

Supplementary Data

This supplementary data is a part of a paper entitled “Synthesis, Thermal, DFT Calculations, HOMO-LUMO, MEP, and Molecular Docking Analysis of New Derivatives of Imidazolin-4-Ones”.

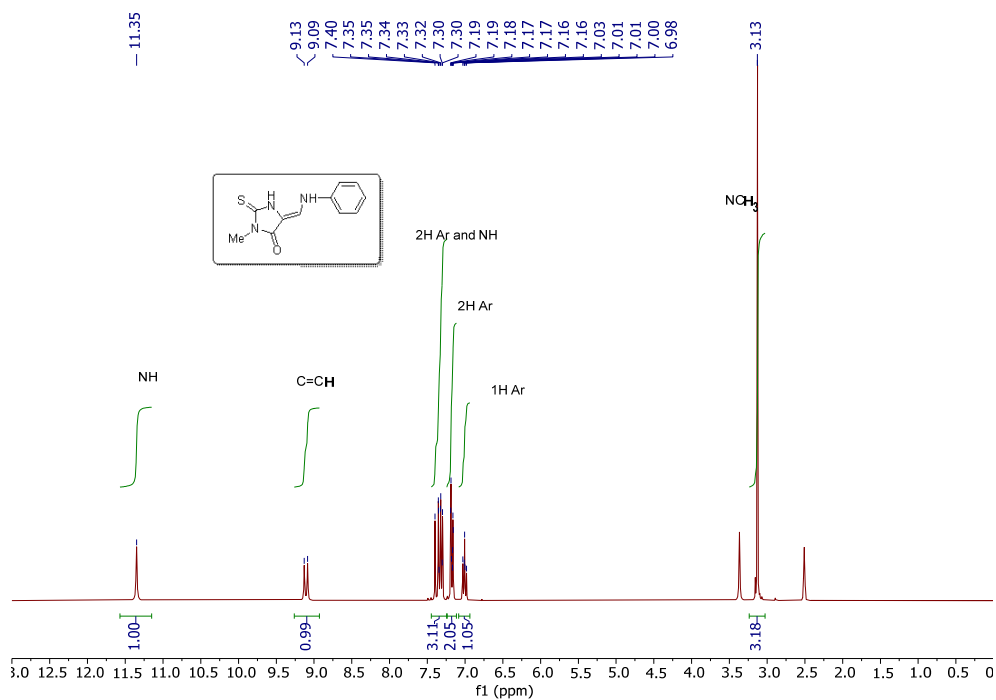


Fig S1. $^1\text{H-NMR}$ spectrum of 3-methyl-5-phenylaminomethylene-2-thioxoimidazolidin-4-one

