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Process and Development of Medicinal Chemistry

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Short Communication

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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 identification, synthesis, and development of new chemical entities suitable for therapeutic use are the focus of medicinal chemistry. It also includes the investigation of currently available drugs, their biological properties, and 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. Compounds used as medicines are typically organic compounds, which are often 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 etc.)

Medicines can also be inorganic and organometallic compounds known as metallodrugs (e.g., platinum, lithium and gallium-based agents such as cisplatin, lithium carbonate and gallium nitrate, respectfully). Medicinal Inorganic Chemistry studies the role of metals in medicine (metallotherapeutics), which includes the study and treatment of diseases and health conditions linked to inorganic metals in biological systems. Several metallotherapeutics have been approved for the treatment of cancer (e.g., Pt, Ru, Gd, Ti, Ge, V, and Ga), antimicrobials (e.g., Ag, Cu, and Ru), diabetes (e.g., V and Cr), broad-spectrum antibiotics (e.g., Bi), and bipolar disorder (e.g., Li). Metallomics, genomics, proteomics, diagnostic agents (e.g., MRI: Gd, Mn; X-ray: Ba, I), and radiopharmaceuticals are also being researched (e.g., 99mTc for diagnostics, 186Re for therapeutics).

Medicinal chemistry, in particular, encompasses synthetic organic chemistry and aspects of natural products, as well as computational chemistry, in close collaboration with chemical biology, enzymology, and structural biology, with the goal of discovering and developing new therapeutic agents. In practice, it entails chemical aspects of identification, followed by systematic, thorough synthetic modification of new chemical entities to make them suitable for therapeutic use.

It entails the synthetic and computational aspects of studying existing drugs and agents in development to their bioactivities (biological activities and properties), i.e., comprehending their structure-activity relationships (SAR) [1]. Pharmaceutical chemistry is concerned with the quality of medicines and the fitness of medicinal products for their intended use .

At the biological interface, medicinal chemistry combines to form a set of highly interdisciplinary sciences, emphasizing 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 practices, systematically oversee altering identified chemical agents such that after phasing out [2,3].

The identification of novel active chemical compounds, often referred to as "hits," which are typically discovered by assaying compounds for a biological activity. Initial hits can be obtained by repurposing existing agents toward new pathologic processes, as well as by observing the biologic effects of new or existing natural products derived from bacteria, fungi, plants, and so on [4].

Furthermore, small molecule are frequently derived from structural observations of "fragments" that bound to therapeutic targets (enzymes, receptors, etc.), where the fragments serve as starting points for the synthesis of more chemically complex forms. Finally, these small molecule generate by mass testing of chemical compounds against biological targets using biochemical or chemo proteomics assays, where the compounds may be from novel synthetic chemical libraries known to have specific properties (kinase inhibitory activity, diversity, or drug-likeness, for example), or from historic chemical compound collections or libraries created through combinatorial chemistry [5,6].

While there are several approaches to identifying and developing molecules, the most successful techniques are based on chemical and biological intuition developed in team environments over years of rigorous practice aimed solely at discovering new therapeutic agents. The final stages of synthetic chemistry involve the creation of a lead compound in sufficient quantity and quality to allow large-scale animal testing, followed by human clinical trials. This includes optimizing the synthetic route for bulk industrial production and identifying the best drug formulation. The former is still the domain of medicinal chemistry, while the latter includes the specialization of formulation science (with its components of physical and polymer chemistry and materials science).

Process synthesis is a synthetic chemistry specialization in medicinal chemistry that aims to adapt and optimize the synthetic route for industrial scale syntheses of hundreds of kilograms or more. It entails thorough knowledge of acceptable synthetic practice in the context of large scale reactions (reaction thermodynamics, economics, safety, etc.). The transition to more stringent Good Manufacturing Practice (GMP) requires materials sourcing, handling, and the chemistry is critical at this stage.

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