The rise of PlayMolecule

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1. Innovation in Modern Biotechnology

Since the earliest virtual models of molecules and simulations, incredible efforts in technology and methodology have brought forth solutions and tools now employed in the understanding of biomolecular interactions and prediction of their properties.
The development and performance of these solutions were challenged by their diversity but have definitely lead to the increased use of computerized methods in a wide range of research fields, from genomics to drug design.

Acellera has acquired a strong expertise in software development and structural studies over the last 10 years. We designed, alone or in collaboration, innovative solutions for the understanding of critical events for molecular recognition like ligand binding and conformational changes of biomolecules, key steps in the drug design process. Complex protocols combined with the need for high performance infrastructure hampered the access and use of such solutions by the whole scientific community dedicated to Drug Discovery.

To overcome these hurdles, we have developed a specific web platform to provide cutting-edge tools based on molecular dynamics and deep learning applications: www.playmolecule.org. It is a unique repository of applications covering the Drug Design and Drug Discovery pipeline, running on distributed resources. With PlayMolecule, we aim to democratize their use among the whole scientific community, to encourage the exploration of novel chemical space and to accelerate the discovery of molecules of interest.

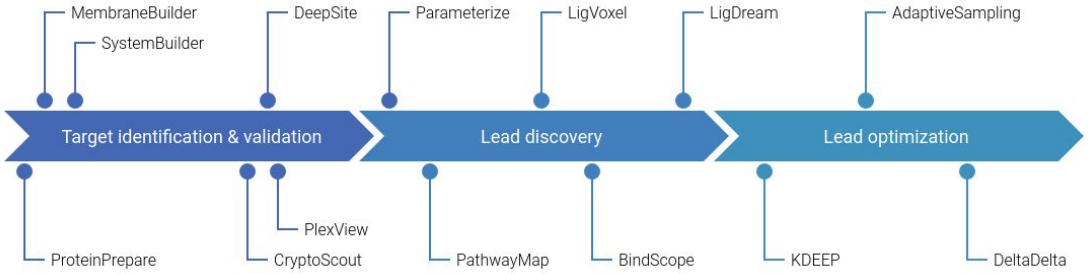

Figure 1 *PlayMolecule applications pipeline*

Miha Skalic, José Jiménez Luna, Davide Sabbadin, and Gianni De Fabritiis; Shape-Based Generative Modeling for de-novo Drug Design, Journal of Chemical Information and Modeling, (2019). https://doi.org/10.1021/acs.jcim.8b00706

José Jiménez, Davide Sabbadin, Alberto Cuzzolin, Gerard Martínez-Rosell, Jacob Gora, John Manchester, José Duca, and Gianni De Fabritiis; PathwayMap: Molecular Pathway Association with Self-Normalizing Neural Networks, Journal of Chemical Information and Modeling, (2018). https://doi.org/10.1021/acs.jcim.8b00711

Miha Skalic, Gerard Martínez-Rosell, José Jiménez, Gianni De Fabritiis; PlayMolecule BindScope: Large scale CNN-based virtual screening on the web, Bioinformatics, (2018) , bty758, https://doi.org/10.1093/bioinformatics/bty758

Miha Skalic, Alejandro Varela-Rial, José Jiménez, Gerard Martínez-Rosell, Gianni De Fabritiis; LigVoxel: Inpainting binding pockets using 3D-convolutional neural networks, Bioinformatics (2018) https://doi.org/10.1093/bioinformatics/bty583

José Jiménez Luna, Miha Skalic, Gerard Martinez-Rosell, and Gianni De Fabritiis. KDEEP: Protein-ligand absolute binding affinity prediction via 3D-convolutional neural networks. Journal of Chemical Information and Modeling. (2018) https://doi.org/10.1021/acs.jcim.7b00650