

Analytical Chemistry

Our Core Capabilities

❖ Spectroscopic Capabilities

- Structure elucidation of small molecules using advanced spectroscopic techniques
- Multi-nuclear NMR analysis using smart probes for nuclei including ^{19}F , ^{31}P , ^{11}B , ^7Li , and ^{29}Si
- Execution of a broad range of 1D and 2D NMR experiments
- MS/MS experiments to aid in molecular characterization
- Specialized NMR experiments such as:
 - ^1H and ^{13}C NMR (APT, DEPT)
 - COSY, HSQC, HMBC, HOESY, NOESY, ROESY
 - ^{15}N – ^1H correlation, NOE, ROE studies for stereochemistry and regioisomer confirmation
 - Variable temperature experiments for assessing rotamers and hydrogen bonding
 - Quantitative NMR (qNMR) for purity estimation
 - Residual solvent analysis, TFA content estimation, and butyllithium purity determination

❖ Chromatographic Capabilities

- Purity assessment of NCEs using reverse- and normal-phase chromatography
- Determination of enantiomeric excess using a diverse array of chiral columns
- HPLC method development using mass-triggered scouting systems for reliable and rapid optimization

❖ Purification Capabilities

- High-throughput purification and isolation of compounds from milligram to gram scale
- Efficient purification support for Parallel Medicinal Chemistry libraries and singleton compounds
- Chiral purification using SFC and normal phase systems, scalable from mg to g

- Specialized methodologies for purification of unstable compounds, including:
 - High-temperature purification setup
 - Focused gradients and multiple column chemistries
 - Techniques like sandwich-mode injection, At Column Dilution (ACD)
 - Use of shorter, wider columns (e.g., 30x100 mm) for high-load, short runtime purifications

❖ **Impurity Profiling Capabilities**

- Isolation and characterization of unknown impurities from APIs and formulations
- Utilization of preparative HPLC, spectroscopic techniques, and structure elucidation expertise

❖ **Chiral Chromatography**

- Fast screening of chiral compounds using SFC, UPC², and normal phase chromatography
- Preparative-scale isolation of enantiomers and diastereoisomers

❖ **Polymorph Screening**

- Screening using DSC, Infrared Spectroscopy, and XRPD (via third-party collaboration)

❖ **Specialized Analytical Assays**

- Chrom Log D and Log P estimation via HPLC
- Experimental polar surface area measurement using SFC
- Amino acid and chloride content analysis using CAD detection

❖ **GLP Capabilities**

- GLP-certified analytical laboratory for method development and validation in alignment with ICH and OECD guidelines
- Support for Kilo-lab activities, including final GMP release testing
- Conduct of short-term and long-term stability studies for APIs and intermediates

❖ **GMP Capabilities**

- USFDA-recognized and NABL-accredited analytical lab infrastructure
- Analytical method validation and transfer as per global regulatory guidelines (ICH/USP/EP)
- Full analytical support for DOE/QbD studies and regulatory submissions
- Timely and accurate response to regulatory queries
- Stability studies (short- and long-term) for APIs and intermediates