Supplementary Information (SI) for New Journal of Chemistry.
This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2025

Supporting Information

Synthesis, photophysical, electrochemical, and spectroelectrochemical properties of the *β*-pyrrole functionalized push-pull porphyrins

Amiy Krishna and Rajneesh Misra*

Department of Chemistry, Indian Institute of Technology Indore

Indore 453552, India

E-mail: rajneeshmisra@iiti.ac.in

1. Cyclic voltammograms

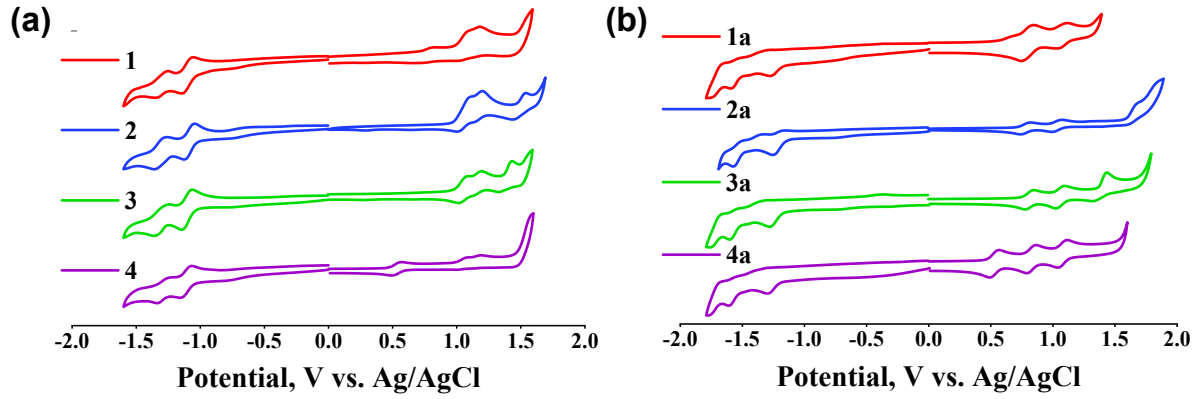

Fig. S1 CVs of the (a) free-base porphyrins (**1**−**4**) and (b) corresponding Zn(II) porphyrins (**1a**−**4a**) in dichloromethane containing 0.1 M n-Bu_4NPF_6 as the supporting electrolyte, recorded at a scan rate of 100 mV/s vs Ag/AgCl.

2. Spectroelectrochemical studies

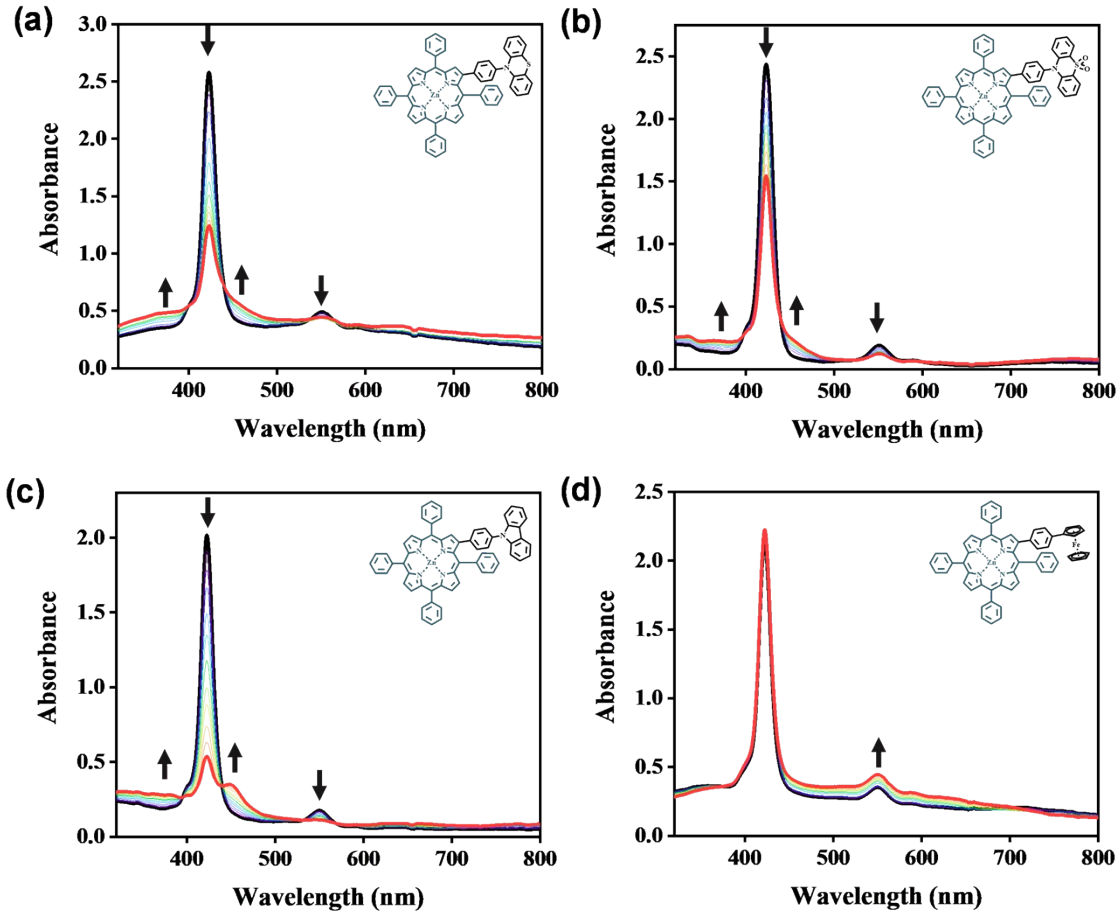

Fig. S2 Spectral changes observed during the first oxidation of the Zn(II) porphyrins **1a**–**4a**.

3. Computational studies

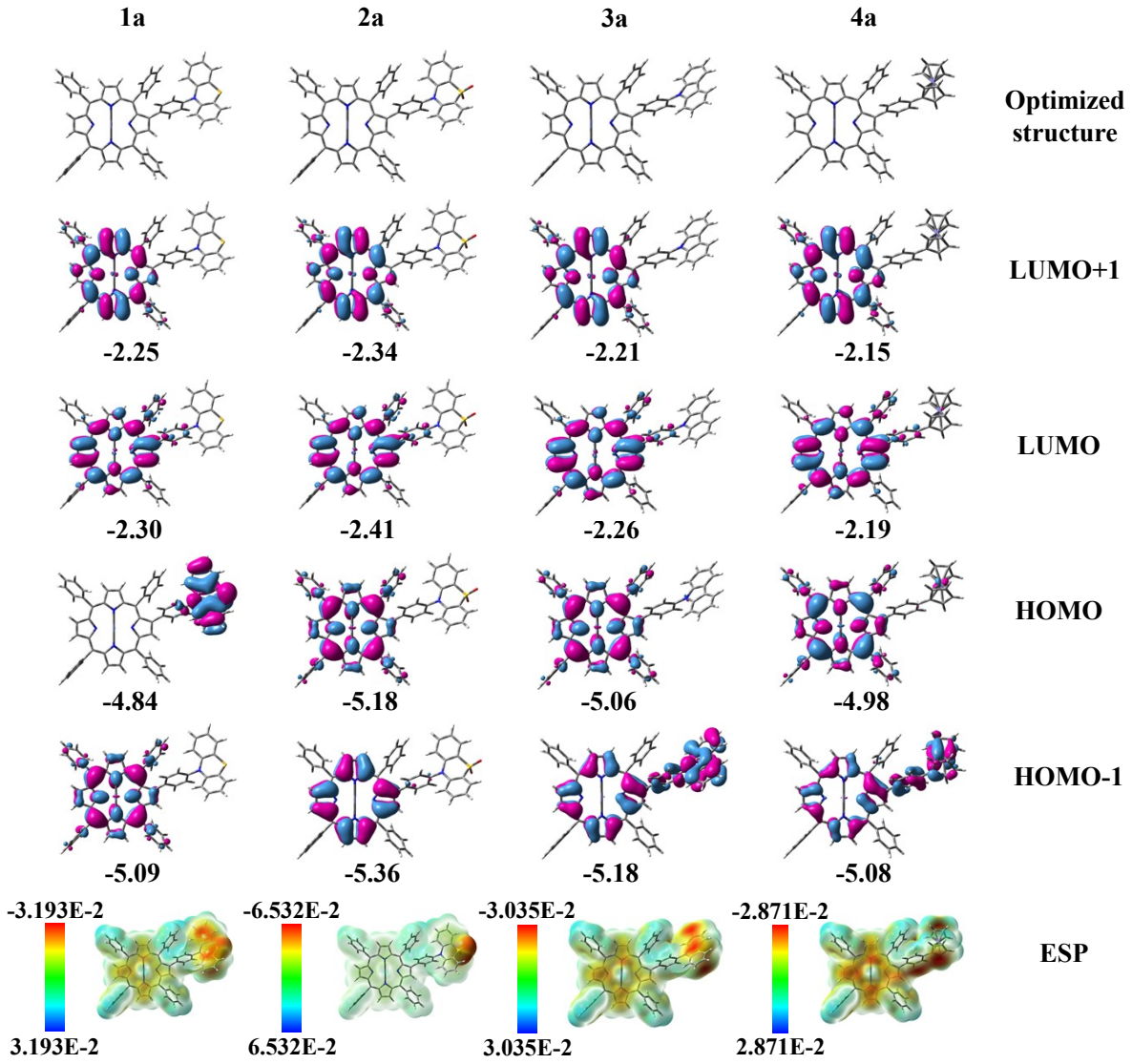

Fig. S3 B3LYP/6-31G (d,p) optimized structure, frontier HOMO-1, HOMO, LUMO and LUMO+1 and electrostatic potential energy maps of the Zn(II) porphyrins **1a**–**4a**.

