



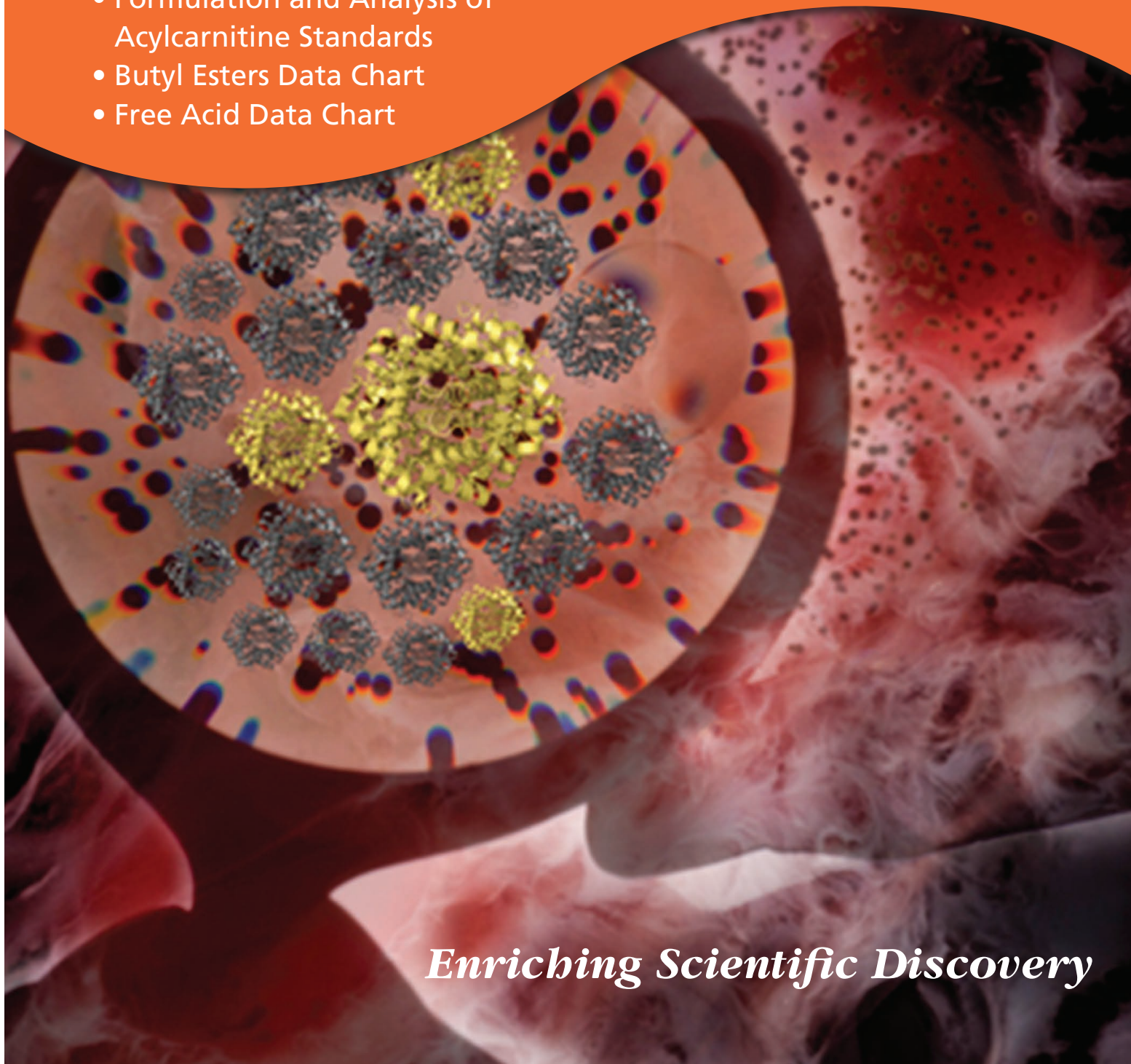
CIL

Cambridge Isotope Laboratories, Inc.  
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RESEARCH PRODUCTS

# MS/MS Standards

- NSK Standards
- Formulation and Analysis of Acylcarnitine Standards
- Butyl Esters Data Chart
- Free Acid Data Chart



*Enriching Scientific Discovery*

Phone: **1.800.322.1174** (North America)  
**1.978.749.8000**

Fax: **1.978.749.2768**

Email: **cilsales@isotope.com**  
**intlsales@isotope.com** (International)

Website: **isotope.com**

CIL Corporate Headquarters:  
**3 Highwood Drive**  
**Tewksbury, MA 01876 USA**

## NSK-A – Amino Acid Reference Standards

This set contains 10 vials of a dry mixture of 12 isotopically labeled amino acids. Accurate and complete reconstitution of the contents of one vial in 1 mL of high purity solvent will produce the concentrations presented in the Standard Concentrations table. Mix well. This solution becomes the concentrated amino acid stock standard.

### Dilution of Reference Standards Concentrated Working Stock

To prepare working stock solutions, one of the following procedures is suggested:

- Dilute 1 mL (reconstituted vial contents per instructions above) of the concentrated amino acid stock standard with pure solvent.
- If Set B (Acylcarnitine Reference Standards) was purchased, mix 1 mL (reconstituted vial contents) of concentrated standards from Set A with 1 mL of the concentrated standards from Set B.

