

Standard Reference Material® 1849b Infant/Adult Nutritional Formula I

CERTIFICATE OF ANALYSIS

Purpose: The certified values delivered by this Standard Reference Material (SRM) are intended for validating methods for determining elements and vitamins in infant and adult nutritional formulas and similar materials and for quality assurance when assigning values to in-house control materials.

Description: A unit of SRM 1849b consists of 10 packets, each containing approximately 10 g of material.

Certified Values: NIST certified values are traceable to the International System of Units (SI) derived unit of mass fraction, expressed as milligrams per kilogram. The values are reported on an as-received basis [1].

Mass Fraction(a) Mass Fraction^(a) (mg/kg) (mg/kg) Chromium (Cr) Molybdenum (Mo) 1.741 ± 0.063 $1.033 \pm$ 0.018 Phosphorus (P) Copper (Cu) $18.96 \pm$ 0.30 3750 ± 130 Iodine (I) $2.03 \pm$ 0.19 Selenium (Se) $0.816 \pm$ 0.025 Iron (Fe) $168.0 \pm$ 7.4 Magnesium (Mg) 1570 30 Cyanocobalamin (Vitamin B₁₂) $0.0497 \pm$ 0.0046

Table 1. Certified Values for Various Measurands in SRM 1849b

Non-Certified Values: Non-certified values for elements, vitamins, carotenoids, fatty acids, proximates, sugars, other nutrients, nucleotides, amino acids, and taurine in SRM 1849b are provided in Appendix A.

Period of Validity: The certified values delivered by **SRM 1849b** are valid within the measurement uncertainty specified until **31 December 2032.** The certified values are nullified if the SRM is stored or used improperly, damaged, contaminated, or otherwise modified.

Maintenance of Certified Values: NIST will monitor this SRM over the period of its validity. If substantive technical changes occur that affect the certification, NIST will issue an amended certificate through the NIST SRM website (https://www.nist.gov/srm) and notify registered users. SRM users can register online from a link available on the NIST SRM website or fill out the user registration form that is supplied with the SRM. Registration will facilitate notification. Before making use of any of the values delivered by this material, users should verify they have the most recent version of this documentation, available through the NIST SRM website (https://www.nist.gov/srm).

Safety: SRM 1849b is intended for research use only; not for human consumption.

Storage and Handling: The original unopened packets of SRM 1849b should be stored at -20 °C or colder. For vitamin B₁₂, the certification only applies to the initial use and the same results are not guaranteed if the remaining powder is used at a later date. For inorganic constituents, an open packet can be reused until the material reaches its expiration date, provided that the open packet is resealed and stored at -20 °C or lower. For all non-certified constituents, the value assignment only applies to the initial use as stability in previously opened packets has not been evaluated.

Carlos A. Gonzalez, Chief Chemical Sciences Division Steven J. Choquette, Director Office of Reference Materials

SRM 1849b Page 1 of 5

Values are expressed as $x \pm U_{95\%}(x)$, where x is the certified value and $U_{95\%}(x)$ is the expanded uncertainty of the certified value. The true value of the analyte lies within the interval $x \pm U_{95\%}(x)$ with 95 % confidence. To propagate this uncertainty, treat the certified value as a normally distributed random variable with mean x and standard deviation $U_{95\%}(x)/2$ [2–6].

Use: Before use, a packet should be allowed to warm to room temperature, and the contents of the packet should be mixed thoroughly by shaking the packet. Allow the contents to settle for one minute prior to opening to minimize the loss of fine particles. For certified values to be valid, test portion size should be based on descriptions of NIST methods [7]. Results obtained should include their own estimates of uncertainty and can be compared to the certified values using procedures described in reference 8.

Source: SRM 1849b is a milk-based, hybrid infant/adult nutritional powder, prepared by a manufacturer of infant formula and adult nutritional products.

Analysis: Measurements used to value assign SRM 1849b values were performed at NIST using a variety of analytical techniques, by the material manufacturer, and by participants of NIST interlaboratory comparison studies [7].

