

Supplementary Material

Fluorinated pyrazolinic thiosemicarbazones: selective synthesis and computational analysis

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1. Infrared Spectroscopy data

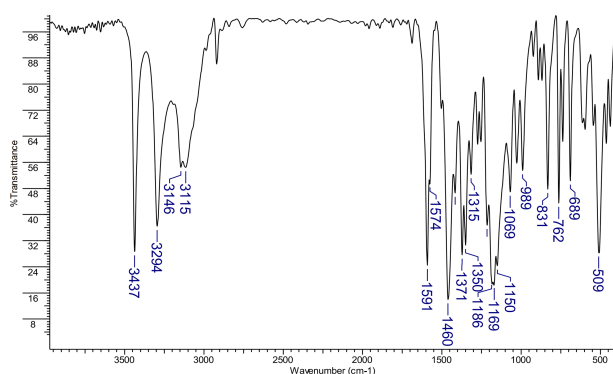


Figure S1. Infrared spectrum of thiosemicarbazone **1**.

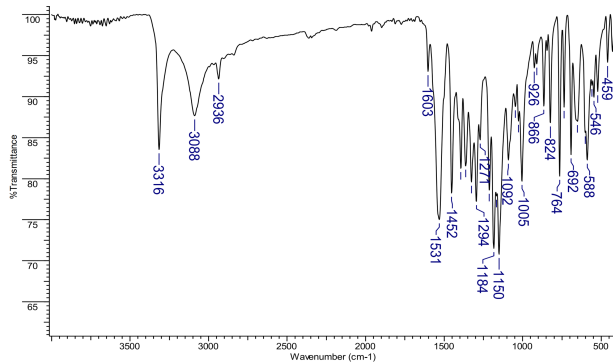


Figure S2. Infrared spectrum of thiosemicarbazone **2**.

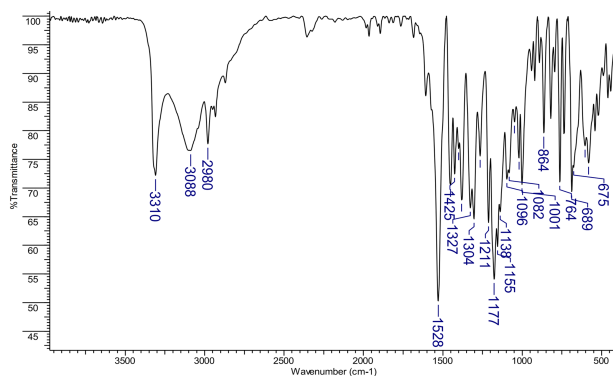


Figure S3. Infrared spectrum of thiosemicarbazone **3**.

2. NMR data

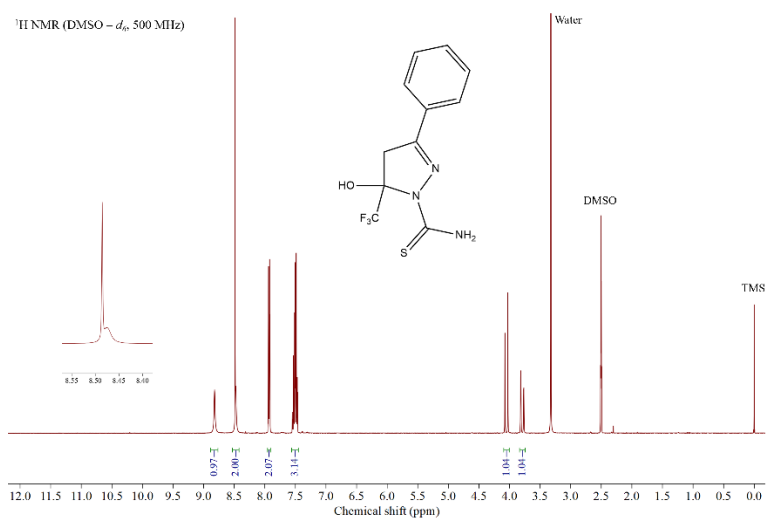


Figure S4. ^1H NMR spectrum of thiosemicarbazone **1**, in $\text{DMSO}-d_6$ solution.