Store the diluted standards in a tightly sealed vial at 4°C. In order to maintain the integrity of the solution, we recommend storing the sealed vials in a second sealed container. We recommend discarding this concentrated working stock solution after ~1 month. Stability data is being obtained.

Standards Concentrations	(nmol/mL)
Reference Standard	Concentration
<sup>15</sup> N; 2- <sup>13</sup> C-Glycine	2500
<sup>2</sup> H <sub>4</sub> -Alanine	500
<sup>2</sup> H <sub>8</sub> -Valine	500
<sup>2</sup> H <sub>3</sub> -Leucine	500
<sup>2</sup> H <sub>3</sub> -Methionine	500
<sup>13</sup> C <sub>6</sub> -Phenylalanine	500
<sup>13</sup> C <sub>6</sub> -Tyrosine	500
<sup>2</sup> H <sub>3</sub> -Aspartate	500
<sup>2</sup> H <sub>3</sub> -Glutamate	500
<sup>2</sup> H <sub>2</sub> -Ornithine	500
<sup>2</sup> H <sub>2</sub> -Citrulline	500
<sup>2</sup> H <sub>4</sub> ; 5- <sup>13</sup> C-Arginine	500

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Not for diagnostic  
purposes.**



## NSK-B – Free Carnitine and Acylcarnitine Reference Standards

This set contains 10 vials of a dry mixture of eight isotopically labeled free carnitine and acylcarnitines. Accurate and complete reconstitution of the contents of one vial in 1 mL of high purity solvent will produce the concentrations presented in the Standard Concentrations table. Mix well. This solution becomes the concentrated acylcarnitine stock standard.

### Dilution of Reference Standards Concentrated Working Stock

To prepare working stock solutions, one of the following procedures is suggested:

- Dilute 1 mL (reconstituted vial contents per instructions above) of the concentrated acylcarnitine stock standard with pure solvent.
- If Set A (Amino Acid Reference Standards) was purchased, mix 1 mL (vial contents) of concentrated standards from Set A with 1 mL of the concentrated standards from Set B.

Store the diluted standards in a tightly sealed vial at 4°C. In order to maintain the integrity of the solution, we recommend storing the sealed vials in a second sealed container. We recommend discarding this concentrated working stock solution after ~1 month. Stability data is being obtained.

Standards Concentrations	(nmol/mL)
Reference Standard	Concentration
<sup>2</sup> H <sub>9</sub> -Carnitine (free carnitine, CN)	152.0
<sup>2</sup> H <sub>3</sub> -Acetylcarnitine (C2)	38.0
<sup>2</sup> H <sub>3</sub> -Propionylcarnitine (C3)	7.6
<sup>2</sup> H <sub>3</sub> -Butyrylcarnitine (C4)	7.6
<sup>2</sup> H <sub>9</sub> -Isovalerylcarnitine (C5)	7.6
<sup>2</sup> H <sub>3</sub> -Octanoylcarnitine (C8)	7.6
<sup>2</sup> H <sub>9</sub> -Myristoylcarnitine (C14)	7.6
<sup>2</sup> H <sub>3</sub> -Palmitoylcarnitine (C16)	15.2

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## NSK-B-G1 – Supplemental Acylcarnitine Reference Standards

This set contains 10 vials of a dry mixture of five isotopically labeled acylcarnitines. Accurate and complete reconstitution of the contents of one vial in 1 mL of high purity solvent will produce the concentrations presented in the Standard Concentrations table. Mix well. This solution becomes the concentrated supplemental acylcarnitine stock standard.

### Dilution of Reference Standards Concentrated Working Stock

To prepare working stock solutions, mix 1 mL (vial contents) of concentrated standards from NSK-A with 1 mL of the concentrated standards from NSK-B and 1 mL of the concentrated standards from NSK-B-G1.

Store the diluted standards in a tightly sealed vial at 4°C. In order to maintain the integrity of the solution, we recommend storing the sealed vials in a second sealed container. We recommend discarding this concentrated working stock solution after ~1 month. Stability data is being obtained.

Note: NSK-B-G1 replaces NSK-B-G with the addition of hydroxypalmitoylcarnitine ( $^2\text{H}_3$ -hydroxypalmitoylcarnitine).

Standards Concentrations	(nmol/mL)
Reference Standard	Concentration
$^2\text{H}_3$ -Glutarylcarnitine	15.20
$^2\text{H}_3$ -Hydroxyisovalerylcarnitine	7.6
$^2\text{H}_9$ -Dodecanoylcarnitine	7.6
$^2\text{H}_3$ -Octadecanoylcarnitine	15.20
$^2\text{H}_3$ -Hydroxypalmitoylcarnitine	15.20

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## NSK-T – Succinylacetone Reference Standards

This set contains 10 vials of isotopically labeled succinylacetone. Accurate and complete reconstitution of the contents of one vial in 1 mL of high purity solvent will produce the concentrations presented in the Standard Concentrations table. Mix well. This solution becomes the concentrated succinylacetone stock standard.

