

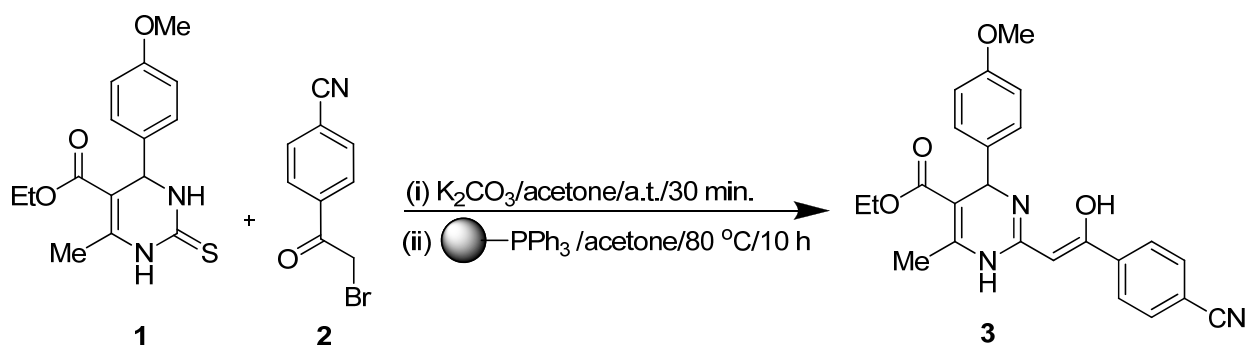
Supplementary Information

Synthesis of 5-Ethoxycarbonyl-6-methyl-4-(4-methoxyphenyl)-2-(2-hydroxy-2-(4-cyanophenyl)vinyl)-1,4-dihydropyrimidine

