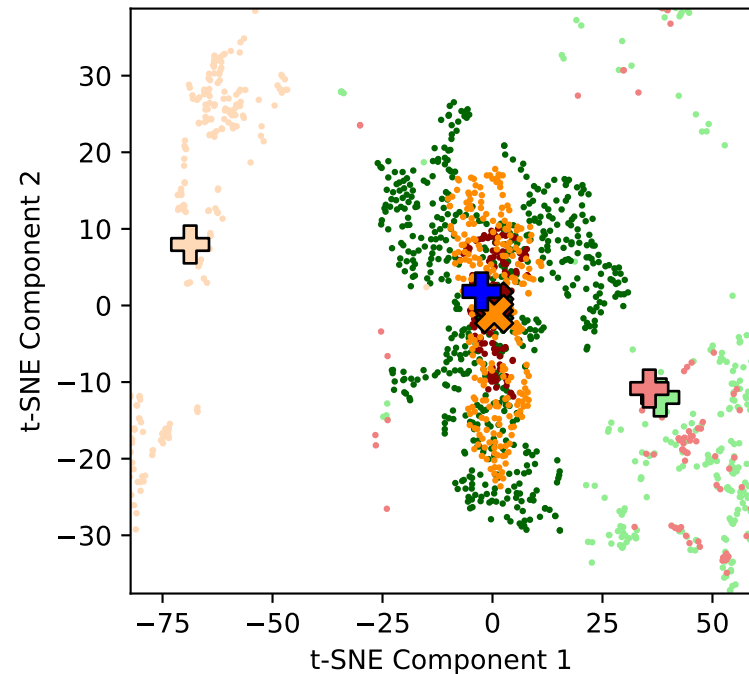
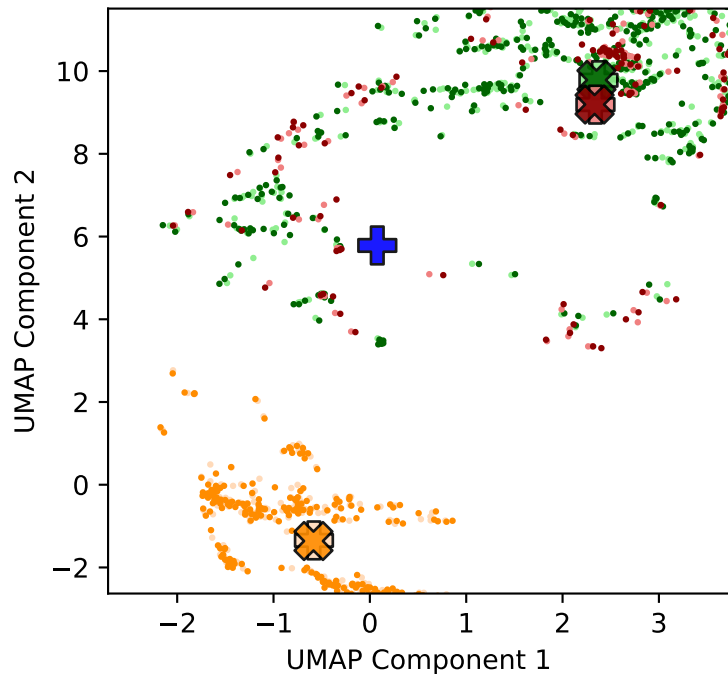


t-SNE Projection



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 | | |