Table S1 Energies of the frontier orbitals on B3LYP/6-31G (d,p) optimized structures in the gas phase.

Compound	HOMO-1 (eV)	HOMO (eV)	LUMO (eV)	LUMO+1 (eV)
1	-5.01	-4.88	-2.37	-2.30
1a	-5.09	-4.84	-2.30	-2.25
2	-5.42	-5.11	-2.48	-2.40
2a	-5.36	-5.18	-2.41	-2.34
3	-5.23	-4.98	-2.33	-2.27
3a	-5.18	-5.06	-2.26	-2.21
4	-5.13	-4.90	-2.24	-2.19
4a	-5.08	-4.98	-2.19	-2.15

4. Copies of ^{1}H-NMR, ^{13}C-NMR and HRMS spectra

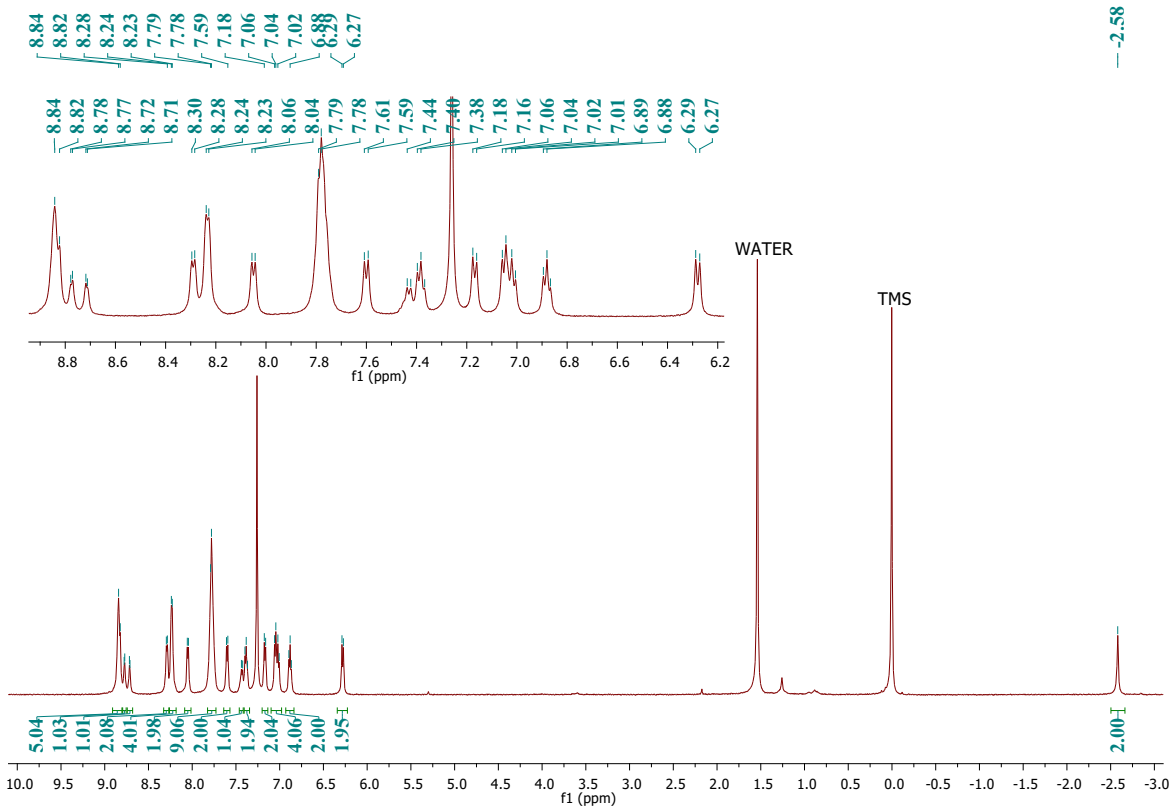

Fig. S4 ^{1}H NMR ($CDCl_3$) spectra of **1**.

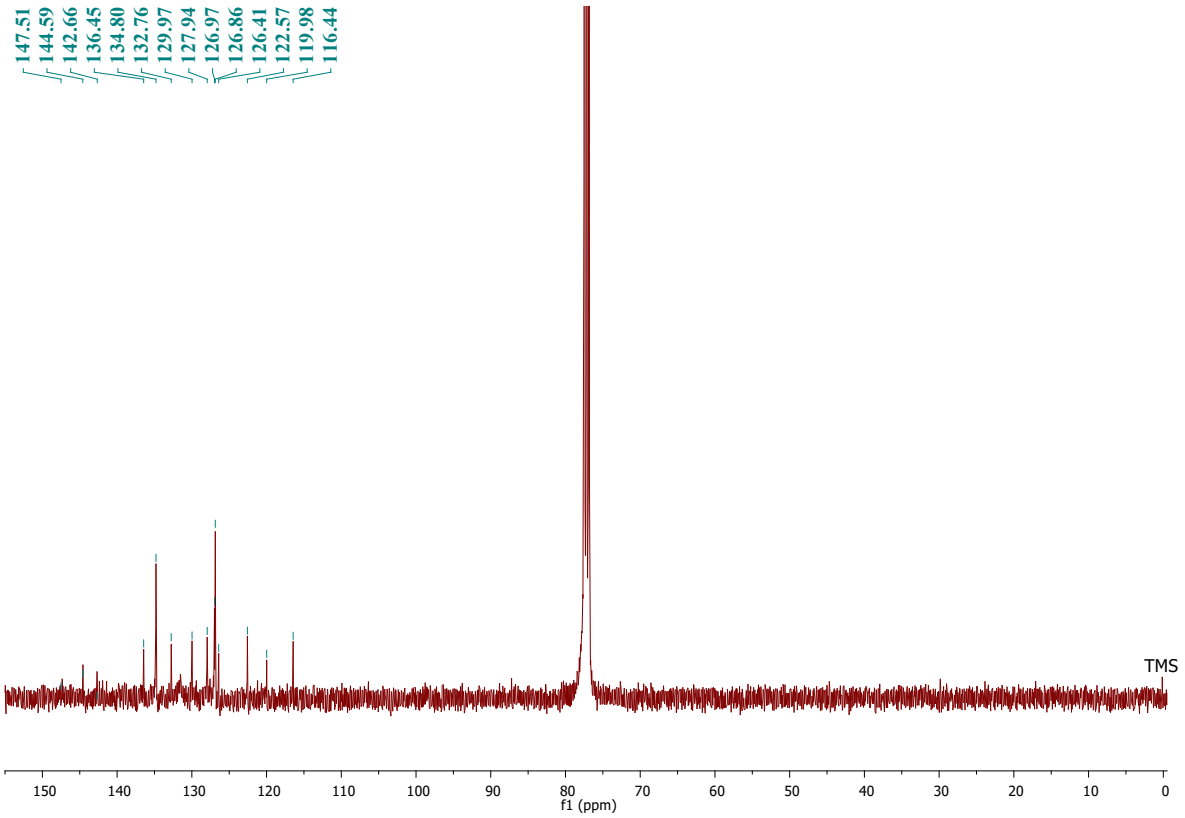

Fig. S5 $^{13}C\{^{1}H\}$ NMR ($CDCl_3$) spectra of **1**.

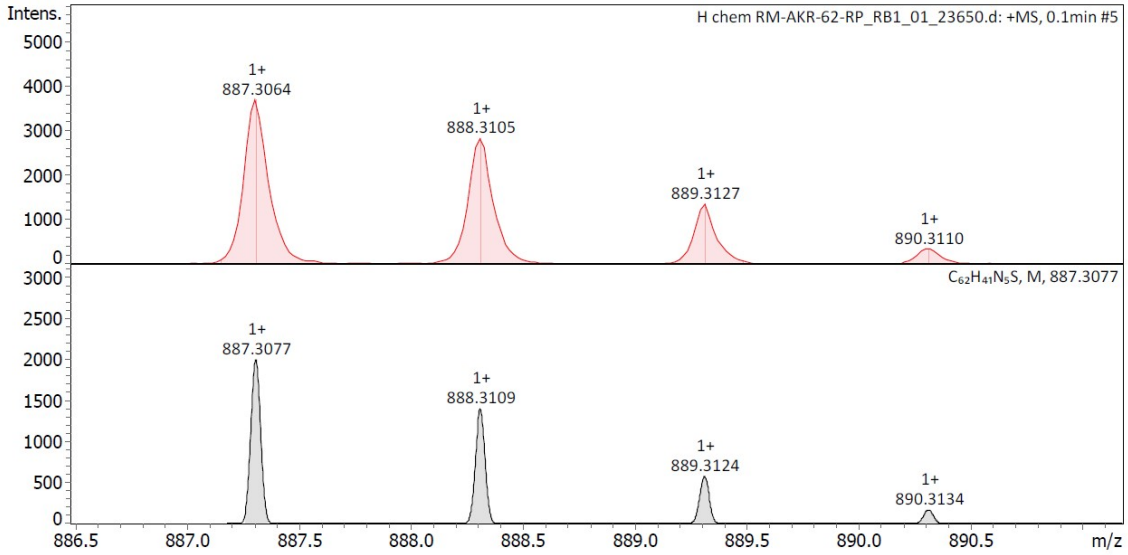

Fig. S6 HRMS of **1**.

