

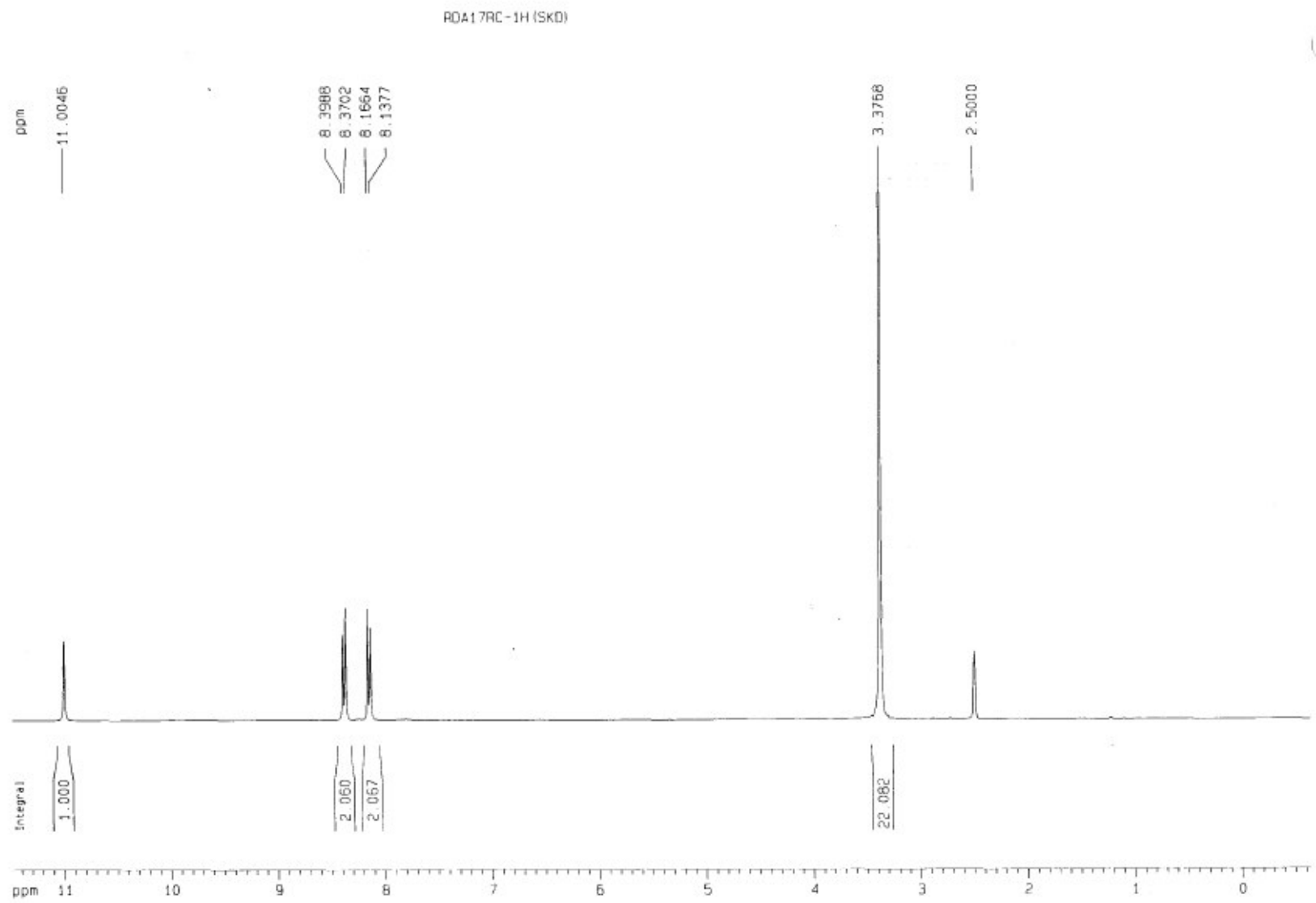
## Supporting Information

### Optical Detection of Sodium Salts of Fluoride, Acetate and Phosphate by a Diacylhydrazine Ligand *via* the Formation of a Colour Alkali Metal Complex

