NIST NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
U.S. DEPARTMENT OF COMMERCE

Date of Issue:
03 February 2026

Standard Reference Material® 3673a
Organic Contaminants in Non-Smokers' Urine
(Frozen)
CERTIFICATE OF ANALYSIS

Purpose: The certified values delivered by this Standard Reference Material (SRM) are intended for use in evaluating analytical methods for the determination of caffeine, creatinine, selected hydroxylated polycyclic aromatic hydrocarbons (hydroxylated PAHs), phthalate, phenol, nicotine, volatile organic compound (VOC), herbicide, and pesticide metabolites in urine. All the constituents for which certified and non-certified values are provided are naturally present in the urine.

Description: A unit of SRM 3673a consists of five vials each containing 5 mL of frozen urine. The development of SRM 3673a was a collaboration between NIST and Division of Laboratory Sciences, Centers for Disease Control and Prevention (CDC).

Certified Values: These values are traceable to International System of Units (SI) unit of mass. The values are reported on an as-received basis [1,2].

Certified Mass Fraction Values in SRM 3673a

Analyte	Mass Fraction[(a)] (µg/g)
Caffeine[(b,d,e)]	1.4476 ± 0.0180
Creatinine[(c,d,f)]	727.1 ± 1.2

[(a)] 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.

[(b)] NIST gas chromatography mass spectrometry (GC-MS) analysis

[(c)] NIST liquid chromatography with tandem mass spectrometry (LC-MS/MS) analysis

[(d)] CDC LC-MS/MS analysis; data were converted from nmol/mL using the density of the materials which was measured to be 1.0074 ± 0.0001 g/mL and the molar mass of caffeine recorded as 194.191 ± 0.005 g/mol.

[(e)] The certified value is the DerSimonian-Laird consensus estimator of µ, $\bar{y}_{DL}$ [3] from two methods. The standard and approximate 95 % level of confidence expanded uncertainties were estimated using the bootstrap method [4]. The standard uncertainty is estimated as the standard deviation of the bootstrap values. A symmetrical expanded uncertainty is estimated as the half-width of the interval from the 2.5th percentile to the 97.5th percentile of the bootstrap values.

[(f)] The certified value is the arithmetic mean from one reference measurement procedure. The standard uncertainty of the mean is the standard deviation divided by the square root of the number of replications. The expanded uncertainty is estimated using the Student's t 0.95 confidence level for n–1 degrees of freedom as the coverage factor.

Non-Certified Values: Non-certified mass fraction values are provided in Appendix A.

Additional Information: Additional information is provided in Appendix B.

Period of Validity: The certified values delivered by **SRM 3673a** are valid within the measurement uncertainty specified until **01 March 2040**. The certified values are nullified if the material 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). 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).

Carlos A. Gonzalez, Chief
Chemical Sciences Division

Steven J. Choquette, Director
Office of Reference Materials

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Safety: This is a human-source material. This material was tested for the presence of blood and found to be negative within the acceptable limits [5]. SRM 3673a is a Biosafety Level 2 material and should be handled according to applicable federal, state, and/or local regulations and according to policies and procedures of recipient's organization.

Storage: The SRM is stored at –80 °C at NIST. The urine is shipped frozen (on dry ice) and, upon receipt, should be stored frozen until ready for use. A freezer temperature of –20 °C is acceptable for storage for up to one week. If a longer storage time is anticipated, the material should be stored at or below –60 °C. The SRM should not be exposed to sunlight or ultraviolet radiation. Storage of thawed material at room or refrigerator temperatures may result in changes to analyte concentrations.

Use: SRM 3673a IS INTENDED FOR RESEARCH USE. Vials of the SRM to be analyzed should be removed from the freezer and thawed completely to room temperature (20 °C to 25 °C). After the material is thawed to room temperature, it should be used immediately. The material should be vortex mixed before aliquots are withdrawn.

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.; Molloy, J.; Nelson, M.A.; Phinney, K.W.; Polakoski, M.; Possolo, A.; Sander, L.C.; Schiel, J.E.; Sharpless, K.E.; 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, 2021 edition; National Institute of Standards and Technology, Gaithersburg, MD (2021); available at https://nvlpubs.nist.gov/nistpubs/SpecialPublications/NIST.SP.260-136-2021.pdf (accessed Feb 2026).

