

Core Technologies

Automation and Compound Management

The goal of the Automation and Compound Management group is to support research activities at NCATS. Specifically, the group:

- Supports NCATS activities in high-throughput screening and assay development and optimization.
- Provides compound management for both small molecules and biologics.
- Offers automated tissue-culture capabilities and high-content screening capabilities.
- Assists in custom instrumentation development and production and offline instrumentation maintenance and support.
- Researches and evaluates next-generation technologies and biological systems.

Visit <https://ncats.nih.gov/preclinical/core/automation> and <https://ncats.nih.gov/preclinical/core/compound> to learn more.

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Analytical Chemistry Core

The Analytical Chemistry Core (ACC) maintains a state-of-the-art laboratory whose mission is to support translational research throughout NCATS by providing analytical chemistry services involving the isolation, purification, identification and analysis of various therapeutic modalities for targeted disease states. A wide variety of instrumentation and equipment is managed to facilitate scientific efforts focused on early-stage drug discovery and development. The ACC also provides expert analysis to both intramural and extramural collaborators throughout all stages of a research program. Furthermore, the ACC develops new and innovative methods, technologies and platforms to improve analysis and workflow for the advancement of translational research. Specifically, the ACC:

- Utilizes an automated liquid chromatography platform for the purification, processing, registration and library incorporation of synthesized and acquired compounds.
- Administers a laboratory information management system for the storage, organization and management of all analytical data.
- Uses nuclear magnetic resonance (NMR) spectroscopy to characterize and verify compound structure; determine chromatographic, chiral and isotopic purity; and identify sample impurities.

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- Uses high-throughput mass spectrometry (MS) screening assays for the identification of biologically relevant compounds against unique disease targets.
- Develops omics-based MS analysis platforms (e.g., proteomics, metabolomics, lipidomics) for the discovery of biomarkers and potential therapeutics.
- Applies NMR-based fragment screening and ligand-target engagement to aid in structural design and as a means of assessing biological activity for advanced candidates.
- Develops structural analysis tools to aid in determining absolute configuration and 3-D conformation of small molecules.

Visit <https://ncats.nih.gov/preclinical/core/chemistry> to learn more.

Informatics

The goal of the Informatics group in NCATS is to enable data-driven decisions that accelerate translation by developing new or enhancing the application of existing methods that prioritize targets and therapeutic opportunities for evaluation; designing novel, fit-for-purpose chemical probes; and assessing the productivity of the translational research process. Specifically, the group:

- Transforms raw numeric data obtained from large-scale experiments into actionable decisions in chemistry and biology.
- Applies techniques from a broad array of disciplines — including cheminformatics, bioinformatics, computational biology and chemistry — to enable experimental decision-making.
- Develops algorithms and software to disseminate research results to the broader community.
- Fosters collaborative relationships with other investigators to develop robust assay designs and analytics.

Visit <https://ncats.nih.gov/preclinical/core/informatics> to learn more.

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Drug Metabolism and Pharmacokinetics Team

The Drug Metabolism and Pharmacokinetics team performs a variety of studies for measuring absorption, distribution, metabolism and excretion (ADME) studies of lead clinical candidates. Specifically, the team:

- Applies pharmacokinetic concepts to drug structure optimization, lead selection, study design for efficacy and safety evaluations and dose regimen forecasts for human clinical trials.
- Develops and implements new techniques for ADME studies.
- Integrates pharmacodynamic and toxicity evaluations of new drug candidates together with ADME studies to increase process optimization.

Visit <https://ncats.nih.gov/trnd> to learn more.

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