Sukhdeep Singh ¹, Andreas Schober ¹ and G. Alexander Groß ^{2,*}

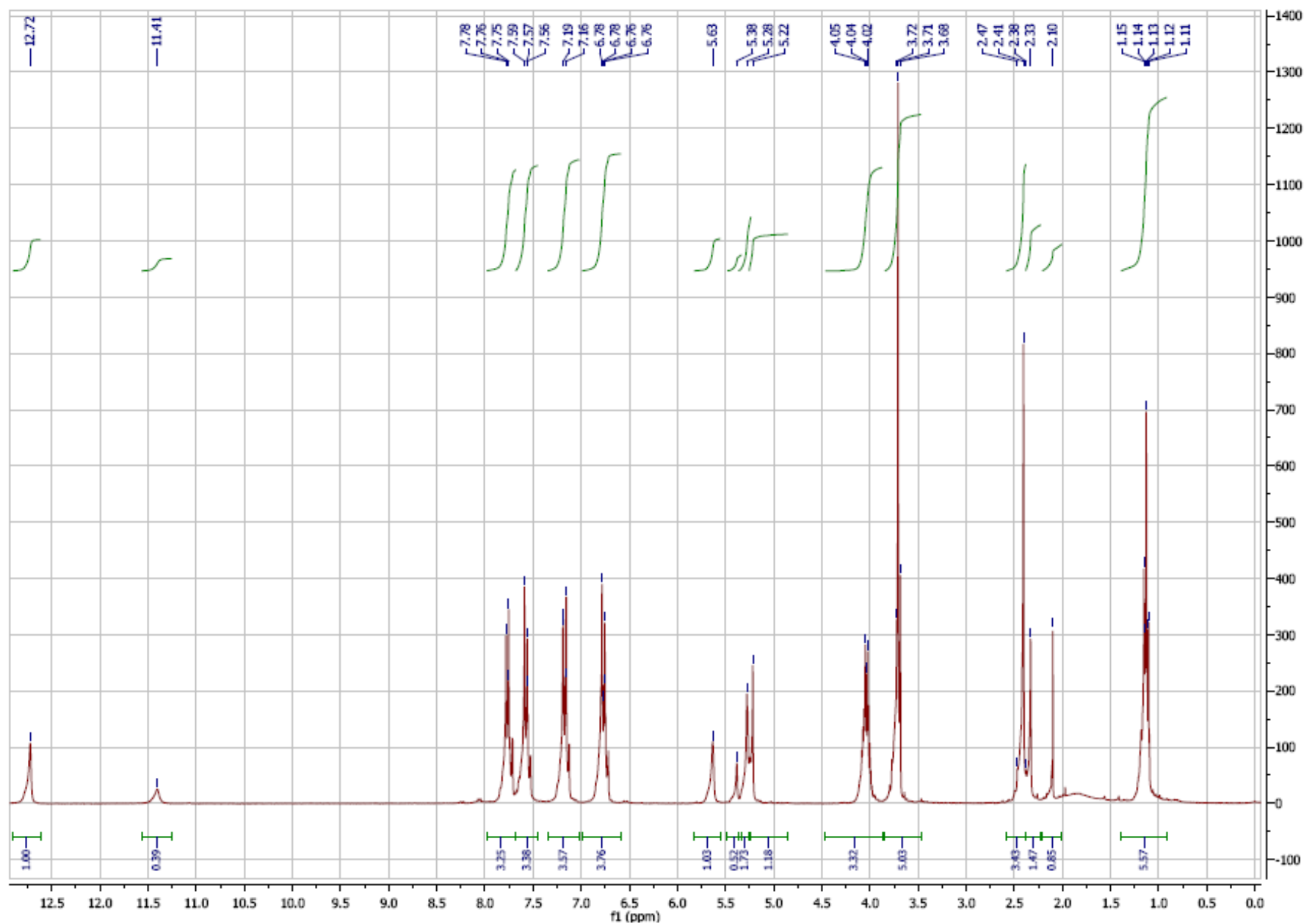
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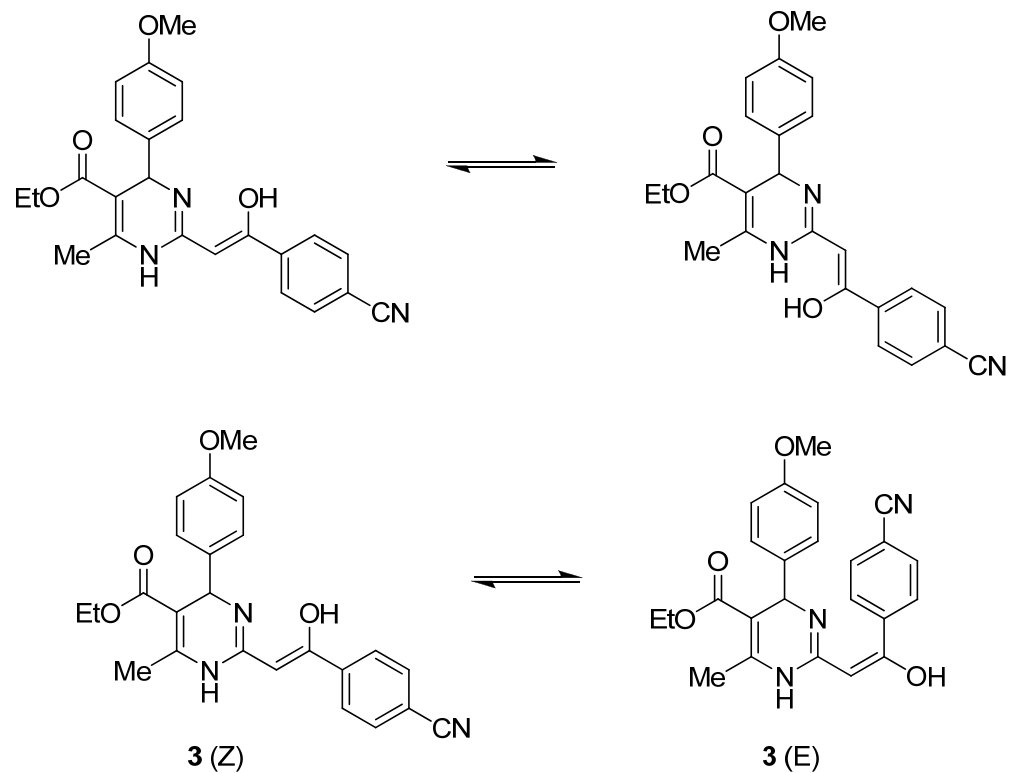
Analytical data for compound 3:

^1H -NMR (300 MHz, CDCl_3) :

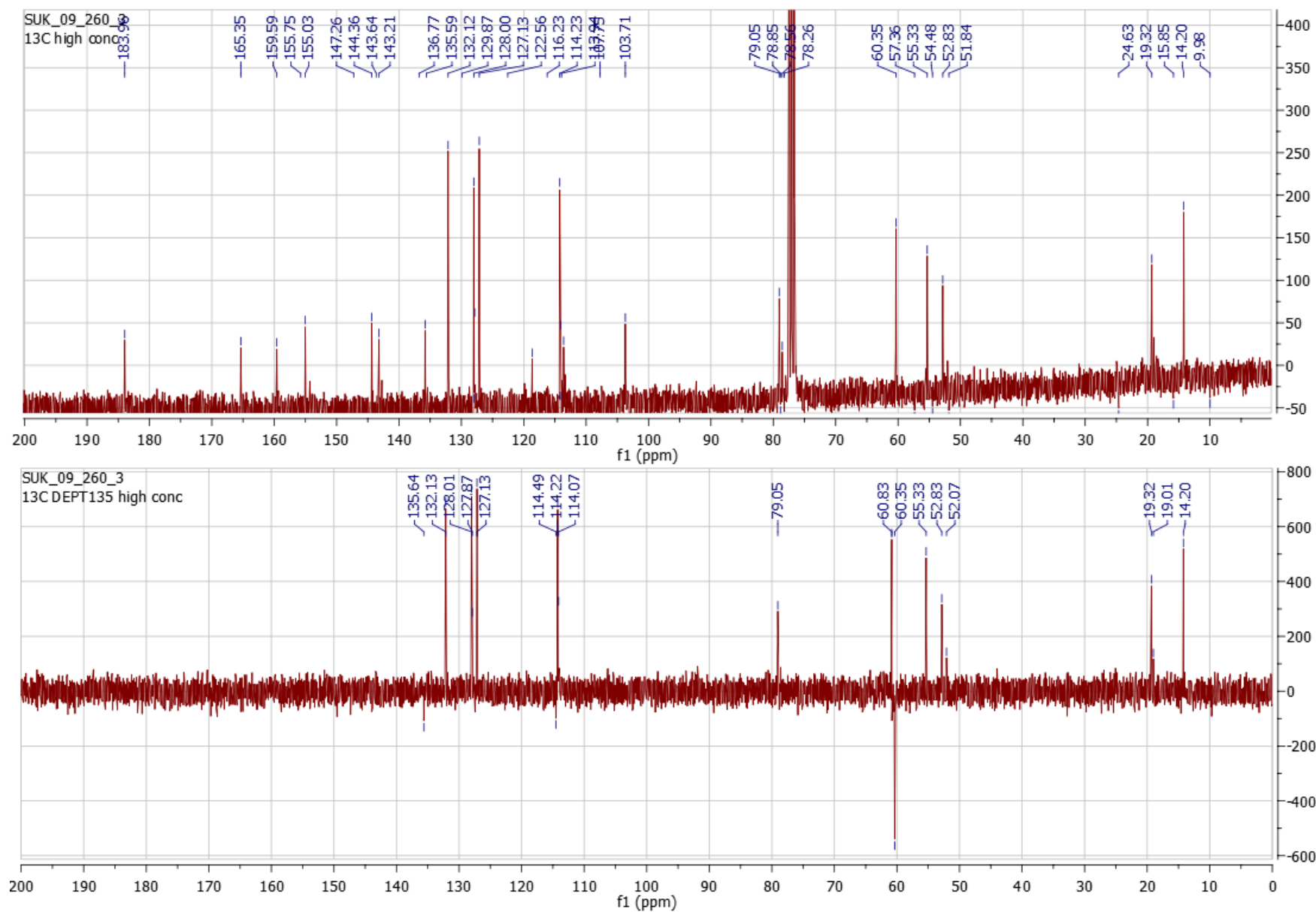


It was observed that the ^1H NMR spectra of **3** show a duplicate set of some signals (approximately 3:1 ratio). We assume that the second set of signals belong to different conformers of **3** as