

March 2010

Editor: Regina R. Montgomery

New NIST SRMs

NIST SRM 2244 Relative Intensity Correction Standard for Raman Spectroscopy Using 1064 nm Excitation



This SRM is the fourth in a series of SRMs (2241, 2242, 2243) that provides relative intensity correction for Raman spectrometers employing laser excitation. Raman spectroscopy is becoming very popular analytical technique because the Raman spectrum of a compound can be used to uniquely identify a material with very little, and in many cases, no sample preparation. In addition, a Raman spectrum can be acquired through common glass containers, making this an ideal technology

for first responders, hazmat teams, TSA examiners, etc., wishing to identify materials through translucent containers without exposing themselves or the instrument to the material. Because Raman scattering is an emission process, the spectra acquired are necessarily convolved with the instrument response. Detector spectral response, grating efficiency, and filter bandpass are among the largest contributors to the unique spectrometer response function. As a result, current Raman libraries are necessarily vendor-, if not instrument-, specific. This makes intercomparison and/or interchange of Raman spectral data from various sources difficult, if not impossible.

The only remedy in the past was to correct the spectra for the unique instrument response by measuring a calibrated irradiance source under the same conditions as the sample. These sources are extremely expensive, very difficult to correctly align with the instrument, and require periodic recalibration. As a result, they are infrequently used for routine calibration of Raman instruments. This special glass SRM replaces the calibrated irradiance source by producing a featureless fluorescence spectrum when illuminated with the Raman excitation laser. NIST provides a mathematical expression describing the "true" fluorescence spectrum of the SRM glass, which was determined using a variety of NIST-calibrated spectrometers and irradiance sources. The irradiance calibration is effectively transferred by the SRM artifact to the user's Raman spectrometer by simply measuring the spectrum of the glass and dividing the measured glass spectrum by the "true" spectrum. The result then represents a correction curve that is unique to the user's spectrometer. Multiplying a Raman spectrum of a sample by this correction curve results in a spectrum that is largely corrected for the instrument-dependent response, enabling comparison between systems or searching of the data in standardized libraries.

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IMPORTANT MESSAGE WHEN ACCESSING THE SRM WEBSITE: http://www.nist.gov/srm PAGE 12

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The SRM does not require recalibration, and alignment issues are minimized as the SRM is placed in the same position as the sample. These are particularly useful for calibration of micro Raman systems, and because the glass is photostable, these standards are useful as day-to-day intensity standards. The standard was originally developed with the pharmaceutical industry in mind as this industry tends to use Fourier transform (FT) spectrometers (1064 nm excitation) for their applications. However recent advances in InGaAs detector array technology enable the use of this excitation wavelength with dispersive spectrometers. Because these tend to be much smaller than FT instruments, homeland security applications of Raman, i.e., identification of explosives and narcotics, are now feasible using this wavelength. The preparation and certification of this SRM was supported in part by the Test & Evaluation and Standards Division, Science and Technology Directorate, of the Department of Homeland Security.

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NIST SRM 2772 Biodiesel (Soy-Based) and SRM 2773 (Animal-Based)

Biodiesel is an alternative fuel produced by transesterification of triglycerides of vegetable oils or animal fat with methanol to form fatty acid methyl esters. Since some of the by-products, if not separated, can cause engine problems, it is important to have reliable concentrations for glycerol, mono- and diacylglycerols, unreacted triglycerides, and fatty acids. The biodiesel industry within the US is increasing at a fast pace, and the industry needs reference materials to benchmark the measurements of the fatty acids and glycerols as well as those for sodium, potassium, calcium, magnesium, sulfur, phosphorous, moisture, and density. To meet this need, NIST, in collaboration with the National Institute of Metrology, Standardization, and Industrial Quality (INMETRO) in Brazil, has produced two biodiesel SRMs, one produced from soybeans (SRM 2772) and one produced primarily from white grease and pork lard (SRM 2773). NIST and INMETRO have provided certified concentration values for fatty acid methyl esters, water, sulfur, density, and kinematic viscosity; reference concentration values for additional fatty acid methyl esters, free glycerol, and additional physical properties; and information values for trace elements other than sulfur, mono-, di-, and triglycerides, and total glycerol. In addition, SRM 2773, the animal-based biodiesel, was used in an ASTM Committee D-2 Interlaboratory Crosscheck Program for analysis of other parameters of interest to the biodiesel industry. The data from the interlaboratory study is summarized in an appendix to the Certificate of Analysis for SRM 2773.

