Pontificia Universidad JAVERIANA Bogotá

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SUPPLEMENTARY MATERIAL 1

Computer-aided design, synthesis, and characterization of molecular hybrids of dihydropyrazoles, aminopyrimidines, and thiazolidin-4-ones as potential inhibitors of the penicillin-binding protein 3 (PBP-3) of *Escherichia coli*

Fabián Orozco-López*[1], Liliana Rocío Guerrero Villalobos[1], Paola Andrea Cuervo Pardo[1]

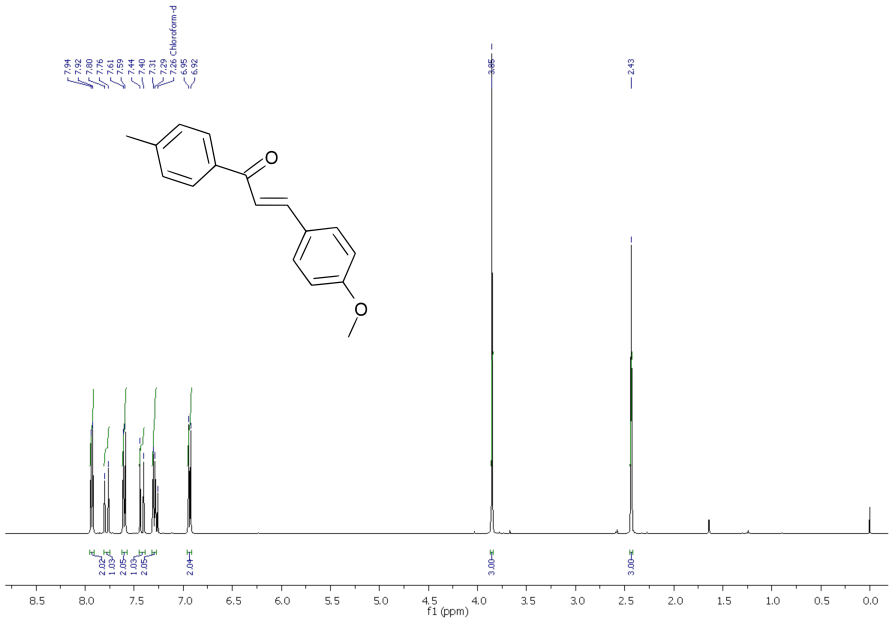
Contents

1. NMR Spectra

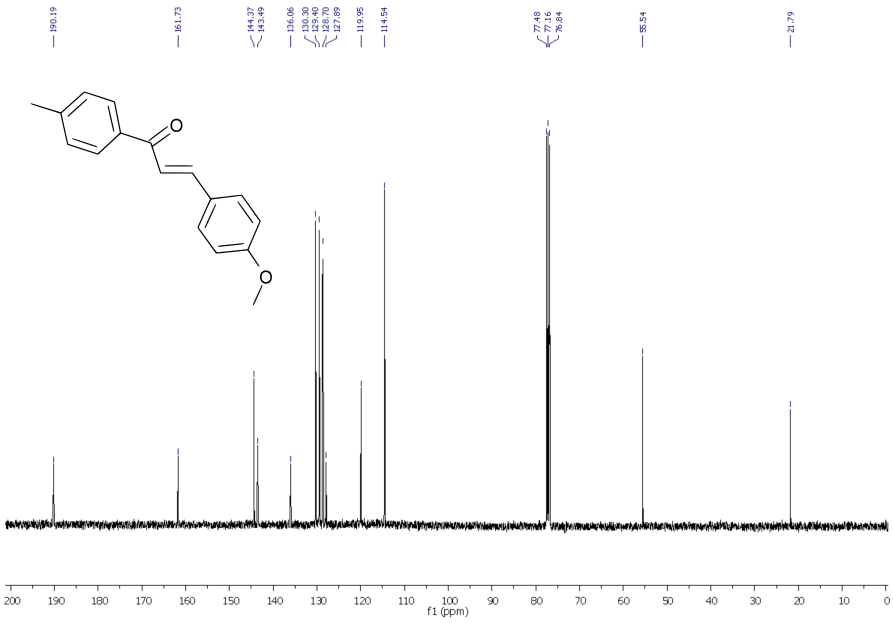
The NMR spectra were recorded on Bruker spectrometer (400MHz, CDCl3 or DMSO d6).

