

Electronic Supplementary Information

Rapid Detection Strategies for the Ultra-level Chemosensing of Uranyl Ions

Selva Kumar R^{a,b}, Vetriarasu V^a, R. Bhaskar^a, S.K. Ashok Kumar^{a*}, Kari Vijayakrishna^c, Akella Sivaramakrishna^a, C.V.S. Brahmmananda Rao^d, N. Sivaraman^d, and Suban K. Sahoo^e

^a Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore-632014, Tamil Nadu, India.

^b Department of Chemistry, Saveetha School of Engineering, Saveetha Institute of Medical and Technological Sciences, (SIMATS), Chennai- 602105, Tamil Nadu, India.

^c School of Basic Sciences, Indian Institute of Technology Bhubaneswar, Bhubaneswar, Odisha 752050, India.

^d Indira Gandhi Centre for Atomic Research, HBNI, Kalpakkam-603102, Tamil Nadu, India.

^e Department of Chemistry, Sardar Vallabhbhai National Institute Technology, Surat-395007, Gujarat, India.

† E-mail: ashok312002@gmail.com.

Contents

Colour space and its conversion

Figure Captions

Figure 1S. FTIR spectrum of **L**

Figure 2S. ¹H NMR spectrum of **L**

Figure 3S. ¹³C NMR spectrum of **L**

Figure 4S. DEPT-135 NMR spectrum of **L**

Figure 5S. HH-COSY NMR spectrum of **L**

Figure 6S. CH-COSY NMR spectrum of **L**

Figure 7S. NOESY NMR spectrum of **L**

Figure 8S. HR-Mass spectrum for **L**

Figure 9S. Stability examination of **L** in DMSO in (8:2, v/v) DMSO:water media

Figure 10S. FMO of Ligand **L** by TDDFT analysis.

Figure 11S. FMO of **L-UO₂²⁺** complex by TDDFT analysis.

Figure 12S. Colour change of **L** with Th⁴⁺ and UO₂²⁺ in CIE 1931 colour space

Figure 13S. Change in RGB values of **L** with respect to UO₂²⁺ concentration.

Table captions

Table 1S. The atomic charges on selected atoms

Table 2S. UV-vis spectra characteristic by experimental and theoretical.

Table 3S. Sensing ability of **L** towards UO₂²⁺ determination with previously reported work

Colour Space and its Conversion

Conversion of smartphone camera image data into the CIE 1931 colour space involves three steps. In which the colour space terms are derived from the conventional RGB values.

At first, the non-linear RGB values are obtained from smartphone must be converted into linear RGB values using the following equations.

$$R_l = (0.055 + R_c / 1.055)^{2.4} \text{ ----- (1)}$$

$$G_l = (0.055 + G_c / 1.055)^{2.4} \text{ ----- (2)}$$

$$B_l = (0.055 + B_c / 1.055)^{2.4} \text{ ----- (3)}$$

Next, the linear RGB values are converted into tristimulus values X, Y, Z by the following relationships.

$$\begin{bmatrix} X \\ Y \\ Z \end{bmatrix} = \begin{bmatrix} 0.607 & 0.174 & 0.200 \\ 0.299 & 0.587 & 0.114 \\ 0.000 & 0.066 & 1.116 \end{bmatrix} \begin{bmatrix} R_l \\ G_l \\ B_l \end{bmatrix} \text{ ----- (4)}$$

Finally, the X, Y, Z tristimulus values are converted into 2-D (x,y) CIE 1931 chromaticity space using the following relationships.

$$x_j = \frac{X}{X + Y + Z} \text{ ----- (5)}$$

$$y_j = \frac{Y}{X + Y + Z} \text{ ----- (6)}$$

The new colour space specified by x, y and Y is represented in 2-D chromaticity diagram. The pure colour is located in boundary curve from blue (380 nm) to red (700 nm), while all the mixed colours are represented within the area enclosed by the curve.