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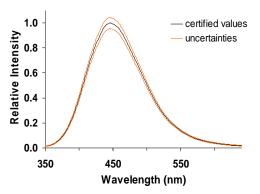


NIST SRM 2943 Relative Intensity Correction Standard for Fluorescence Spectroscopy: Blue Emission

A ready-to-use, fluorescent glass SRM has recently been released by NIST. It enables the relative spectral correction and day-to-day performance verification of fluorescence instruments to be achieved in the blue spectral region with relative ease, even by non-expert users. Luminescence measurements have become the detection methods of choice for many clinical and biochemical assays due to their extraordinary sensitivity and selectivity. These analytical methods are becoming more quantitative, requiring standards for instrument calibration and for method validation as required by quality and regulatory systems. Ideally, users would like to employ the same organic dye probes used for analyte detection as standards for fluorescence intensity and spectral correction. Unfortunately, organic dyes photodegrade quickly, do not have long shelf lives in solution, have environment-dependent fluorescence, and are expensive to produce at high purity.

After studying the characteristics of the different types of fluorescent materials, NIST researchers found metal-ion-doped glasses to be the best choice for use as fluorescence standards for spectral correction and intensity. These glasses are photostable, robust, relatively inexpensive, and can be made to suit most detection formats. SRM 2943 has blue emission that peaks at 445 nm and an effective emission range from 380 nm to 560 nm.

The certified, steady-state emission spectrum is supplied with each SRM, along with estimated total The SRM is highly resistant to uncertainties. photodegradation and is. therefore, also recommended for use as a day-to-day and instrument-to-instrument intensity standard for performance verification. The SRM is provided in the form of a solid glass, standard-sized cuvette $(12.5 \text{ mm} \times 12.5 \text{ mm} \times 45 \text{ mm})$ with three polished long faces for 90-degree detection and one frosted long face for front-face or epifluorescence detection.



The emission range of SRM 2943 is very similar to that of SRM 936a Quinine Sulfate Dihydrate, a dye-based blue emission standard that was recently discontinued. SRM 2943 can replace SRM 936a for many applications and can be used in combination with pre-existing, fluorescent glass SRMs 2940 (orange emission), 2941 (green emission), and 2942 (UV emission). This combination allows the user to cover the UV and visible regions from 320 nm to 780 nm. The high photostability of SRMs 2940 through 2943 make them particularly useful as day-to-day intensity standards, even when spectral correction is not needed or when the excitation wavelength differs from that used for certification.

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NIST SRM 2972 25-Hydroxyvitamin D₂ and D₃ Calibration Solutions

Vitamin D, along with calcium, is generally associated with supporting bone health. Moreover, vitamin D deficiency can lead to rickets in children and osteoporosis in adults. Recent evidence suggests that this vitamin may play an even greater role in optimal health, and studies to determine the recommended levels of vitamin D intake are currently ongoing. There are two forms of vitamin D: vitamin D₂ and vitamin D₃. Exposure to sunlight is the primary source of vitamin D₃ for most individuals, while vitamin D₂ is found in certain dietary supplements and plants. A person's vitamin D status is normally determined through measurement of 25-hydroxyvitamin D [25(OH)D], which is a metabolite of vitamin D. The volume of testing for 25(OH)D has increased dramatically in the past few years, with clinical laboratories performing hundreds of thousands of 25(OH)D tests per year. At the same time, a number of studies have reported inconsistencies between the results of different techniques used to measure 25(OH)D. As a result, accurate diagnosis of vitamin D deficiency has remained problematic.

NIST has developed SRM 2972 25-Hydroxyvitamin D_2 and D_3 Calibration Solutions for use in calibrating instrumentation or techniques used in the measurement of 25(OH)D. This SRM was developed in collaboration with the National Institutes of Health (NIH) Office of Dietary Supplements (ODS). The SRM consists of two separate solutions of the vitamin D metabolites 25(OH)D₂ and 25(OH)D₃ in ethanol. Certified values are provided for the mass fraction (ng/g) and concentration (nmol/L) of 25(OH)D₂ or 25(OH)D₃ in each solution. The solutions have concentrations of 25(OH)D that are approximately ten-fold higher than the levels generally expected in human serum, and they can be diluted by the user to prepare a calibration curve. The new SRM is anticipated to help reduce interlaboratory variability in 25(OH)D measurements through the use of a common calibrator with well-characterized analyte concentrations.

