「EMPOWERING HUMANS: INTEGRATING AI AND ROBOTICS FOR EFFICIENT DRUG DESIGN AND DISCOVERY」

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While significant progress has been made in the drug design and discovery process, it remains an iterative, expensive, and time-consuming process. The manual and segregated nature of the Design, Make, Test, Analyze (DMTA) cycle presents a significant obstacle in drug discovery. Efficiently exploring the vast, drug-like chemical space, while reducing chemist intervention is critical for accelerating this painstaking process. Even more crucial is the need to successfully synthesize proposed compounds in an automated environment. At Iktos, we focus on the close connection between the 'Design' and 'Make' steps, aiming to improve efficiency and reduce costs. To achieve this, we have developed Artificial Intelligence (AI) based tools for design and synthesis planning, integrated with our robotics platform, providing a semi-autonomous DMTA cycle. Our pipeline marries AI with automation, designing novel compounds using our generative AI tool for chemistry (Makya), while enumerating detailed synthetic routes for these compounds with our data-driven retrosynthesis solution (Spaya). By pairing synthetic feasibility (building block availability & cost, named reactions, etc.) with the management of synthesis schedules (factoring in variables including common reaction conditions and building blocks), our smart scheduler (Ilaka) communicates with the robotics platform to carry out a synthesis. This synergistic platform will provide chemists the ability to apply their expert knowledge to guide the drug discovery process. By tethering generative AI to synthetic constraints of a robotics platform, alongside a reaction scheduling interface, Iktos robotics seeks to drastically improve the DMTA iterative cycle, reducing the time and cost of efficient SAR exploration.