Instruments used in analyses:

FT-IR spectra were recorded using a Shimadzu FT-IR spectrometer within the range 400–4000 cm^{-1}. Electronic absorption spectra in DMF were measured utilizing an automated UV/Vis–NIR 3101 PC Shimadzu spectrophotometer. Conductivity meter ORION model 150 of 0.6 cells constant: Molar conductance measurement of 10^{-3}M solutions of compound, DMF (dimethylformamide) was the solvent used. Automatic analyzer CHNS Vario EL III-Elementar, Germany: (C, H and N) elemental analyses. Varian NMR spectrometer (300 MHz): ^{1}H NMR spectra in deuterated dimethylsulfoxide d_6-DMSO were recorded. Cambridge, England, Sherwood Scientific: Molar magnetic susceptibility using the equation $\mu_{eff} = 2.828\ (X_M\ T)^{1/2}$ B.M. at room temperature, Mass-GC-2010 Shimadzu instrument. The thermal measurements were performed using a TGA-50H-Shimadzu thermal analyzer under a nitrogen atmosphere, heating from room temperature to 800^{o}C at a rate of 10^{o}C min^{-1}.

CT-DNA binding

Monitoring DNA gel electrophoresis-induced binding change under the influence of a steady rise in sample concentrations allowed for the determination of DNA binding with the tested sample. The concentration range was (5.00-25.00 µg/ml) in 20 mM of Tris HCl containing 50 mM NaCl at pH 7.3 with 25 µg/ml of CT-DNA and incubated for 2 hrs at 37°C. Agarose gel (1% w/v) was prepared in TBE buffer (1.00 mM EDTA, 45 mM of boric acid, 45 mM Tris, pH 7.30). The binding qualities of the DNA pattern will be impacted by the DNA movement and intensity during the gel electrophoresis procedure. After adding 6x gel loading dye to the reaction mixture to stop the reaction, it was electrophoresed at 60 V for 45 minutes. A UV-transilluminator was used to visualize the gel after it had been stained with ethidium bromide (EB) at 25°C for 5 minutes, and a mobile camera was used to take pictures of the gel.

Bovine serum albumin denaturation inhibition measurement

Screening for protein denaturation inhibitors is crucial in anti-inflammatory screening investigations. A protein denaturation test was performed as described by Gambhire et al [41] with slight modification. In a reaction volume of 5 ml, composed of 200 µl of 1.0 % of BSA (Bovine Serum Albumin) and PBS buffer (4.78 ml, pH 7.4), a sample concentration of 10 µg/ml was utilized. After the reaction solution was

incubated at 37°C for 15 min, the reaction was heated at 70°C for 5 min, the tube was left for cooling and the developed turbidity was measured spectrophotometrically at 660 nm. The control consisted of phosphate buffer solution and BSA without the tested sample. The % inhibition denaturation was calculated based on the following equation:

$$\% \text{ inhibition of denaturation} = \frac{1 - Absorbance\ of\ the\ tested\ sample}{Absorbance\ of\ the\ control} \times 100$$

Computational methods

All calculations were carried out using the DFT/B3LYP approach, as described in Gaussian 09 revision [33,34]. The standard basis sets for AA and VO(II) chelate are B3LYP/6-311G++ and LANL2DZ[35], respectively. The theoretical NMR calculation was performed for the AA ligand. Additionally, computational FT-IR analyses for the free ligand and VO(II) complex are calculated. The binding modes of the α-amylase enzyme and epidermal growth factor receptor with synthesized compounds were investigated with the help of molecular docking using the MOE program 2009. (1PIF and 1m17) PDB files were downloaded from the protein data bank for the structure of α-amylase and EGFR.

