Supporting Information

A Selective, Cell-Permeable Fluorescent Probe for Al^{3+} in Living Cells

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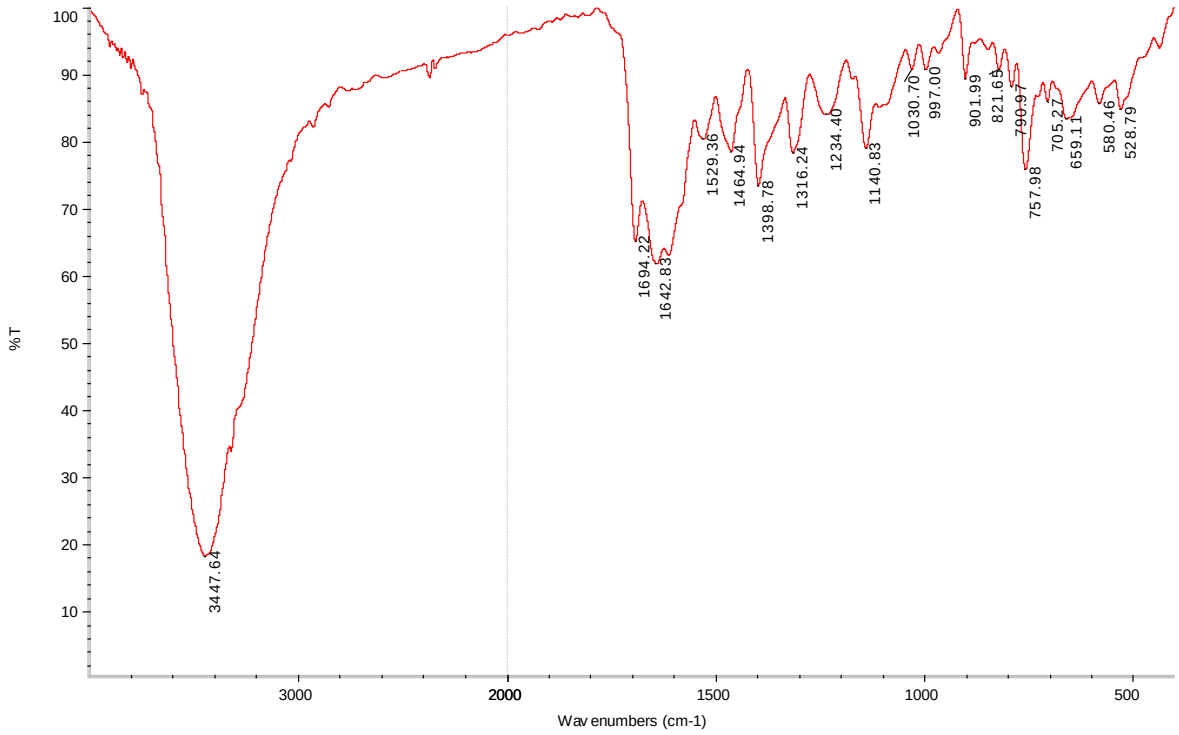
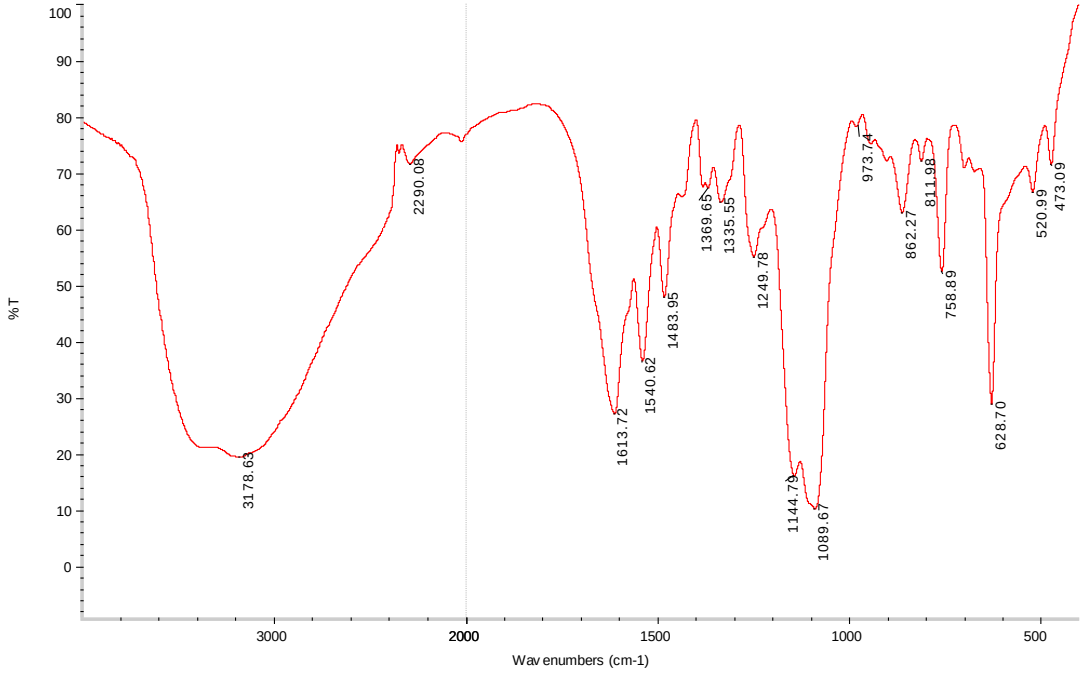
Spectroscopic data

