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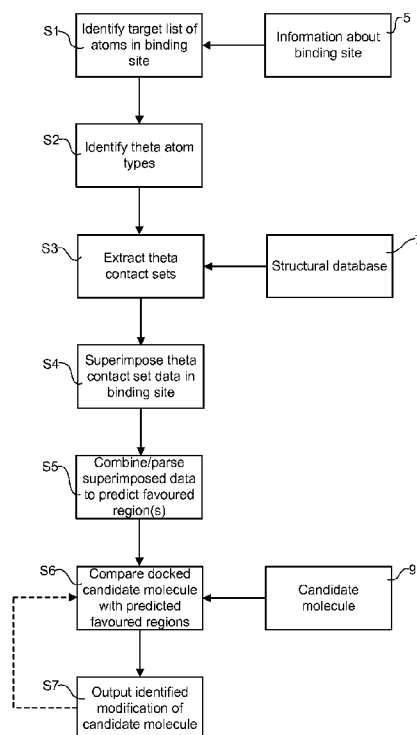
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(54) Title: OBTAINING AN IMPROVED THERAPEUTIC LIGAND

Fig. 7

(57) Abstract: Methods and associated apparatus involving designing a ligand *ab initio* that will bind to a binding site of a macromolecular target, or of identifying a modification to a ligand for improving the affinity of the ligand to a binding site of a macromolecular target, comprising using information about non-bonding, intra-molecular or inter-molecular atom to atom contacts extracted from a database of biological macromolecules to identify favoured regions adjacent to the binding site for particular atom types and modifying a candidate ligand to increase the intersection between atoms of the candidate ligand and the favoured regions. One or more steps of the methods may be performed by a computer.



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