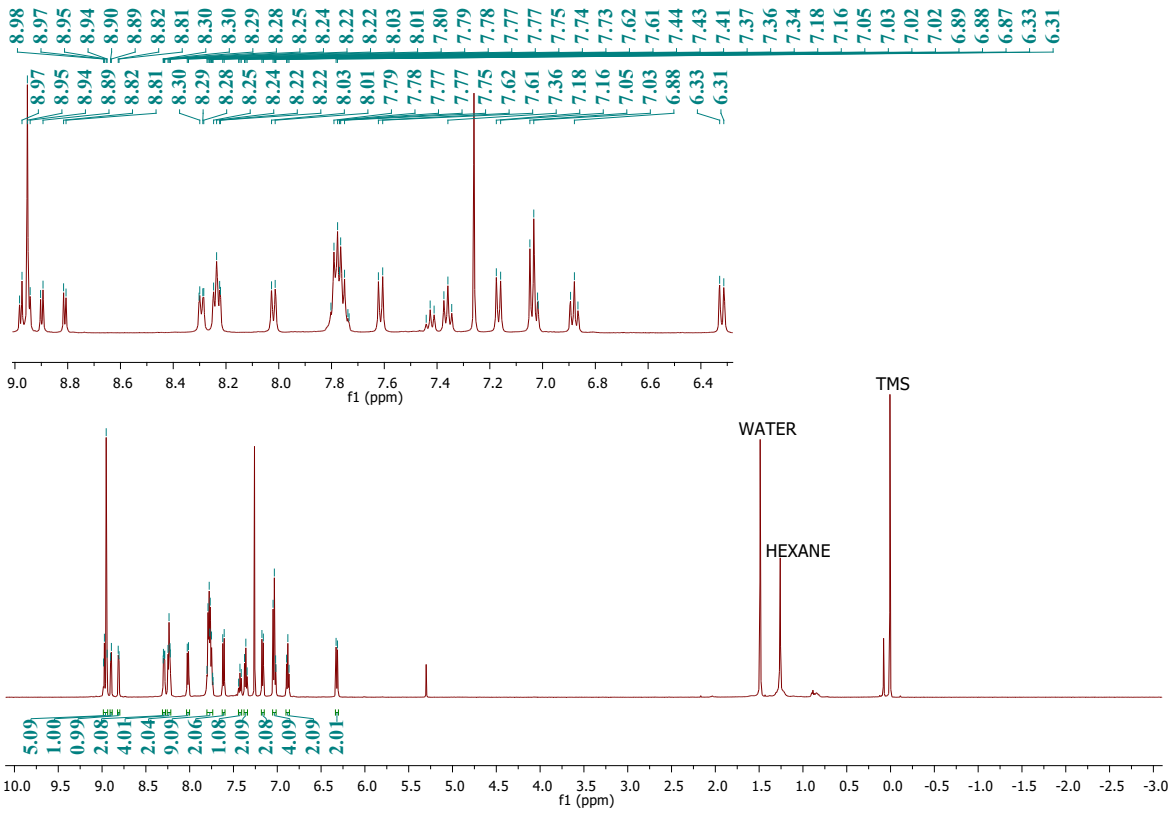

Fig. S7 ^{1}H NMR ($CDCl_3$) spectra of **1a**.

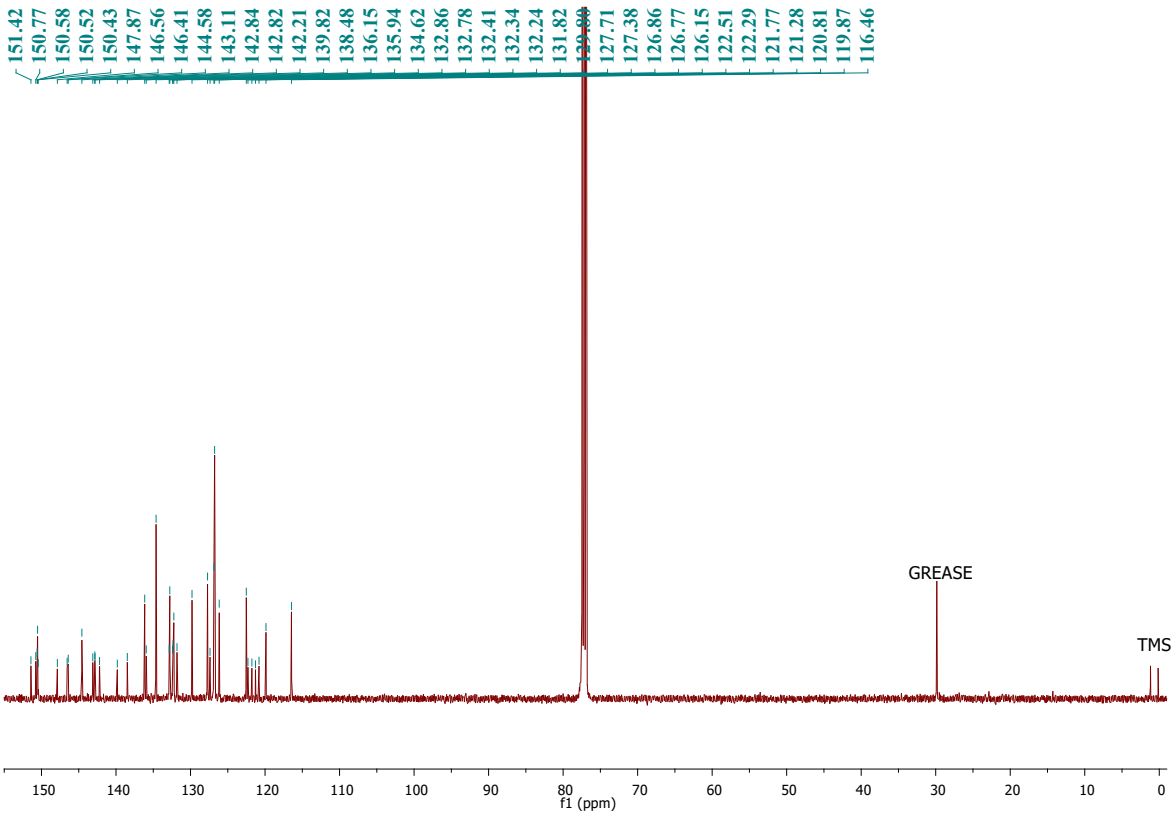

Fig. S8 $^{13}C\{^{1}H\}$ NMR ($CDCl_3$) spectra of **1a**.

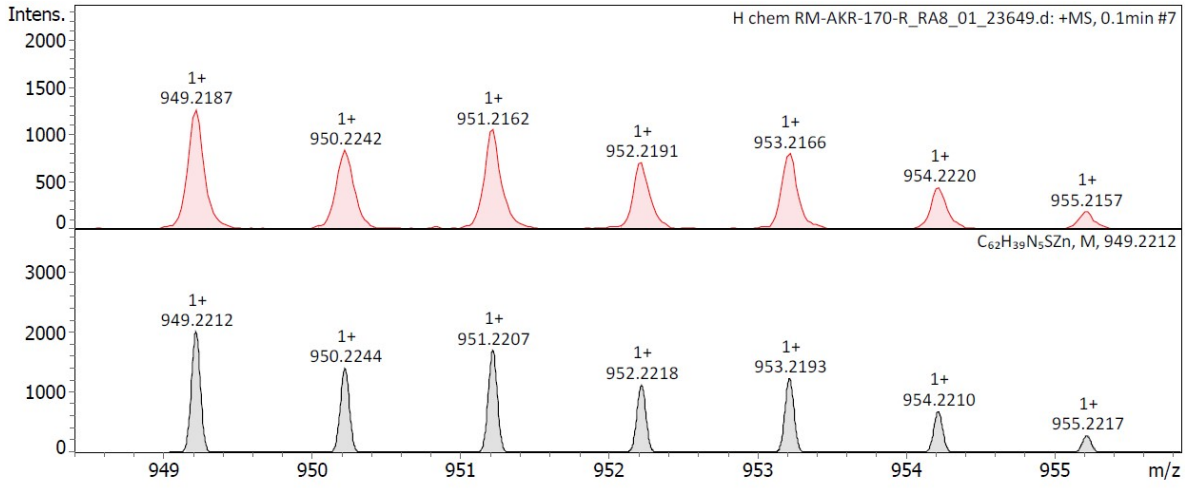

Fig. S9 HRMS of **1a**.

