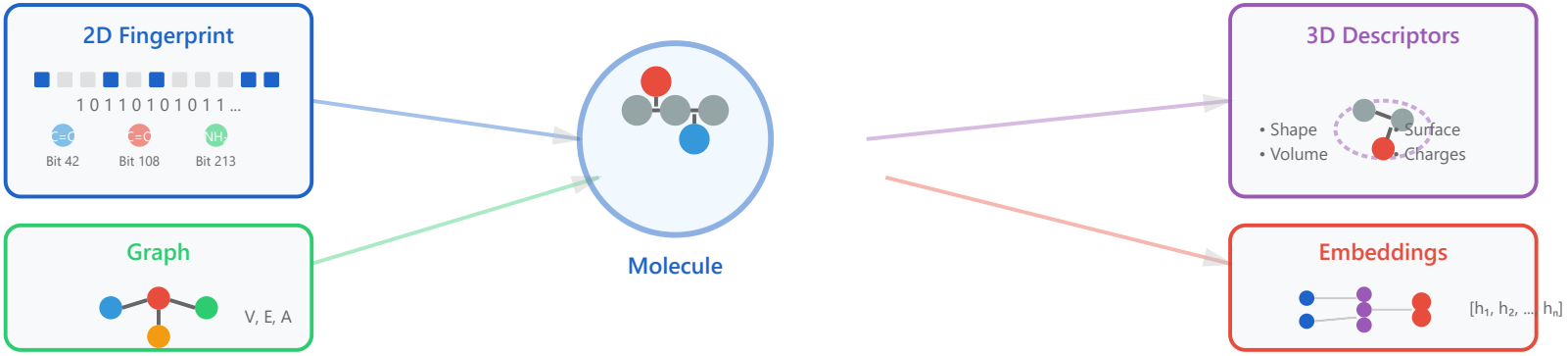
Molecular Representations



2D fingerprints

Binary feature vectors

3D descriptors

Geometric and conformational features

Graph representations

Molecular graph structures

Learned embeddings

Deep learning representations

Multi-view learning

Combining multiple representations