Supporting Information

1-(2-Naphthyl)benzimidazolium based tripod for the fluorescence enhancement based recognition of surfactants in water

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Content

1. UV-Vis and fluorescence behavior of TRI-BINAP-1

Complexation studies of **TRI-BINAP-1** (5 µM) were performed in CH_3CN, DMSO and 95% aqueous DMSO. The UV-Vis and emission spectrum of **TRI-BINAP-1** (5 µM) in both CH_3CN and DMSO exhibits a significant change with 50 µM addition of tetrabutylammonium salts of F^-, AcO^- and $H_2PO_4^-$, whereas all other anions viz. Cl^-, Br^-, I^-, NO_3^-, HSO_4^-, ClO_4^-, CN^- and even sodium salts of alkyl chain (C_3-C_{12}) carboxylates and sulfonates, caused insignificant change in the absorption and emission spectrum of **TRI-BINAP-1** (Figure SI 1, 2).

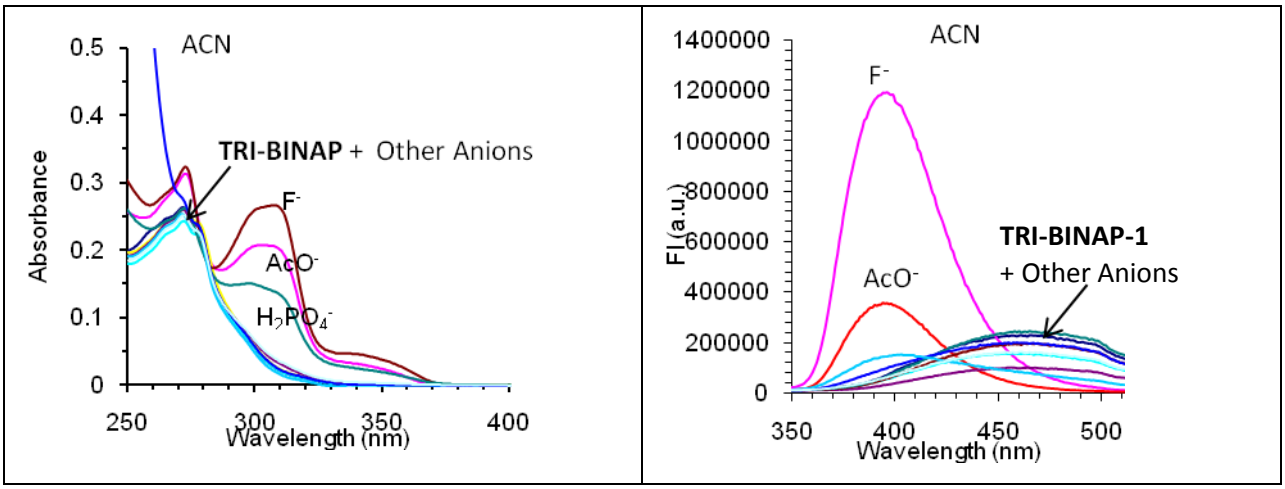


Fig. SI 1. Effect of tetrabutylammonium salts of different anions and sodium salts of alkyl carboxylates and sulfonates on the (a) UV-Vis spectra; (b) Fluorescence spectra of **TRI-BINAP-1** (5 μM) in CH_3CN solutions.

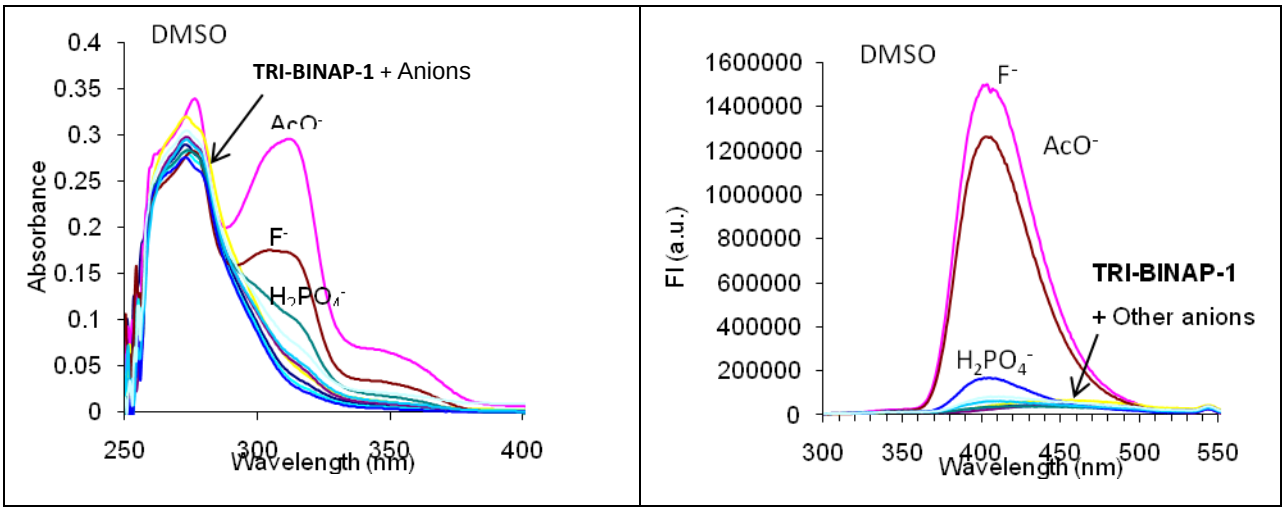


Fig. SI 2. Effect of tetrabutylammonium salts of different anions and sodium salts of alkyl carboxylates and sulfonates on the (a) UV-Vis spectra; (b) Fluorescence spectra of **TRI-BINAP-1** (5 μM) in DMSO solutions.