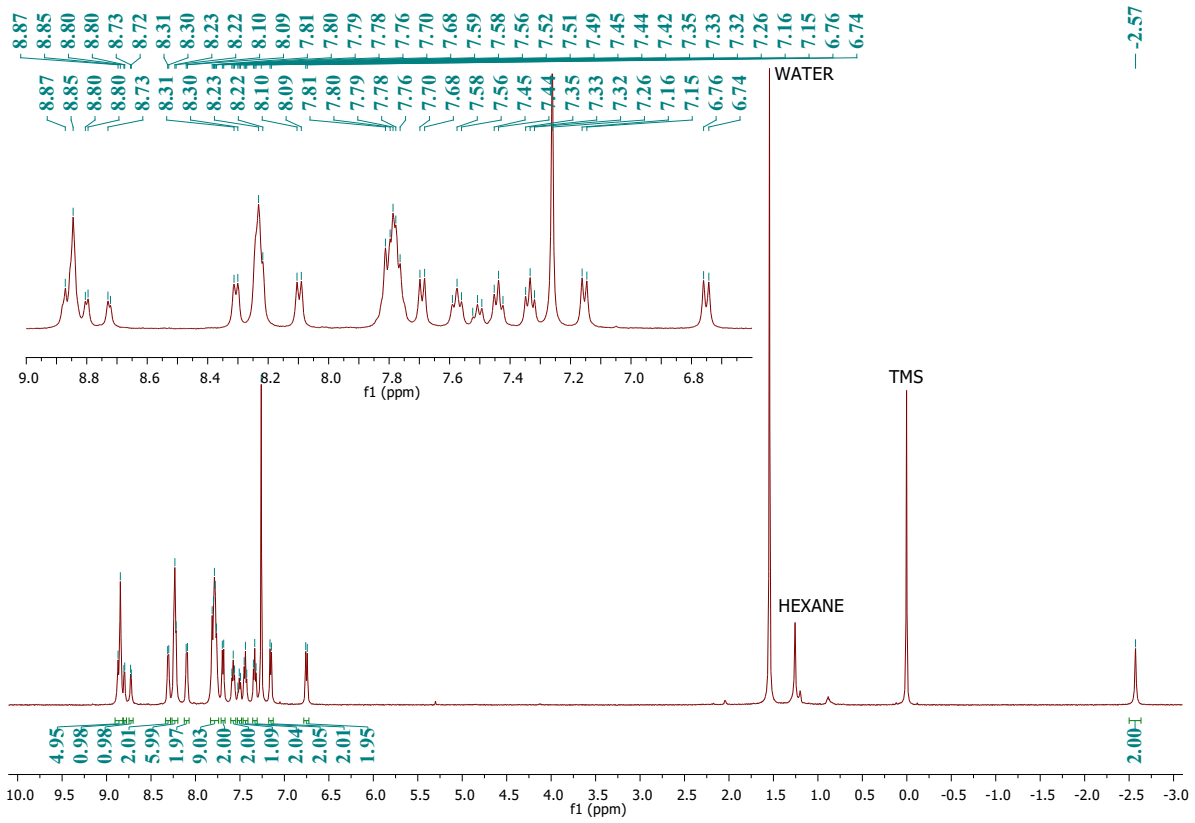

Fig. S10 ^{1}H NMR ($CDCl_3$) spectra of **2**.

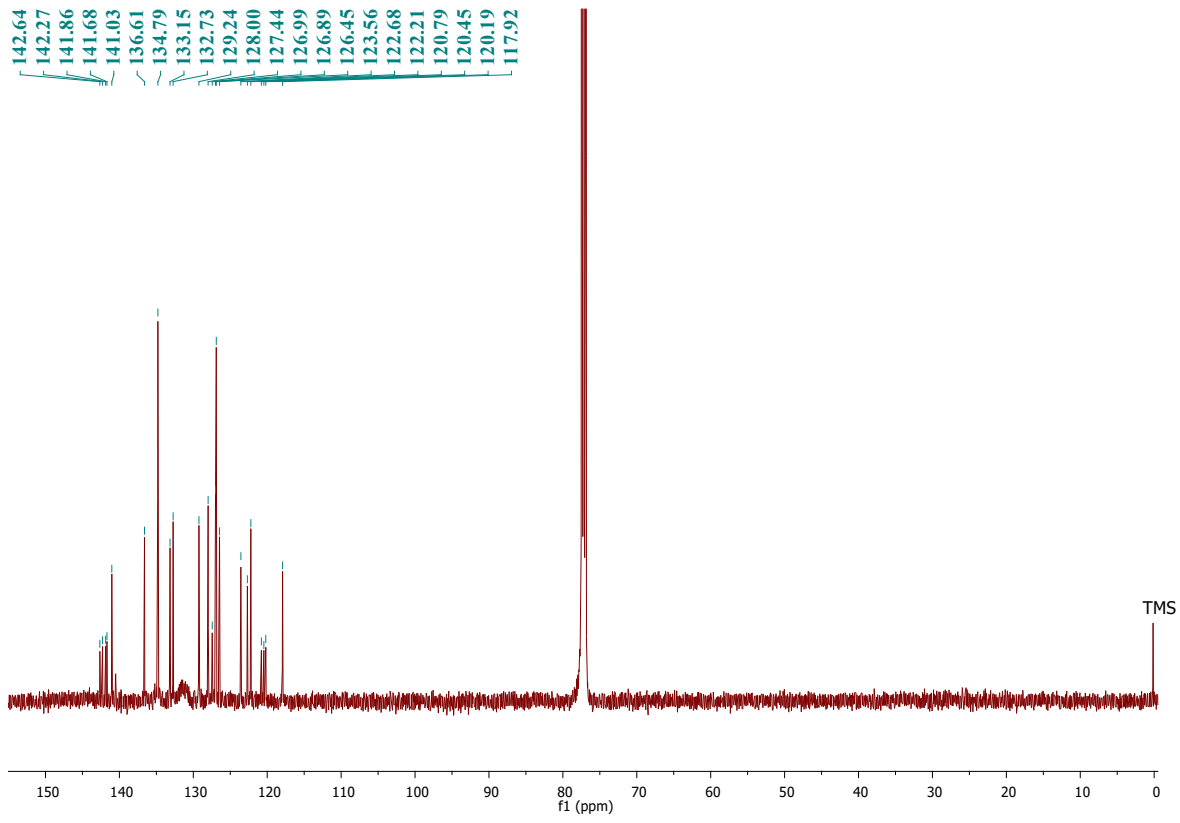

Fig. S11 $^{13}C\{^{1}H\}$ NMR ($CDCl_3$) spectra of **2**.

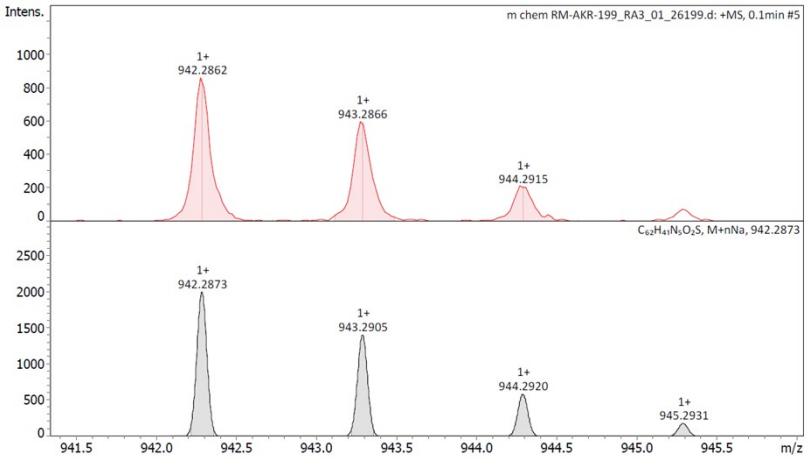

Fig. S12 HRMS of **2**.

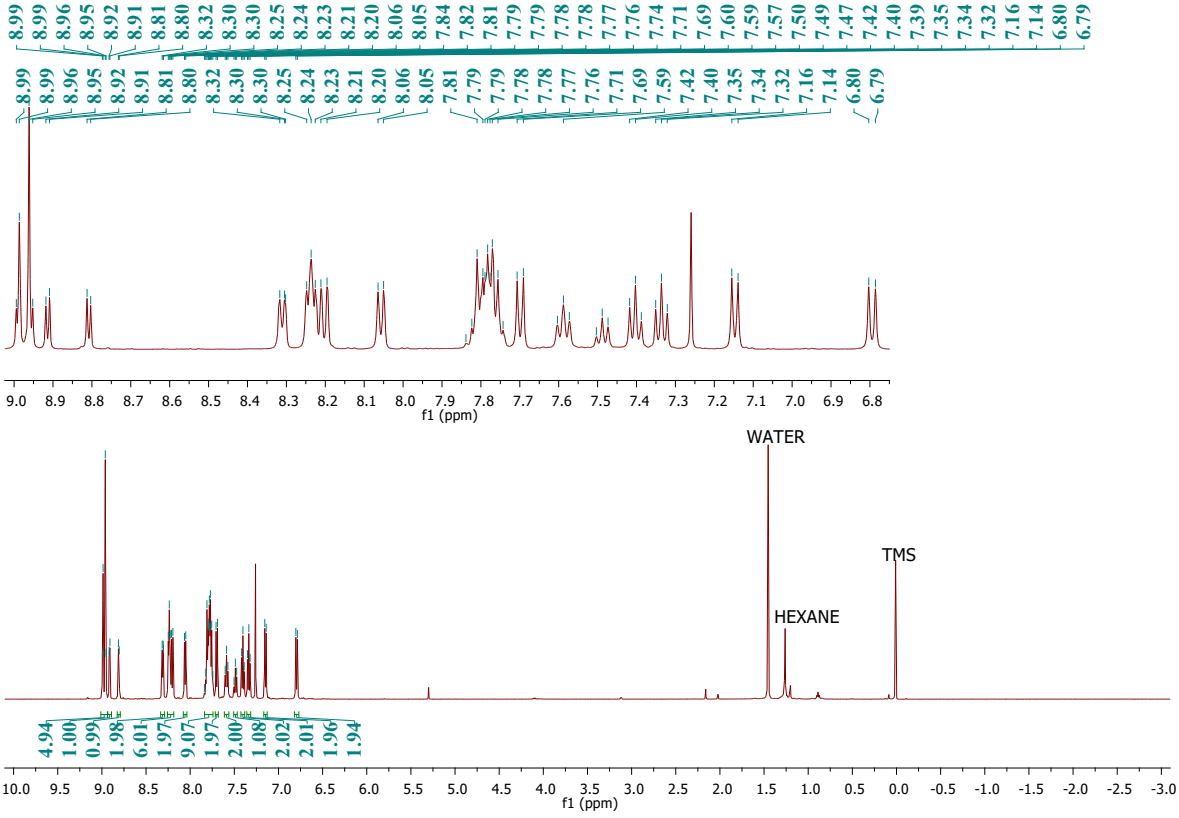

Fig. S13 ^{1}H NMR ($CDCl_3$) spectra of **2a**.