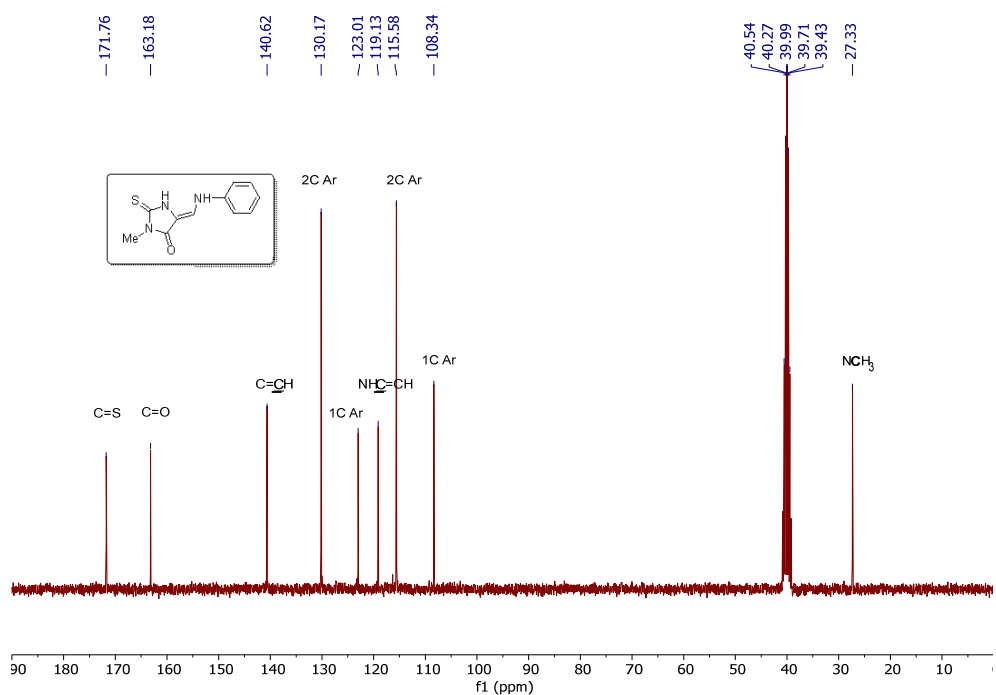
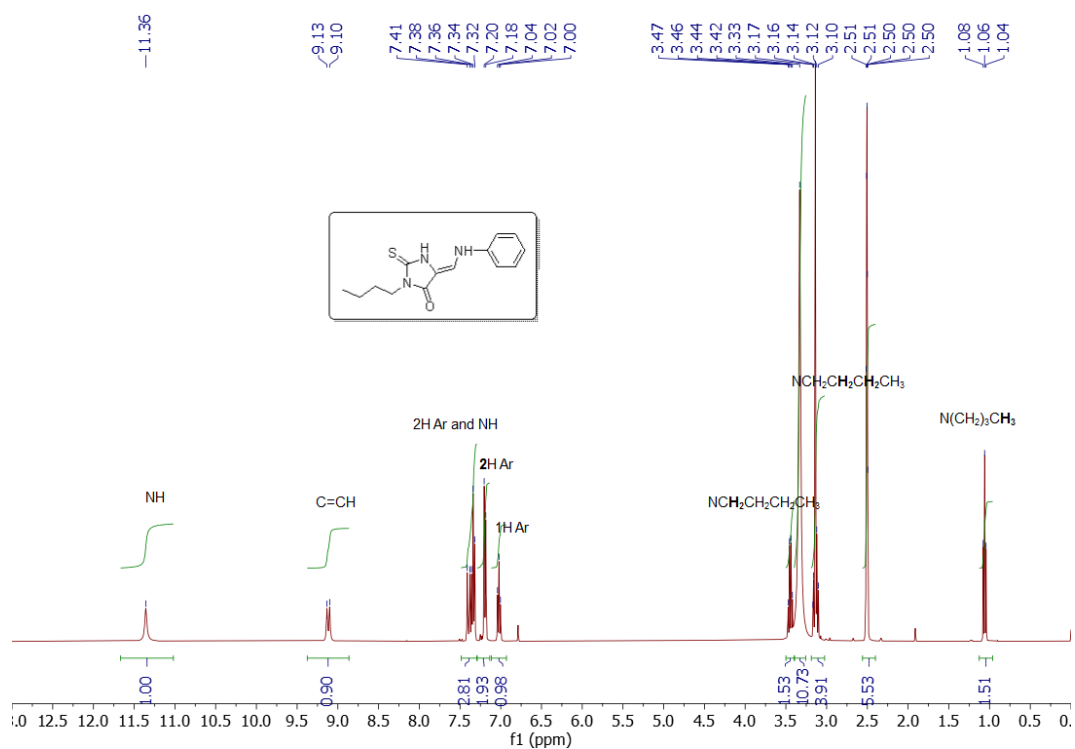