### Dilution of Reference Standards Concentrated Working Stock

To prepare working stock solutions, the following procedure is suggested: dilute 1 mL (reconstituted vial contents per instructions above) of the concentrated succinylacetone standard with pure solvent.

Store the diluted standards in a tightly sealed vial at 4°C. In order to maintain the integrity of the solution, we recommend storing the sealed vials in a second sealed container. We recommend discarding this concentrated working stock solution after ~1 month. Stability data is being obtained.

Standards Concentrations	(nmol/mL)
Reference Standard	Concentration
$^{13}\text{C}_5$ -Succinylacetone	1000

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## NSK-A-TS and NSK-B-TS Tuning Standards

Tandem Mass Spectrometer (MS/MS) Tuning Standards, NSK-A-TS and NSK-B-TS, have been developed to complement quality assurance and quality control (QA/QC) procedures in the laboratory. Use MS/MS Tuning Standards to:

- Ensure MS/MS instrument is operating at peak sensitivity for analysis of amino acids and acylcarnitines prior to analysis.
- Monitor instrument sensitivity from analysis of the first dried blood spot (DBS) to the last, whether samples are from one or several microtiter plates, during and between analysis runs.
- Quickly locate the source of sensitivity loss during an analytical run or between batch analyses.
- Compare performance of multiple instruments within a laboratory or across many laboratories.
- Evaluate performance before and after instrument maintenance.
- Assess MS/MS performance in analysis of amino acids (AA) and acylcarnitines (AC) independent of DBS samples and their preparation.

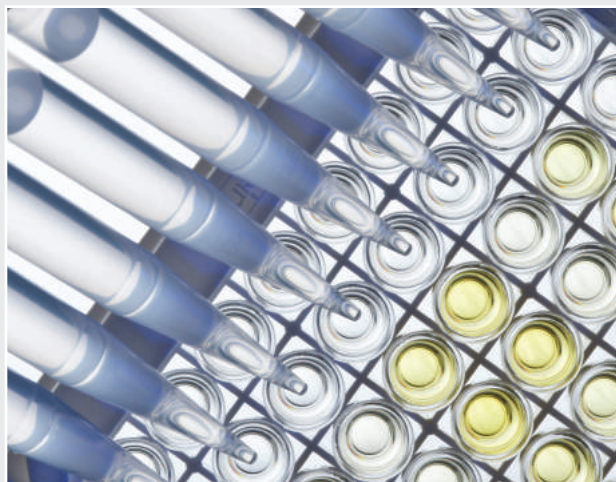
After reconstitution in mobile phase whether as free acids or derivatized as butyl esters, the tuning standards are stable in solution for up to 30 days when stored at 4°C. The prepared solutions are ready for use immediately whether for tuning the instrument as part of regular maintenance, for troubleshooting MS/MS instrument problems or for a quick daily check before each batch run (or as often as a protocol may require). These reconstituted tuning standards are concentrated solutions and do not replace NSK-A and NSK-B reference standards.

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NSK-A-TS		( $\mu\text{M}$ )*
Catalog No.	Amino Acid	Concentration
DLM-250	L-Alanine ( $\text{D}_4$ )	25
CLM-1055	L-Phenylalanine (ring- $^{13}\text{C}_6$ )	25
DLM-3860	L-Citrulline (5,5- $\text{D}_2$ )	25
DLM-335	DL-Glutamic acid (2,4,4- $\text{D}_3$ )	25
DLM-431	L-Methionine (methyl- $\text{D}_3$ )	25

NSK-B-TS		( $\mu\text{M}$ )*
Catalog No.	Carnitine	Concentration
DLM-3555	L-Carnitine ( $\text{D}_9$ , 98%) (CN)	7.6
DLM-3973	O-Propionyl-L-carnitine-HCl ( $\text{D}_3$ ) (C3)	0.38
DLM-755	O-Octanoyl-L-carnitine-HCl ( $\text{D}_3$ ) (C8)	0.38
DLM-1263	O-Palmitoyl-L-carnitine-HCl ( $\text{D}_3$ ) (C16)	0.76

\*When reconstituted in 1 mL solvent.



# NSK-S-CAH – Congenital Adrenal Hyperplasia (CAH)

## Reference Standards

NSK-S-CAH Congenital Adrenal Hyperplasia (CAH) Reference Standards is designed as a calibrator for use in screening, diagnosis and monitoring procedures for metabolic disorders. When used as directed, NSK-S-CAH provides a solution containing steroids at defined concentrations. When combined with techniques such as tandem mass spectrometry (MS/MS), LC/MS, GC/MS, etc., the solution may be used as a calibrator to measure concentrations of steroids in plasma, blood spots, urine and other bodily fluids.

Each vial (packaged as 1 to 10 vials per box) contains only a dry mixture of isotopically labeled steroids. Complete reconstitution in 1 mL of solvent will produce the concentrations presented in the Standards Concentrations table.