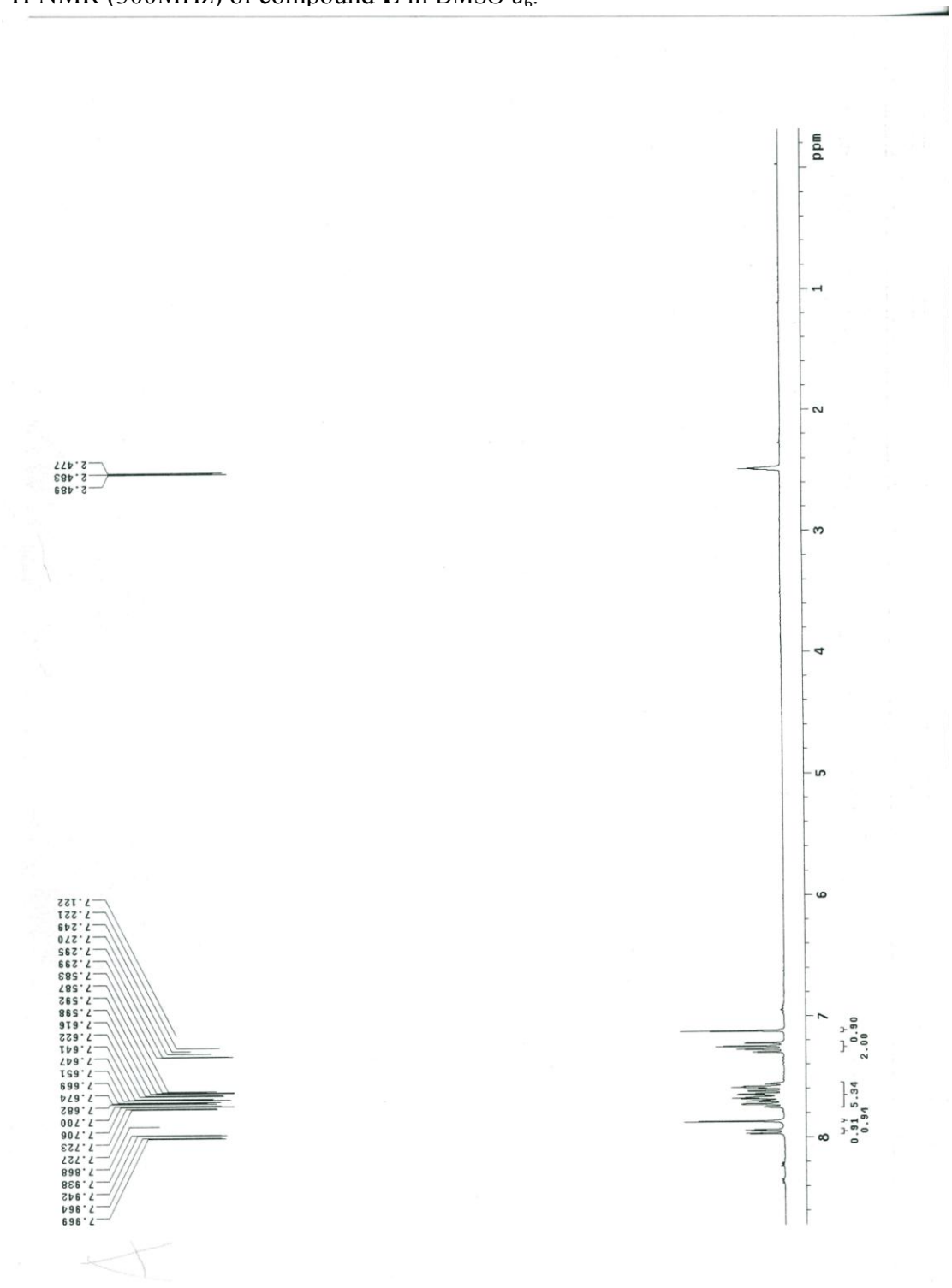
IR spectra of **L**.



