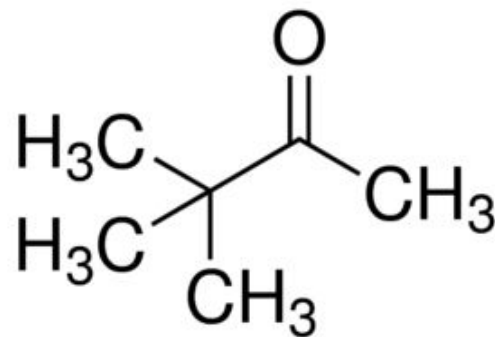


Unknown Project #18

Nancy

Group 1 Section 2

3,3-dimethyl-2-butanone



Transmittance

% Transmittance

IR

Tue Oct 09 16:48:50 2018 (GMT-07:00)

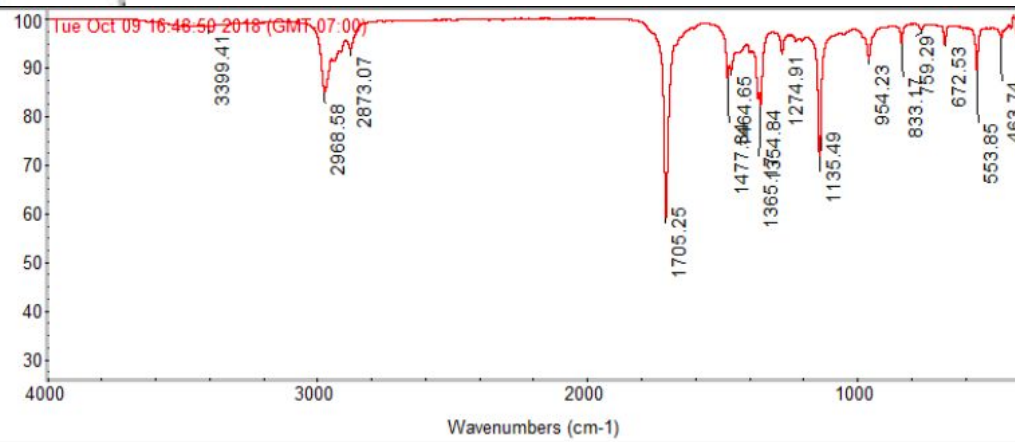
