NMR Structure Elucidation Problems

For each problem use the data provided to predict the structure. You may not need all data provided.

Use the separate worksheet provided to show your work, proposed structure, and assignments.

***HINT**: Calculating degree of unsaturation is key!!!*

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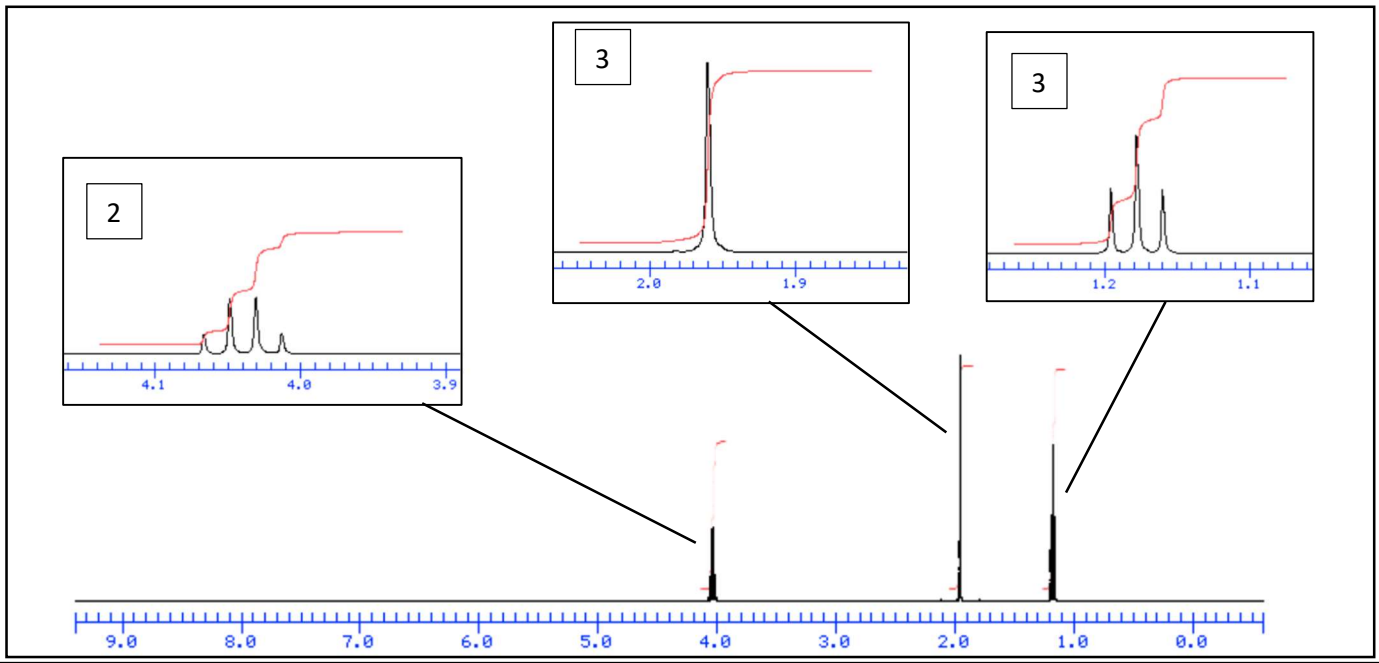
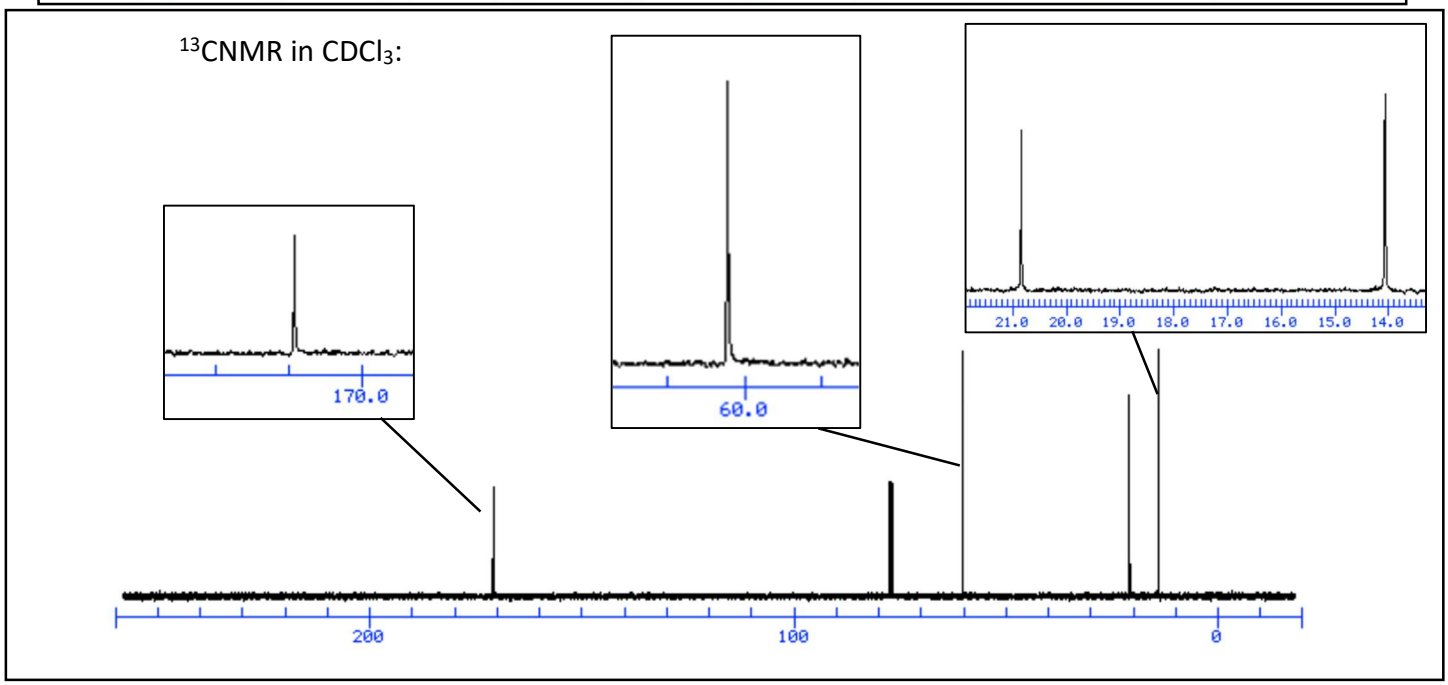
1. Molecular Formula: $C_4H_8O_2$

^{1}HNMR in $CDCl_3$: Integration values provided next to each expanded peak.