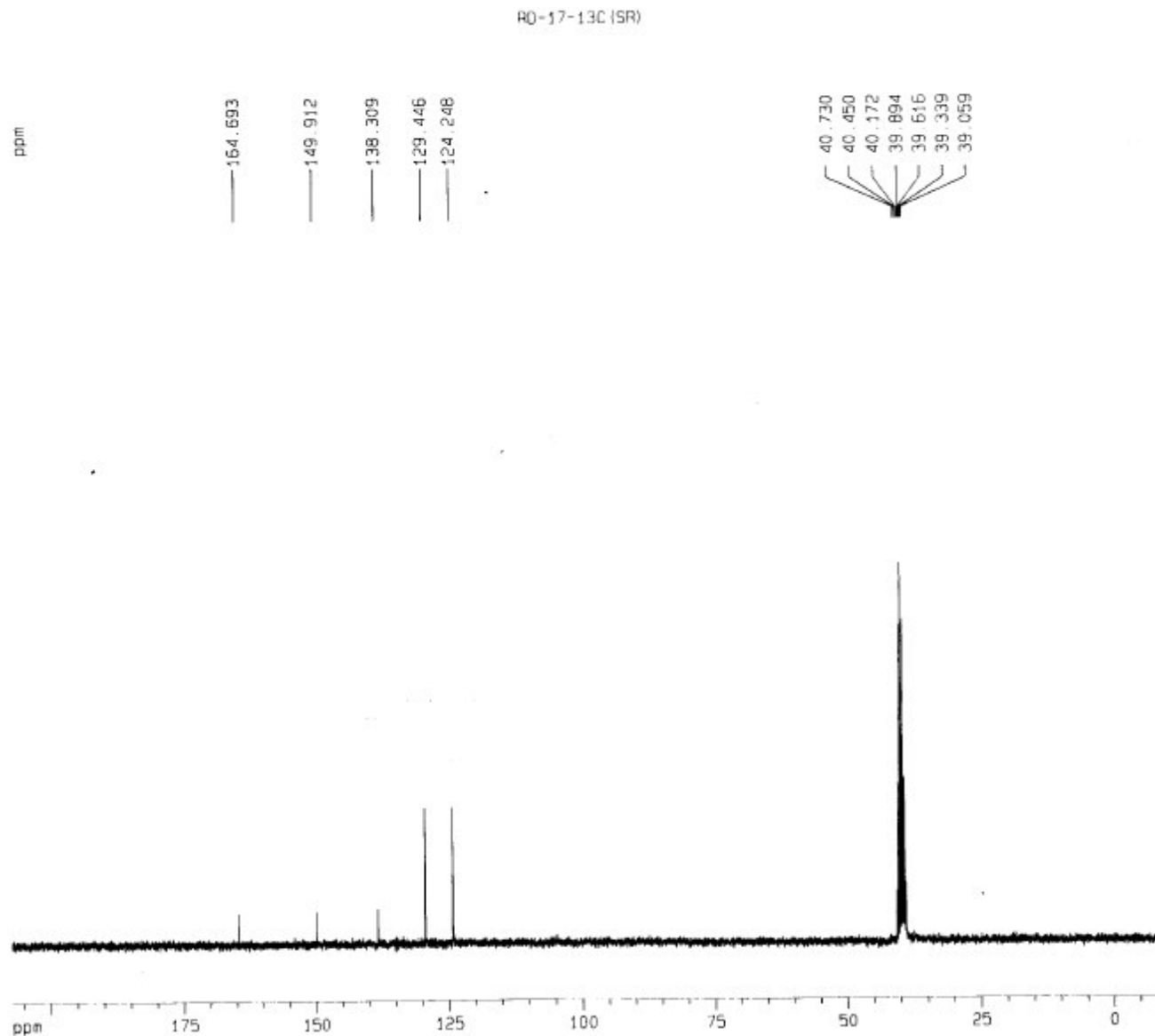
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**Figure S1.**  $^1\text{H}$  NMR spectrum of **L** in  $\text{DMSO-d}_6$ .



