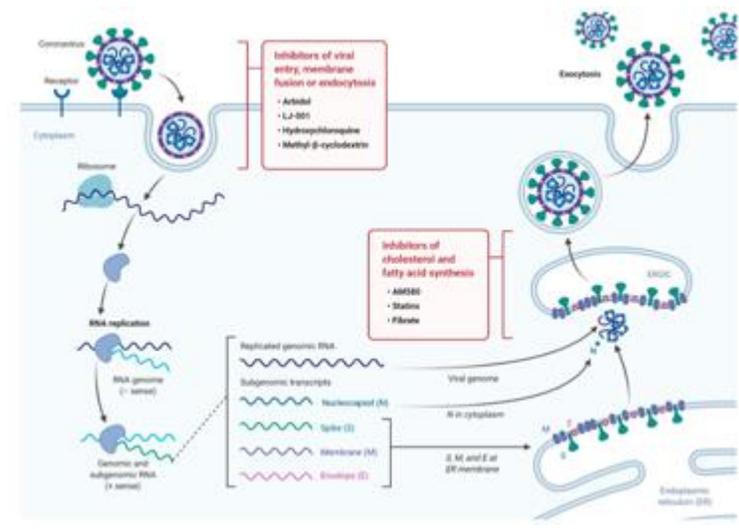


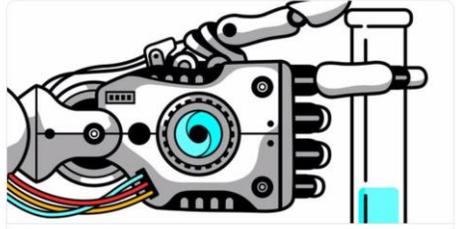
## Structure-based virtual screening of M<sup>Pro</sup>-inhibitors

Design of M<sup>Pro</sup> inhibitors for the treatment of COVID-19



 **Frances Arnold**  
@francesarnold Following

AI in #proteinengineering and drug discovery: chemists who use machines (and #machinelearning) will replace chemists who don't.



**Making New Drugs With a Dose of Artificial Intelligence**  
Researchers at DeepMind, owned by Google's parent company, and other companies are applying their powerful A.I. systems to drug discovery research.  
nytimes.com

7:41 AM - 7 Feb 2019

## Novel prediction methods for small molecule pK<sub>a</sub> values

- ITC-Messungen an der Aspartylprotease Endothiapepsin
- Proteinkristallstrukturbestimmung neuer Endothiapepsin-Ligand-Komplexe
- Covid Moonshot (<https://postera.ai/moonshot>): Neue Wirkstoffe gegen Covid19
- pKa-Messungen und Daten-Analyse von Wirkstoffkandidaten

## Protonation Effects of Endothiapepsin-Fragment Complexes



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