shown below. The possible tautomeric form of **3** was not observed during the NMR experiments. The ^1H NMR as well as the ^{13}C NMR didn't show appropriate signals for the expected aliphatic CH_2 group.

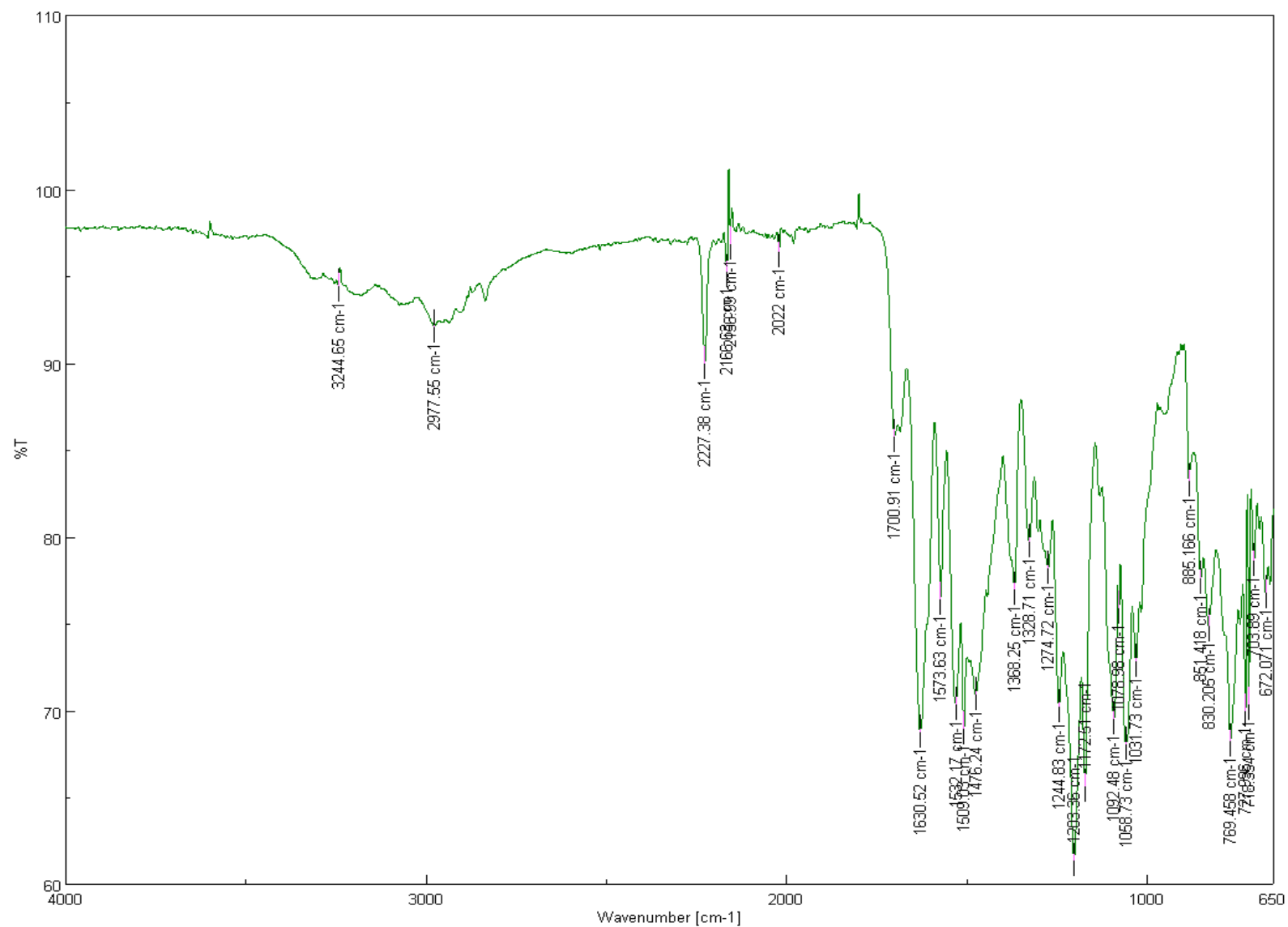
Proposed Conformers:



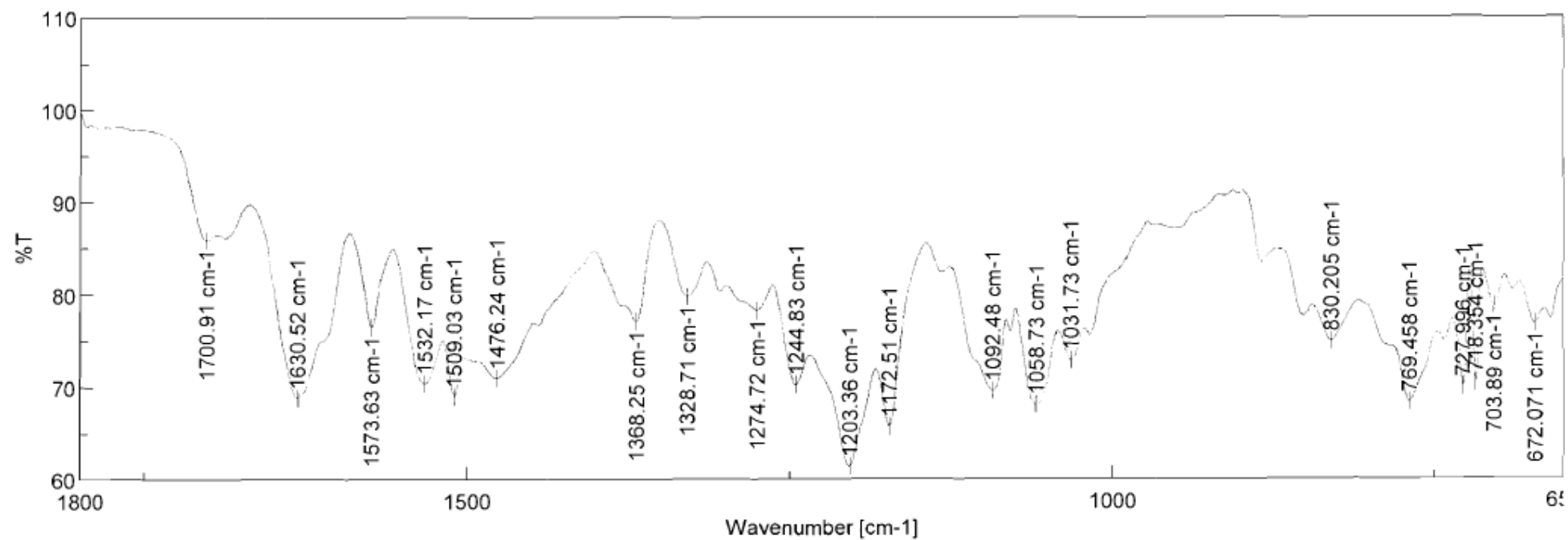
^{13}C -NMR, ^{13}C -DEPT135-NMR (75 MHz, CDCl_3):



