

# Supporting Information 2

## **Design, synthesis and docking study of acyl thiourea derivatives as possible histone deacetylase inhibitors with novel zinc binding group**

Duraïd H. Al-Amily\* and Mohammed H. Mohammed

Address: Pharmaceutical Chemistry Department, College of Pharmacy-University of  
Baghdad, Baghdad, Iraq.

Email: Duraïd H. Al-Amily – colrelated@copharm.uobaghdad.edu.iq

\* Corresponding author

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## FT-IR Spectra

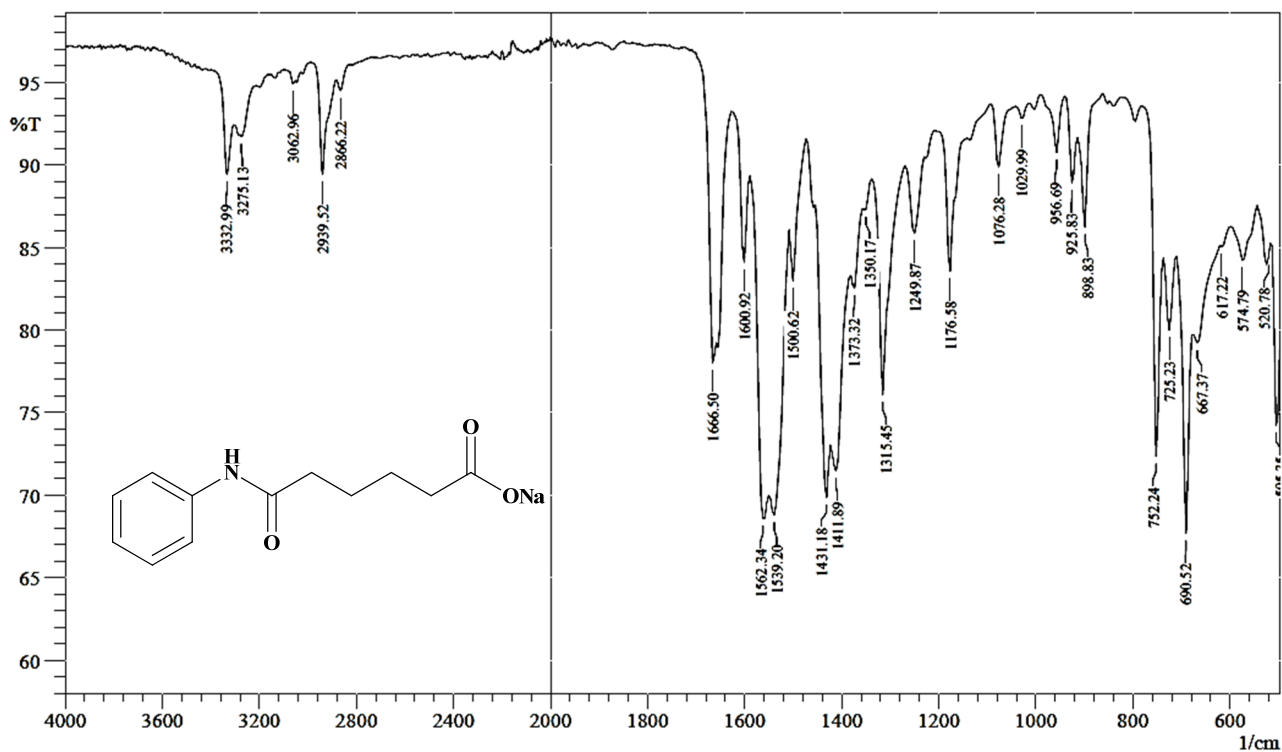


Figure 1: FT-IR spectrum of monosodium adipic monoanilide, **4d**

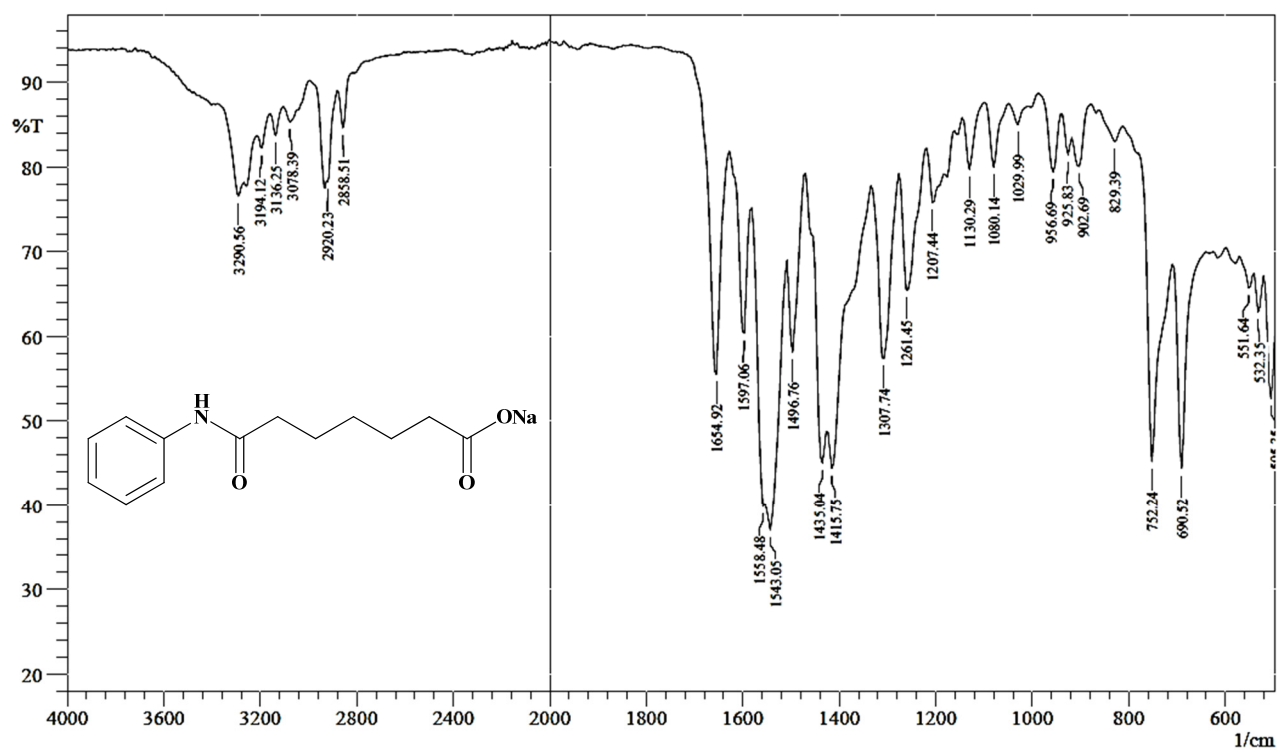


