Supporting Information

Structural Assignment of 6-Oxy Purine Derivatives through Computational Modeling, Synthesis, X-ray Diffraction, and Spectroscopic Analysis

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Running Title: Structures of 6-Oxy Purine Derivatives

Supporting Information Available. Two figures for ¹H NMR and IR spectra of compound **4**. This material is available free of charge *via* the Internet at <u>http://pubs.acs.org</u>.

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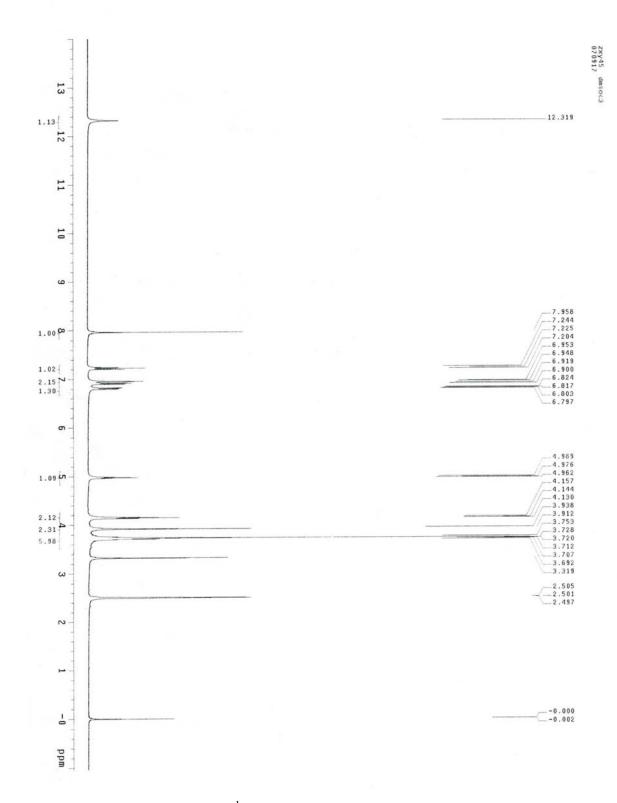


Figure S1. ¹H NMR spectrum of compound 4

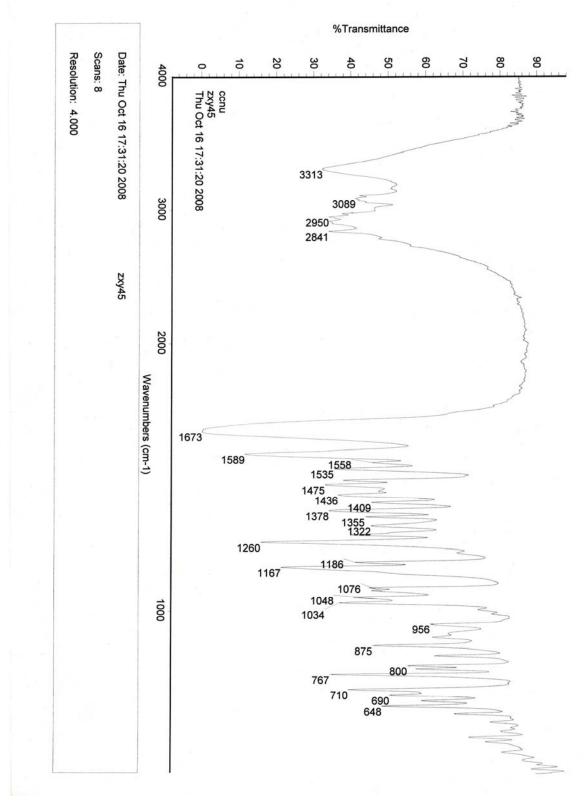


Figure S2. IR spectrum of compound 4