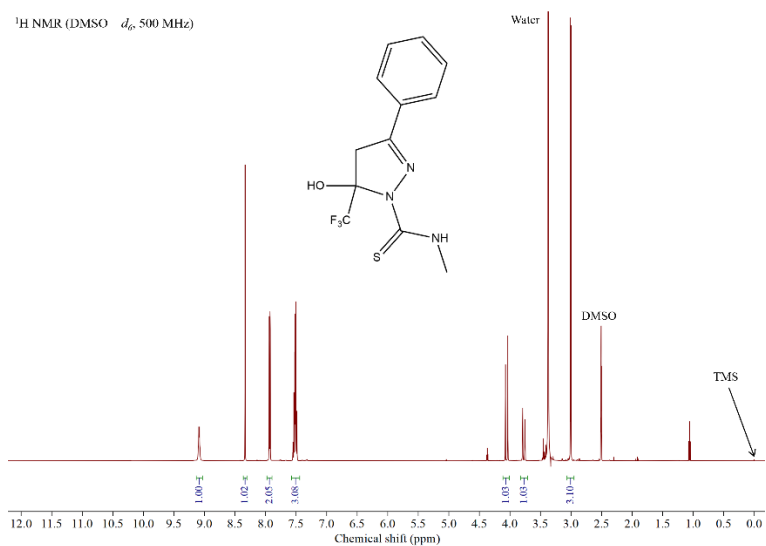


Figure S5. ^1H NMR spectrum of thiosemicarbazone **2**, in DMSO - d_6 solution.

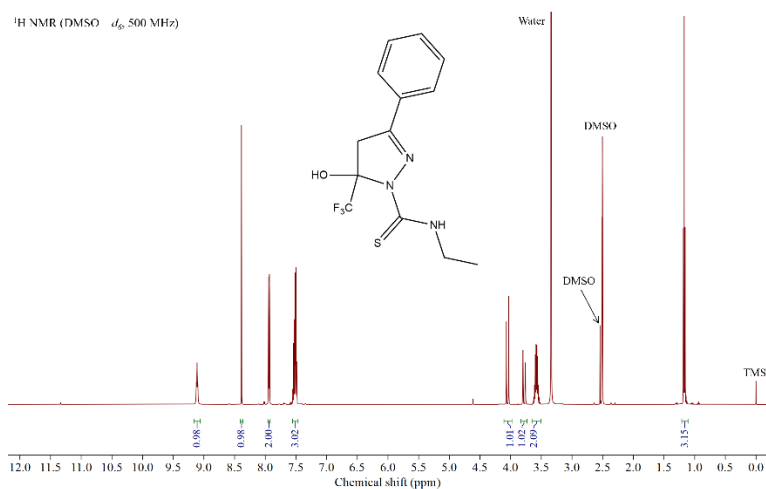


Figure S6. ^1H NMR spectrum of thiosemicarbazone **3**, in DMSO - d_6 solution.

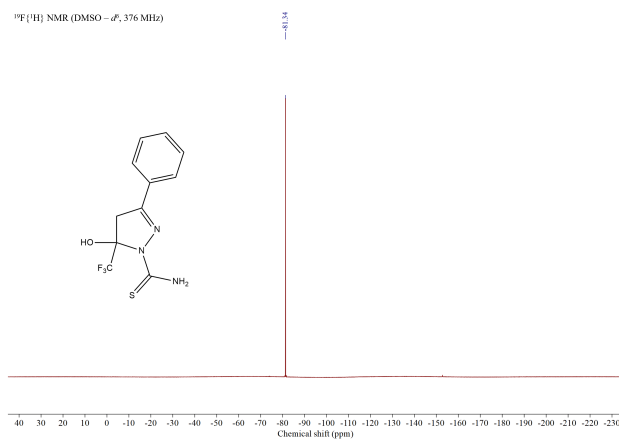


Figure S7. ¹⁹F{¹H} NMR spectrum of thiosemicarbazone **1**, in DMSO – *d*⁶ solution.