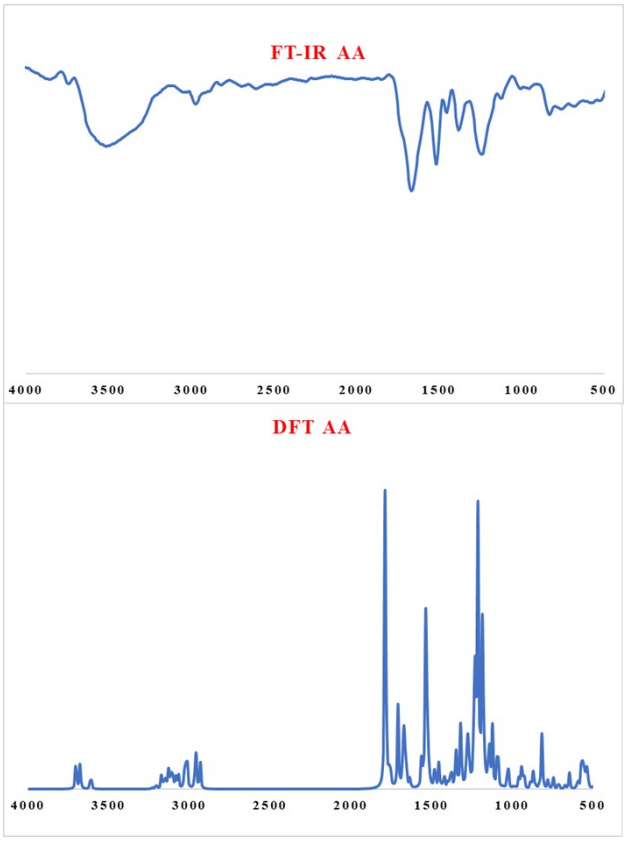


Figure S1a. The experiemental and calculated vibration pattern for the AA ligand, respectively.

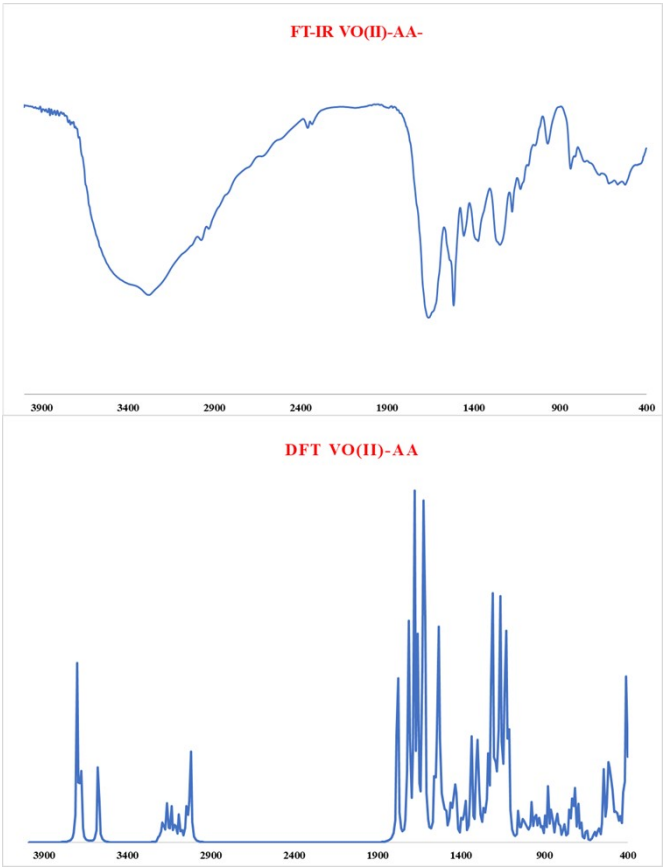


Figure S1b. The experimental and calculated vibration pattern for the $VO(AA)_2$ complex, respectively.