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NIST SRM 3278 Tocopherols in Edible Oils

Vitamin E is of interest to both the food and dietary supplement industry because of its purported health benefits. The four tocopherols (alpha, beta, gamma, and delta) that constitute vitamin E have varying levels of biological activity; alpha-tocopherol has the most. Oils used in cooking are a natural source of tocopherols, and a mixture of edible oils characterized for their tocopherol content has been added to the series of SRMs produced by the National Institute of Standards and Technology (NIST) and the National Institutes of Health's Office of Dietary Supplements (NIH/ODS). Oils were combined to provide approximately equal amounts of alpha-tocopherol and gamma-tocopherol. This entailed blending 10 % soybean oil, 10 % canola oil, 10 % safflower oil, and 70 % sunflower oil (mass fractions). Tocopherols can be added to foods and feeds as antioxidants, and butylated hydroxytoluene (BHT) was added to prevent the tocopherols' oxidation. A unit of this material consists of five ampoules of the blended oil with each ampoule containing approximately 1.2 mL of oil under argon. Certified values are assigned for the alpha-, beta-, gamma-, and delta-tocopherol content. Materials in this suite of SRMs are intended for use as primary control materials when assigning values to in-house (secondary) control materials and for validation of analytical methods.

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Renewals

- SRM 191d pH Standard
- SRM 965b Glucose in Frozen Human Serum
- SRM 967a Creatinine in Frozen Human Serum
- SRM 1640a Trace Elements in Natural Water
- SRM 1680b Carbon Monoxide in Nitrogen (Nominal Amount-of-Substance Fraction, 500 µmol/mol)
- SRM 1762a Low Alloy Steel
- SRM 1884b Portland Cement
- SRM 2092 Low-Energy Charpy V-Notch
- SRM 2096 High-Energy Charpy V-Notch
- SRM 2899a Ethanol-Water Solution (nominal 25 % mass fraction)
- SRM 3110 Cerium Standard Solution
- SRM 3123a Holmium Standard Solution
- SRM 3164 Uranium Standard Solution
- SRM 3186 Phosphate Anion Standard Solution

Revisions

Certificate Revisions—Are You Using These Materials?

This is a list of our most recent certificate revisions. Revisions for the primary purpose of updating the expiration date of a material are not listed below. Users of NIST SRMs should ensure that they have the current certificates. NIST updates certificates for a variety of reasons, such as to extend the expiration date or to include additional information gained from stability testing. If you do not have the current certificate for your material, you can print or view a copy from the website at:

http://www.nist.gov/srm or contact the SRM Program at:

Phone: 301-975-2200 Fax: 301-926-4751 Email: srminfo@nist.gov

SRM 32e Nickel-Chromium Steel (SEA 3140)

Revised Assignments and Values and Editorial Changes

SRM 50c Tungsten-Chromium-Vanadium

Revised Assignments and Values and Editorial Changes

Revisions (continued)

SRM 126c High-Nickel Steel (36 % Ni)

Editorial Changes

SRM 160b Stainless Steel (Cr 18-Ni 12-Mo 2) (AISI 316)

Revised Assignments and Values and Editorial Changes

SRM 166c Stainless Steel, Low-Carbon (AISI 316L)

Revised Assignments and Values and Editorial Changes

SRM 195 Ferrosilicon (75 % Si) Editorial Changes

SRM 927d Bovine Serum Albumin 7 %

Deletion of an Information Value and Editorial Changes

SRM 1155 Stainless Steel (Cr 18-Ni 12-Mo 2) (AISI 316)

Revised Assignments and Values

SRM 1171 Stainless Steel (Cr 17-Ni 11-Ti 0.3) (AISI 321)

Revised Assignments and Values and Editorial Changes

SRM 2298 Sulfur in Gasoline (High Octane)

Addition of Information Values for Density

SRM 2299 Sulfur in Gasoline (Reformulated)

Addition of Information Values for Density

SRM 2585 Organic Contaminants in House Dust Editorial Changes

SRM 2701 Hexavalent Chromium in Contaminated Soil (High Level)

