

**CHEMISTRY SEMINAR 291****Walking in the Woods with Quantum Chemistry—Unexpected Discoveries
in the World of Terpene Biosynthesis**

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Location: COB1 267

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When the steepest descent pathway following a transition state structure for a given reaction splits in two, the reaction is said to involve a post-transition state bifurcation (PTSB). The presence of a PTSB presents complications for predicting product selectivity, in that a single transition state structure allows direct access to two products without any intervening minima (intermediates). Examples of reactions from natural products biosynthesis for which PTSBs have been proposed will be discussed, along with emerging guidelines for predicting the existence of a PTSB and the selectivity that arises from its presence.

About the Speaker

Research in the Tantillo group is driven by puzzling mechanistic questions. The group is particularly interested in elucidating the origins of low activation barriers and high regio- and stereoselectivities for various cascade polycyclization reactions used by Nature and by organic chemists to synthesize complex natural products, in designing new metal-promoted pericyclic reactions, and in applying quantum chemical predictions of NMR spectra to structure elucidation. A synergistic combination of theory and experiment is used to tackle such problems.

For more information, visit :
<https://bit.ly/2ZBDQa6>