Current Data Parameters  
 NAME RD-17-13C  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20090325  
 Time 16 25  
 INSTRUM spect  
 PROBHD 5 mm Multinucl  
 PULPROG zgpg  
 TD 65536  
 SOLVENT DMSO  
 NS 197  
 DS 4  
 SWH 19841.270 Hz  
 FIDRES 0.302754 Hz  
 AQ 1.6515572 sec  
 RG 9195.2  
 DW 25.200 usec  
 DE 6.00 usec  
 TE 883.2 K  
 D1 2.0000000 sec  
 d11 0.0300000 sec  
 MCREST 0.0000000 sec  
 MCNRR 0.0150000 sec

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 NUC1 13C  
 P1 13.00 usec  
 PL1 0.00 dB  
 SFO1 75.4763276 MHz

----- CHANNEL f2 -----  
 PROPRG2 waltz16  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 -6.00 dB  
 PL12 7.00 dB  
 SFO2 300.1312005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.4677534 MHz  
 WDM EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 CY 6.56 cm  
 F1P 207.275 ppm  
 F1 15642.54 Hz  
 F2P -9.552 ppm  
 F2 -720.87 Hz  
 PPMCN 10.84133 ppm/cm  
 HZCM 818.17090 Hz/cm

Figure S2.  $^{13}\text{C}$  NMR spectrum of L in  $\text{DMSO-d}_6$ .

