



# Metabolomics QC Kits

For Untargeted/Targeted  
Mass Spectrometry



Materials for testing assay effectiveness and platform performance are paramount to obtaining quality data. Under routine implementation, such materials can provide a reliable measure of the efficiency of a specific method, while flagging deficiencies or errors in an analytical platform (e.g., LC- or GC-MS/MS). To help aid these performance assessments in MS metabolomics and additionally provide the potential of metabolite quantification, Cambridge Isotope Laboratories, Inc. (CIL) is pleased to offer two metabolomics QC kits (**MSK-QC-KIT**, **MSK-QReSS™-KIT**) for untargeted/targeted MS-based applications.

## MSK-QC-KIT [← Click for additional information](#)

This kit contains the following materials and tools:

- 2 vials of stable isotope-labeled metabolites (dried down)
- Detailed user manual

**Table.** Mix composition. Reconstitution in 1 mL of solvent (e.g., 50% methanol) yields the concentrations specified.

| Description  | Conc. (µg/mL) | Vial |
|--|---------------|------|
| L-Alanine ( <sup>13</sup> C <sub>3</sub> , 99%)                    | 4             | 1    |
| L-Leucine ( <sup>13</sup> C <sub>6</sub> , 99%)                    | 4             | 1    |
| L-Phenylalanine ( <sup>13</sup> C <sub>6</sub> , 99%)              | 4             | 1    |
| L-Tryptophan ( <sup>13</sup> C <sub>11</sub> , 99%)                | 40            | 1    |
| L-Tyrosine ( <sup>13</sup> C <sub>6</sub> , 99%)                   | 4             | 1    |
| Caffeine ( <sup>13</sup> C <sub>3</sub> , 99%)                     | 4             | 2    |
| D-Glucose ( <sup>13</sup> C <sub>6</sub> , 99%)                    | 4             | 2    |
| Sodium benzoate ( <sup>13</sup> C <sub>6</sub> , 99%)              | 4             | 2    |
| Sodium citrate ( <sup>13</sup> C <sub>3</sub> , 99%)               | 4             | 2    |
| Sodium octanoate ( <sup>13</sup> C <sub>8</sub> , 99%)             | 4             | 2    |
| Sodium propionate ( <sup>13</sup> C <sub>3</sub> , 99%)            | 4             | 2    |
| Stearic acid, sodium salt ( <sup>13</sup> C <sub>18</sub> , 98%)   | 0.4           | 2    |
| Succinic acid, disodium salt ( <sup>13</sup> C <sub>4</sub> , 99%) | 4             | 2    |
| D-Sucrose ( <sup>13</sup> C <sub>6</sub> , 98%)                    | 4             | 2    |

*Individual vials and companion unlabeled mixtures may also be available. Please inquire.*

### Example Reference

Barco, S.; Lavarello, C.; Cangelosi, D.; et al. **2022**. Untargeted LC-HRMS based-plasma metabolomics reveals 3-O-methyldopa as a new biomarker of poor prognosis in high-risk neuroblastoma. *Front Oncol*, 12, 845936-845946.

*Chemical purity (CP) is 98% or greater, unless otherwise indicated.  
For research use only. Not for use in diagnostic procedures.*

**Cambridge Isotope Laboratories, Inc.**

## Example Features and Benefits

- Mixes (in neat form) with user manual
- Predominantly <sup>13</sup>C and/or <sup>15</sup>N metabolites
- Offers flexibility in use and application
- Reduces development time and cost
- Provides enhanced reproducibility

## MSK-QReSS-KIT [← Click for additional information](#)

This kit contains the following materials and tools:

- 2 vials of stable isotope-labeled metabolites (dried down)
- Detailed user manual

**Table.** Mix composition. Reconstitution in 1 mL of solvent (e.g., 50% methanol) yields the concentrations specified.

| Description  | Conc. (µg/mL) | Vial |
|--|---------------|------|
| L-Alanine ( <sup>13</sup> C <sub>3</sub> , 99%; <sup>15</sup> N, 99%)            | 100           | 1    |
| 1,4-Butanediamine·2HCl ( <sup>13</sup> C <sub>4</sub> , 99%)                     | 10            | 1    |
| Creatinine (N-methyl-D <sub>3</sub> , 98%)                                       | 100           | 1    |
| Ethanolamine·HCl (1,1,2,2-D <sub>4</sub> , 98%)                                  | 10            | 1    |
| Guanosine·2H <sub>2</sub> O ( <sup>15</sup> N <sub>5</sub> , 96%)                | 2             | 1    |
| Hypoxanthine ( <sup>13</sup> C <sub>5</sub> , 99%)                               | 10            | 1    |
| L-Leucine ( <sup>13</sup> C <sub>6</sub> , 99%)                                  | 5             | 1    |
| L-Phenylalanine (ring- <sup>13</sup> C <sub>6</sub> , 99%)                       | 100           | 1    |
| Thymine (1,3- <sup>15</sup> N <sub>2</sub> , 98%)                                | 20            | 1    |
| L-Tryptophan ( <sup>13</sup> C <sub>11</sub> , 99%)                              | 100           | 1    |
| L-Tyrosine (ring- <sup>13</sup> C <sub>6</sub> , 99%)                            | 100           | 1    |
| Vitamin B <sub>3</sub> ( <sup>13</sup> C <sub>6</sub> , 99%)                     | 5             | 1    |
| Citric acid (1,5,6-carboxyl- <sup>13</sup> C <sub>3</sub> , 99%)                 | 10            | 2    |
| Fumaric acid ( <sup>13</sup> C <sub>4</sub> , 99%)                               | 100           | 2    |
| Indole-3-acetic acid (phenyl- <sup>13</sup> C <sub>6</sub> , 99%)                | 5             | 2    |
| α-Ketoglutaric acid, disodium salt (1,2,3,4- <sup>13</sup> C <sub>4</sub> , 99%) | 100           | 2    |
| Sodium palmitate (U- <sup>13</sup> C <sub>16</sub> , 98%)                        | 10            | 2    |
| Sodium pyruvate ( <sup>13</sup> C <sub>3</sub> , 99%)                            | 100           | 2    |

**Example Reference:** Lipka, K.A.; Aristizabal-Henao, J.J.; Beger, R.D.; et al. **2022**. Reference materials for MS-based untargeted metabolomics and lipidomics: a review by the metabolomics quality assurance and quality control consortium (mQACC). *Metabolomics*, 18(4), 24-52.

**Example Application Note:** Percy, A.J.; Souza, A.; Ntai, I.; et al. **2022**. From QC to quantitation: Utility of QReSS™ metabolites in FBS measurements. (CIL application note #51)