Walking In the Woods with Quantum Chemistry

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Unusual intermediates and transition state structures encountered in our theoretical studies on carbocation cascade polycyclization reactions leading to terpene natural products will be described with an emphasis on the nature of delocalization in these carbocations. The ability of functional groups in enzyme active sites to modulate this delocalization will be highlighted. The use of computed 1H and 13C NMR chemical shifts as a tool to assign the structures of terpene natural products will also be discussed.