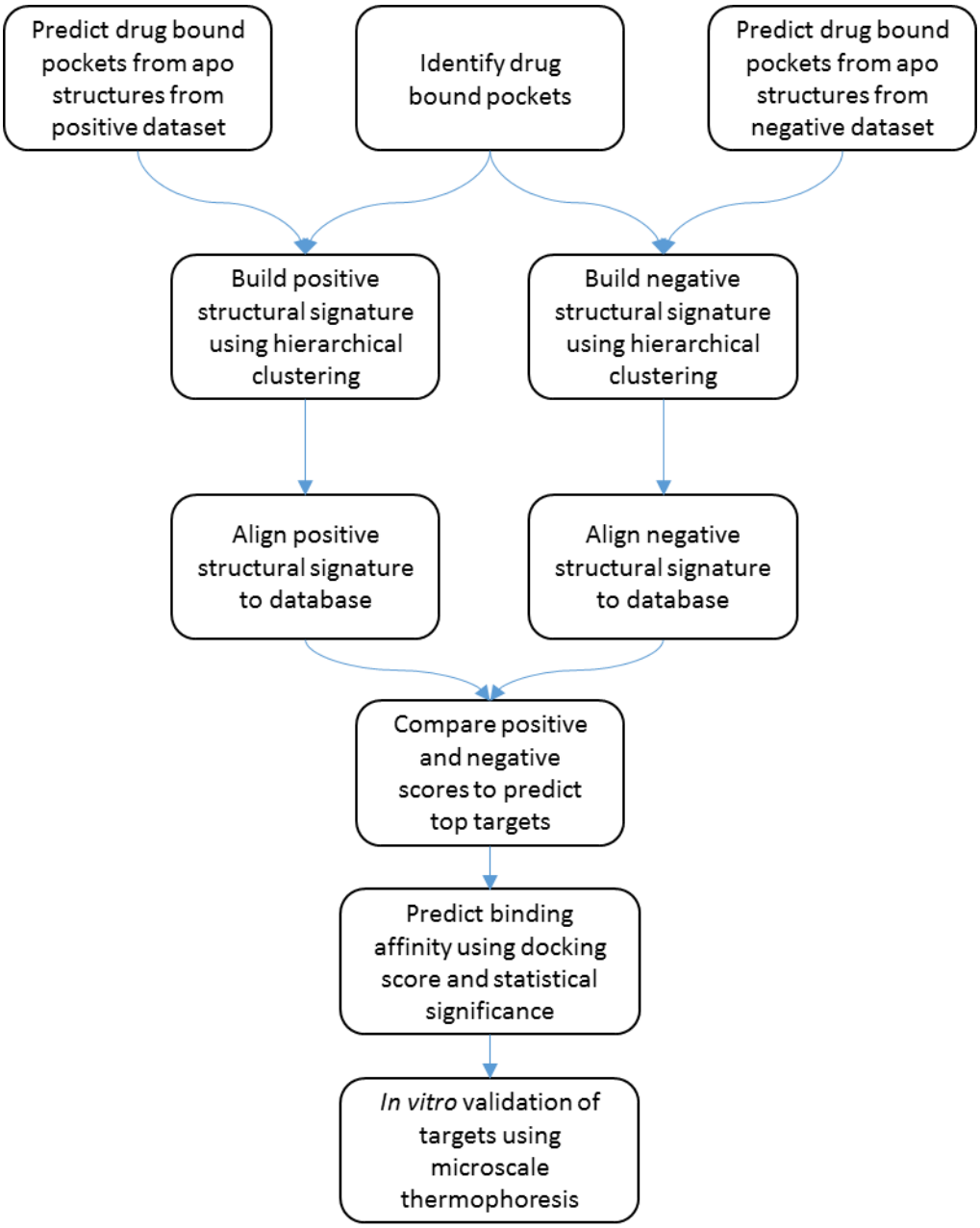
Predict drug bound pockets from apo structures from positive dataset
Identify drug bound pockets
Predict drug bound pockets from apo structures from negative dataset
Build positive structural signature using hierarchical clustering
Build negative structural signature using hierarchical clustering
Align positive structural signature to database
Align negative structural signature to database
Compare positive and negative scores to predict top targets
Predict binding affinity using docking score and statistical significance
In vitro validation of targets using microscale thermophoresis