1.1. Compound 1h

1.1.1. ^{1}H NMR spectrum of compound 1h

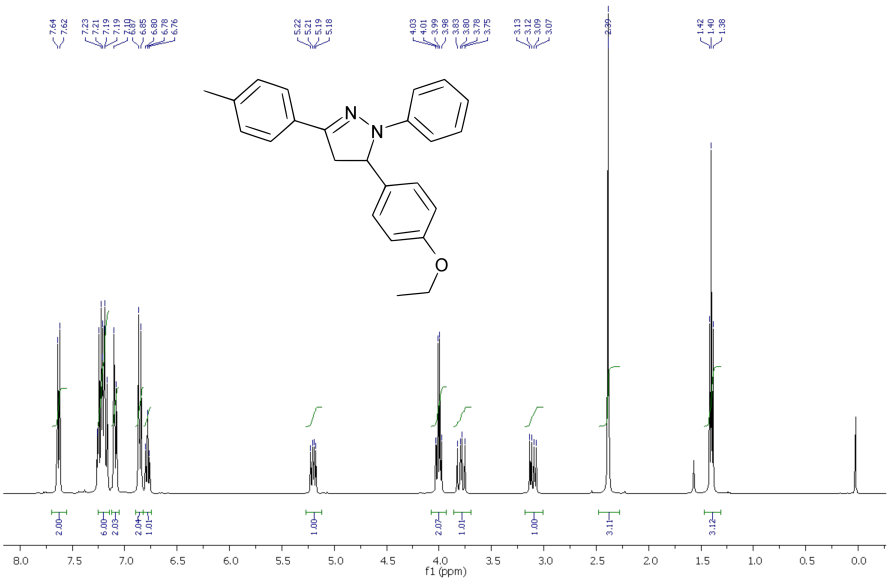


1.1.2. ^{13}C NMR spectrum of compound 1h

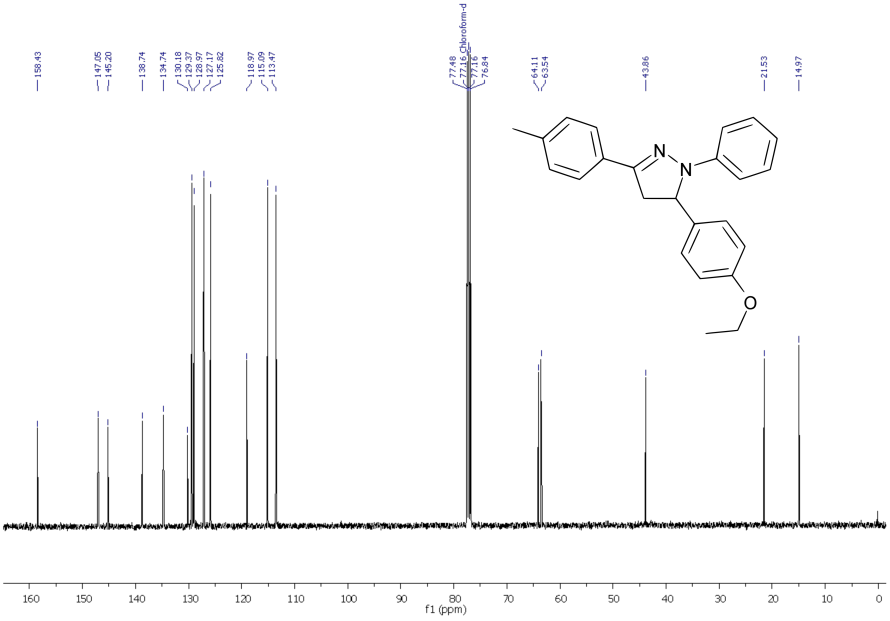


1.2. Compound 2b

1.2.1. ^{1}H NMR spectrum of compound 2b