[2] Boggs, A.S.P.; Blount, B.C.; Botelho, J.C.; Brosius, C.; Burdette, C.Q.; Calafat, A.M.; Camara, J.; Feng J.; Heckert, A.N.; Hoguet, J.C.; Huncik, K.; Morel Espinosa, M.; Ospina, M.; Ragland, J.; Reese, C.; Rybak, M.; Seyler, T.; Valentin-Blasini, L.; Wang, L.; Wood, E.S.C.; Xia, B.; *Certification of Standard Reference Material®s 3672a & 3673a: Organic Contaminants in Smokers' Urine (Frozen) & Organic Contaminants in Non-Smokers' Urine (Frozen)*; NIST Special Publication (NISTSP) 260-256; National Institute of Standards and Technology, Gaithersburg, MD (2025); available at. https://doi.org/10.6028/NIST.SP.260-256r1 (accessed Feb 2026).

[3] DerSimonian, R.; Laird, N.; *Meta-Analysis in Clinical Trials;* Control Clin Trials, Vol. 7(3), pp. 177–188 (1986).

[4] Efron, B.; Tibshirani, R.J.; *An Introduction to the Bootstrap*; Chapman & Hall: London, UK (1993).

[5] United States Department of Labor, Occupational Safety and Health Administration, Standard 1910.1030, Standard Interpretations; *The Potential for the Transmission of HIV from Contact with Urine Specimens*; available at https://www.osha.gov/laws-regs/standardinterpretations/1996-04-15 (accessed Feb 2026).

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

Boggs ASP, Blount BC, Botelho JC, Brosius C, Burdette CQ, Calafat AM, Camara J, Feng J, Heckert AN, Hoguet JC, Huncik K, Morel Espinosa M, Ospina M, Ragland J, Reese C, Rybak M, Seyler T, Valentin-Blasini L, Wang L, Wood ESC, Xia B (2025) Certification of Standard Reference Material® s 3672a & 3673a: Organic Contaminants in Smokers' Urine (Frozen) & Organic Contaminants in Non-Smokers' Urine (Frozen). (National Institute of Standards and Technology, Gaithersburg, MD), NIST Special Publication (NISTSP) 260-256. https://doi.org/10.6028/NIST.SP.260-256r1

Certificate Revision History: 03 February 2026 (Addition of non-certified values; editorial changes); 14 May 2025 (Original certificate date).

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.

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APPENDIX A

Non-Certified Values: Non-certified values are suitable for use in method development, method harmonization, and process control but do not provide metrological traceability to the SI or other higher-order reference system. Non-certified mass fraction values are provided below.

Table A1. Non-Certified Mass Fraction Values for Selected Phthalate, Terephthalate, and 1,2-cyclohexane dicarboxylic acid diisononyl ester Metabolites in SRM 3673a

Analyte	Abbreviation	Mass Fraction ng/g[(a)]
mono-ethyl phthalate[(b,c,d)]	MEP	21.6 ± 2.2
mono-n-butyl phthalate[(b,c,d)]	MBP	6.11 ± 0.32
mono-isobutyl phthalate[(b,c,d)]	MiBP	4.055 ± 0.091
monobenzyl phthalate[(b,c,d)]	MBzP	1.43 ± 1.10
mono-hydroxyisobutyl phthalate[(c,e)]	MHiBP	1.153 ± 0.030
mono-2-ethyl-5-hydroxyhexyl phthalate[(b,c,d)]	MEHHP	3.103 ± 0.059
mono-2-ethyl-5-oxohexyl phthalate[(b,c,d)]	MEOHP	3.2 ± 2.5
monooxononyl phthalates[(c,e)]	MONP	0.771 ± 0.026
mono-2-ethyl-5-carboxypentyl phthalate[(b,c,d)]	MECPP	4.39 ± 1.22
monocarboxyisooctyl phthalate isomers[(c,e)]	MCOP	3.001 ± 0.101
mono-carboxyisononyl phthalate isomers[(c,e)]	MCNP	1.772 ± 0.059
mono-2-ethyl-5-hydrohexyl terephthalate[(c,e)]	MEHHTP	11.84 ± 0.25
mono-2-ethyl-5-carboxypentyl terephthalate[(c,e)]	MECPTP	95.35 ± 1.44
cyclohexane-1,2-dicarboxylic acid monohydroxy isononyl ester[(c,e)]	MHiNCH	0.764 ± 0.038