REFERENCES

- [1] Beauchamp, C.R.; Camara, J.E.; Carney, J.; Choquette, S.J.; Cole, K.D.; DeRose, P.C.; Duewer, D.L.; Epstein, M.S.; Kline, M.C.; Lippa, K.A.; Lucon, E.; Phinney, K.W.; Polakoski, M.; Possolo, A.; Sharpless, K.E.; Sieber, J.R.; Toman, B.; Winchester, M.R.; Windover, D.; *Metrological Tools for the Reference Materials and Reference Instruments of the NIST Material Measurement Laboratory*; NIST Special Publication 260-136; U.S. Government Printing Office: Washington, DC (2020); available at https://nvlpubs.nist.gov/nistpubs/SpecialPublications/NIST.SP.260-136-2020.pdf (accessed Mar 2023).
- [2] JCGM 100:2008; Evaluation of Measurement Data Guide to the Expression of Uncertainty in Measurement (GUM 1995 with Minor Corrections); Joint Committee for Guides in Metrology (2008); available at https://www.bipm.org/en/committees/jc/jcgm/publications accessed Feb 2023); see also Taylor, B.N.; Kuyatt, C.E.; Guidelines for Evaluating and Expressing the Uncertainty of NIST Measurement Results; NIST Technical Note 1297; U.S. Government Printing Office: Washington, DC (1994); available at https://www.nist.gov/pml/nist-technical-note-1297 (accessed Mar 2023).
- [3] JCGM 101:2008; Evaluation of Measurement Data Supplement 1 to the "Guide to the Expression of Uncertainty in Measurement" Propagation of Distributions Using a Monte Carlo Method; Joint Committee for Guides in Metrology (JCGM) (2008); available at https://www.bipm.org/en/committees/jc/jcgm/publications (accessed Mar 2023).
- [4] Efron, B.; Tibshirani, R.J.; An Introduction to the Bootstrap; Chapman & Hall: London, UK (1993).
- [5] Searle, S.; Casella, G.; McCulloch, C.; Variance Components; John Wiley: Hoboken, NJ (1992).
- [6] Rukhin, A.L.; Possolo, A.; *Laplace Random Effects Models for Interlaboratory Studies*; Comput. Stat. Data Anal.; Vol. 55, pp. 1815–1827 (2011).
- [7] Phillips, M.M.; Wood, L.J.; Barber, C.A.; Scruggs, B.E.; Sieber, J.R.; Yen, J.H.; Yu, L.L.; *Value Assignment of Standard Reference Material*® *1849b Infant/Adult Nutritional Formula I*; NIST Special Publication 260-233; National Institute of Standards and Technology, Gaithersburg, MD; available at https://nvlpubs.nist.gov/nistpubs/SpecialPublications/NIST.SP.260-233.pdf (accessed Mar 2023).
- [8] Sharpless, K.E.; Duewer, D.L.; Standard Reference Materials for Analysis of Dietary Supplements; J AOAC Int., Vol. 91, pp. 1298–1302 (2008).

If you use this SRM in published work, please reference:

Phillips MM, Wood LJ, Barber CA, Scruggs BE, Sieber JR, Yen JH, Yu LL (2022) Value Assignment of Standard Reference Material[®] 1849b Infant/Adult Nutritional Formula I. (National Institute of Standards and Technology, Gaithersburg, MD), NIST Special Publication (SP) 260-233. https://doi.org/10.6028/NIST.SP.260-233

Certain commercial equipment, instruments, or materials may be identified in this Certificate of Analysis to adequately specify the experimental procedure. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

Users of this SRM should ensure that the Certificate of Analysis in their possession is current. This can be accomplished by contacting the Office of Reference Materials 100 Bureau Drive, Stop 2300, Gaithersburg, MD 20899-2300; telephone (301) 975-2200; e-mail srminfo@nist.gov; or the Internet at https://www.nist.gov/srm.

* * * * * * * * * * * * * End of Certificate of Analysis * * * * * * * * * * * *

SRM 1849b Page 2 of 5

APPENDIX A

Non-Certified Values: Non-certified values are suitable for use in method development, method harmonization, and process control but do not meet the NIST criteria for certification [1] nor provide metrological traceability to the International System of Units (SI) or other higher-order reference system. They are the best estimates of the true values based on available data. The values are provided with an uncertainty that may reflect only measurement reproducibility, may not include all sources of uncertainty, and/or may reflect a lack of sufficient statistical agreement among multiple analytical methods.

