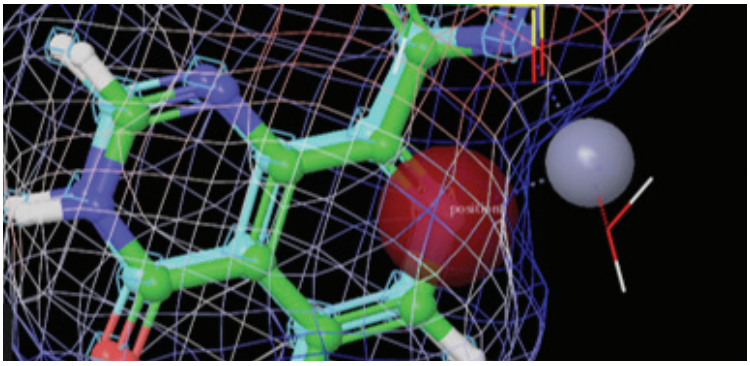
Cayman Services

In Silico Drug Design

Cayman's Medicinal Chemistry and Structural Biology Service groups have decades of experience in *in silico* drug design and selectivity assessment. We offer a full suite of customizable services including homology modeling, virtual screening, lead optimization and development, and protein-protein docking using Schrödinger Maestro 11.

Virtual Screening



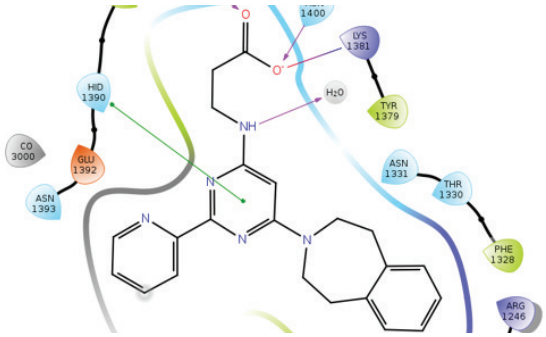
Ligand in 5F32 (PDB ID) active site

- Virtual Library Screening
  - *vHTS of >12 million compounds from the Enamine® Stock Screening Compounds Collection and the MilliporeSigma Aldrich Market Select® Screening Collection Phase databases*
  - *Fragments, drug-like, near drug-like, and lead-like compounds*
  - *Customized/on-demand*
- Binding Site Characterization
- Ligand Preparation and pKa Predictions
- Advanced Screening Technology
  - *Shape-based screening*
  - *Pharmacophore modeling*
  - *Glide docking*
  - *MM-GBSA and FEP analysis*

Protein Modeling

- Accurate Protein Structure Prediction and Refinement
- Homology Modeling
- Study Protein-Protein Interactions
- Visualize Electron Density from X-ray or Cryo-EM

Lead Optimization & Development



Key interactions between ligand and active site residues (PDB ID 4ASK)

- Enumerate Hits
  - *Reaction-based*
  - *Core hopping*
  - *Bioisostere replacement*
- Identify Key Interactions
  - *Induced-fit docking*
  - *Molecular dynamics*
- Model Pharmacophores (QSAR)
- Physiochemical and ADME/Tox Property Predictions

Learn more about our *In Silico* Drug Design Services or request a quote at **www.caymanchem.com/medchem**

Cayman Services

Contract Services

Cayman Contract Services provides discovery and preclinical development services to the global pharmaceutical, biotechnology, and academic research markets. Our diverse suite of services leverages a team of over 150 highly skilled scientists with expertise in medicinal chemistry, structural biology, complex multi-step organic synthesis, analytical chemistry, sample analysis, and custom assay development. We offer a personalized, flexible approach that enables our clients to accelerate their drug discovery and development through a single-source partner, from novel drug design and synthesis to target identification and validation.

Our Contract Services Division provides expertise in:

01	02	03	04
Bioanalysis & Assay Development	Medicinal Chemistry & Structural Biology	Analytical Chemistry	Chemical Synthesis

Why Cayman?

We offer comprehensive solutions to drive your projects to completion. With prompt quotations, competitive prices, quality science, and personalized customer service, our team is committed to our mission to help make research possible.

- Maintain complete control of your study with phase-based, flexible project design.
- Consult with our cross-functional team of scientists with expertise in diverse research areas and technical skill sets.
- Access our state-of-the-art laboratories with dedicated resources to support your project needs.

To learn more about Cayman Contract Services,
visit **www.caymanchem.com/services**

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