

Supplementary data

Anion selective chromogenic and fluorogenic chemosensor and its application in breast cancer live cell imaging

Darshna Sharma^a, Anuradha Moirangthem^b, Suban K Sahoo^{a*}, Anupam Basu^{b*},

Sutapa M. Roy^a, Ranjan K. Pati^a, Ashok Kumar SK^c, Jitendra P. Nandre^d, Umesh D

Patil^d

^aDepartment of Applied Chemistry, S.V. National Institute of Technology (SVNIT), Surat, Gujarat, India.

^bMolecular Biology and Human Genetics Laboratory, Department of Zoology, The University of Burdwan, Burdwan (WB), India.

^cSchool of Advanced Sciences, VIT University, Vellore (TN), India.

^dSchool of Chemical Sciences, North Maharashtra University, Jalgaon (MS), India.

*Corresponding author (Dr SK Sahoo): E-mail: suban_sahoo@rediffmail.com; Mob: +91-9662620556; (Dr A Basu): E-mail: abasu@zoo.buruniv.ac.in; Mob: +919734029333.

FIGURES

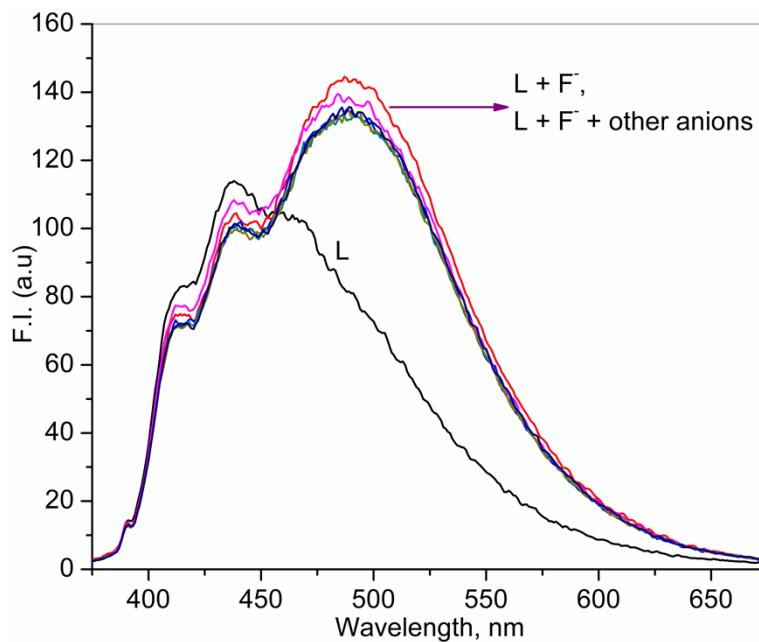


Fig. S1. Interference study of **L** for the detection of F⁻ in DMSO (2 mL solution of **L** of 5 x 10⁻⁵ M was mixed with 100 µL of F⁻ and 100 µL of other anions of 1 x 10⁻³ M, except AcO⁻).

