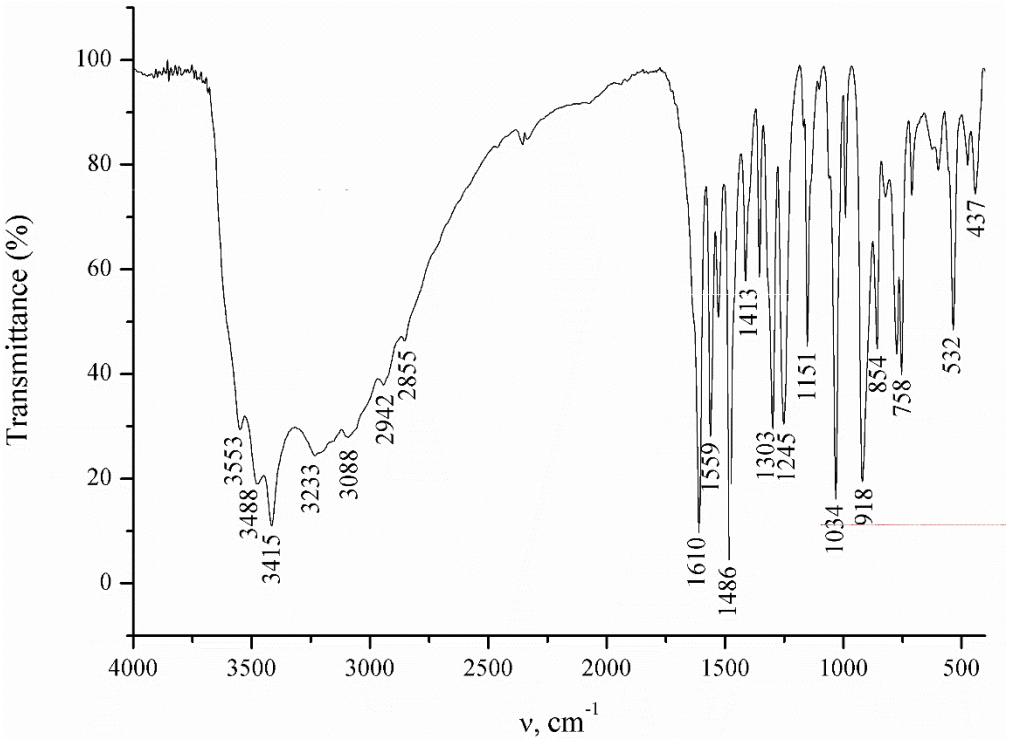

Transmittance (%)
ν, cm-1
3262
3059
2934
2855
2680
1617
1544
1471
1406
1275
1107
1034
794
751
714

(b)

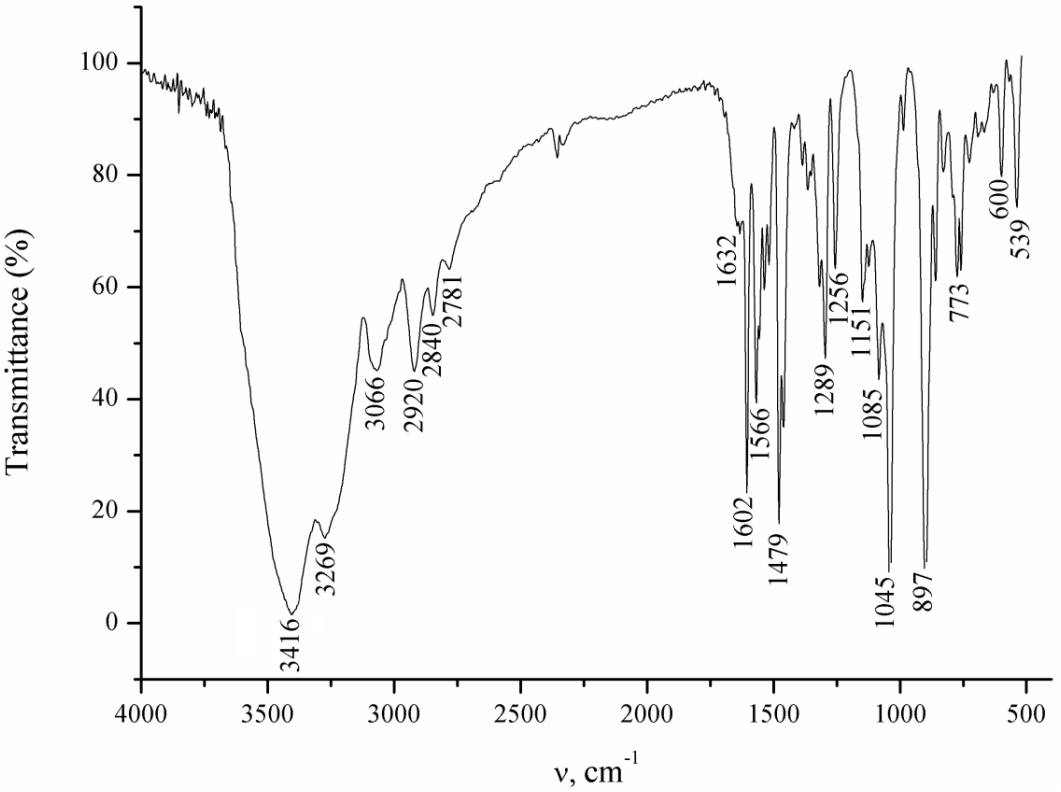


(c)