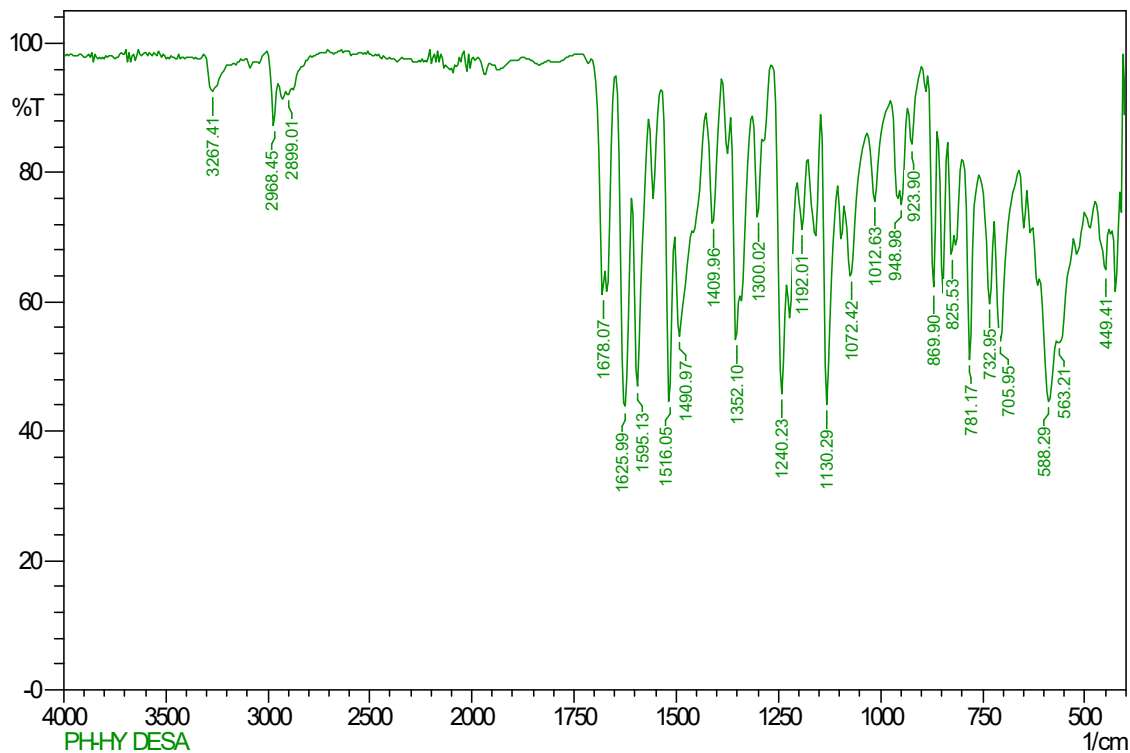


Figure 1S. FTIR spectrum of L

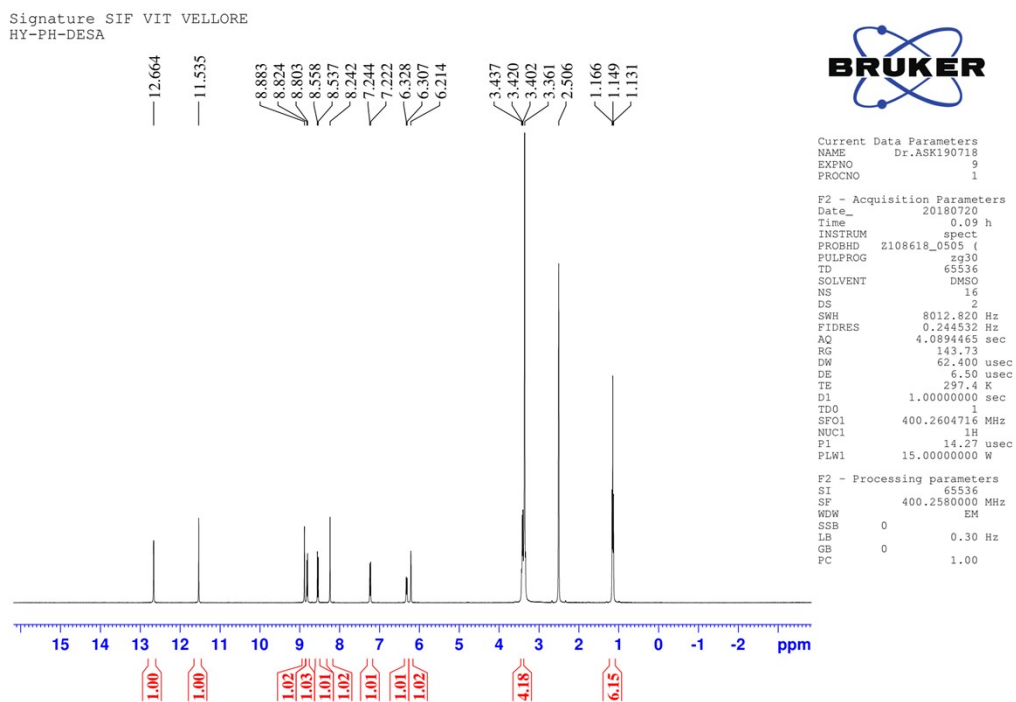
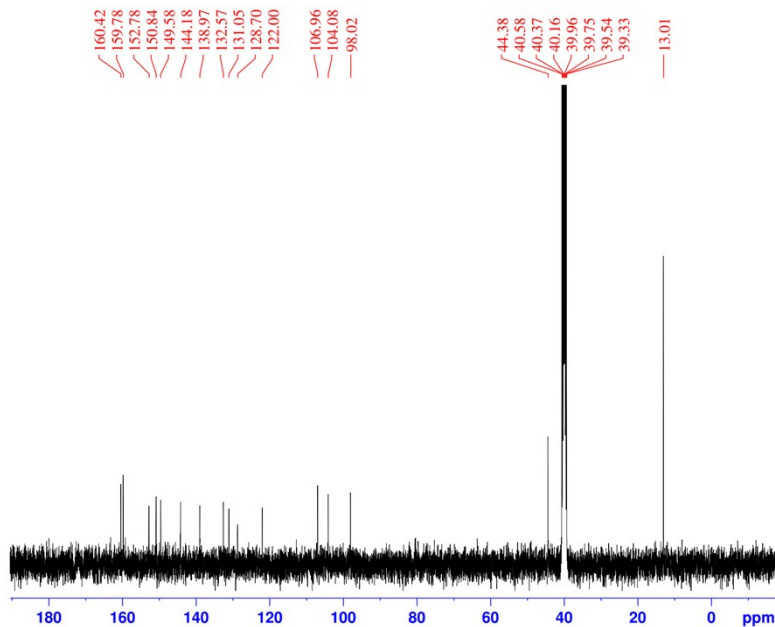