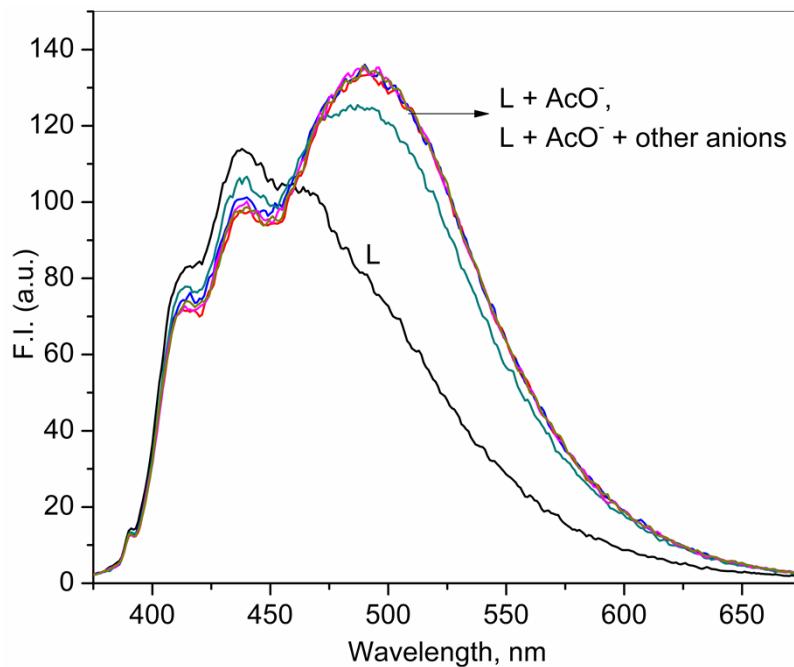


Fig. S2. Interference study of **L** for the detection of AcO⁻ in DMSO (2 mL solution of **L** of 5 x 10⁻⁵ M was mixed with 100 µL of AcO⁻ and 100 µL of other anions of 1x10⁻³ M, except F⁻).

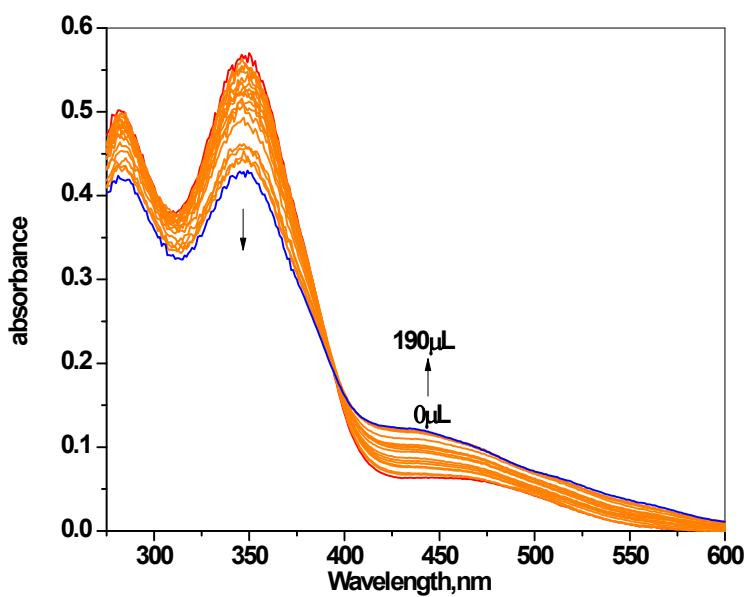


Fig. S3. Absorption titration of **L** (5×10^{-5} M) upon incremental addition of TBAAcO (1 X 10^{-3} M).

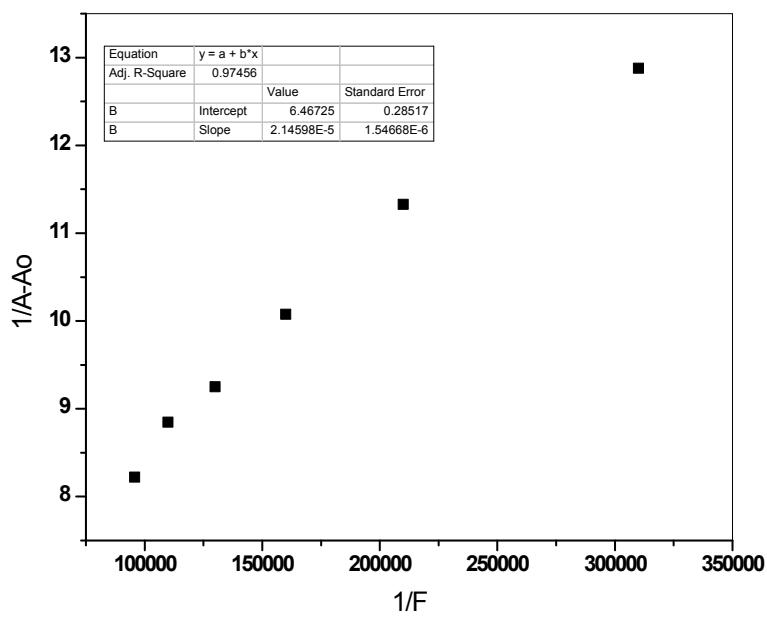


Fig. S4. BH plot for **L** with Fluoride, $K = 3.01 \times 10^5 \text{ M}^{-1}$.