Editorial Changes

PITTCON 2010 Program – NIST Presentations ORLANDO, FL FEBRUARY 28-MARCH 5, 2010

DATE	NIST STAFF	EVENT TITLE & NUMBER	TIME	LOCATION
2/28/2010	Samuel P. Forry, Peter C. Thomas, Laurie Locascio	Microfluidic Cell Culture with Dissolved Gas Control	1:00pm	Rm 307D
3/1/2010	Presentation of Dal Nogare Award to Lane C. Sander	Lane C. Sander will receive the Dal Nogare Award for 2010, presented by the Chromatography Forum of Delaware Valley. The award recognizes Dr. Sander's development of polymeric and other novel stationary phases for liquid chromatography.	8:00am	Rm 206A
3/1/2010	Lane C. Sander	Progress Towards an Understanding of Shape Recognition in Liquid Chromatography #290-1	8:10am	Rm 206A
3/1/2010	Stephen A. Wise, Michele Miller Schantz, Karen W. Phinney, Lane C. Sander	The Role of Chromatography in the Development of Standard Reference Materials for Environmental, Clinical, and Nutritional Measurements #290-2	8:45am	Rm 206A
3/1/2010	Gary W. Kramer	Introductory Remarks	8:00am	Rm 205C
3/1/2010	Gary W. Kramer	Introductions to AnIML:What It Is and Where We're At	8:05am	Rm 205C
3/1/2009	Michele M. Schantz, W. Clay Davis, John Kucklik, Jessica Reiner, Stacy van derPol, Stephen Wise, Rolf Zeisler	New SRMs for Organic Contaminants in Air Particulate and Mussel Tissue #430-5	9:35am	Rm 308D
3/1/2010	Paul DeRose	POSTER: Realizing Fluorescence Standardization - New Guidelines and Reference Materials for Fluorometer Qualification	10:00am	Blue Area, Hall A2
3/2/2010	Stephen A. Wise	Introductory Remarks	8:00am	Rm 308A
3/2/2010	Catherine A. Rimmer	National Institute of Standards and Technology: SRMs for Analysis of Foods and Dietary Supplements #1130-1	8:05am	Rm 308A
3/2/2010	Karen W. Phinney, Nathan G. Dodder, Daniel W. Bearden, Stephen E. Long, Lane C. Sander, Michele M. Schantz, Katherine E. Sharpless, Stephen E. Stein, Gregory C. Turk, Stephen A. Wise	Development of a Standard Reference Material for Metabolomics #1130-2	8:40am	Rm 308A
3/2/2010	Michele M. Schantz	Characterization of Two Biodiesel SRMs: SRM 2772 B100 Biodiesel (Soy-Based) and SRM 2773 B100 Biodiesel (Animal-Based) #1130-3	9:15am	Rm 308A
3/2/2010	Stephen E. Long	Fossil Fuel SRMs to Support the Transportation and Electric Utility Sectors #1130-4	10:05am	Rm 308A

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DATE	NIST STAFF	EVENT TITLE	TIME	LOCATION
3/2/2010	Elizabeth A. Mackey, Stephen E. Long, Gregory C. Turk, Michael R. Winchester, Rolf Zeisler	Standard Reference Materials for Quality Assurance in Environmental Regulatory Compliance #1130-5	10:40am	Rm. 308A
3/2/2010	Mary Bedner, Lane C. Sander, Katherine Sharpless	Determination of Catechins in Green Tea Dietary Supplement Standard Reference materials Using LC-UV and LC-MS #1220-1	8:00am	Rm 309AB
3/2/2010	John L. Molloy, John Sieber	Development of Reference Materials Containing Lead in Paint	3:35pm	Rm 205B
3/2/2010	Janelle D. Newman, Mark S. Lowenthal, Karen W. Phinney	Advances in the Quantitation of Thiolated-poly(ethylene glycol) in Gold Nanoparticle Preparations #1730-6P	1:00 - 3:00pm	Hall B4, Aisles 3400-3900
3/2/2010	Catherine A. Rimmer, Kevin D. Krueger, Lane C. Sander, Katherine E. Sharpless, Stephen A. Wise, Mark S. Lowenthal	Procyanidin Fingerprints in Food and Dietary Supplement Standard Reference Materials #1590-1	2:00pm	Rm 309B
3/2/2010	Melissa M. Phillips, Catherine A. Rimmer, Lane C. Sander, Katherine E. Sharpless, Stephen A. Wise	Determination of Vitamins in NIST Food-Matrix SRMs #1590-3	2:40pm	Rm 309AB
3/2/2010	Melody V. Smith, John C. Travis, Steven Choquette	POSTER: Prototype Reference Materials for UV/Visible/NIR Spectrophotometry	10:00am	Blue Area, Hall A2
3/3/2010	Michael R. Winchester	Achieving Extraordinary Accuracy and Precision Using "Off the Shelf" Atomic Spectroscopy Instrumentation	3:15pm	Rm 205C
3/3/2009	Michael E. Kelley, Gerald D. Mitchell	How Close to Zero Is Your Zero Gas?	3:35pm	Rm 310A
3/3/2009	Lyn Gameson	Accurate Quantification of Multi-Component Protocol Gases	4:15pm	Rm 310A
3/4/2010	Katrice A. Lippa, Catherine A. Rimmer, Lane C. Sander	Novel Reversed-Phase Liquid Chromatography Stationary Phases Designed for Molecular Shape Recognition #2560-4	9:00am	Rm 311C
3/4/2010	Steven Choquette, Melody V. Smith, John C. Travis, David L. Duewer	POSTER: Traceable Photometric Certification Measurements	10:00am	Gray Area, Hall B4
3/4/2010	Justin M. Zook, Wyatt N. Vreeland	Microfluidic Hydrodynamic Focusing to Study the Effects of Formation Temperature and Phase Transition Temperature on Liposome Formation and Size	3:00pm	Rm 307B
3/4/2010	William A. MacCrehan, Stephanie Moore, Michele M. Schantz	Assuring the Quality of Trace Explosives Measurements with NIST Standard Reference Materials (SRMs)	4:15pm	Rm 311A