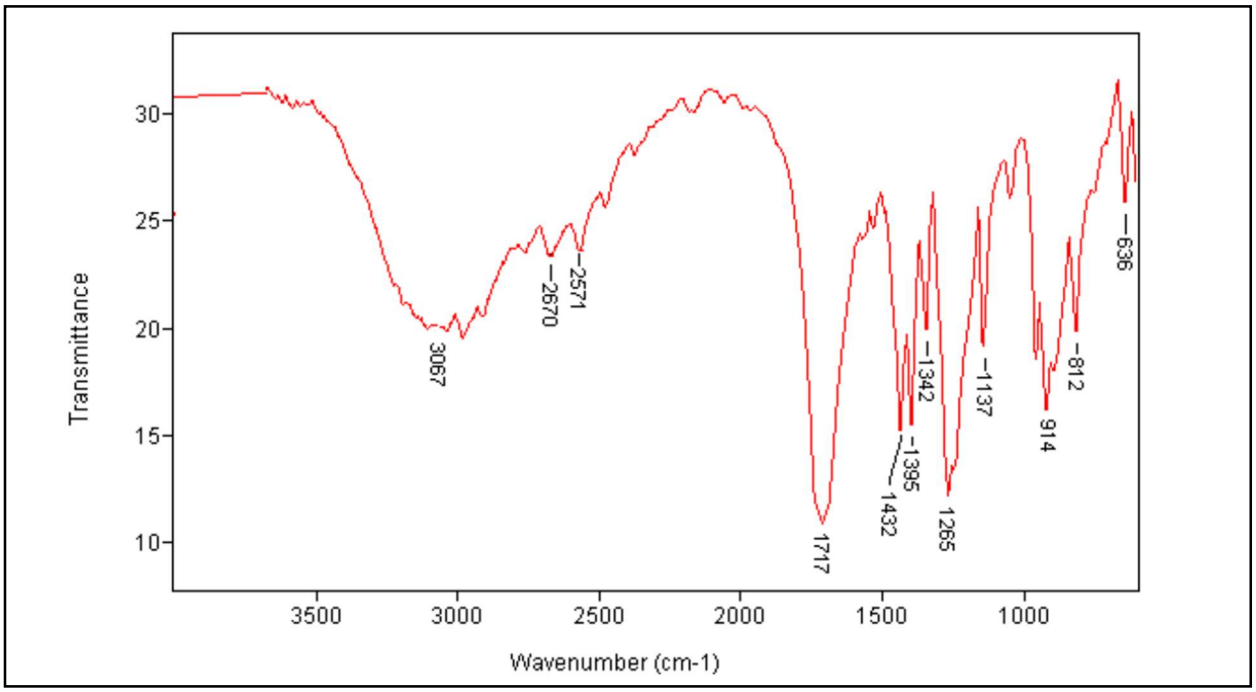
^{13}CNMR in $CDCl_3$:



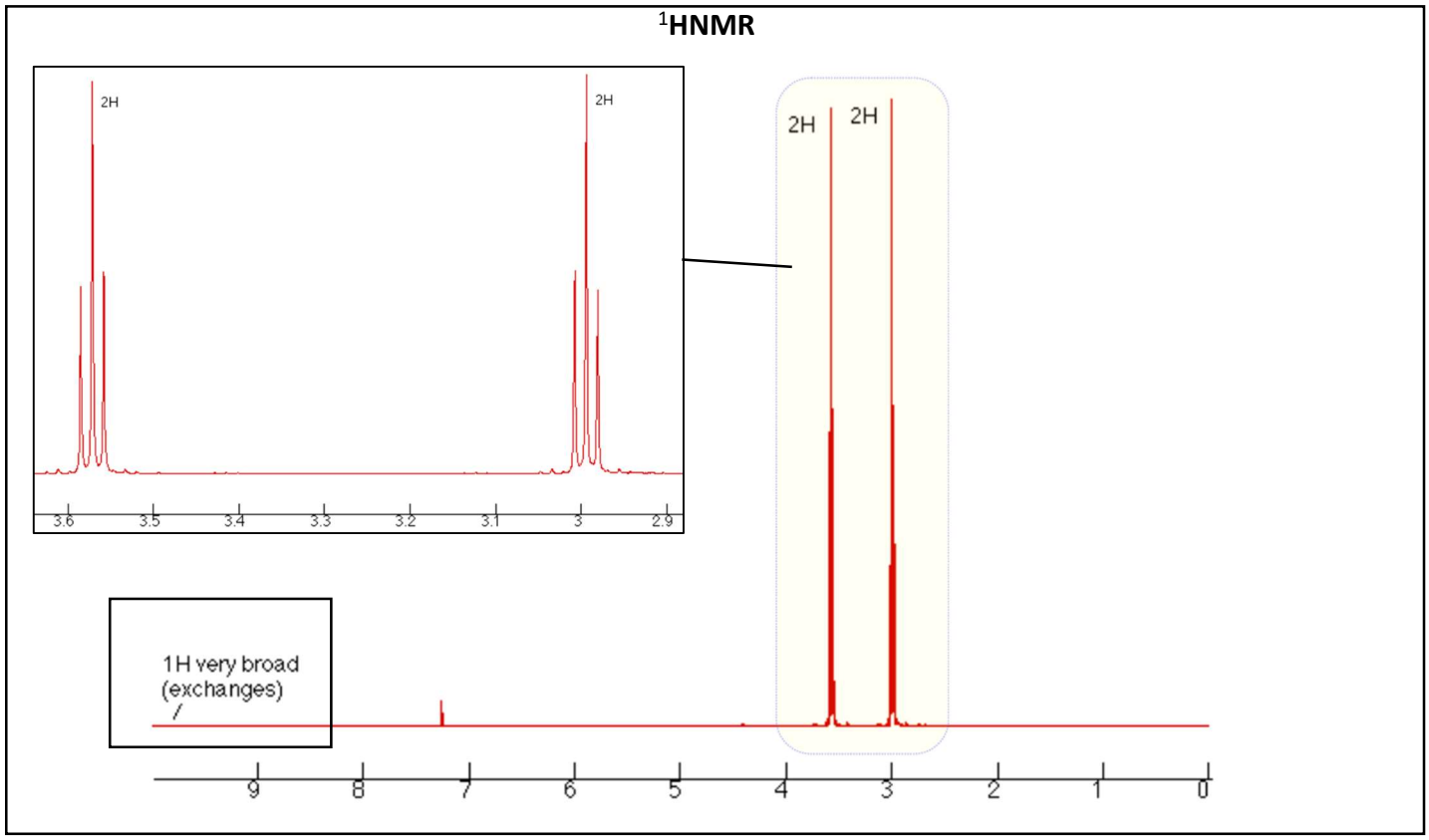
2.