sp³ C-H
stretch

sp³ C-H
bend

C-C
alkane

C-CO-C
bend

C=O Ketone
Stretch



4000

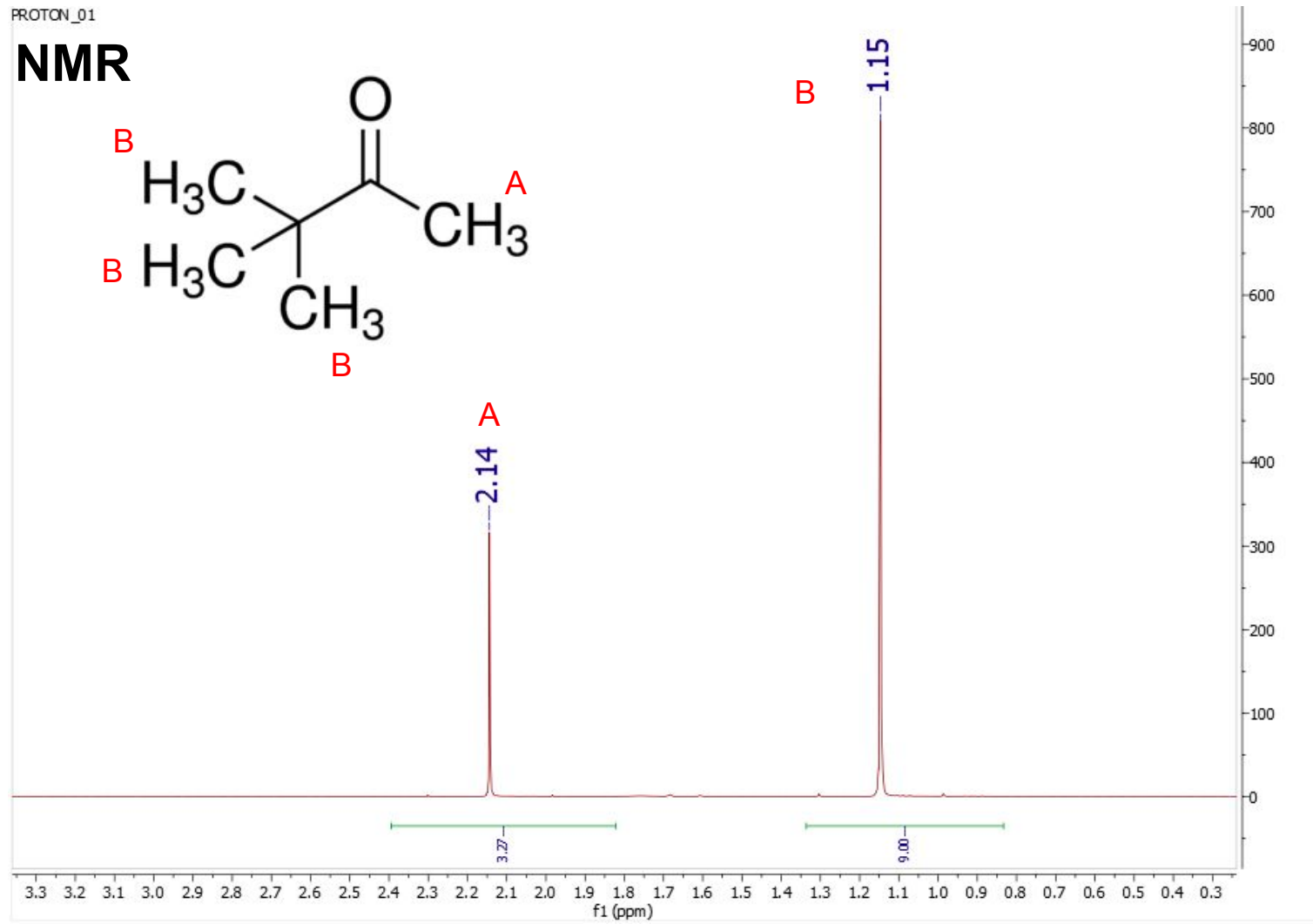
3000

2000

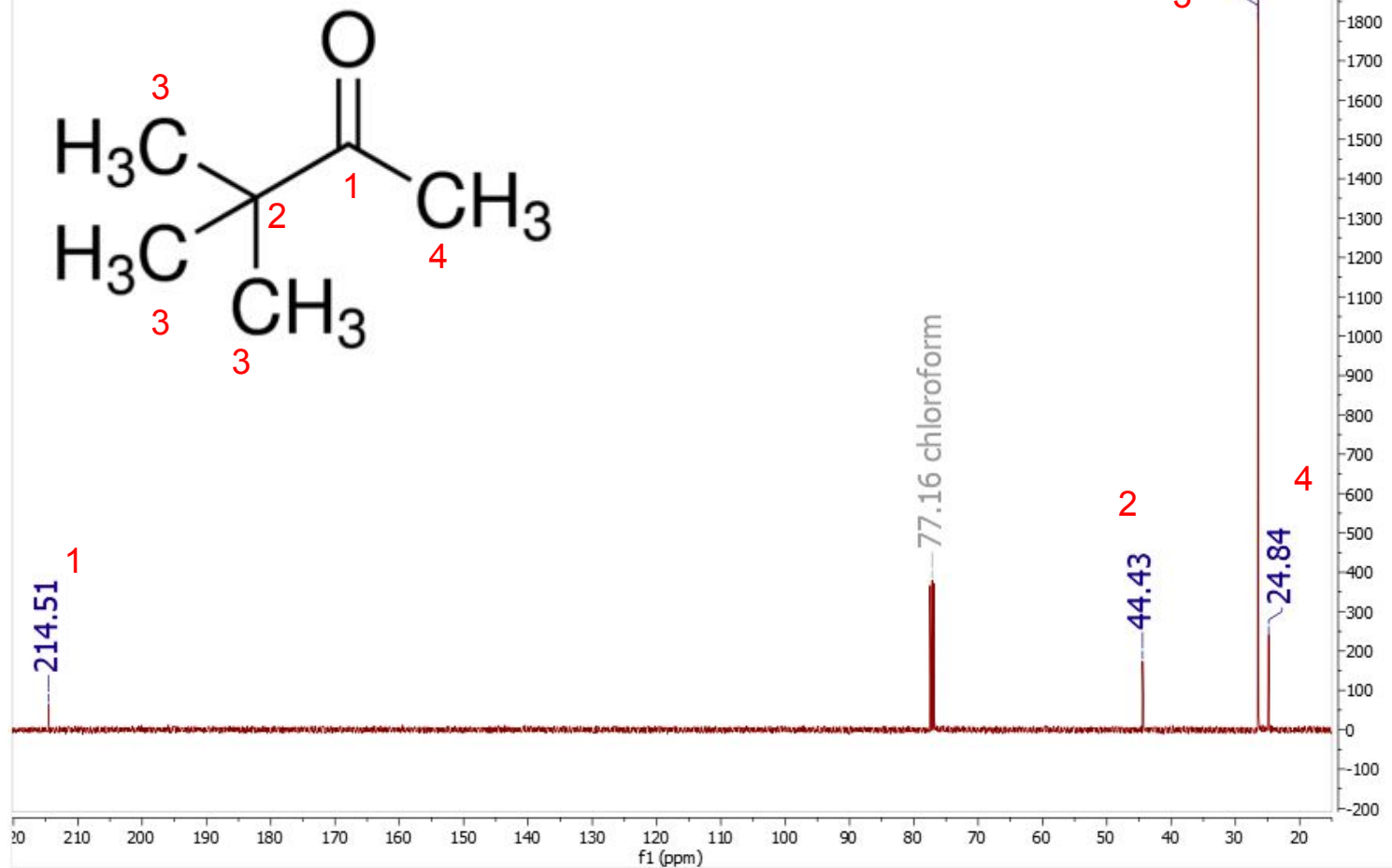
1000

Wavenumbers (cm⁻¹)