[(a)] These values are expressed as $x \pm 2u(x)$, where x is a mean value and $u(x)$ is its associated standard uncertainty. While the best estimate of measurand mass fraction lies within the interval $x \pm 2u(x)$, neither the purity nor the identity of the calibrants used have been determined by NIST. For purposes of harmonization and process control, the imprecision and homogeneity components of uncertainty can be propagated as $u(x)/x$ relative standard deviations.

[(b)] NIST LC-MS/MS analysis

[(c)] CDC LC-MS/MS analysis; data were converted from ng/mL using the density of the materials which was measured to be 1.0074 g/mL ± 0.0001 g/mL.

[(d)] The non-certified value is the DerSimonian-Laird consensus estimator of μ, $\bar{y}_{DL}$ [3] from two methods. The standard and approximate 95 % level of confidence expanded uncertainties were estimated using the bootstrap method [4]. The standard uncertainty is estimated as the standard deviation of the bootstrap values. A symmetrical expanded uncertainty is estimated as the half-width of the interval from the 2.5th percentile to the 97.5th percentile of the bootstrap values.

[(e)] The non-certified value is the arithmetic mean from one procedure. The standard uncertainty of the mean is the standard deviation divided by the square root of the number of replications. The expanded uncertainty is estimated using the Student's t 0.95 confidence level for n–1 degrees of freedom as the coverage factor.

Table A2. Non-Certified Mass Fraction Values for Selected Polyaromatic Mono-Hydroxylated Hydrocarbons in SRM 3673a

Analyte	Abbreviation	Mass Fraction ng/g[(a)]
1-hydroxynaphtholene[(b,c,d)]	1-NAP	2.30 ± 0.28
2-hydroxynaphtholene[(b,c,d)]	2-NAP	9.970 ± 0.152
2-hydroxyfluorene[(b,c,d)]	2-FLU	0.0860 ± 0.0100
3-hydroxyfluorene[(c,e)]	3-FLU	0.03742 ± 0.00161
2-hydroxyfluorene + 3-hydroxyfluorene[(b,e)]	2&3-FLU	0.1567 ± 0.0078
1-hydroxyphenanthrene[(c,e)]	1-PHE	0.05918 ± 0.00189
2-hydroxyphenanthrene[(b,e)]	2-PHE	0.0361 ± 0.0022
3-hydroxyphenanthrene[(b,e)]	3-PHE	0.0474 ± 0.0027
2-hydroxyphenanthrene + 3-hydroxyphenanthrene[(b,c,d)]	2&3-PHE	0.0853 ± 0.0060
4-hydroxyphenanthrene[(b,e)]	4-PHE	0.01892 ± 0.00120
1-hydroxypyrene[(b,c,d)]	1-PYR	0.0411 ± 0.0048

[(a)] These values are expressed as $x \pm 2u(x)$, where x is a mean value and $u(x)$ is its associated standard uncertainty. While the best estimate of measurand mass fraction lies within the interval $x \pm 2u(x)$, neither the purity nor the identity of the calibrants used have been determined by NIST. For purposes of harmonization and process control, the imprecision and homogeneity components of uncertainty can be propagated as $u(x)/x$ relative standard deviations.

[(b)] NIST LC-MS/MS analysis

[(c)] CDC LC-MS/MS analysis; data were converted from ng/mL using the density of the materials which was measured to be 1.0074 g/mL ± 0.0001 g/mL.