Molecular Formula: $C_3H_5BrO_2$ MW = 152

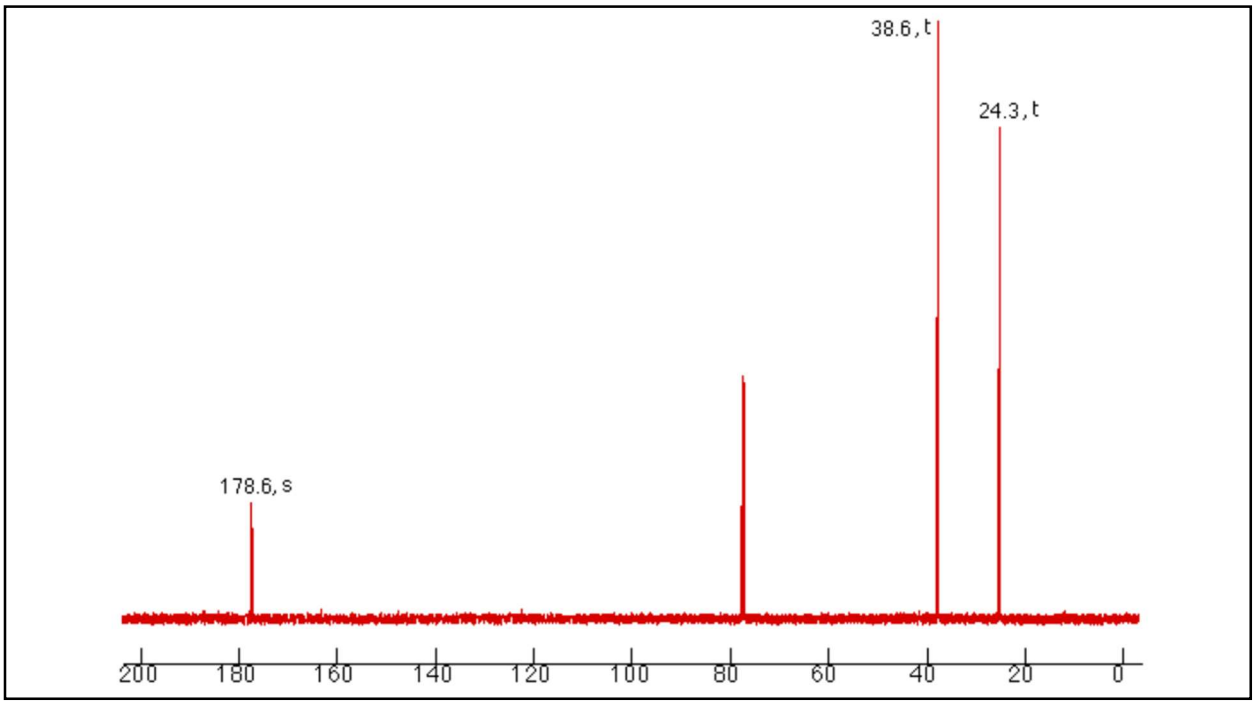
IR



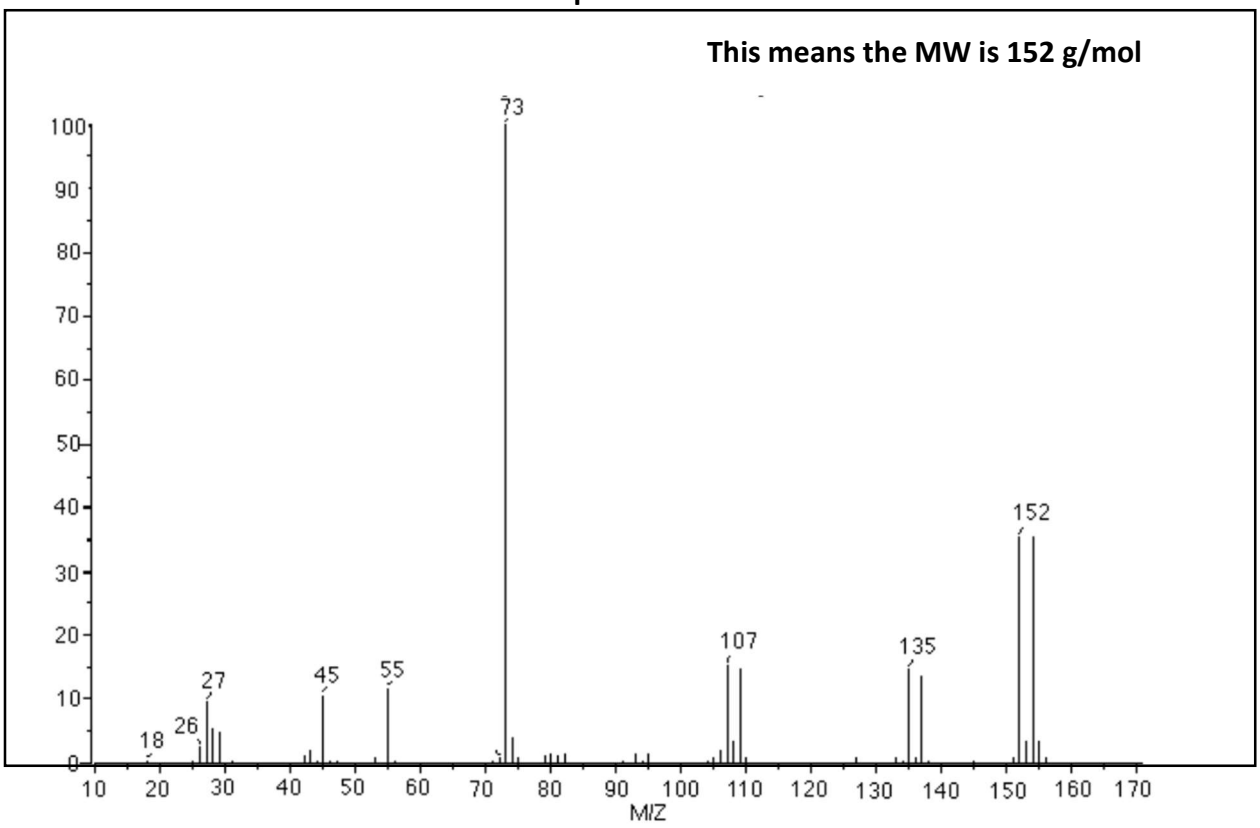
^{1}HNMR



^{13}CNMR

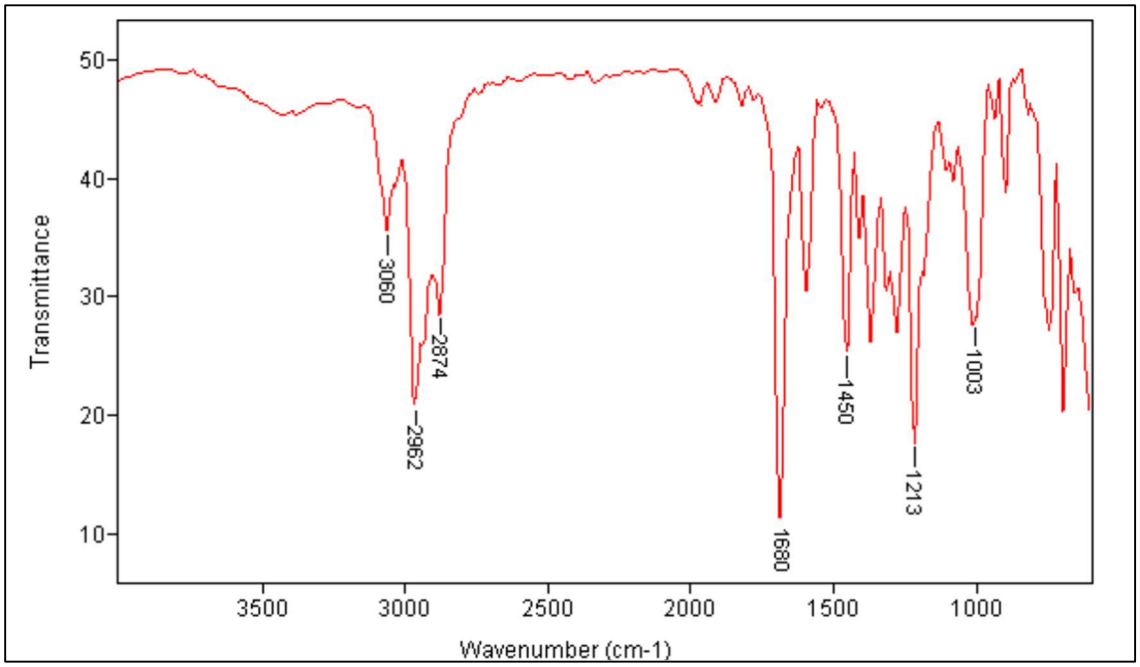


