Credentialed *E. coli* Cell Extract Kit

For Benchmarking and Optimizing Untargeted MS Methods

An exceeding challenge in optimizing metabolomic methodologies toward improved metabolome coverage has been the difficulty in comparing the number of metabolites profiled in each. This evaluation is complicated by artifactual signals. Artifacts can arise from sample contamination during metabolite extraction, background instrument noise, or misannotation of data during bioinformatic processing. While efforts to minimize artifacts have been extended, it is generally not possible to completely remove these from the features list nor desirable to do so without well characterized extracts and proper software tools designed to effectively filter biogenics from artifacts.

Cambridge Isotope Laboratories, Inc. (CIL) is pleased to offer a Credentialed *E. coli* Cell Extract Kit (MSK-CRED-KIT, MSK-CRED-DD-KIT) that can assist the user in developing and optimizing methodologies for untargeted metabolomic profiling.

The kit contents are as follows:

- 13C-labeled (at ≥98%) *E. coli* cell extract (dried down or 100 µL)
- Unlabeled *E. coli* cell extract (dried down or 100 µL)
- Detailed user manual (contains instructions on solution/sample preparation and data analysis with Credentialing software)

The supplied extracts require simple preparation prior to mixing (at defined ratios), LC-MS analysis, and bioinformatic processing. This latter processing is facilitated by a well validated, informatic workflow, which is designed to effectively discriminate biological from artifactual features on the basis of isotopic spacing and intensity ratios. Overall, this kit helps streamline method optimization/evaluation in untargeted microbial metabolomics and provides a robust metric for performance comparisons between different metabolomic methods and instrument platforms.

**Kit Features and Benefits**

- Credentialing yields 100s of standards
- Effective biogenic vs. artifact signal discrimination
- Preserves low-intensity signals
- Platform-independent metabolite analysis
- Enables interlaboratory method comparison
- Allows method optimization and benchmarking

**NEW!** The Credentialing tool is now available in Compound Discoverer 3.0 software.

**Note:** The cells are *E. coli* K12 strain MG1655; extracts are generated from 2.5 mg lyophilized cells. Other sizes may be available. Please inquire.

**References**