

# AI-Seeded Modeling and Simulations of Chemoreceptor Mechanisms

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Taste and smell are intriguing biological systems in which an array of chemically diverse molecules is recognized by receptor repertoires. Chemosensory receptors, including odorant receptors, trace amine-associated receptors, bitter taste receptors, sweet and umami taste receptors, are the most numerous members of the G protein-coupled receptor (GPCR) superfamily. Despite its high relevance and representation, the chemosensory-GPCRome is structurally poorly characterized and the receptive range of most chemosensory receptors is unknown [1]

Advances in artificial intelligence (AI) are ushering in a new era in molecular modeling [2]. In my talk, I will highlight how AI breakthroughs are advancing our understanding of the molecular mechanisms of chemosensory perception. I will introduce AI-driven protein modeling applications to characterize the binding process of chemosensory GPCRs [3, 4], enabling the discovery of novel chemoreceptor modulators, and, overall, providing new insights into the chemistry and biology of chemosensation.

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