



Service package 3: Drug discovery and design

SP3

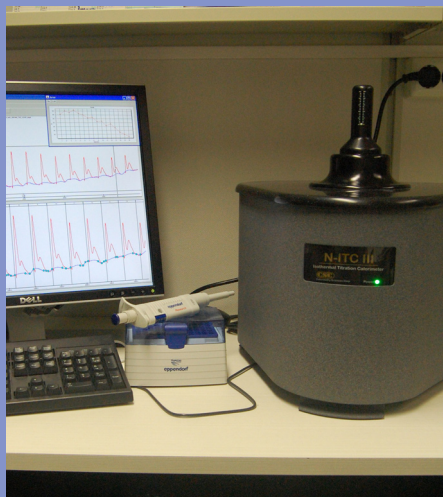
Drug discovery and design

NorStruct will through SP3 offer a new service package that covers ligand discovery and design using a combination of biophysical, computational and crystallographic techniques.

Thermodynamics

Standard services includes characterization of ligand-receptor complexes using ultrasensitive calorimetric techniques:

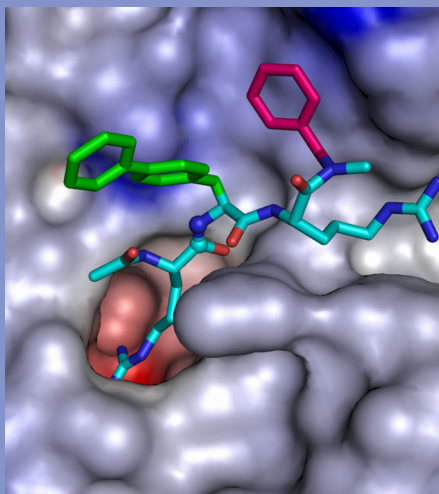
- Calorimetric investigations using both Isothermal Titration (ITC) and Differential Scanning Calorimetry (DSC)
- Optimization of experimental condition suitable for calorimetry
- Complete thermodynamic characterization including determination of ΔG , ΔH , ΔS and the stoichiometry for binding reactions.



Summary NorStruct Services

NorStruct will continue to offer state of the art services and collaboration in structural biology techniques to the Norwegian research community. High quality expertise and services will be assured via in-house research projects and national and international partnerships.

The services will be organized in three different service packages (SPs), whereby the services ordered are tailored to the customer's specific needs. The three SPs will be "Protein production" (SP1), "Structure determination" (SP2), and "Drug discovery and design" (SP3).



Computer modeling

A service package for computational modeling of ligand-receptor complexes may include:

- Library construction and virtual screening
- Prediction of ADME properties
- Pharmacophore modeling
- Lead optimization using sophisticated free energy calculations.

SP1

Subcloning, small-scale expression and purification
Large scale expression and purification
Protein expression optimization and refolding

SP2

Crystallization
Quality control and buffer optimization
Data collection and structure determination

SP3

Protein ligand complexes
Molecular modeling/docking and virtual screening
Protein-ligand thermodynamic studies

Crystallography

NorStruct will offer a service on structural investigations in conjunction with drug design and lead optimization covering:

- High throughput structure determination of multiple ligand-receptor complexes
- Identification of weakly binding low molecular weight ligands using fragment screening for appropriate targets
- Structural studies of off-target effects, primarily serum albumin interactions
- Structure determination of putative ligands using chemical crystallography.

