Supplementary information for

Greener Synthesis, In-silico and theoretical analysis of hydrazides as potential antituberculosis agents (Part 1)

Experimental details:

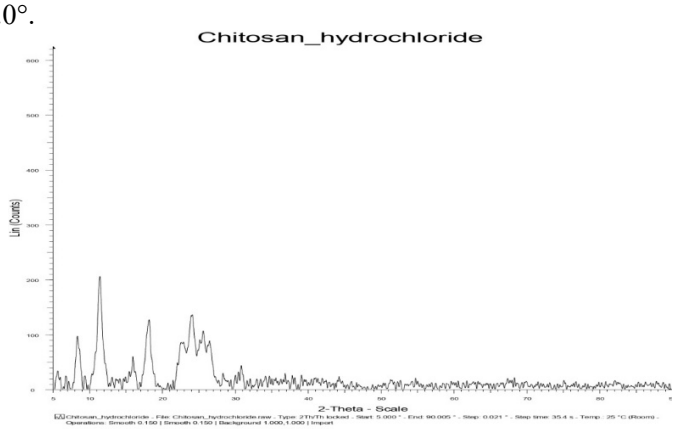
Materials and methods

All the aldehydes were purchased from Sigma-Aldrich. NMR spectra were recorded on a Bruker-400 MHz NMR spectrometer. Column chromatography was performed using silica gel (100-200 mesh) purchased from SRL, India and mixtures of hexane-ethyl acetate were used for elution. TLC was carried out using Merck Silica Gel 60/UV254 either by UV fluorescence or by iodine chamber.

1. **Characterization of Chitosan Catalyst**

XRD Analysis

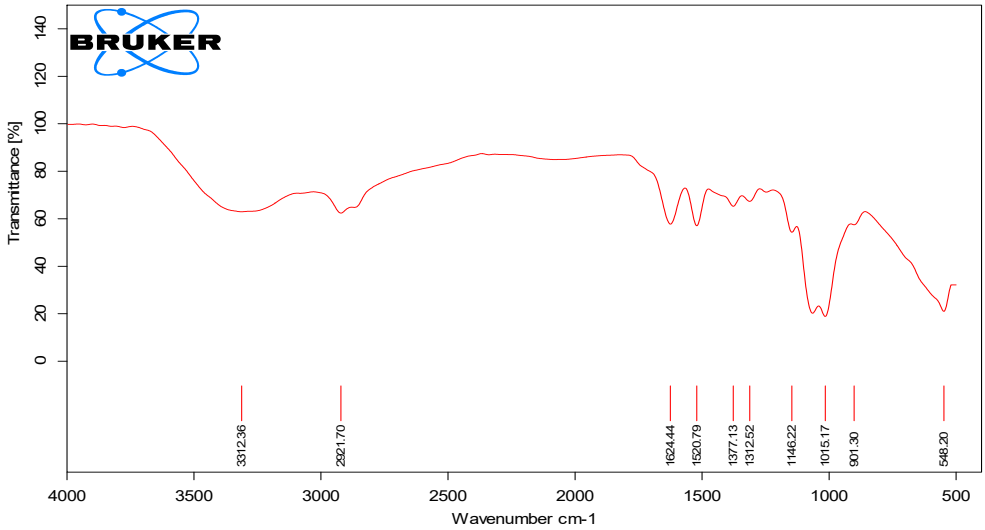
The XRD pattern of the as prepared chitosan hydrochloride (Figure-6) appeared four peak at 2θ value 8.5, 12.6, 15.8, 18.5 and 24.0°.