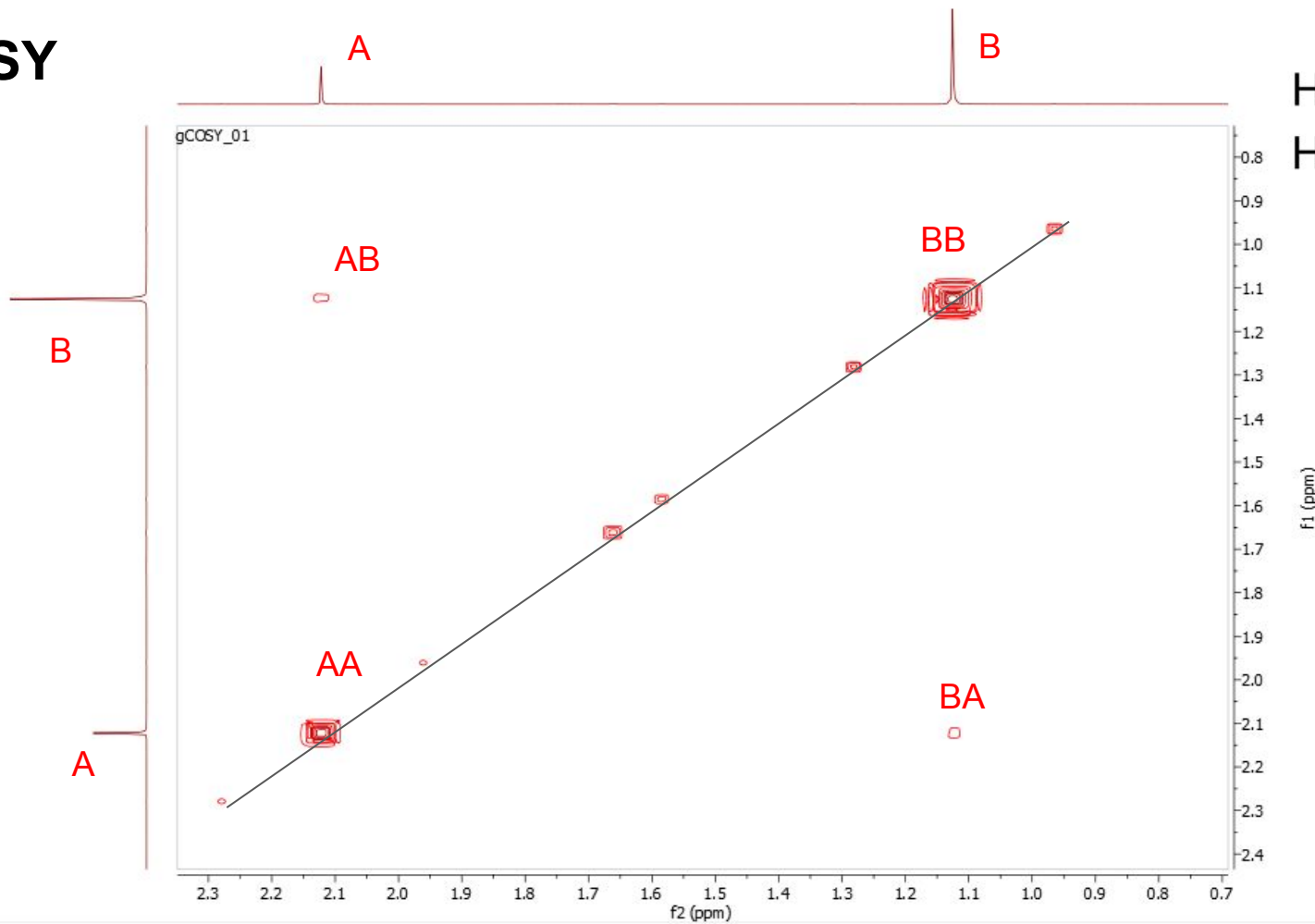
Proton NMR



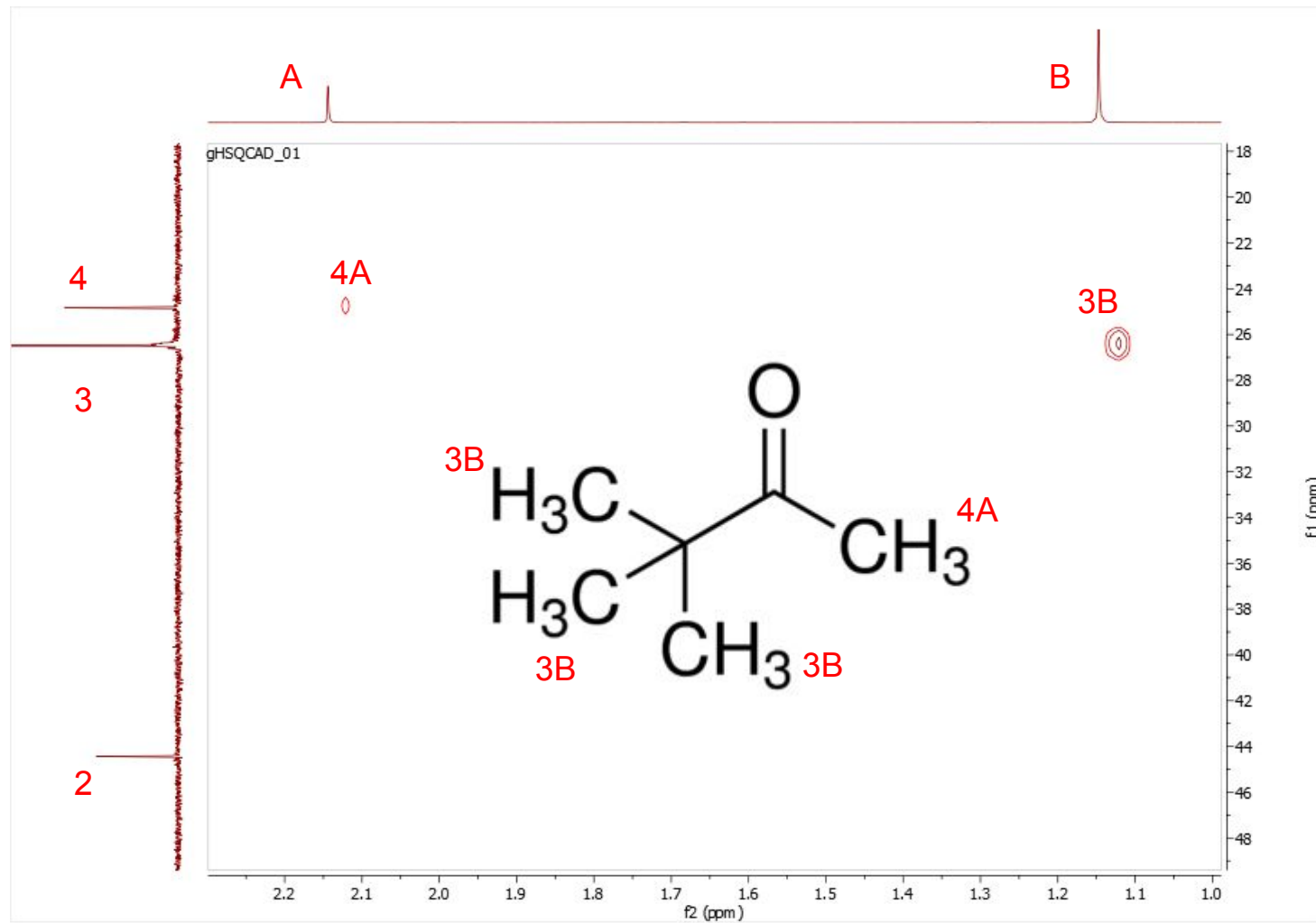
Carbon NMR



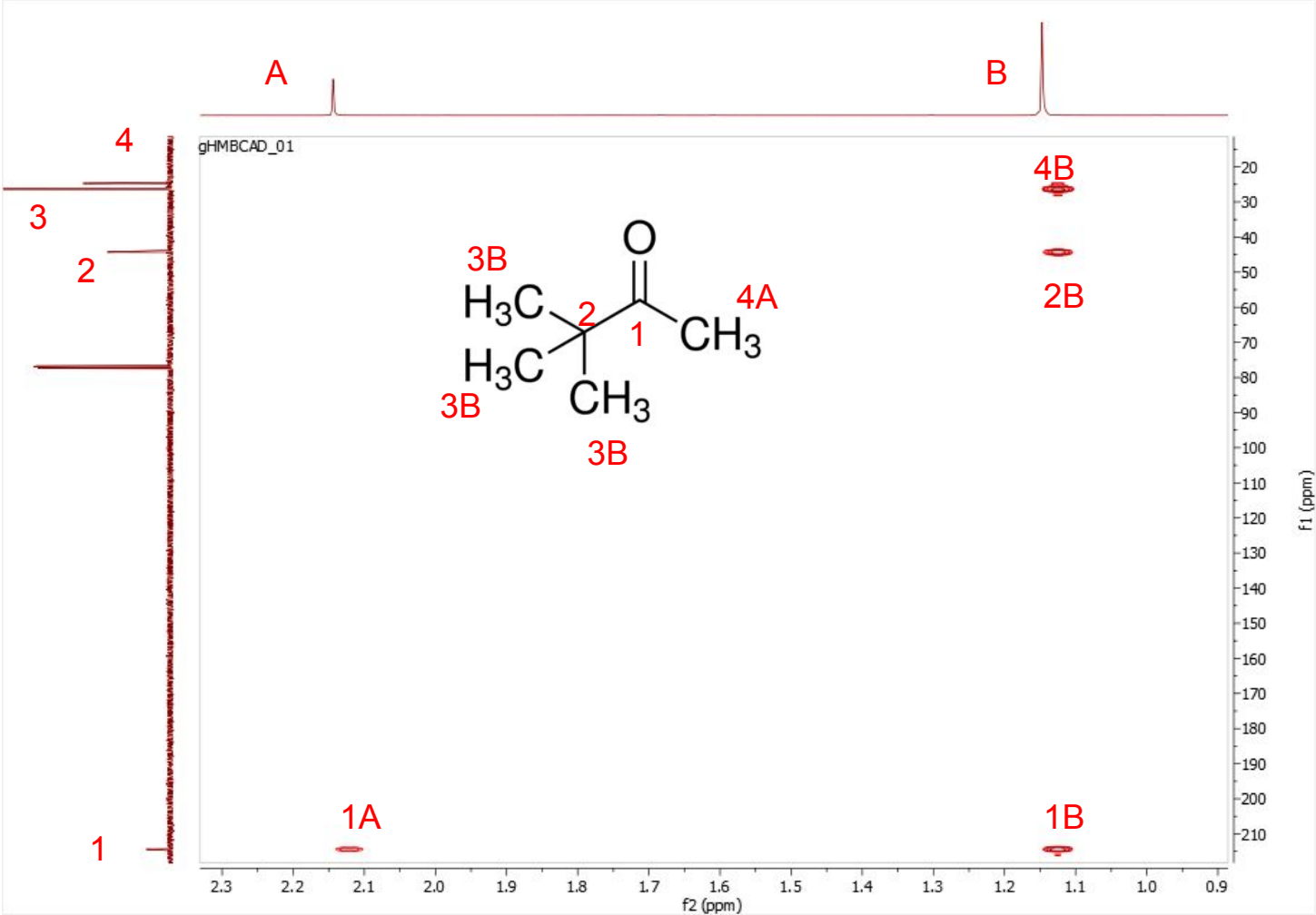
COSY



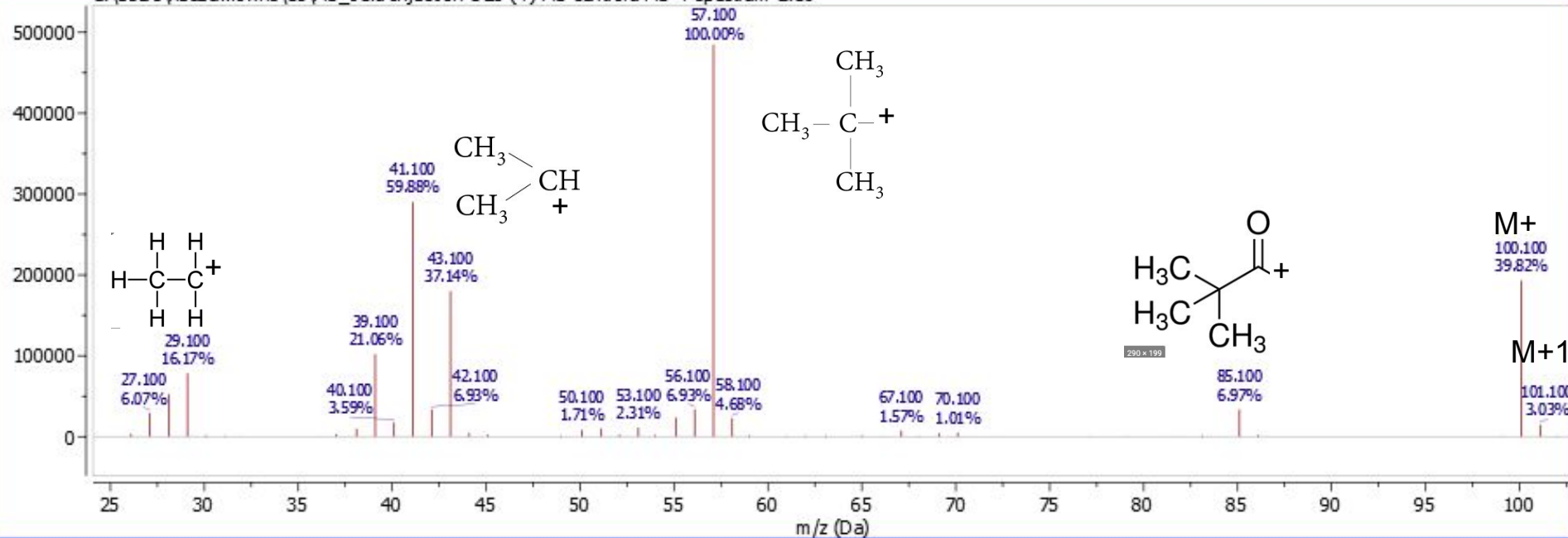
HSQC