### Instructions for Use/ Method of Reconstitution

To reconstitute the NSK-S-CAH Congenital Adrenal Hyperplasia (CAH) Reference Standards solution, the following procedure is suggested: add 1 mL of purified methanol or suitable solvent to the dry mixture in the vial. Vortex the vial manually for one minute then auto-vortex for 30 minutes or until solids are dissolved. Use the same day or store the reconstituted standards in a tightly sealed vial in a freezer. In order to maintain the integrity of the solution, we recommend storing the sealed vial in a second sealed container. We recommend discarding the solution after one month.

Standards Concentrations		(nmol/mL)
Reference Standard	Concentration	
17 $\alpha$ -Hydroxyprogesterone (2,2,4,6,6,21,21,21-D <sub>8</sub> )	20.0	
4-Androstene-3,17-dione (2,2,4,6,6,16,16-D <sub>7</sub> )*	20.0	
11-Deoxycortisol (2,2,4,6,6-D <sub>2</sub> )	20.0	
21-Deoxycortisol (2,2,4,6,6,21,21,21-D <sub>8</sub> )	20.0	
Cortisol (9,11,12,12-D <sub>4</sub> )	100.0	

### Handling, Storage and Disposal Instructions

Sealed vials, as received, can be stored at room temperature away from light with a recommended shelf life of two years. The recommended shelf life for methanol solutions is one month when kept in a freezer and away from light. The product should be disposed of properly: in the dry form, as a steroid and in solution as solvent waste.

### Second-Tier Testing for Congenital Adrenal Hyperplasia (CAH)

The use of standards similar to the NSK-S-CAH Congenital Adrenal Hyperplasia (CAH) Reference Standards has been well documented in the scientific literature with detailed examples in the journal articles referenced below.

**For research use only. Not for diagnostic purposes. \*Controlled substance. CIL has a DEA exemption for this product.**

Lacey, J.M.; Minutti, C.Z.; Magera, M.J.; Tauscher, A.L.; Casetta, B.; McCann, M.; Lymp, J.; Hahn, S.H.; Rinaldo, P.; Matern, D. **2004**. Improved Specificity of Newborn Screening for Congenital Adrenal Hyperplasia by Second-Tier Steroid Profiling Using Tandem Mass Spectrometry. *Clin Chem*, 50, 621-625.

Janzen, N.; Sander, S.; Terhardt, M.; Steuerwald, U.; Peter, M.; Das, A.M.; Sander, J. **2011**. Rapid steroid hormone quantification for congenital adrenal hyperplasia (CAH) in dried blood spots using UPLC liquid chromatography-tandem mass spectrometry. *Steroids*, 76, 1437-1442.

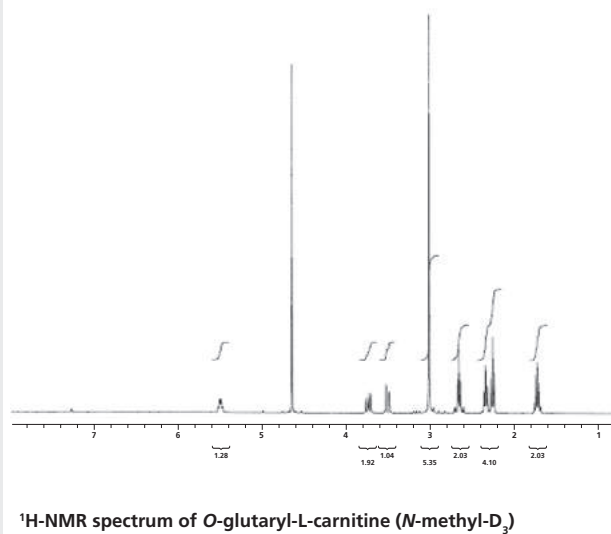
Dhillon, K.; Ho, T.; Rich, P.; Xu, D.; Lorey, F.; She, J.; Bhandal, A. **2011**. An automated method on analysis of blood steroids using liquid chromatography-tandem mass spectrometry: Application to population screening for congenital adrenal hyperplasia in newborns. *Clin Chim Acta*, 412, 2076-2084.

Rossi, C.; Calton, L.; Brown, H.A.; Gillingwater, S.; Wallace, A.M.; Petrucci, F.; Ciavardelli, D.; Urbani, A.; Sacchetta, P.; Morris, M. **2011**. Confirmation of congenital adrenal hyperplasia by adrenal steroid profiling of filter paper dried blood samples using ultra-performance liquid chromatography-tandem mass spectrometry. *Clin Chem Lab Med*, 49, 677-684.

## Formulation and Analysis of Acylcarnitine Standards

**Cambridge Isotope Laboratories, Inc. (CIL) provides *O*-acylcarnitines of high chemical purity as individual components and kits. As part of this program, CIL offers:**

- Straight-chain *O*-acylcarnitines from C<sub>0</sub> to C<sub>26</sub> in high chemical purity with D<sub>3</sub>, D<sub>6</sub>, or D<sub>9</sub> labeling.
- Branched-chain and other substituted *O*-acylcarnitines, including glutaryl, isovaleryl, 3-hydroxyisovaleryl, and 2-decenoyl carnitines, also with D<sub>3</sub>, D<sub>6</sub>, or D<sub>9</sub> labeling.
- High-purity unlabeled reference standards corresponding to all labeled analogs.
- Kits prepared under batch record control, analyzed against certified standards with excellent reproducibility and quality assurance.