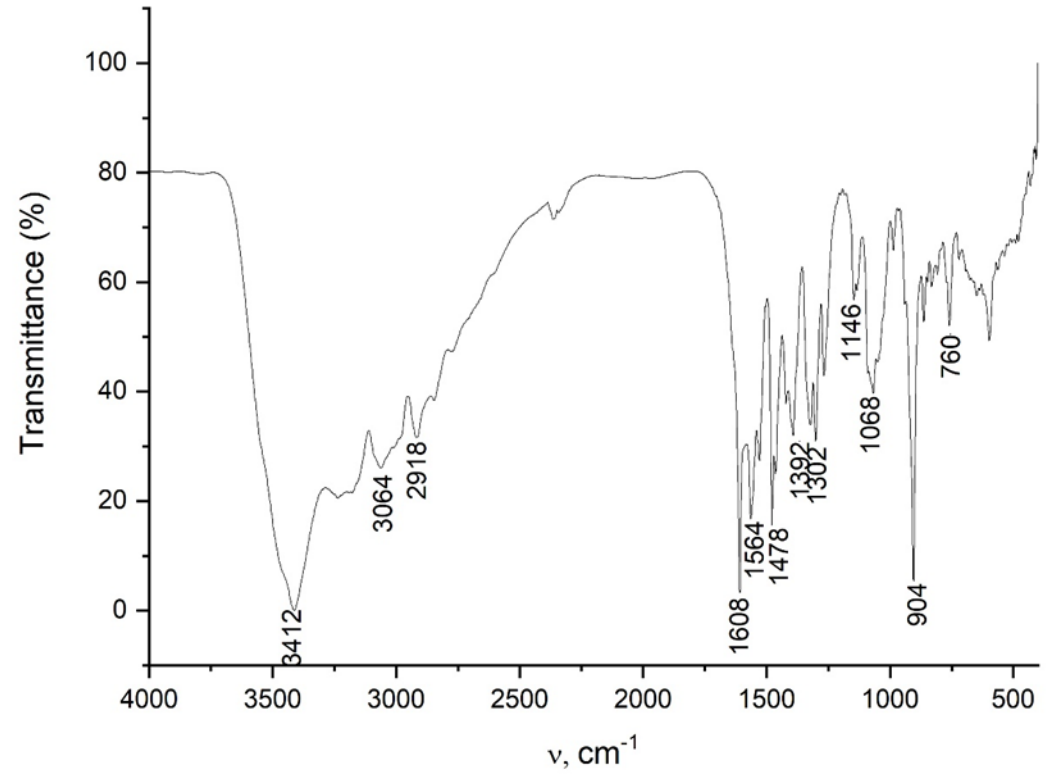
Fig. S9. IR spectra of $\mathbf{H_2L^1}$ (a), $\mathbf{H_2L^2}$ (b) and $\mathbf{H_2L^3}$ (c) in KBr.



(a)



(b)



(c)

Fig. S10. IR spectra of **1** (a), [**2**–4DMF] (b) and **3** (c) in KBr.

Table S3. Selected geometric parameters (Å, º) for **1** and **2**[a]