Figure 2: FT-IR spectrum of monosodium pimelic monoanilide, **5d**

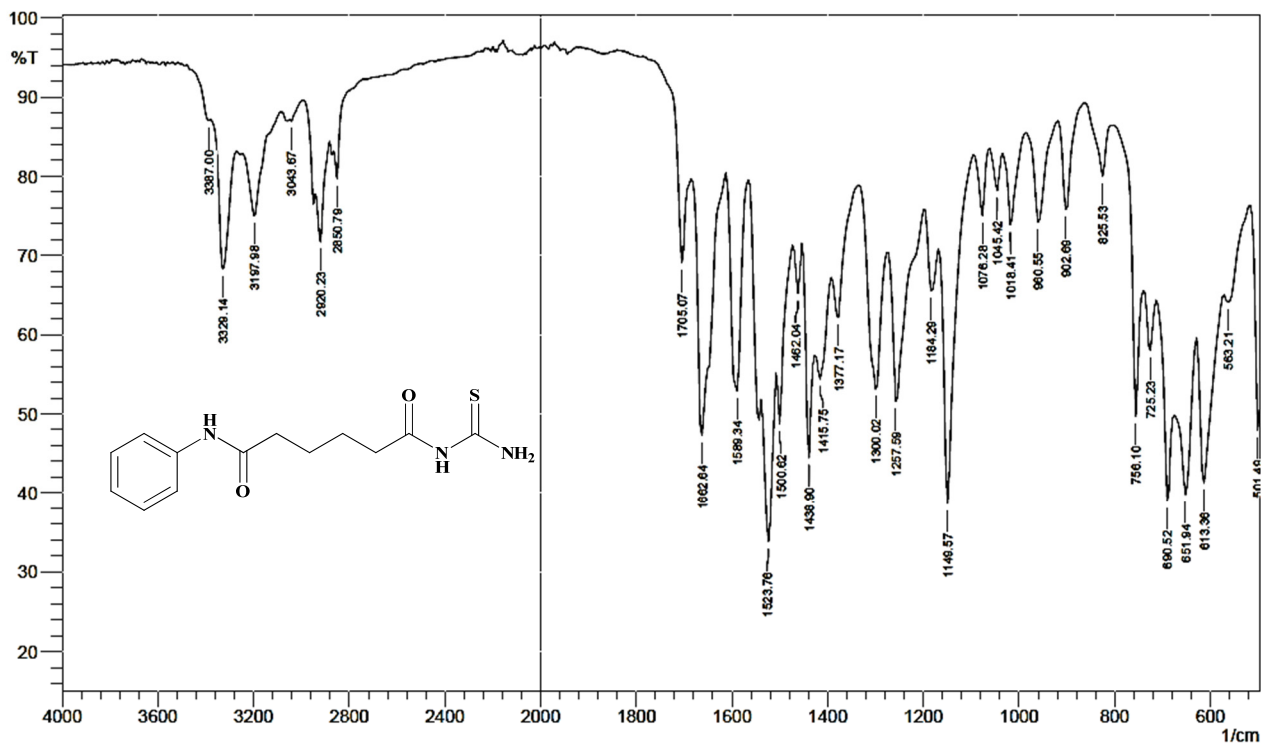


Figure 3: FT-IR spectrum of *N*-adipoyl monoanilide thiourea, 4

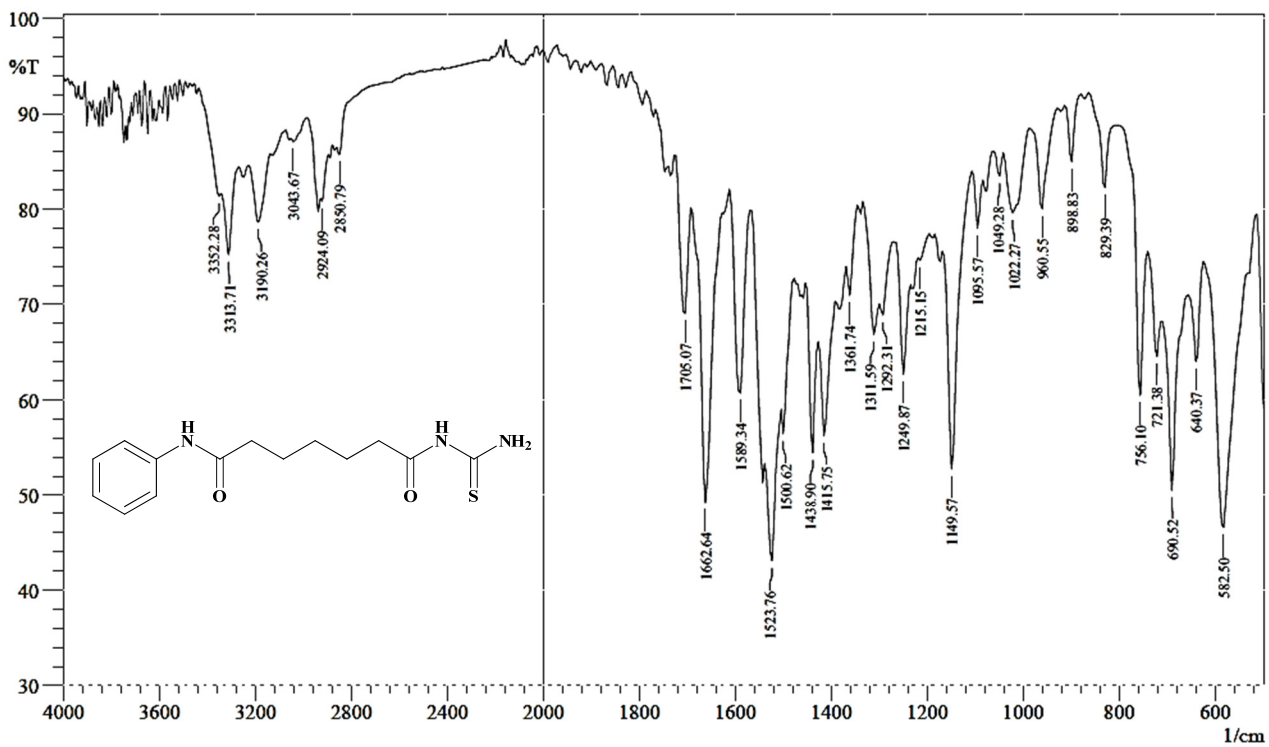