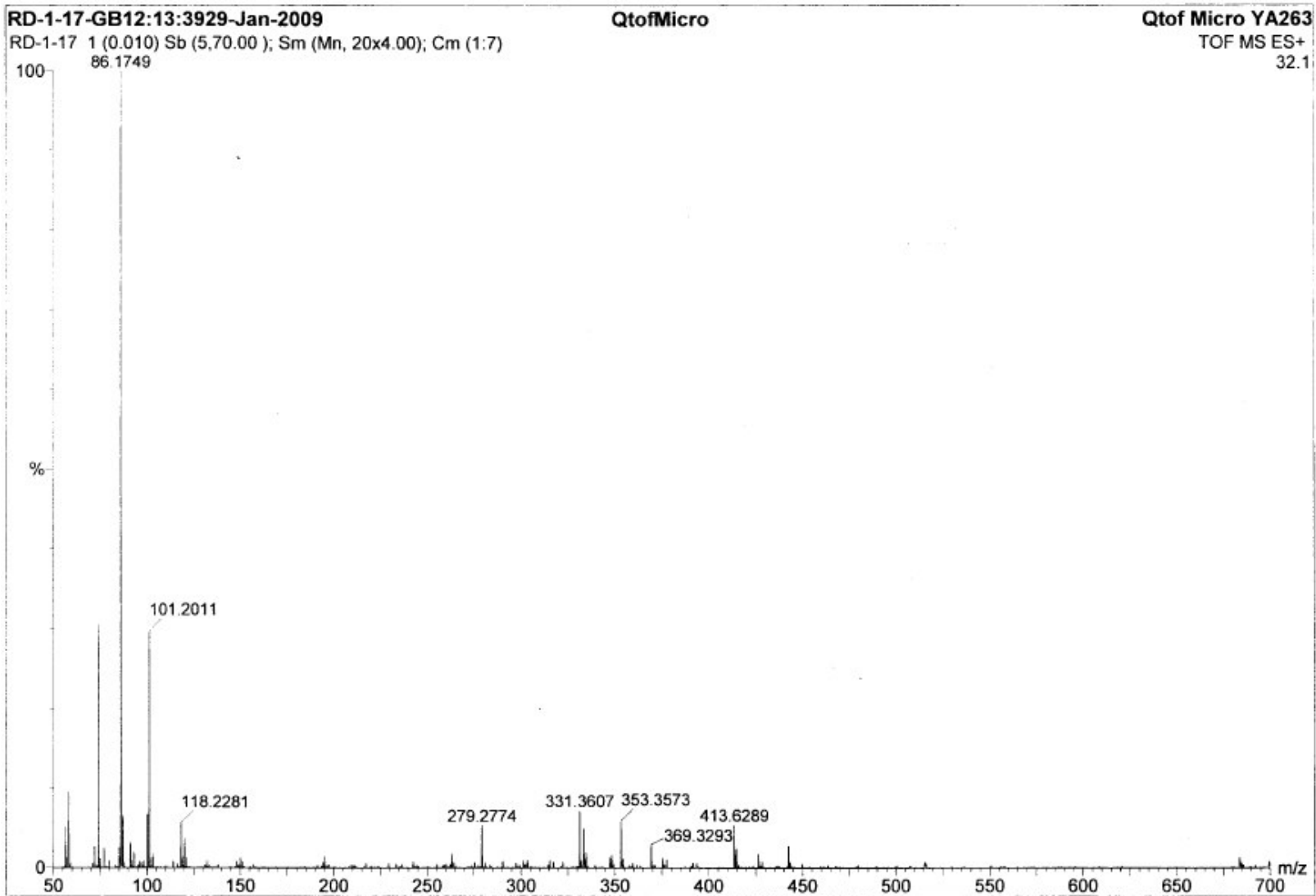
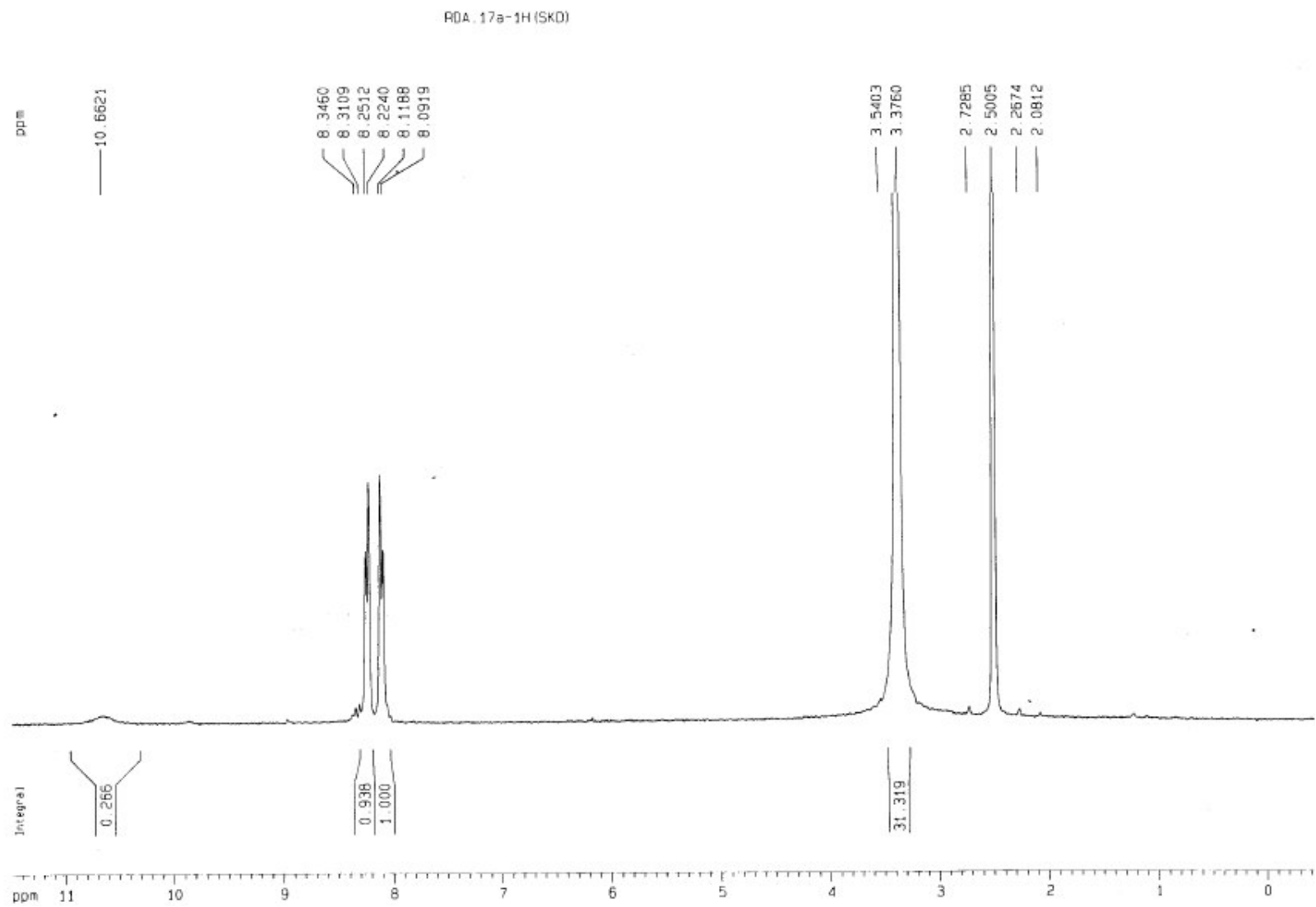
