**Abstract**

A unique software configuration was assembled to facilitate the discovery of novel bioactive compounds in natural products extracts and to accelerate the translation of the findings to clinical use. The suite of tools includes the Beilstein Natural Products Database, the Beilstein STR, CN, INP databases, and ISIS/Base. These databases are integrated with high-throughput biological screening, fast chromatographic methods, and robotic sample preparation to improve the discovery and development of new antibiotics.

**Materials and Methods**

1. **Chromatographic Analysis**
   - The multidimensional HPLC system, which provides a fingerprint of the sample, is controlled by Waters Millennium ²³² software and operates in a tripartite-chromatographic mode. The data generated is recorded by an Array Detector. The Mass Directed Autopurification is achieved through the use of Waters Fraction Lynx v3.5 Application Manager.

2. **Preparative HPLC Column**
   - Daughter plates at 250 ul in each well. Three of these daughter plates are 96 well polypropylene flat bottom containing 250 mm x 21 mm Dynamax 60A C-18 phase bonded column eluted with acetonitrile/20 mM NH₄OAc pH 4.0 at 15 ml/min.

3. **Data Mining for Novel Active Compounds – ISIS/Base Interface**
   - ISIS/Base Interface is a powerful tool for the identification of novel lead compounds in natural products extracts. It allows merging of Beilstein STR, CN, INP databases and biological data into a unified database.

**Computer and Database Tools for the Identification of Novel Lead Compounds in Natural Products Extracts**

Paul Klausmeyer*, T. Luke Simmons, Thomas G. McCloud
SAIC-Frederick, Inc., National Cancer Institute at Frederick, Frederick, MD

**Introduction**

The NCI is collaborating with SAIC-Frederick, Inc., to discover antibiotics from natural sources for the purpose of combating antibiotic-resistant pathogens. The suite of tools includes the Beilstein Natural Products Database, the Beilstein STR, CN, INP databases, and ISIS/Base. These databases are integrated with high-throughput biological screening, fast chromatographic methods, and robotic sample preparation to improve the discovery and development of new antibiotics.

**Conclusion**

The NCI is collaborating with SAIC-Frederick, Inc., to discover antibiotics from natural sources for the purpose of combating antibiotic-resistant pathogens. The suite of tools includes the Beilstein Natural Products Database, the Beilstein STR, CN, INP databases, and ISIS/Base. These databases are integrated with high-throughput biological screening, fast chromatographic methods, and robotic sample preparation to improve the discovery and development of new antibiotics.