SI. Figure 1 - XRD Analysis of Chitosan Hydrochloride

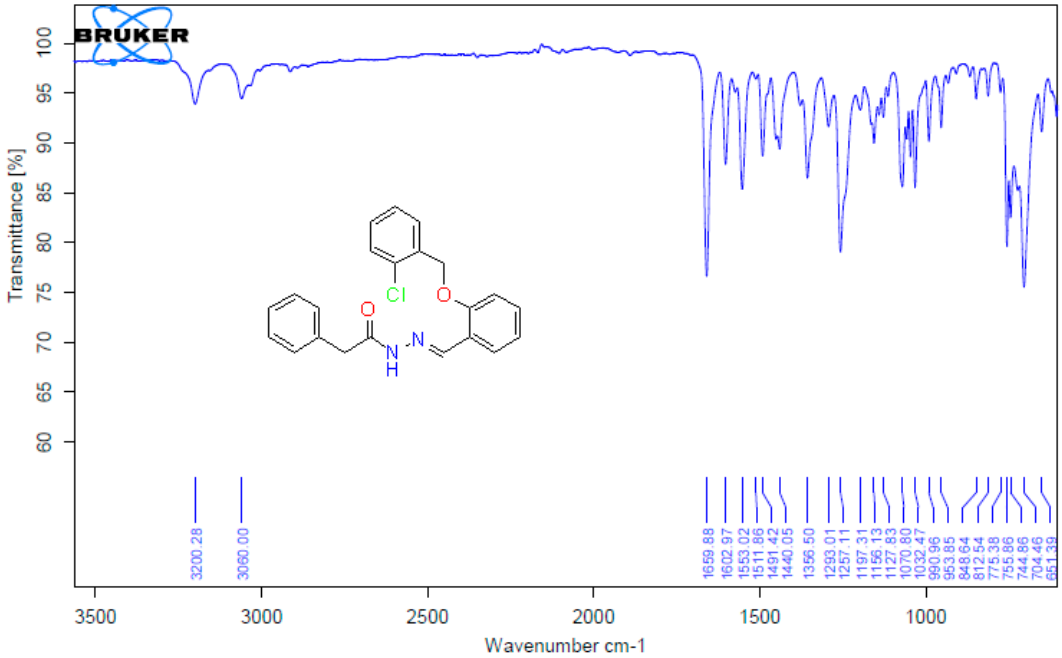
FTIR Analysis

The FT-IR spectra of chitosan hydrochloride are shown in (SI Figure -2). The following peaks were observed in the FT-IR spectrum of chitosan hydrochloride. The peak at 3312 cm^{-1} indicates the broad vibration of O−H band. The peaks appeared at 2921, 1624, 1520, confirmed the presence of C-H stretching, C=O group in amide respectively. Peaks appeared at 1377 and 1312 cm^{-1} indicating CH_2 bending and peaks appeared at 1146, 1050, 901 indicating C−O stretching, respectively.

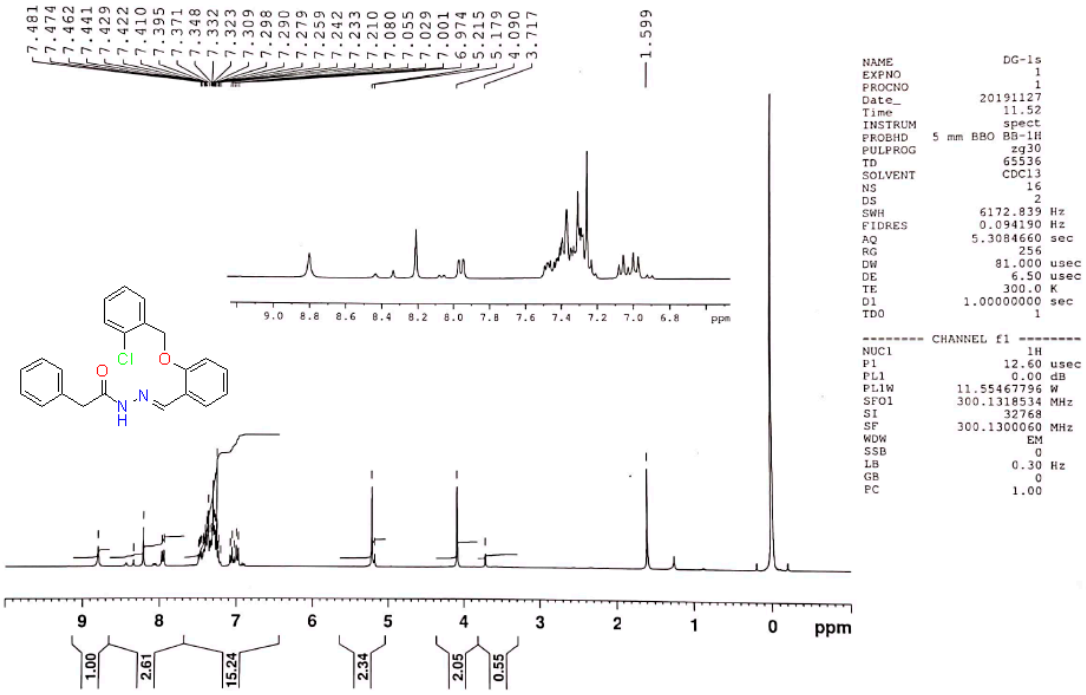


SI. Figure 2 - FTIR Analysis of Chitosan Hydrochloride.

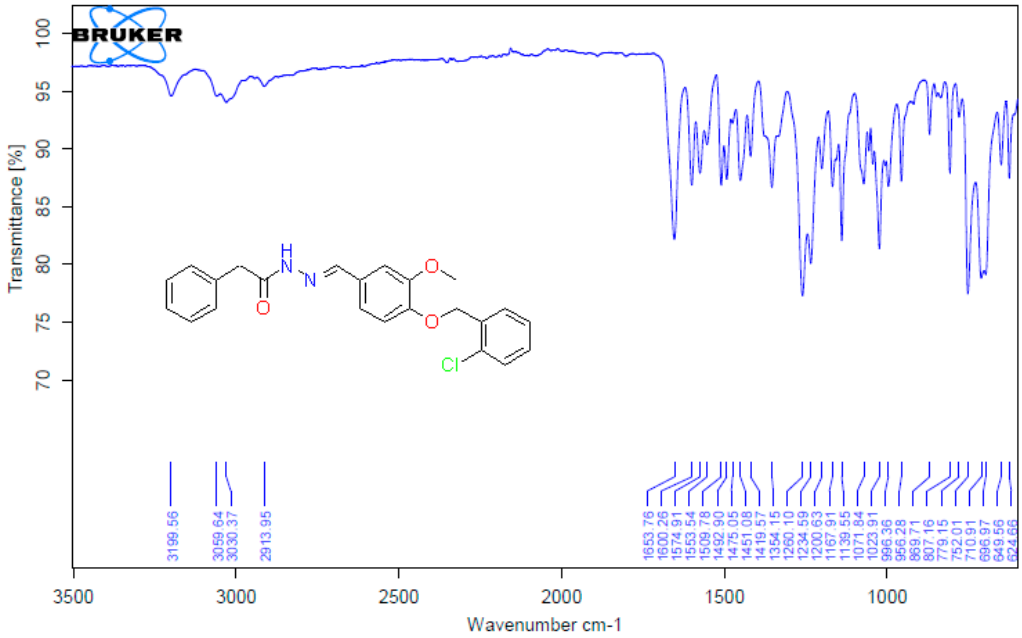
FT-IR spectra of (E)-N'-(2-((2-chlorobenzyl)oxy)benzylidene)-2-phenylacetohydrazide (3a):



