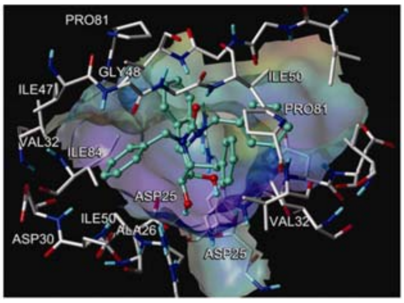
In this issue

Utility of customized scoring functions

Structure-based and ligand-based virtual screening of large chemical libraries plays a key role in lead identification and optimization in rational approaches to pharmaceutical drug discovery. While the former techniques (e.g. 3D-QSAR) lead to good local models that rationalize the structure–activity relations (SAR) in



a given series, they provide limited insights into receptor–ligand interactions. Structure-based methods (e.g. automated docking) depend on scoring functions that are typically not functionalized to reproduce local SAR while doing a good job of producing accurate poses and enriching actives seeded in a decoy set. Govardhan A. Balaji *et al.* (**page 86**) have employed the ability to customize the scoring function associated with Surflex-dock technology to develop HIV-1 protease inhibitor-specific scoring functions using a well-defined training set of cyclic urea compounds. These scoring functions are developed using the top-ranked docked poses of the training set ligands which are qualitatively consistent with experimental data, in that they possess all the key hydrogen bonding (with backbone NH of Ile150 and side chain carboxylates of Asp25) and hydrophobic interactions with the active site residues. The study highlights the significance of various docking features such as protein flexibility, fragment-based core constraints and sampling of the docking space in optimization of docking scores. Applying customized scoring functions improved correlation between experimental and computed docking scores and thus enabled better rationalization of SAR. In addition, the tuned scoring functions show utility in recovery of actives in enrichment studies. Such studies lend themselves to identification of novel ligands as potential HIV-1 inhibitors from the pool of chemical libraries whose activities against HIV-1 Protease are unknown.

Role of boron in plants

The exciting developments in boron research in the past few years greatly contributed to better understanding of the role of boron in plants. Its essentiality as a micronutrient for plants was provided way back in 1923 by Warington. Globally boron deficiency has widely been recognized among micronutrients. Pertaining to its role in plants, a close relationship has been observed between the primary cell wall and boron nutrition. Besides, boron also plays an important role in maintaining plasma membrane integrity, possibly by linking glycoprotein and glycolipid components of the plasma membrane bilayer through its ability to complex OH-containing polysaccharides or through its involvement in enzyme systems, such as ATPases or esterases, which become active on pollen hydration. Unlike vegetative growth, it has been observed that in most plant species the boron requirement for reproductive growth is much higher. Boron may be involved in carbohydrate or phenolic metabolism which is central to pollen tube growth. Whatever the mechanism, the role of boron in reproductive growth is particularly striking. It is now well documented that in fruit plants boron is involved in a number of metabolic pathways and can act in the regulation of metabolic processes like photosynthesis, respiration, cell-wall formation, membrane and membrane-associated reactions, reproduction, pollination, pollen germination and pollen tube growth which is likely to increase fruit set, yield and fruit quality. See **page 76**.

India's higher engineering education

Soon after political independence, Prime Minister Jawaharlal Nehru recognized the importance of good engineering education to achieve economic independence. Quickly, five Indian Institutes of Technology were set up, patterned after Massachusetts Institute of Technology. Over the next half century, these IITs produced undergraduate engineers as good as, or even better than, any institution in the world. The great demand for engineers led to an unprecedented mushrooming of the number of institutions and students, mostly in the private sector. This resulted in a sharp decrease in quality, partly due to shortage of qualified teachers and infrastructure. No Indian engineering institution is among the top 200 in the world today, a really pathetic, challenging dilemma. Concerted efforts are urgently needed to provide liberal funding, total autonomy and academic leadership to a few select institutions to encourage world-class postgraduate engineering education, with emphasis on high quality research leading to cited publications, exploitable patents, innovations and entrepreneurship. The goal is to enable some Indian institutions to be among the top 50, later among the top 10 world-class academia, which alone can propel India to be among the three top economies of the world. A case is made out here that it is doable if determined efforts are made: Substantial increase in the number and quality of engineering Ph Ds; Markedly differential salaries for star professors, based on demonstrated competence; Strong research linkages with leading universities abroad including exchange of faculty and students; Purposeful, mutually beneficial academia–industry bonds. See **page 55**.