1		**2**, molecule **A**		**2**, molecule **B**	
U1–O1	1.777(3)	U1A–O1A	1.770(6)	U1B–O1B	1.790(6)
U1–O2	1.789(2)	U1A–O2A	1.781(6)	U1B–O2B	1.783(5)
U1–O3	2.304(2)	U1A–O3A	2.237(6)	U1B–O3B	2.220(6)
U1–O4	2.404(2)	U1A–O4A	2.453(5)	U1B–O4B	2.440(6)
U1–O4^{1}	2.381(2)	U1A–O4A^{2}	2.317(5)	U1B–O4B^{3}	2.333(6)
U1–O5	2.401(2)	U1A–N1A	2.563(6)	U1B–N1B	2.593(7)
U1–N1	2.463(3)	U1A–N4A	2.506(7)	U1B–N4B	2.493(7)
U1–U1^{1}	3.97423(17)	U1A–U1A^{2}	3.9569(7)	U1B–U1B^{3}	3.9378(7)
O1–U1–O2	176.88(10)	O1A–U1A–O2A	178.7(3)	O1B–U1B–O3B	90.3(2)
O1–U1–O3	91.39(10)	O1A–U1A–O3A	91.4(3)	O1B–U1B–O4B	94.3(2)
O1–U1–O4	93.41(10)	O1A–U1A–O4A^{2}	88.8(2)	O1B–U1B–O4B^{3}	90.1(2)
O1–U1–O4^{1}	90.52(10)	O1A–U1A–O4A	95.3(2)	O1B–U1B–N1B	90.8(2)
O1–U1–O5	89.74(10)	O1A–U1A–N1A	93.8(2)	O1B–U1B–N4B	89.0(2)
O1–U1–N1	89.72(11)	O1A–U1A–N4A	88.8(3)	O2B–U1B–O1B	177.0(3)
O2–U1–O3	87.26(10)	O2A–U1A–O3A	89.7(3)	O2B–U1B–O3B	90.2(2)
O2–U1–O4	89.56(10)	O2A–U1A–O4A	84.1(2)	O2B–U1B–O4B^{3}	92.9(2)
O2–U1–O4^{1}	89.72(10)	O2A–U1A–O4A^{2}	91.9(2)	O2B–U1B–O4B	86.4(2)
O2–U1–O5	87.23(10)	O2A–U1A–N1A	85.8(2)	O2B–U1B–N1B	86.5(2)
O2–U1–N1	92.38(10)	O2A–U1A–N4A	89.9(3)	O2B–U1B–N4B	88.6(2)
O3–U1–O4	133.48(8)	O3A–U1A–O4A^{2}	89.3(2)	O3B–U1B–O4B^{3}	87.8(2)
O3–U1–O4^{1}	158.55(8)	O3A–U1A–O4A	156.1(2)	O3B–U1B–O4B	156.2(2)
O3–U1–O5	77.61(8)	O3A–U1A–N1A	72.2(2)	O3B–U1B–N1B	70.4(2)
O3–U1–N1	68.24(8)	O3A–U1A–N4A	139.5(2)	O3B–U1B–N4B	139.3(2)
O4^{1}–U1–O4	67.67(9)	O4A^{2}–U1A–O4A	67.9(2)	O4B^{3}–U1B–O4B	68.8(2)
O4^{1}–U1–O5	81.04(8)	O4A–U1A–N1A	129.99(19)	O4B–U1B–N1B	132.7(2)
O4–U1–N1	65.55(8)	O4A^{2}–U1A–N1A	161.4(2)	O4B^{3}–U1B–N1B	158.2(2)
O4^{1}–U1–N1	133.14(8)	O4A^{2}–U1A–N4A	131.1(2)	O4B–U1B–N4B	64.3(2)
O5–U1–O4	148.56(8)	O4A–U1A–N4A	63.7(2)	O4B^{3}–U1B–N4B	132.9(2)
O5–U1–N1	145.82(8)	N4A–U1A–N1A	67.4(2)	N4B–U1B–N1B	68.9(2)

[a] Symmetry codes: ^{i} –*x*, –*y*+2, –*z*+2 (**1**); ^{i} –*x*, –*y*+1, –*z*+3; ^{ii} –*x*+1, –*y*+1, –*z*+4 (**2**).

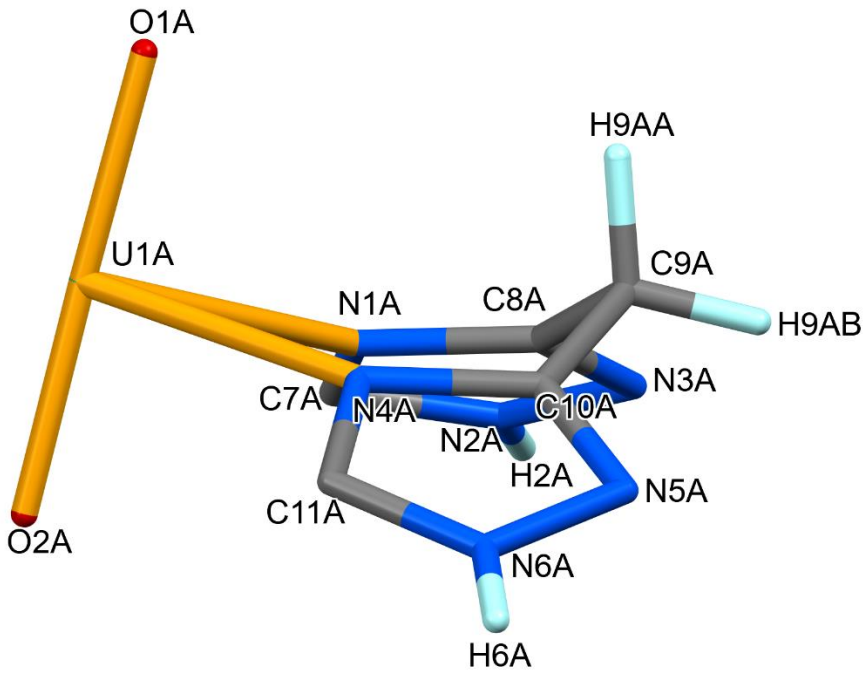


Fig. S11. Fragment of molecule **A** of complex **2** showing a boat conformation of the six-membered metallacycle.