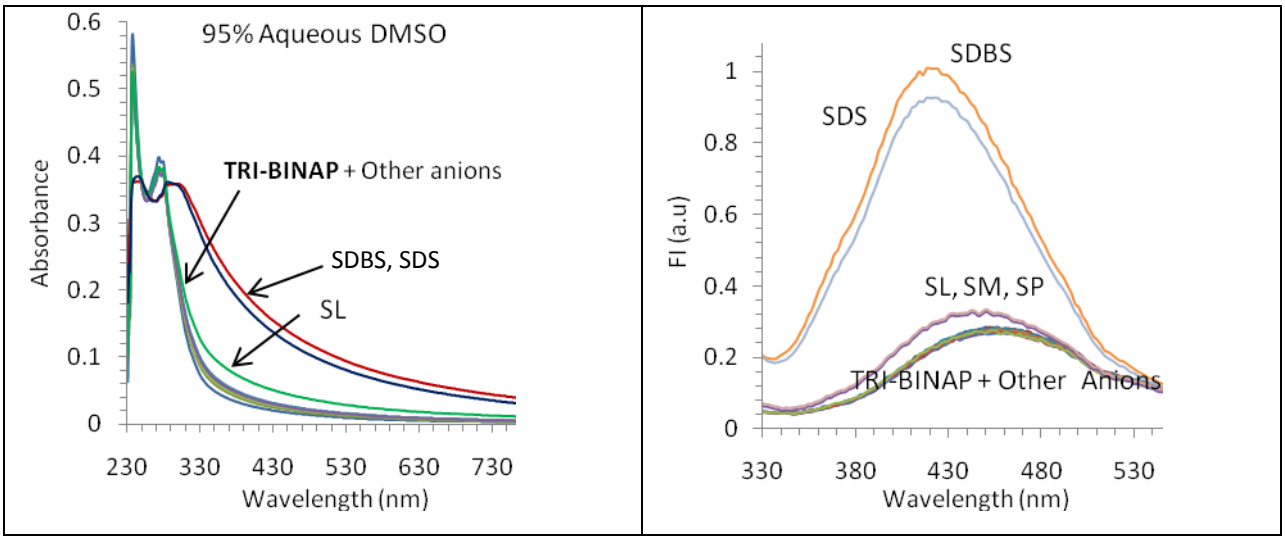


Figure SI 3. Effect of tetrabutylammonium salts of different anions and sodium salts of carboxylates and sulfonates on the (a) UV-Vis spectrum; (b) Fluorescence spectrum of **TRI-BINAP-1** (5 μM) in 95% aqueous DMSO solutions.

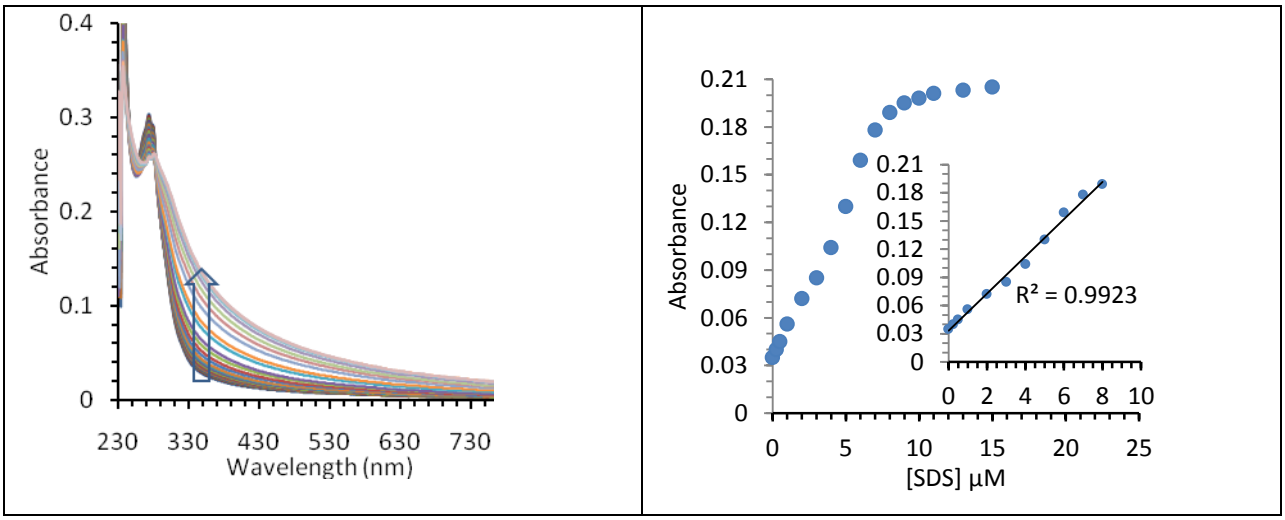


Figure SI 4. (a) Effect of gradual addition of SDS on the absorption spectrum of **TRI-BINAP-1** (5 μM) in 95% aqueous DMSO solution.

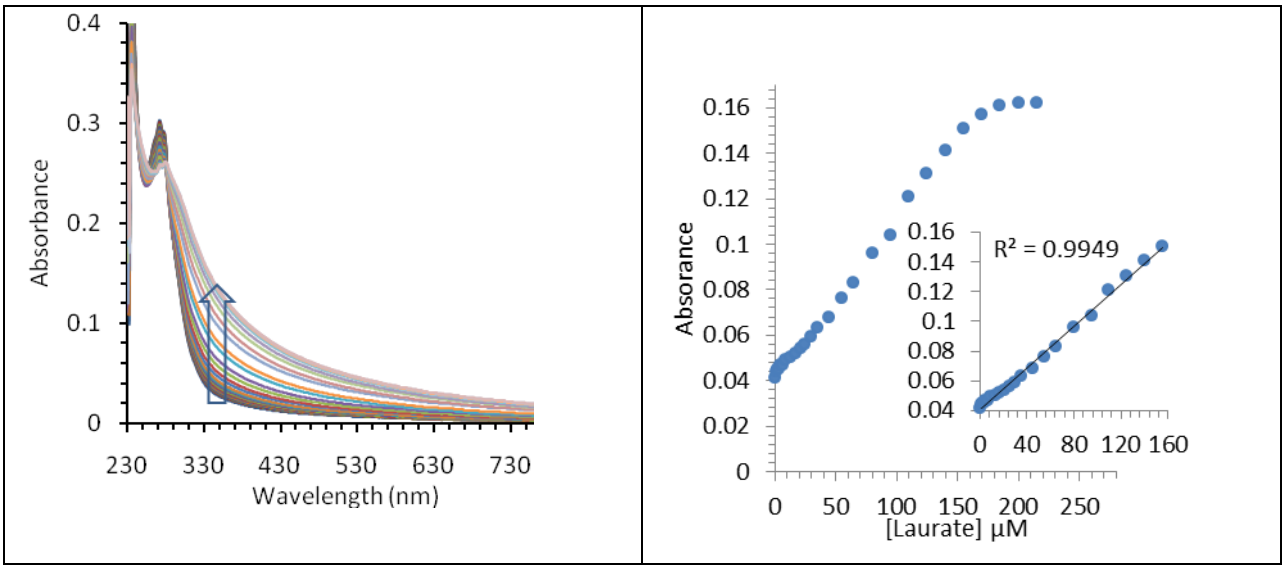


Figure SI 5. Effect of gradual addition of sodium laurate (SL) solution to the absorption spectra of **TRI-BINAP-1** (5 µM) in 95% Aqueous DMSO solution.

