Electronic Supplementary Information

Lead ion induced chemodosimeter approach of a tripodal hydroxyl-quinoline based phospho-ester through P-O bond cleavage

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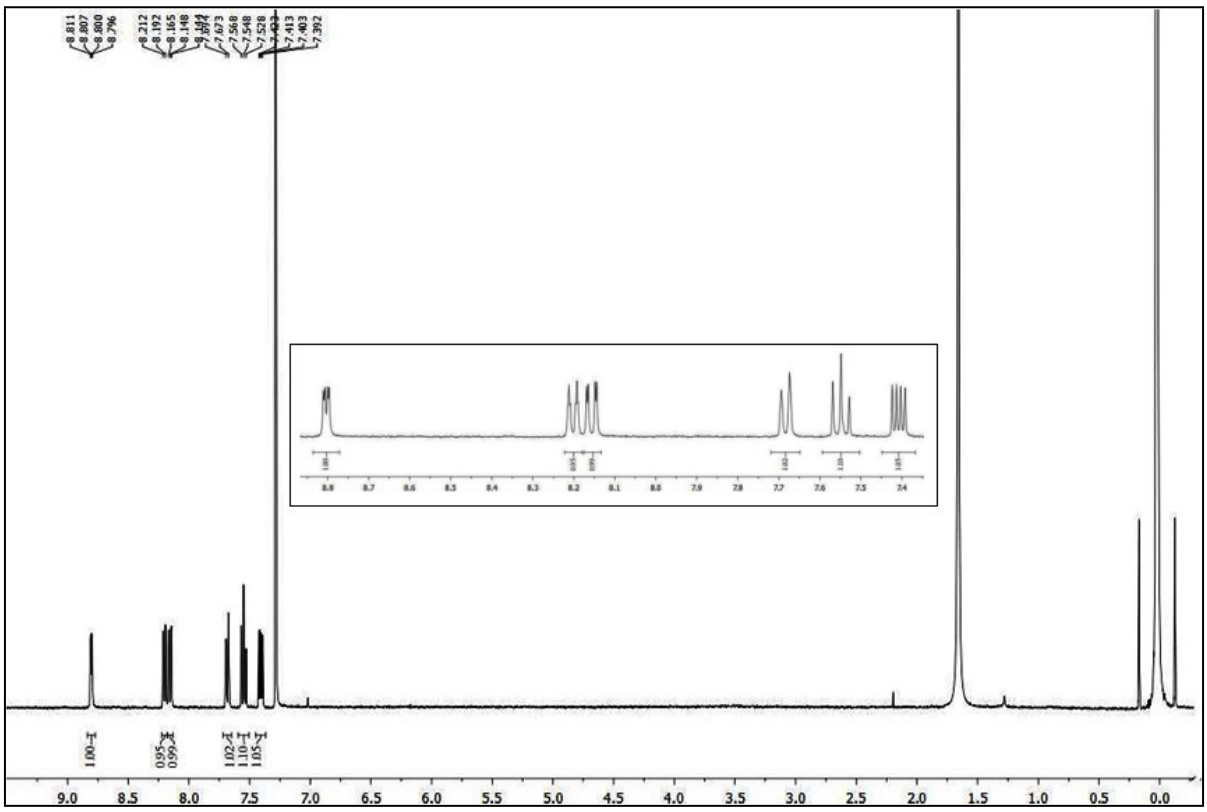
Table S1: ***Crystallographic data for HQP, NP and $Pb_4(HQ)_6(ClO_4)_2$:***

