



Metabolomics QReSS™ Kits

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 Mix 1
MSK-QReSS2-1	Metabolomics QReSS Standard Mix 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, high-flow 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 (see app note #49 for example overview).

Table. Mix compositions. Reconstituting each vial in 1 mL of solvent (e.g., 50% methanol) will yield the specified concentrations.

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

Application Note

Percy, A.J.; Proos, R.; Demianova, Z.; Backiel, K.; Ubhi, B.K. **2021.** Standardizing quantitative metabolomics analyses through the QReSS™ kit. (CIL note #49)

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