[(d)] The non-certified value is the DerSimonian-Laird consensus estimator of μ, $\bar{y}_{DL}$ [3] from two or three methods. The standard and approximate 95 % level of confidence expanded uncertainties were estimated using the bootstrap method [4]. The standard uncertainty is estimated as the standard deviation of the bootstrap values. A symmetrical expanded uncertainty is estimated as the half-width of the interval from the 2.5th percentile to the 97.5th percentile of the bootstrap values.

[(e)] The non-certified value is the arithmetic mean from one procedure. The standard uncertainty of the mean is the standard deviation divided by the square root of the number of replications. The expanded uncertainty is estimated using the Student's t 0.95 confidence level for n-1 degrees of freedom as the coverage factor.

Table A3. Non-Certified Mass Fraction Values for Selected Caffeine Metabolites in SRM 3673a

Analyte	Mass Fraction μg/g[(a)]
Paraxanthine[(b,c,d)]	3.33 ± 0.20
Theobromine[(b,c,d)]	5.07 ± 0.60
Theophylline[(b,c,d)]	0.3130 ± 0.0176

[(a)] These values are expressed as $x \pm 2u(x)$, where x is a mean value and $u(x)$ is its associated standard uncertainty. While the best estimate of measurand mass fraction lies within the interval $x \pm 2u(x)$, neither the purity nor the identity of the calibrants used have been determined by NIST. For purposes of harmonization and process control, the imprecision and homogeneity components of uncertainty can be propagated as $u(x)/x$ relative standard deviations.

[(b)] NIST LC-MS/MS analysis

[(c)] CDC LC-MS/MS analysis; data were converted from ng/mL using the density of the materials which was measured to be 1.0074 g/mL ± 0.0001 g/mL.

[(d)] The non-certified value is the DerSimonian-Laird consensus estimator of μ, $\bar{y}_{DL}$ [3] from two methods. The standard and approximate 95 % level of confidence expanded uncertainties were estimated using the bootstrap method [4]. The standard uncertainty is estimated as the standard deviation of the bootstrap values. A symmetrical expanded uncertainty is estimated as the half-width of the interval from the 2.5th percentile to the 97.5th percentile of the bootstrap values.

Table A4. Non-Certified Mass Fraction Values for Selected Benzene and Furfural Metabolites in SRM 3673a

Analyte	Abbreviation	Mass Fraction ng/g[a]
t,t-Muconic acid [b,c]	MUCA	124.6 ± 2.2
N-Acetyl-S-(phenyl)-L-cysteine [b,c]	PhMA	0.1931 ± 0.0090
N-2-Furoylglycine [b,c]	N2FG	7423 ± 61
5-Hydroxymethyl-2-furancarboxylic acid[b,c]	HMFA	3507 ± 188
5-Hydroxymethyl-2-furoylglycine [b,c]	HMFG	464.1 ± 19.7

[a] These values are expressed as $x \pm 2u(x)$, where x is a mean value and $u(x)$ is its associated standard uncertainty. While the best estimate of measurand mass fraction lies within the interval $x \pm 2u(x)$, neither the purity nor the identity of the calibrants used have been determined by NIST. For purposes of harmonization and process control, the imprecision and homogeneity components of uncertainty can be propagated as $u(x)/x$ relative standard deviations.

[b] CDC LC-MS/MS analysis; data were converted from ng/mL using the density of the materials which was measured to be 1.0074 g/mL ± 0.0001 g/mL.

[c] The non-certified value is the arithmetic mean from one procedure. The standard uncertainty of the mean is the standard deviation divided by the square root of the number of replications. The expanded uncertainty is estimated using the Student's t 0.95 confidence level for n–1 degrees of freedom as the coverage factor.

