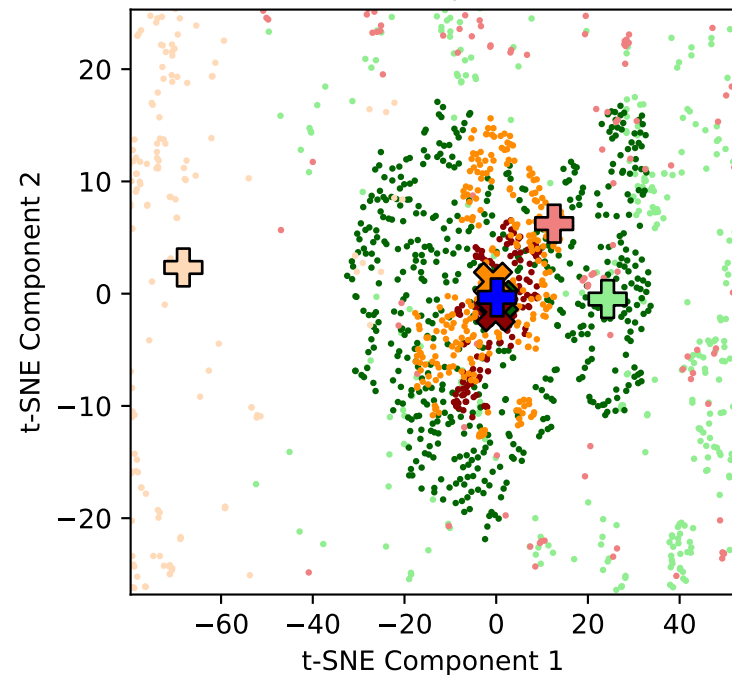
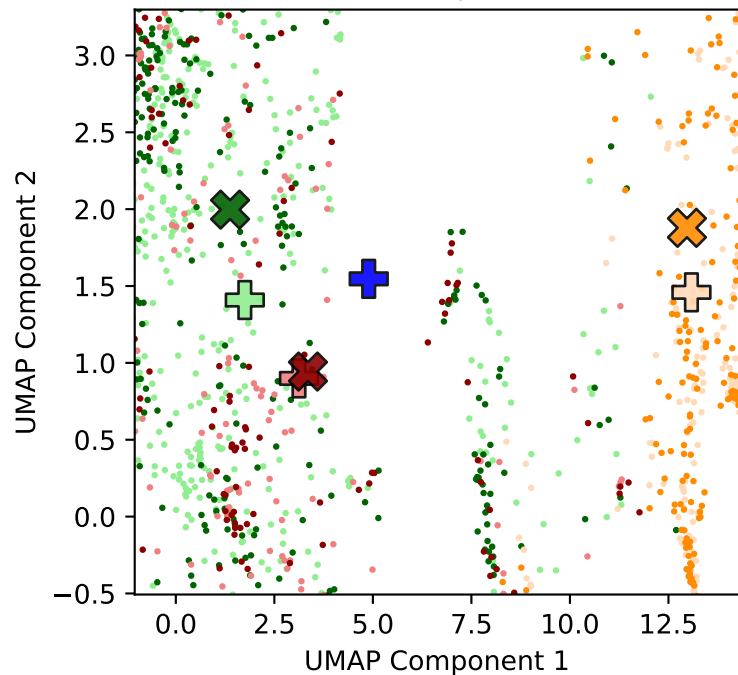


t-SNE Projection



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