Adsorption and Corrosion Inhibition Potentials of Salicylaldehyde-based Schiff Bases of Semicarbazide and *p*-Toluidine on Mild Steel in Acidic Medium: Experimental and Computational Studies

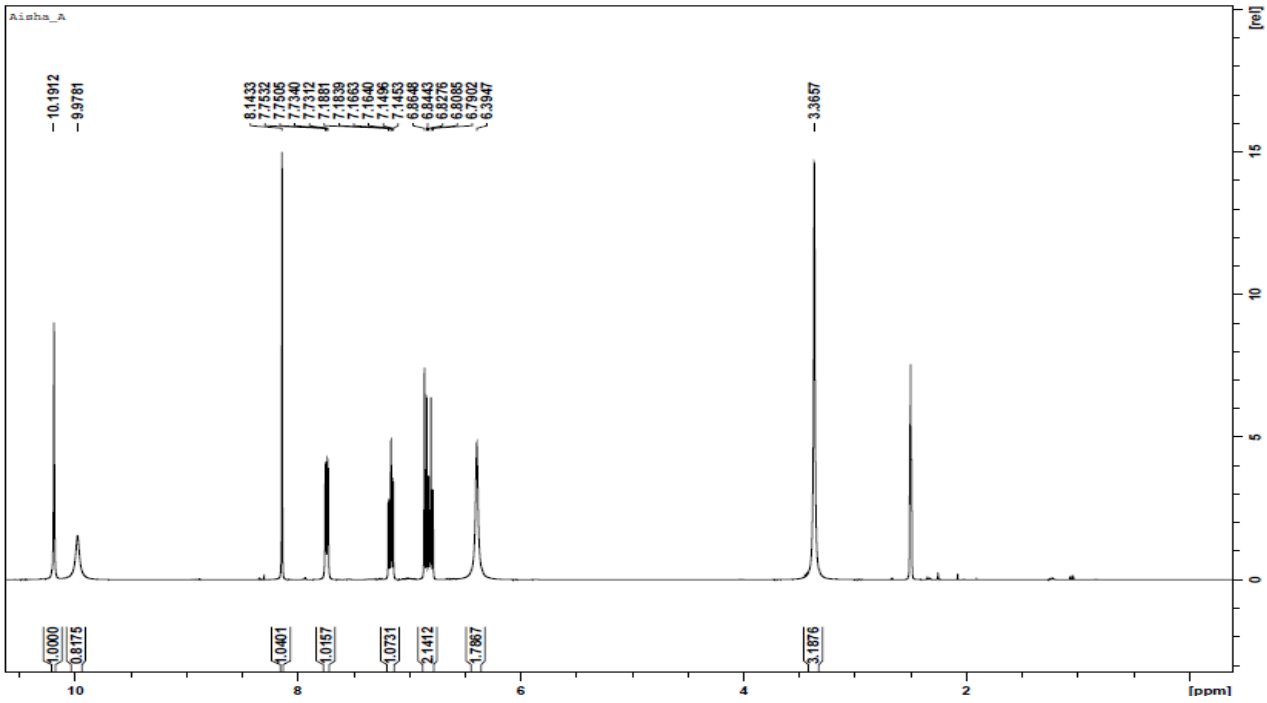
Supplementary Material

Lukman O. Olasunkanmi[a,b], Aishat O. Idris[a], Adetola H. Adewole[c], Olaide O. Wahab[d], and Eno E. Ebenso[b,e]

[a]Department of Chemistry, Faculty of Science, Obafemi Awolowo University, Ile-Ife 220005, Nigeria
[b]Materials Science Innovation & Modelling (MaSIM) Research Focus Area, Faculty of Natural and Agricultural Sciences, North-West University, Private BagX2046, Mmabatho 2735, South Africa
[c]Department of Chemistry, Faculty of Natural and Agricultural Sciences, University of Pretoria, Pretoria 0002, South Africa
[d]Department of Chemistry, Faculty of Pure and Applied Sciences, Nigerian Army University Biu, Nigeria
[e]Institute for Nanotechnology and Water Sustainability, College of Science, Engineering and Technology, University of South Africa, Johannesburg, South Africa

* Corresponding author - E-mail address: waleolasunkanmi@gmail.com (L.O. Olasunkanmi).

