ChemPartner
Dedicated to LifeScience

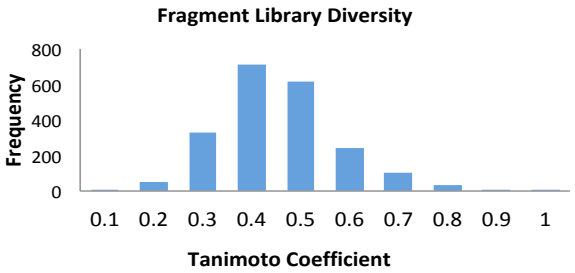
FRAGMENT-BASED LEAD GENERATION

CAPABILITIES OVERVIEW

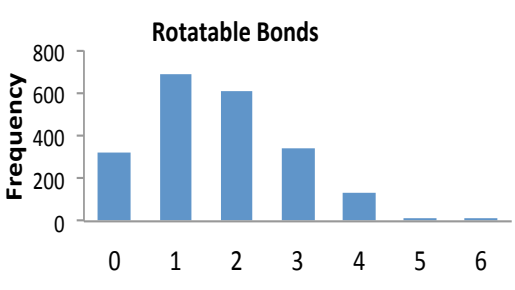
- **Screening**
  - » Ligand observe NMR methods: STD, wLOGSY, CPMG
- **Library Preparation**
  - » Identity, solubility, purity
  - » Automated smart pooling
- **Follow-up Analysis**
  - » Validation (follow-up singletons)
  - » Rank-order; cluster
- **Target Generation**
  - » Protein generation and 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

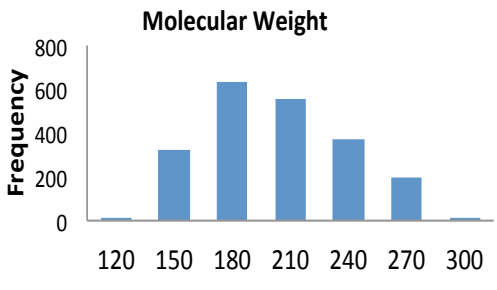
LIBRARY SCREENING OPTIONS

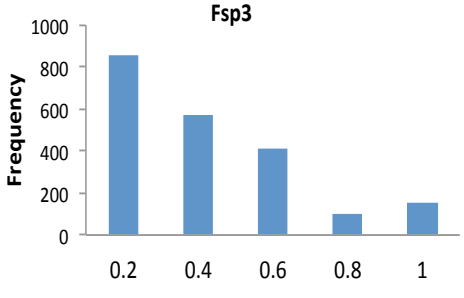
- **Fragment Library**
- **Commercial and Proprietary**
  - » Fragment sets from internal small molecule collections
  - » Fragment sets designed from FDA approved drugs
  - » ^{19}F- containing fragments
  - » Covalent fragments
  - » Commercial fragments
- **External libraries**
  - » Client-provided
  - » Client-selected commercial libraries
  - » Custom commercial libraries



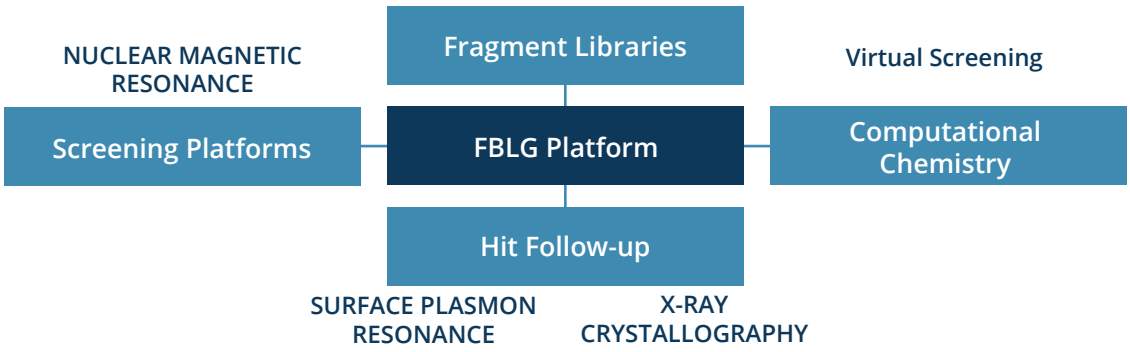
SELECT FRAGMENT LIBRARY PROPERTIES





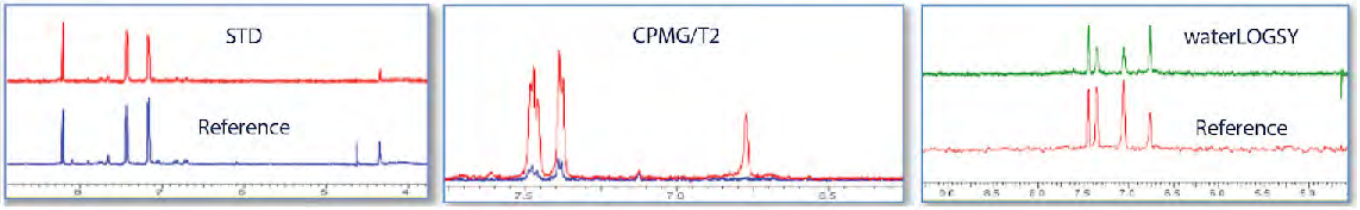


CUTTING EDGE SCREENING PLATFORM



VERSATILE BIOPHYSICAL SCREENING METHODS

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



Addtional Screening Methods

^{19}F NMR

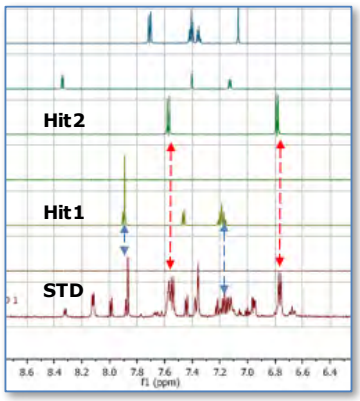
TSA

SPR

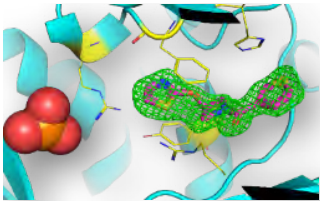
CASE STUDY: FRAGMENT-BASED DRUG DESIGN OF NOVEL NAMPT SCAFFOLDS

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

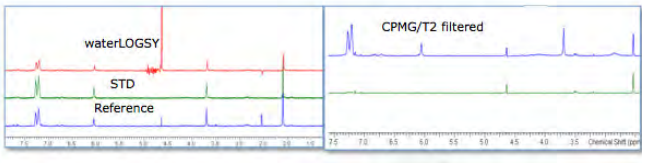
Primary Screening: STD NMR of 1000 fragments in 100 pools. Hits were selected based on structural diversity, virtual screening and the strength of the STD signals from the primary screen



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



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



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

Validated Novel Scaffold for NAMPT

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