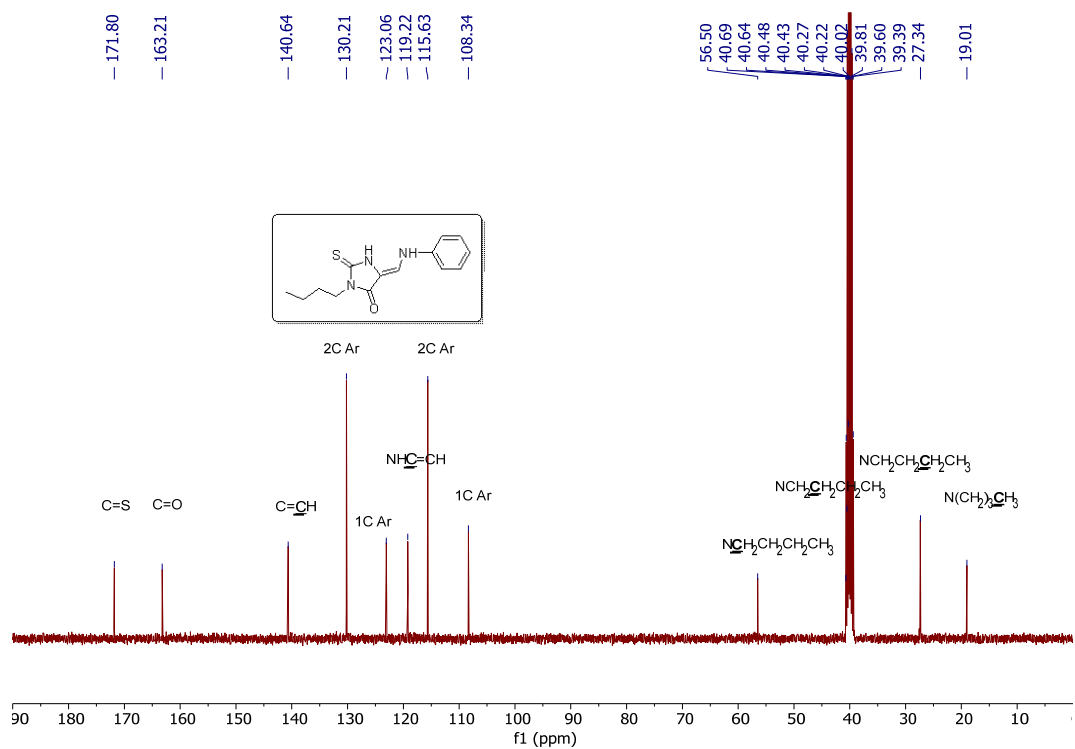