(I)



(II)

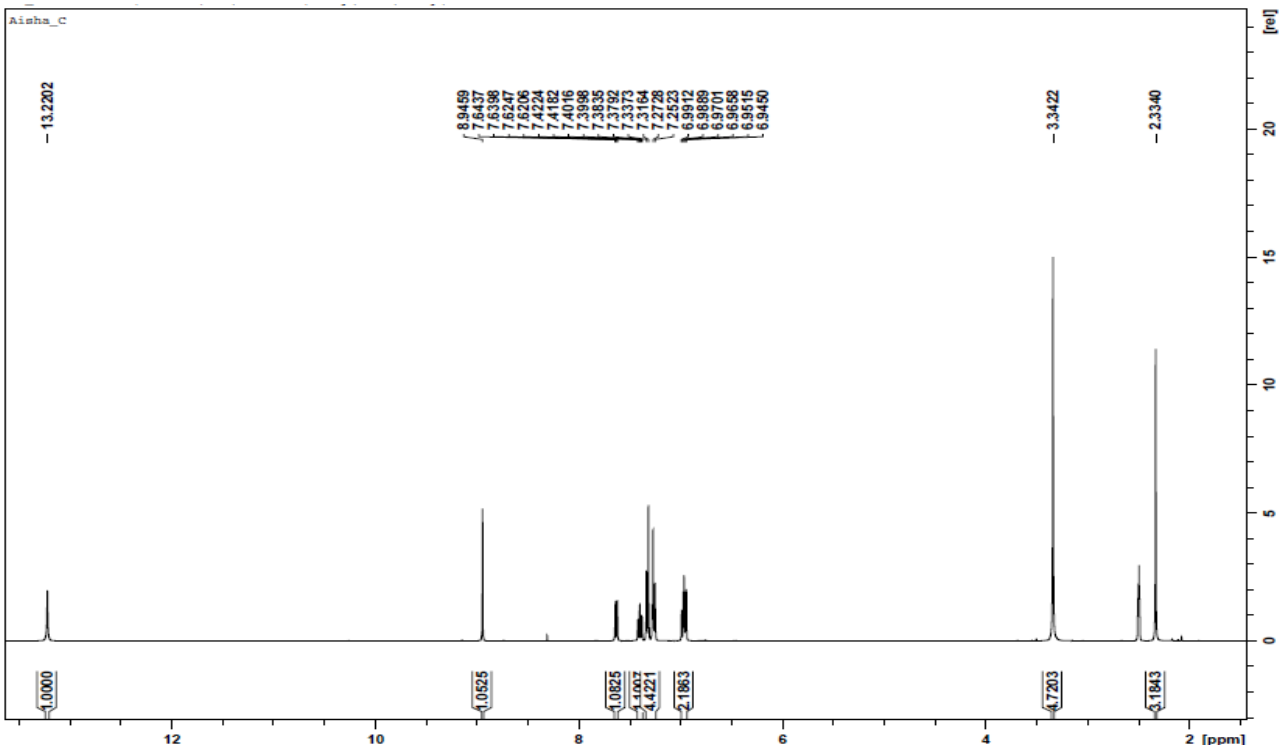