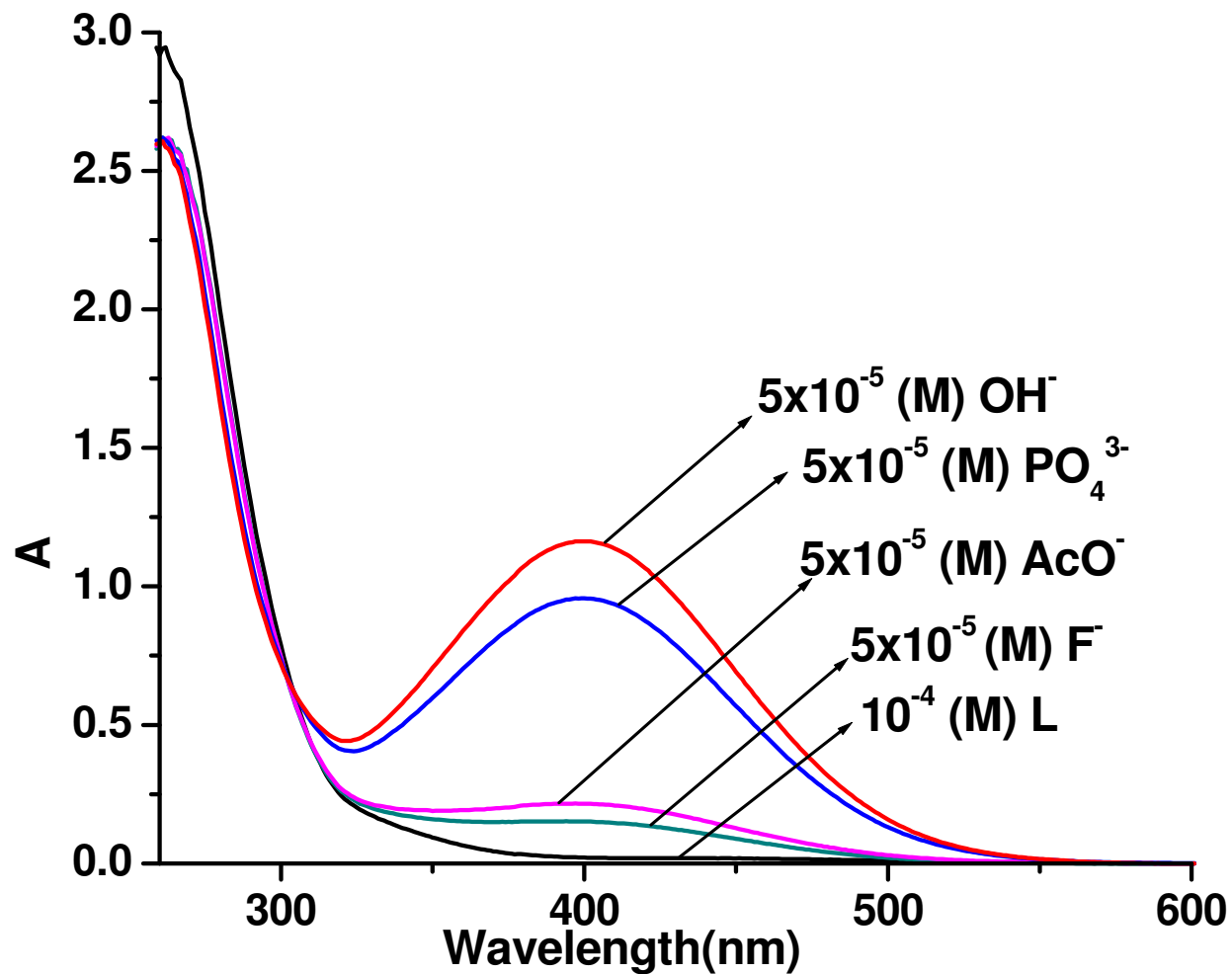


