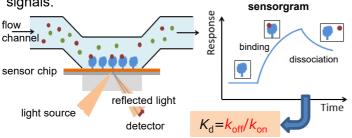
## Intermolecular Interaction Analysis (SPR, ITC)

In the R&D of drugs, diagnostic medicines, and others, interaction analysis of developing molecules and their targets is essential. Toray Research Center can evaluate the interaction analysis from various perspectives using our intermolecular interaction instruments such as ITC, NMR, MS and the latest SPR. The following are the features of SPR and ITC.

## Surface Plasmon Resonance (SPR)

SPR detects a slight mass change caused by the interaction between the molecules on the sensor chip and the molecules flowing in the flow channel as SPR signals.



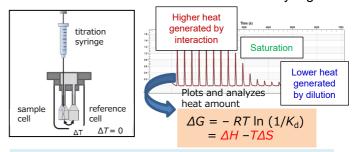
Binding kinetics and dissociation kinetics information is obtained.

Example of research

Faster binding rate: Rapid testing for diagnosis etc. Slower dissociation rate: Sustained efficacy of drug etc.

## Isothermal Titration Calorimetry (ITC)

ITC detects a slight thermal change caused by the interaction between the molecules in the sample cell and the molecules titrated from the titration syringe.



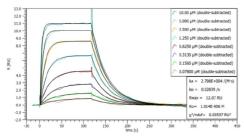
Binding modes (entropy/enthalpy) and binding ratio information is obtained.

Enthalpy predominance: hydrogen bond and/or

electrostatic interaction

Entropy predominance: hydrophobic interaction

## Analysis example: Interaction analysis of carbonic anhydrase (30 kDa) and sulfamoylbenzoic acid (201 Da)



The dissociation constants were confirmed to be equivalent.

Even when  $K_d$  is the same, binding and dissociation kinetics differs by compound. SPR has high throughput performance, making comparison and examination easier.

K <sub>d</sub> (mol/L)	1.014×10 <sup>-6</sup>
k <sub>on</sub> (L/mol·s)	2.798×10 <sup>4</sup>
k <sub>off</sub> (1/s)	0.02839

K <sub>d</sub> (mol/L)	1.398×10 <sup>-6</sup>	
n	0.807	
ΔH (kJ/mol)	-46.76	
<i>-TΔS</i> (kJ/mol)	13.34	

Slight deactivation of protein is indicated.
The binding mode that enthalpy is predominant.

Method	SPR	ITC
Immobilization/ Labeling	Immobilization is required	unnecessary
Molecular weight restriction	>100 Da	none
Required volume	Approx. 10 μg	1 mg or more

ITC does not require immobilization or labeling, and interaction analysis can be conducted under more natural conditions.

To save samples, it is recommended to first analyze by SPR, and then by ITC to obtain the validity of the results and further information.

We propose to perform interaction analysis using an optimum method for your purpose.