



# Metabolomics QReSS Kit

For Untargeted and Targeted  
Mass Spectrometric Analysis



To ensure high-quality metabolomics results, the method and instrument system must be qualified as being fit for purpose. This involves testing for losses or errors in the analytical workflow. **To aid such performance assessments in MS metabolomics and enable metabolite quantification, Cambridge Isotope Laboratories, Inc. (CIL) is pleased to offer the QReSS (Quantification, Retention, and System Suitability) kit.** Its potential use could also extend to other applications, such as metabolite retention indexing.

The kit contains the following materials and tools:

- 2 Vials of stable isotope-labeled metabolite mixes (lyophilized)
- User manual (with example procedures and LC-MS methods)

Catalog No.	Description
MSK-QReSS-KIT	Metabolomics QReSS Kit
MSK-QReSS1-1	Metabolomics QReSS Standard 1
MSK-QReSS2-1	Metabolomics QReSS Standard 2

**Note:** Unlabeled mixes are also available. Please inquire.

This kit, through collaboration with Sciex, was validated in different matrices (e.g., plasma, urine, CHO cells) using a single injection, microflow UHPLC-MRM/MS method (QTRAP® 6500+). Note that the mixes can also be extended to alternate LC-MS platforms. Procedurally, after reconstituting and mixing the kit vials, a working aliquot can be applied in various ways for use in metabolomic LC-MS/MS exercises. This enables the analytical performance to be evaluated and quantitative determinations of metabolites to be made.

**Table.** Mix compositions. Reconstituting each vial in 1 mL of solvent (e.g., water:methanol) will yield the specified concentrations.

Description	Chemical Formula	MW (Da)	Conc. (µg/mL)	Vial
L-Alanine ( <sup>13</sup> C <sub>3</sub> , 99%; <sup>15</sup> N, 99%)	<sup>13</sup> C <sub>3</sub> H <sub>7</sub> <sup>15</sup> N <sub>2</sub> O <sub>2</sub>	93.07	100	1
1,4-Butanediamine (putrescine)-2HCl ( <sup>13</sup> C <sub>4</sub> , 99%)	<sup>13</sup> C <sub>4</sub> H <sub>12</sub> N <sub>2</sub> ·2HCl	92.10	10	1
Creatinine (N-methyl-D <sub>3</sub> , 98%)	C <sub>4</sub> H <sub>4</sub> D <sub>3</sub> N <sub>3</sub> O	116.14	100	1
Ethanolamine-HCl (1,1,2,2-D <sub>4</sub> , 98%)	C <sub>2</sub> H <sub>3</sub> D <sub>4</sub> NO·HCl	65.11	10	1
Guanosine-2H <sub>2</sub> O ( <sup>15</sup> N <sub>5</sub> , 96-98%)	C <sub>10</sub> H <sub>13</sub> <sup>15</sup> N <sub>5</sub> O <sub>5</sub>	288.21	2	1
Hypoxanthine ( <sup>13</sup> C <sub>5</sub> , 99%)	<sup>13</sup> C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O	141.08	10	1
L-Leucine ( <sup>13</sup> C <sub>6</sub> , 99%)	<sup>13</sup> C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub>	137.13	5	1
L-Phenylalanine (ring- <sup>13</sup> C <sub>6</sub> , 99%)	<sup>13</sup> C <sub>6</sub> C <sub>3</sub> H <sub>11</sub> NO <sub>2</sub>	171.15	100	1
Thymine (1,3- <sup>15</sup> N <sub>2</sub> , 98%)	C <sub>5</sub> H <sub>6</sub> <sup>15</sup> N <sub>2</sub> O <sub>2</sub>	128.10	20	1
L-Tryptophan ( <sup>13</sup> C <sub>11</sub> , 99%)	<sup>13</sup> C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	215.14	100	1
L-Tyrosine (ring- <sup>13</sup> C <sub>6</sub> , 99%)	<sup>13</sup> C <sub>6</sub> C <sub>3</sub> H <sub>11</sub> NO <sub>3</sub>	187.14	100	1
Vitamin B <sub>3</sub> (nicotinamide) ( <sup>13</sup> C <sub>6</sub> , 99%)	<sup>13</sup> C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O	128.08	5	1
Citric acid (1,5,6-carboxyl- <sup>13</sup> C <sub>3</sub> , 99%)	<sup>13</sup> C <sub>3</sub> C <sub>3</sub> H <sub>8</sub> O <sub>7</sub>	195.10	10	2
Fumaric acid ( <sup>13</sup> C <sub>4</sub> , 99%)	<sup>13</sup> C <sub>4</sub> H <sub>4</sub> O <sub>4</sub>	120.04	100	2
Indole-3-acetic acid (phenyl- <sup>13</sup> C <sub>6</sub> , 99%)	<sup>13</sup> C <sub>6</sub> C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub>	181.14	5	2
α-Ketoglutaric acid, disodium salt (1,2,3,4- <sup>13</sup> C <sub>4</sub> , 99%) CP 97%	<sup>13</sup> C <sub>4</sub> CH <sub>4</sub> Na <sub>2</sub> O <sub>5</sub>	194.03	100	2
Sodium palmitate (U- <sup>13</sup> C <sub>16</sub> , 98%)	<sup>13</sup> C <sub>16</sub> H <sub>31</sub> O <sub>2</sub> Na	294.29	10	2
Sodium pyruvate ( <sup>13</sup> C <sub>3</sub> , 99%)	<sup>13</sup> C <sub>3</sub> H <sub>3</sub> O <sub>3</sub> Na	113.02	100	2

**Please inquire for pricing and companion unlabeled mixtures.**

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