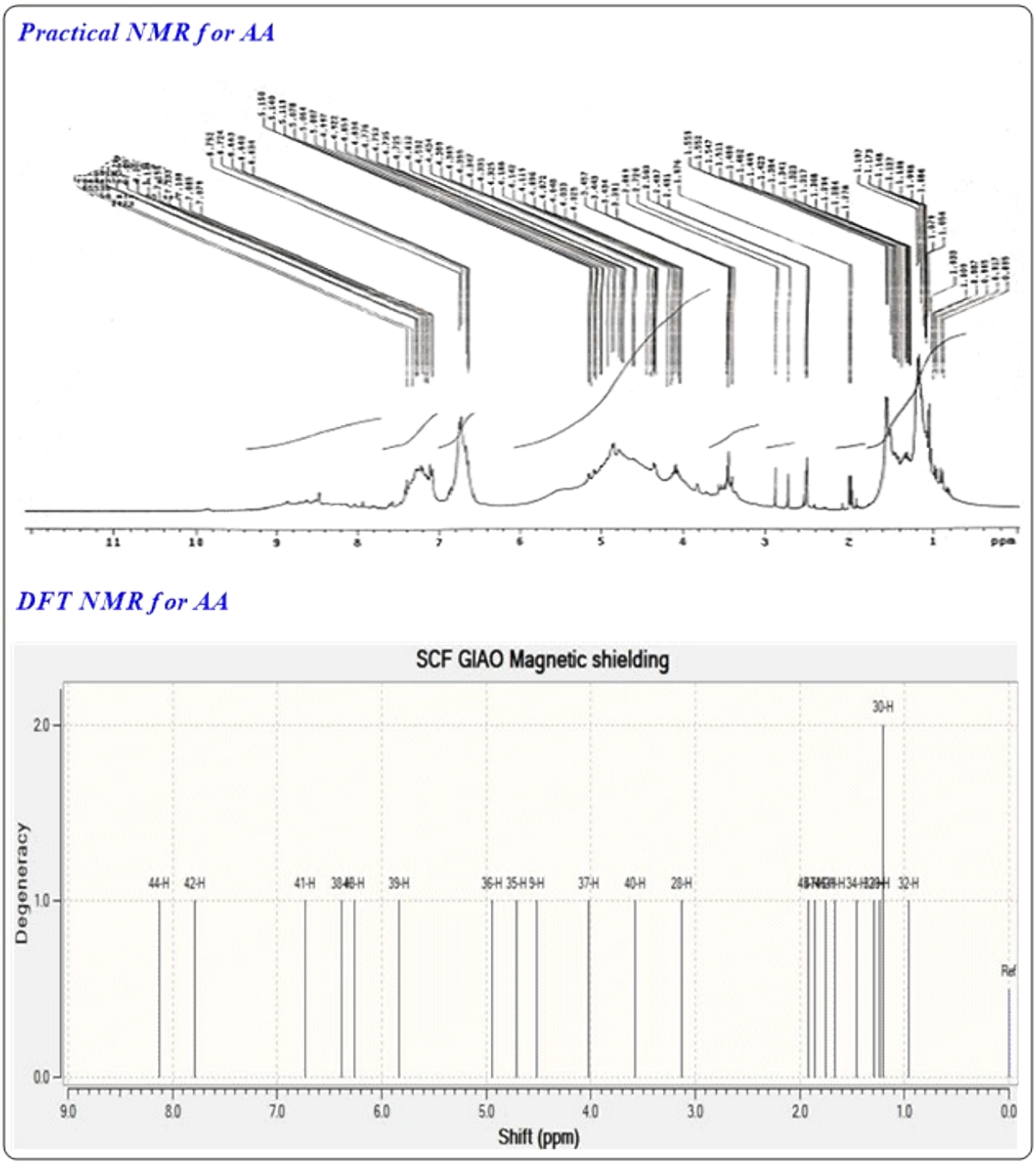
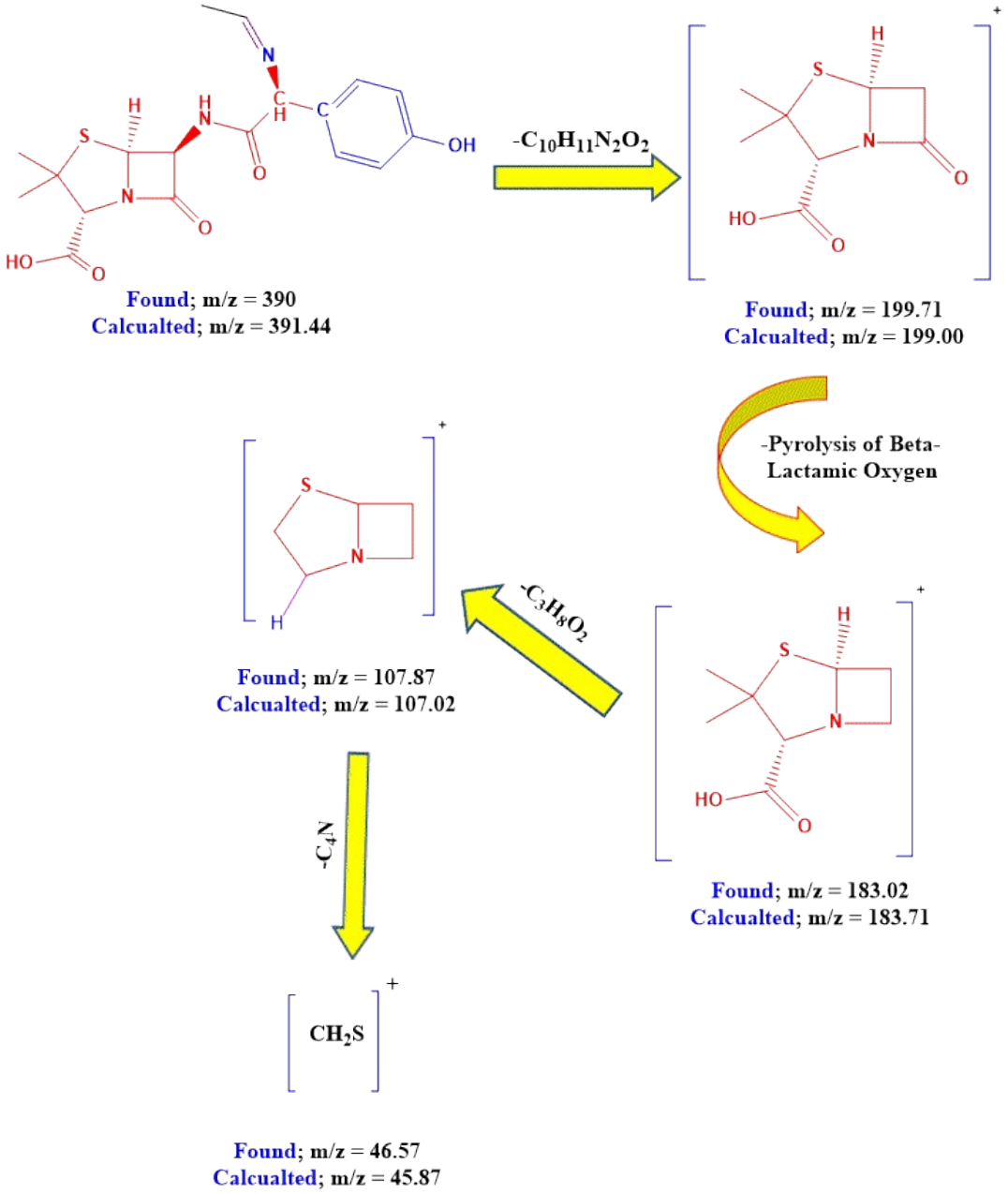
