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Graph theoretical techniques in exploring selectivity and mechanism in terpene synthases.

The Chemical Abstracts Service reports that over 60 million compounds have been produced through synthetic chemistry over the past 20 years and the combined academic and commercial collections of small molecules worldwide are at an estimate of above 100 million. A point to note however is that these large numbers cannot ascertain efficacy, absence of side effects and toxicity, thus the need for computational drug design to search for innovative structures that may display better selectivity and efficacy. However due to the restrictive population space of algorithm application the innovative potential is limited. Various mechanism on the formation of terpenes have been presented, however this information is not suffice to address the whole reaction mechanism. In consideration, the establishment of the GDB-17 database a huge chemical database has demonstrated that graph theoretic approaches are powerful. It is therefore in the light of the principles of the graph theory, that the interest of this research seeks to employ and modify such techniques so as to perform a rigorous graph theory method, generating a library of monoterpene carbocation which will then be explored in the presence of an enzyme active site via docking and other molecular dynamics(MD), molecular mechanics(MM) and Quntum mechanics(QM) techniques. As a result of the heavy computational power needed to process the compounds generated, the CHPC will be used to, run calculations and establish accurate geometries for the generated compounds in the library through Gausian. Extension of this work will be considered to accommodate monoterpenoid ketones such as camphor, verbenone and fenchone. It is expected that a library of above 800,000-11,000,000 compounds will be generated, and possible reaction mechanisms for terpene formation resolved.

Keywords: Graph theory; reaction mechanism; terpene; docking,

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