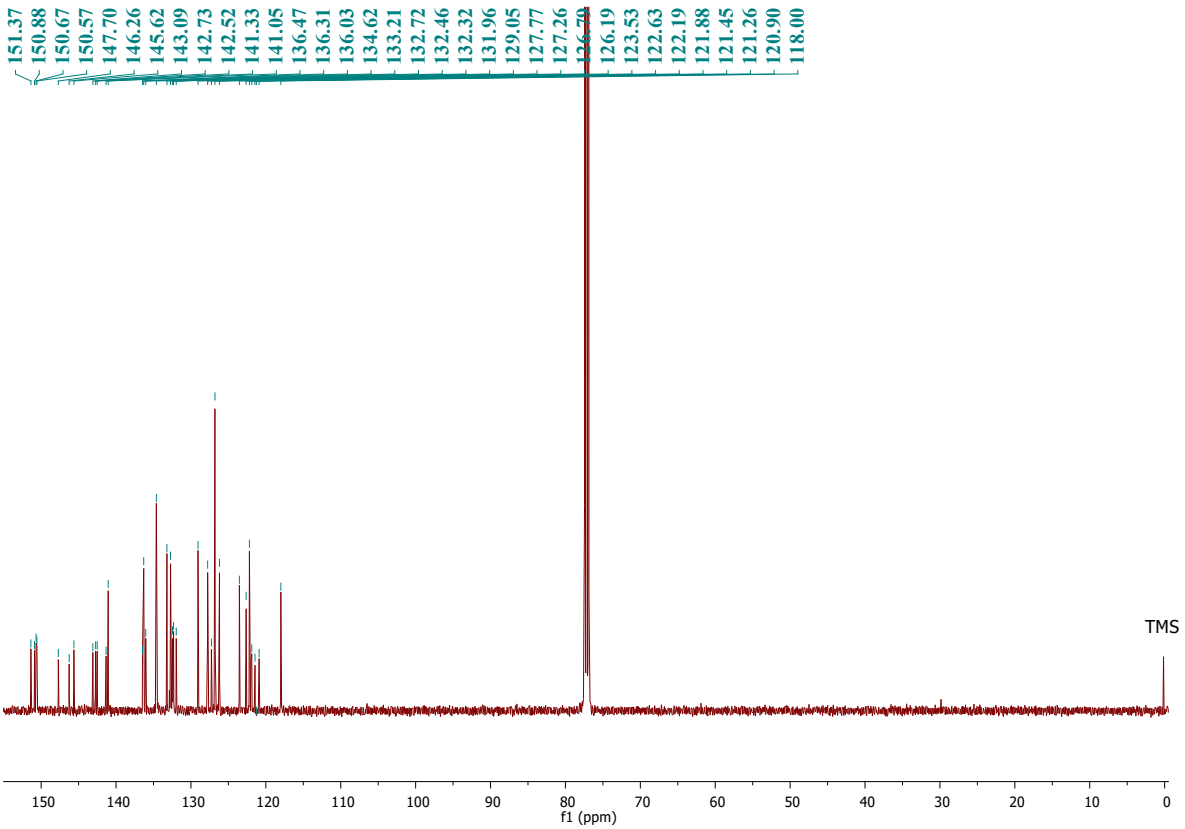

Fig. S14 $^{13}C\{^{1}H\}$ NMR ($CDCl_3$) spectra of **2a**.

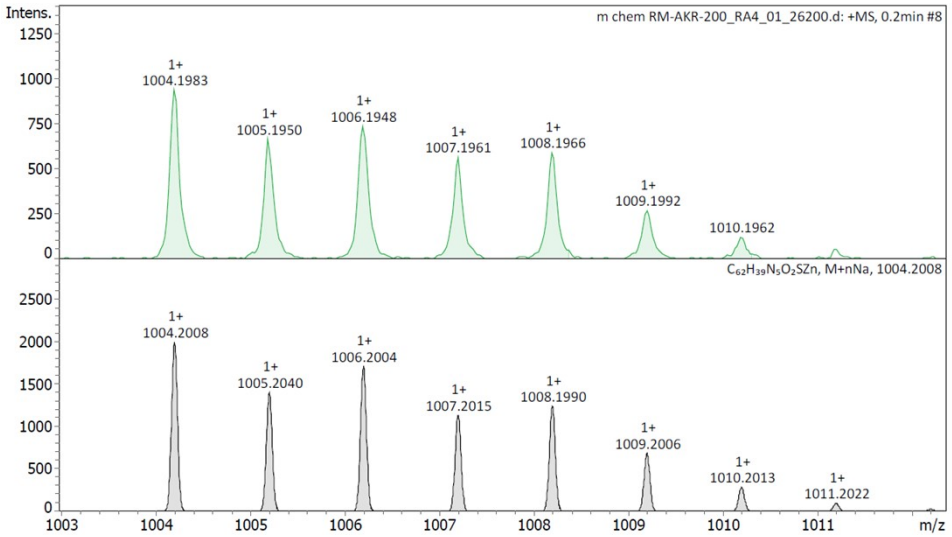

Fig. S15 HRMS of **2a**.

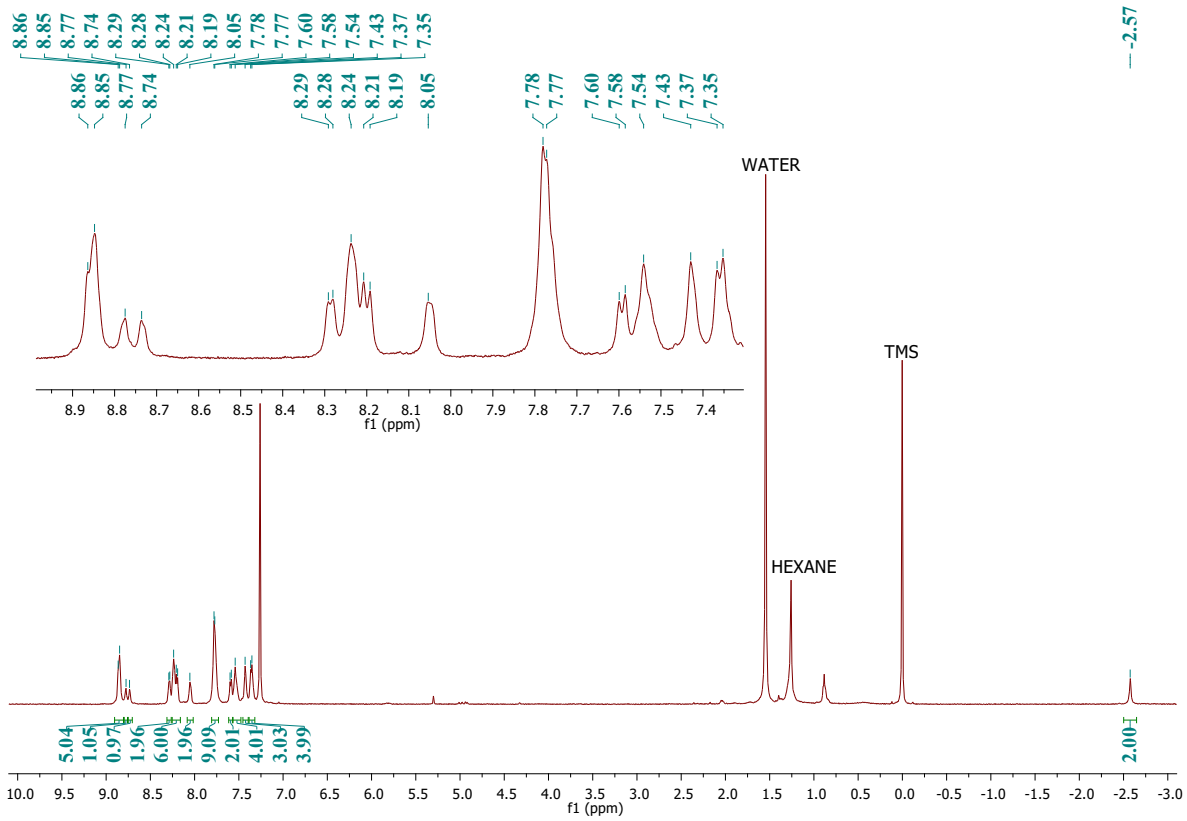

Fig. S16 ^{1}H NMR ($CDCl_3$) spectra of **3**.