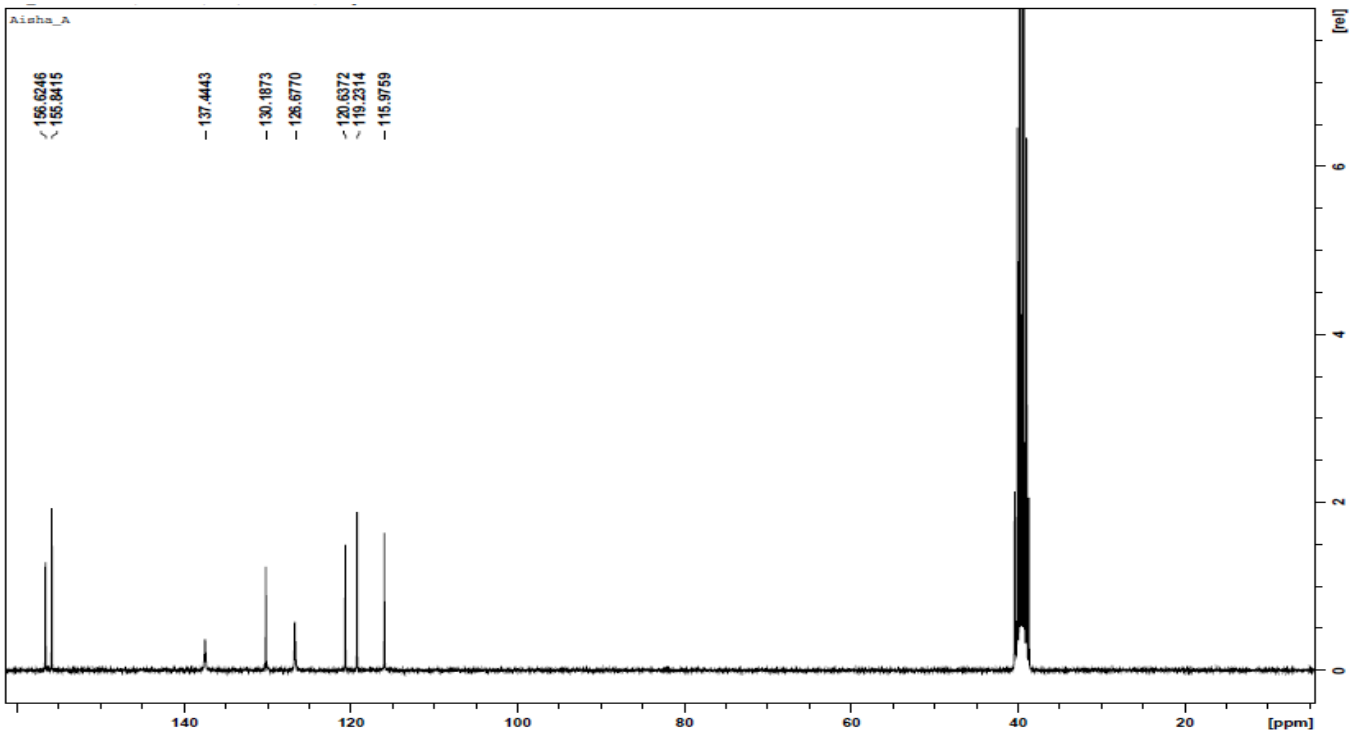