Figure S3. HRMS spectrum of L.

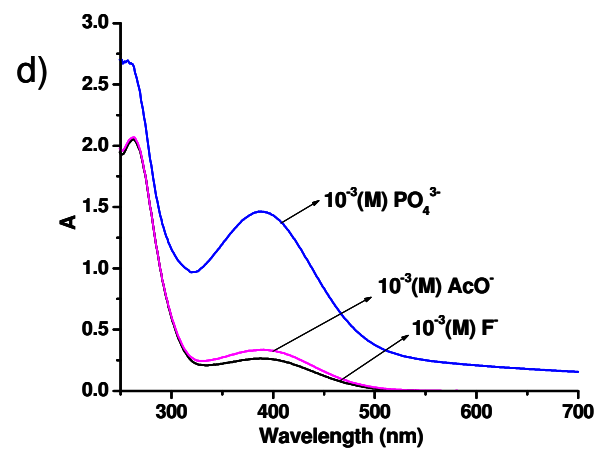
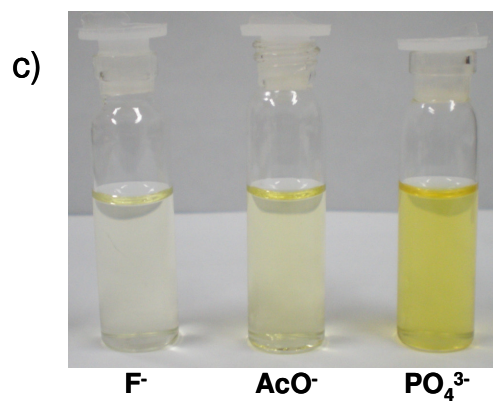
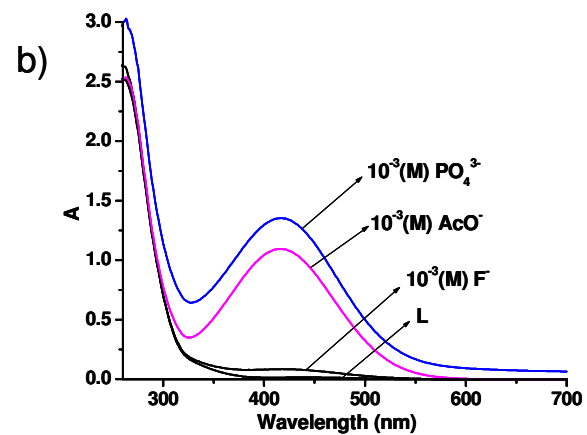
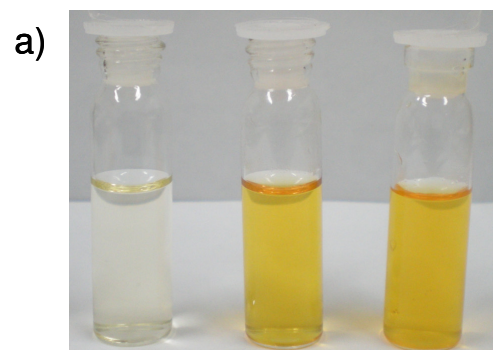


**Figure S4.**  $^1\text{H}$  NMR spectrum of complex **1** in  $\text{DMSO-d}_6$ .

a)



**Figure S5.** Changes in optical spectra of L ( $1.0 \times 10^{-4}$  M) in MeCN/DMF(4.9:0.1)(v/v) upon addition 0.3 ml of  $5 \times 10^{-4}$  M each anion solution.