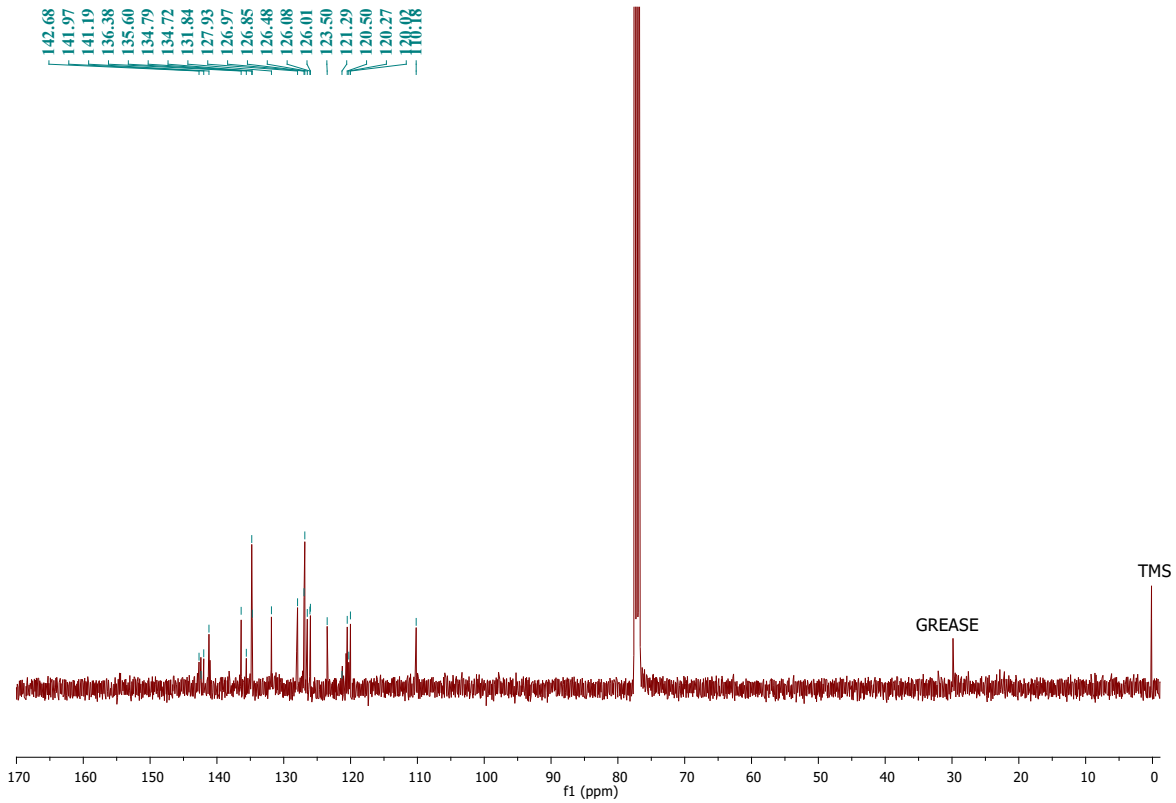

Fig. S17 $^{13}C\{^{1}H\}$ NMR ($CDCl_3$) spectra of **3**.

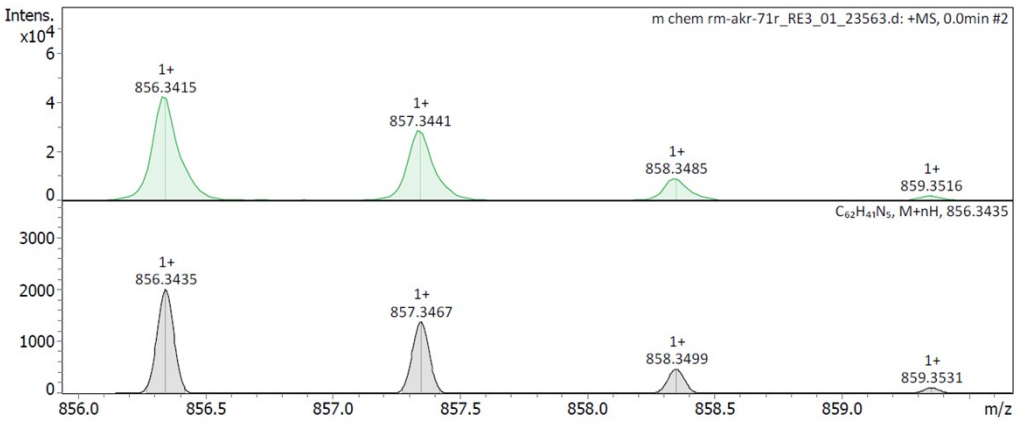

Fig. S18 HRMS of **3**.

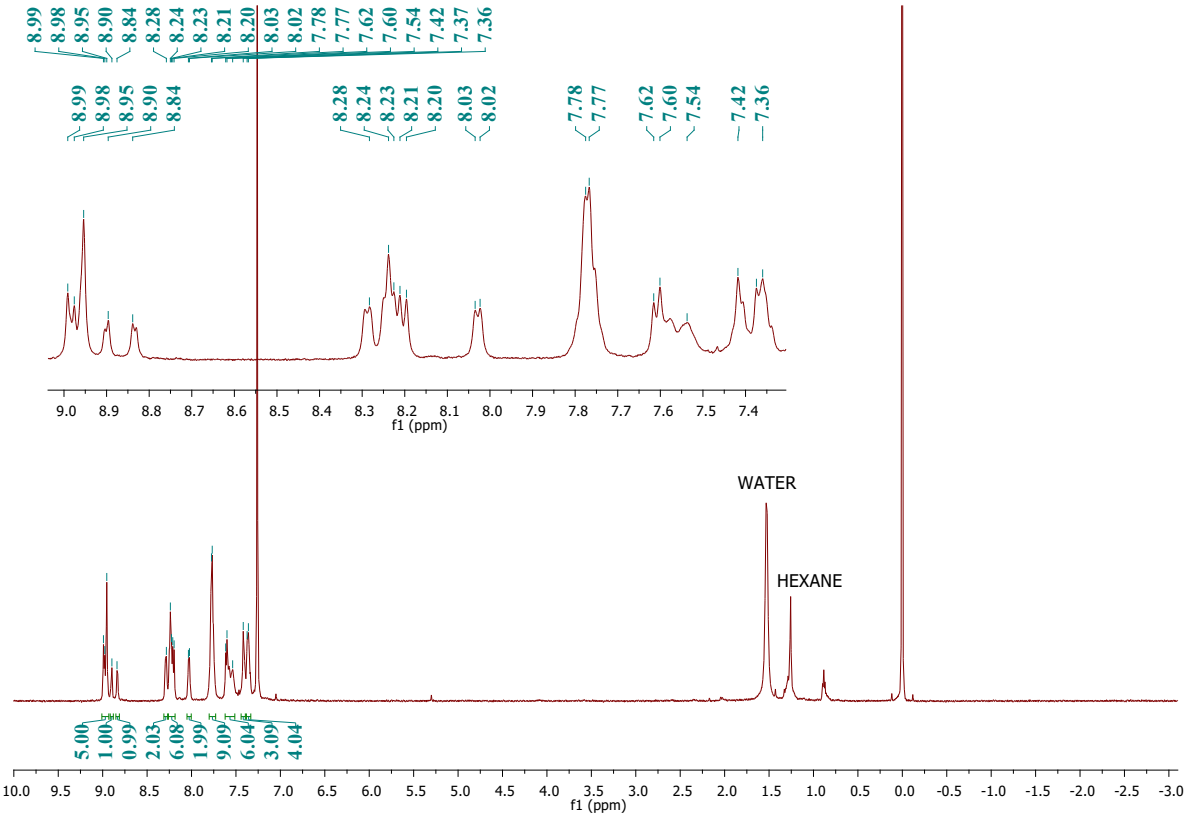

Fig. S19 ^{1}H NMR ($CDCl_3$) spectra of **3a**.

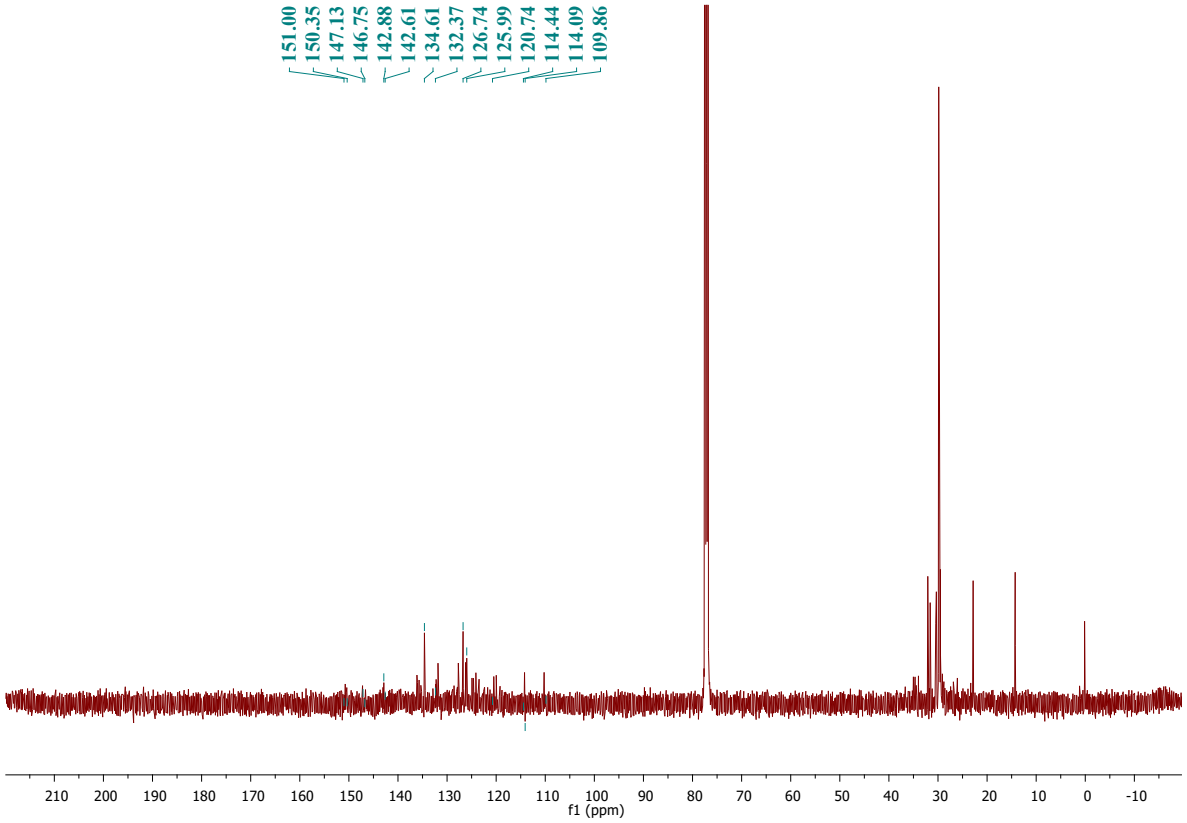

Fig. S20 $^{13}C\{^{1}H\}$ NMR ($CDCl_3$) spectra of **3a**.

