# MARTS-DB: The Mechanisms And Reactions of Terpene Synthases DataBase

Engst Martin1,2, Brokeš Martin1,2, Čalounová Tereza1, Tajovská Adéla1, Perković Milana1, Samusevich Raman1, Chatpatanasiri Ratthachat 3, Pluskal Tomáš1

1 Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Flemingovo náměstí 2, Prague, Czech Republic

2 Faculty of Chemical Technology, University of Chemistry and Technology Prague, Technická 5, Prague, Czech Republic

3 *Czech Institute of Informatics, Robotics and Cybernetics (CIIRC), Czech Technical University, Jugoslávských partyzánů 1580/3, 160 00 Prague, Czech Republic*

Terpene synthases (TPS) are enzymes that catalyze some of the most complex reactions in nature, the cyclizations of terpenes, the carbon backbones to the largest group of natural products, terpenoids. On average, more than half of the carbon atoms in a terpene scaffold undergo a change in connectivity or configuration during these enzymatic cascades. Understanding TPS reaction mechanisms remains challenging, often requiring intricate computational modeling and isotopic labeling studies. Moreover, the relationship between TPS sequence and catalytic function is difficult to decipher, and data-driven approaches remain limited due to the lack of comprehensive, high-quality data sources. To address this gap, we introduce the Mechanisms And Reactions of Terpene Synthases DataBase (MARTS-DB)—a manually curated, structured, and searchable database that integrates TPS enzymes, the terpenes they produce, and their detailed reaction mechanisms. MARTS-DB includes over 2,600 reactions catalyzed by 1,334 annotated enzymes from across all domains of life. Where available, reaction mechanisms are mapped as stepwise cascades. Accessible at https://www.marts-db.org, the database provides advanced search functionality and supports full dataset download in machine-readable formats. It also encourages community contributions to promote continuous growth. By enabling systematic exploration of TPS catalysis, MARTS-DB opens new avenues for computational analysis and machine learning, as recently demonstrated in the prediction of novel terpene synthases.