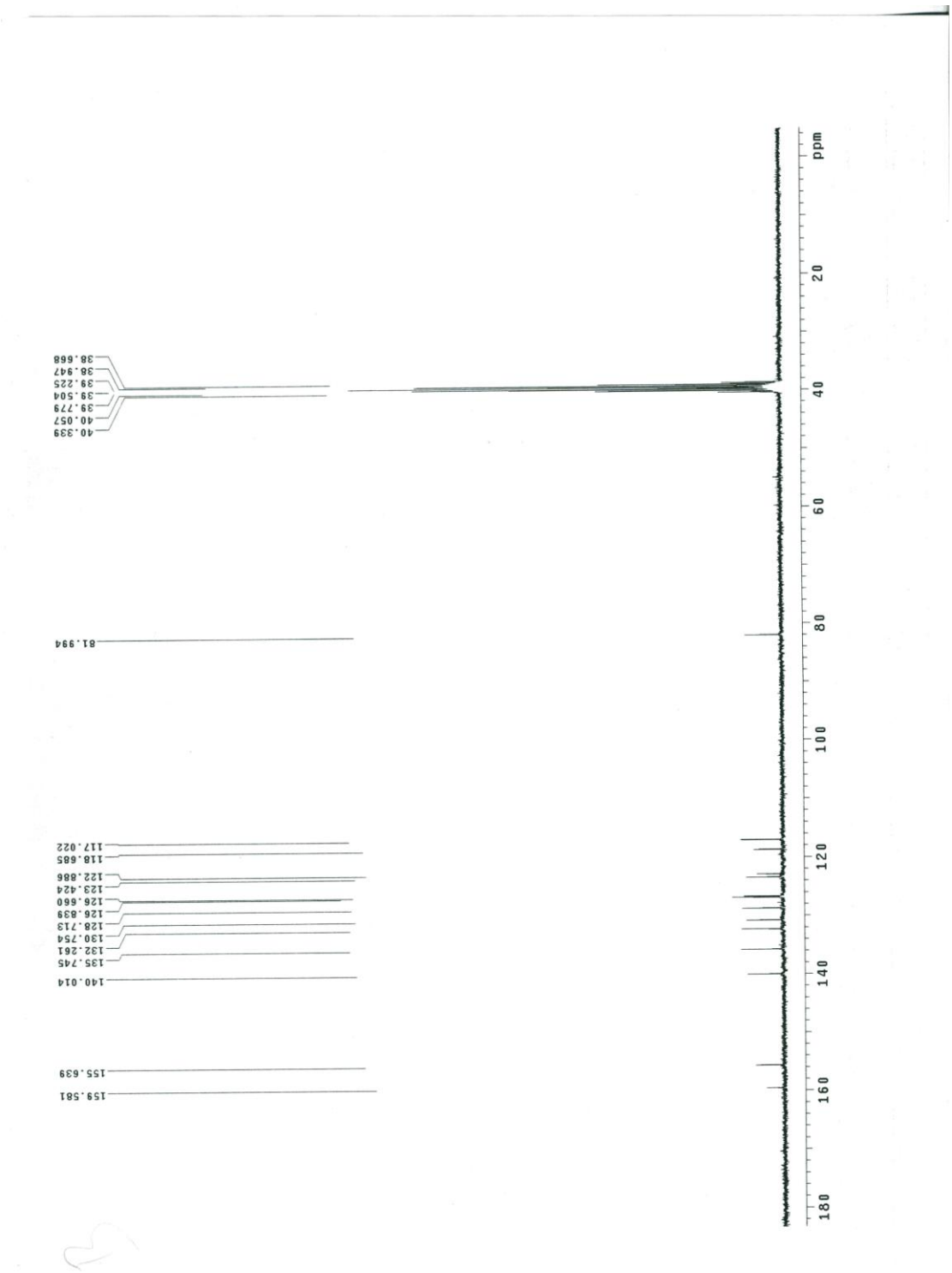
IR spectra of complex **L**-$Al(ClO_4)_3$.