Figure 2S. ¹H NMR spectrum of L

Signature SIF VIT VELLORE
HY-PH-DESA



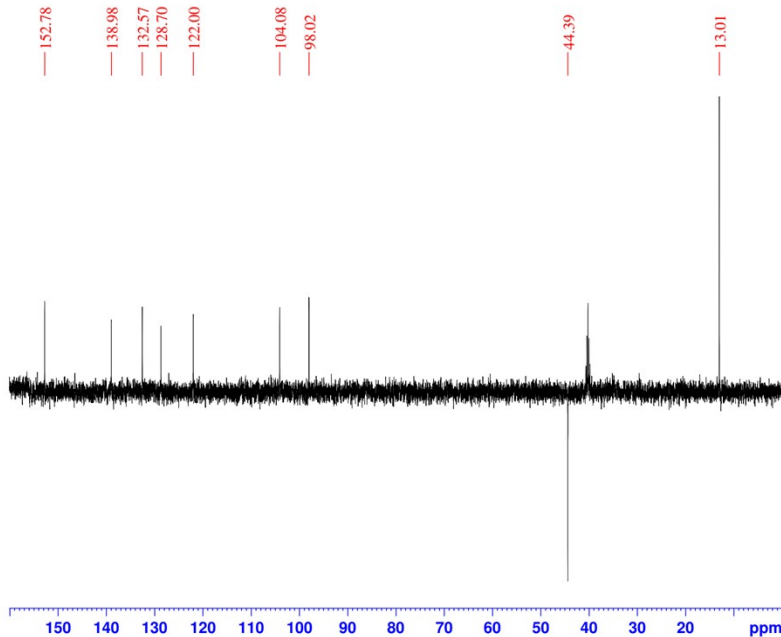
Current Data Parameters
NAME Dr.ASK190718
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180720
Time 0.39 h
INSTRUM spect
PROBHD z108618_0505 ()
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 127.79
DW 20.800 usec
DE 6.50 usec
TE 297.8 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1
SFO1 100.6550186 MHz
NUC1 13C
P1 9.80 usec
PLW1 58.0000000 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.0000000 W
PLW12 0.37709999 W
PLW13 0.18968000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 3S. ¹³C NMR spectrum of L

Signature SIF VIT VELLORE
PH-HY-DESA



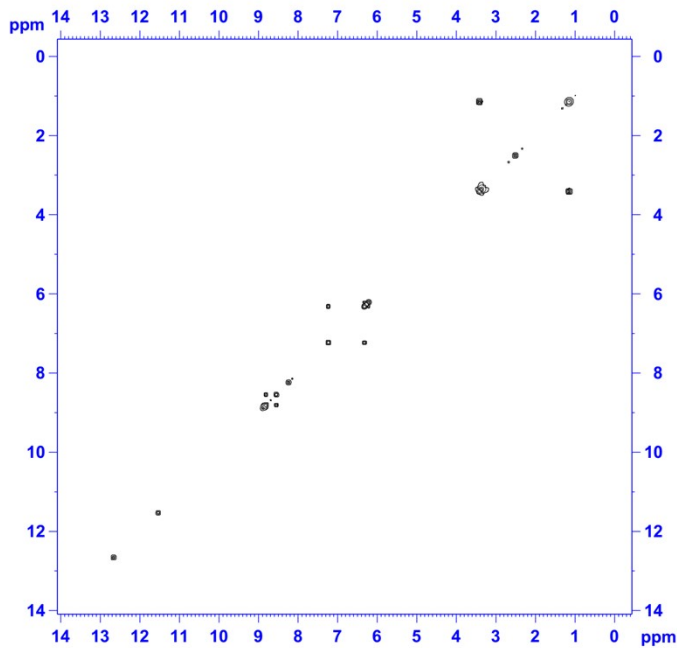
Current Data Parameters
NAME Dr.ASK260718
EXPNO 26
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180727
Time 9.28 h
INSTRUM spect
PROBHD z108618_0505 ()
PULPROG deptsp135
TD 65536
SOLVENT DMSO
NS 256
DS 8
SWH 16129.032 Hz
FIDRES 0.482219 Hz
AQ 2.0316160 sec
RG 199.6
DW 31.000 usec
DE 6.50 usec
TE 298.1 K
CNST2 145.0000000
D1 2.0000000 sec
D2 0.0034828 sec
D12 0.0000200 sec
TDO 1
SFO1 100.6530057 MHz
NUC1 13C
P1 9.80 usec
P13 2000.00 usec
PLW0 0 W
PLW1 58.0000000 W
SPNAM[5] Crp60comp.4
SFOAL5 0 Hz
SPW5 8.51080036 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
F3 14.27 usec
F4 28.54 usec
PCPD2 90.00 usec
PLW2 15.0000000 W
PLW12 0.37709999 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 4S. DEPT-135 NMR spectrum of L

