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Synthetic Analysis, Processing and its Development of a Medicinal Drug Discovery

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Opinion Article

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DESCRIPTION

Medicinal or pharmaceutical chemistry is a scientific discipline that combines chemistry and pharmacy to design and develop pharmaceutical drugs. The discovery, synthesis, and development of new chemical entities with therapeutic potential is the focus of medicinal chemistry. It also entails studying existing drugs, their biological properties, and their Quantitative Structure-Activity Relationships (QSAR). Organic chemistry is combined with biochemistry, computational chemistry, pharmacology, molecular biology, statistics, and physical chemistry to form the highly interdisciplinary science of medicinal chemistry. Organic compounds used as medicines are typically classified as small organic molecules (e.g., atorvastatin, fluticasone, clopidogrel) and "biologics" (infliximab, erythropoietin, insulin glargine), the latter of which are typically medicinal preparations of proteins (natural and recombinant antibodies, hormones, and so on). Metalloid drugs are inorganic and organometallic compounds that can be used as medicines. Examples include platinum, lithium, and gallium-based agents such as cisplatin, lithium carbonate, and gallium nitrate. Medicinal Inorganic Chemistry studies the role of metals in medicine (metallotherapeutics), which includes the study and treatment of diseases and health conditions caused by inorganic metals in biological systems.

Medicinal chemistry, in its most common form, includes synthetic organic chemistry and natural product aspects, as well as computational chemistry in close collaboration with chemical biology, enzymology, and structural biology, all with the goal of discovering and developing new therapeutic agents.

In practise, it entails chemically identifying new chemical entities, followed by systematic, comprehensive synthetic modification to make them suitable for therapeutic use. It entails studying existing drugs and agents in development in terms of their bioactivities (biological activities and properties), i.e., understanding their Structure-Activity Relationships (SAR). Pharmaceutical chemistry is concerned with medicine quality and pharmaceutical product suitability for their intended use. At the biological interface, medicinal chemistry combines to form a set of highly interdisciplinary sciences emphasising organic, physical, and computational emphases alongside biological areas such as biochemistry, molecular biology, pharmacognosy and pharmacology, toxicology, and veterinary and human medicine; these, in conjunction with project management, statistics, and pharmaceutical business practises, systematically oversee changing identified chemical agents susceptibility.

Medicinal drug discovery

Discovery: The discovery of novel active chemical compounds, also known as "hits," which are typically discovered by assaying compounds for a desired biological activity. Initial hits can be obtained by repurposing existing agents towards new pathologic processes, as well as by observing the biologic effects of new or existing natural products derived from bacteria, fungi, plants, and other sources. Furthermore, structural observations of small molecule "fragments" bound to therapeutic targets (enzymes, receptors, etc.) are frequently used to generate hits, with the fragments serving as starting points for the synthesis of more chemically complex forms.

Hit to lead and lead optimization: More chemistry and analysis are required, first to identify "triage" compounds that do not provide series with suitable SAR and chemical properties associated with long-term development potential, and then to improve remaining hit series in terms of the desired primary activity, as well as secondary activities and physiochemical properties, so that the agent will be useful when administered in real patients.

Process chemistry and development: The final stages of synthetic chemistry involve the production of a sufficient quantity and quality of a lead compound to allow large-scale animal testing, followed by human clinical trials. This includes identifying the best drug formulation and optimizing the synthetic route for bulk industrial production. The former is still the domain of medicinal chemistry, whereas the latter includes formulation science (which includes physical and polymer chemistry as well as materials science).

Synthetic analysis: Traditional organic synthesis is not constrained in the same way that medicinal chemistry's synthetic methodology is. Because of the possibility of scaling the preparation, safety is critical. The potential toxicity of reagents affects methodology.

Structural analysis: Pharmaceutical structures are assessed in a variety of ways, including efficacy, stability, and accessibility predictions. Lipinski's rule of five focuses on a compound's number of hydrogen bond donors and acceptors, number of rotatable bonds, surface area, and lipophilicity. Medicinal chemists also use synthetic complexity, chirality, flatness, and aromatic ring count to evaluate or classify their compounds.