# AHoJ: Rapid, tailored search and retrieval of apo and holo protein structures

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Studying protein – ligand interactions can provide insights into diverse but fundamental topics in structural biology. Understanding the induced fit model, observing conformational shifts upon binding, or exploring the promiscuity of a binding site, often requires access to a bound (holo) and an unbound (apo) state of the protein. There is currently no dataset or tool available, capable of generating lists of apo and holo conformations for a target protein structure on demand.

Here we present Apo-Holo Juxtaposition (AHoJ), a web application, that given a user-specified protein structure and one or more ligands that bind to it, marks the position of these ligands, identifies and aligns other structures that belong to the same protein, and classifies them as apo or holo depending on the presence of ligands in the previously marked positions. The search can also start with structures that do not bind any ligands. Results are visualised in the browser and locally through PyMOL. AHoJ also features a multiple input mode, allowing it to generate customised apo-holo datasets.