CAPABILITIES OVERVIEW

• Screening
  » Ligand observe NMR methods: STD, wLOGSY, CPMG

• Library Preparation
  » Identity, solubility, purity
  » Automated smart pooling

• Follow-up Analysis
  » Validation (follow-up singletons)
  » Rank-order; cluster

• Target Generation
  » Protein generation and purification

• Target Preparation
  » Screen design; sample optimization; experimental conditions optimization

• Complimentary Capabilities
  » Orthogonal methods (SPR)
  » X-Ray Crystallography
  » Computational Chemistry
  » Chemical elaboration to support optimization
  » Biological assay design and support

LIBRARY SCREENING OPTIONS

• Fragment Library

• Commercial and Proprietary
  » Fragment sets from internal small molecule collections
  » Fragment sets designed from FDA approved drugs
  » 19F- containing fragments
  » Covalent fragments
  » Commercial fragments

• External libraries
  » Client-provided
  » Client-selected commercial libraries
  » Custom commercial libraries

SELECT FRAGMENT LIBRARY PROPERTIES
CUSING EDGE SCREENING PLATFORM

VERSATILE BIOPHYSICAL SCREENING METHODS

Primary Screening via Ligand Observe NMR: STD, wLOGSY and CPMG

NAMPT (nicotinamide phosphoribosyltransferase): An oncology target in the cellular metabolism pathway.

**Primary Screening:** STD NMR of 1000 fragments in 100 pools. Hits were selected based on structural diversity, virtual screening and the strength of the STD signals from the primary screen.

**Confirmation:** The top hits from the primary screen were screened as singletons and confirmed via STD NMR, waterLOGSY and CPMG experiments.

**Validation:** X-ray co-crystal structures confirm multiple screening hits as true binders to NAMPT.

**Orthogonal Methods:** SPR and biochemical assays to confirm binding and functional enzyme inhibition.

**Validated Novel Scaffold for NAMPT**