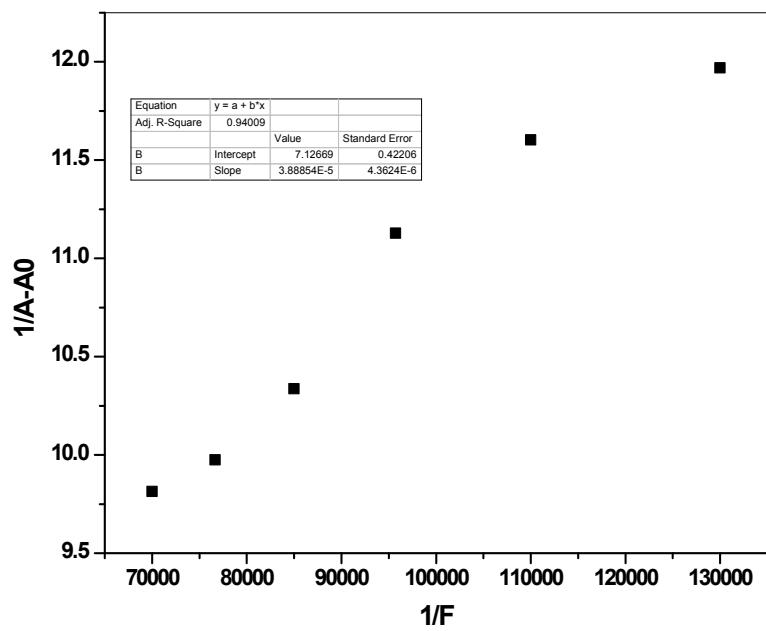


Fig. S5. BH plot for **L** with acetate, $K = 1.83 \times 10^5 \text{ M}^{-1}$.

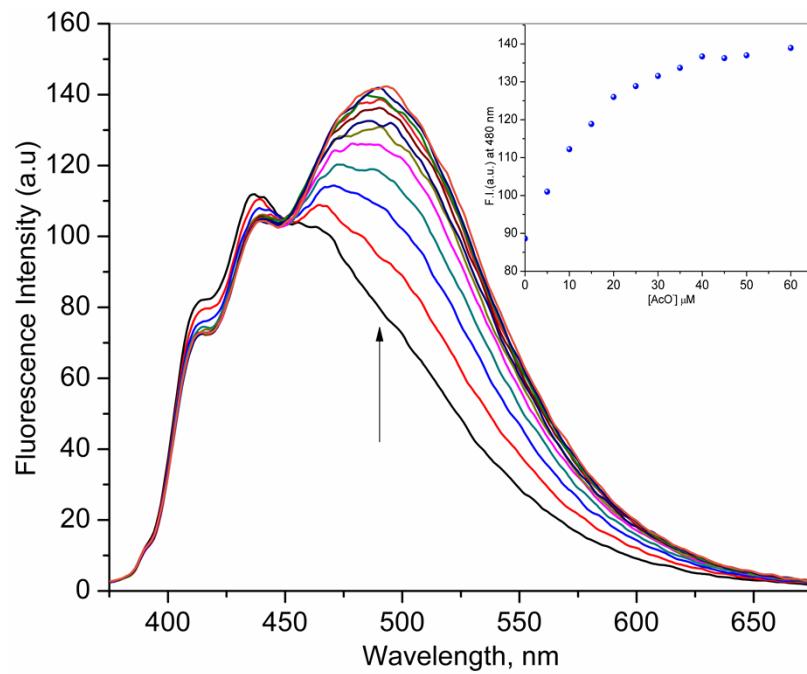


Fig. S6. Fluorescence spectral changes of **L** ($1.0 \times 10^{-5} \text{ M}$, $\lambda_{\text{exc}} = 350 \text{ nm}$) upon incremental addition of TBAAcO in DMSO. Inset showing the $[\text{AcO}^-]$ vs. F.I. at 480 nm.