Signature SIF VIT VELLORE
PH-HY-DESA



```
Current Data Parameters
NAME      Dr.ASK260718
EXPNO     24
PROCNO    1

F2 - Acquisition Parameters
Date_     20180727
Time      8.50 h
INSTRUM   spect
PROBHD    Z108618_0505 (
PULPROG   cosypppqr4e
TD         6548
SOLVENT   DMSO
NS         1
DS         16
SWH        5813.954 Hz
FIDRES     5.677689 Hz
AQ         0.1761280 sec
RG         63.11
DM         86.000 usec
DE         6.50 usec
TE         297.8 K
D0         0.0000300 sec
D1         2.02047990 sec
D11        0.03000000 sec
D12        0.00002000 sec
D13        0.00000400 sec
D16        0.00020000 sec
IND        0.00017200 sec
TDav      400.2607318 MHz
SFO1       1H
NUC1       1H
PQ         14.27 usec
PL1        14.27 usec
P17        2500.00 usec
PLM1       15.00000000 W
PLM10      3.39389992 W
GPRM(1)    SMSG10_100
GF21       10.00 %
PF6        1000.00 usec

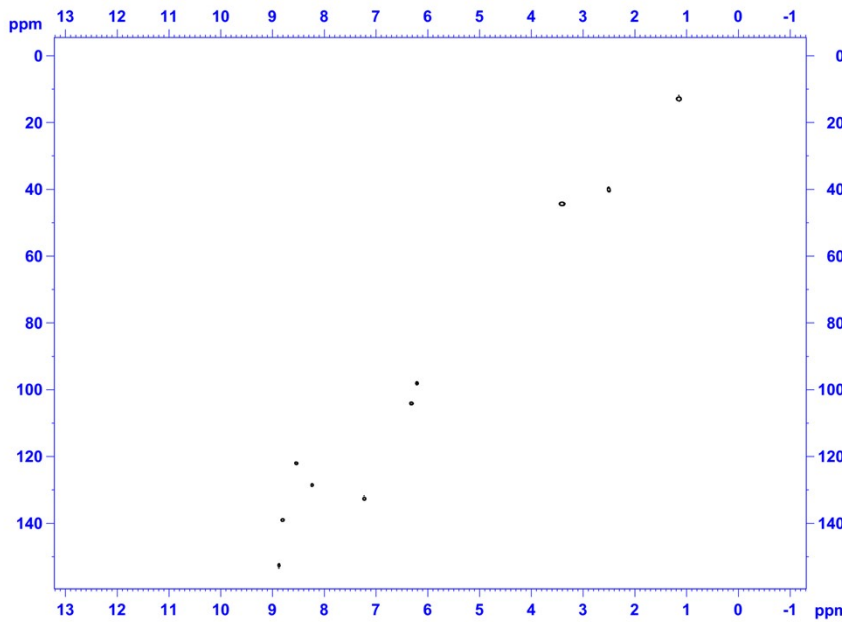
F1 - Acquisition parameters
TD         128
SFO1       400.2607 MHz
FIDRES     90.849025 Hz
SW         14.525 ppm
FHM00E     QF

F2 - Processing parameters
SI         1024
SF         400.2580000 MHz
WDW        QSIING
SSB         0
LB         0 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
NUC2       1H
SF         400.2580000 MHz
WDW        QSIING
SSB         0
LB         0 Hz
GB         0
```

