Structural Elucidation

Capabilities & Expertise

J-Star provides high quality scientific and technical ability in small molecule problem solving including impurity/degradant isolation and structure elucidation. We have over 85 years of cumulative expertise in NMR/MS data acquisition and interpretation and are equipped with state-of-the-art instrumentation typically seen only in Big Pharma. We achieve results through a unique blend of highly integrated scientists among many interdisciplinary branches (structure elucidation/chemistry/analytical) who work efficiently together to achieve results.

At J-Star, we also have in house capabilities on par with Big Pharma. For instance, we work cross-functionally on impurity isolation for unambiguous structure elucidation. This allows our structure elucidation and analytical scientists to work individually or together on data acquisition using state of the art instrumentation, analysis, interpretation. Together, we arrive at unambiguous structures based on the data and mechanistic understanding of the impurity/degradant formation to provide highly confident structure elucidation.

Once the unambiguous structure is determined, if desired, chemistry can work on synthetic route proposal with proof of concept to produce milligram/gram quantities of the authentic impurity. The chemistry work is aided by interaction with structure elucidation and analytical scientists to guide the route scouting to produce the authentic impurity. All this takes place quickly and efficiently under one roof.

Capabilities

- 4 NMRs (1 x 500 MHz, 2 x 400 MHz and 1 x 300 MHz) and 3 NMR spectroscopists
- HRMS Orbitrap Elite Mass Spectrometer with MSn capabilities
- Multiple LCMS systems and preparative HPLC with mass-directed isolation capabilities
- Single Crystal X-ray Diffractometer (Bruker D8 Quest)
- New – Varian proton/fluorine cryoprobe at 500 MHz

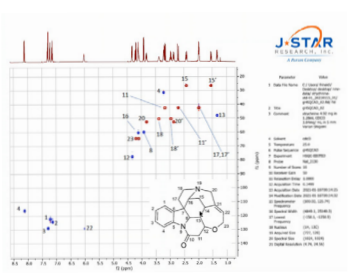
Experts in identifying and characterizing low levels (e.g. 0.1%) of impurities in chemical intermediates and APIs

Connect With Us

Visit jstar-research.com
Call (877) 56-JSTAR

Cranbury Location
6 Cedarbrook Dr,
Cranbury Township, NJ 08512

J-STAR RESEARCH, Inc.



Partnering with the Pharmaceutical Industry to Make New Therapies Possible

The Industry Leader in Small Molecule Process Research & Crystallization R&D

Identifying Unknown Impurities and Metabolites

Our mission at J-STAR Research is to help pharmaceutical small molecule R&D programs succeed in all phases of development.

The marriage of significant analytical capabilities with the experience of our scientific personnel allows for the isolation and characterization of sub-microgram quantities of chemical impurities/degradants for unambiguous structure elucidation.

Structural Elucidation Scope of Services

We employ a highly integrated team of experts to identify and confirm molecular structures of chemical impurities/degradants. Our experts use multi-dimensional orthogonal data sets for unambiguous structure elucidation of impurities and degradants from pharmaceutical, chemical and agricultural processes.

We enable impurity and degradant structural identification:

- Automated Impurity Enrichment & Isolation
- NMR & LCMS Data Acquisition
- Orthogonal Spectroscopic/ Spectrometry Analysis
- Experienced NMR/ MS Interpretation
- Highly Confident Structural Formula
- Impurity Synthesis & Route Scouting (optional)

Structure Elucidation

- Waters ZQ/2487 mass and/or UV triggered auto purification.
- Enrich impurities for quick isolation: use existing mother liquors,normal phase (ISCO/Biotage) to extract material rich in impurities, force degradation, crystallization to reject main compound.
- NEW Varian proton/fluorine cryoprobe at 500 MHz - 1D/2D structure elucidation experiments, H-C, H-N and F-C 2D on as little as 100 -300 micrograms
- Bruker 400 MHz multi nuclear probe detects: ^{13}C, ^{19}F, ^{31}P and more exotic nuclei such as Pt, Cl, Na, etc.
- LC-MS in parallel with NMR analysis: parent and fragment ions orthogonal data for unambiguous structure elucidation.
- HRMS Orbitrap Elite Mass Spectrometer with MSn capabilitiesSingle
- Crystal X-ray Diffractometer (Bruker D8 Quest)
- Isolated compound can be saved for use as HPLC marker.
- Quick and easy isolated compound synthesis all under one roof!

Experts in identifying and characterizing low levels (e.g. 0.1%) of impurities in chemical intermediates and APIs

Structure Elucidation

Our experienced scientists use state of the art instrumentation and orthogonal data analysis for highly confident impurity/degradant structure elucidation.

Fast & Efficient, State-of-the-Art Workflow cuts weeks from Program Timeline

Mass-Directed Automatic Impurity Isolation capable of handling a wide variety of crude mixtures

Mass-Directed Automatic Impurity Isolation efficiently isolates chromatographically overlapped peaks, giving purer isolate for easy analysis

Orthogonal NMR and LC-MS data acquisition and interpretation for faster elucidation and highly confident structures