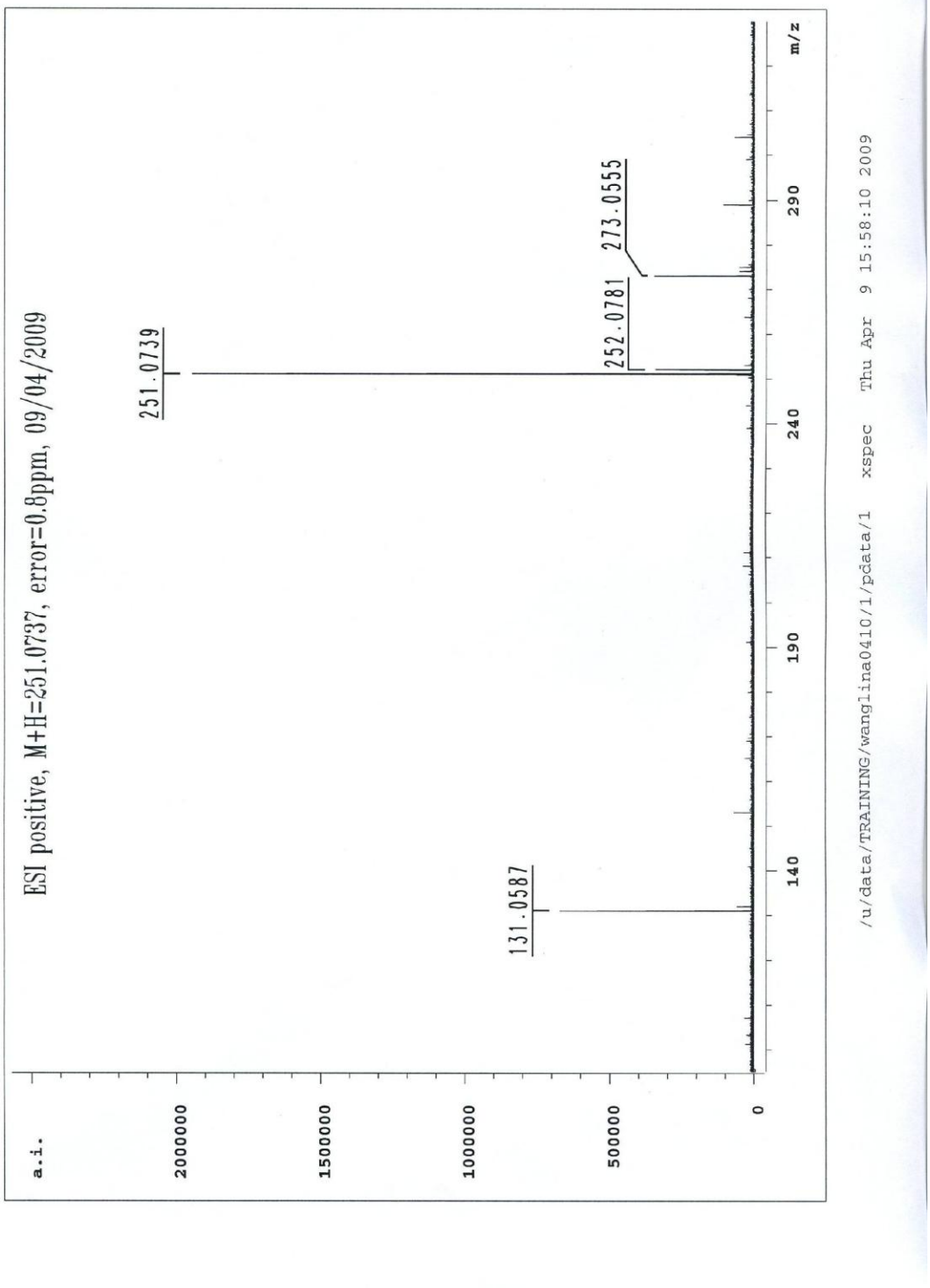
^{1}H NMR (300MHz) of compound **L** in DMSO-d_6.