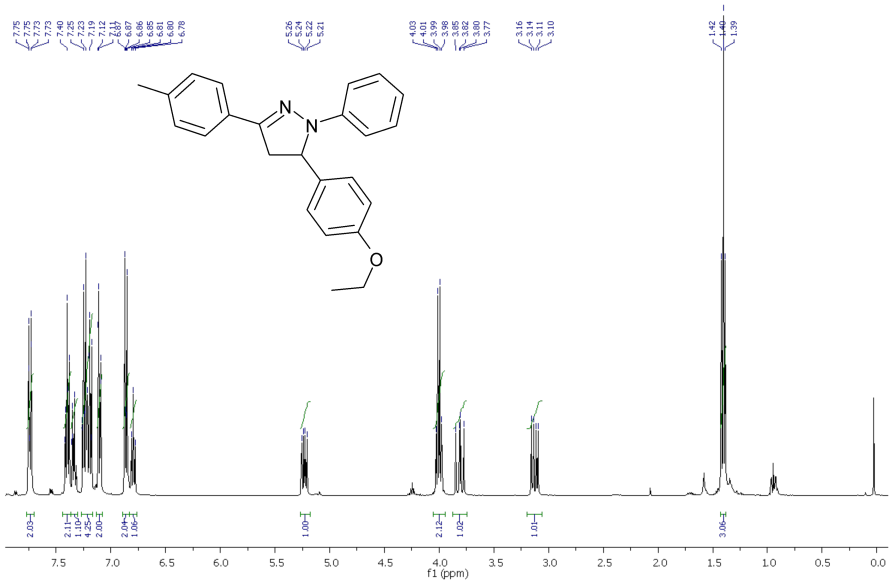


1.2.2. ^{13}C NMR spectrum of compound 2b

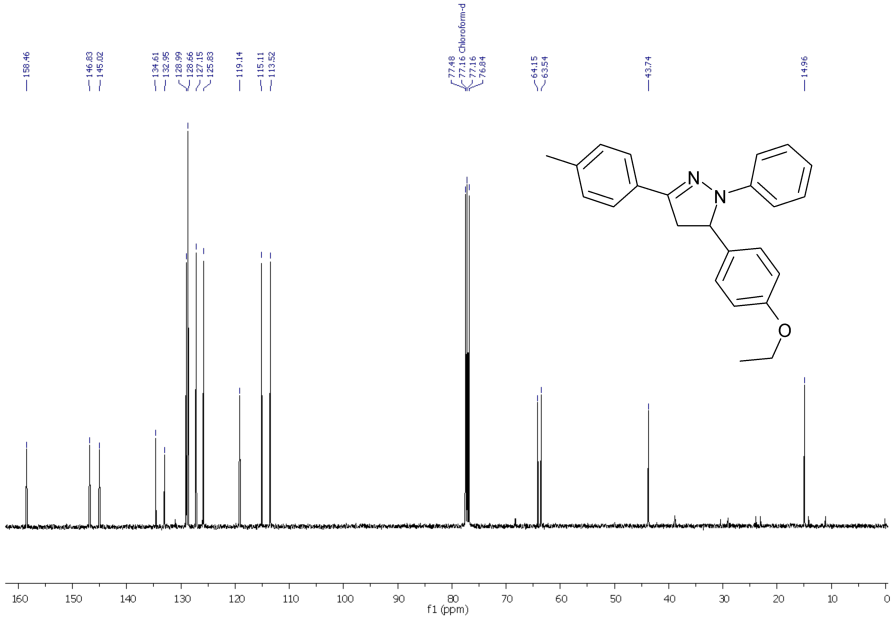


1.3. Compound 2c

1.3.1. ^{1}H NMR spectrum of compound 2c

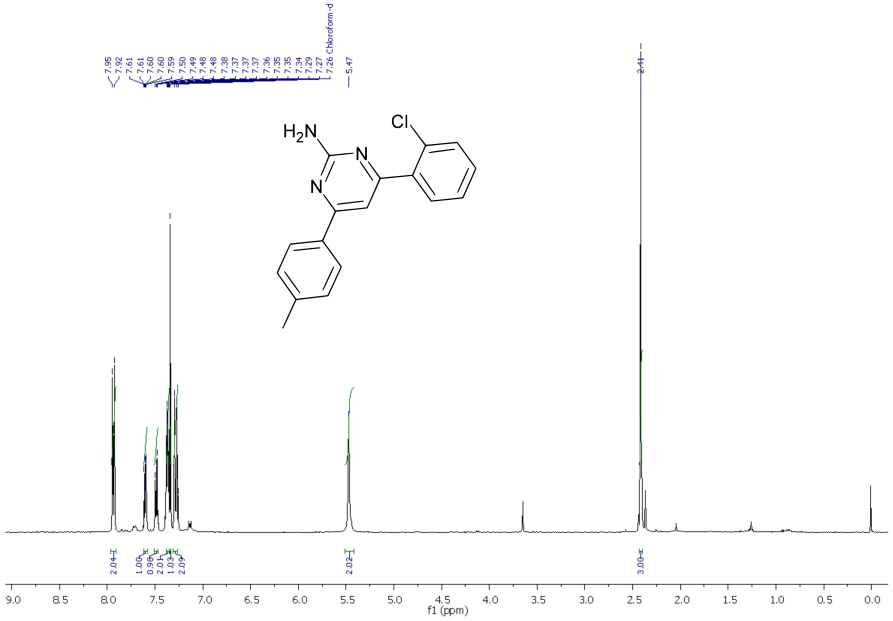