FYI: Mass Spectrum Positive Ion

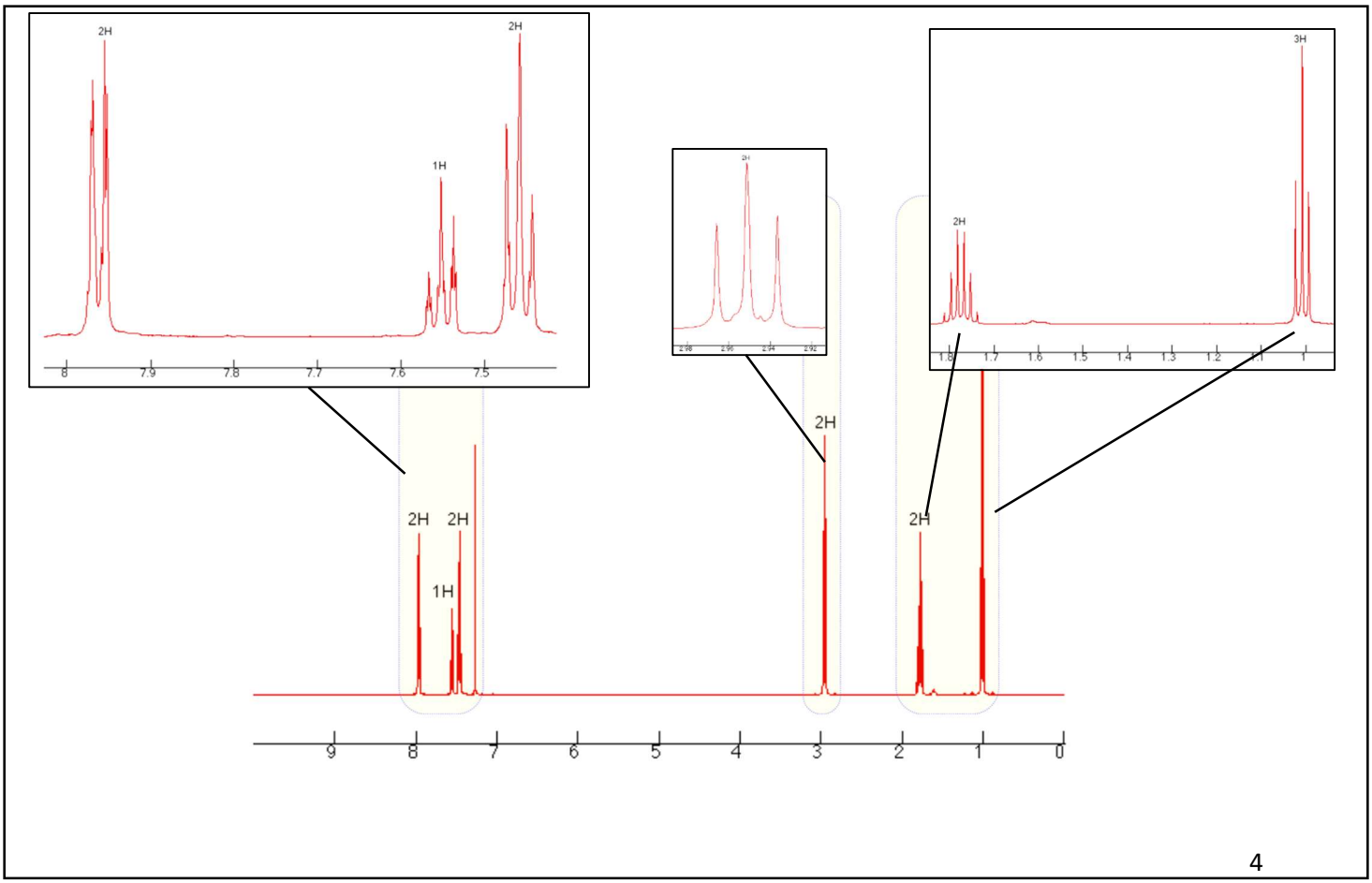


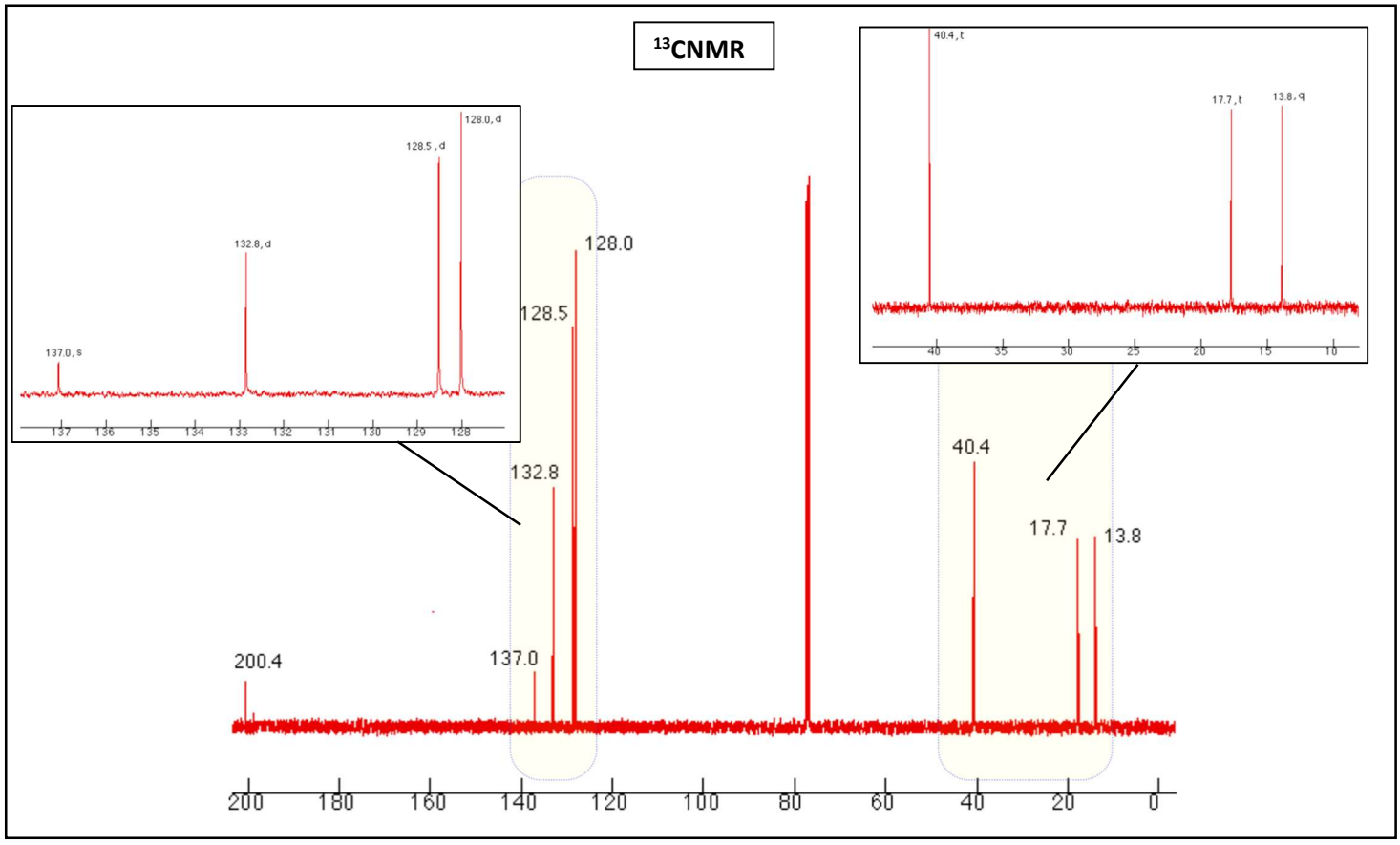
3. Molecular Formula: $C_{10}H_{12}O$ MW = 148