ORDER NIST SRMS ONLINE

You can now order NIST SRMs through our new online ordering system, which is constantly being updated. **PLEASE NOTE:** Purchase orders and credit cards may be used when ordering an SRM online. This system is efficient, user-friendly, and secure. Our improved search picks up keywords on the detail page along with the words in the title of each SRM.

In addition, we are in the midst of a project to add numerous certificate references for each SRM online. Please also note we are adding many historical archive certificates online for your convenience.

https://www-s.nist.gov/srmors

Users of NIST SRMs should ensure that they have the most recent certificates.

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January 2010 Standard Reference Materials Catalog



If you would like a copy of our new January 2010 SRM Marketing Catalog, Price List, or a CD, please call, fax, or email us at:

> Ph: 301-975-2200 Fax: 301-948-3730 Email: srminfo@nist.gov

NIST SRM 2010 Exhibit Schedule



Pittsburgh Conference (PITTCON) *March 1-4, 2010* Booth #2820 & 2821 Orange County Convention Ctr Orlando, FL

American Chemical Society (ACS) *March 21-25, 2010* San Francisco Convention Ctr San Francisco, CA

Analytica 2010

March 23-26, 2010 Booth #A2-509 Munich Trade Fair Centre Munich, Germany

NOBCChE

March 29-April 3, 2010 Booth #405-407 Marriott Marquis Hotel Atlanta, GA

Materials Research Society Spring Meeting (MRS) April 5-9, 2010 Moscone West San Francisco, CA Clearwater Clean Coal Conference June 6-10, 2010 Sheraton Sand Key Clearwater, FL

IFT – Food Expo July 18-20, 2010 McCormick Place South Booth #3329 Chicago, IL

NCSL Symposium July 25-29, 2010 Booth #625-627 Rhode Island Convention Ctr Providence, RI

AACC Clinical Lab Expo July 27-29, 2010 Anaheim Convention Ctr Anaheim, CA

American Chemical Society (ACS)

August 22-26, 2010 Boston Convention and Exhibition Ctr Boston, MA **Dioxin 2010** September 12-17, 2010 Marriott Rivercenter San Antonio, TX

Analytica China September 15-17, 2010 Shanghai, China

Association of Analytical Communities (AOAC) September 26-29, 2010 Booth #505 Royal Pacific Resort Orlando, FL

MS&T

October 17-21, 2010 Booth #421 George R. Brown Convention Ctr Houston, TX

Materials Research Society Fall Meeting (MRS)

November 30-December 2, 2010 Hynes Convention Ctr Boston, MA



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PLEASE NOTE: New security settings to protect your private information have been mandated by the U.S. government. The following are instructions to upgrade your browser settings so you can view SRM documents, perform searches, and order online.

If you are using Mozilla Firefox

- 1) You must have the most current version 3.0.5
- 2) You must enable SSL 3.0
- 3) You must enable TLS 1.0

To enable SSL 3.0 and TLS 1.0

- 1) Go to Tools Options Advanced
- 2) Click the encryption tab
- 3) Under Protocols, ensure that both boxes are checked

If you are using Internet Explorer

- 1) You must have the most current version IE 6.0 or IE 7.0
- 2) You must enable SSL 3.0
- 3) You must enable TLS 1.0

To enable SSL 3.0 and TLS 1.0

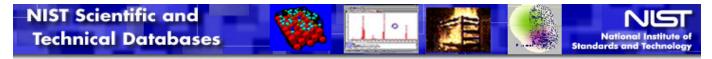
- 1) Go to Tools Internet Options Advanced
- 2) Scroll down to security
- 3) Ensure that both SSL 3.0 and TLS 1.0 are checked

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Other NIST Measurement Services Websites of Interest



Standard Reference Materials www.nist.gov/srm Historical Archived Certificates/Reports of Investigation https://www-s.nist.gov/srmors/certArchive.cfm



NIST Scientific and Technical Databases http://www.nist.gov/srd

NIST Data Gateway http://www.srdata.nist.gov/gateway



Calibrations Services http://www.nist.gov/calibrations

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