1.3.2. ^{13}C NMR spectrum of compound 2c

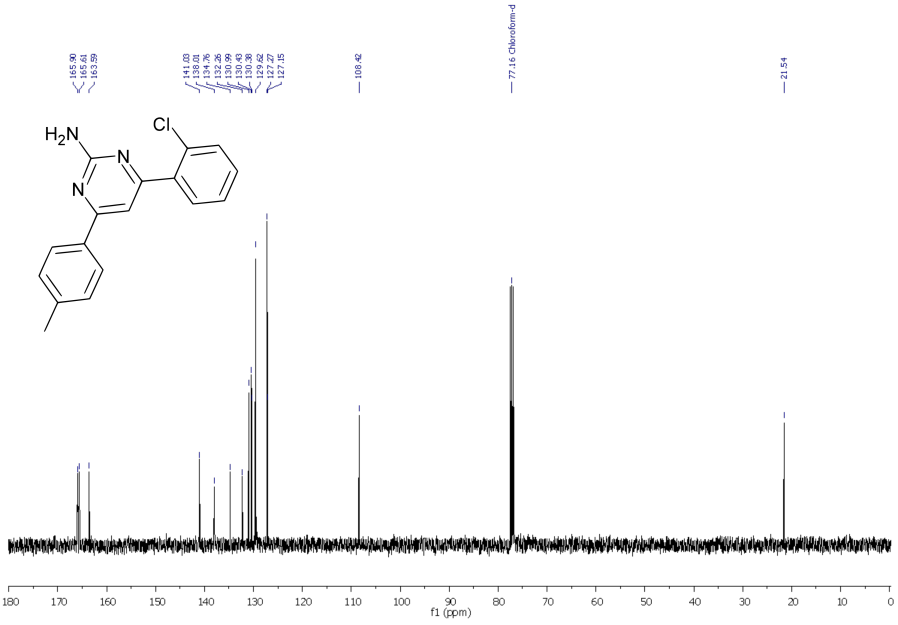


1.4. Compound 3a

1.4.1. ^{1}H NMR spectrum of compound 3a

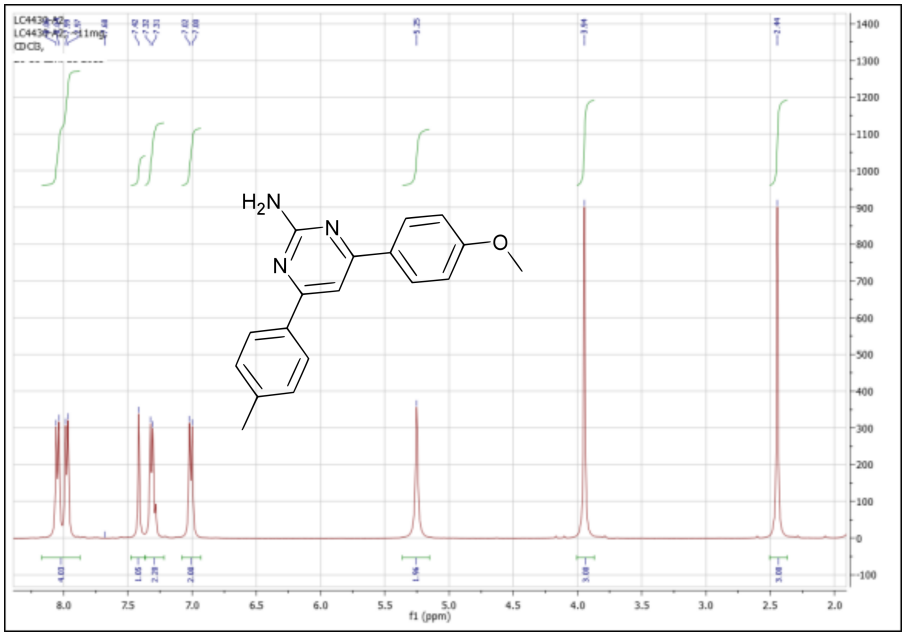


1.4.2. ^{13}C NMR spectrum of compound 3a