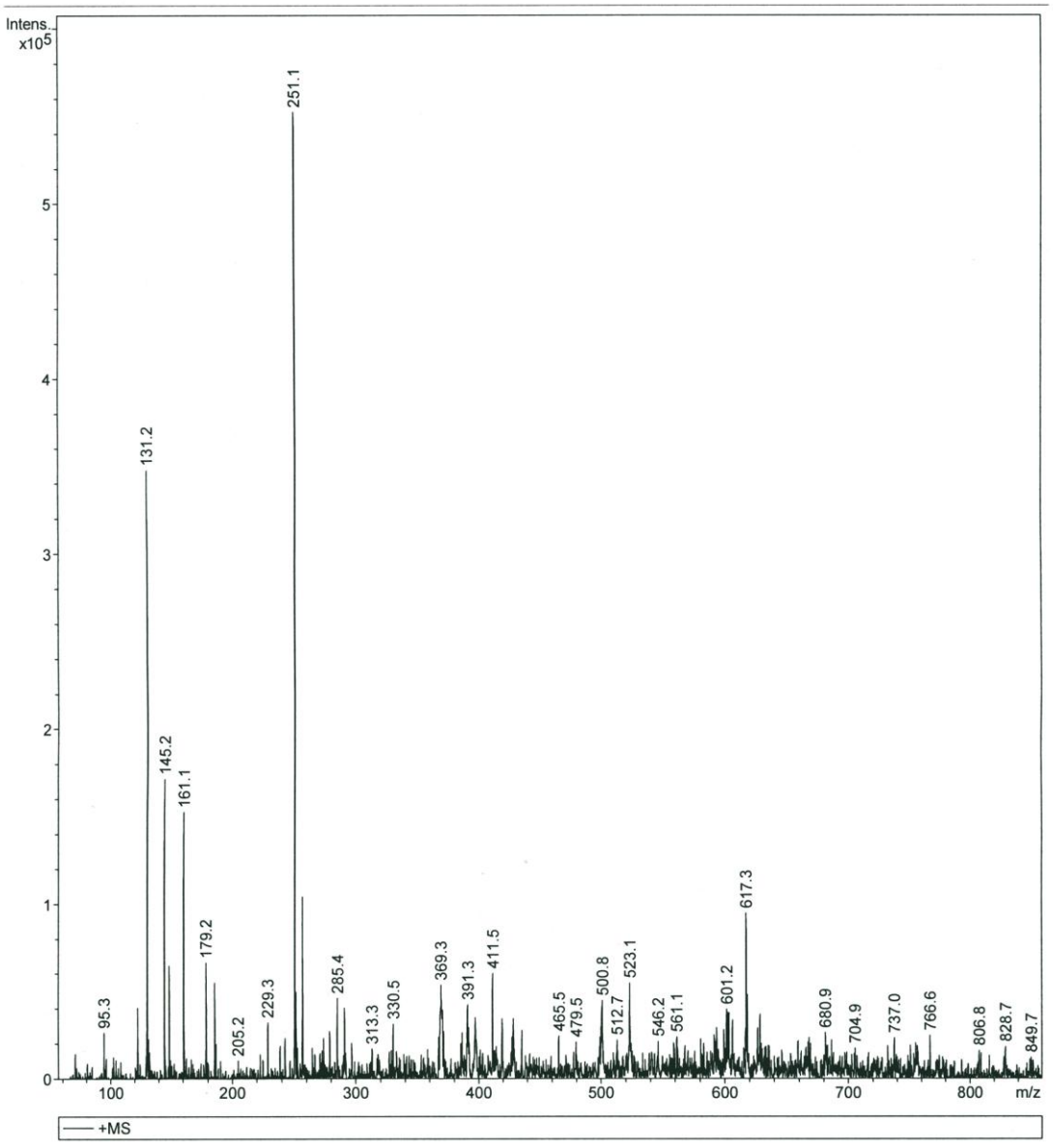
^{13}C NMR (75MHz) of compound **L** in DMSO-d_6.