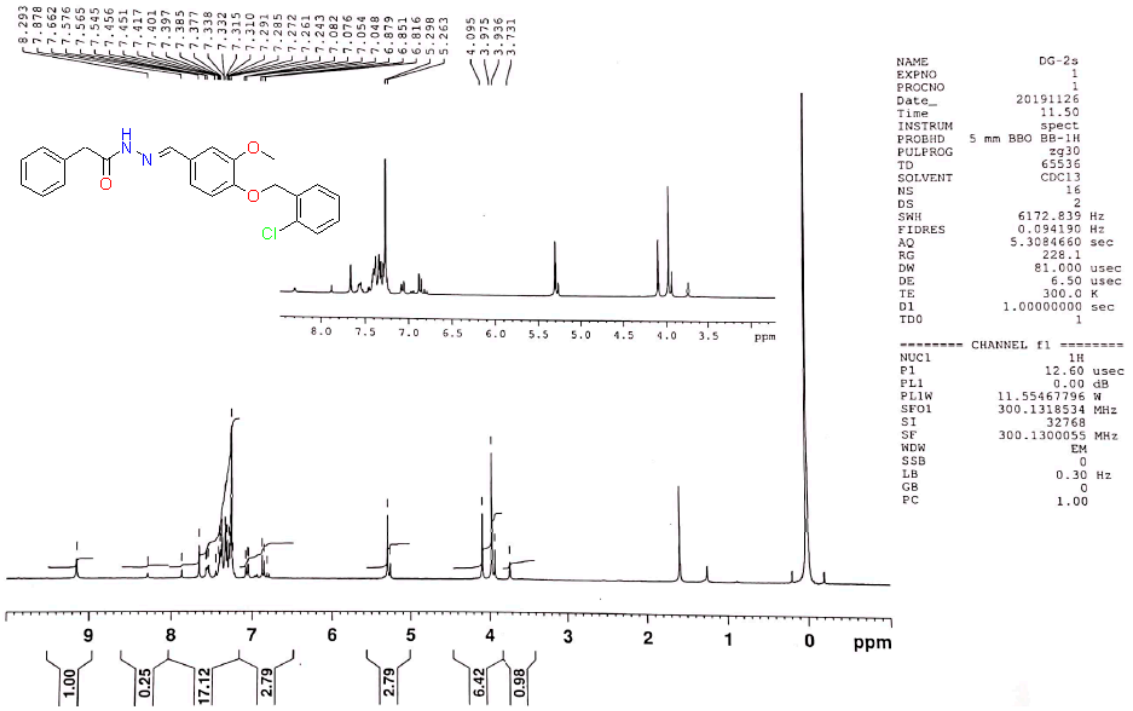
^{1}H-NMR spectra of (E)-N'-(2-((2-chlorobenzyl)oxy)benzylidene)-2-phenylacetohydrazide (3a):



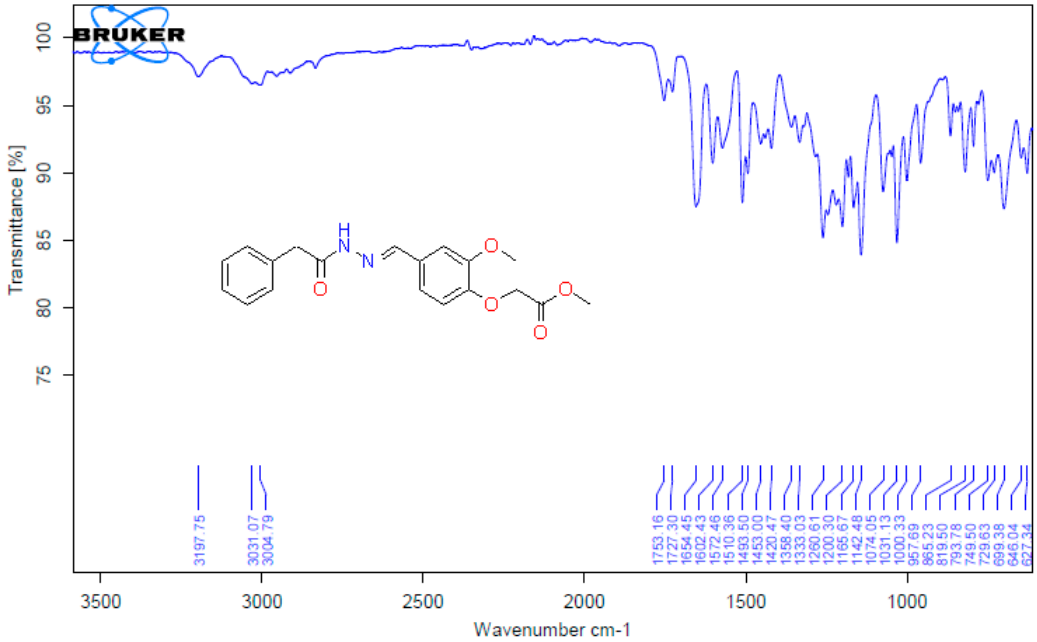
FT-IR spectra of (E)-N'-(4-((2-chlorobenzyl)oxy)-3-methoxybenzylidene)-2-phenylacetohydrazide (3b)