	HQP	**NP**	***$Pb_4(HQ)_6(ClO_4)_2$***
CCDC ref. no.	**1413010**	**1413012**	**1413011**
Formula	$C_{27}H_{18}N_3O_4P$	$C_{30}H_{21}O_4P$	$C_{54}H_{36}Cl_2N_6O_{14}Pb_4$
Formula Weight	479.41	476.44	1892.55
Crystal size (mm)	0.16 x 0.14 x 0.10	0.24 x 0.17 x 0.11	0.20 x 0.14 x 0.10
Temperature (K)	293(2)	293(2)	293(2)
Crystal System	Cubic	Monoclinic	Triclinic
Space group	P 213	P 21/c	P -1
a (Å)	13.3936(15)	13.7844(15)	10.247
b (Å)	13.3936(15)	9.8719(11)	11.756
c (Å)	13.3936(15)	21.2839(19)	12.669
α (°)	90.00	90.00	65.39
β (°)	90.00	125.688(5)	75.83
γ (°)	90.00	90.00	82.73
V [Å]^3	2402.7(5)	2352.4(4)	1344.8
Z	4	4	1
D_{calc} [g/cm^3]	1.325	1.345	2.337
μ(Mo-Kα) [mm^{-1}]	0.153	0.153	12.654
F(000)	992	992	876
Radiation [Å]: Mo-Kα	0.71073	0.71073	0.71073
$\theta_{Min-Max}$ [°]:	5.49, 27.41	0.982, 27.64	0.959, 27.00
Dataset:	-3≤ h ≤ 11	-17≤ h ≤ 17	-12≤ h ≤ 13
	-3 ≤ k ≤ 17	-11 ≤ k ≤ 12	-15 ≤ k ≤ 14
	-15 ≤ l ≤17	-27 ≤ l ≤ 27	-15 ≤ l ≤ 16
Total reflections	1636	5372	5615
Unique reflections	1299	3275	3795
Observed data [I > 2σ(I)]	1299	3275	3795
Refinement: N_{ref}, N_{par}	1636, 106	5372, 316	5615, 361
R (int)	0.0490	0.0487	0.0383
wR2 (all data), S	0.1293, 0.854	0.1083, 1.016	0.0790, 1.050
Max. & Av. Shift/Error	0.045, 0.010	0.000, 0.000	0.000, 0.000
Resd. Dens. [e/ Å^3]	-0.209, 0.196	-0.278, 0.273	-1.989, 1.345

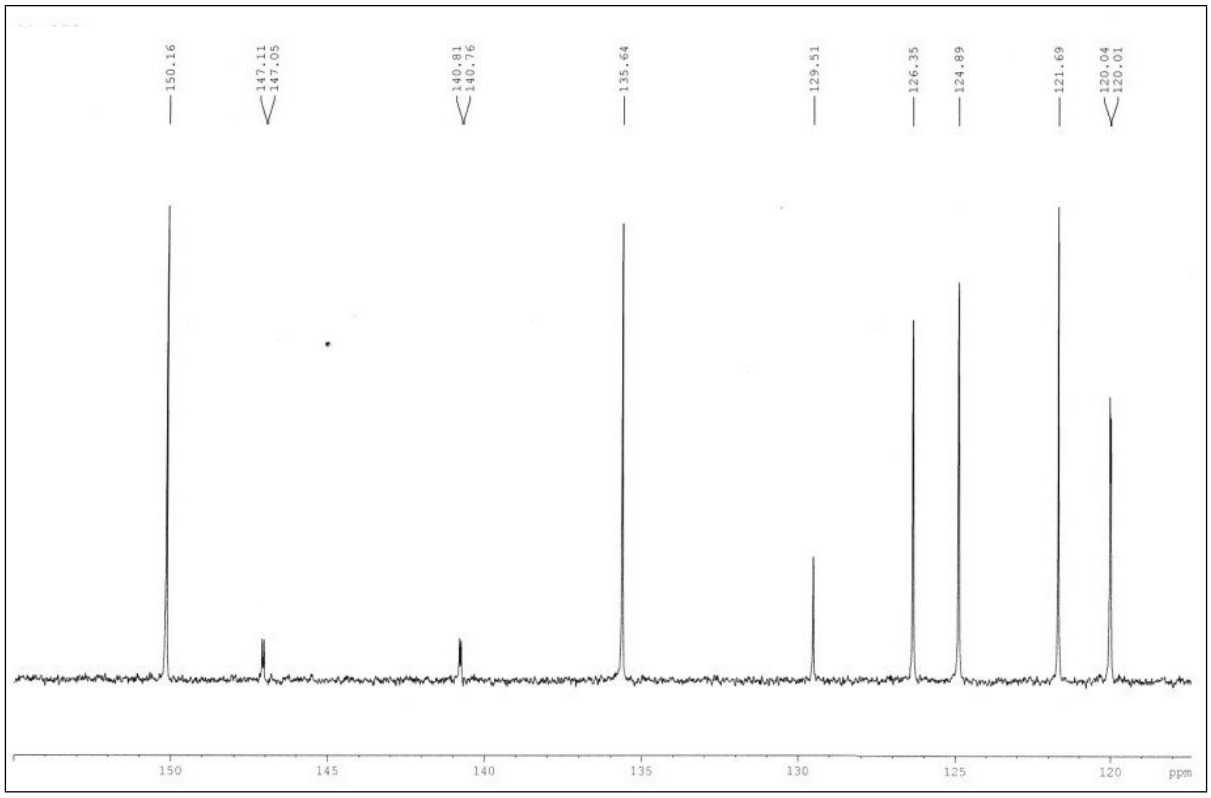
Table S2: Short contacts (Å) for the structure of ***$Pb_4(HQ)_6(ClO_4)_2$***.