Table A5. Non-Certified Mass Fraction Values for Selected Mercapturic Acid and Related Biomarkers in SRM 3673a

Analyte	Abbreviation	Mass Fraction ng/g[a]
N-Acetyl-S-(2-carbamoylethyl)-L-cysteine[b,c]	2CaEMA	60.59 ± 0.89
N-Acetyl-S-(N-methylcarbamoyl)-L-cysteine[b,c]	MCaMA	49.3 ± 3.4
N-Acetyl-S-(benzyl)-L-cysteine[b,c]	BzMA	4.012 ± 0.126
N-Acetyl-S-(n-propyl)-L-cysteine[b,c]	1PMA	5.44 ± 0.59
N-Acetyl-S-(2-carboxyethyl)-L-cysteine[b,c]	2CoEMA	98.0 ± 3.0
N-Acetyl-S-(2-cyanoethyl)-L-cysteine[b,c]	2CyEMA	6.83 ± 0.22
N-Acetyl-S-(2-hydroxypropyl)-L-cysteine[b,c]	2HPMA	32.51 ± 0.37
N-Acetyl-S-(3-hydroxypropyl)-L-cysteine[b,c]	3HPMA	274.0 ± 12.5
N-Acetyl-S-(3-hydroxypropyl-1-methyl)-L-cysteine[b,c]	3HMPMA	163.0 ± 2.1
2-Methylhippuric acid[b,c]	2MHA	12.87 ± 0.96
3-Methylhippuric acid + 4-Methylhippuric acid[b,c]	3MHA + 4MHA	61.1 ± 2.9
Mandelic acid[b,c]	MADA	96.9 ± 11.3
Phenylglyoxylic acid[b,c]	PhGA	132.02 ± 1.86
2-Aminothiazoline-4-carboxylic acid[b,c]	2ATCA	82.5 ± 9.1
2-Thioxothiazolidine-4-carboxylic acid[b,c]	TTCA	39.21 ± 1.95

[a] These values are expressed as $x \pm 2u(x)$, where x is a mean value and $u(x)$ is its associated standard uncertainty. While the best estimate of measurand mass fraction lies within the interval $x \pm 2u(x)$, neither the purity nor the identity of the calibrants used have been determined by NIST. For purposes of harmonization and process control, the imprecision and homogeneity components of uncertainty can be propagated as $u(x)/x$ relative standard deviations.

[b] CDC LC-MS/MS analysis; data were converted from ng/mL using the density of the materials which was measured to be 1.0074 g/mL ± 0.0001 g/mL.

[c] The non-certified value is the arithmetic mean from one procedure. The standard uncertainty of the mean is the standard deviation divided by the square root of the number of replications. The expanded uncertainty is estimated using the Student's t 0.95 confidence level for n–1 degrees of freedom as the coverage factor.

Table A6. Non-Certified Mass Fraction Values for Selected Phenolic Metabolites in SRM 3673a

Analyte	Abbreviation	Mass Fraction ng/g[(a)]		
2,4-Dichlorophenol[(b,c)]	2,4-DCP	0.414	±	0.043
2,5-Dichlorophenol[(b,c)]	2,5-DCP	17.72	±	0.31
Methyl Paraben[(b,c)]	M-PB	28.70	±	0.67
Ethyl Paraben[(b,c)]	E-PB	5.708	±	0.109
Propyl Paraben[(b,c)]	P-PB	4.583	±	0.122
Benzophenone-3[(b,c)]	BP-3	210.8	±	5.1
Dihydroxyavobenzone	DHAVO	0.099267	±	0.000058
Bisphenol F[(b,c)]	BPF	0.811	±	0.078
Bisphenol S[(b,c)]	BPS	0.745	±	0.057

[(a)] These values are expressed as $x \pm 2u(x)$, where x is a mean value and $u(x)$ is its associated standard uncertainty. While the best estimate of measurand mass fraction lies within the interval $x \pm 2u(x)$, neither the purity nor the identity of the calibrants used have been determined by NIST. For purposes of harmonization and process control, the imprecision and homogeneity components of uncertainty can be propagated as $u(x)/x$ relative standard deviations.

[(b)] CDC LC-MS/MS analysis; data were converted from ng/mL using the density of the materials which was measured to be 1.0074 g/mL ± 0.0001 g/mL.

[(c)] The non-certified value is the arithmetic mean from one procedure. The standard uncertainty of the mean is the standard deviation divided by the square root of the number of replications. The expanded uncertainty is estimated using the Student's t 0.95 confidence level for n–1 degrees of freedom as the coverage factor.