Fluorescence titration profile of TRI-BINAP (5 µM) with SDS in 95% aqueous solution.

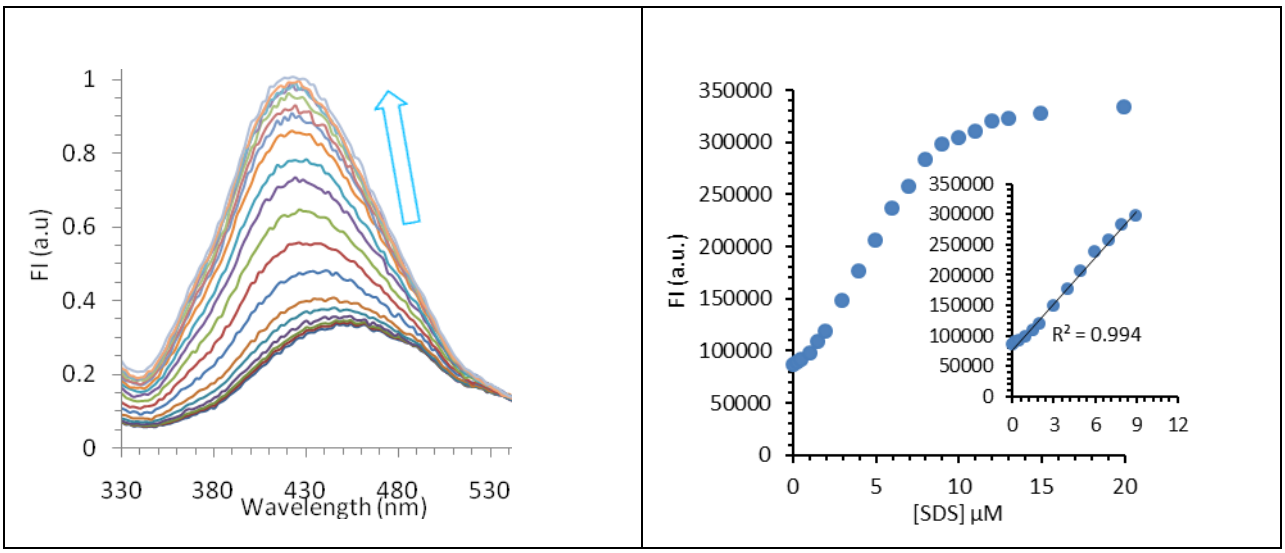


Figure SI 6. (a) Effect of gradual addition of SDS to the emission spectra of **TRI-BINAP-1** (5 µM) in 95% aqueous DMSO solution. (b) FI vs. conc. plot of **TRI-BINAP-1** titration with SDS.

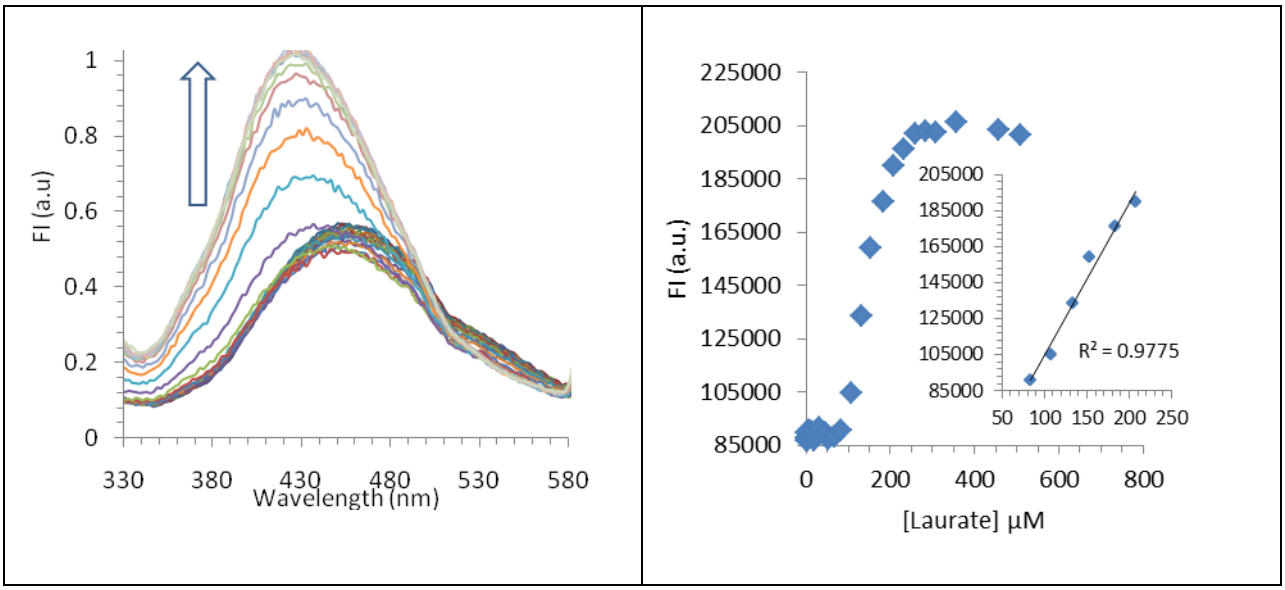


Figure SI 7. (a) Effect of gradual addition of sodium laurate (SL) to the emission spectra of **TRI-BINAP-1** (5 µM) in 95% aqueous DMSO solution. (b) FI vs. conc. plot of **TRI-BINAP-1** titration with SL.

