

Pocket-PLE and Pocket-POE comparison using overlapping scores

The overlapping between pocket-PLE and pocket-POE is quantified by three scores: Score of Overlapping (SO), Relative Overlap (RO) and Mutual Overlap (MO). RO and MO are calculated from atom solvent-accessibility.⁷

$$SO = \frac{N_{POE} \cap N_{PLE}}{N_{POE} \cup N_{PLE}}$$

where N_{POE} and N_{PLE} are the number of atoms of pockets estimated by POE and PLE, $(N_{POE} \cap N_{PLE})$ is the number of common atoms in pockets estimated by POE and PLE, $N_{POE} \cup N_{PLE} = N_{POE} + N_{PLE} - N_{POE} \cap N_{PLE}$. SO is between 0 and 1, a score close to 1 indicates a maximal overlapping between the paired pocket estimates.

$$RO = \frac{RSA_{POE} \cap RSA_{PLE}}{RSA_{PLE}}$$

$$MO = \frac{RSA_{POE} \cap RSA_{PLE}}{RSA_{POE}}$$

where RSA_{POE} and RSA_{PLE} are the number of solvent accessibility atoms in pocket-POE and pocket PLE, $(RSA_{POE} \cap RSA_{PLE})$ the sum of solvent accessibility atoms present in both pockets. More the MO and RO are close to 1, more the pocket-POE overlaps the pocket-PLE and more the binding site is included in the pocket.