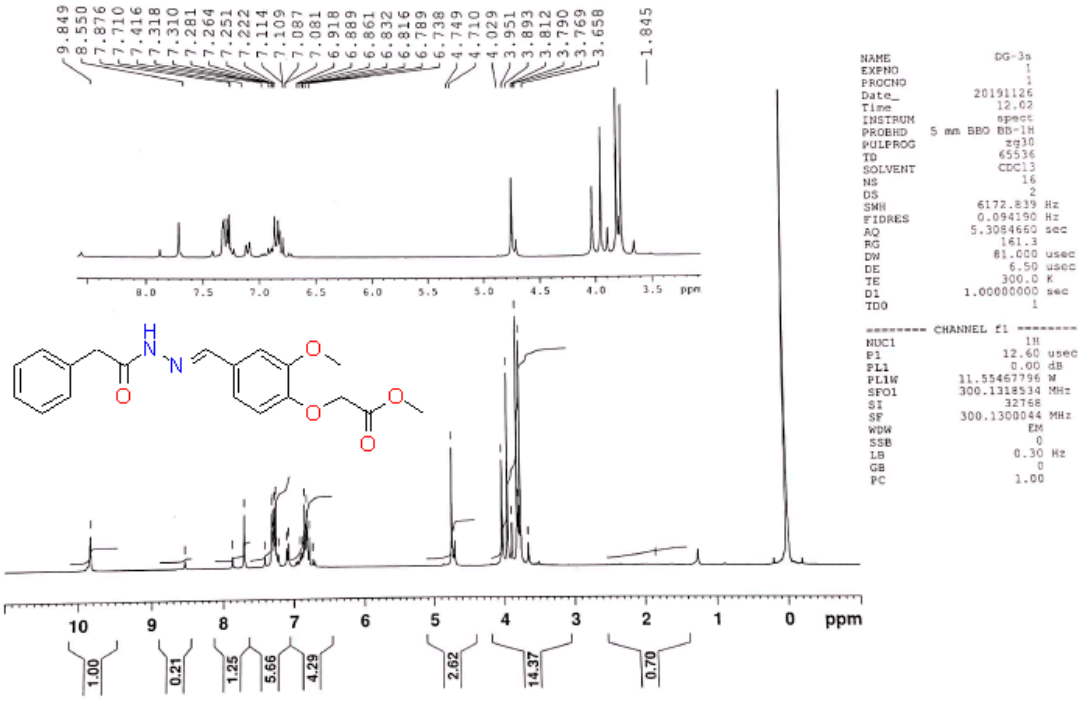
^{1}H-NMR spectra of (E)-N'-(4-((2-chlorobenzyl)oxy)-3-methoxybenzylidene)-2-phenylacetohydrazide (3b):



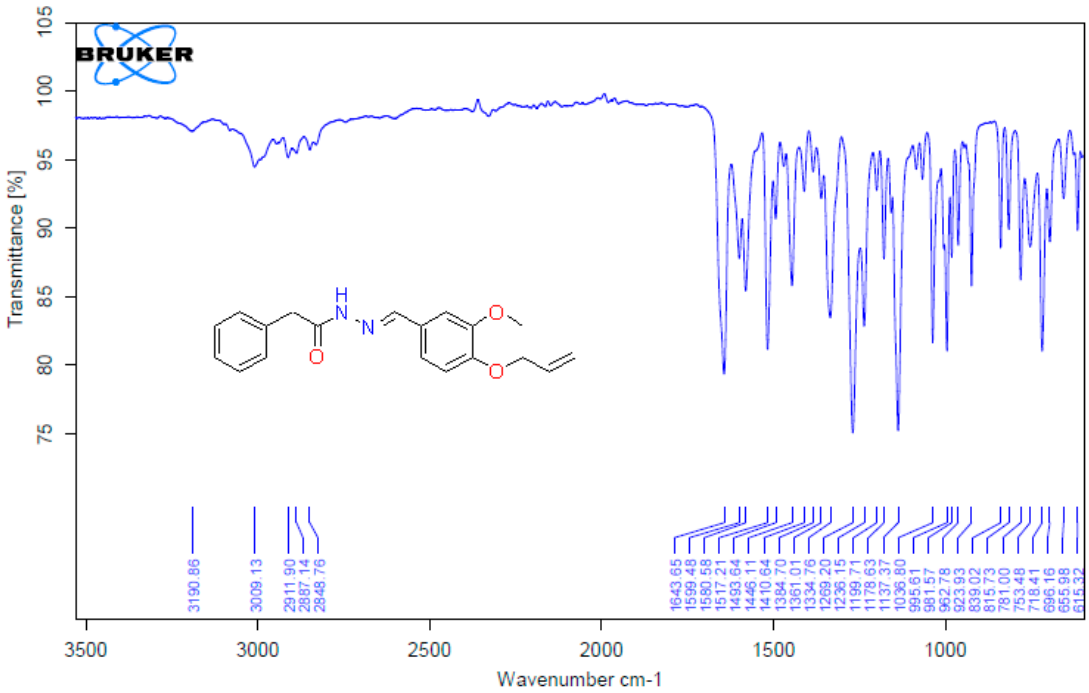
FT-IR spectra of methyl (E)-2-(2-methoxy-4-((2-(2-phenylacetyl)hydrazono)methyl)phenoxy)acetate (3c)