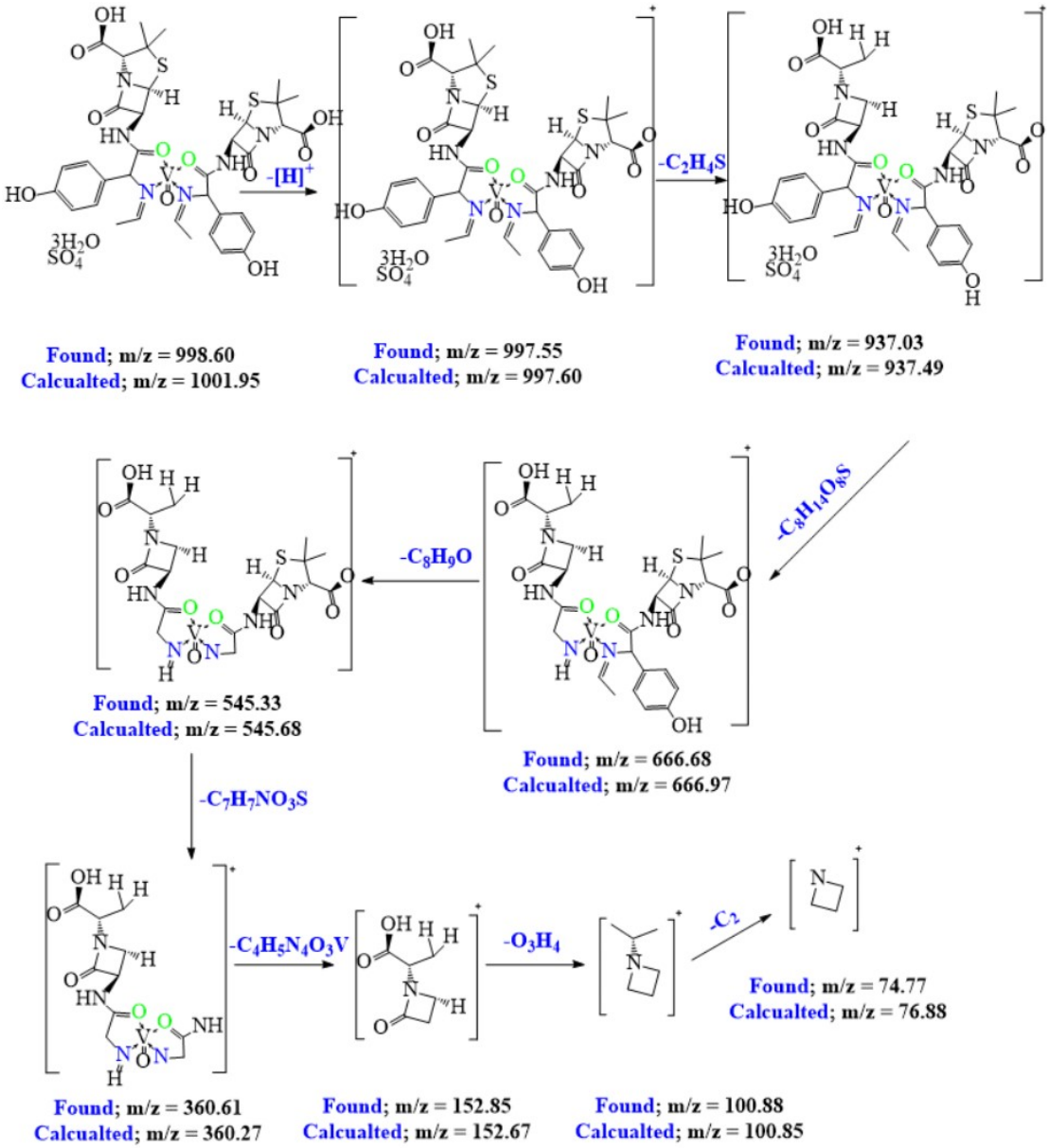