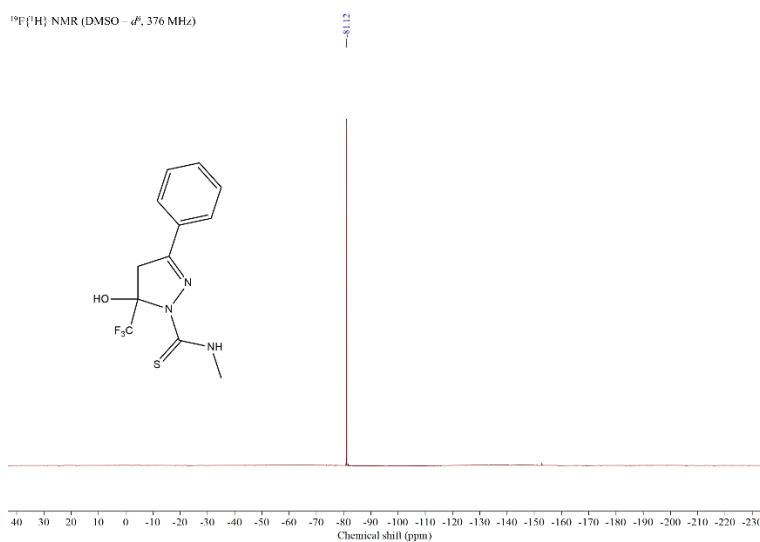


Figure S8. ¹⁹F{¹H} NMR spectrum of thiosemicarbazone **2**, in DMSO – *d*⁶ solution.

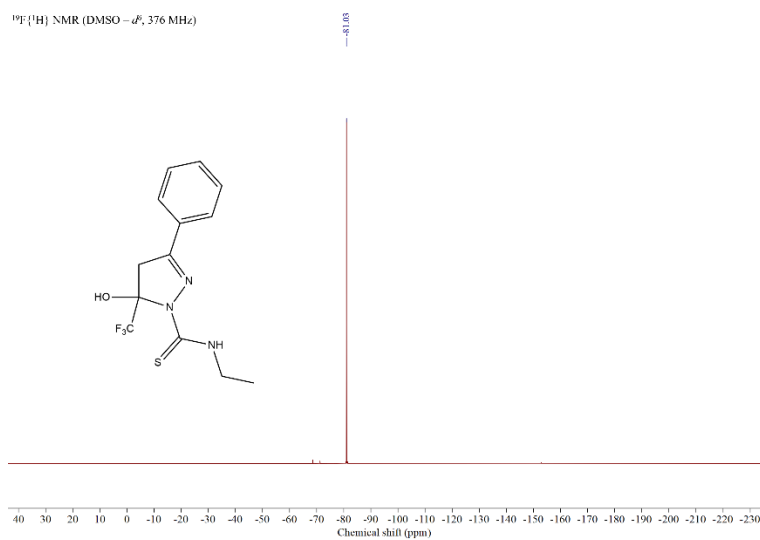


Figure S9. ¹⁹F{¹H} NMR spectrum of thiosemicarbazone **3**, in DMSO – *d*⁶ solution.