Figure 5S. HH-COSY NMR spectrum of L

Signature SIF VIT VELLORE
PH-HY-DESA



```
Current Data Parameters
NAME      Dr.ASK260718
EXPNO     25
PROCNO    1

F2 - Acquisition Parameters
Date_     20180727
Time      8.56 h
INSTRUM   spect
PROBHD    Z108618_0505 (
PULPROG   hugeteqp
TD         1024
SOLVENT   DMSO
NS         1
DS         16
SWH        9813.054 Hz
FIDRES     11.353378 Hz
AQ         0.08800400 sec
RG         199.6
DM         86.000 usec
DE         6.50 usec
TE         297.8 K
D0         0.0000300 sec
D1         1.51023994 sec
D4         0.0017414 sec
D11        0.03000000 sec
D12        0.00002000 sec
IND        0.00003010 sec
TDav      400.2607318 MHz
SFO1       13C
NUC1       13C
PQ         14.27 usec
PL1        28.54 usec
P17        1000.00 usec
PLM1       15.00000000 W
PLM10      100.4535021 MHz
NUC2       13C
CPROG(2)   gwhf
P3         9.80 usec
P4         19.40 usec
PCF02      80.00 usec
PLM2       58.00000000 W
PLM21      0.87030000 W
GPRM(1)    SMSG10_100
GF21       10.00 %
GF22       SMSG10_100
GF23       01.10 %
PF6        1000.00 usec

F1 - Acquisition parameters
TD         256
SFO1       100.6255 MHz
FIDRES     129.737574 Hz
SW         165.036 ppm
FHM00E     EchoAnticlock

F2 - Processing parameters
SI         1024
SF         400.2580000 MHz
WDW        QSIING
SSB         2
LB         0 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
NUC2       echoAnticlock
SF         100.4449452 MHz
WDW        QSIING
SSB         2
LB         0 Hz
GB         0
```

