

Title: Phenylisoxazole - 3/5 – carbaldehyde isonicotinohydrazide derivatives : Synthesis Characterization, and antituberculous activity

Autors: Fernando Carrasco, Wilfredo Hernández, Oscar Chupayo, Patricia Sheen, Mirko Zimic, Jorge Coronel, Celedonio M. Álvarez, Sergio Ferrero, Sandra Oramas-Royo, Evgenia Spodine, Jesus M. Rodilla, Juan Z. Dávalos.

Description of Supporting Information:

- **Table S1.** Computational results, at B3LYP/6-311++G(d,p) for **1** to **8** synthesized compounds. Relative enthalpies (ΔH) of stable conformers and their equilibrium molar fractions (populations).
- **Figure 1.** Linear Correlation of vibrational frequencies (given as wave numbers σ , in cm^{-1}) between experimental IR data and the corresponding to B3LYP/6-311++G(d,p) theoretical values for **1** to **8** synthesized compounds.
- **Compound 1**
 - ^1H NMR spectra
 - ^{13}C NMR spectra
 - Two-dimensional NMR spectroscopy (^1H - ^1H DQF COSY)
 - Two-dimensional NMR spectroscopy (^1H - ^1H NOESY)
 - Two-dimensional NMR spectroscopy (^1H - ^{13}C HSQC)
 - Mass spectra
 - Infrared spectra
- **Compound 2**
 - ^1H NMR spectra
 - ^{13}C NMR spectra
 - Two-dimensional NMR spectroscopy (^1H - ^1H DQF COSY)
 - Two-dimensional NMR spectroscopy (^1H - ^{13}C HMBC)
 - Two-dimensional NMR spectroscopy (^1H - ^{13}C HSQC)
 - Mass spectra
 - Infrared spectra

- **Compound 3**
 - ^1H NMR spectra
 - ^{13}C NMR spectra
 - Mass spectra
 - Infrared spectra
- **Compound 4**
 - ^1H NMR spectra
 - ^{13}C NMR spectra
 - Mass spectra
 - Infrared spectra
- **Compound 5**
 - ^1H NMR spectra
 - Mass spectra
 - Infrared spectra
- **Compound 6**
 - ^1H NMR spectra
 - ^{13}C NMR spectra / DEPT 45, DEPT 90 spectra
 - Two-dimensional NMR spectroscopy (^1H - ^1H COSY)
 - Two-dimensional NMR spectroscopy (^1H - ^{13}C HMBC)
 - Two-dimensional NMR spectroscopy (^1H - ^{13}C HSQC)
 - Infrared spectra
- **Compound 7**
 - ^1H NMR spectra
 - ^{13}C NMR spectra
 - Two-dimensional NMR spectroscopy (^1H - ^1H DQF COSY)
 - Two-dimensional NMR spectroscopy (^1H - ^{13}C HMBC)
 - Two-dimensional NMR spectroscopy (^1H - ^{13}C HSQC)
 - Infrared spectra

- **Compound 8**
 - ^1H NMR spectra
 - ^{13}C NMR spectra
 - Mass spectra
 - Infrared spectra