IR

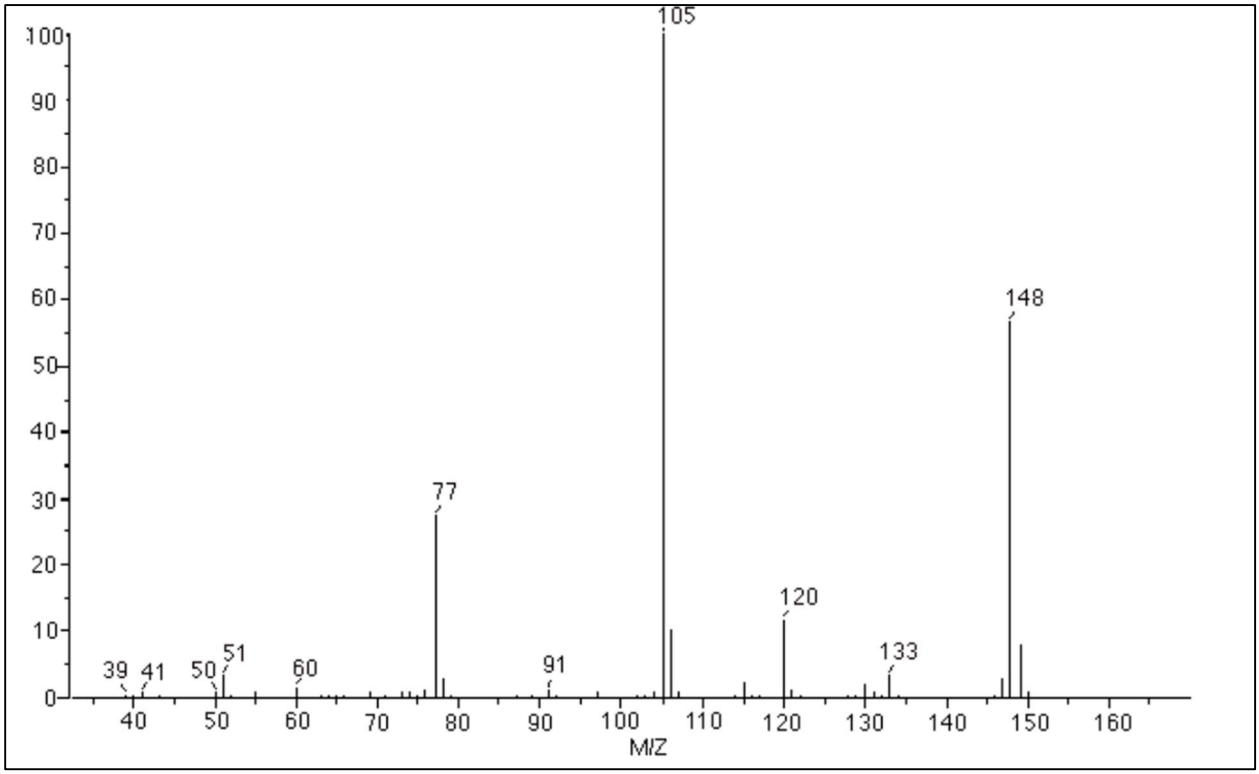


^{1}HNMR



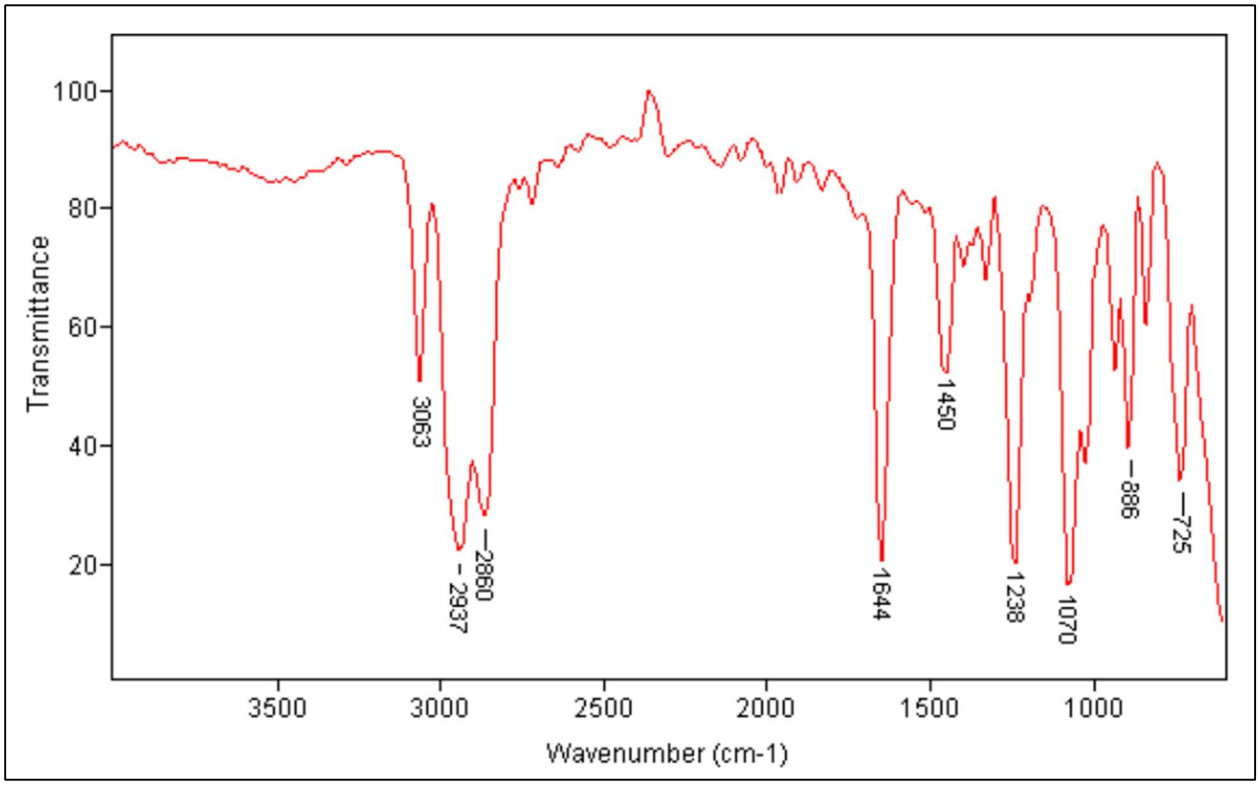


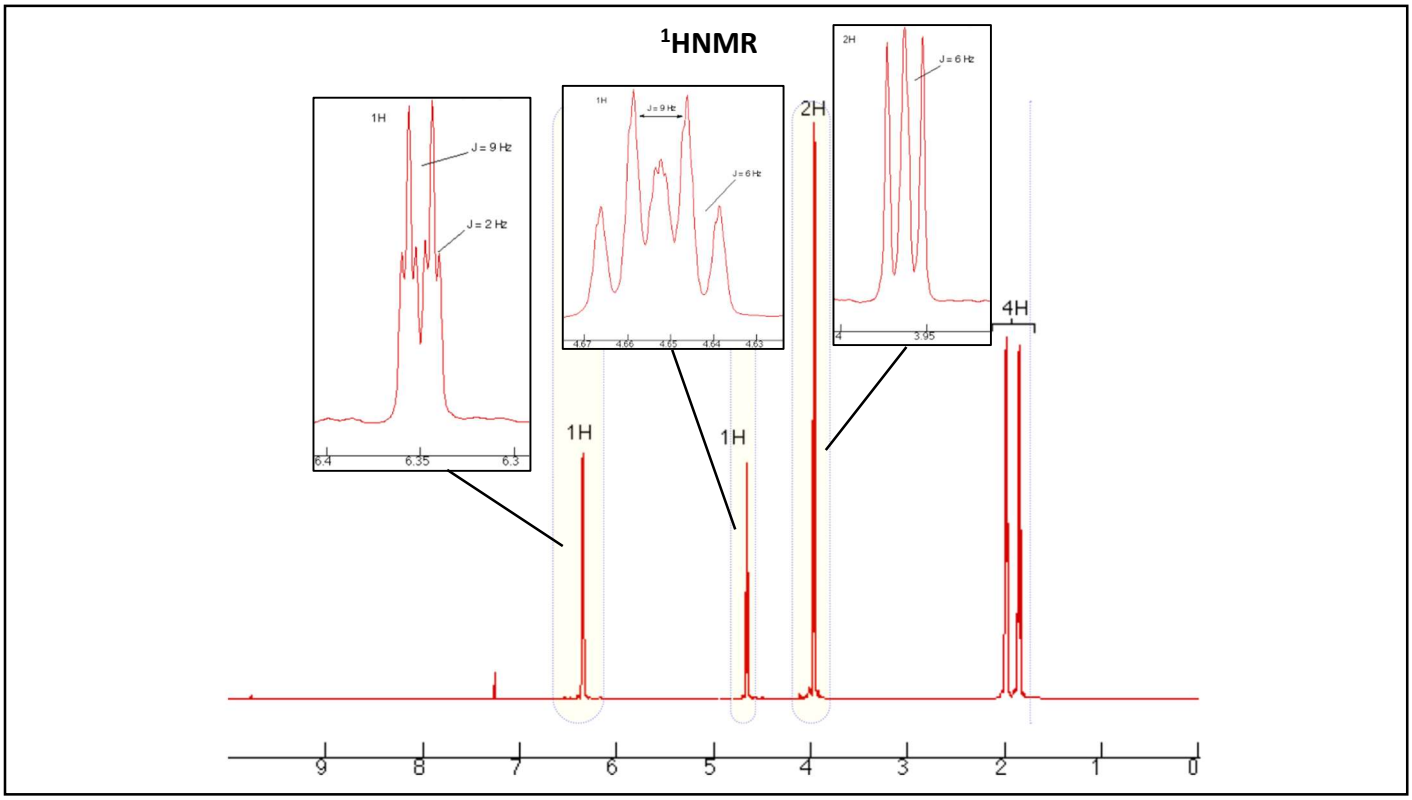