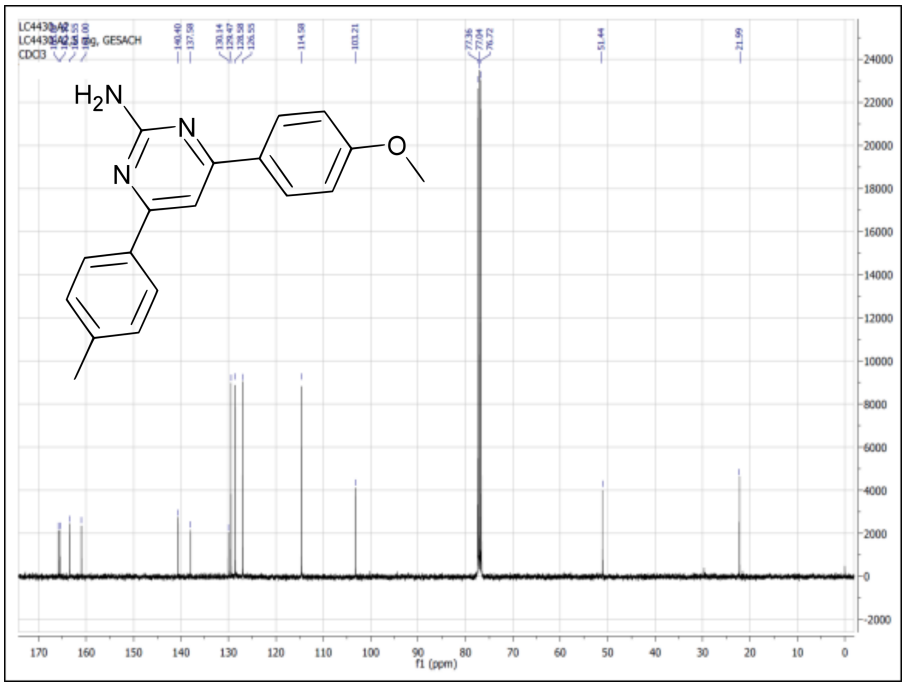


1.5. Compound 3h

1.5.1. ^{1}H NMR spectrum of compound 3h

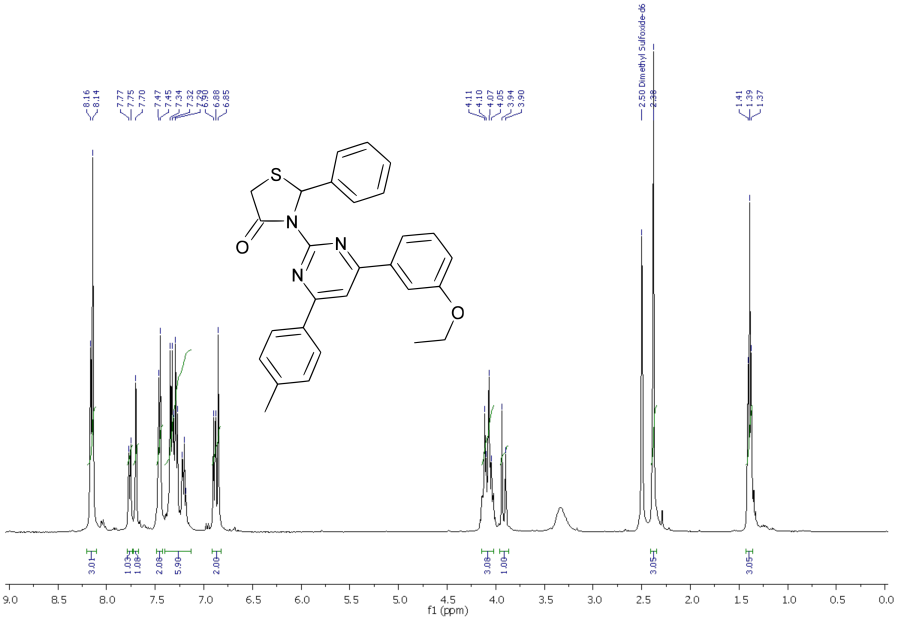


1.5.2. ^{13}C NMR spectrum of compound 3h

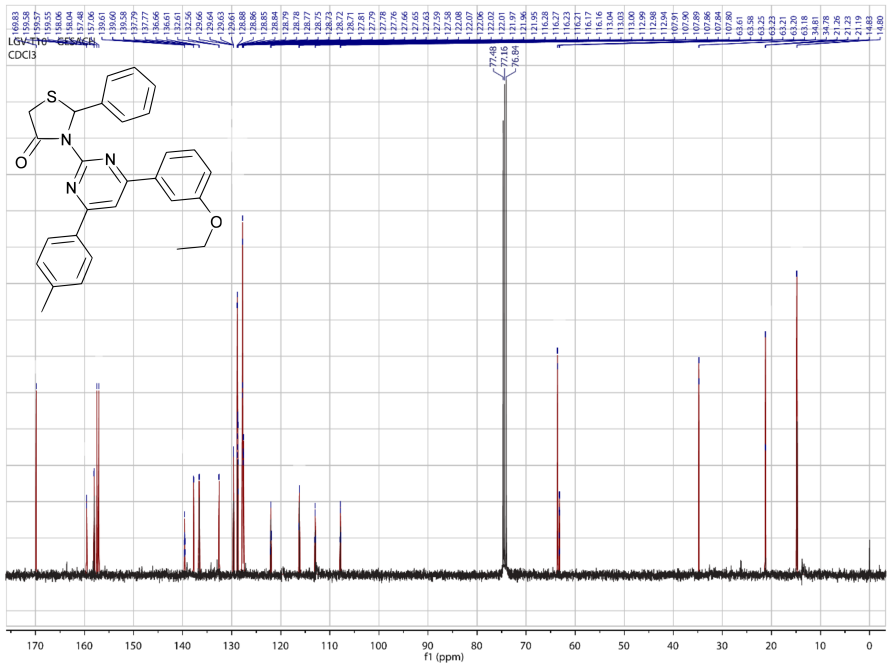


1.6. Compound 4g