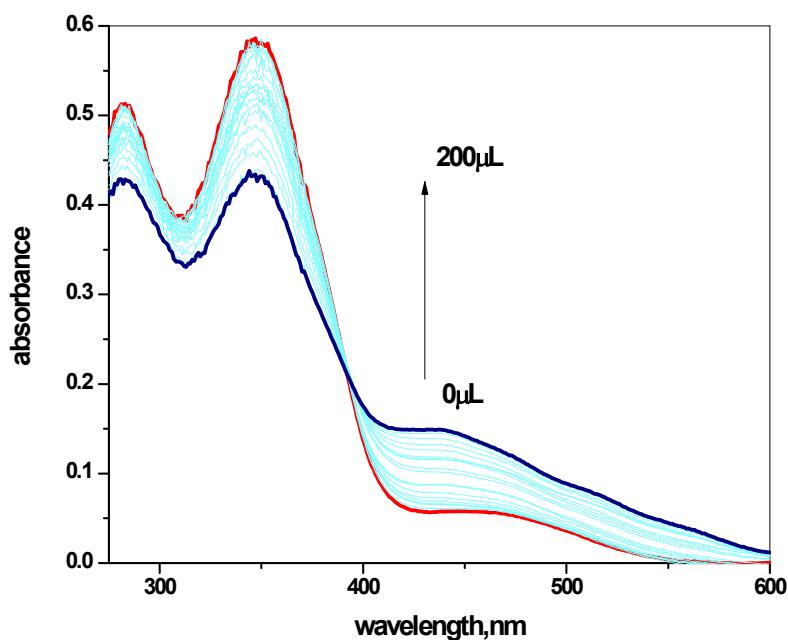


Fig. S7. Absorption titration of **L** (5×10^{-5} M) upon incremental addition of TBAOH (1×10^{-3} M).

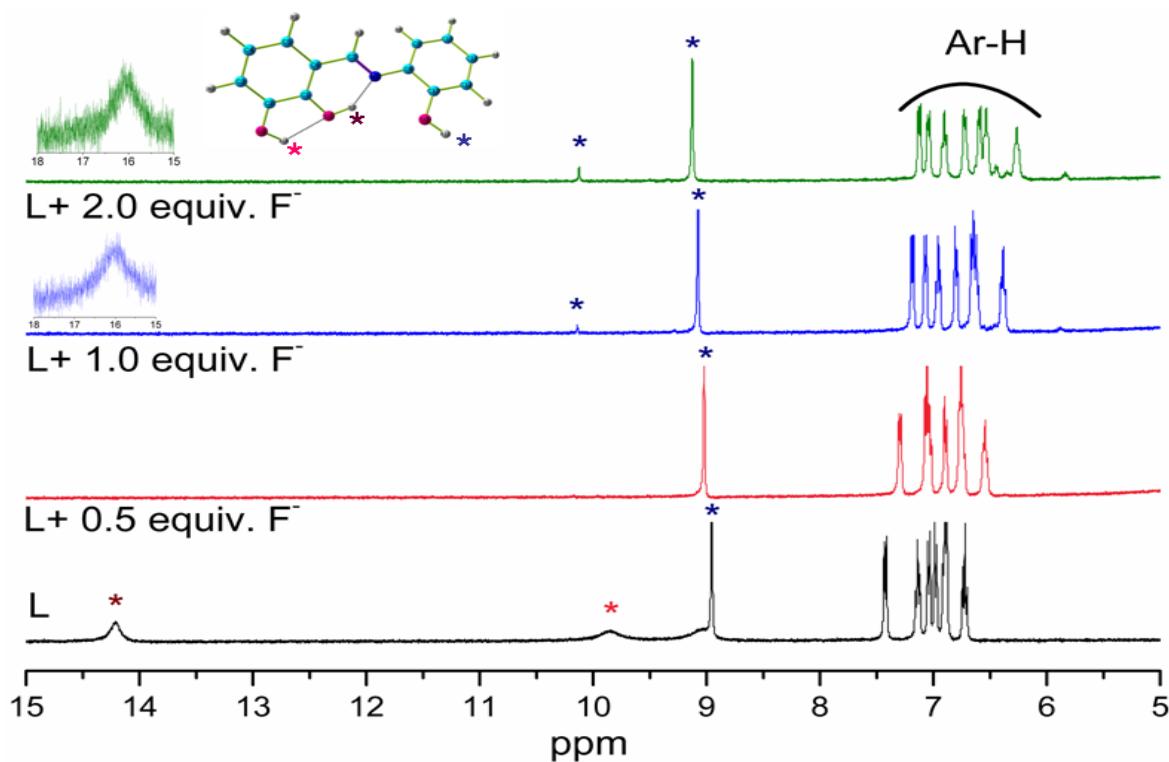


Fig. S8. ^1H NMR titration of **L** upon addition of different equivalents of TBAF in $\text{DMSO}-d_6$.

