Colorado State University

CHEM 431 Instrumental Analysis Laboratory

Notes for Determination of Grape Juice Fermentation Using Gas Chromatography-Mass Spectrometry

The following is a set of short notes to outline the experiment in question and to provide helpful guidance to those executing the experiment.

- **A.** Gas chromatography-mass spectrometry (GCMS) is a powerful analytical technique used to separate mixtures for reliable identification of components. The progression of fermentation in grape juice/wine can be tracked through the production of certain chemical species (KEY REFERNCE) identified using GCMS.
- **B.** Develop a procedure for the separation of the species in the mixture that is ten minutes or less in length. Additionally take note of the identification of the species in the mixture.
- **C.** Make five multicomponent standards containing four key chemical species that will fall within the linear range of the instrument? (What resources do you have to determine what you expect to be a reasonable estimate of the linear range?) You will also be presented with three solutions containing grape juice extracts to analyze for the unknown concentrations of your key chemical species.
- **D.** Perform and present a quantitative analysis of the standards and samples. Demonstrate practical use of figures of analytical merit and effectively communicate the level of confidence in the obtained results. At what relative point in the fermentation process are each of the three unknowns?
- **E.** Identify what fragments are **most likely** to have produced the three largest peaks in the **library spectrum** for each of the four of your identified compounds making use of thermochemical data (appearance energy and/or bond energies) to help support your hypotheses. Provide chemical reaction scheme for the formation of each fragment.