3. Mass spectrometry data

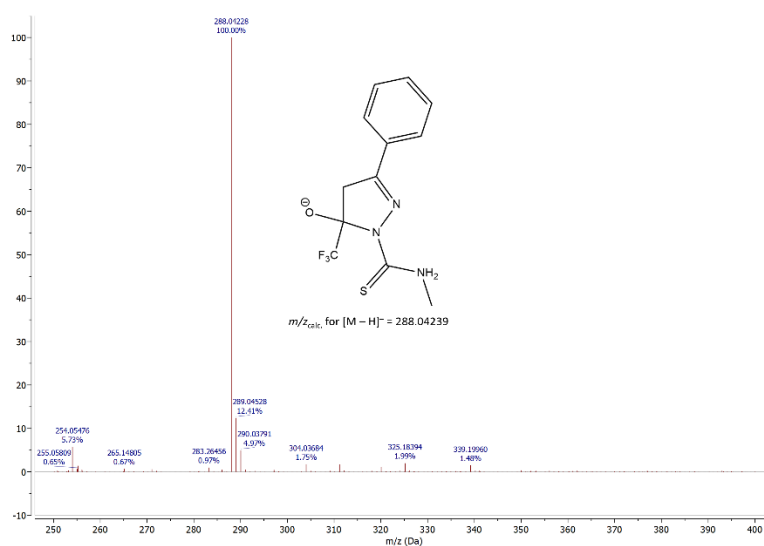


Figure S10. Negative mode mass spectrum of thiosemicarbazone **1**, in acetonitrile solution.

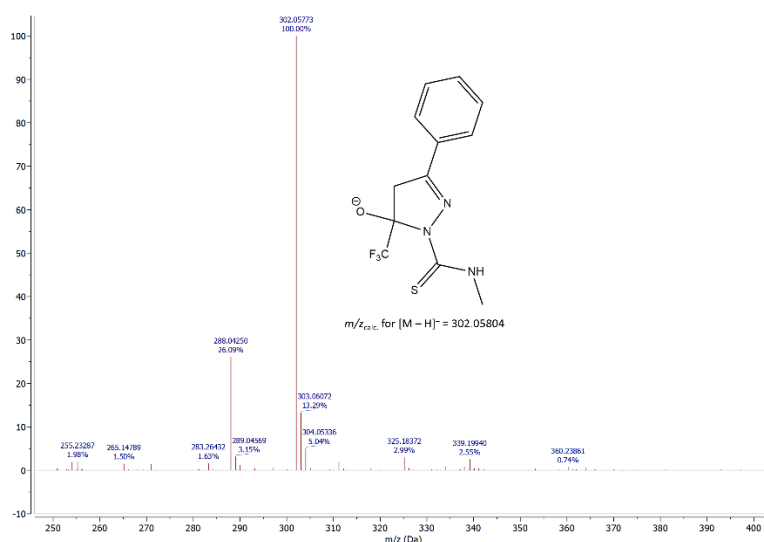


Figure S11. Negative mode mass spectrum of thiosemicarbazone **2**, in acetonitrile solution.

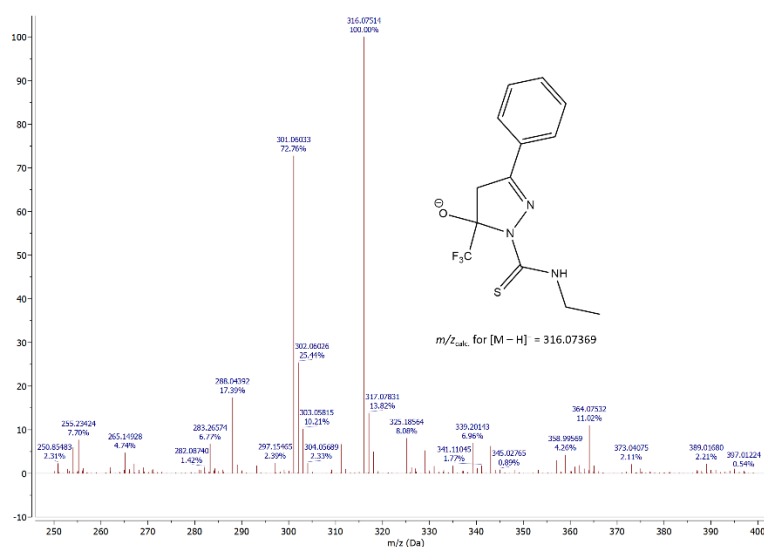


Figure S12. Negative mode mass spectrum of thiosemicarbazone **3**, in acetonitrile solution.

