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Improving the Mass Spectrometric Analysis of Volatile Components Hyphenated by Gas Chromatography by using AMDIS Deconvolution Software and a Retention Index Database

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Improving the Mass Spectrometric Analysis of Volatile Components Hyphenated by Gas Chromatography by using AMDIS Deconvolution software and a Retention Index database.

A Proposal for the Research and Creative Experience for Undergraduates (RCEU) Program, Summer 2016

Faculty Sponsor: Bernhard Vogler, Department of Chemistry, MSB 321. Phone: 6267

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Project Summary:

In the Natural Products group we have been analyzing samples of aroma plants containing volatile components for a number of years. One of the key issues is to quickly recognize and confirm individual components. Samples often contain 100 or more volatile compounds that with similar structure. Deconvolution of co-eluting compounds is more the rule than the exception. The identification of similar compounds is typically tricky and only achievable by using multiple pieces of information, like mass spectrometry and retention time (retention indices), simultaneously. Thus a robust protocol with simultaneous access to these data is necessary.

Student Duties:

Build a database with reference compounds from existing GC-MS experiments. Improve this database with literature retention indices.

Develop a working protocol to implement AMDIS, **A**utomated **M**ass Spectral **D**econvolution & **I**dentification **S**ystem, a software freely available from NIST, National Institute of Standards and Technology. This software has been demonstrated to be successfully used for the analysis of drug samples and other complex mixtures.

Tentative plan for the 10 week schedule:

Week 1/2: familiarization with GC-MS, GC-MS analysis software such as Chemstation, OpenChrom, and AMDIS.

Week 3/4: building of retention time data files.

Week 5/6: building of in-house target compound libraries from existing GC-MS data sets.

Week 7/8: building of internal standards library.

Week 9/10: Analysis of results.

Establishing measurement parameters:

The RCEU participant will use old data sets to get familiarized with measurements and software. After establishing appropriate measurement parameters we will be building datasets as described above.

Manuscript preparation:

Dr. Vogler encourages all undergraduate student researchers to write up their results in the form of a manuscript for publication. The RCEU participant, under the supervision of Dr. Vogler, will help prepare the manuscript(s), which may include data from other undergraduate or graduate Students.

Expected results and deliverables:

The student will be exposed to important instrumental techniques such as mass spectrometric analysis, gas chromatographic analysis, preparation of samples in smallest concentrations, error analysis, literature studies. Exposure to state of the art instrumental techniques will greatly enhance any students' career chances in chemistry or related disciplines. Instrumental skills are highly regarded.

Faculty Supervision and Mentoring:

GC-MS measurements will be supervised by Dr. Vogler. Manuscript preparation will be supervised by Dr. Vogler. We will hold regular group meetings weekly. The student will have access to the instructor at least once a day. Students that already have completed Organic Chemistry class will be preferred. Other classes are not needed as a prerequisite.