Table S4. Selected geometric parameters (Å, º) for **3**

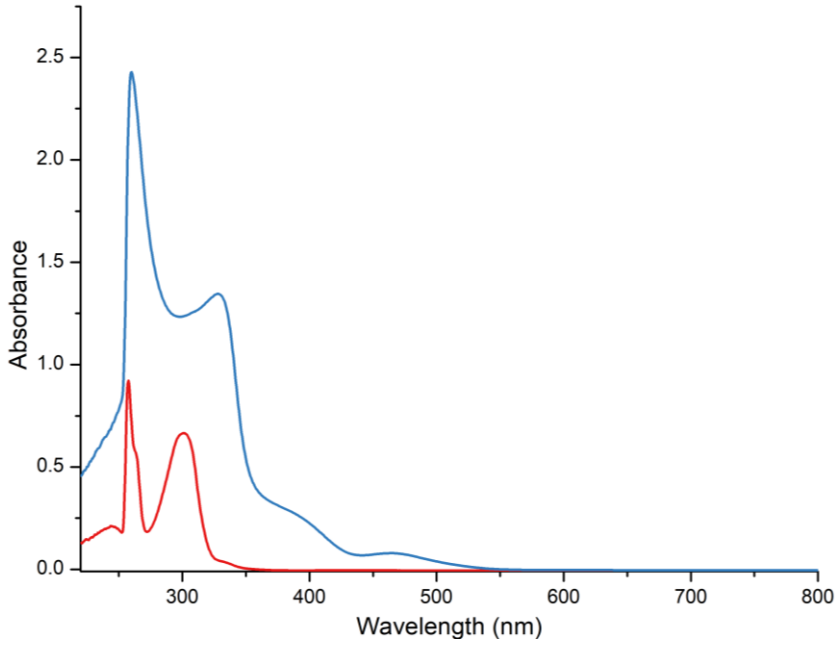
U1–O1	1.772(3)	U1–N1	2.558(3)
U1–O2	1.774(3)	U1–N4	2.588(3)
U1–O3	2.230(3)	U1–N7	2.559(4)
U1–O5	2.331(3)		
O1–U1–O2	177.26(15)	O3–U1–O5	79.07(11)
O1–U1–O3	88.24(13)	O3–U1–N1	69.94(11)
O1–U1–O5	94.86(13)	O3–U1–N4	139.20(11)
O1–U1–N1	93.13(13)	O3–U1–N7	151.48(12)
O1–U1–N4	93.81(13)	O5–U1–N1	147.69(10)
O1–U1–N7	84.26(13)	O5–U1–N4	140.99(10)
O2–U1–O3	94.34(13)	O5–U1–N7	74.22(11)
O2–U1–O5	86.55(13)	N1–U1–N4	69.26(11)
O2–U1–N1	86.90(13)	N1–U1–N7	137.82(11)
O2–U1–N4	83.64(13)	N7–U1–N4	68.93(11)
O2–U1–N7	93.87(13)		