Table A7. Non-Certified Mass Fraction Values for Nicotine and Smoking Related Metabolites in SRM 3673a

Analyte	Abbreviation	Mass Fraction ng/g[(a)]		
Total (-)-Cotinine[(b,c)]	COTT-total	0.586	±	0.026
Free (-)-Cotinine[(b,d)]	COTF-free	0.2751	±	0.0095
Total (-)-trans-3′-Hydroxycotinine [(b,c)]	HCTT-total	0.816	±	0.049
Free (-)-trans-3′-Hydroxycotinine[(b,d)]	HCTF-free	0.600	±	0.033
Total 4-(Methylnitrosamino)-1-(3 Pyridyl)-1-butanol[(b,c)]	NNAL-total	0.001000	±	0.000124
Total (-)-menthol β-D-glucuronide[(b,c)]	MEG	2028	±	116
Total 8-iso-prostaglandin F2α [(b,c)]	8PGFT-total	0.1856	±	0.0046
Free 8-iso-prostaglandin F2α [(b,c)]	8PGFF-free	0.11738	±	0.00192

[(a)] These values are expressed as $x \pm 2u(x)$, where x is a mean value and $u(x)$ is its associated standard uncertainty. While the best estimate of measurand mass fraction lies within the interval $x \pm 2u(x)$, neither the purity nor the identity of the calibrants used have been determined by NIST. For purposes of harmonization and process control, the imprecision and homogeneity components of uncertainty can be propagated as $u(x)/x$ relative standard deviations.

[(b)] CDC LC-MS/MS analysis; data were converted from ng/mL using the density of the materials which was measured to be 1.0074 g/mL ± 0.0001 g/mL.

[(c)] The non-certified value is the arithmetic mean from one procedure. The standard uncertainty of the mean is the standard deviation divided by the square root of the number of replications. The expanded uncertainty is estimated using the Student's t 0.95 confidence level for n–1 degrees of freedom as the coverage factor.

[(d)] The non-certified value is the DerSimonian-Laird consensus estimator of μ, $\bar{y}_{DL}$ [3] from two methods. The standard and approximate 95 % level of confidence expanded uncertainties were estimated using the bootstrap method [4]. The standard uncertainty is estimated as the standard deviation of the bootstrap values. A symmetrical expanded uncertainty is estimated as the half-width of the interval from the 2.5th percentile to the 97.5th percentile of the bootstrap values.

Table A8. Non-Certified Mass Fraction Values for Thiocyanate in SRM 3673a

Analyte	Abbreviation	Mass Fraction ng/g[a]
Thiocyanate[b,c]	SCN	442.4 ± 7.4

[a] These values are expressed as $x \pm 2u(x)$, where x is a mean value and $u(x)$ is its associated standard uncertainty. While the best estimate of measurand mass fraction lies within the interval $x \pm 2u(x)$, neither the purity nor the identity of the calibrants used have been determined by NIST. For purposes of harmonization and process control, the imprecision and homogeneity components of uncertainty can be propagated as $u(x)/x$ relative standard deviations.

[b] CDC LC-MS/MS analysis; data were converted from ng/mL using the density of the materials which was measured to be 1.0074 g/mL ± 0.0001 g/mL.

[c] The non-certified value is the arithmetic mean from one procedure. The standard uncertainty of the mean is the standard deviation divided by the square root of the number of replications. The expanded uncertainty is estimated using the Student's t 0.95 confidence level for n–1 degrees of freedom as the coverage factor.

Table A9. Non-Certified Mass Fraction Values for Organophosphate Esters Metabolites and Dialkylphosphates in Urine in SRM 3673a

Analyte	Abbreviation	Mass Fraction ng/g[a]
Bis(1,3-dichloro-2propyl) phosphate[b,c]	BDCIPP	0.784 ± 0.047
Diphenyl phosphate[b,c]	DPHP	1.122 ± 0.166
Diethylphosphate[b,c]	DEP	3.53 ± 0.38
Dimethyldithiophosphate[b,c]	DMDTP	0.2396 ± 0.0151
Dimethylphosphate[b,c]	DMP	0.934 ± 0.061
Dimethylthiophosphate[b,c]	DMTP	0.752 ± 0.052

[a] These values are expressed as $x \pm 2u(x)$, where x is a mean value and $u(x)$ is its associated standard uncertainty. While the best estimate of measurand mass fraction lies within the interval $x \pm 2u(x)$, neither the purity nor the identity of the calibrants used have been determined by NIST. For purposes of harmonization and process control, the imprecision and homogeneity components of uncertainty can be propagated as $u(x)/x$ relative standard deviations.