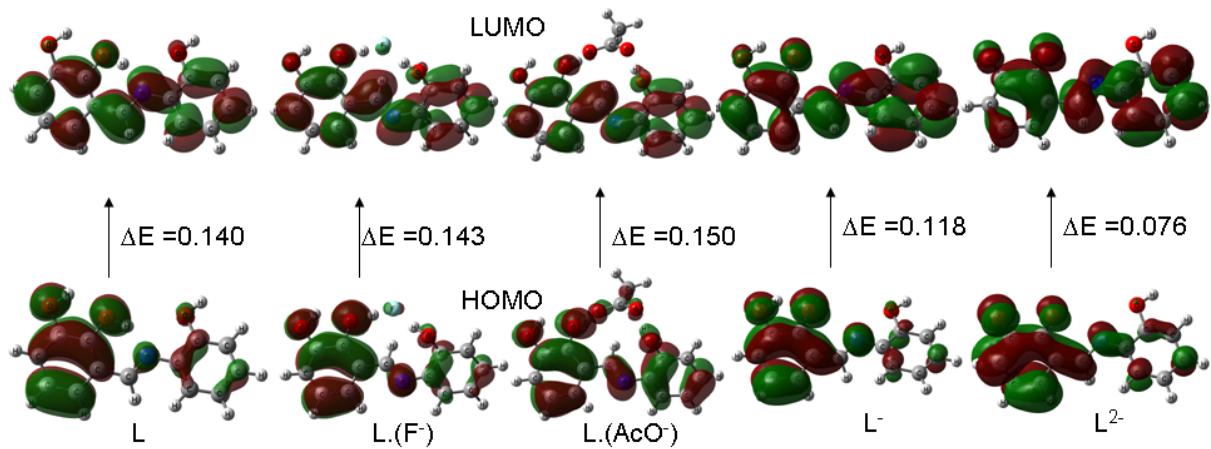


Fig. S9. DFT computed highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of different species of **L**.

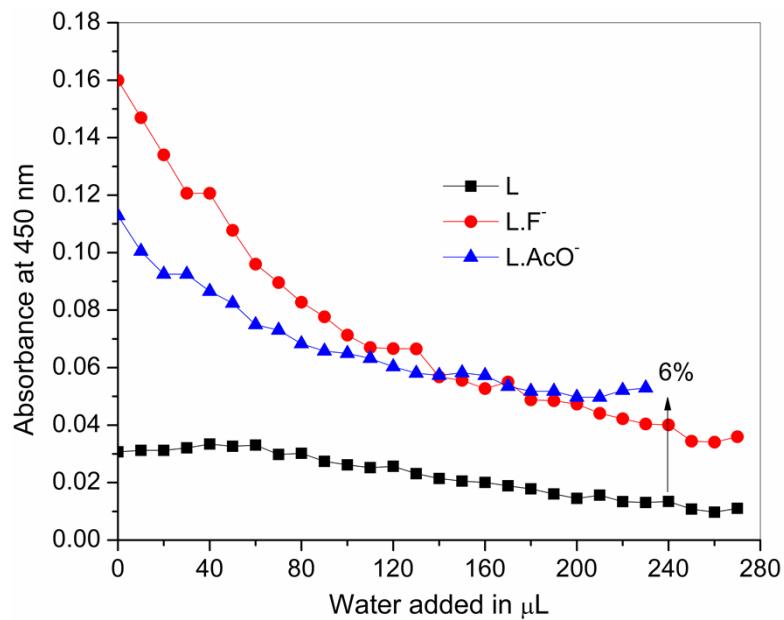


Fig. S10. Changes in the absorbance spectrum of **L** (2 mL, 5.0×10^{-5} M, in DMSO) and in the presence of five equivalents of F^- and AcO^- upon addition of incremental amounts (10 μL) of water.

