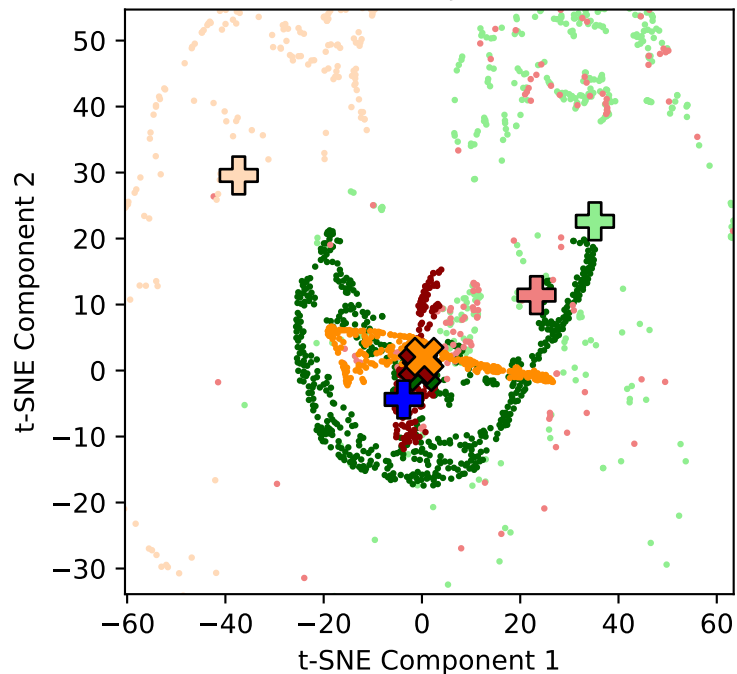
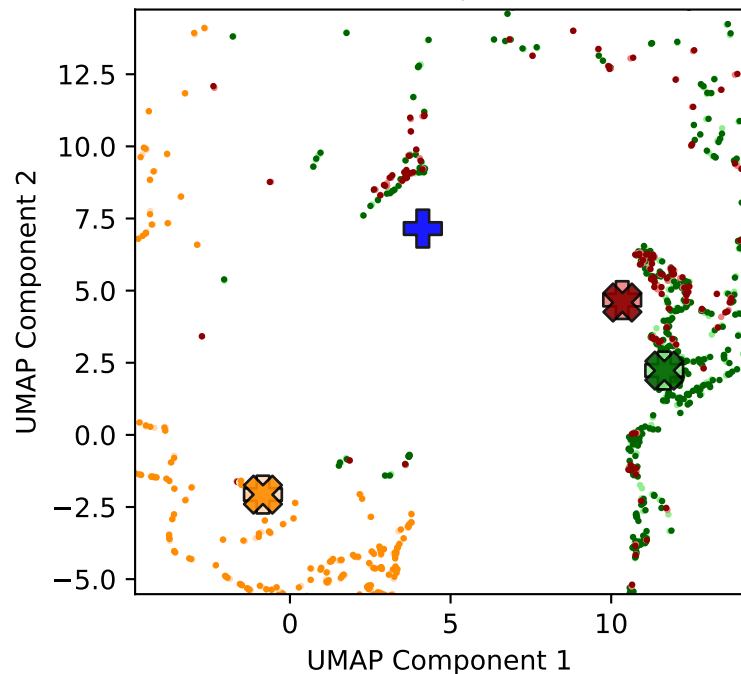


t-SNE Projection



UMAP Projection



- |                             |                                  |                              |
|-----------------------------|----------------------------------|------------------------------|
| • 20 Atom Test Set          | • Validation Set with TTA        | ⊗ NH2 Test Centroid with TTA |
| • 20 Atom Test Set with TTA | + 20 Atom Test Centroid          | + Train Centroid             |
| • NH2 Test Set              | ⊗ 20 Atom Test Centroid with TTA | + Val Centroid               |
| • NH2 Test Set with TTA     | + NH2 Test Centroid              | ⊗ Val Centroid with TTA      |
| • Validation Set            |                                  |                              |