16 potential organophosphorus poisoning **antidotes** were chosen from drugs present in ChEMBL database.

Repurposing Pharmaceuticals for Organophosphorus Poisoning

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1 Intro

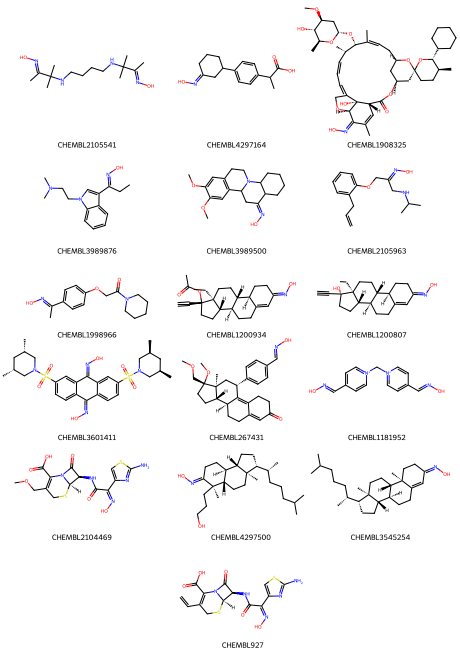
- little interest in developing new therapies
- current drugs poorly penetrate blood-brain-barrier
- what if there are proper chemicals among other drugs?

2 Methods

- training data from PubChem (n=62)
- molecular descriptors, MACCS keys (RDKit)
- LightGBM, LOOCV
- molecules containing oxime moiety from ChEMBL (n=34)

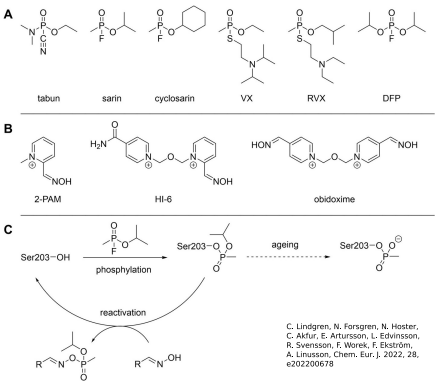
3 Results

- LOOCV ROC AUC = 0.92
- recall = 0.90

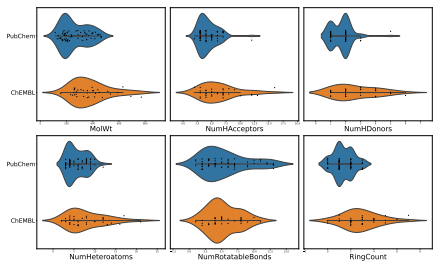


Extra figures

- OP compounds (A), known reactivators (B), inhibition, ageing and reactivation reaction (C)



- chemical space analysis



Next steps

- molecular docking
- molecular dynamics
- QM/MM
- in-vitro evaluation

Interested? Get in touch ↓
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