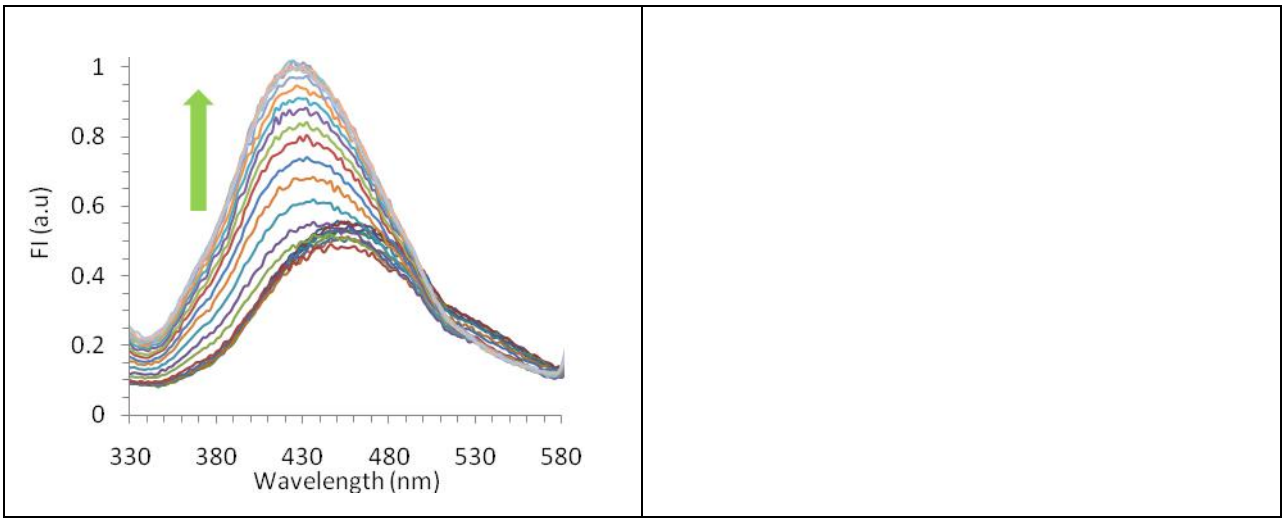


Figure SI 8. (a) Effect of gradual addition of sodium myristate (SM) on the emission spectrum of **TRI-BINAP-1** (5 µM) in 95% aqueous DMSO solution.

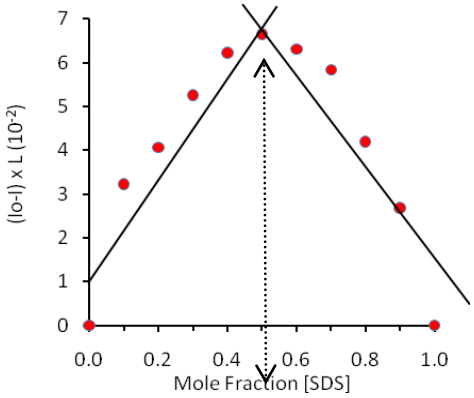


Figure SI 9. Job's plot[2] analysis of **TRI-BINAP-1** titration with SDS in 95% aqueous DMSO solution.

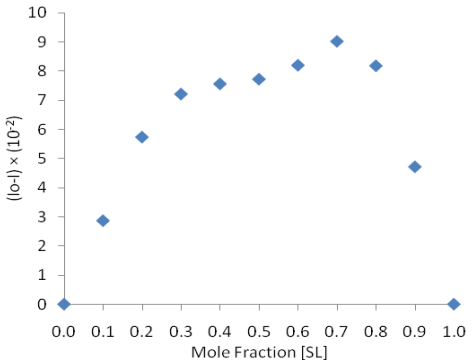


Figure SI 10. Job's plot analysis of **TRI-BINAP-1** titration with sodium laurate in 95% aqueous DMSO solution.

2. Evaluation of Thermodynamic parameters:

To evaluate thermodynamic parameters i.e. enthalpy and entropy, responsible for binding of **TRI-BINAP-1** with SDBS/SDS, the UV-Vis titrations of **TRI-BINAP-1** at four different temperatures 20, 30, 35 and 40 ^{o}C were performed.

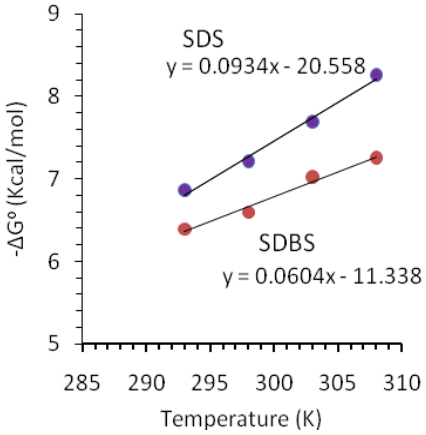


Figure SI 11. Free energy change vs. temperature plots of **TRI-BINAP-1** against SDBS and SDS.

