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Differential binding force: A new physicochemical parameter for drug design

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The optimization of drug structures has conventionally used the binding constant, which corresponds to the Gibbs free energy, as the physicochemical parameter to quantitatively measure the binding efficiency. Recent studies have questioned whether this is the best criterion; enthalpy instead has been considered an alternative parameter, supported by several drug-developing paths. However, it remains difficult to experimentally obtain enthalpy that is specific to the drug binding process because of the limitations of micro-calorimetry. We propose to use the differential binding force (DBF) as a new parameter to quantify the binding efficiency and stability of drug candidates. DBF is defined as the difference between the binding forces of ligand-receptor pairs with and without drug interactions. The binding forces are determined by force-induced remnant magnetization spectroscopy (FIRMS). The experimental scheme is that one of the ligand-receptor pairs is immobilized on the surface, while the other is labeled with magnetic beads. The magnetic signal is measured by an atomic magnetometer as a function of an external mechanical force. The binding force is given as the external force at which there is a decrease in the magnetic signal due to the dissociation of the ligand-receptor bonds. Because of the high force resolution and detection efficiency, DBF of drugs can be obtained more precisely than any other techniques. This method has been applied for various drug-DNA systems and revealed an unusual mutual selectivity between drug chirality and DNA sequence. Future applications and further technological development will be discussed.

Biography

Shoujun Xu obtained his PhD in Chemistry from the Johns Hopkins University and received Post-doctoral training in Caltech and University of California at Berkeley. His expertise includes magnetic detection, spectroscopy and technology development. He invented the force-induced remnant magnetization spectroscopy (FIRMS) technique. Its high force resolution has enabled a wide range of applications in biochemical research. Multiple papers on prestigious scientific journals have been produced, and several patents have been either awarded or pending.

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