Positive EI Mass Spectrum



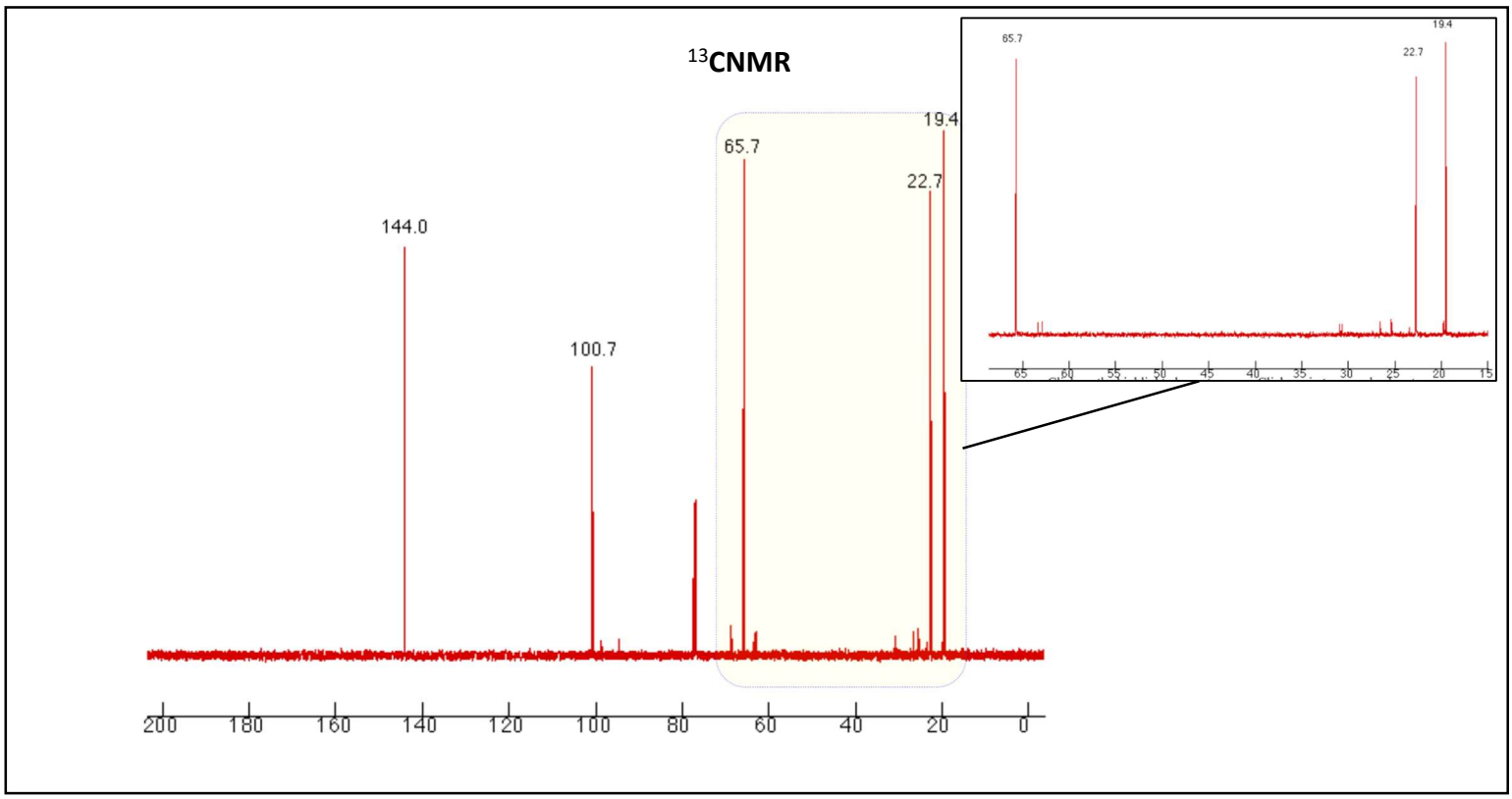
4. Molecular Formula: C_5H_8O MW = 84

IR

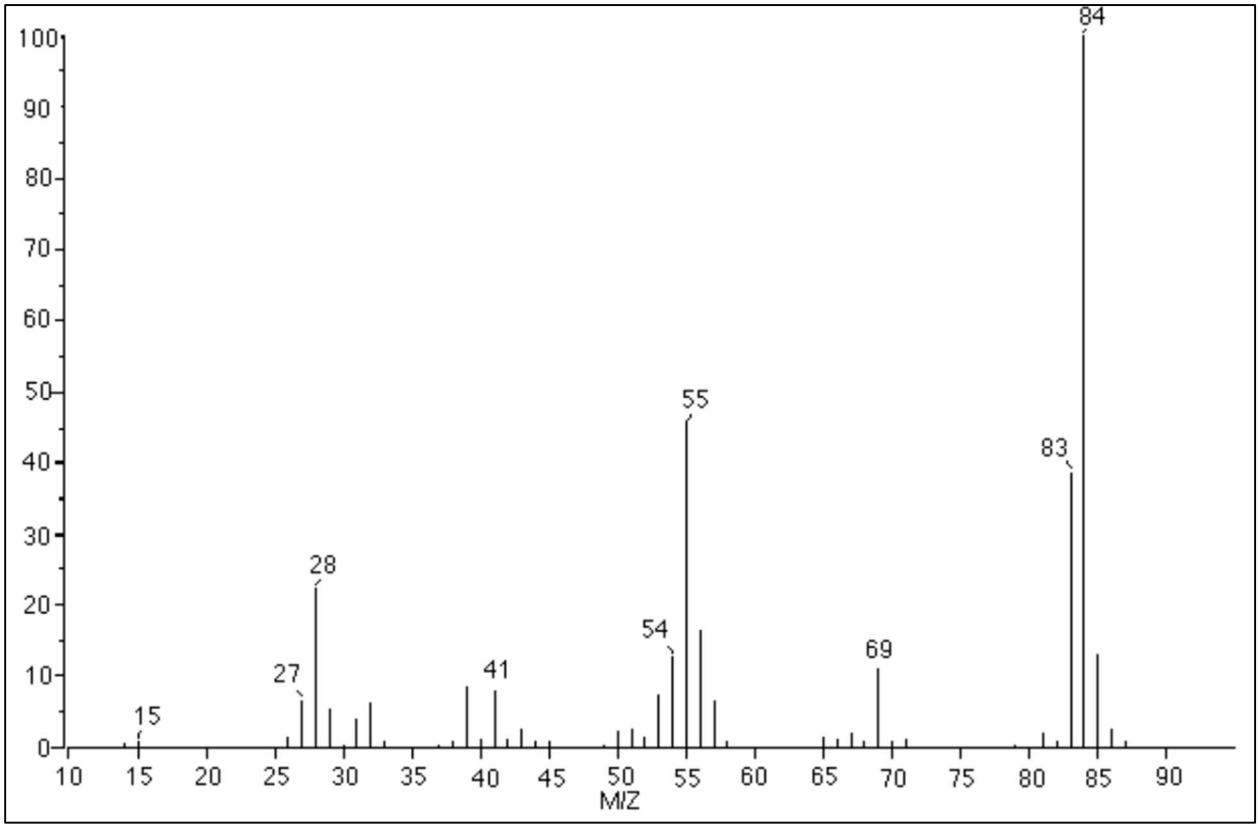




