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Editorial: Insights in silico methods and artificial intelligence for drug discovery: 2022

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Editorial on the Research Topic
Insights in silico methods and artificial intelligence for drug discovery: 2022

Entering the third decade of the 21st Century, artificial intelligence (AI) continues to offer significant advances in drug discovery (Jiménez-Luna et al., 2021; Jayatunga et al., 2022). When used rationally beyond the hype, AI offers clear promise to advance further basic and applied research (Medina-Franco et al., 2021). At the same time, AI faces challenges to address at different levels. The present Research Topic brings together experts worldwide from industry, academic, not-for-profit, and governmental settings to openly discuss novel insights, recent advances, latest discoveries, and current challenges in the field of In silico Methods and Artificial Intelligence for Drug Discovery.

From an industry point of view, DiNuzzo presents a perspective on how AI enables the modeling and simulation of biological networks to accelerate drug discovery. He emphasizes that the proper combination of the predictive capability of AI with the mechanistic knowledge of modeling and simulation is expected to provide a major contribution to the pharmaceutical industry. DiNuzzo also concludes that AI will be a key player in analyzing biological networks that will deliver substantial progress towards the improvement of drug target identification and validation, qualify potentially associated side-effects, identify the efficacy and toxicity of biomarkers, aid with hypothesis generation, optimal experimental design, and testing for disease understanding and identification of disease biomarkers. McDermott et al. discuss a platform based on AI that aids in the discovery of DNA damaging agents for ultra-rare cancer atypical teratoid rhabdoid tumors (ATRT). Specifically, the authors showed the power of using the public USA's National Cancer Institute (NCI)'s CellMiner Cross Database and Lantern Pharma's proprietary AI and machine learning (ML) RADR® platform to uncover biological insights and potentially new target indications for the acylfulvene derivative drugs LP-100 (Irofulven) and LP-184. Lantern's AI and ML RADR® platform was used to develop a model to test, computationally, if LP-184 would be effective in ATRT patients. RADR® suggested that ATRT would be sensitive to LP-184, which was then validated *in vitro* and *in vivo*. Namba-Nzanguim et al. review how AI is helping to advance antiviral drug discovery in low-resourced settings. Authors shared their perspectives on the benefits, limitations, and pitfalls of AI/ML tools in the discovery of novel antivirals. Namba-Nzanguim et al. also present current and novel data sharing models, including intellectual property-preserving AI/ML. Authors concluded that AI/ML provides a cost-effective solution for developing antivirals, but AI/ML tools depend on improved access to viral assays data and better data integration protocols. Schmitz et al.

introduce a novel methodology to include three-dimensional information on ligands in AI/ML in lead optimization. In their contribution, the authors described their recent work employing the BIOVIA Generative Therapeutics Design application, which is prepared to take advantage of the pharmacophoric representation of desired features in ligand-protein interactions. Schmitz et al. also discuss how the novel Generative Therapeutics Design application can be arranged to generate molecules incorporating characteristics from multiple unrelated molecule series.

In all, the authors, Topic Editor, and the journal of Frontiers in Drug Discovery expect that this special edition Research Topic contributes to shedding light on the progress made in the past decade in the In silico Methods and Artificial Intelligence for Drug Discovery field and on its future challenges. It is anticipated that the article Research Topic will inform, motivate, and offer direction to the scientific community, including researchers and students in the field.

Author contributions

The author confirms being the sole contributor of this work and has approved it for publication.

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Conflict of interest

The author declares that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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