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2 Isothermal Titration Calorimetry: A Tutorial

2.1 Introduction; 2.2 Thermodynamic characterization; 2.3 Instrumentation; 2.4 Raw data; 2.5 Basic considerations for experimental set-up; 2.6 Data analysis; 2.7 Summary; Application notes; Acknowledgement; References; 3 The Application of Isothermal Titration Calorimetry to Drug Discovery; 3.1 Introduction; 3.2 Overview of the drug discovery process; 3.3 Experimental measurement of thermodynamic binding parameters; 3.4 ITC in drug discovery; 3.5 Summary; References; 4 Dissecting the Thermodynamics of DNA-Protein Interactions; 4.1 Introduction; 4.2 Model systems; 4.3 Comparison with the hydrophobic effect; 4.4 Protonation and charged-charged hydrogen bonds; 4.5 Dissection of the binding entropy; 4.6 Entropy contributions to the Sso7d-DNA interaction; 4.7 Entropy contributions to the GCN4-DNA interaction; 4.8 Discussion; Acknowledgements; References; 5 Salt Effects in Ribonuclease-Ligand Interactions: Screening or Competitive Binding?; 5.1 Introduction; 5.2 Anion binding to a protein-protein complex; 5.3 Charge-charge interactions in ribonuclease binding; 5.4 Conclusions; Acknowledgement; References; 6 Thermodynamics-Structure Correlations of Sulfonamide Inhibitor Binding to Carbonic Anhydrase; 6.1 Introduction; 6.2 Identification of protonation reactions occurring upon binding; 6.3 Observed thermodynamics of inhibitor binding to CA; 6.4 Energetics of inhibitor protonation; 6.5 Sulfonamide 'anion' binding thermodynamics; 6.6 Correlations between structures and the thermodynamics of sulfonamide binding to CA; 6.7 Conclusions; References; 7 Energetics of the Interaction of Human Acidic Fibroblast Growth Factor with Heparin and the Functional Analogue Myo-Inositol Hexasulfate; 7.1 Introduction; 7.2 Thermodynamic parameter derived from ITC experiments

Sommario/riassunto

Over the last decade, high-sensitivity calorimetry has developed from a specialist method used mainly by dedicated experts to a major, commercially available tool in the arsenal directed at understanding molecular interactions and stability. Calorimeters have now become commonplace in bioscience laboratories. As a result, the number of those proficient in experimentation in this field has risen dramatically, as has the range of experiments to which these methods have been applied. Applications extend from studies in small molecule and solvent biophysics, through drug screening to whole cell as