Table S5. Hydrogen-bond geometry (Å, º) for **1**–**3**

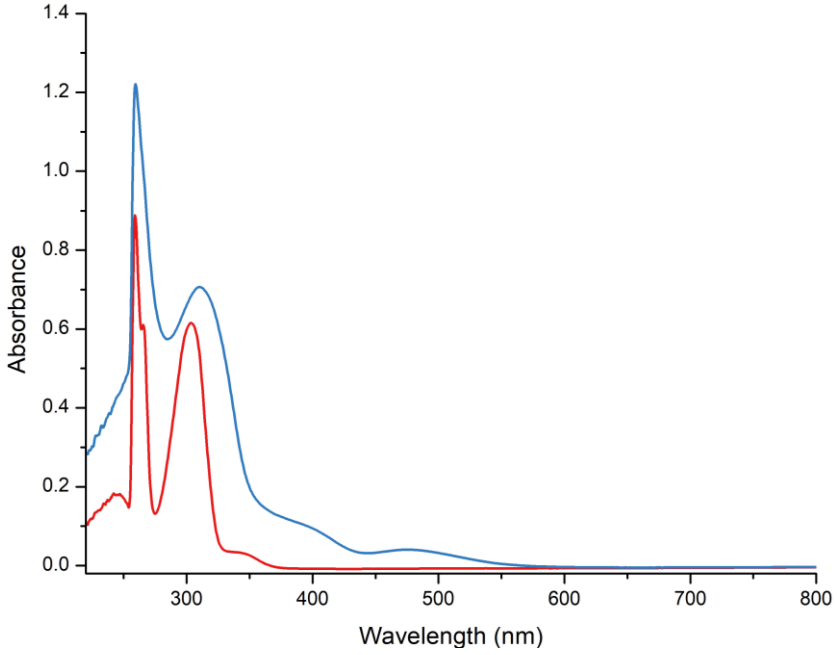
D–H···*A*	*D*–H	HC*A*	*D*···*A*	*D*–H···*A*	Symmetry codes
1					
O5–H···O3[1]	0.854(9)	1.732(10)	2.582(3)	173(2)	[1]–*x*, –*y*, 1–*z*
O6–H···O2[2]	0.82	2.05	2.833(4)	160.1	[2]1–*x*, 1–*y*, 1–*z*
N2–H···O6	0.86	1.89	2.732(4)	167.6	-
C9–H···O5[3]	0.97	2.53	3.037(4)	112.6	[3]1–*x*, –*y*, 1–*z*
C11–H···O1[4]	0.96	2.51	3.307(6)	140.0	[4]+*x*, 1+*y*, +*z*
2					
N2*A*–H2*A*···O3[1]	0.88	1.83	2.694 (16)	167.7	[1] *x*+1, *y*–1, *z*–1
N2*A*–H2*A*···O3*X*[1]	0.88	1.93	2.799 (17)	169.6	[1] *x*+1, *y*–1, *z*–1
N6*A*–H6*A*···O4[2]	0.88	1.78	2.626 (10)	161.3	[2] –*x*+1, –*y*+1, –*z*+1
N2*B*–H2*B*···O1[3]	0.88	1.93	2.770 (10)	160.4	[3] –*x*+1, –*y*+2, –*z*+1
N5*B*–H5*B*···O2[2]	0.88	1.86	2.708 (9)	160.4	[2] –*x*+1, –*y*+1, –*z*+1
C1–H1···N4*B*	0.95	2.64	3.447 (12)	142.8	-
C3–H3*C*···O2*B*	0.98	2.60	3.513 (12)	155.0	-
C5–H5*E*···O1*A*[2]	0.98	2.59	3.283 (12)	127.4	[2] –*x*+1, –*y*+1, –*z*+1
C7–H7···O2*A*[4]	0.95	2.64	3.55 (2)	161.5	[4] *x*, *y*+1, *z*+1
C8–H8*C*···O2*A*[2]	0.98	2.47	3.45 (2)	177.1	[2] –*x*+1, –*y*+1, –*z*+1
C12–H12*E*···O4*B*[2]	0.98	2.59	3.39 (4)	138.1	[2] –*x*+1, –*y*+1, –*z*+1
C12–H12*G*···O1*B*[2]	0.98	2.63	3.44 (3)	140.7	[2] –*x*+1, –*y*+1, –*z*+1
C9*A*–H9*AA*···O3*A*[5]	0.99	2.63	3.572 (11)	159.3	[5] –*x*+2, –*y*+1, –*z*
C9*B*–H9*BA*···O1*B*[2]	0.99	2.40	3.382 (10)	171.8	[2] –*x*+1, –*y*+1, –*z*+1
C12*B*–H12*D*···N5*A*[6]	0.99	2.70	3.501 (12)	138.5	[6] *x*–1, *y*, *z*
C7*X*–H7*X*···O2*A*[4]	0.95	2.41	3.30 (2)	155.7	[4] *x*, *y*+1, *z*+1
C8*X*–H8*XA*···O2*A*[2]	0.98	2.65	3.26 (2)	120.5	[2] –*x*+1, –*y*+1, –*z*+1
C9*X*–H9*XB*···O3*X*[7]	0.98	2.49	3.19 (3)	128.5	[7] –*x*+1, –*y*+2, –*z*+2
C12*X*–H12*H*···O4*B*[2]	0.98	2.44	3.41 (4)	168.0	[2] –*x*+1, –*y*+1, –*z*+1
3					
O1W–H···O4[1]	0.86	2.19	2.865(5)	135.2	[1]–1/2+*x*,3/2–*y*,1–*z*
O1W–H···O6	0.85	1.87	2.699(5)	165.9	-
O4–H···O6[2]	0.82	1.90	2.705(5)	169.3	[2]1–*x*,1–*y*,1–*z*
O7–H···O3	0.82	2.10	2.884(5)	160.6	-
N2–H···N5[3]	0.86	2.15	2.984(5)	163.8	[3]–1/2+*x*,+*y*,1/2–*z*
N6–H···O1W[4]	0.86	1.88	2.685(6)	156.1	[4]1+*x*,+*y*,+*z*
N9–H···O7[5]	0.86	1.96	2.796(6)	164.7	[5]1/2+*x*,3/2–*y*,1–*z*
C9–H···O2[6]	0.97	2.43	3.399(5)	179.1	[6]3/2–*x*,1/2+*y*,+*z*
C12–H···O1[7]	0.97	2.65	3.600(5)	166.2	[7]3/2–*x*,–1/2+*y*,+*z*

C12–H···N8[8]	0.97	2.61	3.340(5)	132.2	[8]2–*x*,1–*y*,1–*z*
C15–H···O5	0.97	2.43	3.209(6)	137.2	-
C18–H···O1W[9]	0.96	2.55	3.484(9)	165.5	[9]1/2–*x*,1/2+*y*,+*z*

[a] Symmetry codes: [1] –*x*+1, –*y*, –*z*+1; [2] –*x*+1, –*y*+1, –*z*; [3] –*x*, –*y*+1, –*z*+1.

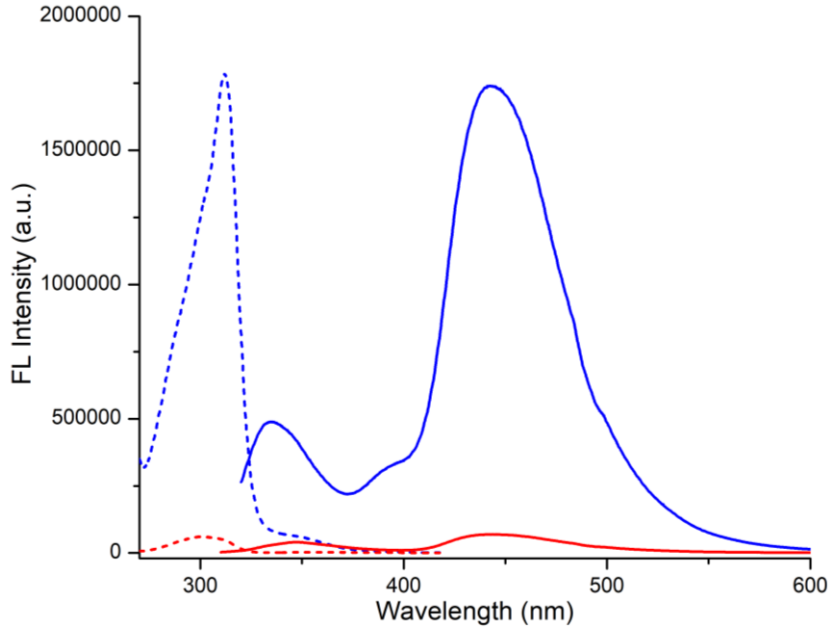


(a)

