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Quantitative Structure-Property Relationships: Gas Chromatographic Retention Indices of Sesquiterpenoids

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A Proposal for the Research or Creative Experience for Undergraduates (RCEU) Program
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Project Summary: The overall goal of this research is to establish a quantitative structure property relationship (QSPR) between volatile sesquiterpenoids and their gas chromatographic retention indices (RI). The chemical components of essential oils are typically determined using gas chromatography – mass spectrometry (GC-MS). In this technique, both the mass spectral fragmentation patterns as well as the retention properties on the gas chromatographic column are used to reliably determine the identity of a particular compound. We have several essential oils that contain sesquiterpenoid components that are not in our mass spectral fragmentation / retention index database (*i.e.*, they are unidentified sesquiterpenoid components).

The research will involve building the structures (using the molecular modeling program SPARTAN) of sesquiterpenoids for which both chemical structure and retention indices are known (from our database of essential oil components) and carrying out a conformational analysis using SPARTAN to determine the lowest-energy conformation in the gas phase. The three-dimensional structures will then be used to determine a set of molecular descriptors to correlate with the retention indices of the sesquiterpenoids to arrive at a quantitative structure-property relationship. The QSPR so developed will then be used to help identify the likely structures of the unidentified sesquiterpenoid components in our essential oils: Potential structural candidates, based on mass spectral fragmentation, will be constructed using Spartan and the QSPR used to calculate the RI for these structures, which can then be compared to experimentally determined RI values from our GC-MS measurements. ***We are experienced in QSAR/QSPR***[1] ***as well as GC-MS analysis of essential oil components***.[2]

Student Prerequisites: There are no coursework or academic standing prerequisites. We will instruct and oversee all the student needs to carry out the project. This project does molecular modeling of organic compounds; some understanding of organic chemistry and use of computers would be beneficial.

Student Duties:

Structure and Conformational Analysis of Sesquiterpenoids. The student will use the SPARTAN molecular modeling program to construct and and carry out conformational analyses of the sesquiterpenoids contained in the Adams library of essential oil components.[3]

Determination of the Quantitative Structure-Property Relationship. The student will use the Molegro Modeller software to determine the appropriate chemical descriptors and develop the quantitative structure-property relationship to correlate molecular structures of sesquiterpenoids with gas chromatographic retention indices.

Identification of Unknown Sesquiterpenoid Structures. The student will build the structures of likely sesquiterpenoid candidates using SPARTAN and apply the QSPR to calculate RI values for the structures. Based on this information, tentative identification of unknown sesquiterpenoid structures can be made.

Manuscript Preparation. Dr. Setzer 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. Setzer, will help prepare the manuscript(s), which may include data from other undergraduate or graduate students.

Expected Results and Deliverables. Familiarization with the SPARTAN software, building sesquiterpenoid structures and conformational analysis will take approximately one month. Familiarization with the Molegro Modeller software and development of the QSPR will probably take two weeks. Analysis (building likely structures and RI calculation) of unidentified sesquiterpenoid components will be ongoing until the end of the summer term. The results of this molecular modeling / QSPR project will be a useful addition to our toolkit for identification of essential oil components.

Mentor Supervision and Interaction: All computational work, software familiarization, and data analysis will be supervised by Dr. Setzer and computational chemistry collaborator, Dr. Kendall Byler. Manuscript preparation will be supervised by Dr. Setzer. We will hold regular group meetings each week. The student will be supervised by Dr. Setzer every day during the conduct of this research. Dr. Setzer's office (MSB 315) is next door to the departmental computer facility (MSB 317), so he will be available at all times during the day and evenings for consultation. The student's work will fit directly into our overall efforts in chemical compositions of essential oils. In addition, the project is ideal in terms of scope for an undergraduate summer research project. Dr. Setzer has a good track record in working with undergraduate researchers (more than 170 individuals at UAH) and publishing their results (56 peer-reviewed publications based on undergraduate research have appeared since 2010).

References

1. Yongye AB, Byler K, Santos R, Martinez-Mayorga K, Maggiora GM, Medina-Franco JL. Consensus models of activity landscapes with multiple chemical, conformer, and property representations. *Journal of Chemical Information and Modeling*, **2011**, *51*, 1259-1270.
2. da Silva JKR, Gomes MVS, Dosoky NS, Maia JGS, Setzer WN. Chemical composition and biological activities of essential oil chemotypes of *Licaria rigida* (Kosterm.) Kosterm. (Lauraceae). *International Journal of Applied Research in Natural Products*, **2016**, *9*(3), 1-9.
3. Adams RP. *Identification of Essential Oil Components by Gas Chromatography / Mass Spectrometry*, 4th Ed. Allured Publishing, Carol Stream, Illinois, 2007.