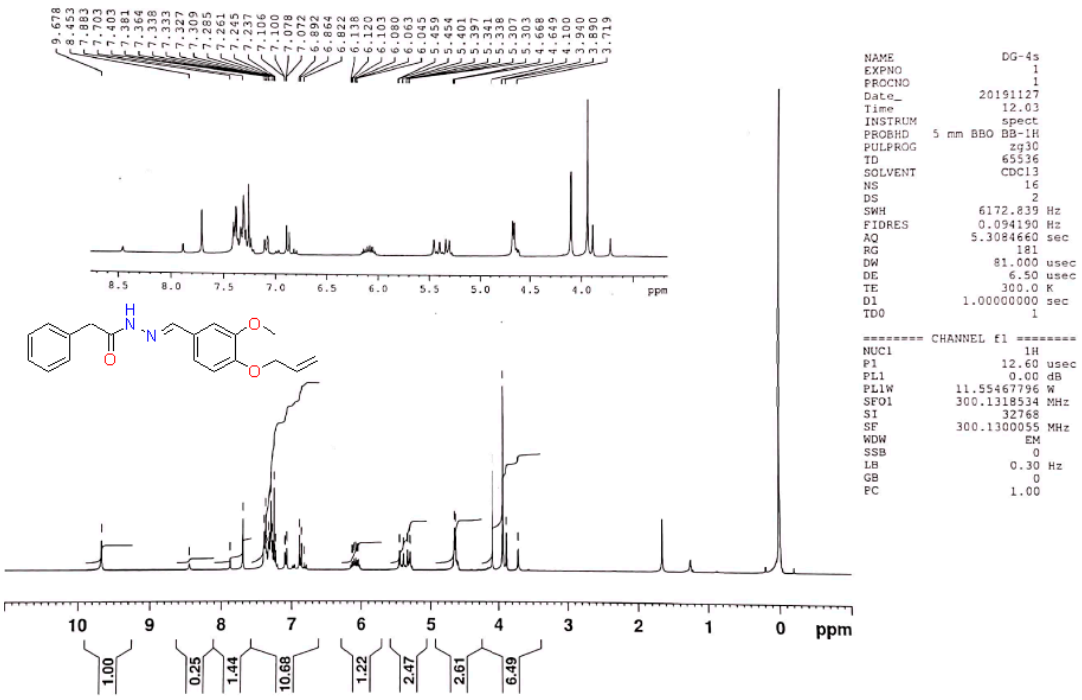
^{1}H-NMR spectra of methyl (E)-2-(2-methoxy-4-((2-(2-phenylacetyl)hydrazono)methyl)phenoxy)acetate (3c):



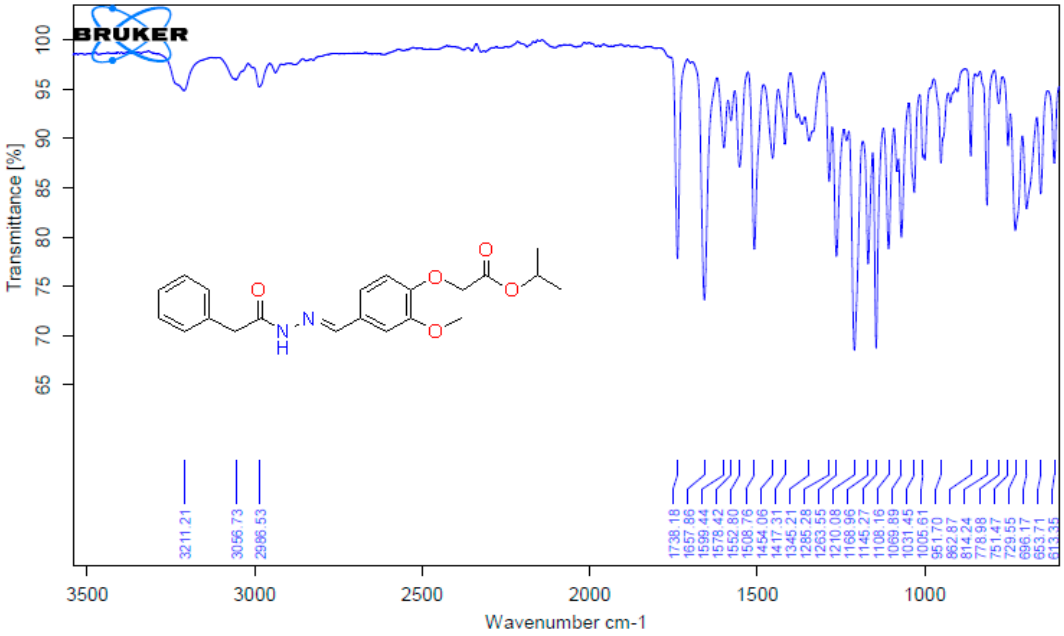
FT-IR spectra of (E)-N'-(4-(allyloxy)-3-methoxybenzylidene)-2-phenylacetohydrazide (3d):



