Structural Biology in Drug Discovery Through the (Orange) Years

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Structural Biology has significantly influenced drug discovery and development over the past few decades. The use of structural information to design and improve drug molecules trace back to the early 1980s, following the advent of macromolecular X-ray crystallography. In the 1990s significant advancements in computational power and algorithms greatly enhanced the capability of Structure Based Drug Design (SBDD). In the following years, integration of structural information with high-throughput screening, computational chemistry, and chemical biology underscored the potential of SBDD to produce highly effective and specific drugs. Most recently, the incorporation of cryo-electron microscopy (cryo-EM) as structural tool has enabled high-resolution structure determination of systems previously inaccessible thus expanding the space of accessible targets and the breadth of structure-based drug design

The transformation of SBDD from a niche approach to a mainstream strategy in drug discovery can be clearly seen through the several SBDD courses held in Erice (TP) since 1983 as part of the International School of Crystallography. This presentation will provide an overview of the advancements in SBDD (from small molecule design to integration with AI) and will cover pivotal moments in its history as conveyed through these educational sessions, showcasing its transformation and its significant impact on modern therapeutic development.