**Figure S6.** Colour changes of **L** ( $1.0 \times 10^{-4}$  M) in MeCN/DMF(4.9:0.1)(v/v) upon addition of a) 0.06 ml of  $5 \times 10^{-2}$  M and c) 0.6 ml of  $5 \times 10^{-3}$  M anion solution respectively. b) and d) are the optical spectra of corresponding solutions respectively.

**Table S1. Table of Crystallographic parameters.**

| <b>Parameters</b>                                 | <b>Complex 1</b>            |
|---|-----------------------------|
| <b>Empirical formula</b>                          | $C_{28}H_{34}N_8Na_2O_{20}$ |
| <b>Formula weight</b>                             | 848.61                      |
| <b>crystal system</b>                             | Triclinic                   |
| <b>Space group</b>                                | P-1                         |
| <b><i>a</i> (Å)</b>                               | 7.761(9)                    |
| <b><i>b</i> (Å)</b>                               | 9.182(11)                   |
| <b><i>c</i> (Å)</b>                               | 13.791(17)                  |
| <b><i>α</i> (deg)</b>                             | 73.221(11)                  |
| <b><i>β</i> (deg)</b>                             | 86.963(12)                  |
| <b><i>γ</i> (deg)</b>                             | 74.063(12)                  |
| <b><i>V</i> (Å<sup>3</sup>)</b>                   | 904.4(19)                   |
| <b><i>Z</i></b>                                   | 1                           |
| <b><i>d</i><sub>calc</sub> (g/cm<sup>3</sup>)</b> | 1.558                       |
| <b>Crystal size (mm<sup>3</sup>)</b>              | 0.40 x 0.10 x 0.08          |
| <b>Diffractometer</b>                             | Smart CCD                   |
| <b><i>F</i>(000)</b>                              | 440                         |
| <b><i>μ</i> MoKα (mm<sup>-1</sup>)</b>            | 0.153                       |
| <b><i>T</i> (K)</b>                               | 120 (2)                     |
| <b><i>θ</i> max</b>                               | 25.00                       |
| <b>Observed Reflections</b>                       | 7279                        |
| <b>Parameters refined</b>                         | 298                         |
| <b>R<sub>1</sub>; WR<sub>2</sub></b>              | 0.0699 ; 0.2052             |
| <b>GOF (F2)</b>                                   | 1.080                       |



**Table S2. Selected geometric parameters (Å , °)**

|                   |            |
|-------------------|------------|
| Na25...N12        | 2.660(5)   |
| Na25...O15        | 2.334(4)   |
| Na25...O26        | 2.365(4)   |
| Na25...O27        | 2.348(5)   |
| Na25...O28        | 2.360(4)   |
| Na25...O28'       | 2.543(4)   |
| O15...Na25...O26  | 99.14(10)  |
| O15...Na25...O28  | 83.53(10)  |
| O15...Na25...N12  | 65.85(10)  |
| O15...Na25...O28' | 81.95(10)  |
| O26...Na25...O27  | 91.93(11)  |
| O26...Na25...O28  | 171.74(12) |
| O26...Na25...N12  | 81.87(10)  |
| O26...Na25...O28' | 85.07(10)  |
| O27...Na25...O28  | 83.60(11)  |
| O27...Na25...N12  | 130.67(12) |
| O27...Na25...O28' | 84.55(12)  |
| O28...Na25...O12  | 106.31(11) |
| O28...Na25...O28' | 87.59(10)  |
| O28'...Na25...N12 | 142.55(10) |