Figure 4: FT-IR spectrum of *N*-pimeloyl monoanilide thiourea, 5

# NMR spectra

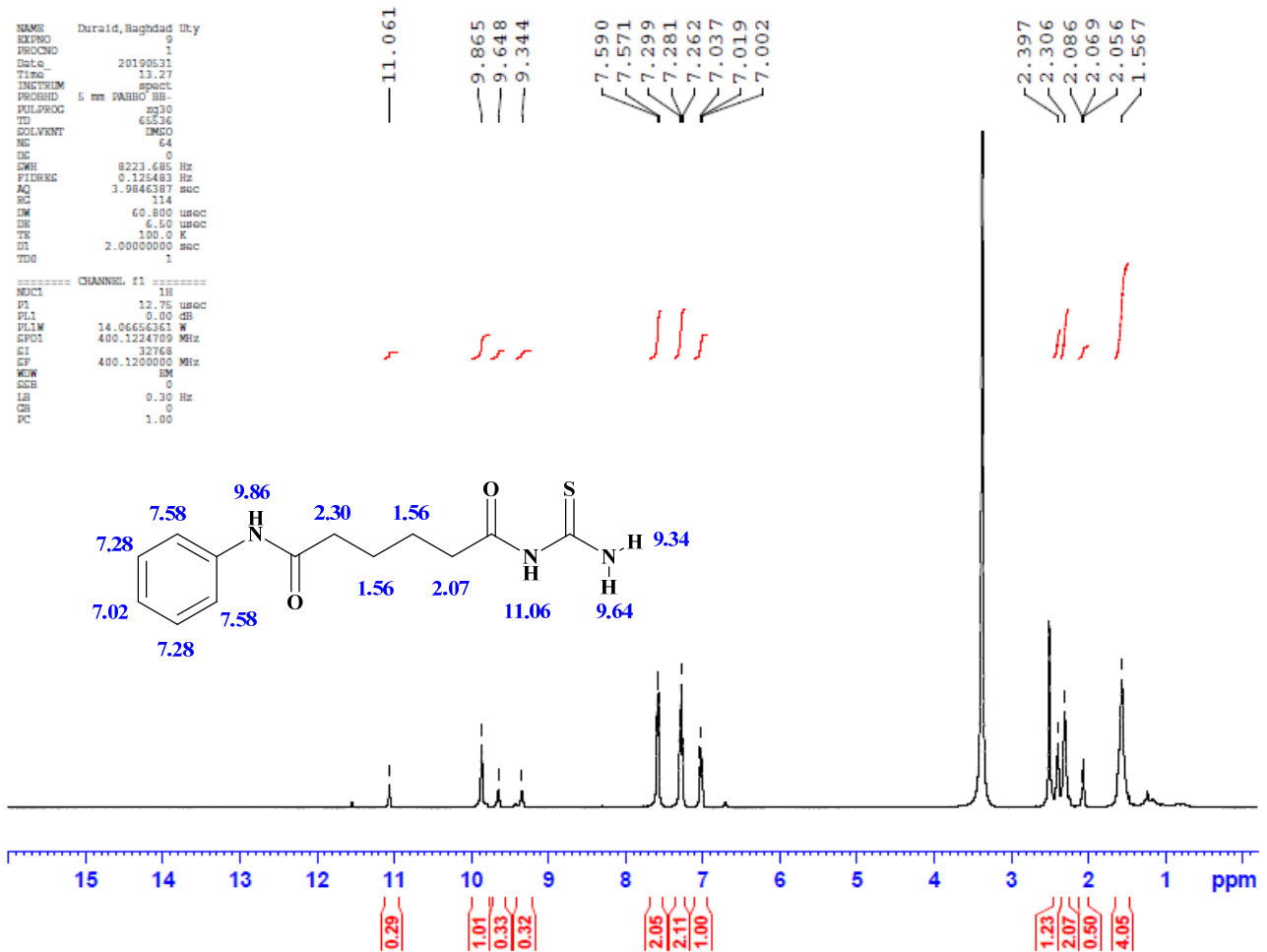


Figure 5: <sup>1</sup>H-NMR spectrum of *N*-adipoyl monoanilide thiourea, 4

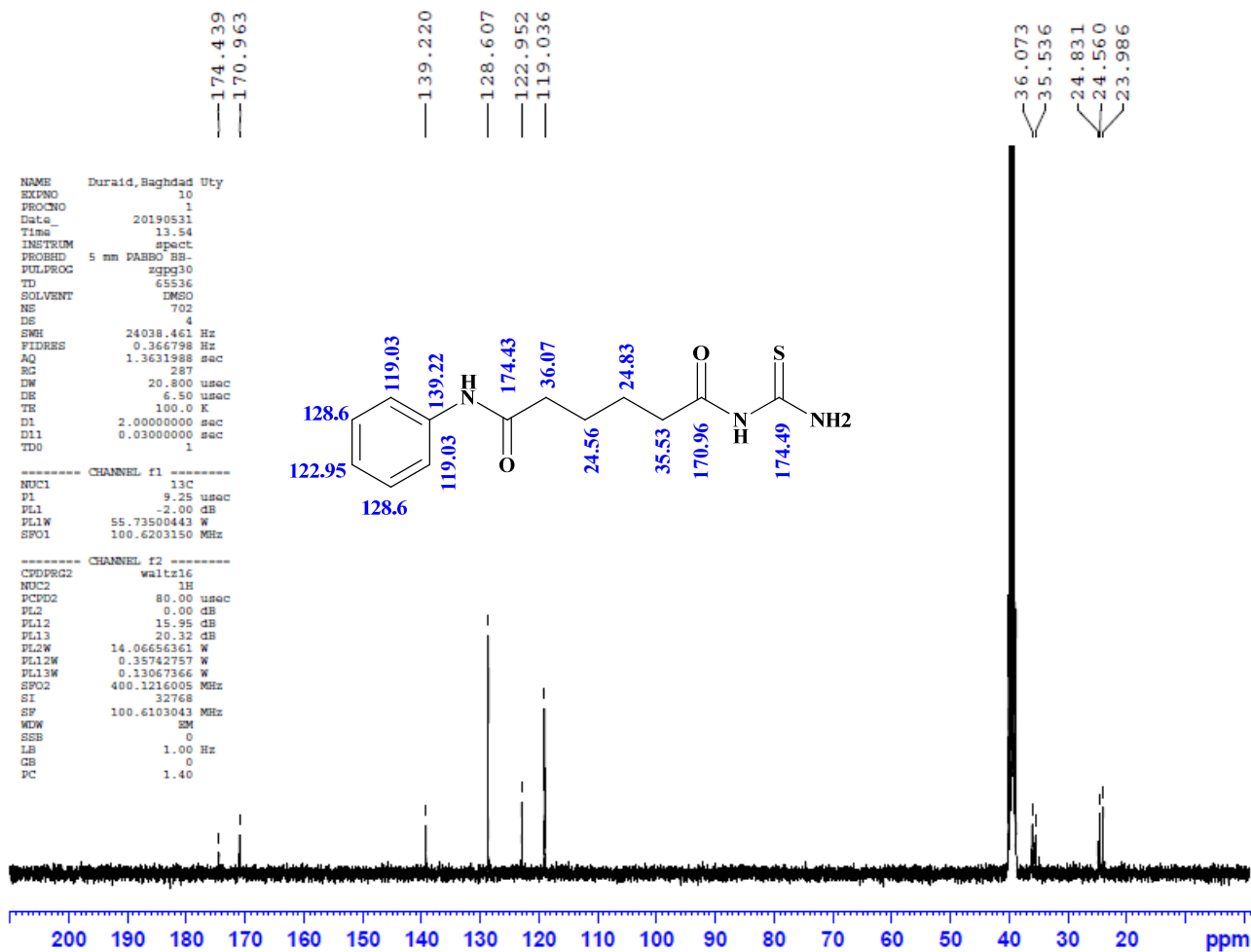


