第399回触媒科学研究所コロキウム

Development of Catalysts, Drugs and Biomaterials: Insights from Theoretical Studies

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Theoretical and computational techniques are used to study complex processes that are required in a wide range of biological, biotechnological and industrial applications. We have applied these techniques to investigate the mechanisms of peptide hydrolysis by aspartyl protease (beta-secretase) and mono- and binuclear metal center containing metalloproteases (insulin degrading enzyme and leucine aminopeptidase, respectively) and their synthetic analogues. In the first step, we have investigated the roles of organic cofactors, metal ions, ligands, second coordination shell residues and the protein environment in the catalytic functioning of these enzymes. In the next step, the knowledge of the roles of metal ions and the ligand environment in the mechanisms of existing synthetic analogues (Pd(II), Cu(II) and Co(III) metal center containing complexes) of enzymes have been combined with the information acquired in the previous step to design more efficient synthetic analogues of peptide cleaving enzymes. Additionally, interactions of small drug like molecules such as activators of insulin degrading enzyme and inhibitors of beta-secretase and Alzheimer's amyloid beta (Aβ) aggregation with their receptors have been investigated.

Self-assembling, bio-inspired fibrous materials that span the nano-to-meso scales provide an exciting opportunity to reinterpret the building blocks used to engineer devices with desired physico-chemical and biomimetic properties. Aβ peptides are biomolecules that are capable of forming a rich variety of materials under diverse conditions. We have created structures of varying length of Aβ fibrils and computed their mechanical properties such as Young's modulus and ultimate tensile strength. It was found that these fibrils possess mechanical properties comparable to the most robust natural polymers (spider silk) and in some cases are comparable to the strongest known materials, such as steel. Due to their mechanical rigidity, strength, and elasticity, biomaterials formed by amyloid fibrils can be used for novel Bio-Nano-Med applications.

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Ph.D. in 2003 at Stockholm University, Stockholm Sweden and postdoctoral training from 2003-2006 at Emory University, Atlanta, USA. He started his independent research career in 2006 at the University of Miami, Miami, USA. In 2013, he became associate professor at the University of Miami. He has received the Wiley Young Investigator Award in 2011 and a fellowship from the Japanese Society of Promotion of Science (JSPS) in 2016. He is an author of 66 scientific articles and 3 book chapters and has given 48 invited talks.