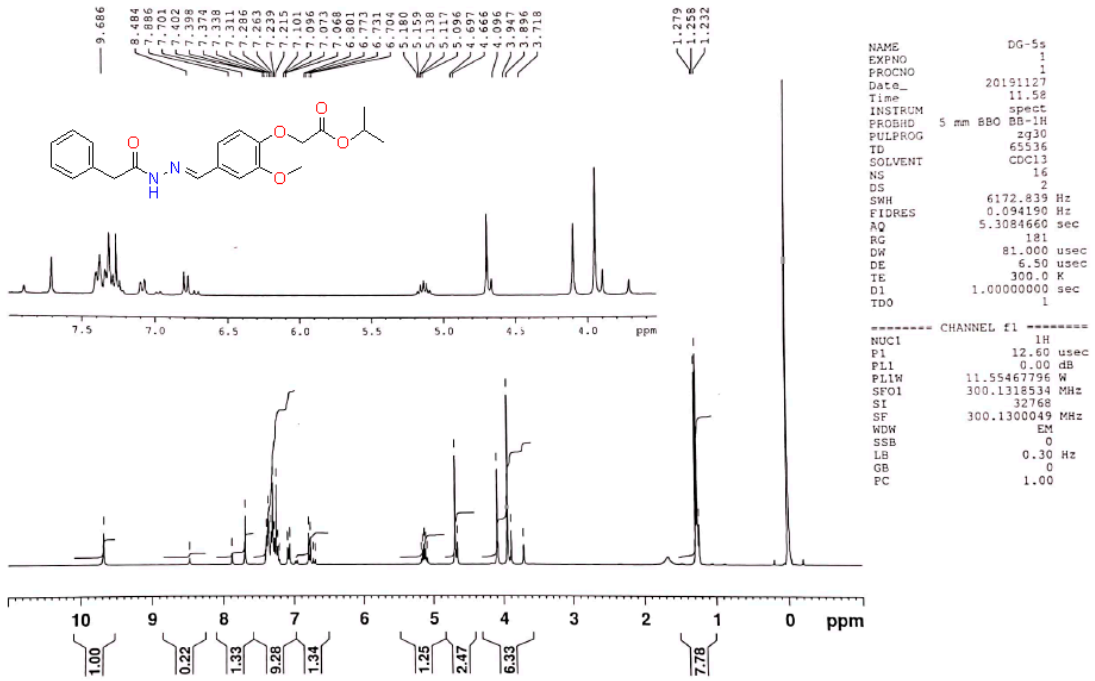
^{1}H-NMR spectra of (E)-N'-(4-(allyloxy)-3-methoxybenzylidene)-2-phenylacetohydrazide (3d):



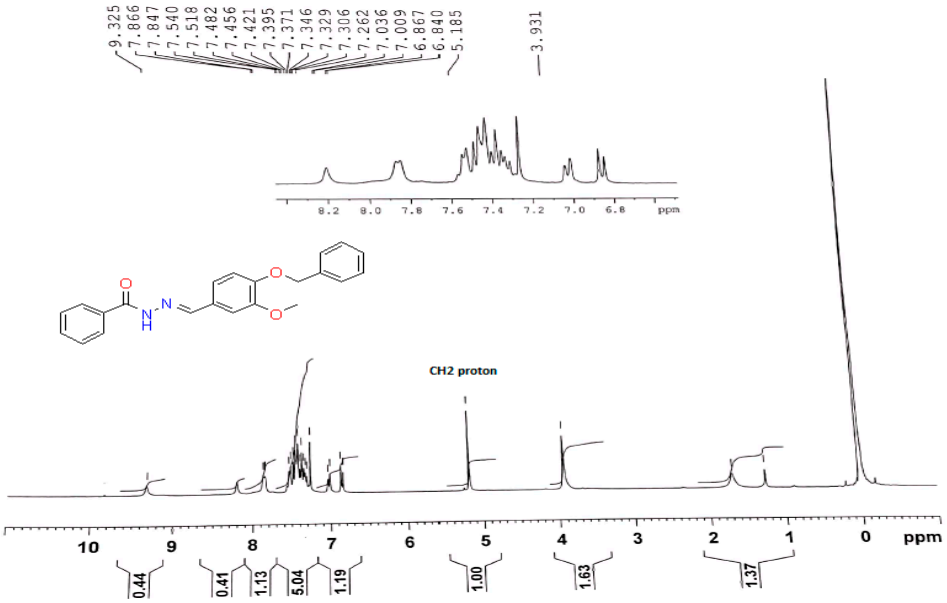
FT-IR spectra of isopropyl (E)-2-(2-methoxy-4-((2-(2-phenylacetyl)hydrazono)methyl)phenoxy)acetate (3e):