Figure 6:  $^{13}\text{C}$ -NMR of *N*-adipoyl monoanilide thiourea, 4

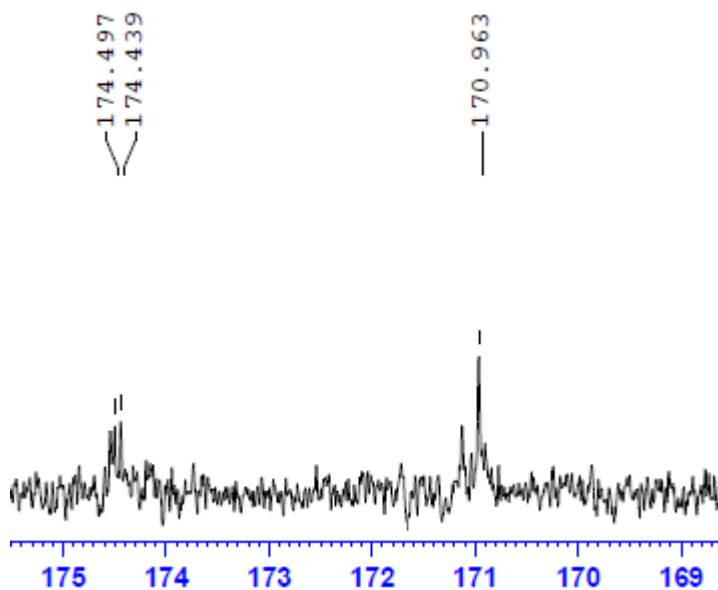


Figure 7: A magnified  $^{13}\text{C}$ -NMR spectrum of *N*-adipoyl monoanilide thiourea, 4