^{13}CNMR

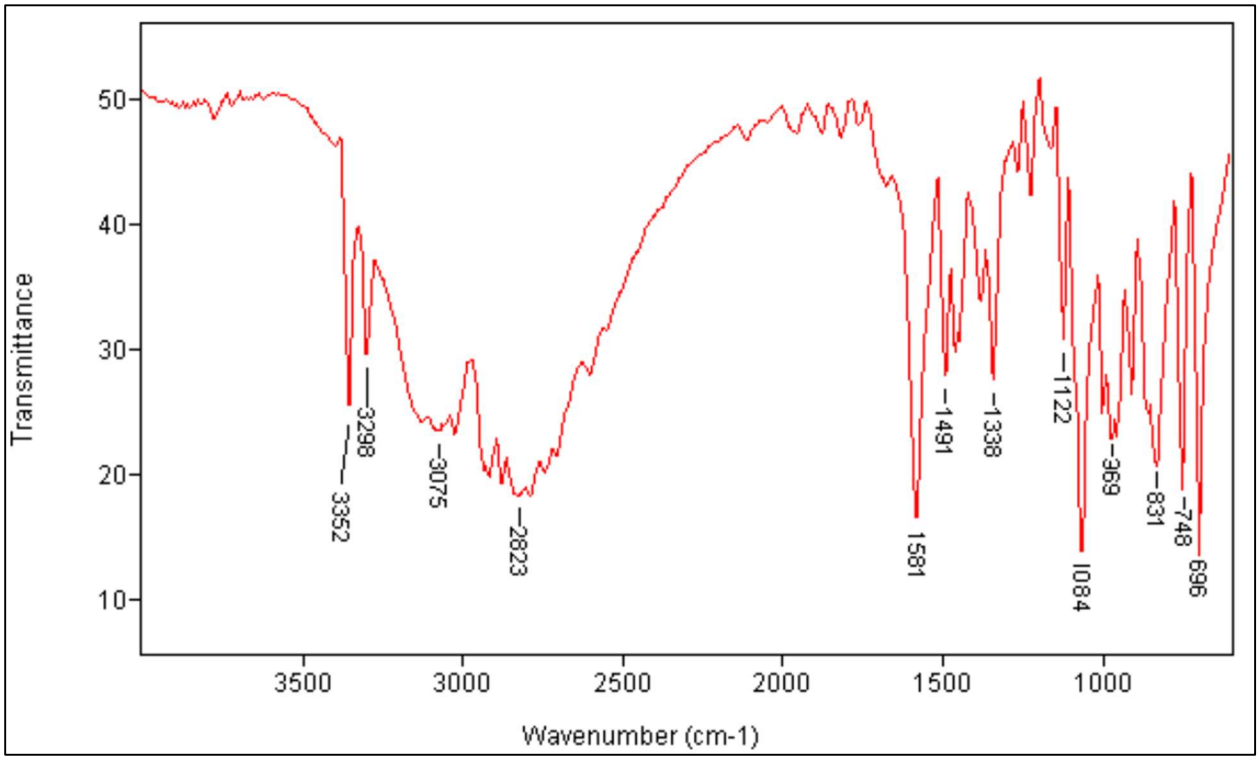


Mass Spec Positive Ion

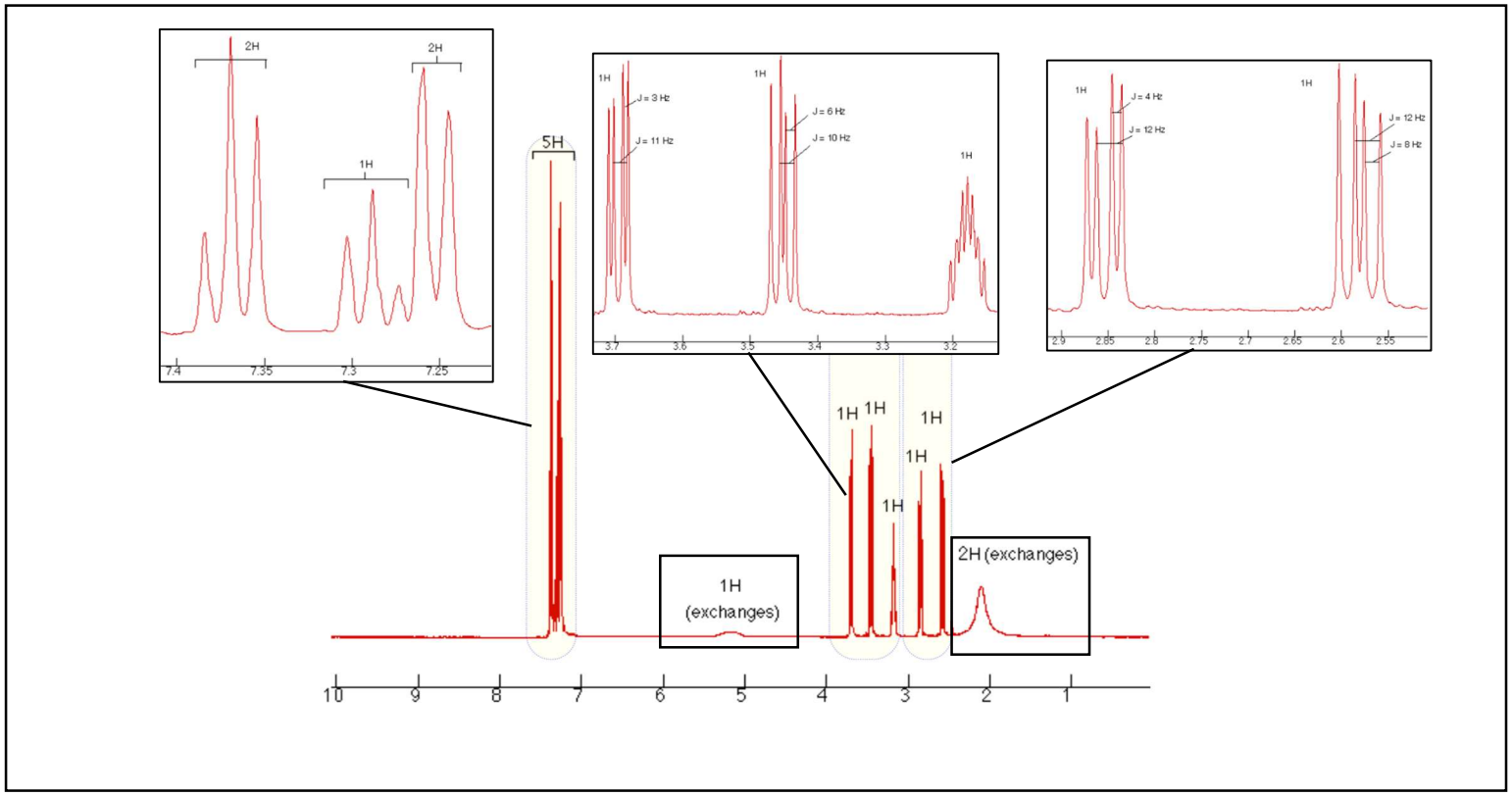