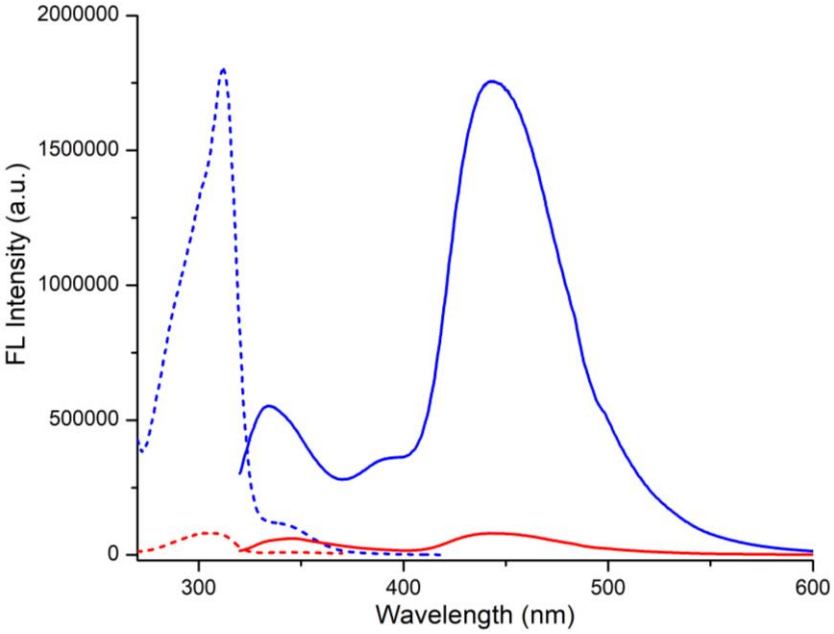


(b)

Fig. S12. Absorption spectra of (a) **H_2L^1** (red) and complex **1** (blue); (b) **H_2L^3** (red) and complex **3** (blue) in DMSO at r.t. $C_{Ligand} = C_{Complex} = 5 \times 10^{-5}$ M.



(a)



(b)

Fig. S13. Excitation (dotted) and emission spectra (solid) of ligands (blue) and their complexes (red) in DMSO at r.t.: (a) **H_2L^2** and [**2**–4DMF]; (b) **H_2L^3** and **3**. $C_{Ligand} = C_{Complex} = 1 \times 10^{-5}$ M.

Listing S1. Cartesian coordinates of the optimized molecular structures of $\mathbf{H_2L^{1–3}}$ and complexes **1–3** in DMSO medium (SMD continuum solvation model).

Complex [**1**–2CH_3OH]:

U	-1.082808	8.970621	-0.587447
U	-4.776343	9.758808	0.617199
O	0.554982	10.868402	-0.253811
O	0.828627	8.048651	-1.398670
N	-1.404141	6.593052	-1.230906
O	-0.641331	8.466637	1.071324
O	-1.478388	9.533848	-2.237663
O	-3.325274	8.065725	-0.225504
O	-2.533965	10.663365	0.258878
O	-6.414825	7.859209	0.293046
O	-6.691087	10.681689	1.421278
N	-4.464106	12.145288	1.237389
O	-5.216771	10.253134	-1.044640
O	-4.380485	9.205314	2.270665
H	1.208056	10.727232	0.446526
C	1.142729	11.676847	-1.297490
C	1.296089	7.157552	-2.235159
C	-0.682684	5.703476	-1.916543
C	-2.518248	5.935694	-0.826907
C	-3.514750	6.683270	-0.002144
C	-2.343961	12.043961	0.024731
H	-7.073349	8.006193	-0.401012
C	-7.001835	7.060587	1.344763
C	-7.171796	11.591117	2.229800
C	-5.192707	13.043641	1.904001
C	-3.347725	12.798974	0.833471
H	0.363909	11.865106	-2.031652
H	1.487588	12.623020	-0.879960
H	1.972156	11.146978	-1.766736
C	2.547811	7.359070	-2.850551
C	0.597684	5.954335	-2.541208
N	-1.375630	4.554169	-1.905751
N	-2.549357	4.684974	-1.222869
H	-3.365333	6.433602	1.057109
H	-4.526499	6.371979	-0.271343
H	-2.484463	12.284044	-1.037962
H	-1.334788	12.358574	0.299700
H	-6.216121	6.858965	2.067978
H	-7.368310	6.120474	0.932055
H	-7.815634	7.604200	1.825466
C	-8.431904	11.401714	2.832148
C	-6.479796	12.802306	2.518206
N	-4.500933	14.193577	1.883609
N	-3.321466	14.055015	1.212409
C	3.078059	6.428090	-3.722745
H	3.085293	8.270103	-2.618242
C	1.157706	5.026372	-3.429258
H	-1.131670	3.667686	-2.323313
C	-8.975631	12.351337	3.675456
H	-8.965146	10.484969	2.613031
C	-7.053434	13.749116	3.377238
H	-4.749426	15.085814	2.285930
C	2.385748	5.251184	-4.021039
H	4.041905	6.617191	-4.180870
H	0.613283	4.120653	-3.669116
C	-8.289196	13.535850	3.956902
H	-9.945739	12.171200	4.123881
H	-6.513665	14.661114	3.603143
H	2.800894	4.526765	-4.709182
H	-8.715060	14.275128	4.622329