Fig S2. $^{13}\text{C-NMR}$ spectrum of 3-methyl-5-phenylaminomethylene-2-thioxoimidazolidin-4-one

Fig. S3. ^1H -NMR spectrum of 3-butyl-5-phenylaminomethylene-2-thioxoimidazolidin-4-oneFig S4. ^{13}C -NMR spectrum of 3-butyl-5-phenylaminomethylene-2-thioxoimidazolidin-4-one

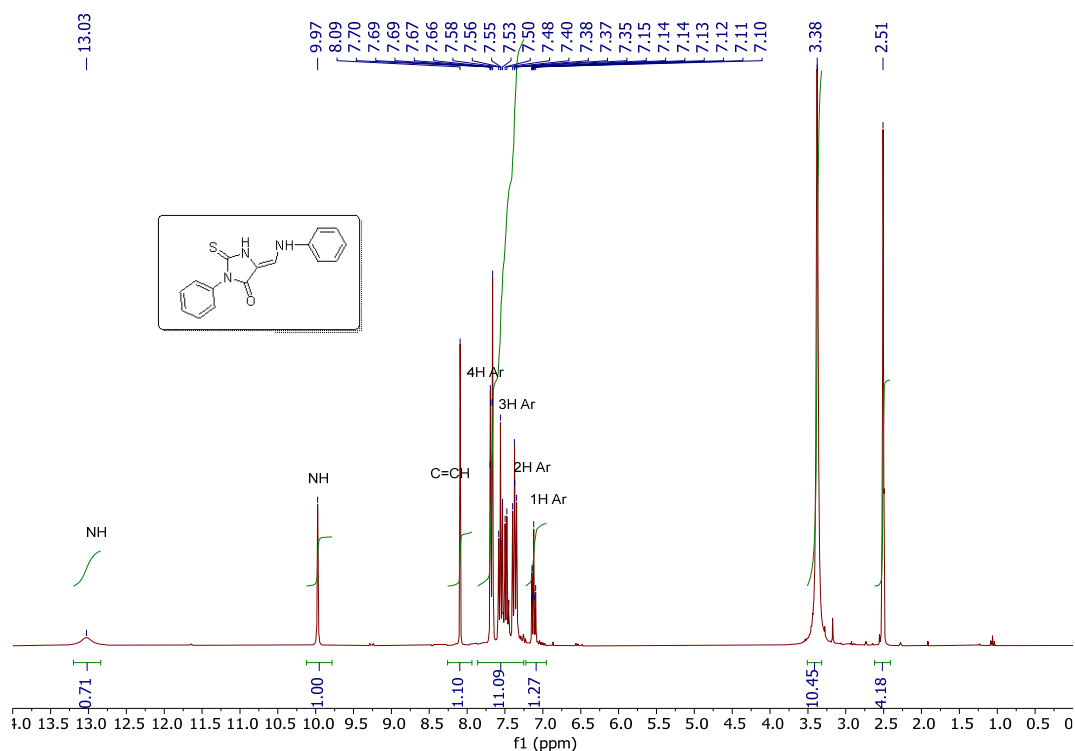


Fig S5. ^1H -NMR spectrum of 3-phenyl-5-phenylaminomethylene-2-thioxoimidazolidin-4-one

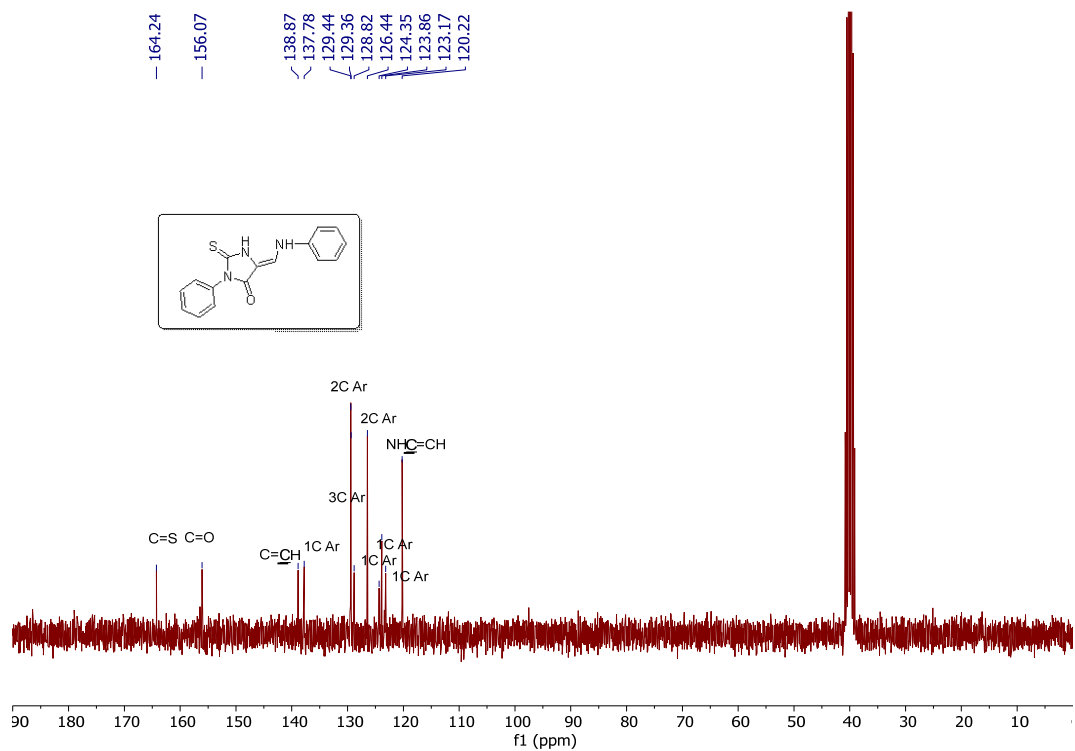


Fig S6. ^{13}C -NMR spectrum of 3-phenyl-5-phenylaminomethylene-2-thioxoimidazolidin-4-one

