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Peruselab: Improving onscreen chemistry - A comprehensive chemical informatics system

Statement of the Problem: There's a deluge of chemical software available off the shelf or online. Majority of them perform well in addressing the targeted functionality the developers of the respective software intended to solve. Some are good in letting you draw structures of molecules and chemical reactions. Some let you plan and/or search for chemical reactions while some let you conduct a patent search. The list goes on. The lack of comprehensiveness is a consistent gap between all those products. Our ambitious goal is to develop a software to help you – draw publication quality molecular structures, draw chemical reactions & mechanisms, reuse drawings of molecules and reactions that are already drawn, and create illustrations for presentation and publication. The application's core focus is also to help you search for chemical information by all types of names, molecular formula, keyword, generic terms, properties (chemical, physical, spectral, effects, etc.), and any digitized information. Searching by structures includes – identical, substructure, super-structure, and similar structure. The third goal is to help you conduct online analytics to – identify hidden relations between molecular structures and their properties, identify structural fragments or complete structure, to aid structure elucidation. Our last goal is to let chemists, students, and teachers of chemistry, laboratories, and scientists exchange rich information on chemicals and share knowledge. The software is currently in development and an initial version of it will be available by the first week of July. It's an always available rich web application and will run on any device that can run a modern internet browser.

Biography

Velusamy K. Velu obtained his PhD in physical chemistry from the Indian Institute of Technology, Roorkee, India. His research topic was "Kinetic Studies, Mechanism and Micellar Effects on Substitution Reactions of Some O-Substituted Oximes". He later joined Prof Morton E Munk as a Post-Doctoral fellow to research and develop computer applications in chemistry at Arizona State University, Tempe, Arizona, USA. He developed INFERCNMR, an automated 13C NMR spectrum library search and interpretation system. After that he became a fulltime software developer to develop applications for banks to manage hedge funds and electricity utility companies to manage smart meters. During this period, he gained substantial experience in developing applications using modern techniques, tools and usability improvement guidelines. Currently his focus is to combine his training, knowledge, experience, and expertise to develop a comprehensive chemical informatics system that is intuitive, accessible, and economical.

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