

Invited Talk

Chemistry meets Biology: Chemogenomics in Drug Discovery

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Chemical biology, chemical genetics, and chemogenomics are recent strategies in drug discovery. Although definitions in literature are somehow diffuse and not consistent, a differentiation of the terms shall be attempted here: Chemical biology may be defined as the study of biological systems, e.g. whole cells, under the influence of chemical libraries. If a new phenotype is discovered by the action of a certain substance, the next step is the identification of the responsible target. Chemical genetics is the dedicated study of protein function, e.g. signaling chains, under the influence of ligands which bind to certain proteins or interfere with protein-protein interaction; sometimes orthogonal ligand-protein pairs are generated to achieve selectivity for a certain protein. Chemogenomics defines, in principle, the screening of the chemical universe, i.e. all possible chemical compounds, against the target universe, i.e. all proteins and other potential drug targets. Whereas this task can never be achieved, due to the almost infinite size of the chemical universe, the systematic screening of libraries of congeneric compounds against members of a target family offers unprecedented chances in the search for compounds with significant target or subtype specificity. The presentation will focus on chemogenomics applications in the search for active and highly selective ligands within families of proteases, GPCRs, nuclear receptors, transporters, and kinases.