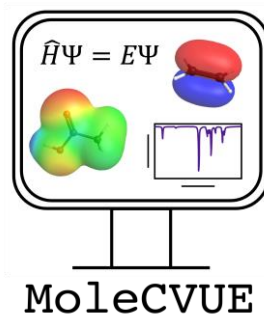




Talk Title or Theme: **Bringing Computational Chemistry into the Classroom**



Speakers Names: Heidi Hendrickson, Carl Salter, Lorena Tribe

Speaker Affiliation: Lafayette College, Moravian University, Penn State University Berks

Speaker Biographical Information: See speaker website links, below.

<https://sites.lafayette.edu/hendrihe/>

<https://www.moravian.edu/chemistry/faculty/salter>

<https://berks.psu.edu/person/lorena-tribe>

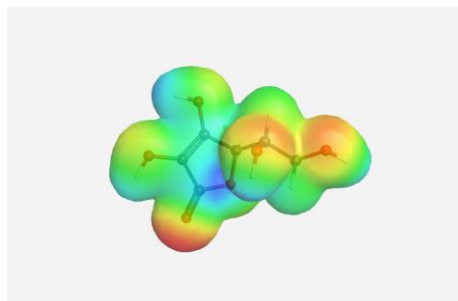
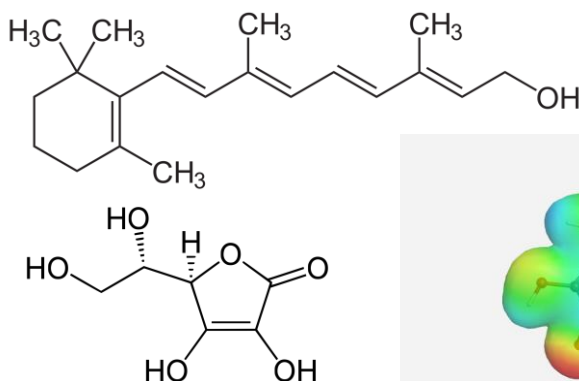
Talk Abstract or Program Description: The program will be an introduction on the use of WebMO and Gaussian calculations in the chemistry classroom. In the past, semi-empirical and *ab initio* calculations were often tied to computers programs with software locks, or to desktops computers with licenses. Those days are over! Thanks to WebMO, now calculations can be done over the web, and all students need is a computer or tablet running a browser. Bring your laptop as we show you how to do three simple computational activities that are appropriate for General and Organic Chemistry classes. We'll investigate a periodic trend, the bond angle in H₂O, H₂S, and H₂Se; we'll look at the solubility of vitamins, and we'll predict the energy change that takes place in simple reactions involving electron or proton addition.

Our presentation follows the outline of the MoleCVUE workshop given at the BCCE meeting at Purdue last August. The suite of activities can be found at <https://sites.google.com/view/molecvue/bcce2022>

For more about WebMO see <https://www.webmo.net/>

For more about Gaussian see <https://gaussian.com/>

Meeting Organizer Contact Information: Carl Salter salterc@moravian.edu



Solubility of Vitamins