Figure 6S. CH-COSY NMR spectrum of L

Signature SIF VIT VELLORE
PH-HY-DESA

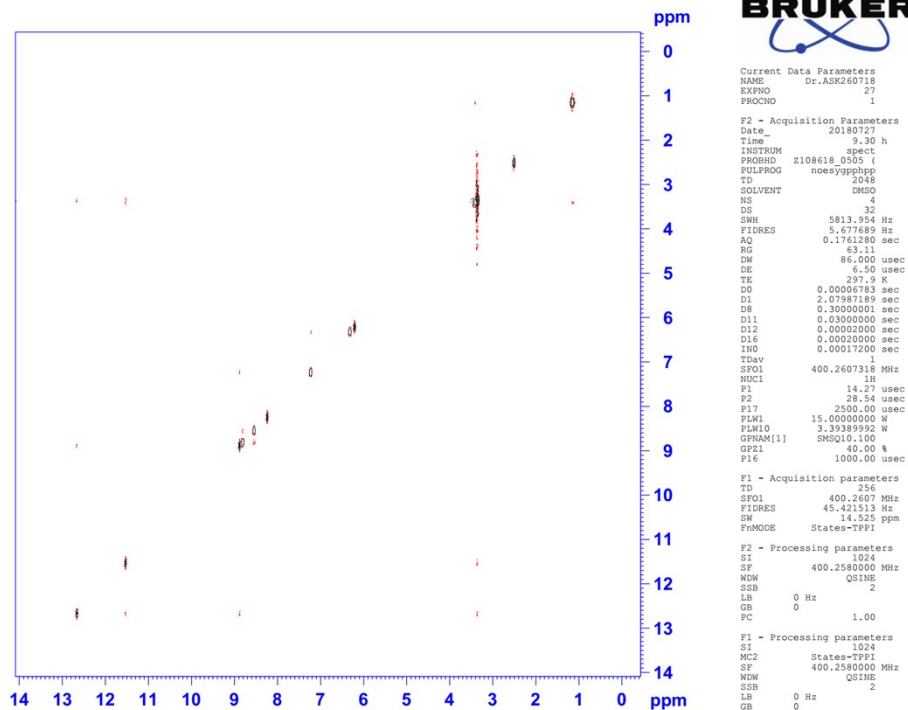


Figure 7S. NOESY NMR spectrum of L

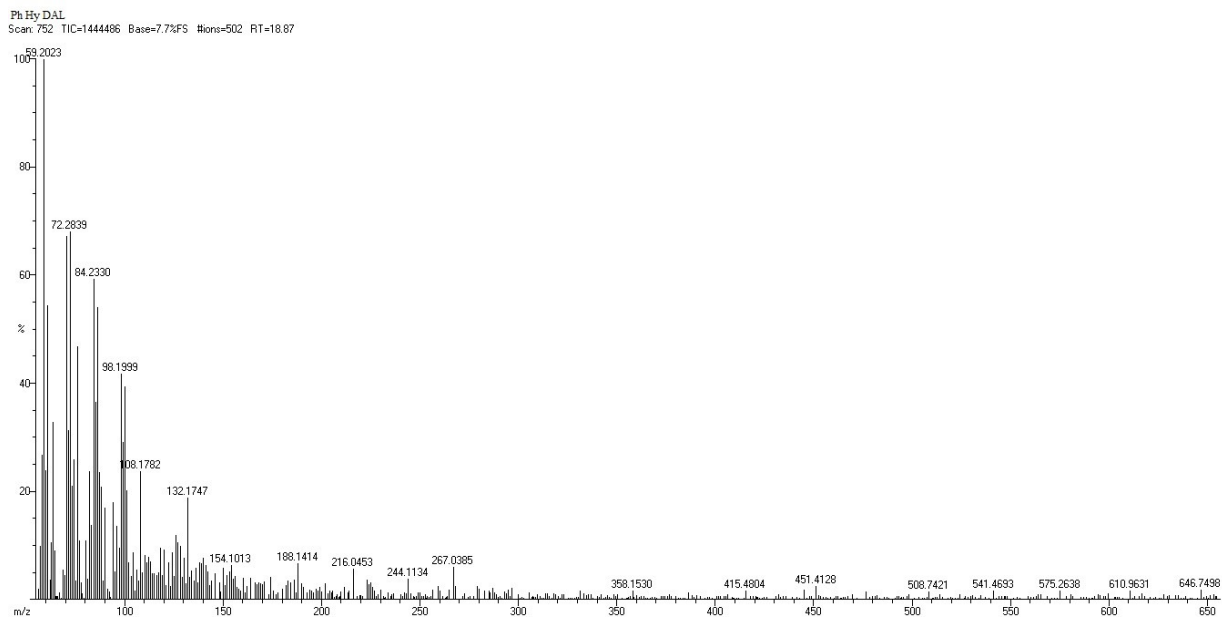


Figure 8S. HR-Mass spectrum for L

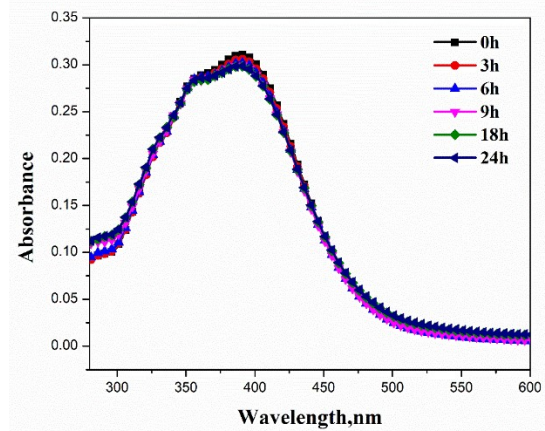


Figure 9S. Stability examination of L in DMSO in (8:2, v/v) DMSO:water media

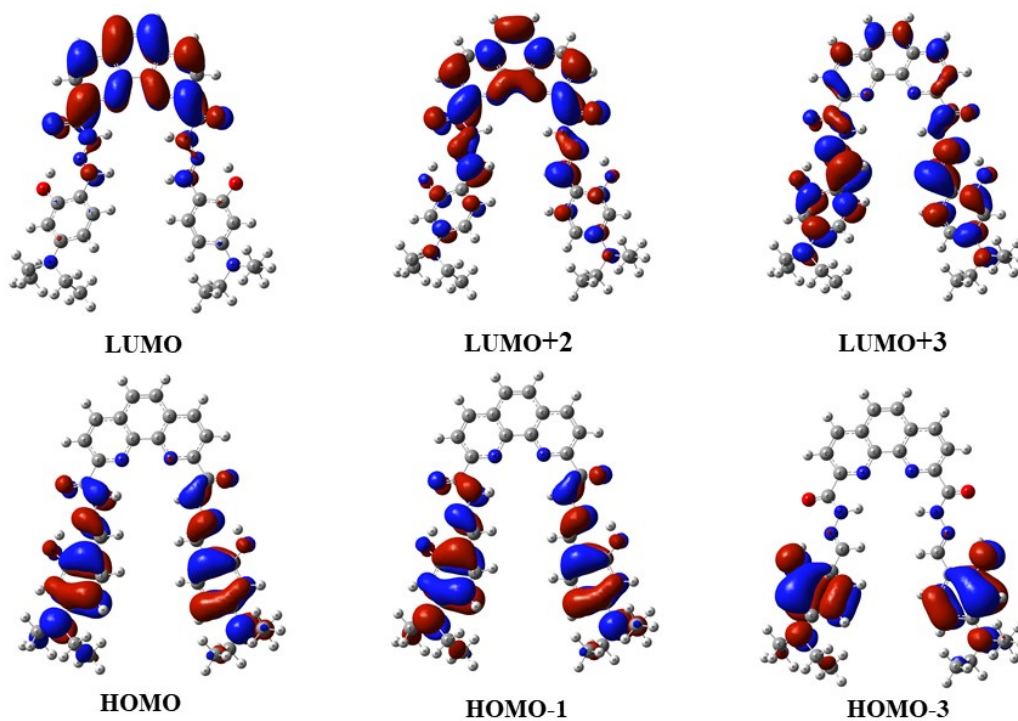


Figure 10S. FMO of L by TDDFT analysis.