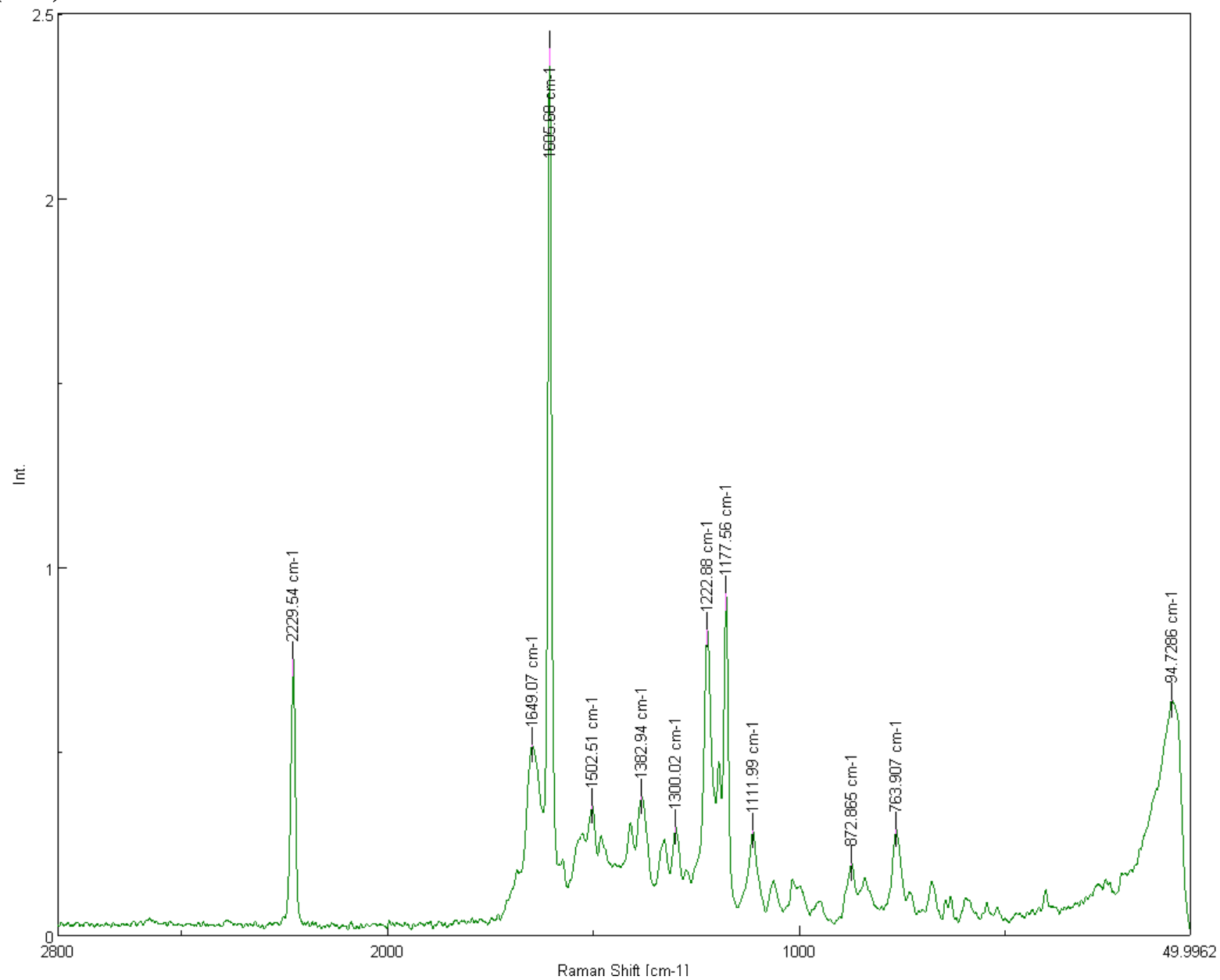
IR-spectra (KBr Pressling):