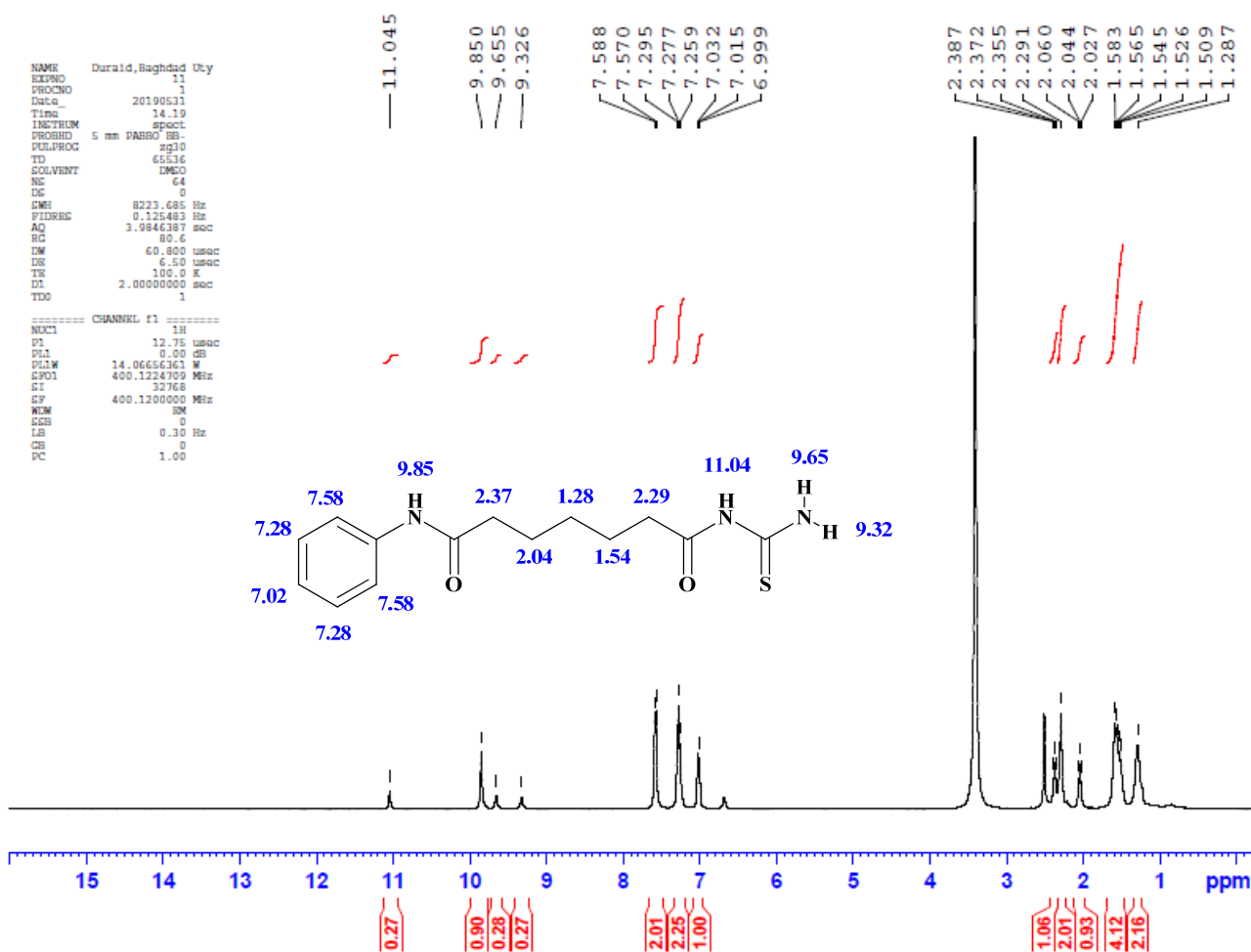


Figure 8:  $^1\text{H-NMR}$  spectrum of *N*-pimeloyl monoanilide thiourea, **5**