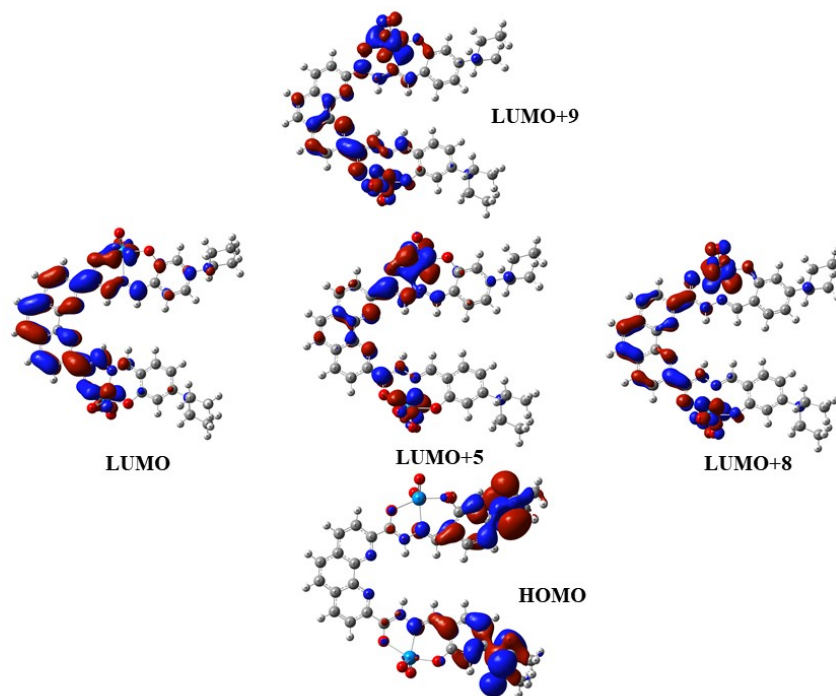


Figure 11S. FMO of L-UO₂²⁺ complex by TDDFT analysis.