Figure S1: ^{1}H-NMR spectrum of SEMISCAD (I) and p-TOLUSCAD (II)

(I)



(II)

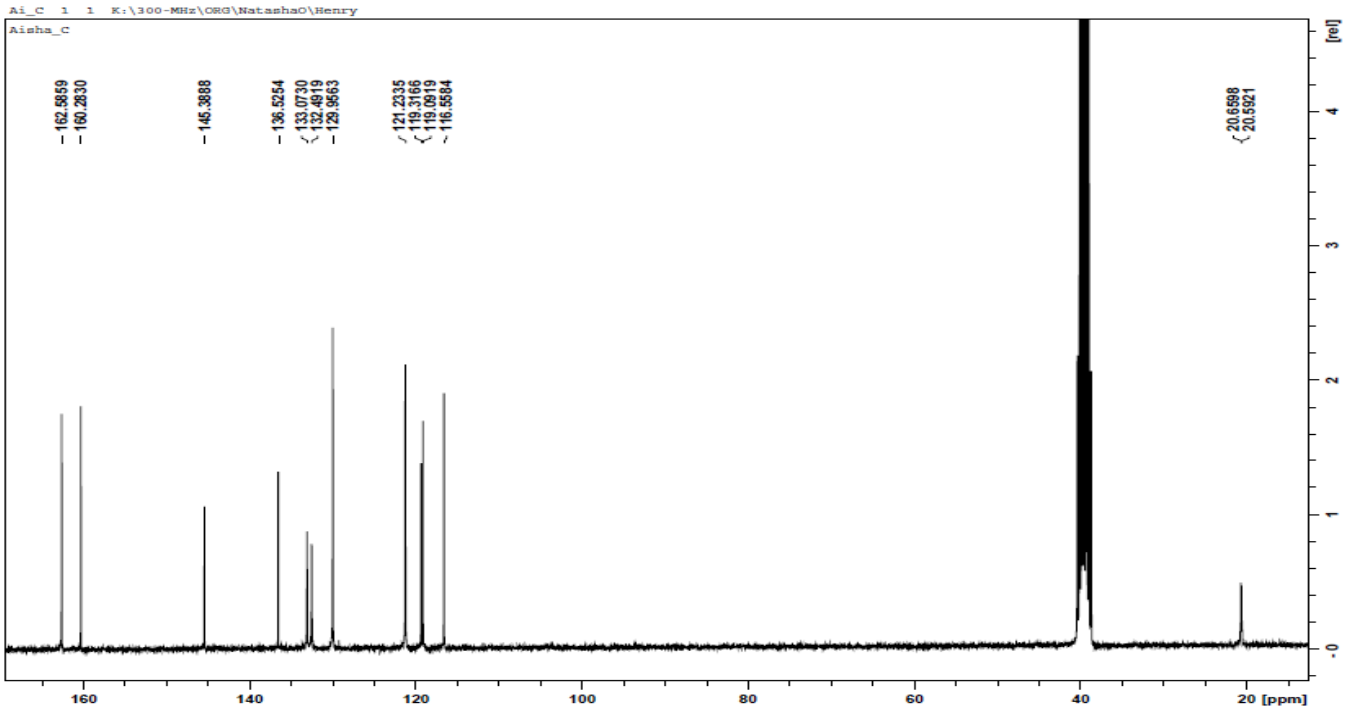
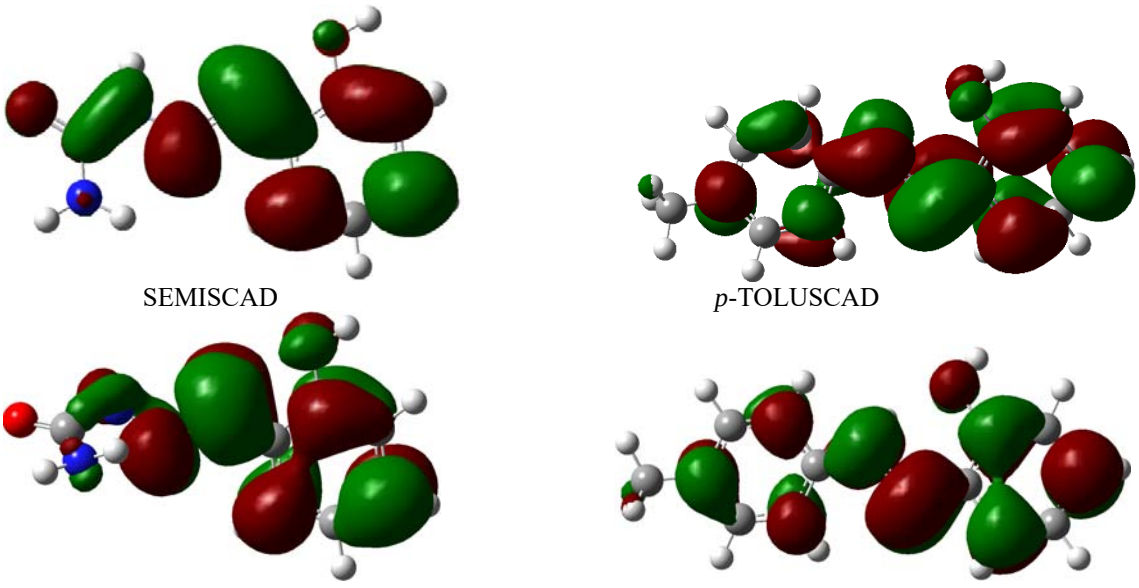


Figure S2: ^{13}C-NMR spectrum of SEMISCAD (I) and p-TOLUSCAD (II) showing assignment of chemical shift.



SEMISCAD *p*-TOLUSCAD

[SEMISCAD-H]$^+$ [*p*-TOLUSCAD-H]$^+$

Figure S3: LUMO electron density isosurfaces of neutral and protonated species of SEMISCAD and *p*-TOLUSCAD (in the gas phase).