### Reference Materials

Before isotopically labeled carnitine standard solutions can be formulated and tested, corresponding unlabeled (“native”) reference materials must be purified and characterized. We have observed that unlabeled materials available from other manufacturers are often of insufficient purity to use as reference standards. At CIL, we independently synthesize and purify each of these reference materials. The identity and purity of native carnitines are established using quantitative nuclear magnetic resonance (NMR) spectroscopy, high-performance liquid chromatography (HPLC), and melting-point determinations. Quantitative NMR is the primary analytical technique, using a common reference material for all the carnitines analyzed.

With pure, well-characterized reference materials in hand, we take similar steps to synthesize, purify, and analyze labeled carnitines. Enrichment, the amount of stable isotope incorporation, is measured relative to native analogs by NMR or liquid chromatography mass spectrometry (LC/MS) techniques. The <sup>1</sup>H-NMR spectrum of *O*-glutaryl-L-carnitine (*N*-methyl-D<sub>3</sub>) is shown above.

### Unlabeled Standard Solutions

The gravimetry is traceable to US National Institute of Standards and Technology (NIST) standards. The weights and balances are calibrated on a regular schedule. Class A volumetric glassware is used. These rigorous procedures allow us to control and calculate the uncertainty for concentrations of the unlabeled certified standard solutions, according to EURACHEM/CITAC guidelines.

### NSK-B Formulation and Dispensing

Labeled carnitine standard solutions are formulated using similar procedures. Once the concentration of the labeled carnitine solution has been verified against the unlabeled standard (described in detail, below), the solution is metered into vials using a calibrated pipette. The mass of solution added to each vial (and hence the amount of labeled standard) is individually verified. The transfer process is organized into discrete blocks, referred to as “dispenses,” to enhance traceability. The solutions in the individual vials are evaporated under vacuum in a carefully controlled environment.

### Sampling and Analysis

Samples of the finished product are taken to verify the reconstituted concentrations of the carnitines. Quality-control samples are drawn according to American National Standards Institute/American Society for Quality Control (ANSI/ASQC) sampling guidelines.

Certified carnitine standards are formulated at five concentrations, bracketing the target concentrations for the product (0.750x, 0.875x, 1.000x, 1.250x, 1.500x). The carnitines are analyzed by HPLC, using an evaporative light-scattering detector (LSD), which is sensitive to a wide range of materials, including carnitines, at low concentrations. Other typical HPLC detectors (e.g., ultraviolet, UV, RI) are not sensitive enough to analyze carnitines at the required concentrations. As with many analytical detectors, the response is nonlinear. Quadratic or cubic equations are fitted to the calibration curves, with typical correlation coefficients ranging