3. NMR Spectral analysis of TRI-BINAP-1 with SDS and SDBS

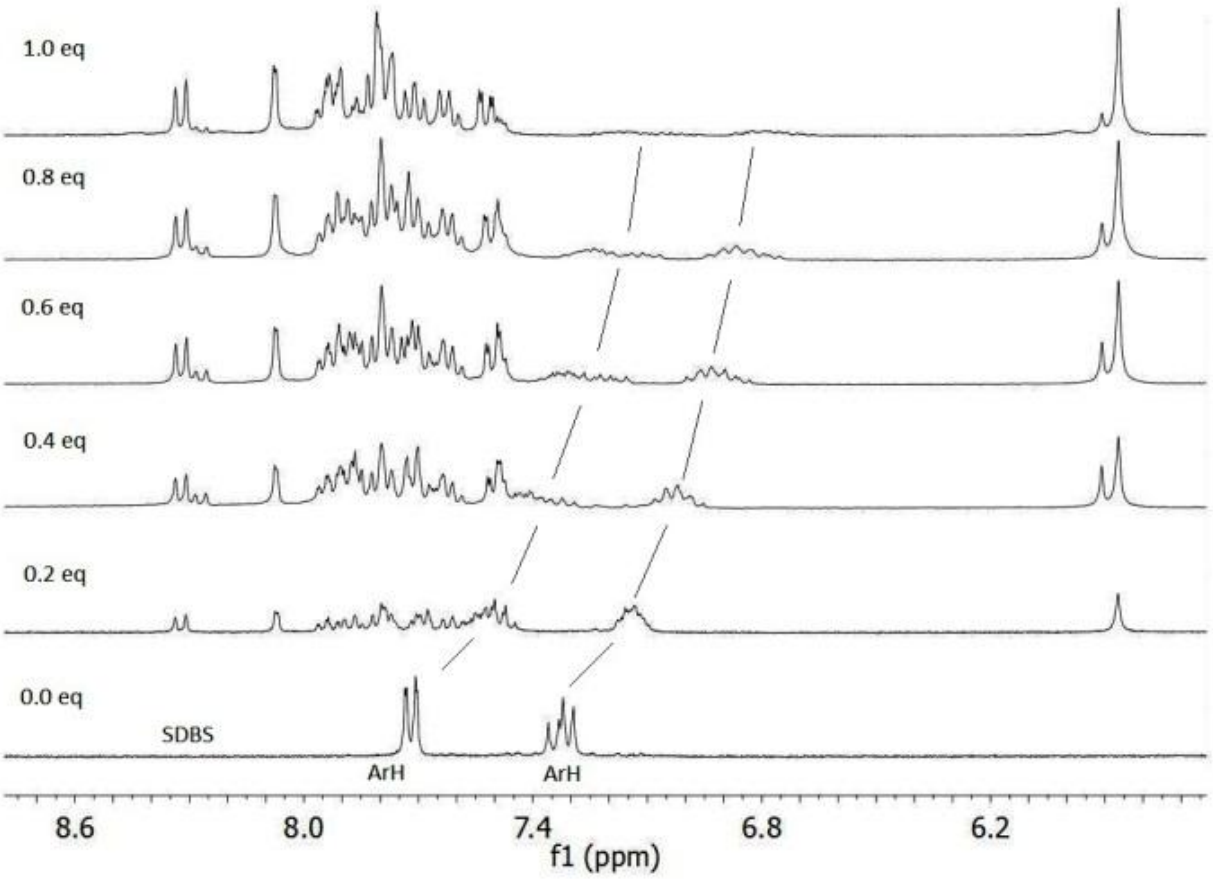


Figure SI 12. ^{1}H NMR titration of SDBS (5 mM) with gradual addition of **TRI-BINAP-1** up to 5 mM in CD_3CN-D_2O (1:1) solutions.

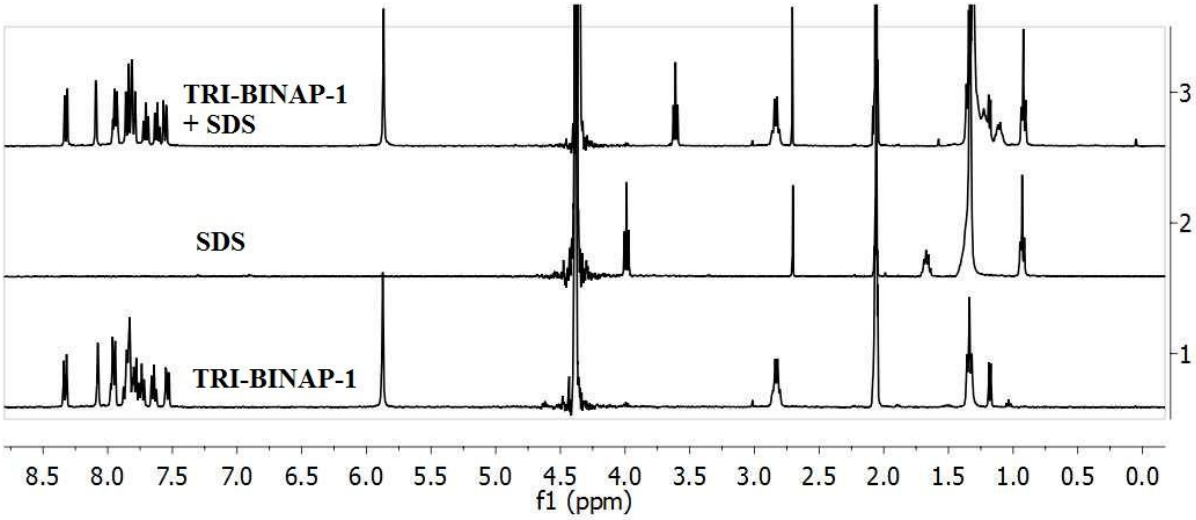


Figure SI 13. ^{1}H NMR spectrum of (1) **TRI-BINAP-1** (5 mM); (2) SDS (5 mM); and (3) **TRI-BINAP-1** + SDS (1:1) in CD_3CN-D_2O (1:1).

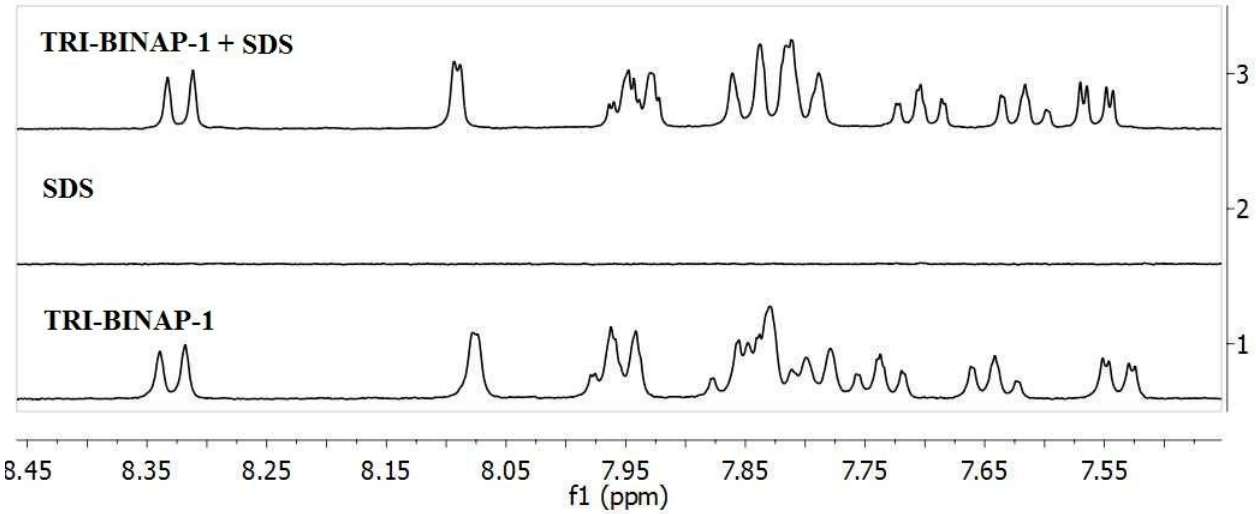


Figure SI 14. ^{1}H NMR spectrum showing expansion of aromatic part. Aromatic protons of **TRI-BINAP-1** showed a change in their chemical shift values on addition of one equivalent SDS.

