MCKENSIE MASON#, THEUNIS VAN AARDT, and JON SERRA, Department of Natural Sciences and Mathematics, West Liberty University, West Liberty, WV, 26074. **Quantum mechanical structure elucidation of the aldol transition state**.

The reaction between methyl 2-methoxyphenylacetate and 4-methoxy-2-O-methoxymethylbenzaldehyde to form the aldol product methyl 3-hydroxy-2-(2”-methoxyphenyl)-3-(2’-O-methoxymethyl-4’-methoxyphenyl)propanoate is significant in the current study of the synthesis of trans-pterocarpans, a non-naturally occurring isomer of an isoflavonoid with potentially increased steroid-like properties. The aldol reaction is believed to first involve the transformation of one carbonyl compound by base into its enolate ion, and then form a six-membered ring transition state involving the two carbonyl compounds and a metal ion, which dictates the stereochemistry of the product. To investigate the energetic favorability of such a transition state, Spartan 14 molecular modeling software was used with the B3LYP theoretical model and 6-31G* basis set, selected for their accuracy with large organic molecules and molecular charges as well as reasonable calculation time. Equilibrium geometry optimization and energy profile calculations of models of the connecting phenylacetate compound, represented both as a carbonyl and as an ylide species, with the benzaldehyde compound showed a lowest-energy conformation with the two oxygen anions in a syn orientation, consistent with the orientation necessary for the proposed transition state. Furthermore, a geometry optimization containing a six-membered ring with a lithium cation successfully converged in a boat conformation.