5. Molecular Formula: $C_9H_{13}NO$ MW = 151

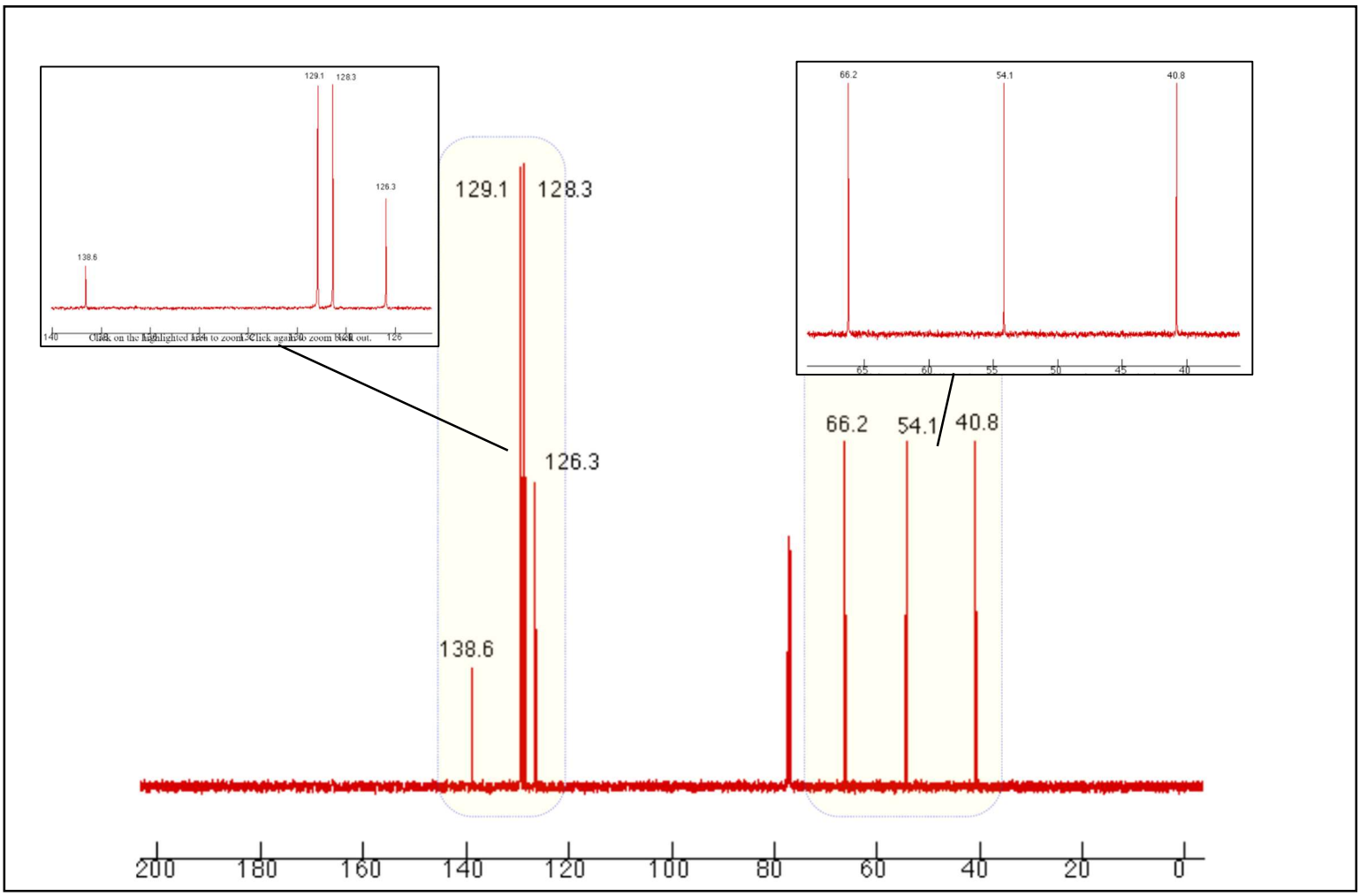
IR



^{1}HNMR



^{13}CNMR



Mass Spec Positive Ion