Supplementary Information

Triply phenoxo bridged Eu(III) and Sm(III) complexes with 2,6-diformyl-4-methylphenol di(benzoylhydrazone) : Emission, EPR, antimicobacterial and cytotoxicity study on different human cell lines

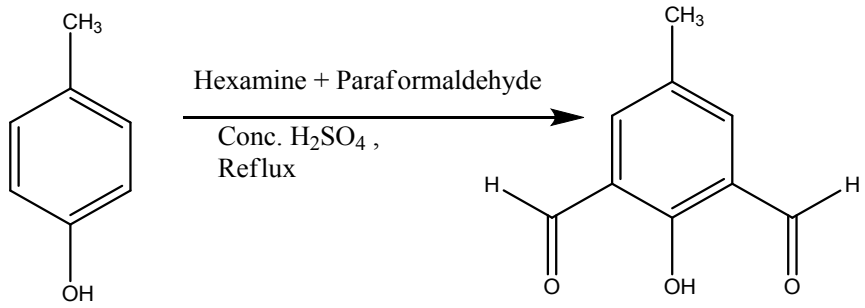
Kuheli Das, Soumendra Nandi, Sudipa Mondal, Tulin Askun, Zerrin Cantürk, Pinar Celikboyun, Chiara Massera, Eugenio Garribba, Amitabha Datta,* Chittaranjan Sinha,* Takashiro Akitsu

Synthesis of 2,6-diformyl-4-methylphenol-di(benzoylhydrazone), H_3L

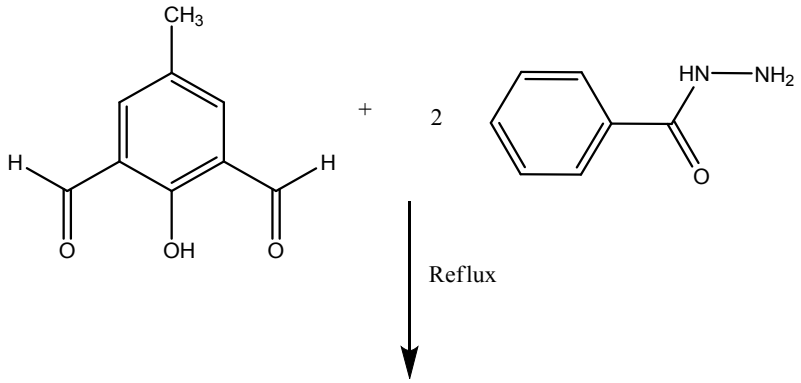
The ligand was synthesized according to literature procedure [19] (**Scheme 1**). 4-Methylphenol in glacial acetic acid was reacted with *p*-formaldehyde and hexamethylene tetraamine to synthesize 2,6-diformyl-4-methylphenol. It was then condensed with benzhydrazide in methanol to isolate 2,6-diformyl-4-methylphenol-di(benzoylhydrazone) (H_3L) in good yield (80%).

^{1}H NMR, 300 MHz, d_6-DMSO: 12.31 (1-OH s); 7.55 (4,6-H s); 8.7 (8,8'-H s); 12.13 (10,10'-NH s); 7.93 (13,13',17,17'-H d, J = 7.2); 7.59 (15,15'-H e); 7.51 (14,14' ,16,16'-H e); 2.31(5-CH_3 s) (s, singlet; d, doublet; e, multiplet).

Step 1:


CH3
OH
Hexamine + Paraformaldehyde
Conc. H2SO4 ,
Reflux
CH3
H
O
OH
O
H

Step 2:


CH3
H
O
OH
O
H
+
2
HN
NH2
O
Reflux

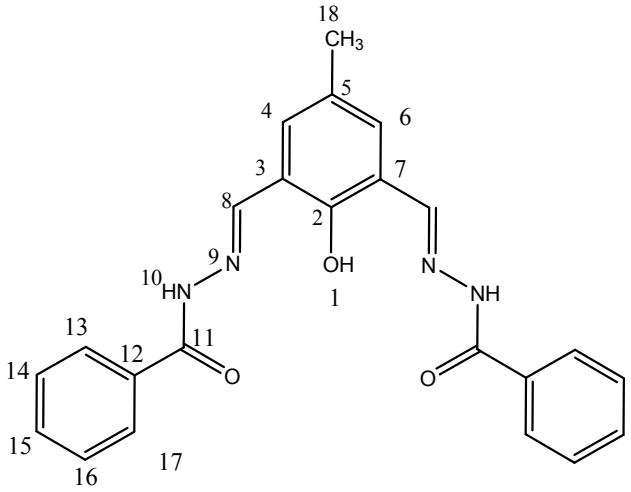

18
CH3
5
4
6
3
7
8
2
9
N
OH
N
10
HN
1
NH
13
11
12
O
14
O
15
17
16

Figure S1

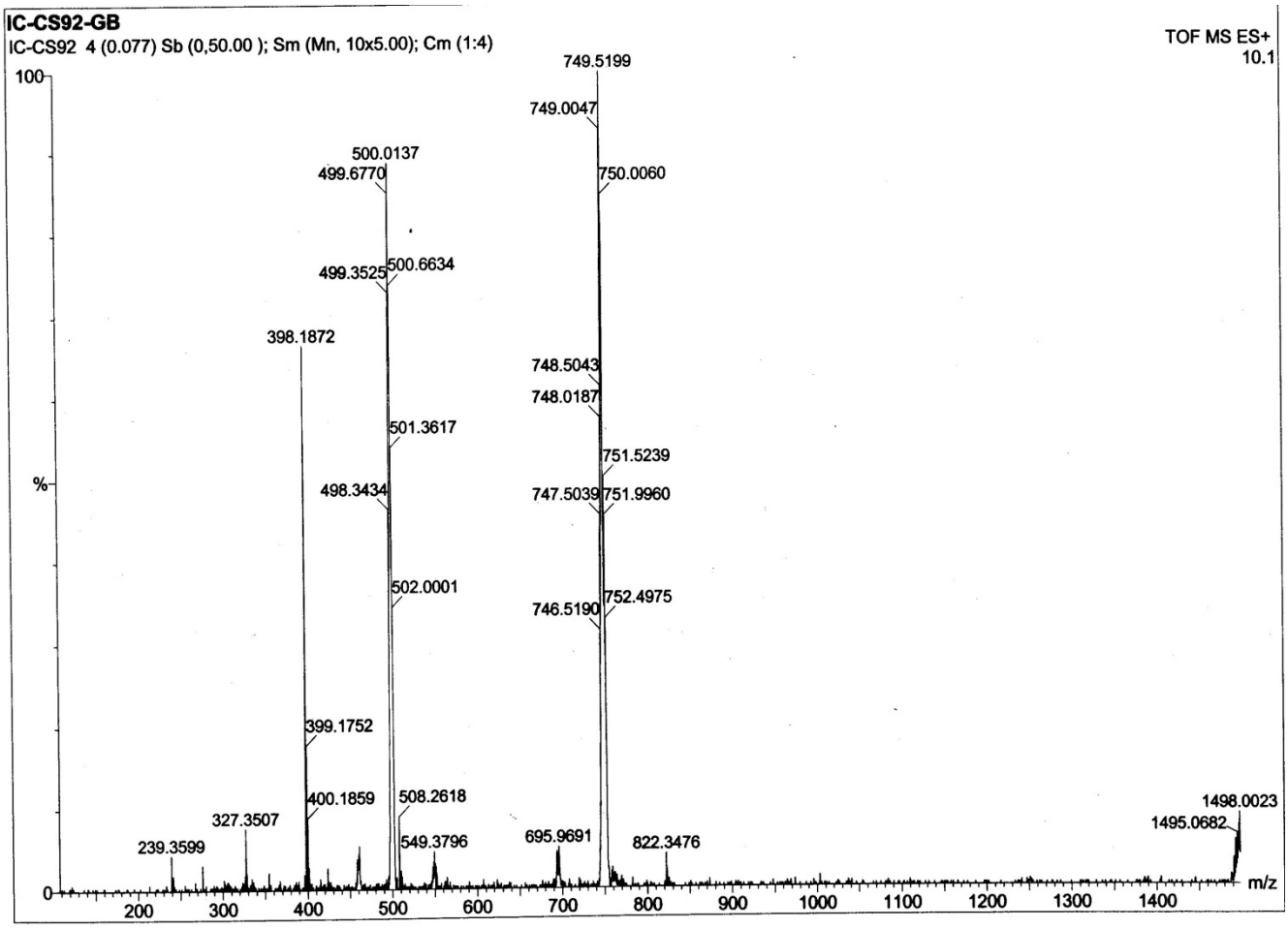
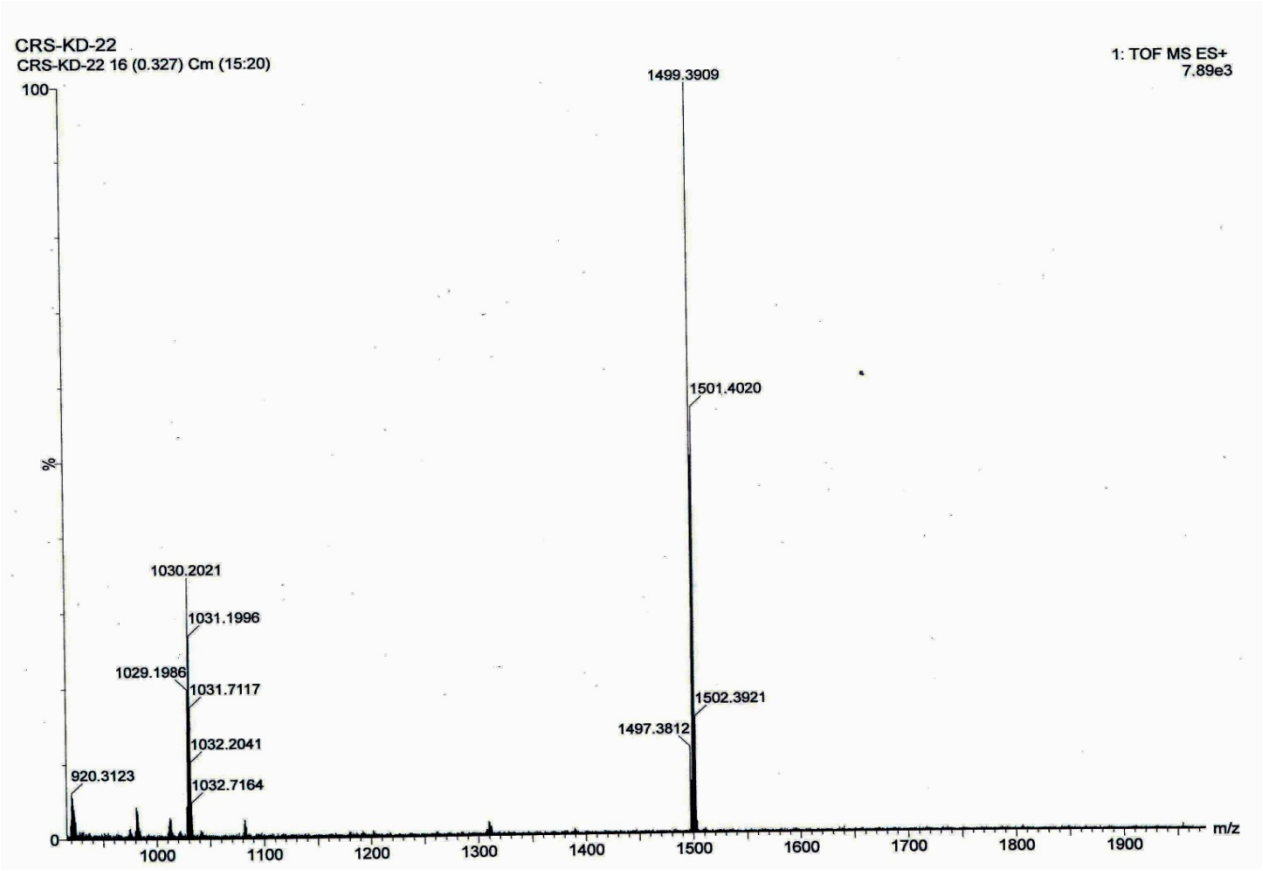


Figure S2


CRS-KD-22
CRS-KD-22 16 (0.327) Cm (15:20)
1: TOF MS ES+
7.89e3
100
%
0
1499.3909
1501.4020
1030.2021
1031.1996
1029.1986
1031.7117
1502.3921
1497.3812
1032.2041
920.3123
1032.7164
1000
1100
1200
1300
1400
1500
1600
1700
1800
1900
m/z