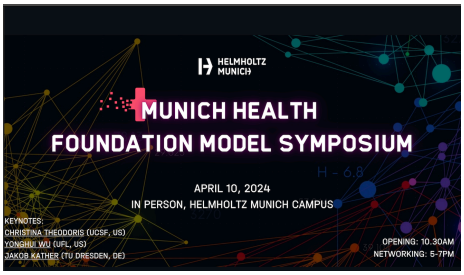

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Pre-trained molecular representations enable antimicrobial discovery

The rise in antimicrobial resistance poses a worldwide threat, reducing the efficacy of common antibiotics. Yet, determining the antimicrobial activity of new chemical compounds through experimental methods is still a time-consuming and costly endeavor.
Compound-centric deep learning models hold the promise to speed up the
search and prioritization process. Here, we introduce a lightweight computational strategy for antimicrobial discovery that builds on MolE
(Molecular representation through redundancy reduced Embedding).
MolE is a non-contrastive self-supervised Graph Neural Network framework
that leverages unlabeled chemical structures to learn task-independent molecular representations. We find that MolE enhances the performance of machine learning algorithms in various molecular property prediction tasks, and fine-tuning the representation for specific applications improves Graph Neural Network-based schemes. By combining a pre-trained MolE representation with experimentally validated compound-bacteria activity data, we build an antimicrobial prediction model that re-discovers recently reported growth-inhibitory compounds that are structurally distinct from current antibiotics. Using the model as a compound prioritization strategy, we identify and experimentally confirm three human-targeted drugs as growth-inhibitors of Staphylococcus aureus, highlighting MolE's potential to accelerate the discovery of new antibiotics.

Primary author: OLAYO ALARCON, Roberto (Institute for Statistics, LMU Munich)

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