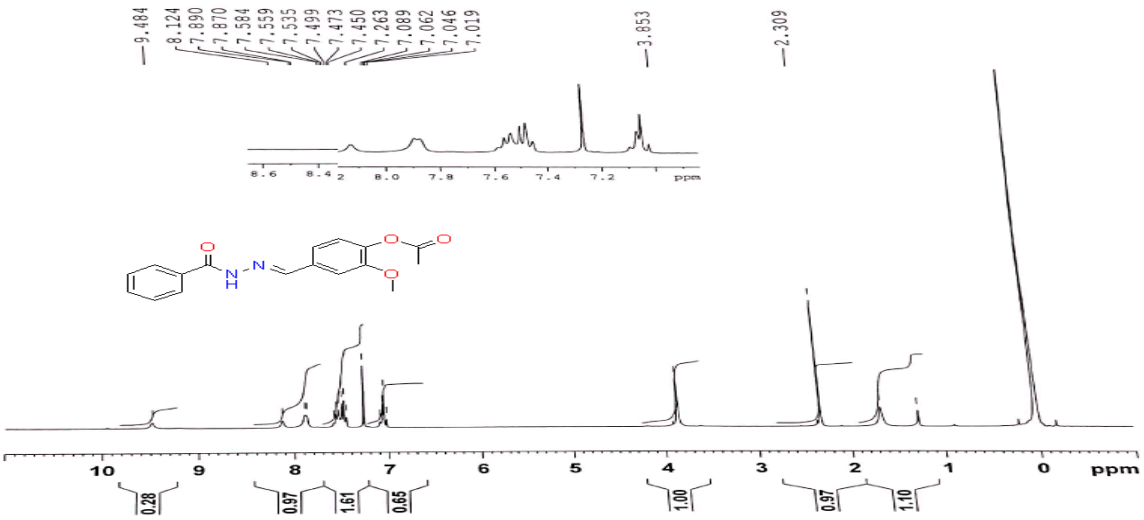
^{1}H-NMR spectra of isopropyl (E)-2-(2-methoxy-4-((2-(2-phenylacetyl)hydrazono)methyl)phenoxy)acetate (3e):



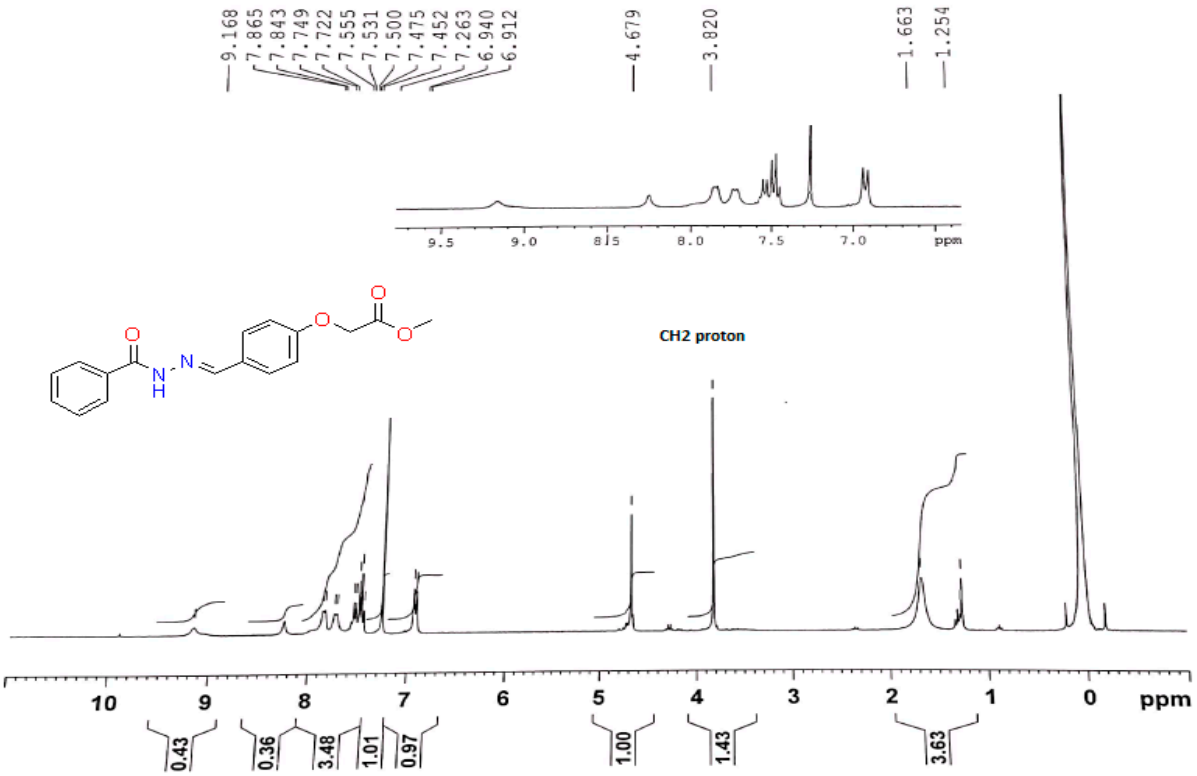
NMR spectra of (E)-N'-(4-(benzyloxy)-3-methoxybenzylidene)benzohydrazide (3f):