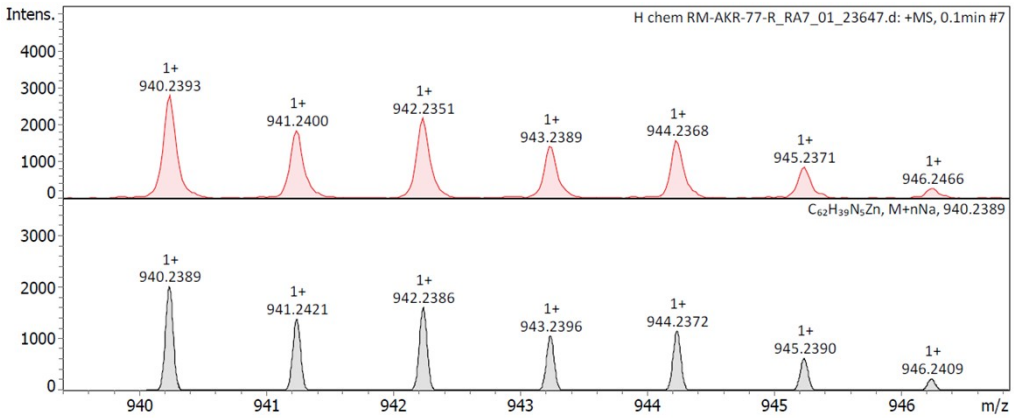

Fig. S21 HRMS of **3a**.

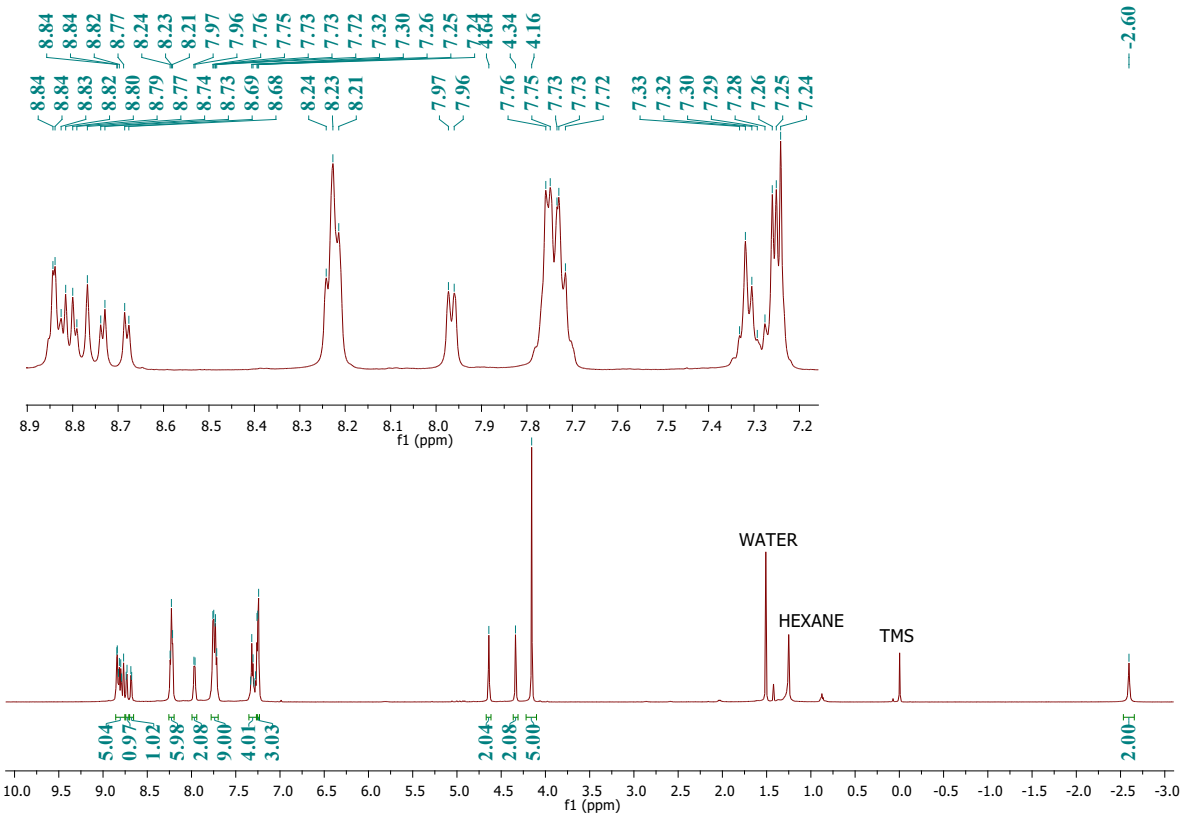

Fig. S22 ^{1}H NMR ($CDCl_3$) spectra of **4**.

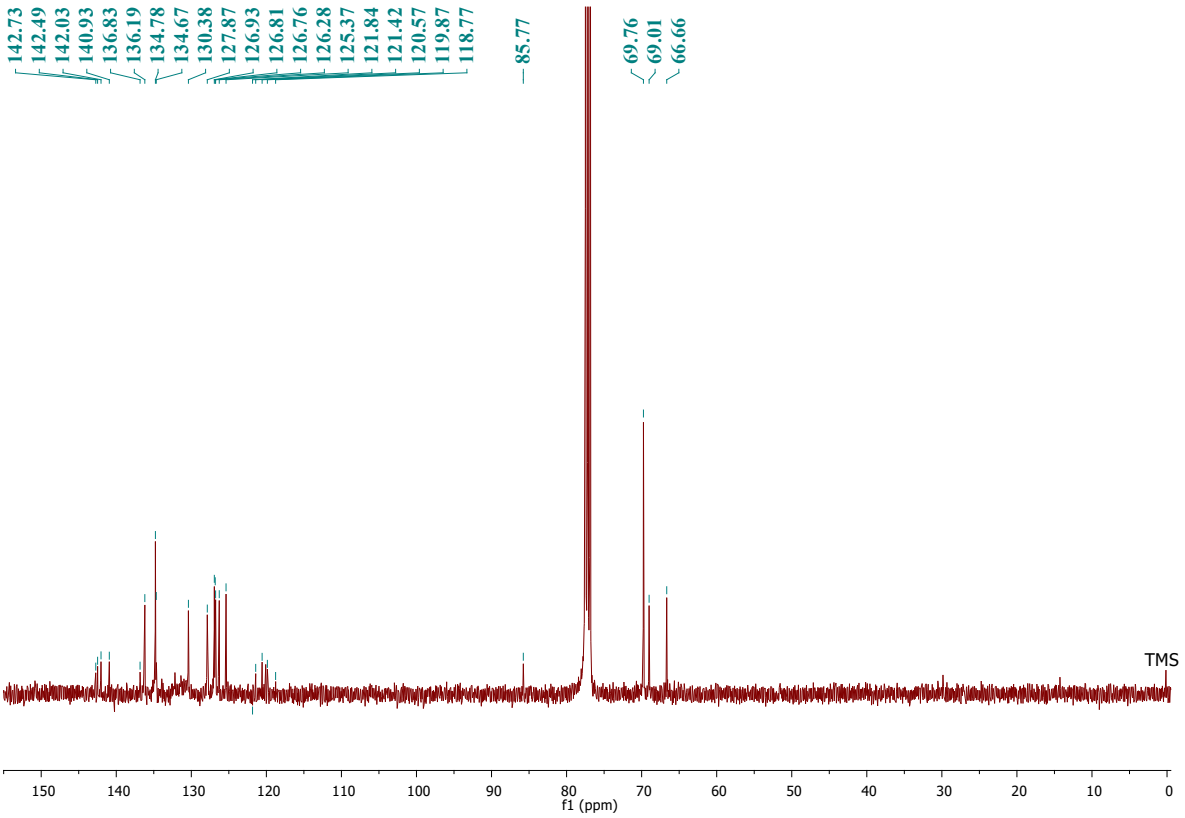

Fig. S23 $^{13}C\{^{1}H\}$ NMR ($CDCl_3$) spectra of **4**.

