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A CAMBRIDGE ISOTOPE LABORATORIES COMPANY

RESEARCH PRODUCTS

Credentialed *E. coli* Cell Extract Kit

For Benchmarking and Optimizing 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 that can assist the user in developing and optimizing methodologies for untargeted metabolomic profiling.

The kit contents are as follows:

- ^{13}C-labeled (at ≥98%) *E. coli* cell extracts (lyophilized)
- Unlabeled *E. coli* cell extracts (lyophilized)
- Detailed user manual with troubleshooting guide
- Credentialing software (download details in user manual)

Note: The cells are *E. coli* K12 strain MG1655; they are available in 5, 25, and 100 mg quantities.

Alternate amounts may be available. Please inquire.

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

The supplied extracts require simple rehydration 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.[1,2] 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. Taken together, this kit paves the way toward the generation of a reference metabolome for *E. coli*.

References

1. Benton, H.P.; Ivanisevic, J.; Mahieu, N.G.; Kurczy, M.E.; et al. **2015**. Autonomous Metabolomics for Rapid Metabolite Identification in Global Profiling. *Anal Chem, 87(2),* 884-891.
2. Mahieu, N.G.; Huang, X.; Chen, Y.; Patti, G.J. **2014**. Credentialing Features: A Platform to Benchmark and Optimize Untargeted Metabolomic Methods. *Anal Chem, 86(19),* 9583-9589.