Table A1. Non-Certified Values for Various Measurands in SRM 1849b

| | Mass Fraction ^(a) (mg/kg) | | | Mass Fraction ^(a) (mg/kg) | |
|---|--------------------------------------|----------------|--|--------------------------------------|--------------|
| Calaium (Ca) | | ±220 | Thiaming (Vitamin P.) | | <u>± 1.4</u> |
| Calcium (Ca) | 5050 | | Thiamine (Vitamin B ₁) | 14.4 | |
| Chlorine (Cl) | 6580 | ± 110 | Riboflavin (Vitamin B ₂) | 16.9 | \pm 1.0 |
| Fluoride (F) | 1.610 | ± 0.064 | Niacinamide (Vitamin B ₃) | 109.7 | \pm 6.5 |
| Manganese (Mn) | 46.4 | ± 2.1 | Pantothenic Acid (Vitamin B ₅) | 72.6 | \pm 2.3 |
| Potassium (K) | 9014 | ± 90 | Pyridoxine (Vitamin B ₆) | 14.8 | ± 1.2 |
| Sodium (Na) | 4155 | ±100 | Biotin | 2.08 | \pm 0.11 |
| Zinc (Zn) | 141.9 | ± 3.9 | Folic Acid | 2.55 | \pm 0.26 |
| | | | Ascorbic Acid (Vitamin C) | 969 | ± 45 |
| Adenosine Monophosphate | 128.8 | ± 1.2 | Retinol ^(c) | 10.13 | \pm 0.10 |
| Cytidine Monophosphate | 350.9 | ± 1.1 | Retinyl Acetate | 7.1 | ± 1.2 |
| Guanosine Monophosphate | 190.36 | \pm 0.54 | Retinyl Palmitate | 7.803 | ± 0.078 |
| Uridine Monophosphate | 177.00 | \pm 0.67 | Ergocalciferol (Vitamin D ₂) | 0.1162 | ± 0.0018 |
| Total Nucleotide Equivalents ^(b) | 847.0 | \pm 2.0 | Cholecalciferol (Vitamin D ₃) | 0.1056 | ± 0.0011 |
| | | | α-Tocopherol (Free) | 55.0 | ± 9.2 |
| β-Carotene | 0.545 | 2 ± 0.0068 | α-Tocopherol (Total) | 202 | ± 26 |
| Lutein | 2.478 | ± 0.015 | α-Tocopheryl Acetate | 147 | ± 30 |
| Lycopene | 1.733 | \pm 0.020 | β-Tocopherol | 4.79 | \pm 0.71 |
| | | | γ-Tocopherol | 115.7 | ± 7.2 |
| Total Choline | 1014 | ± 32 | δ-Tocopherol | 35.0 | ± 5.8 |
| Total Carnitine | 160.1 | ± 2.4 | Phylloquinone (Vitamin K ₁) | 0.96 | \pm 0.16 |
| myo-Inositol | 448.9 | ± 5.1 | | | |
| | | | Cholesterol | 1.3455 | ± 0.0097 |

⁽a) Values are expressed as $x \pm U_{95\%}(x)$, where x is the estimated value and $U_{95\%}(x)$ is the expanded uncertainty of the value. The method-specific value of the analyte lies within the interval $x \pm U_{95\%}(x)$ with 95 % confidence.

SRM 1849b Page 3 of 5

⁽b) The value for total nucleotide equivalents does not include inosine monophosphate.

Retinol was added to SRM 1849b as retinyl acetate and retinyl palmitate. This non-certified value is expressed as retinol equivalents obtained by experimental saponification of these esters or conversion through multiplication using the ratio of the relative molecular masses of retinol and each ester. The value represents total (*cis* + *trans*) retinol. No correction is made for differences in biological activity of the *cis* and *trans* forms.

Table A2. Non-Certified Values for Various Measurands in SRM 1849b

| Mass Fraction ^(a) | | | Mass | Fraction ^(a) | |
|------------------------------|--------------|--------|-------------------------------|-------------------------|-------------|
| (g/100 g) | | | (g/100 g) | | |
| Alanine | 0.4701 ± | 0.0038 | Ash | 4.49 | ± 0.010 |
| Arginine | $0.4275 \pm$ | 0.0099 | Protein | 12.86 | \pm 0.14 |
| Aspartic Acid | $1.0536\pm$ | 0.0062 | Fat (extracted) | 27.93 | \pm 0.40 |
| Cystine | $0.130 \pm$ | 0.016 | Solids | 97.826 | \pm 0.087 |
| Glutamic Acid | $2.503 \pm$ | 0.031 | Carbohydrates | 53.4 | \pm 2.3 |
| Glycine | $0.2465 \pm$ | 0.0011 | Galactooligosaccharides (GOS) | 2.575 | \pm 0.055 |
| Histidine | $0.2969\pm$ | 0.0084 | Glucose | 0.863 | \pm 0.011 |
| Isoleucine | $0.6885\pm$ | 0.0087 | Lactose | 47.34 | \pm 0.38 |
| Leucine | $1.2764 \pm$ | 0.0069 | Total Sugars | 48.20 | \pm 0.39 |
| Lysine | $0.919 \pm$ | 0.040 | | | |
| Methionine (Free) | $0.1100\pm$ | 0.0010 | | Energy | |
| Methionine (Total) | $0.4523 \pm$ | 0.0044 | | $(kcal/100 g)^{(a,b)}$ | |
| Phenylalanine | $0.5760\pm$ | 0.0035 | Calories | 518 | ± 10 |
| Proline | $1.191 \pm$ | 0.011 | | | |
| Serine | $0.658 \pm$ | 0.012 | | | |
| Taurine | $0.3596 \pm$ | 0.0031 | | | |
| Threonine | $0.6338 \pm$ | 0.0036 | | | |
| Tryptophan | $0.1774\pm$ | 0.0037 | | | |
| Tyrosine | $0.5845 \pm$ | 0.0049 | | | |
| Valine | $0.7449 \pm$ | 0.0075 | | | |

⁽a) Values are expressed as $x \pm U_{95\%}(x)$, where x is the estimated value and $U_{95\%}(x)$ is the expanded uncertainty of the value. The method-specific value of the analyte lies within the interval $x \pm U_{95\%}(x)$ with 95 % confidence.

