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Development and mining of a volatile organic compound database

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Volatile organic compounds (VOCs) are small molecules that exhibit high vapor pressure under ambient conditions and have low boiling points. Although VOCs contribute only a small proportion of the total metabolites produced by living organisms, they play an important role in chemical ecology specifically in the biological interactions between organisms and ecosystems. VOCs are also important in the health care field as they are presently used as a biomarker to detect various human diseases. Information on VOCs is scattered in the literature until now; however, there is still no available database describing VOCs and their biological activities. To attain this purpose, we have developed KNApSAcK Metabolite Ecology Database, which contains the information on the relationships between VOCs and their emitting organisms. The KNApSAcK Metabolite Ecology is also linked with the KNApSAcK Core and KNApSAcK Metabolite Activity Database to provide further information on the metabolites and their biological activities. Other than database development, we also applied several data mining algorithms to the accumulated data. We show that VOC based classification of microorganisms is consistent with their classification based on pathogenicity. Furthermore, we show that VOCs of similar chemical structure have similar biological activities. Additionally, in this talk we will discuss briefly about the KNApSAcK family databases and graph clustering algorithms called DPClus and DPClusO, which we have developed, in our laboratory.

Biography

Md. Altaf-Ul-Amin received BSc degree in Electrical and Electronic Engineering from Bangladesh University of Engineering and Technology (BUET), Dhaka, MS degree in Electrical, Electronic and Systems Engineering from Universiti Kebangsaan Malaysia (UKM) and PhD degree from Nara Institute of Science and Technology (NAIST), Japan. He received the best student paper award in the IEEE 10th Asian Test Symposium. Also, he received two other best paper awards as a co-author of journal articles. He previously worked in several universities in Bangladesh, Malaysia and Japan. Currently, he is working as an Associate Professor in Computational Systems Biology Lab of NAIST. He is conducting research on network biology, systems biology, cheminformatics and biological databases.

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