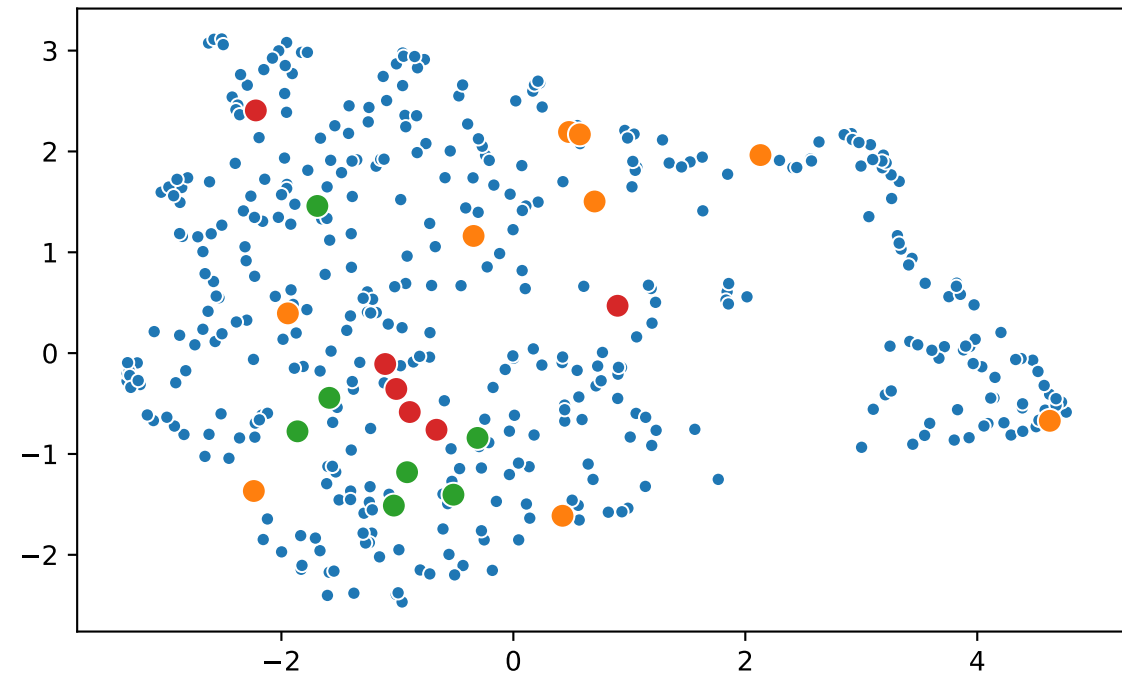
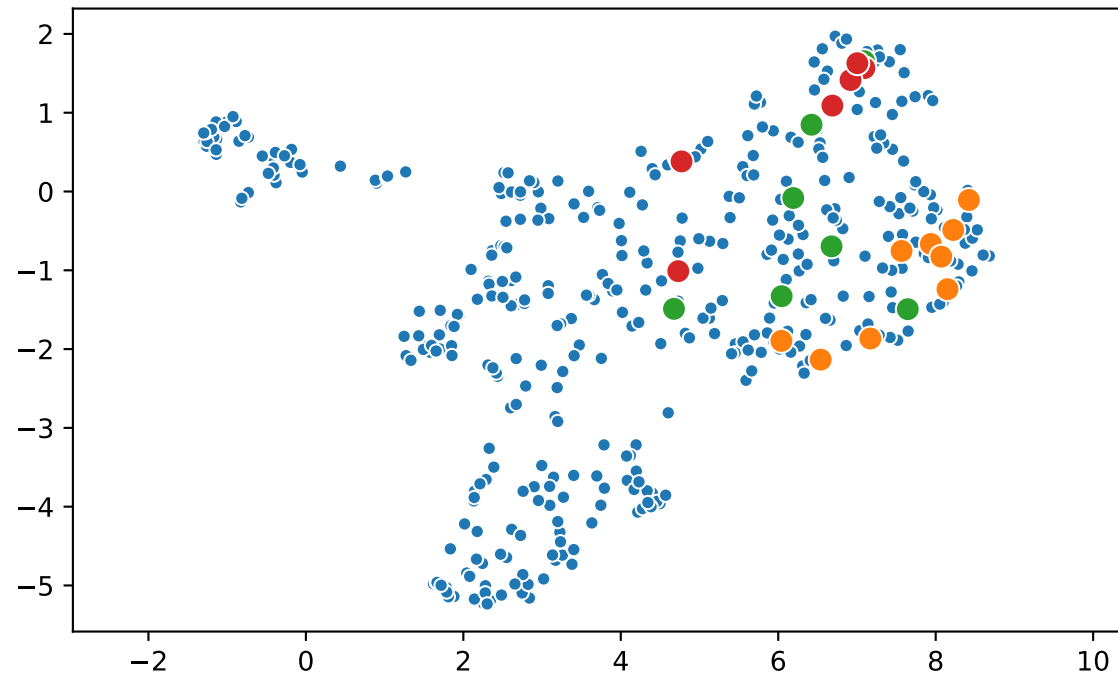


Location in Embedding Space of Drugs with Top 3 Mechanisms

Chemprop PCBA Embeddings



Aligned Chemical Embeddings



● Serotonin receptor antagonist ● Glutamate receptor antagonist ● Cyclooxygenase inhibitor