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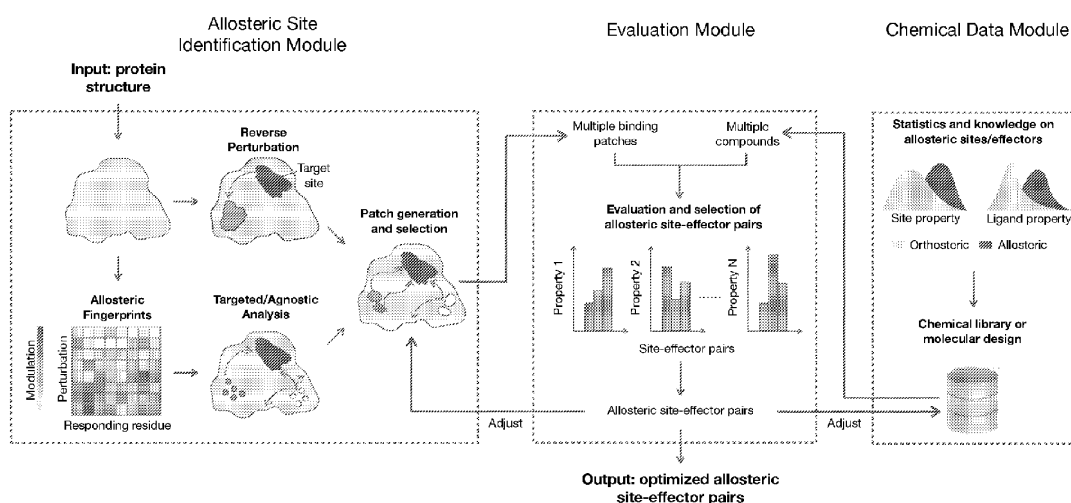
(54) **Title:** COMPUTATIONAL FRAMEWORK FOR RATIONAL DESIGN OF ALLOSTERIC DRUG CANDIDATES

Figure 2

(57) **Abstract:** A high-throughput generic computational framework for rational design of allosteric drug candidates is described here. This present invention discloses identifying allosteric sites/ effectors on the bases of protein dynamics and utilising knowledge on the physicochemical properties of known allosteric sites and effectors. By requiring a bare minimum of a 3D structure information of a protein of interest, Allosteric Fingerprints are computed by perturbing residues or segments of the protein and quantifying allosteric signalling. A set of binding patches of interest is identified from analysing Allosteric Fingerprints, and one or more compounds are then identified based on allosteric modulation value and predicted binding free energy, resulting in one or more allosteric site-effector pairs, which provide desirable allosteric modulation of targeted function. Further optimization of site-effector pairs is achieved by simultaneous and mutual adjustments between binding sites and effectors, in respective identification and prioritization steps.

[Continued on next page]

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