Figure S2. The experimental and calculated ^{1}H-NMR for the (AA) ligand, respectively.



Scheme S2. Fragmentation of AA ligand.



Scheme S3. Fragmentation of VO(II) chelate.

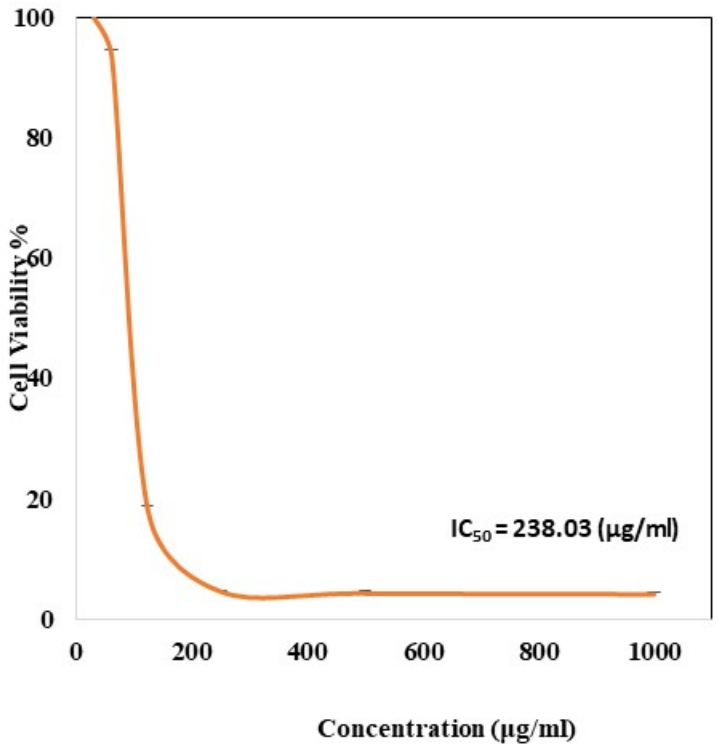


Figure S3. MTT assay of ($[VO(AA)_2]SO_4$) against normal cell line WI-38.