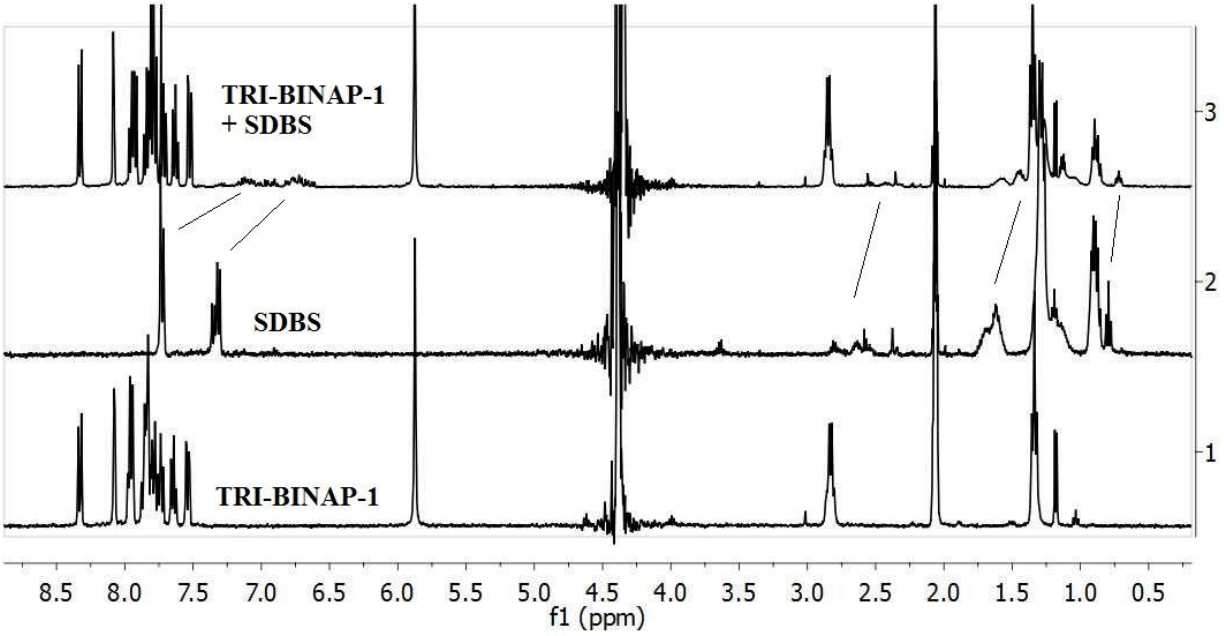


Figure SI 15. ^{1}H NMR spectrum of (1) **TRI-BINAP-1** (5 mM); (2) SDBS (5 mM); and (3) **TRI-BINAP-1** + SDBS (1:1) in CD_3CN-D_2O (1:1).

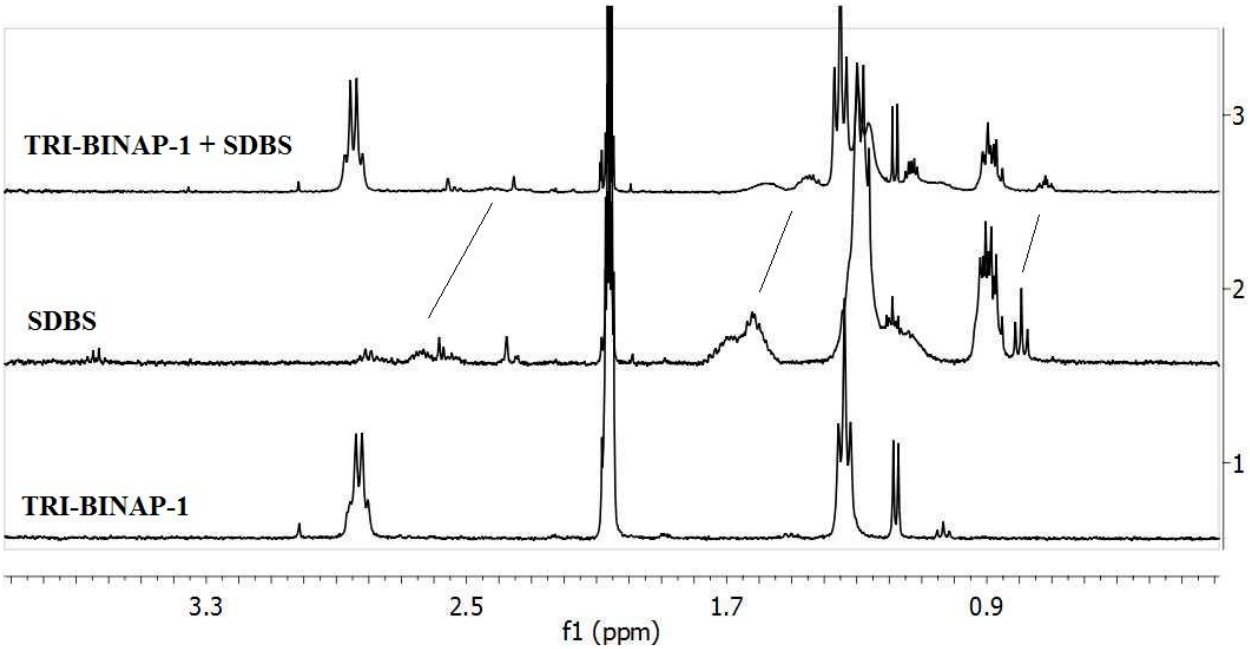


Figure SI 16. ^{1}H NMR spectrum showing up-field shift aliphatic protons of SDBS in **TRI-BINAP-1** + SDS (1:1) in CD_3CN-D_2O (1:1).