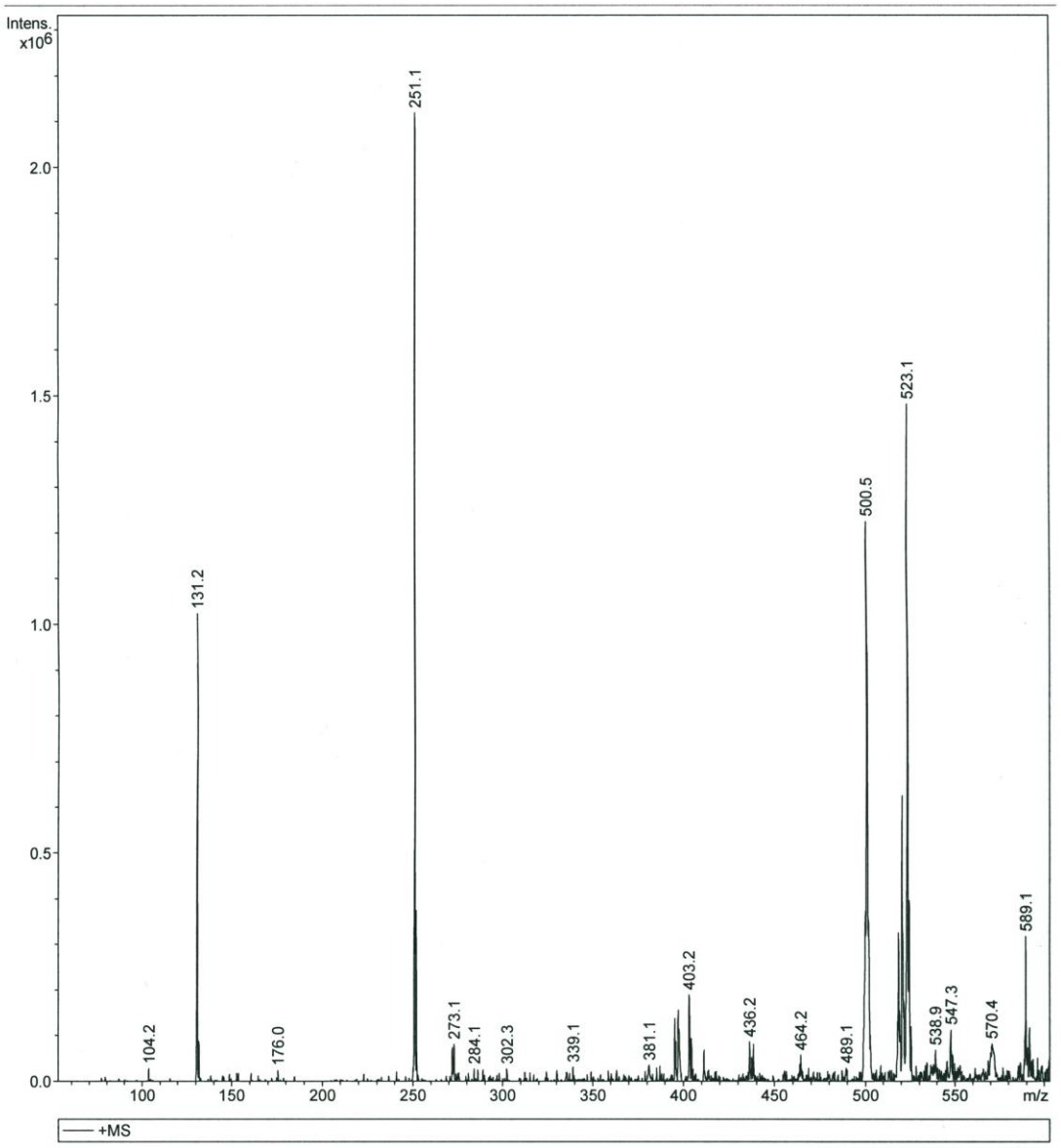
Electrospray ionization (ESI) mass spectrum of **L**.



Electrospray ionization (ESI) mass spectrum of Al-$(L)_2$-$(CH_3CH_2O)_2$.



Electrospray ionization (ESI) mass spectrum of Al-$(L)_2$-$(CH_3O)_2$.



Theoretical modeling

The geometry optimizations were carried out in vacuum using the hybrid density functional Becke-3-Lee-Yang-Parr (B3LYP) potential in conjuration with a 6-31G* basis set for the H, C, N, O atoms, and a LANL2DZ effective core potential (ECP) basis set for the Al atom. All the calculation implemented in GAUSSIAN 98 software package.[1] Frequency calculations were also implemented for the optimized structure to ensure that the optimized structure was the one which has the lowest energy.

(1) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski,; J. A. Montgomery, Jr., R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. A. Ortiz, A. G. Baboul, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres, C. Gonzalez, M. Head–Gordon, E. S. Replogle and J. A. Pople, *Gaussian 98*, Revision A.9; Gaussian, Inc.: Pittsburgh, PA, 1998.