Short Contacts	Distance (Å)
Cl1−O6 ⋯ Pb2	**3.000**
Cl1−O6 ⋯ Pb1	**3.153**
Cl1−O7 ⋯ Pb1	**3.232**
Cl1−O7 ⋯ H1−C1	**2.528**
Cl1−O6 ⋯ H7−C7	**2.637**

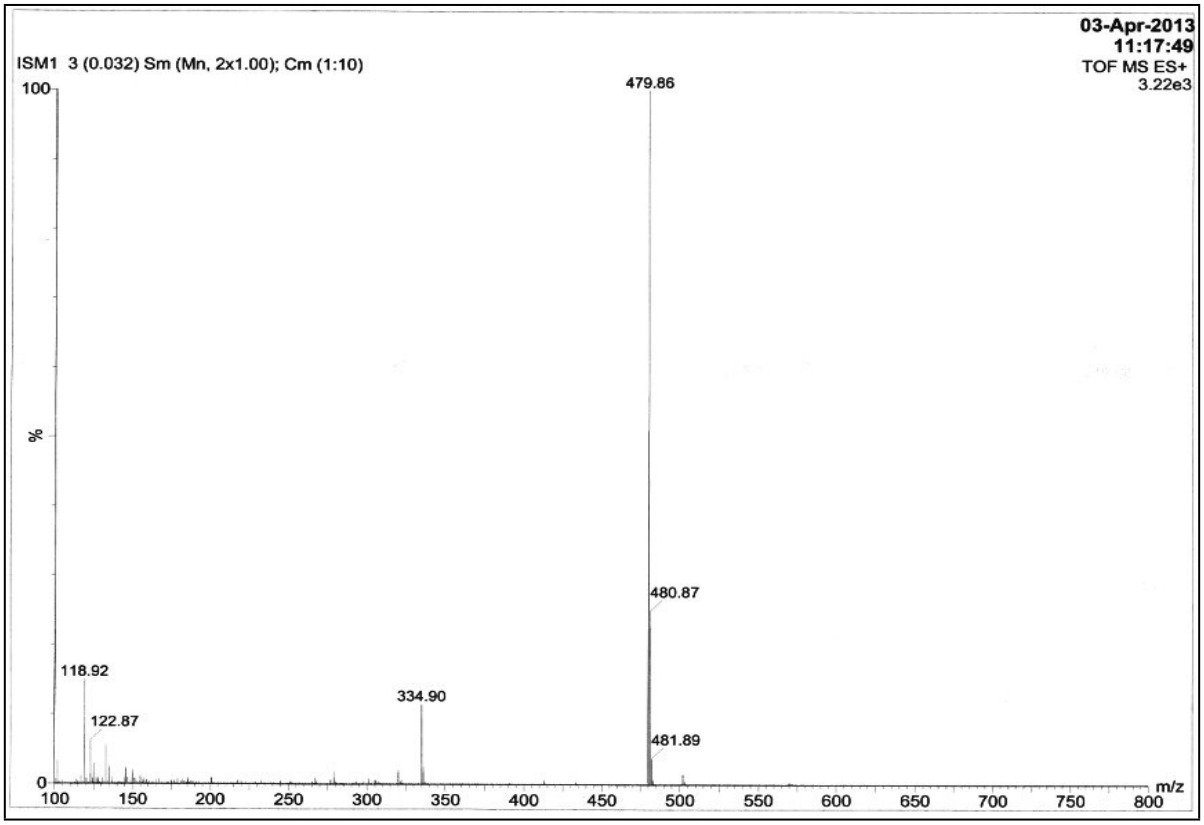
^{1}H NMR spectrum of HQP:



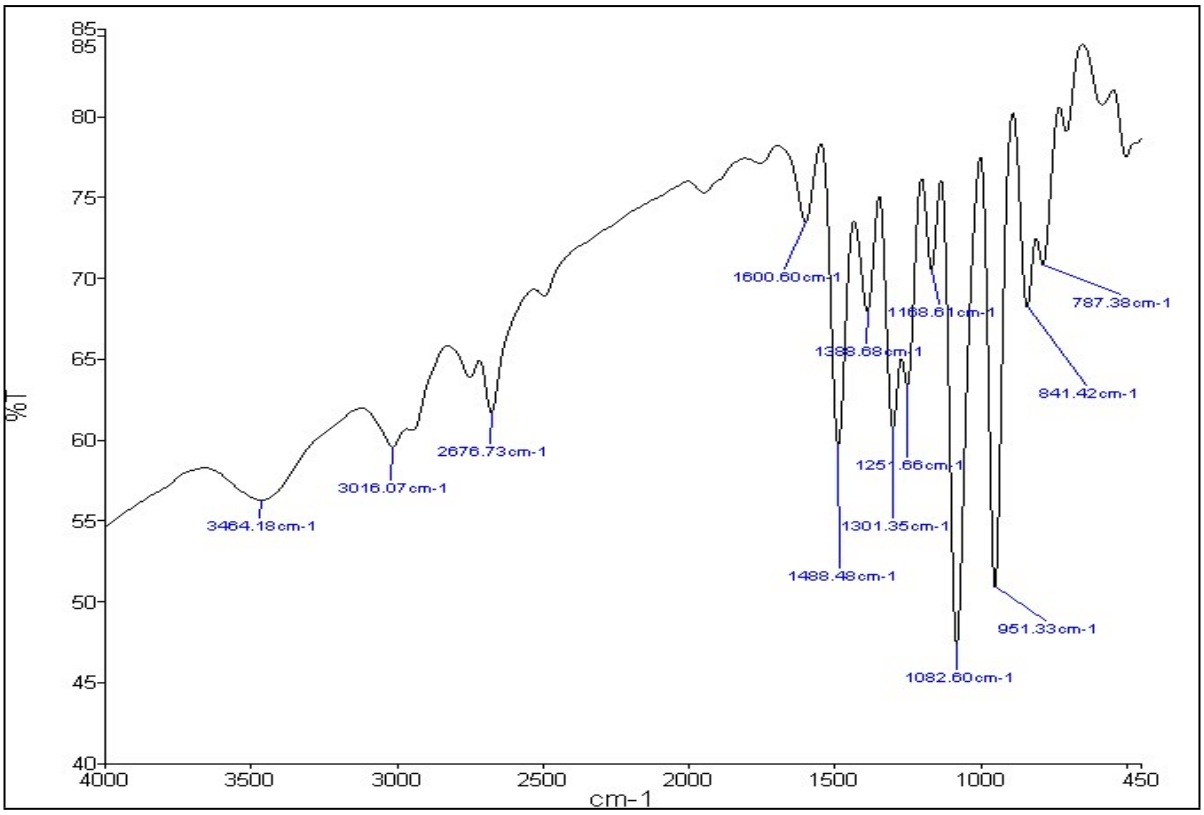
^{13}C NMR spectrum of HQP:



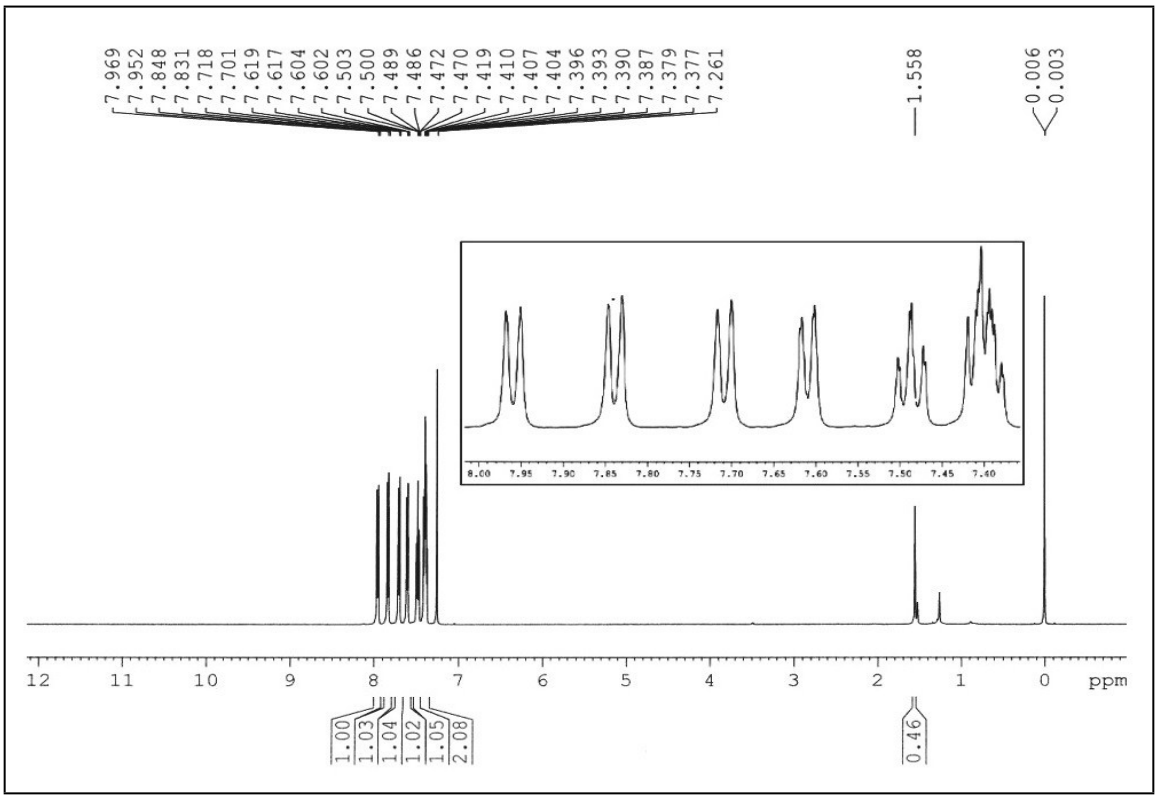
Mass spectrum of HQP:



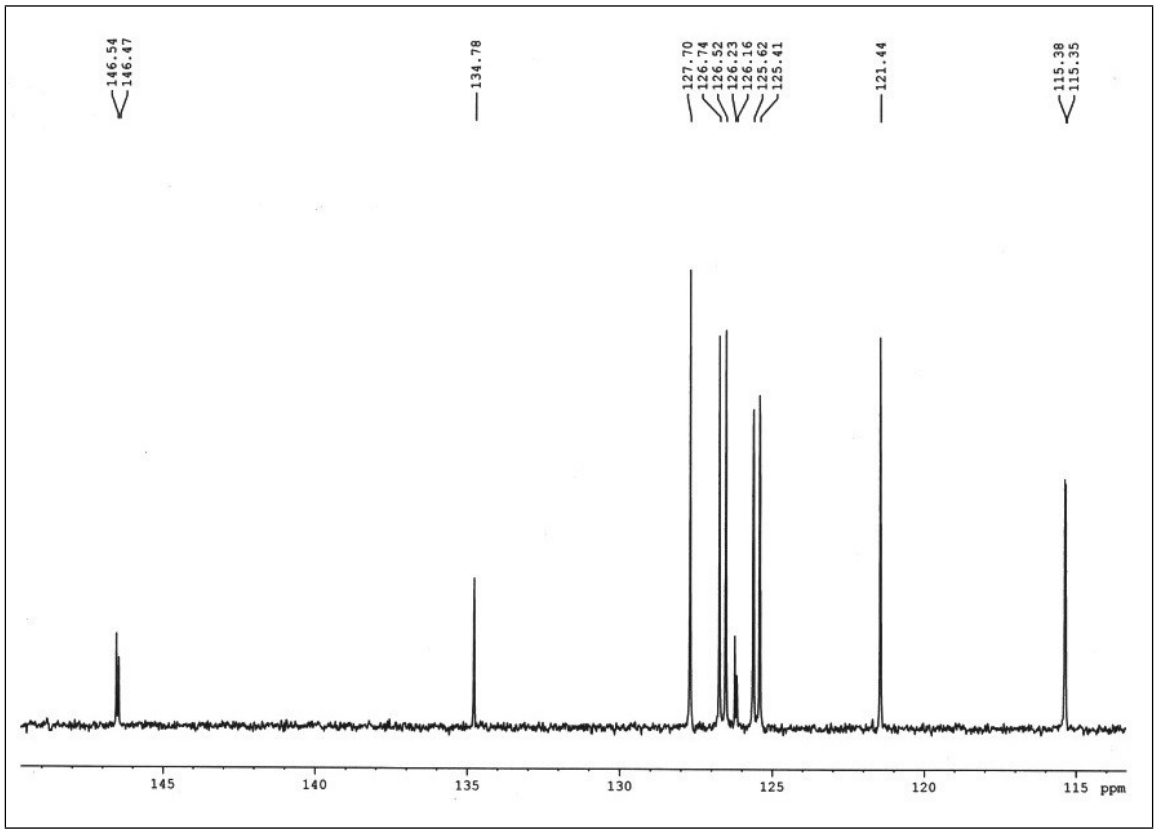
IR spectrum of HQP:



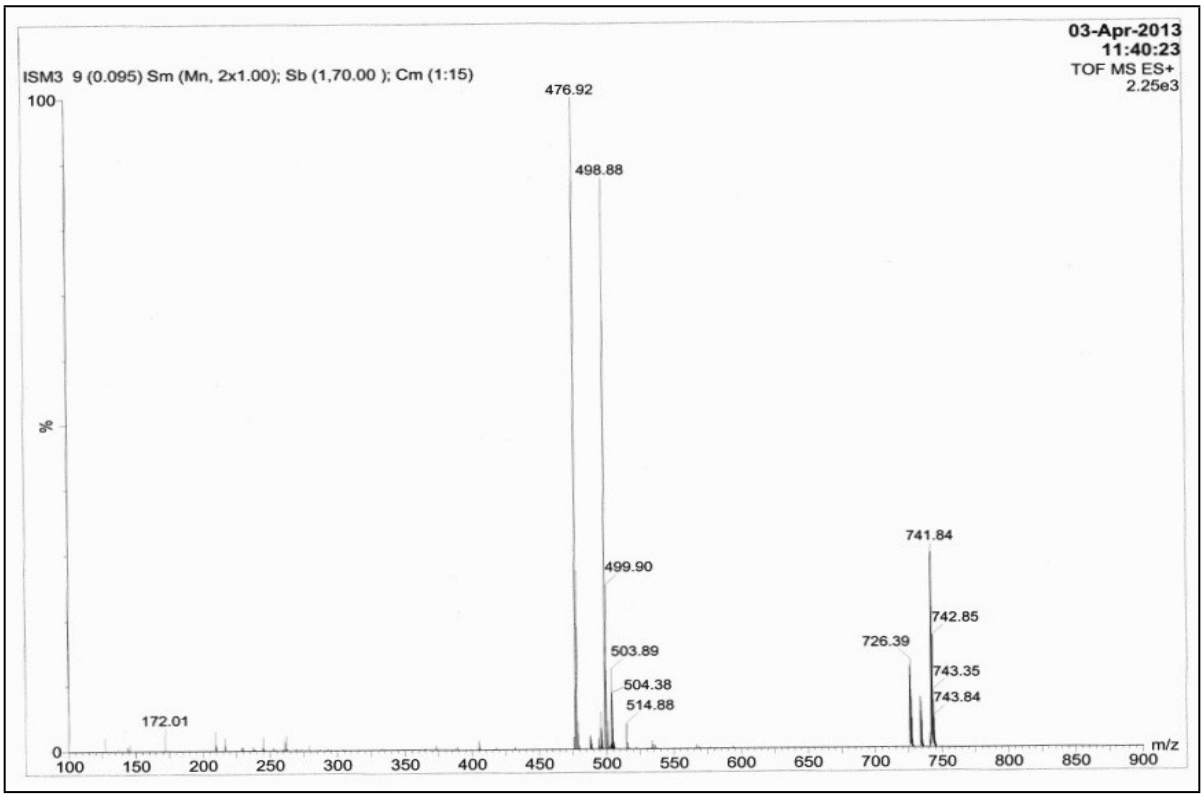
^{1}H NMR spectrum of NP:



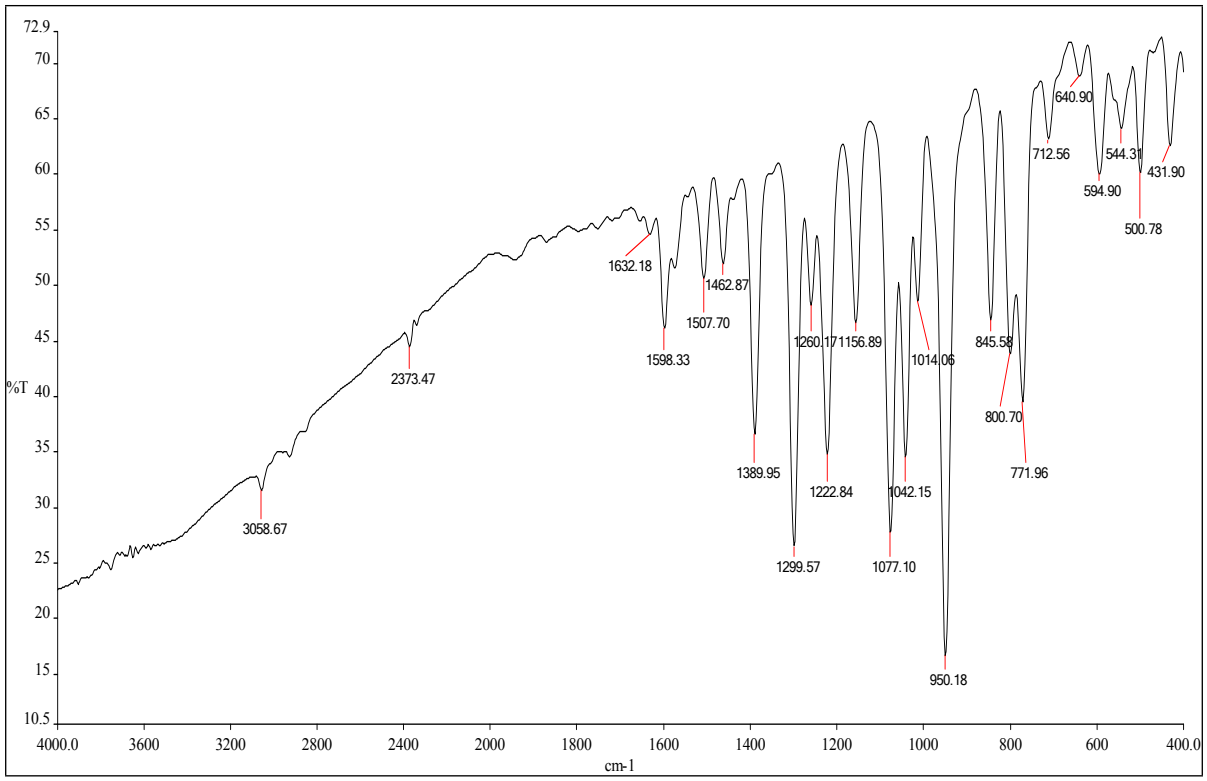
^{13}C NMR spectrum of NP:



Mass spectrum of NP:



IR spectrum of NP:



Calculation of limit of detection (LOD):

The detection limit of **HQP** for Pb^{2+} was calculated on the basis of fluorescence titration. To determine the standard deviation for the fluorescence intensity, the emission intensity of **HQP** without any anion was measured by 10 times and the standard deviation of blank measurements was calculated.

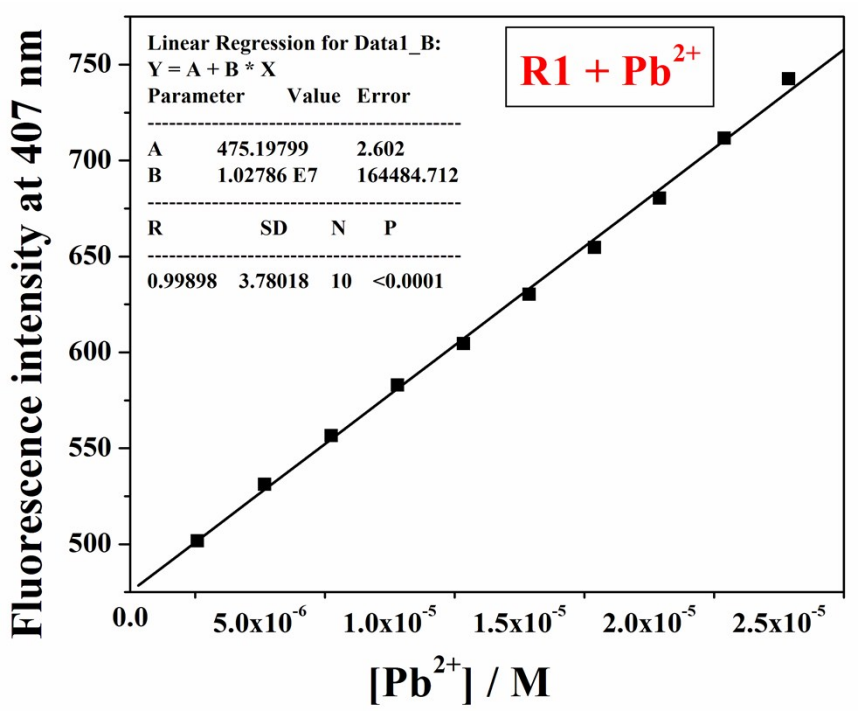
The limit of detection (LOD) of **HQP** for sensing Pb^{2+} was determined from the following equation:

$LOD = K \times SD/S$

Where K = 2 or 3 (we take 3 in this case); SD is the standard deviation of the blank receptor (**HQP**) solution; S is the slope of the calibration curve.

For HQP with Pb^{2+}:

From the linear fit graph we get slope = 1.02786×10^{7}, and SD value is 0.50284. Thus using the above formula we get the Limit of Detection = 1.467×10^{-7} M i.e. **HQP** can detect Pb^{2+} up to this very lower concentration by fluorescence techniques.



Calculation of association constant (K):

Association constant of **HQP** with **Pb^{2+}** ($K = 1.23 \times 10^5\ M^{-1}$) from UV titration data using non-linear method [following non-linear curve fitting equation: **$Y = (I_0 + A.K.X) / (1+ K.X)$**, where $X = [Pb^{2+}]$, Y= intensity of UV Vis absorption, I_0= initial intensity of HQP].