1.6.1. ^{1}H NMR spectrum of compound 4g

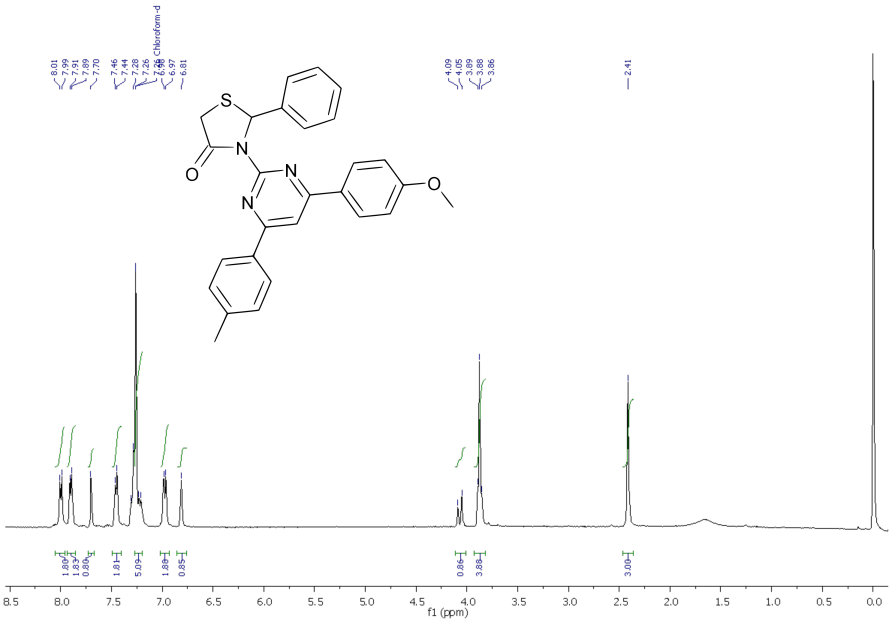


1.6.2. ^{13}C NMR spectrum of compound 4g



1.7. Compound 4h

1.7.1. ^{1}H NMR spectrum of compound 4h



1.7.2. ^{13}C NMR spectrum of compound 4h