Cambridge Isotope Laboratories, Inc.
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RESEARCH PRODUCTS

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:

- Vials of stable isotope-labeled metabolite mixes (lyophilized)
- User manual (with example procedures, methods, and results)

Catalog No.	Description
MSK-QReSS-KIT	Metabolomics QReSS Kit
MSK-QReSS1	Metabolomics QReSS Standard Mix 1
MSK-QReSS2	Metabolomics QReSS Standard Mix 2
COMING SOON! MSK-QReSS-EXP-KIT	Expanded Metabolomics QReSS Kit (contains MSK-QReSS1, MSK-QReSS2, and MSK-QC2)

Note: Unlabeled mixes/kits may be 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%)	$^{13}C_3H_7{}^{15}NO_2$	93.07	100	1
1,4-Butanediamine (putrescine)·2HCl ($^{13}C_4$, 99%)	$^{13}C_4H_{12}N_2\cdot 2HCl$	165.04	10	1
Creatinine (*N*-methyl-D_3, 98%)	$C_4H_4D_3N_3O$	116.14	100	1
Ethanolamine·HCl (1,1,2,2-D_4, 98%)	$C_2H_3D_4NO\cdot HCl$	101.57	10	1
Guanosine·$2H_2O$ ($^{15}N_5$, 96-98%)	$C_{10}H_{13}{}^{15}N_5O_5$	288.21*	2	1
Hypoxanthine ($^{13}C_5$, 99%)	$^{13}C_5H_4N_4O$	141.08	10	1
L-Leucine ($^{13}C_6$, 99%)	$^{13}C_6H_{13}NO_2$	137.13	5	1
L-Phenylalanine (ring-$^{13}C_6$, 99%)	$^{13}C_6C_3H_{11}NO_2$	171.15	100	1
Thymine (1,3-$^{15}N_2$, 98%)	$C_5H_6{}^{15}N_2O_2$	128.10	20	1
L-Tryptophan ($^{13}C_{11}$, 99%)	$^{13}C_{11}H_{12}N_2O_2$	215.14	100	1
L-Tyrosine (ring-$^{13}C_6$, 99%)	$^{13}C_6C_3H_{11}NO_3$	187.14	100	1
Vitamin B_3 (nicotinamide) ($^{13}C_6$, 99%)	$^{13}C_6H_6N_2O$	128.08	5	1
Citric acid (1,5,6-carboxyl-$^{13}C_3$, 99%)	$^{13}C_3C_3H_8O_7$	195.10	10	2
Fumaric acid ($^{13}C_4$, 99%)	$^{13}C_4H_4O_4$	120.04	100	2
Indole-3-acetic acid (phenyl-$^{13}C_6$, 99%)	$^{13}C_6C_4H_9NO_2$	181.14	5	2
α-Ketoglutaric acid, disodium salt (1,2,3,4-$^{13}C_4$, 99%) CP 97%	$^{13}C_4CH_4Na_2O_5$	194.03	100	2
Sodium palmitate (U-$^{13}C_{16}$, 98%)	$^{13}C_{16}H_{31}O_2Na$	294.29	10	2
Sodium pyruvate ($^{13}C_3$, 99%)	$^{13}C_3H_3O_3Na$	113.02	100	2

**Anhydrous*

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

Application Notes

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)

Percy, A.J.; Proos, R.; Demianova, Z.; et al. **2021**. Standardizing quantitative metabolomics analyses through the QReSS™ kit. (CIL application note #49)

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MET_RSCH_QReSS (5/2/23) Supersedes all previously published literature