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BACKGROUND

- Butyrylcholinesterase (BChE) is a nonspecific enzyme known to hydrolyze acetylcholine, a neurotransmitter associated with memory and learning functions,[1] making BChE associated with Alzheimer's Disease and dementia-like symptoms.
- One of our previous studies,[2] focused on simulations of thirteen organophosphate inhibitor-projects in complex with BChE, but failed to address and solve heuristic problems with the *k*-means clustering algorithm,[3]which clusters BChE-inhibitor complexes into binding modes, or average conformations.
- Our last published study addressed the *k*-means' heuristic shortcomings using an intuitive statistical approach that will overcome the heuristic tendencies of k-means clustering and qualitatively validate clustering efficacy using internal metrics based on inter- and intra-cluster similarity.
- **Goal:** The study herein will revisit the thirteen organophosphate inhibitor projects and present reproducible and more accurate tabulations of contacts and interactions for each binding mode.

METHODS

- Models:
  - BChE model PDBID# 1P0I
  - Inhibitors modeled & docked with ICM Pro
- Softwares & O 97>BD25pM0[illegible]051498 0 3456 2stud