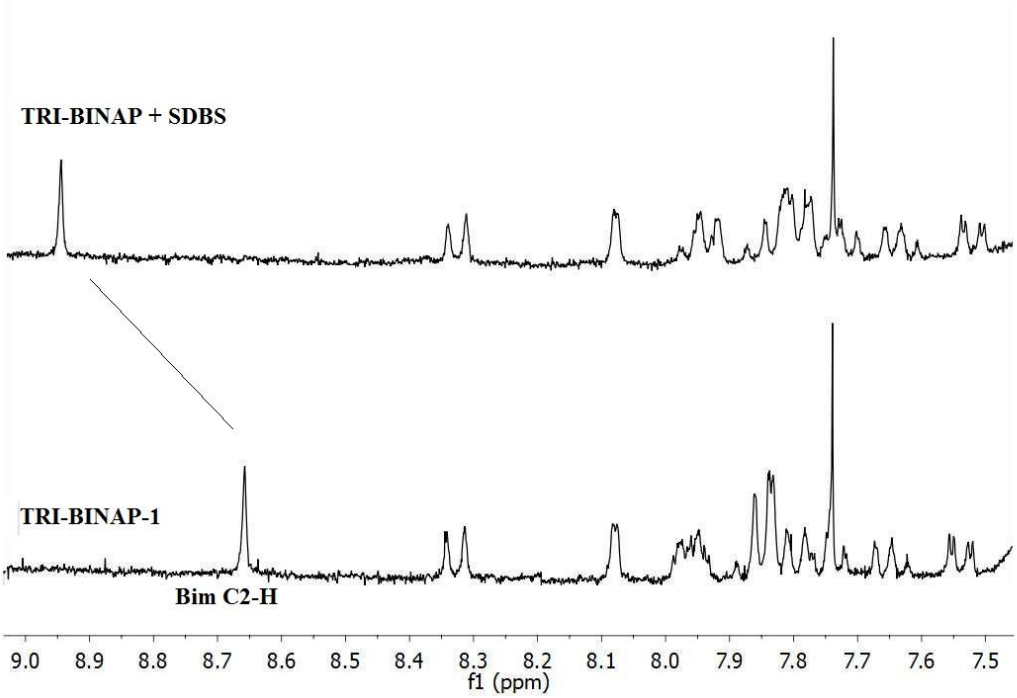


Figure SI 17. ^{1}H NMR spectrum showing down-field shift of BimC2-H protons in **TRI-BINAP-1** + SDBS (1:1) in CD_3CN-H_2O (1:1).

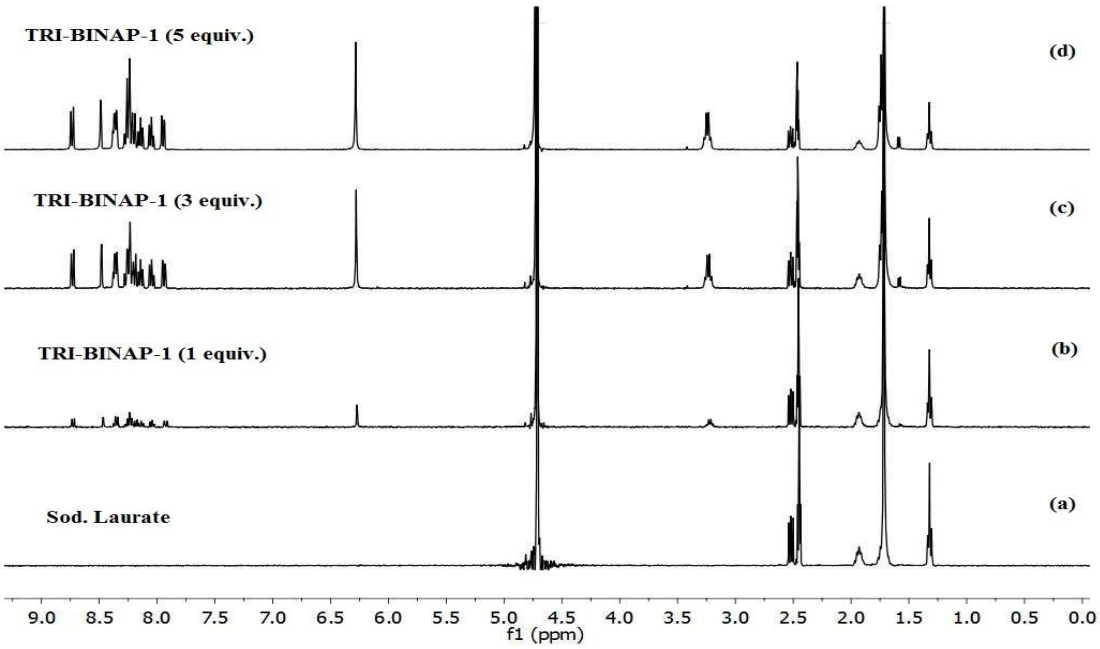


Figure SI 18. ^{1}H NMR spectrum showing no change in the aliphatic protons of Sodium Laurate with gradual addition of **TRI-BINAP-1** in CD_3CN-D_2O (1:1).