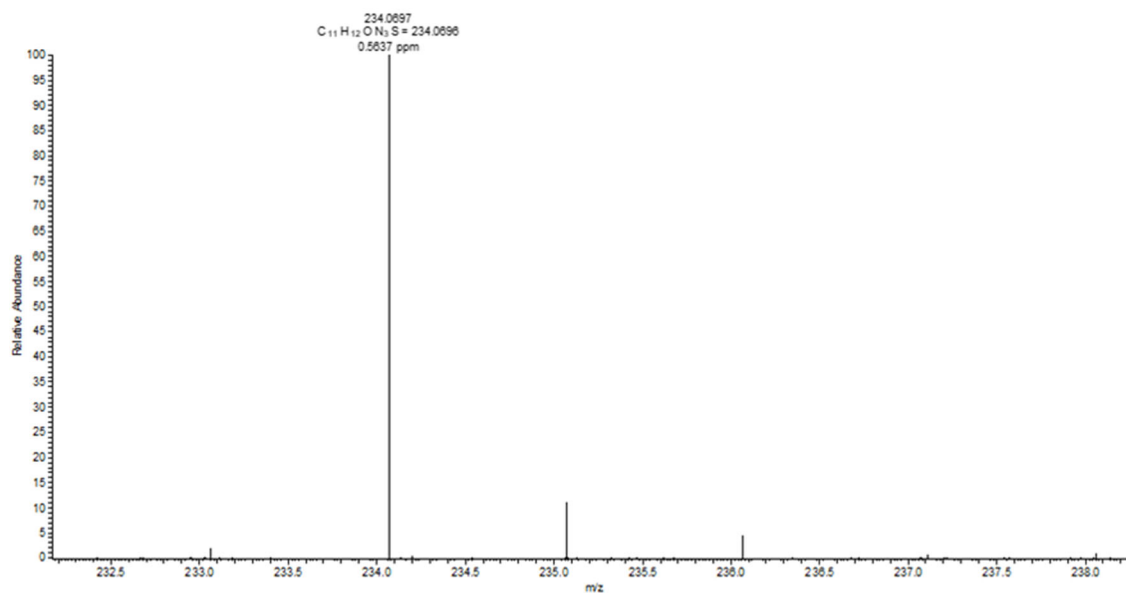


Fig S7. MS spectrum of 3-methyl-5-phenylaminomethylene-2-thioxoimidazolidin-4-one