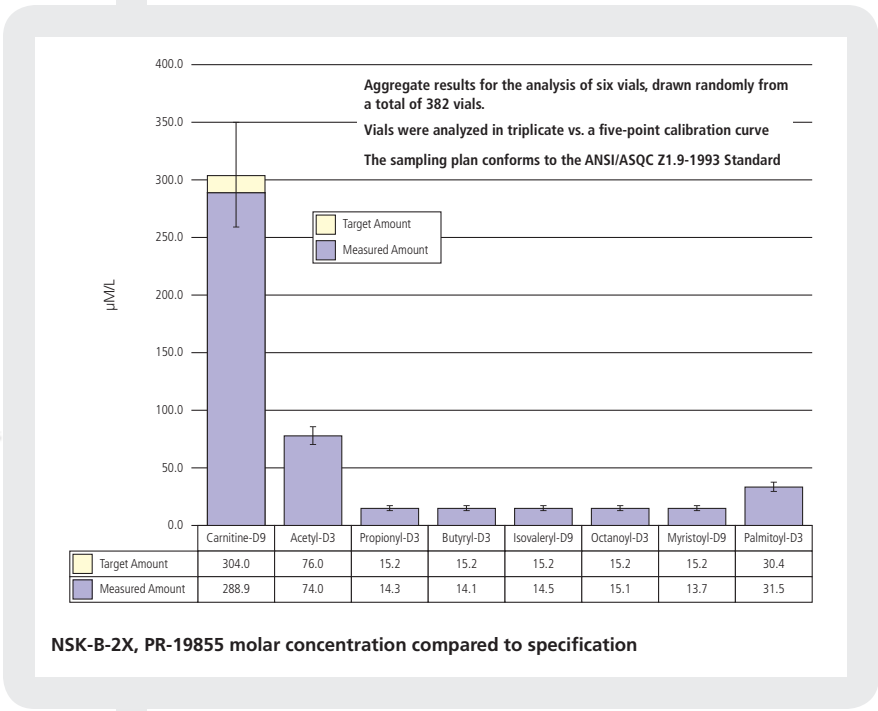
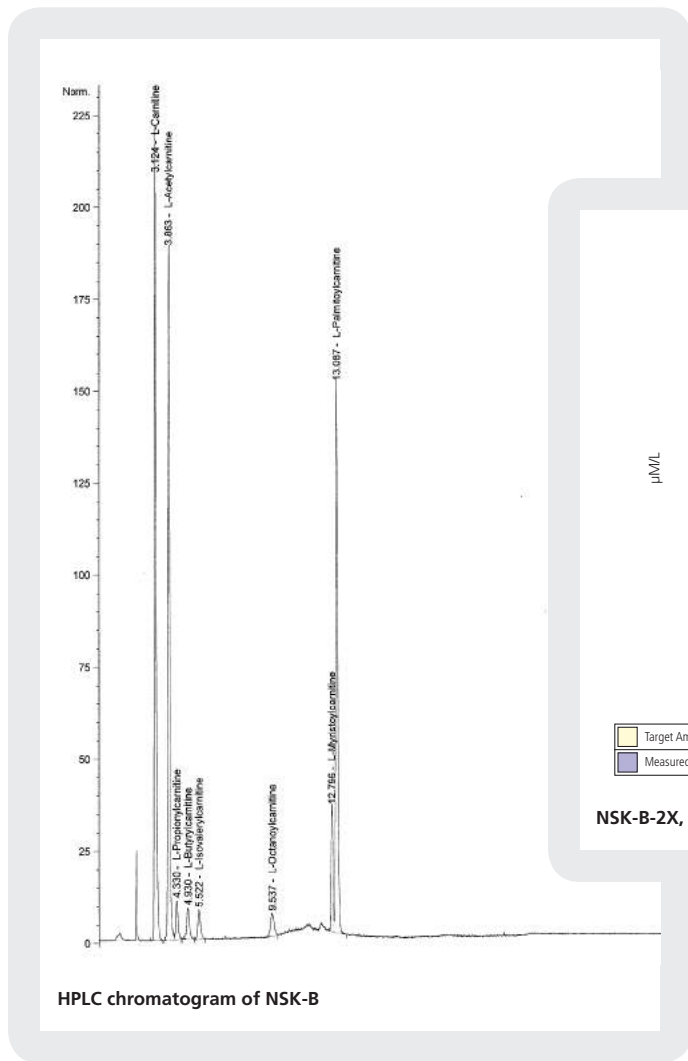
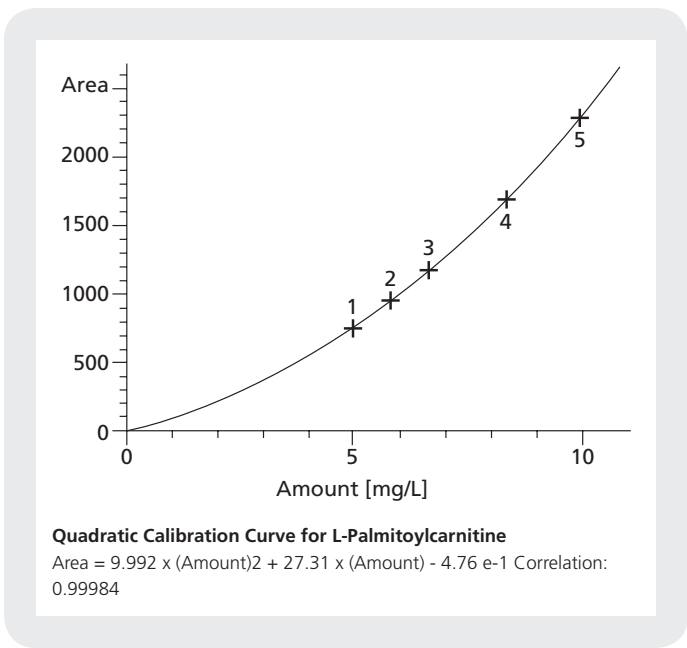
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## Formulation and Analysis of Acylcarnitines (continued)

from 0.99995 to 0.99911. Calibration standards are run, interspersed among the product samples with typically five standard concentrations before each set of 5 (or 6) samples.

### Calculations and Results

The ELSD measures concentrations by weight (mg/L). To compare these values to the specification, the concentrations are converted to micro-moles per liter (µM/L). The measured molar concentrations compare well to the corresponding targets. The upper and lower bounds represent the target concentration +/- 15%.





# Butyl Esters

Neutral and Acidic Amino Acids (NSK- A)			
m/z	Compound	Abbr.	Comments (NL 102)
132	Glycine	Gly	
<b>134</b>	<b>*Glycine</b>	<b>*Gly</b>	<sup>13</sup> C <sub>15</sub> N
146	Alanine	Ala	
<b>150</b>	<b>*Alanine</b>	<b>*Ala</b>	D <sub>4</sub>
162	Serine	Ser	
172	Proline	Pro	
174	Valine	Val	
176	Threonine	Thr	
<b>182</b>	<b>*Valine</b>	<b>*Val</b>	D <sub>8</sub>
186	Glutamine	Gln	(Glu – NH <sub>3</sub> )
188	Leucine+	Leu+	Isoleucine, HydroxyProline, Allo-Ile
<b>191</b>	<b>*Leucine</b>	<b>*Leu</b>	D <sub>3</sub>
206	Methionine	Met	
<b>209</b>	<b>*Methionine</b>	<b>*Met</b>	D <sub>3</sub>
212	Histidine	His	
222	Phenylalanine	Phe	
<b>228</b>	<b>*Phenylalanine</b>	<b>*Phe</b>	<sup>13</sup> C <sub>6</sub>
238	Tyrosine	Tyr	
<b>244</b>	<b>*Tyrosine</b>	<b>*Tyr</b>	<sup>13</sup> C <sub>6</sub>
246	Aspartic Acid	Asp	
<b>249</b>	<b>Aspartic Acid</b>	<b>*Asp</b>	D <sub>3</sub>
260	Glutamic Acid	Glu	
<b>263</b>	<b>Glutamic Acid</b>	<b>*Glu</b>	D <sub>3</sub>