SRM 1849b Page 4 of 5

⁽b) The non-certified value for calories is the median of lab mean caloric calculations from the interlaboratory comparison exercise. If the mean proximate values from Table A2 are used for calculation, with caloric equivalents of 9, 4, and 4 for fat (extracted), protein, and carbohydrate, respectively, the mean caloric content is 516.4 kcal/100 g.

Table A3. Non-Certified Mass Fraction Values for Values for Fatty Acids as Free Fatty Acids in SRM 1849b

Mass Fraction(a) (g/100 g)Hexanoic Acid (C6:0) Caproic Acid 0.04590 ± 0.00069 Octanoic Acid (C8:0) Caprylic Acid 0.5086 ± 0.0025 Decanoic Acid (C10:0) Capric Acid ± 0.0012 0.4101 Dodecanoic Acid (C12:0) Lauric Acid 3.1977 ± 0.0041 Tetradecanoic Acid (C14:0) Myristic Acid 1.3479 ± 0.0030 Hexadecanoic Acid (C16:0) Palmitic Acid 2.1674 ± 0.0034 (Z)-9-Hexadecenoic Acid (C16:1 n-7) Palmitoleic Acid 0.02286 ± 0.00058 Heptadecanoic Acid (C17:0) Margaric Acid 0.01433 ± 0.00058 Octadecanoic Acid (C18:0) Stearic Acid 0.7816 ± 0.0017 (Z)-9-Octadecenoic Acid (C18:1 n-9) Oleic Acid 10.370 ± 0.032 (Z,Z)-9,12-Octadecadienoic Acid (C18:2 n-6) Linoleic Acid 5.724 ± 0.011 Total trans-C18:1 and -C18:2 Fatty Acids 0.06927 ± 0.00064 (Z,Z,Z)-6,9,12-Octadecatrienoic Acid (C18:3 n-6) γ -Linolenic Acid 0.01139 ± 0.00060 (Z,Z,Z) and (Z,Z,E)-9,12,15-Octadecatrienoic Acid (C18:3 n-3) α-Linolenic Acid ± 0.0015 0.5553 Eicosanoic Acid (C20:0) Arachidic Acid 0.07688 ± 0.00063 Eicosenoic Acid (C20:1) 0.07424 ± 0.00064 Eicosatrienoic Acid (C20:3 n-6) Homo-y-Linolenic Acid 0.01467 ± 0.00064 (Z,Z,Z,Z)-5,8,11,14-Eicosatetraenoic Acid (C20:4 n-6) Arachidonic Acid 0.16311 ± 0.00066 Docosanoic Acid (C22:0) Behenic Acid 0.06556 ± 0.00063 (Z,Z,Z,Z,Z)-4,7,10,13,16,19-Docosahexaenoic Acid (C22:6 n-3) DHA 0.0559 ± 0.0012 Tetracosanoic Acid (C24:0) Lignoceric Acid 0.03691 ± 0.00062 Nervonic Acid (Z)-15-Tetracosenoic Acid (C24:1 n-9) 0.02030 ± 0.00058 Monounsaturated Fatty Acids 10.700 ± 0.030 \pm 0.013 Polyunsaturated Fatty Acids 6.501 Saturated Fatty Acids 8.655 ± 0.011 Fat (as the sum of fatty acids as triglycerides) 27.245 ± 0.055

Maintenance of Non-Certified Values: NIST will monitor this material to the end of its period of validity. If substantive technical changes occur that affect the non-certified values during this period, NIST will update this Certificate of Analysis and notify registered users. SRM users can register online from a link available on the NIST SRM website or fill out the user registration form that is supplied with the SRM. Registration will facilitate notification. Before making use of any of the values delivered by this material, users should verify they have the most recent version of this documentation, available through the NIST SRM website (https://www.nist.gov/srm).

* * * * * * * * * * * End of Appendix A * * * * * * * * * *

SRM 1849b Page 5 of 5

Values are expressed as $x \pm U_{95\%}(x)$, where x is the estimated value and $U_{95\%}(x)$ is the expanded uncertainty of the value. The method-specific value of the analyte lies within the interval $x \pm U_{95\%}(x)$ with 95 % confidence.