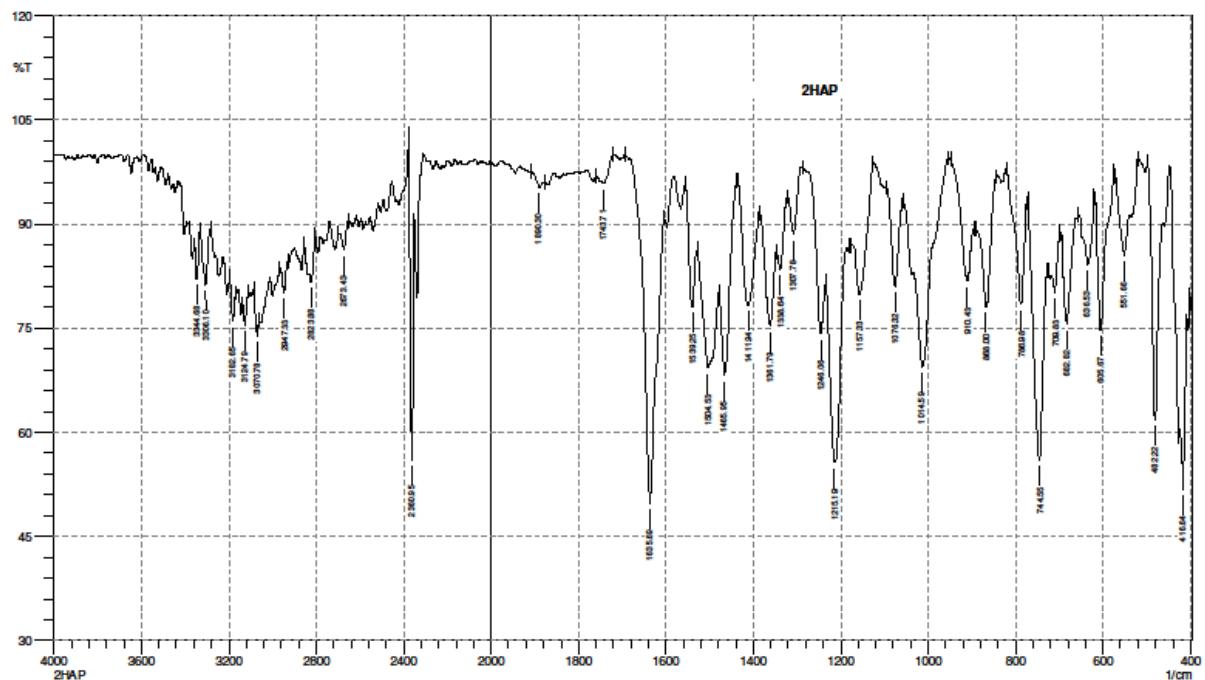


Fig. S11. FTIR spectrum of the receptor **L**.

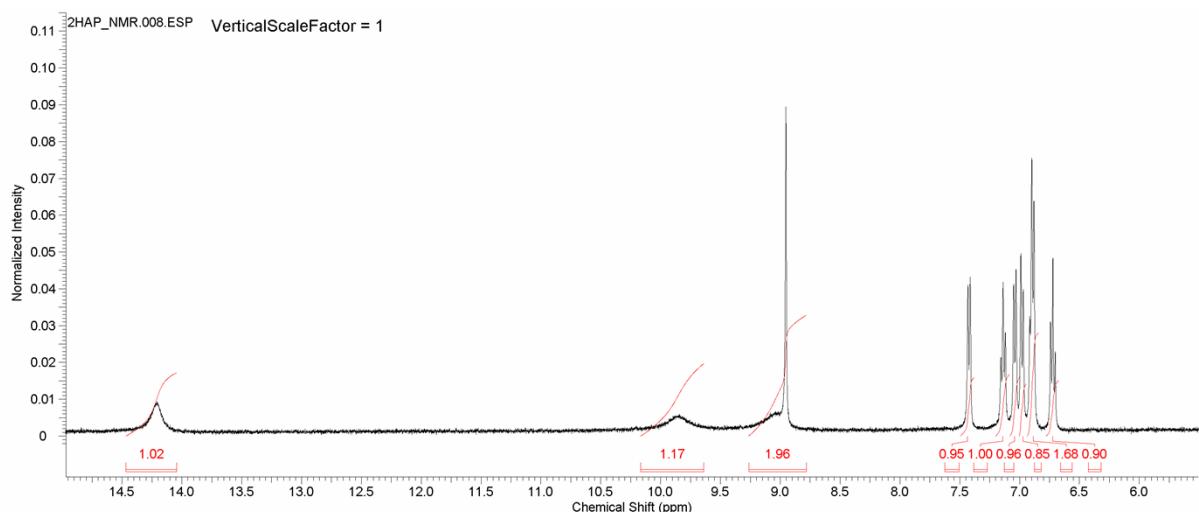


Fig. S12. ^1H NMR spectrum of the receptor **L** in DMSO-d_6 .