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A New Approach to the Isothermal Titration Calorimetric Measurements: Impact on the Validation of the Ligand-Docking. Isothermal titration calorimetry (ITC) has great advantages for the measurement of the thermodynamic parameters of interactions between two molecular species. However, it is relatively new in the field of drug discovery, and many validation issues have to be addressed prior to its use. This work deals with the impact of the fundamental premises underlying the method on the validation of potential drug-target interactions, in particular the need of having the target in its active conformation. A validation methodology was developed based on the ITC principles and, for the first time, was used to validate a docked complex, a pharmacophore-based lead, and its molecular complex with human serum albumin. The validation was made possible because it is independent from the catalytic activity of the target, given that the catalytic activity of the target in this case is taken for granted. Besides, the methodology allows for extracting the stoichiometry of the whole interaction, which is given in the form of an isothermal dose response relationship, instead of the conventional stoichiometry for a single binding event. Results corroborate the hypothesis that the ability of a molecular complex to discriminate a different conformation of the target accounts for