4. HRMS of 1:1 solutions of TRI-BINAP with SDBS and SDS

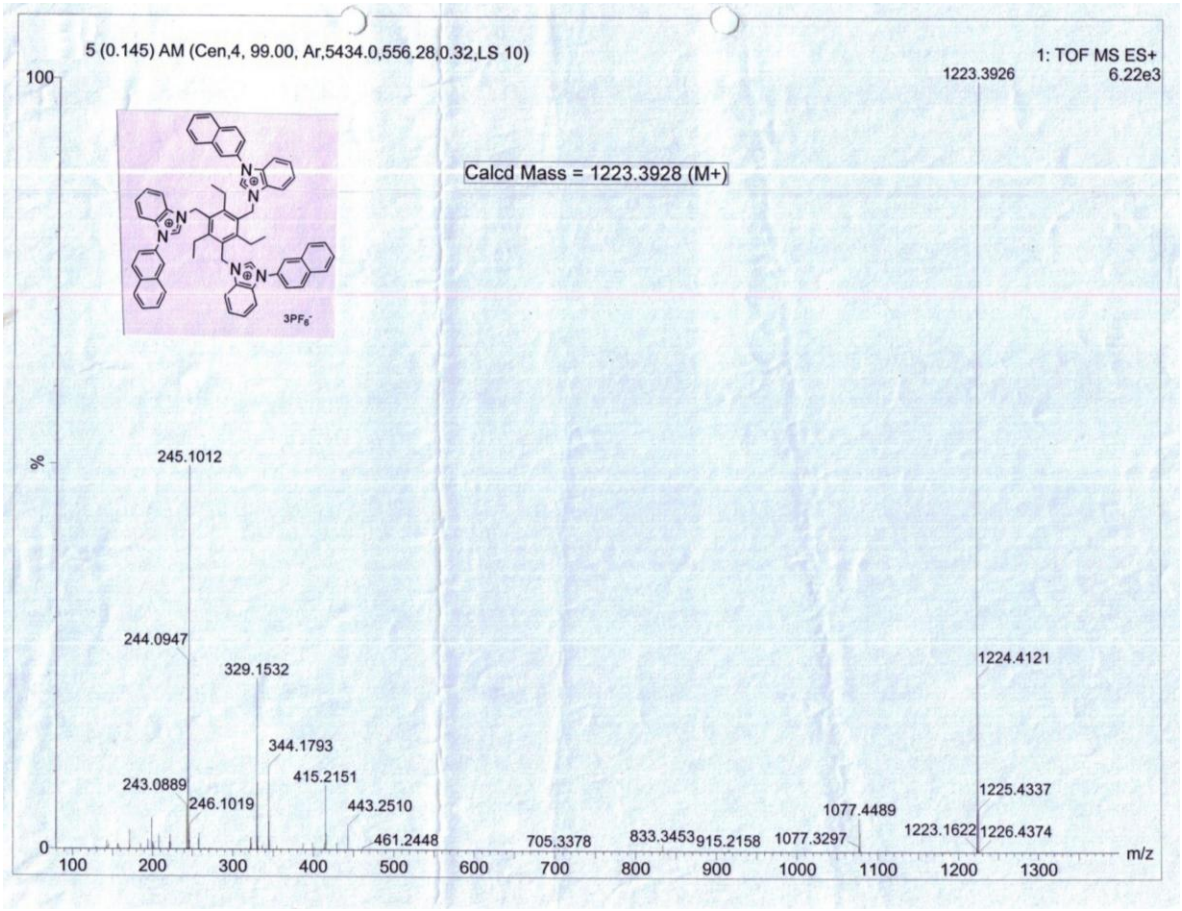


Figure SI 19. HRMS spectrum of **TRI-BINAP-1**

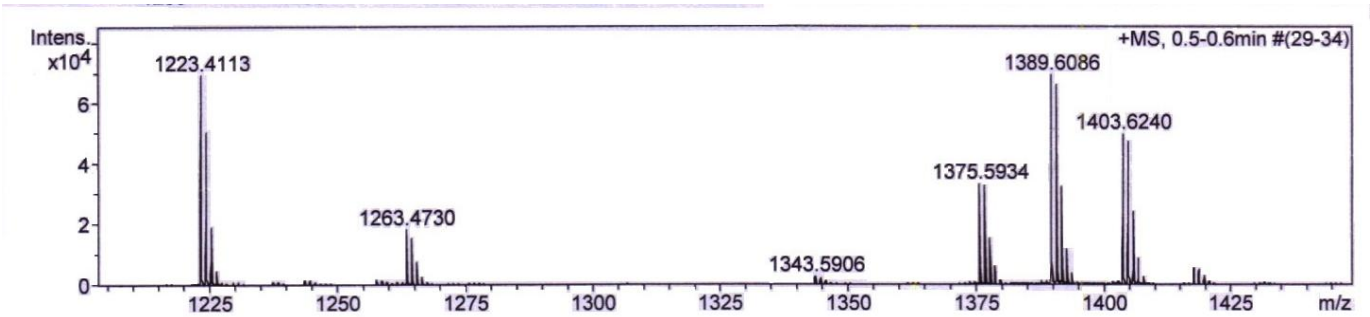
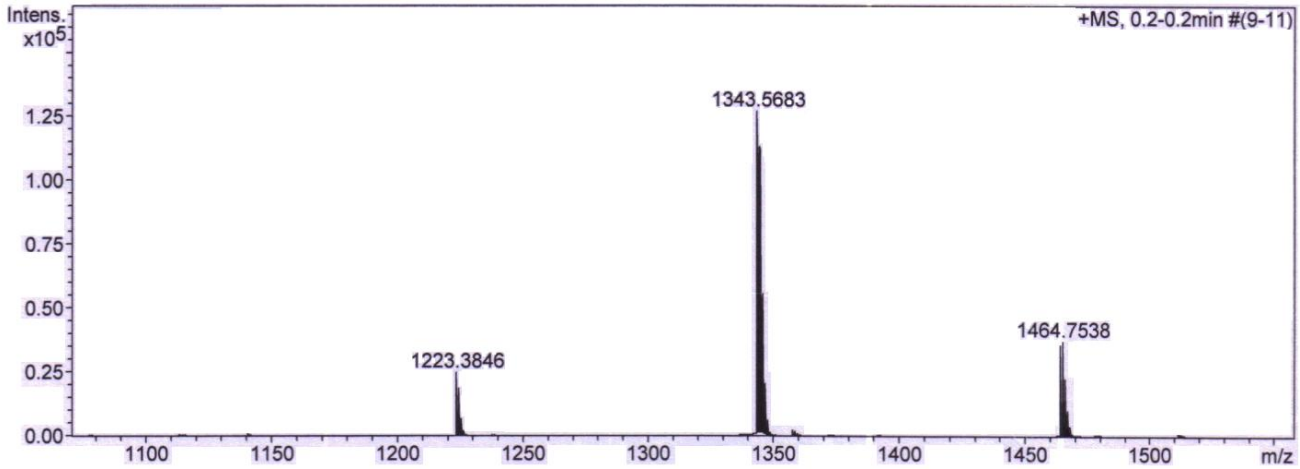


Figure SI 20. HRMS spectrum of 1:1 solution of **TRI-BINAP-1** and SDBS



SI 21. HRMS spectrum of 1:1 solution of **TRI-BINAP-1** and SDS

References:

1. (a) C. Zhang, L. Liheng and Z. Chen, *Chem. Phys. Lett.*, 2006, **420**, 330. (b) Z. Chen, C. Zhang and L. Feng, *Spectrochim Acta, Part A: Mol. Biomol. Spect.*, 2005, **62**, 592. (c) A. K. Verma, J. Singh, V. K. Sankar, R. Chaudhary and R. Chandra, *Tetrahedron Lett*. 2007, **48**, 4207.
2. P. Job, *Ann. Chim.* 1928, **9**, 113.