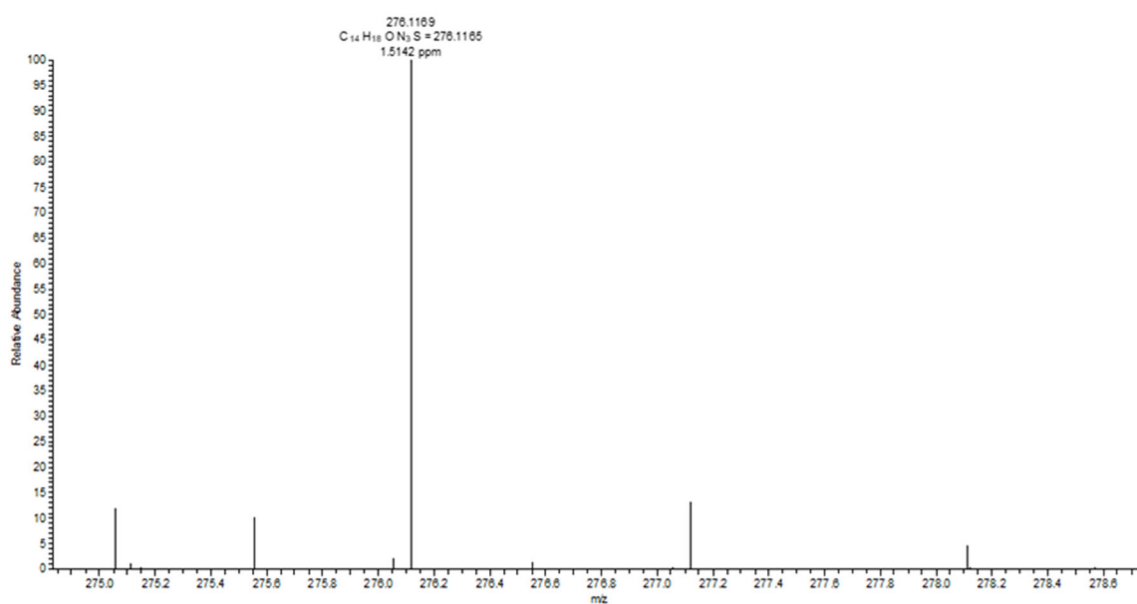


Fig S8. MS spectrum of 3-butyl-5-phenylaminomethylene-2-thioxoimidazolidin-4-one

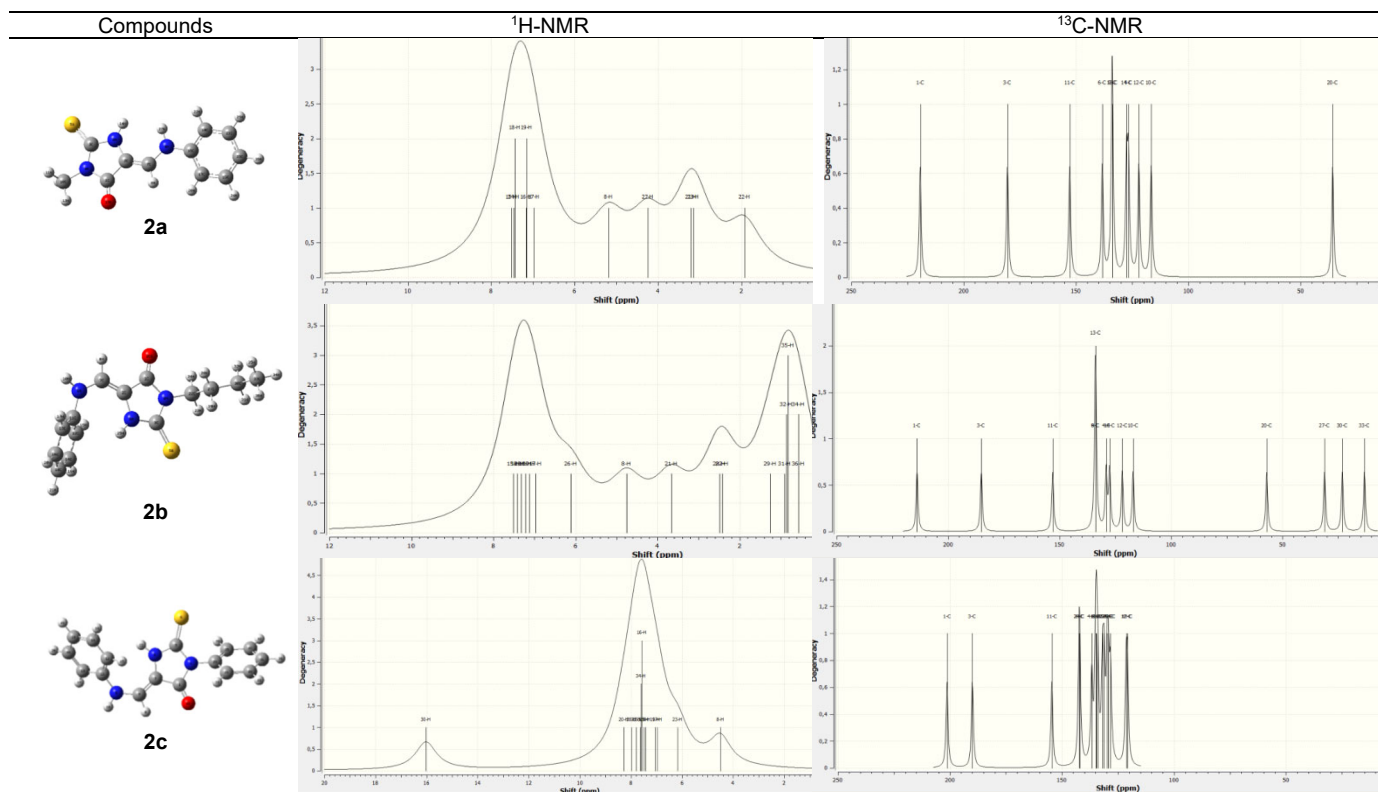


Fig S9. Theoretical NMR spectra of compounds 2a-c