Ligand $\mathbf{H_2L^1}$:

O	-1.12842	12.88327	0.20960
O	-6.19085	10.42101	2.64294
N	-4.27926	12.00029	1.77114
C	-1.92604	11.91928	0.88622
C	-6.94527	11.52333	2.84026
C	-5.14579	13.03493	2.00815
C	-3.19265	12.58507	1.29460
H	-1.42074	11.53656	1.77951
H	-2.16255	11.06388	0.24480
C	-8.23164	11.34573	3.35478
C	-6.48549	12.82461	2.54858
N	-4.63862	14.21680	1.69264
N	-3.39987	13.90238	1.24520
C	-9.05462	12.43556	3.58079
H	-8.56703	10.33914	3.57152
C	-7.33738	13.90990	2.78639
C	-8.60995	13.72726	3.29695
H	-10.04895	12.27856	3.98092
H	-6.98115	14.90716	2.56261
H	-9.25256	14.57991	3.47421
H	-5.31473	10.70582	2.28163
H	-0.22883	12.53879	0.14522
H	-2.76707	14.61917	0.91941

Complex [**2**–4DMF]:

H	3.595401	-0.136663	16.428358

U	-0.842609	2.485800	20.739918
U	2.689751	0.684143	20.770643
O	-1.734142	0.977197	20.372390
O	-0.010409	4.039921	21.041875
O	-2.076537	2.780101	22.594259
O	1.133959	1.838430	19.416003
O	0.693196	1.294048	22.078006
N	-2.902194	3.980787	20.188195
N	-0.922623	3.055868	18.271466
O	3.541404	2.219317	21.120612
O	1.897129	-0.893715	20.485047
O	3.943574	0.390389	18.930321
N	4.786013	-0.743543	21.363402
N	2.770775	0.152618	23.249972
C	-2.468399	3.875694	23.207338
C	1.487509	2.567316	18.266374
C	0.348061	0.565301	23.230070
C	-3.473410	4.776265	21.106017
C	-3.551988	4.269961	19.022626
C	-1.842311	3.495239	17.371883
C	0.225063	3.016315	17.607791
C	4.365509	-0.707339	18.341073
C	5.388647	-1.535293	20.462827
C	5.442225	-0.986331	22.536022
C	3.697709	-0.242531	24.162444
C	1.617687	0.164023	23.905274
C	-2.231418	4.037209	24.584217
C	-3.158428	4.906680	22.519449
H	2.074162	1.960781	17.570010
H	2.092680	3.449443	18.516305
H	-0.265731	1.159400	23.913491
H	-0.225560	-0.337743	22.980726
N	-4.422410	5.487405	20.481576
N	-4.482410	5.186737	19.164271
C	-3.289163	3.613743	17.705749
N	-1.319910	3.737136	16.189751
N	-0.004935	3.420608	16.362326
C	4.135485	-0.904711	16.967864
N	6.361079	-2.199141	21.103042
N	6.405957	-1.870971	22.414411
C	5.149849	-0.316286	23.839557
N	3.174990	-0.484380	25.344487
N	1.851505	-0.214317	25.158126
H	-1.710753	3.243883	25.105941
C	-2.644623	5.174245	25.251897
C	-3.564090	6.051906	23.219946
H	-5.065387	6.157348	20.878285
H	-3.803723	4.170126	16.925057
H	-3.719505	2.606424	17.724451
H	7.031553	-2.850310	20.720735
H	5.678771	-0.840195	24.632994
H	5.544452	0.705103	23.804780
H	1.193447	-0.312541	25.919455
H	-2.441321	5.274455	26.311599
C	-3.313577	6.194195	24.571534
H	-4.065277	6.853530	22.691611
H	4.380512	-2.173597	15.268303
H	6.036031	-3.631633	18.924818
H	-3.626626	7.090081	25.091341
C	5.080869	-1.704813	19.052038
C	4.579204	-2.045087	16.325805
C	5.516776	-2.854514	18.377709
C	5.272471	-3.032600	17.029189
H	5.608768	-3.931562	16.529636

Ligand **H_2L^2**:

