東京大学グローバル COE 特別セミナー

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演題：Computational Approaches to the Elucidation of Olfactory Receptor Structure and the Discovery of Novel Chemosensory Ligands

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Vertebrates recognize and discriminate thousands of odorants of diverse molecular structure. How is this process of molecular recognition accomplished? The identification of an odorant's chemical structure is thought to occur through the combinatorial integration from multiple odorant receptors, each tuned to recognize different molecular features. Thus, by elucidating the molecular specificities of the odorant receptors we will gain a better understanding how information is processed in the olfactory system. In addition, knowledge of the molecular principles underlying odorant recognition will illuminate how these receptors are tuned to bind and discriminate odorous ligands. As an approach to addressing these issues, we have focused on the properties of the "C family" G protein-coupled receptors expressed in the vertebrate olfactory system. This receptor family includes the putative pheromone-sensing receptors of the mammalian vomeronasal system and the amino acid sensing receptors of the fish olfactory system. Our studies utilize computational modeling approaches to reveal the ligand-receptor interactions in amino acid receptors expressed in the fish olfactory system. In addition, we have developed and implemented a high-throughput computational screening strategy to identify novel high affinity receptor agonists. Such ligands provide useful tools for probing the molecular architecture of the receptor ligand binding pocket. Significantly, the top compounds identified in this computational screen also display robust activities as odorants in vivo. Our virtual screening approach should be applicable to the identification of new bioactive molecules for probing the structure of chemosensory receptors and the function of chemosensory systems in vivo.

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