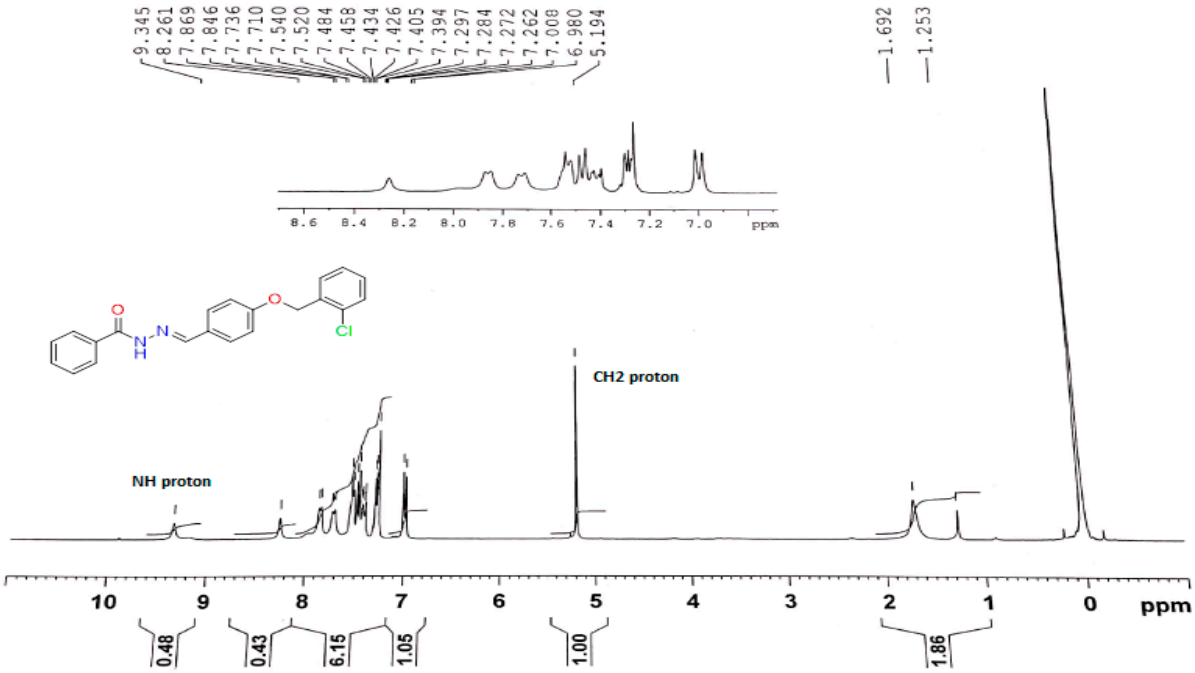
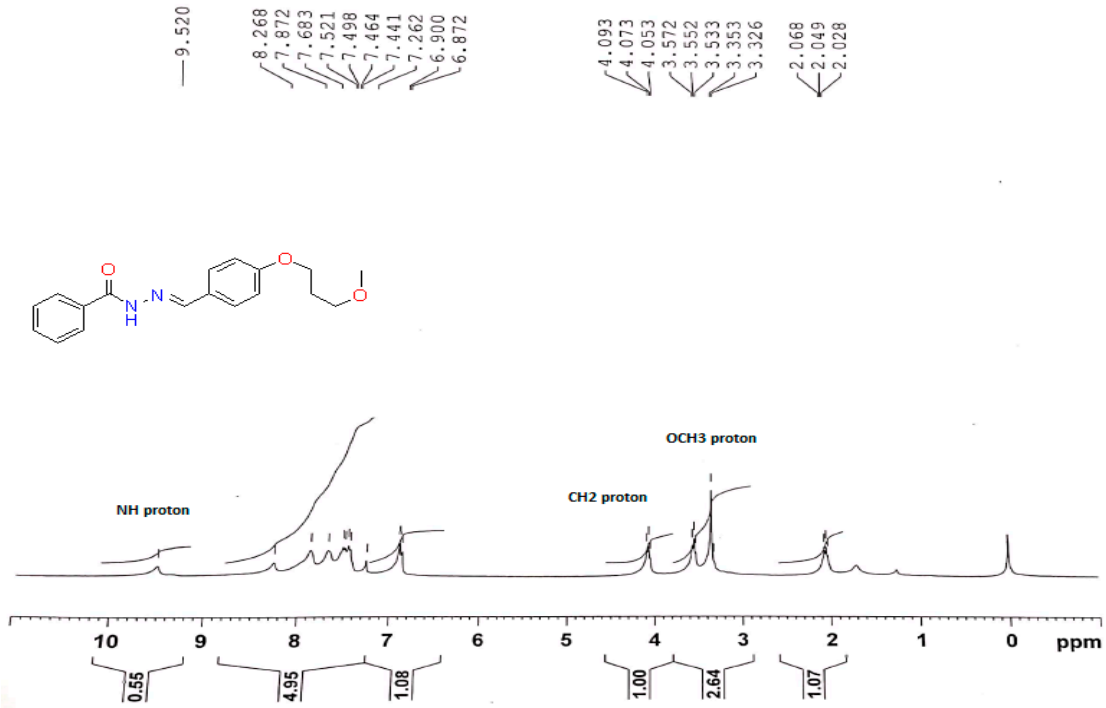
NMR spectra of (E)-4-((2-benzoylhydrazono)methyl)-2-methoxyphenyl acetate (3g):



NMR spectra of methyl (E)-2-(4-((2-benzoylhydrazono)methyl)phenoxy)acetate (3h):



NMR spectra of (E)-N'-(4-((2-chlorobenzyl)oxy)benzylidene)benzohydrazide (3i):



NMR spectra of (E)-N'-(4-(3-methoxypropoxy)benzylidene)benzohydrazide (3j):