C	-1.23372	10.78408	1.19908
O	-5.91394	12.29912	4.95011
N	-4.33146	12.04728	2.87096
C	-1.95196	11.47465	2.31194
C	-6.89987	12.65204	4.09790
C	-5.41107	12.41521	2.11284
C	-3.35929	11.85305	1.99192
H	-1.40738	12.38630	2.58220
H	-1.95219	10.83869	3.19602
C	-8.15112	12.95370	4.64043
C	-6.71057	12.72437	2.70174
N	-5.14315	12.45177	0.81630
N	-3.83998	12.09406	0.76906
C	-9.20280	13.32224	3.81911
H	-8.27722	12.89249	5.71423
C	-7.79017	13.09917	1.89329
C	-9.02695	13.39685	2.43704
H	-10.16614	13.55268	4.25769
H	-7.64140	13.15369	0.82256
H	-9.84863	13.68504	1.79423
H	-5.09705	12.11881	4.41997
H	-3.32837	12.02280	-0.10343
N	-0.44586	9.74415	1.40071
N	0.00031	9.46536	0.15342
C	-0.51552	10.31837	-0.73695
N	-1.30560	11.17430	-0.10311
C	-0.26026	10.29319	-2.20885
O	-1.46868	10.18759	-2.95421
H	0.34772	9.42439	-2.45985
H	0.29853	11.19108	-2.49243
H	-1.99649	10.97837	-2.77592
H	0.63529	8.69531	-0.00922
H	0.650672	3.508743	15.597672

Complex [**3**–CH_3OH,H_2O]:

U	8.02284	10.65977	27.77746
O	6.19342	10.70560	26.47676
O	6.58738	11.33672	29.39886
N	9.47358	10.85300	29.98411
N	10.60870	10.30356	27.36265
N	8.54994	9.97101	25.30770
O	8.37534	12.36459	27.37036
O	7.80010	8.93386	28.19445
C	5.89189	11.36062	25.38034
C	6.04670	12.44353	29.83924
C	10.67053	11.49720	30.11825
C	9.18614	10.43972	31.21666
C	11.25281	9.45688	26.50754
C	11.58288	11.02662	27.90864
C	9.51488	9.15424	24.79977
C	7.85504	10.38384	24.23841
C	4.73862	12.16356	25.31729
C	6.69499	11.25328	24.21669
O	4.89369	12.77088	29.59850
C	6.94947	13.29225	30.70847
N	11.12066	11.51326	31.35136
C	11.41322	12.06908	28.95767
N	10.15933	10.84072	32.03156
C	8.01036	9.63779	31.67269
N	12.55655	9.62421	26.49884
C	10.53599	8.47515	25.64758
N	12.74233	10.61966	27.39992
N	9.46876	9.04298	23.49203
N	8.41298	9.82311	23.15673
H	4.12179	12.24066	26.20356
C	4.40541	12.83909	24.15793
C	6.33574	11.94347	23.05218
H	7.83939	13.58436	30.14826
H	6.42819	14.18431	31.05090
H	7.28361	12.71497	31.57318
H	10.86019	12.91300	28.53714
H	12.38483	12.43223	29.28690
H	10.23637	10.68272	33.02679
O	7.95654	9.56974	33.09067
H	8.11836	8.61593	31.30229
H	7.10179	10.05208	31.23626
H	11.25050	7.95781	25.01129
H	10.04569	7.72932	26.27992
H	13.66995	10.96342	27.61069
H	3.51576	13.45775	24.13933
C	5.20290	12.73552	23.01542
H	6.96346	11.87159	22.17199
H	7.47458	10.34229	33.41576
H	4.94301	13.27261	22.11274
H	8.12091	9.89751	22.19255

Ligand **H_2L^3**:

C	-6.00285	0.55857	-0.57773
C	-5.11547	-0.19250	-1.34915
C	-3.75762	-0.09972	-1.10697
C	-3.25540	0.73547	-0.10000
C	-4.16349	1.48707	0.67705
C	-5.53259	1.38980	0.42341
O	-3.76732	2.31366	1.66530
C	-1.82931	0.85244	0.15334
N	-0.83593	0.27519	-0.54103
N	0.37104	0.63494	-0.04002
C	0.05709	1.42469	0.96794
N	-1.28351	1.58847	1.12393
C	1.08473	2.06545	1.84640
C	0.70605	3.46072	2.21650
N	0.32517	4.39341	1.30404
C	-0.00681	5.44265	2.04000
N	0.19081	5.14924	3.33150
N	0.64150	3.87921	3.46854
C	-0.68384	6.67488	1.55058
C	-2.13055	6.38699	1.27120
N	-2.94585	7.21075	0.56225
C	-4.10689	6.56570	0.54399
N	-3.97301	5.41174	1.21412
N	-2.71800	5.27787	1.68508
C	-5.38533	7.02960	-0.07359
O	-6.06021	8.00424	0.72498
H	-7.06854	0.49402	-0.75983
H	-5.48350	-0.84407	-2.13061
H	-3.07476	-0.68668	-1.70813
H	-6.21340	1.97572	1.02807
H	-0.88801	-0.32573	-1.35079
H	2.04225	2.04725	1.32242
H	1.20638	1.48488	2.76344
H	0.01811	5.72776	4.14178
H	-0.20429	7.02320	0.63489
H	-0.59532	7.47553	2.28840
H	-4.64853	4.67219	1.35391
H	-6.02831	6.16693	-0.27018
H	-5.16303	7.51569	-1.02263
H	-6.39783	7.56321	1.51654
H	-2.77783	2.29879	1.71940