Basic Amino Acids (NSK- A)			
m/z	Compound	Abbr.	Comments
189	Ornithine	Orn	NL 119
<b>191</b>	<b>*Ornithine</b>	<b>*Orn</b>	D <sub>2</sub>
232	Citrulline	Cit	NL 119
<b>234</b>	<b>*Citrulline</b>	<b>*Cit</b>	D <sub>2</sub>
231	Arginine	Arg	NL 161
<b>236</b>	<b>*Arginine</b>	<b>*Arg</b>	D <sub>4</sub> <sup>13</sup> C

NL = Neutral Loss

Legend: NSK-A = blue, NSK-B = green, NSK-B-G = red

Free Carnitine (NSK- B)			
m/z	Compound	Abbr.	Comments (Pre 85)
218	Free Carnitine	C0, FC	Pre 85 and Pre 103
221	*Hydro-Free Carnitine	*Hydro-FC	Hydrolyzed D <sub>3</sub> AC STDS
<b>227</b>	<b>*Free Carnitine</b>	<b>*FC</b>	D <sub>9</sub>
Acylcarnitines (NSK- B, NSK- B-G)			
m/z	Compound	Abbr.	Comments
260	Acetyl-	C2	(+ glutamic acid)
<b>263</b>	<b>*Acetyl-</b>	<b>*C2</b>	D <sub>3</sub> (+ D <sub>3</sub> -Glu)
274	Propionyl-	C3	
<b>277</b>	<b>*Propionyl-</b>	<b>*C3</b>	D <sub>3</sub>
288	Butyryl-	C4	
<b>291</b>	<b>*Butyryl-</b>	<b>*C4</b>	D <sub>3</sub>
300	Tiglyl-	C5:1	
302	Isovaleryl-	C5	Methylbutyryl-
304	Hydroxybutyryl-	C4OH	
<b>311</b>	<b>*Isovaleryl-</b>	<b>*C5</b>	D <sub>9</sub>
316	Hexanoyl-	C6	
318	Hydroxyisovaleryl-	C5OH	
<b>321</b>	<b>*Hydroxyisovaleryl-</b>	<b>*C5OH</b>	D <sub>3</sub>
344	Octanoyl-	C8	
<b>347</b>	<b>*Octanoyl-</b>	<b>*C8</b>	D <sub>3</sub>
360	Malonyl-	C3DC	
368	Decadienoyl-	C10:2	
370	Decenoyl-	C10:1	
372	Decanoyl-	C10	
374	Methylmalonyl-	C4DC	
388	Glutaryl-	C5DC	
<b>391</b>	<b>*Glutaryl</b>	<b>*C5DC</b>	D <sub>3</sub>
400	Dodecanoyl-	C12	
<b>409</b>	<b>*Dodecanoyl</b>	<b>*C12</b>	D <sub>9</sub>
426	Tetradecenoyl-	C14:1	
428	Tetradecanoyl-	C14	
<b>437</b>	<b>*Tetradecanoyl-</b>	<b>*C14</b>	D <sub>9</sub>
456	Palmitoyl-	C16	
<b>459</b>	<b>*Palmitoyl-</b>	<b>*C16</b>	D <sub>3</sub>
472	Hydroxypalmitoyl-	C16OH	
482	Octadecenoyl-	C18:1	
484	Octadecanoyl-	C18	
<b>487</b>	<b>*Octadecanoyl-</b>	<b>*C18</b>	D <sub>3</sub>
498	Hydroxyoctadecenoyl-	C18:1 OH	
500	Hydroxyoctadecanoyl-	C18OH	

Note: Customers can request a laminated copy of this chart by contacting us at [cilmkt@isotope.com](mailto:cilmkt@isotope.com).

