



# 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 three metabolomics QC kits (**MSK-QC-KIT**, **MSK-QReSS™-KIT**, **MSK-QReSS-EXP-KIT**) for untargeted/targeted MS-based applications.

### 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-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.**

North America: 1.800.322.1174 cilsales@isotope.com | International: +1.978.749.8000 intl@isotope.com | fax: 1.978.749.2768 | isotope.com

### 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> , 96-98%)	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%) CP 97%	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:** Lippa, 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)

## MSK-QReSS-EXP-KIT Coming Soon!

This kit contains the following materials and tools:

- 3 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
<b>MSK-QRESS1</b>		
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> , 96-98%)	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
<b>MSK-QRESS2</b>		
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%) CP 97%	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

Description	Conc. (µg/mL)	Vial
<b>MSK-QC2</b>		
Caffeine ( <sup>13</sup> C <sub>3</sub> , 99%)	4	3
D-Glucose ( <sup>13</sup> C <sub>6</sub> , 99%)	4	3
Sodium benzoate ( <sup>13</sup> C <sub>6</sub> , 99%)	4	3
Sodium citrate ( <sup>13</sup> C <sub>3</sub> , 99%)	4	3
Sodium octanoate ( <sup>13</sup> C <sub>8</sub> , 99%)	4	3
Sodium propionate ( <sup>13</sup> C <sub>3</sub> , 99%)	4	3
Stearic acid, sodium salt ( <sup>13</sup> C <sub>18</sub> , 98%)	0.4	3
Succinic acid, disodium salt ( <sup>13</sup> C <sub>4</sub> , 99%)	4	3
D-Sucrose ( <sup>13</sup> C <sub>6</sub> , 98%)	4	3