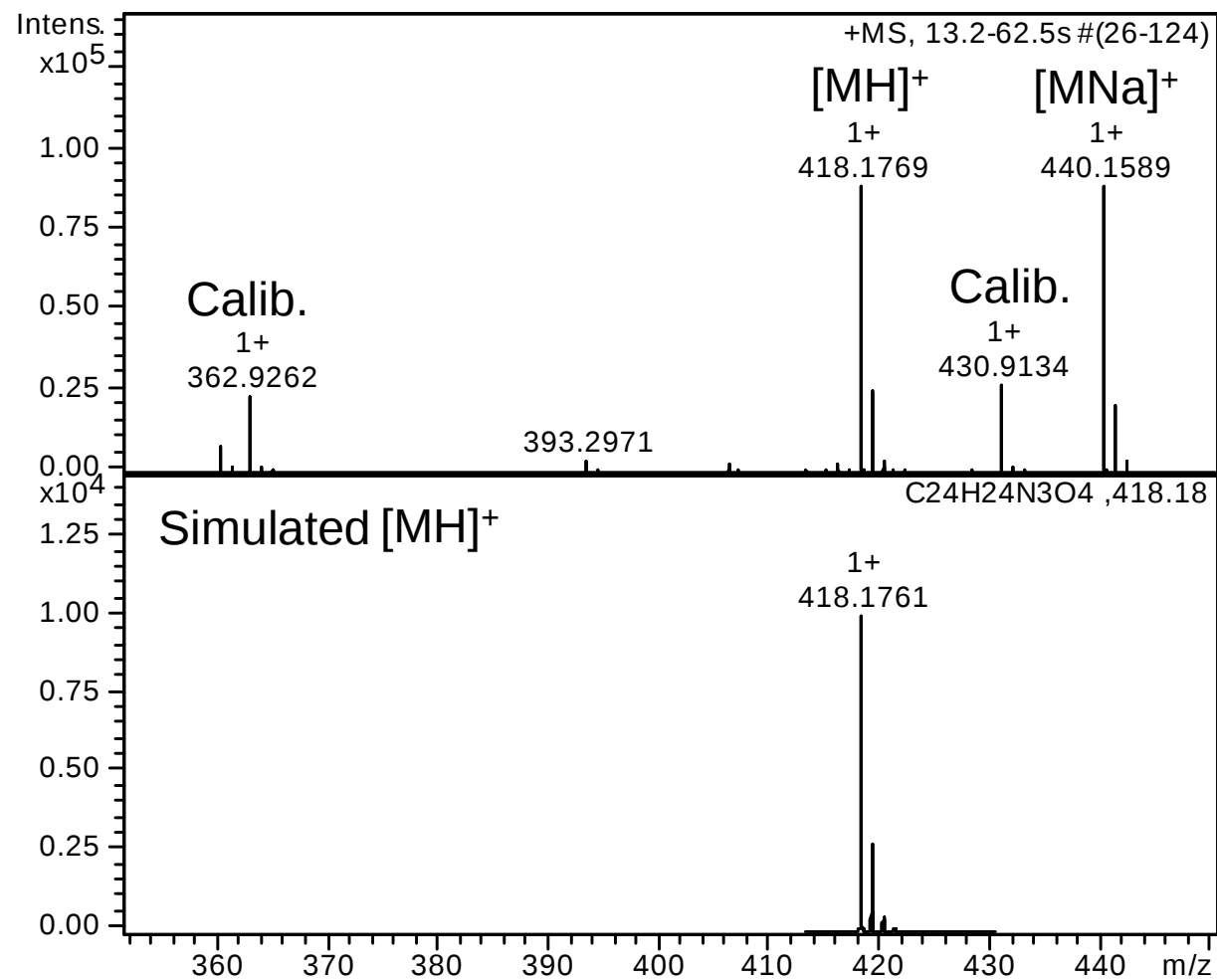
IR-spectra (KBr Pressling):



Raman-spectra (ATR):



HR-ESI-Q-TOF-MS (Sodium-formate calibrant):



UV-Vis (CH_3CN):