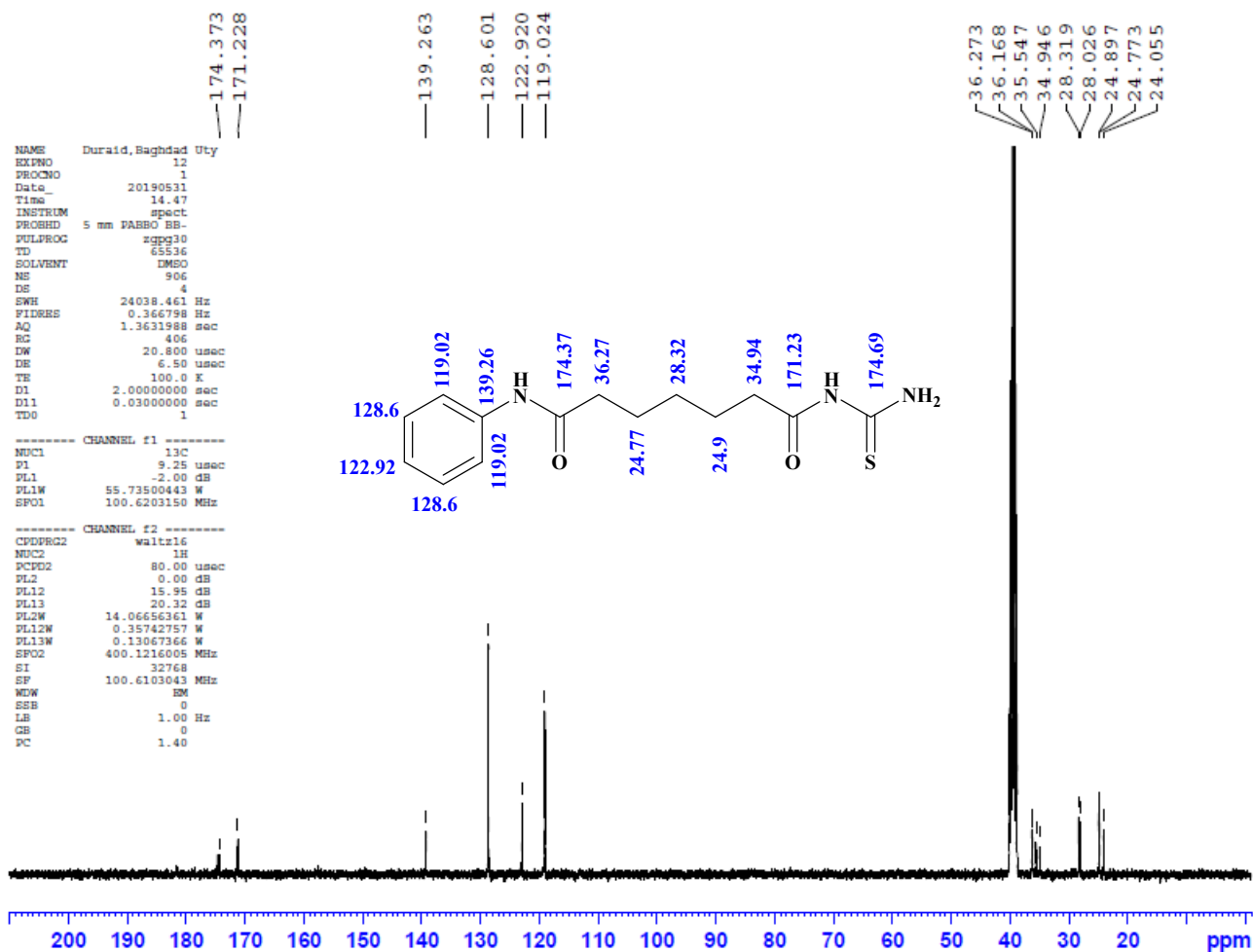


Figure 9:  $^{13}\text{C}$ -NMR spectrum of *N*-pimeloyl monoanilide thiourea, 5

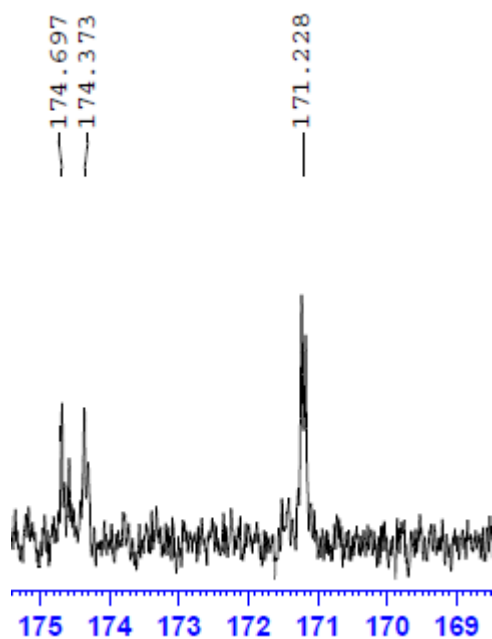


Figure 10: A magnified  $^{13}\text{C}$ -NMR spectrum of *N*-pimeloyl monoanilide thiourea, 5