4. Theoretical data

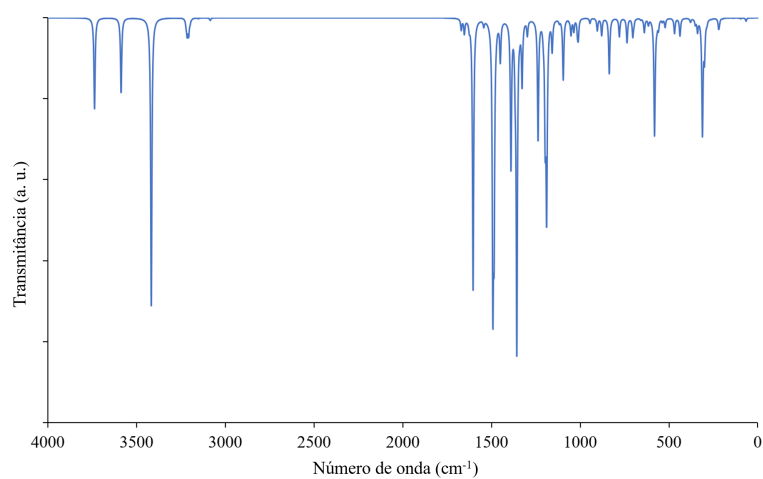


Figure S13. Calculated IR spectrum on thiosemicarbazone 1.

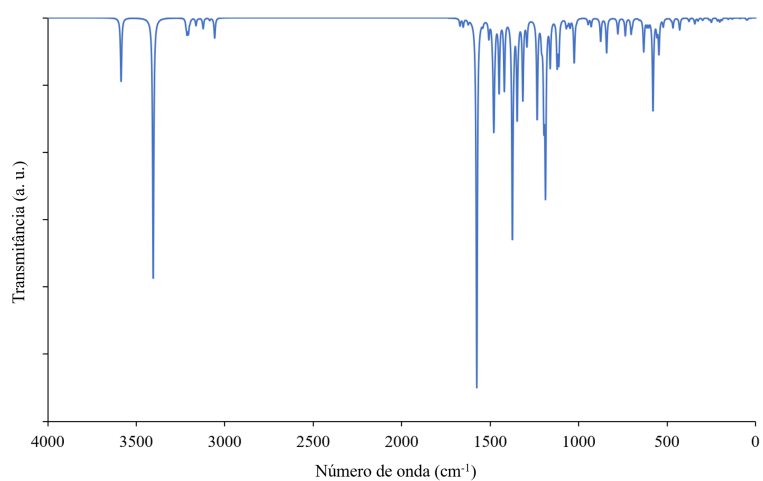


Figure S14. Calculated IR spectrum on thiosemicarbazone 2.

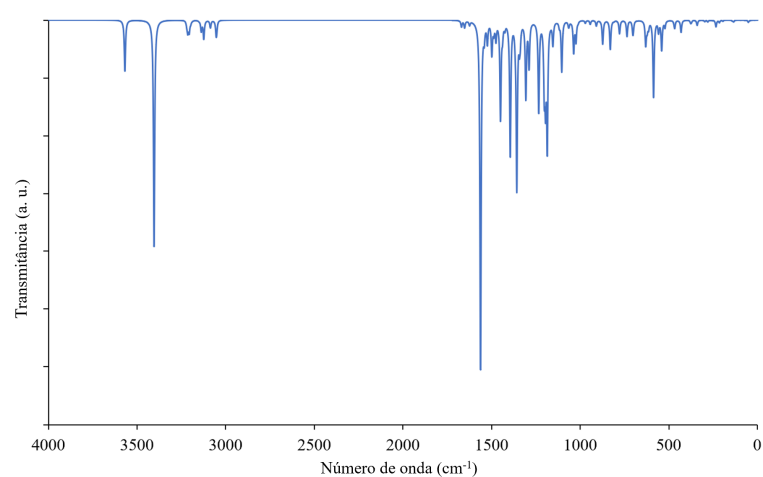


Figure S15. Calculated IR spectrum on thiosemicarbazone 3.