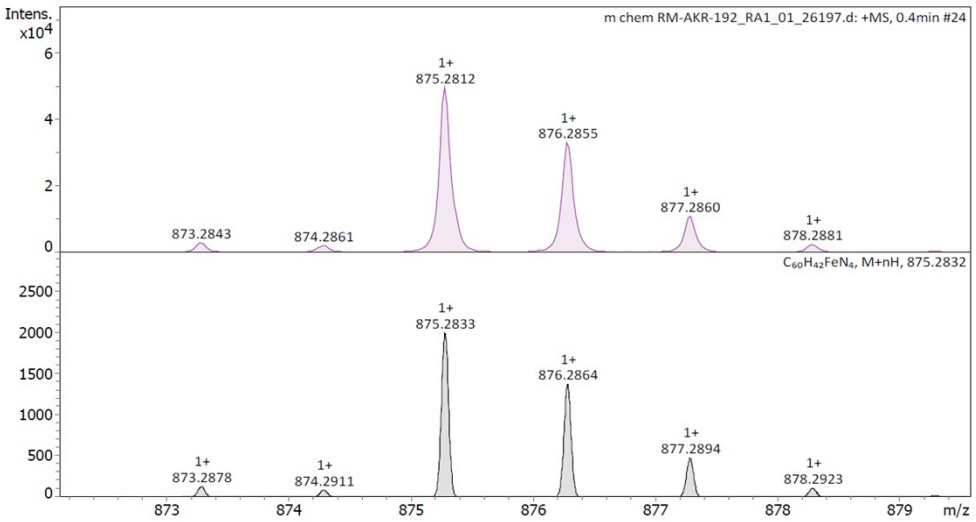

Fig. S24 HRMS of **4**.

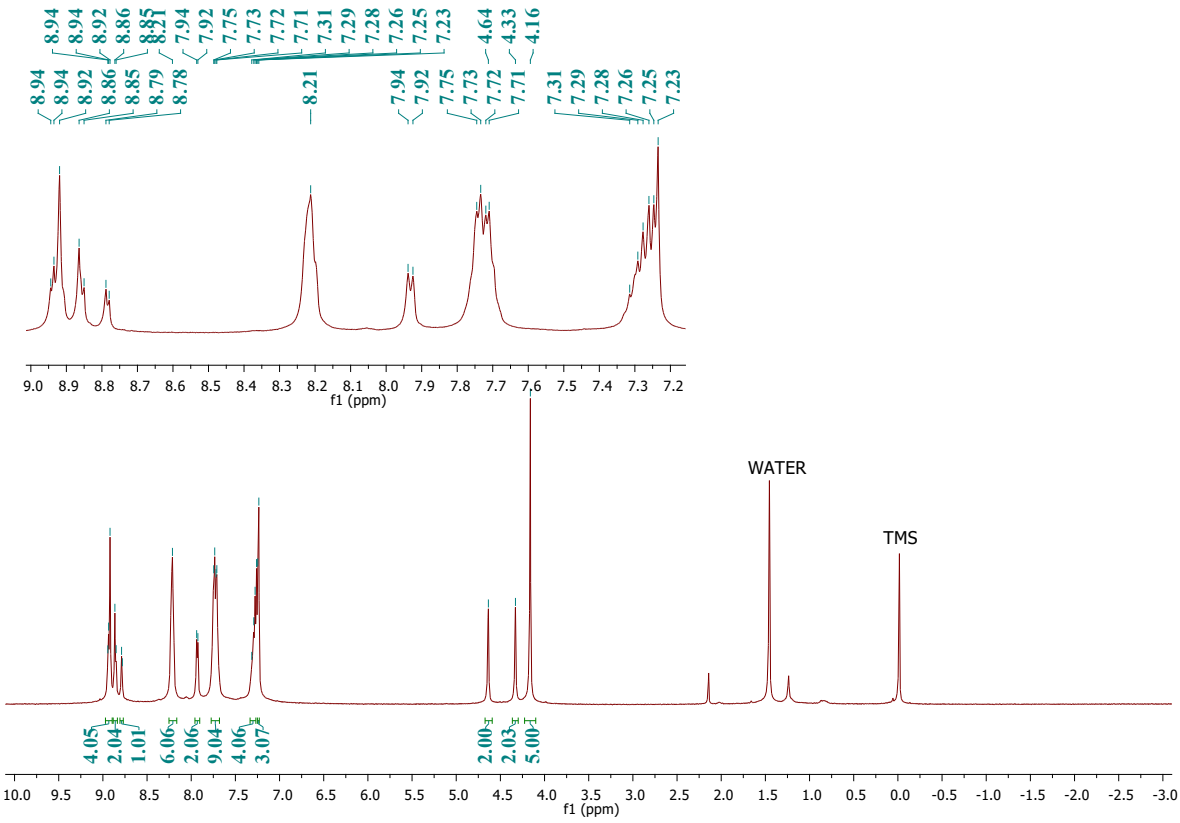

Fig. S25 ^{1}H NMR ($CDCl_3$) spectra of **4a**.

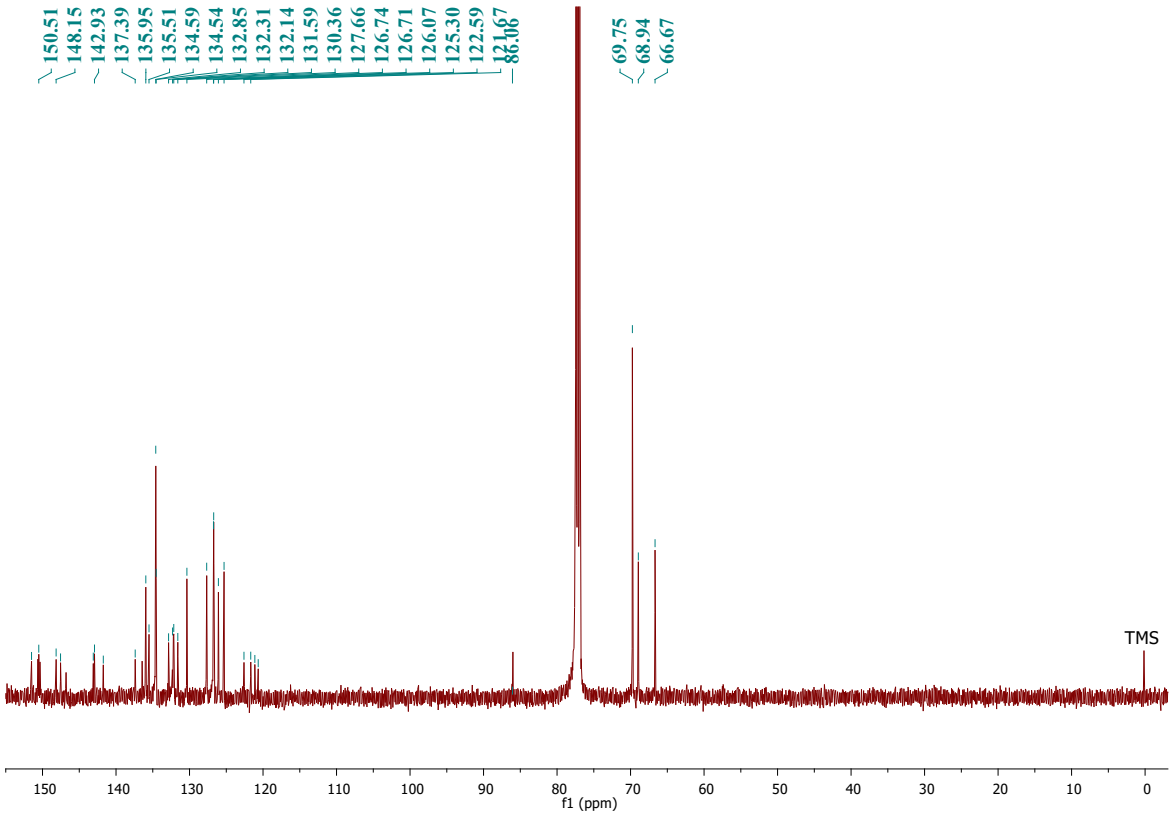

Fig. S26 $^{13}C\{^{1}H\}$ NMR ($CDCl_3$) spectra of **4a**.

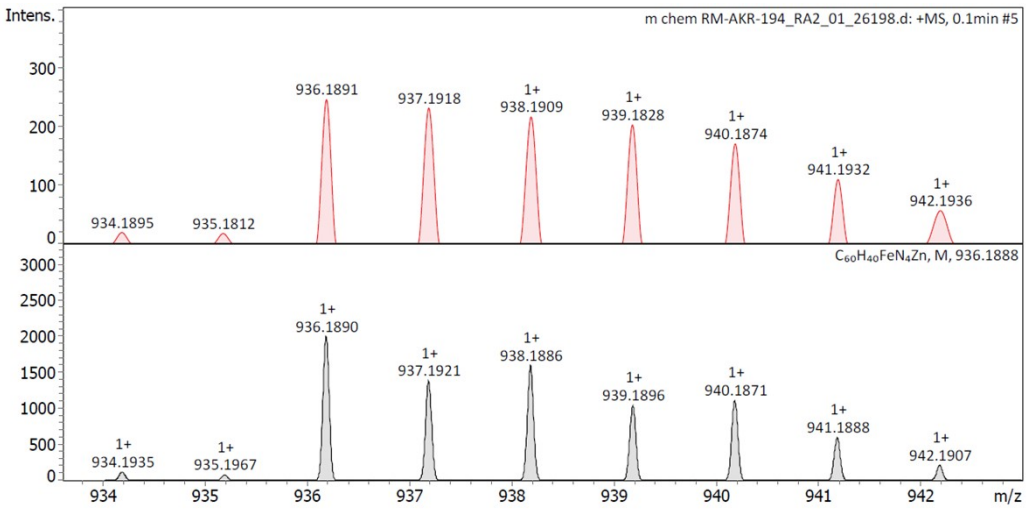

Fig. S27 HRMS of **4a**.