(continued)

## Free Acid (non-derivatized)

Neutral and Acidic Amino Acids (NSK- A)			
m/z	Compound	Abbr.	Comments (NL 46)
76	Glycine	Gly	
<b>78</b>	<b>*Glycine</b>	<b>*Gly</b>	<b><sup>13</sup>C<sup>15</sup>N</b>
90	Alanine	Ala	
<b>94</b>	<b>*Alanine</b>	<b>*Ala</b>	<b>D<sub>4</sub></b>
106	Serine	Ser	
116	Proline	Pro	
118	Valine	Val	
120	Threonine	Thr	
<b>126</b>	<b>*Valine</b>	<b>*Val</b>	<b>D<sub>8</sub></b>
130	Glutamine	Gln	(Glu – NH <sub>3</sub> )
132	Leucine+	Leu+	Isoleucine, HydroxyProline, Allo-Ile
<b>135</b>	<b>*Leucine</b>	<b>*Leu</b>	<b>D<sub>3</sub></b>
150	Methionine	Met	
<b>153</b>	<b>*Methionine</b>	<b>*Met</b>	<b>D<sub>3</sub></b>
156	Histidine	His	
166	Phenylalanine	Phe	
<b>172</b>	<b>*Phenylalanine</b>	<b>*Phe</b>	<b><sup>13</sup>C<sub>6</sub></b>
182	Tyrosine	Tyr	
<b>188</b>	<b>*Tyrosine</b>	<b>*Tyr</b>	<b><sup>13</sup>C<sub>6</sub></b>
134	Aspartic Acid	Asp	
<b>137</b>	<b>Aspartic Acid</b>	<b>*Asp</b>	<b>D<sub>3</sub></b>
148	Glutamic Acid	Glu	
<b>151</b>	<b>Glutamic Acid</b>	<b>*Glu</b>	<b>D<sub>3</sub></b>

Basic Amino Acids (NSK- A)			
m/z	Compound	Abbr.	Comments
133	Ornithine	Orn	NL 63
<b>135</b>	<b>*Ornithine</b>	<b>*Orn</b>	<b>D<sub>2</sub></b>
176	Citrulline	Cit	NL 63
<b>178</b>	<b>*Citrulline</b>	<b>*Cit</b>	<b>D<sub>2</sub></b>
175	Arginine	Arg	NL 105
<b>180</b>	<b>*Arginine</b>	<b>*Arg</b>	<b>D<sub>4</sub><sup>13</sup>C</b>

NL = Neutral Loss

Legend: NSK-A = blue, NSK-B = green, NSK-B-G = red

Note: Customers can request a laminated copy of this chart by contacting us at [cilmkt@isotope.com](mailto:cilmkt@isotope.com).

Free Carnitine (NSK- B)			
m/z	Compound	Abbr.	Comments (Pre 85)
162	Free Carnitine	C0, FC	Pre 85 and Pre 103
165	*Hydro-Free Carnitine	*Hydro-FC	Hydrolyzed D <sub>3</sub> AC STDS
<b>171</b>	<b>*Free Carnitine</b>	<b>*FC</b>	<b>D<sub>9</sub></b>
Acylcarnitines (NSK- B, NSK- B-G)			
m/z	Compound	Abbr.	Comments
204	Acetyl-	C2	
<b>207</b>	<b>*Acetyl-</b>	<b>*C2</b>	<b>D<sub>3</sub></b>
218	Propionyl-	C3	
<b>221</b>	<b>*Propionyl-</b>	<b>*C3</b>	<b>D<sub>3</sub></b>
232	Butyryl-	C4	
<b>235</b>	<b>*Butyryl-</b>	<b>*C4</b>	<b>D<sub>3</sub></b>
244	Tiglyl-	C5:1	
246	Isovaleryl-	C5	Methylbutyryl-
248	Hydroxybutyryl-	C4OH	Malonyl-
<b>255</b>	<b>*Isovaleryl-</b>	<b>*C5</b>	<b>D<sub>9</sub></b>
260	Hexanoyl-	C6	
262	Hydroxyisovaleryl-	C5OH	Methylmalonyl-
<b>265</b>	<b>*Hydroxyisovaleryl-</b>	<b>*C5OH</b>	<b>D<sub>3</sub></b>
288	Octanoyl-	C8	
<b>291</b>	<b>*Octanoyl-</b>	<b>*C8</b>	<b>D<sub>3</sub></b>
248	Malonyl-	C3DC	Hydroxybutyryl-
312	Decadienoyl-	C10:2	
314	Decenoyl-	C10:1	
316	Decanoyl-	C10	
262	Methylmalonyl-	C4DC	Hydroxyisovaleryl-
276	Glutaryl-	C5DC	
<b>279</b>	<b>*Glutaryl</b>	<b>*C5DC</b>	<b>D<sub>3</sub></b>
344	Dodecanoyl-	C12	
<b>353</b>	<b>*Dodecanoyl</b>	<b>*C12</b>	<b>D<sub>9</sub></b>
370	Tetradecenoyl-	C14:1	
372	Tetradecanoyl-	C14	
<b>381</b>	<b>*Tetradecanoyl-</b>	<b>*C14</b>	<b>D<sub>9</sub></b>
400	Palmitoyl-	C16	
<b>403</b>	<b>*Palmitoyl-</b>	<b>*C16</b>	<b>D<sub>3</sub></b>
416	Hydroxypalmitoyl-	C16OH	
426	Octadecenoyl-	C18:1	
428	Octadecanoyl-	C18	
<b>431</b>	<b>*Octadecanoyl-</b>	<b>*C18</b>	<b>D<sub>3</sub></b>
442	Hydroxyoctadecenoyl-	C18:1 OH	
444	Hydroxyoctadecanoyl-	C18OH	

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