O1-3

An Enhanced Machine Learning Models for Predicting Retrosynthesis Accessibility

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O2-3

Dynamical interaction analysis of Remdesivir with SARS-CoV-2 RNA-dependent RNA polymerase by MD and FMO calculations

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O3-2

Lipid composition is critical for accurate membrane permeability prediction of large cyclic peptides by molecular dynamics simulations

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O4-2

Hit Identification for SARS-CoV-2 Main Protease Using Convolutional Neural Network

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O5-5

SmilesFormer: Language Model for Molecular Design

Joshua OWOYEMI, Nazim MEDZHIDOV

Elix Inc.

O6-2

Development of protein-ligand binding affinity evaluation method by combining classical MD and FMO calculations

Hiromu MATSUMOTO, Tsuyohiko FUJIGAYA, Koichiro KATO

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O7-2

Force measurement of kinesin-propelled microtubules in swarming using electromagnetic tweezers

Mst Rubaya RASHID[1], Mousumi AKTER[2], Arif Md. Rashedul KABIR[2], Jakia Jannat KEYA[2], Kazuki SADA[1, 2], Akira KAKUGO[1, 2]

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