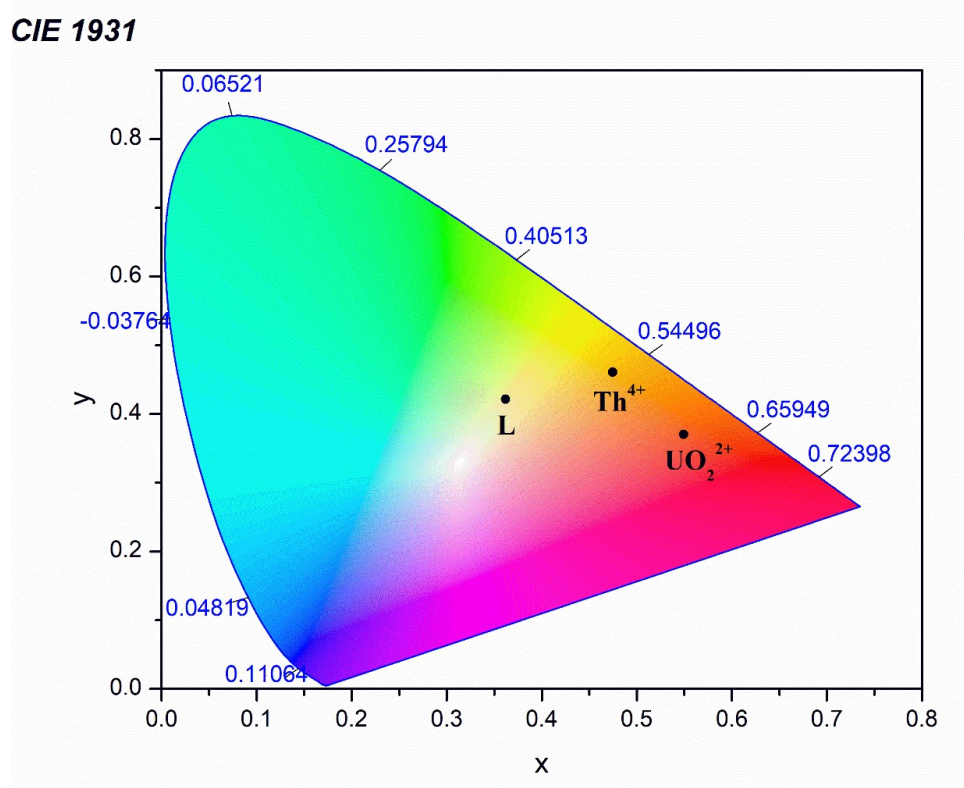


Figure 12S. Colour change of L with Th⁴⁺ and UO₂²⁺ in CIE 1931 colour space

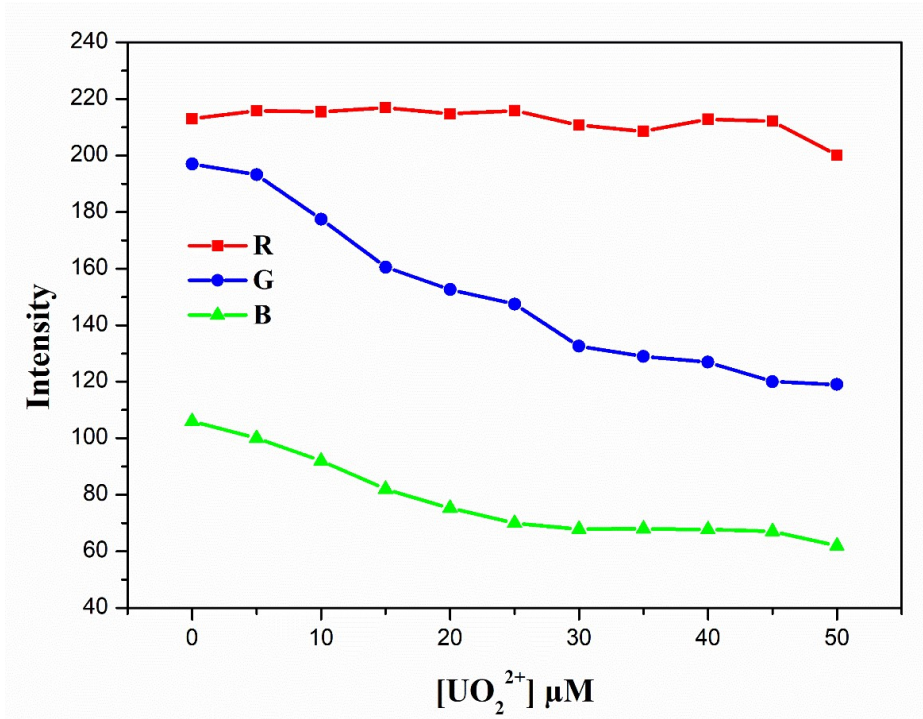


Figure 13S. Change in RGB values of L with respect to UO₂²⁺ concentration.

Table 1S. The atomic charges on selected atoms

Atom	L		L-UO ₂ ²⁺	
	Mullikan charge	NBO charge	Mullikan charge	NBO charge
C=O	-0.336	-0.591	-0.570	-0.633
Imine-N	-0.283	-0.334	-0.484	-0.425
Nap-OH	-0.384	-0.690	-0.603	-0.641
U	-	-	1.637	1.877

Table 2S. UV-vis spectra characteristic by experimental and theoretical.

	Experimental		Theoretical			
	λ_{\max} (nm)	ϵ (L M ⁻¹ cm ⁻¹)	Excitation energy (nm)	Oscillator strength	Excited state	Key transitions
L	353	47460	329.29	0.5454	S ₀ → S ₁₃	H-1 → L+3 (89%)
	389	50500	388.96	0.3238	S ₀ → S ₆	H → L+2 (71%), H-3 → L (27%)
L-UO₂²⁺	482	55275	488.24	0.0538	S ₀ → S ₂₅	H → L+8 (65%), H → L+9 (20%), H→L+5 (2%)

*H- HOMO, L-LUMO

Table 3S. Comparison of the sensing ability of **L** towards UO_2^{2+} determination with previously reported work.

Sensors	UV-Vis	Test Strip	RGB	LOD	pH	Solvent media used	Interference
DNAzyme-functionalized magnetic beads-AuNP ⁵⁴	Yes	NR	NR	74 pM	7.5	TMB-H ₂ O ₂	Fe ³⁺ , Ni ²⁺
DNAzyme modulator ⁵⁵	Yes	NR	NR	2 nM	3.5	TMB-H ₂ O ₂	Mn ²⁺ , Al ³⁺
DNAzyme-functionalized magnetic beads ⁵⁶	Yes	NR	NR	0.33 nM	7.5	TMB-H ₂ O ₂	Mg ²⁺ , Mn ²⁺ , Th ⁴⁺ , La ³⁺
Terbium (III)-based MOF ⁵⁷	Yes	NR	NR	0.9 μg/L	4.0	H ₂ O-suspension	NR
Quinoxolinol Salen ⁵⁸	Yes	NR	NR	1.9 μM	NR	DMF:H ₂ O (8:2, v/v)	Cu ²⁺ , Ni ²⁺
O-phosphoryl ethanolamine-functionalized gold nanoparticles ⁵⁹	Yes	NR	NR	0.084 μM	4.0	H ₂ O-suspension	Co ²⁺
2-(5-Bromo-2-pyridylazo)-5-(diethylamino) phenol in CTA nana fiber ⁶⁰	Yes	Yes	Yes	0.185 μM	6.0	Solid Phase	Fe ²⁺ , Cu ²⁺
This work (L)	Yes	Yes	Yes	73 nM	2-10	DMSO:H ₂ O (8:2, v/v)	No interference

NR= not reported, TMB - 3,3',5,5'-tetramethylbenzidine sulfate,
