Survey of SARS-CoV, main protease assays for creating machine-learning models

Goal is to identify CoV related biochemical assay datasets. Other sources of data from NCATS, PubChem Bioassays, CheMBL had been identified and are being reviewed by ATOM team.

- Identification of SARS-CoV-2 3CL Protease Inhibitors by a Quantitative High-throughput Screening

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- A Fluorescence-based High Throughput-Screening assay for the SARS-CoV RNA synthesis complex

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- Structure of papain-like protease from SARS-CoV-2 and its complexes with non-covalent inhibitors

Jerzy Osipiuk, Saara-Anne Azizi, Steve Dvorkin, Michael Endres, Robert Jedrzejczak, Krysten A. Jones, Soowon Kang, Rahul S. Kathayat, Youngchang Kim, Vladislav G. Lisnyak, Samantha L. Maki, Vlad Nicolaescu, Cooper A. Taylor, Christine Tesar, Yu-An Zhang, Zhiyao Zhou, Glenn Randall, Karolina Michalska, Scott A. Snyder, Bryan C. Dickinson, Andrzej Joachimiak
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- Lead compounds for the development of SARS-CoV-2 3CL protease inhibitors

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- A drug repurposing screen identifies hepatitis C antivirals as inhibitors of the SARS-CoV-2 main protease

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