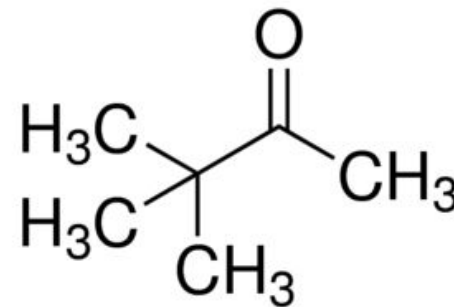
HMBC



C:\Users\mbaba...owns\18\MS_01.d Injection 1 EI (+) MS centroid MS + spectrum 2.16



Mass Spectrum



MS Calculations

Carbon:

$$(3.03/39.82) \times 100\% = 1.1\% (\#C)$$

$$\#C = 6C$$

Nitrogen:

since M^+ is an even value, $\#N$ has to be even

$$(3.03/39.82) \times 100\% = 1.1\%(6) + 0.36\% (\#N)$$

$\#N = 3$, this cannot be therefore, $N=0$

Oxygen:

There is not visible $M+2$ to calculate oxygen.

$$100.1 - 6(12) = 28 \text{ therefore, } 1 \text{ O.}$$

Degree of saturation: $6 - (12/2) + 1 = 1$ carbonyl π bond

Molecular formula: $100.1 - 6(12) - 16 = 12 \text{ H}$, therefore, $MF = C_6H_{12}O$