[b] CDC LC-MS/MS analysis; data were converted from ng/mL using the density of the materials which was measured to be 1.0074 ± 0.0001 g/mL.

[c] The non-certified value is the arithmetic mean from one procedure. The standard uncertainty of the mean is the standard deviation divided by the square root of the number of replications. The expanded uncertainty is estimated using the Student's t 0.95 confidence level for n–1 degrees of freedom as the coverage factor.

Table A10. Non-Certified Mass Fraction Values for Glyphosate in Urine in SRM 3673a

Analyte	Abbreviation	Mass Fraction ng/g[a]
Glyphosate[b,c]	GLYP	0.3560 ± 0.0171

[a] These values are expressed as $x \pm 2u(x)$, where x is a mean value and $u(x)$ is its associated standard uncertainty. While the best estimate of measurand mass fraction lies within the interval $x \pm 2u(x)$, neither the purity nor the identity of the calibrants used have been determined by NIST. For purposes of harmonization and process control, the imprecision and homogeneity components of uncertainty can be propagated as $u(x)/x$ relative standard deviations.

[b] CDC LC-MS/MS analysis; data were converted from ng/mL using the density of the materials which was measured to be 1.0074 ± 0.0001 g/mL.

[c] The non-certified value is the arithmetic mean from one procedure. The standard uncertainty of the mean is the standard deviation divided by the square root of the number of replications. The expanded uncertainty is estimated using the Student's t 0.95 confidence level for n–1 degrees of freedom as the coverage factor.

Table A11. Non-Certified Mass Fraction Values for Neonicotinoid and N,N-diethyl-meta-toluamide (DEET) Metabolites Urine in SRM 3673a

Analyte	Abbreviation	Mass Fraction ng/g[(a)]
3-(ethylcarbamoyl)benzoic acid	ECBA	1.102 ± 0.043
3-(diethylcarbamoyl)benzoic acid	DCBA	3.904 ± 0.120
5-Hydroxyimidacloprid	5-OH-IMI	0.360 ± 0.023
Acetamiprid-N-desmethyl	NDAC	0.4361 ± 0.0144
Flupyradifurone	FLUP	0.0698 ± 0.0059
Sulfoxaflor Isomer 1	SULF1	0.0897 ± 0.0047
Sulfoxaflor Isomer 2	SULF2	0.0871 ± 0.0032

[(a)] These values are expressed as $x \pm 2u(x)$, where x is a mean value and $u(x)$ is its associated standard uncertainty. While the best estimate of measurand mass fraction lies within the interval $x \pm 2u(x)$, neither the purity nor the identity of the calibrants used have been determined by NIST. For purposes of harmonization and process control, the imprecision and homogeneity components of uncertainty can be propagated as $u(x)/x$ relative standard deviations.

[(b)] CDC LC-MS/MS analysis; data were converted from ng/mL using the density of the materials which was measured to be 1.0074 ± 0.0001 g/mL.

[(c)] The non-certified value is the arithmetic mean from one procedure. The standard uncertainty of the mean is the standard deviation divided by the square root of the number of replications. The expanded uncertainty is estimated using the Student's t 0.95 confidence level for n–1 degrees of freedom as the coverage factor.

Table A12. Non-Certified Mass Fraction Values for Selected Nonpersistent Pesticide Metabolites in Urine in SRM 3673a

Analyte	Abbreviation	Mass Fraction ng/g[(a)]
2,4-dichlorophenoxyacetic acid	2,4-D	0.3143 ± 0.0142
3-phenoxybenzoic acid	3-PBA	0.519 ± 0.031
para-nitrophenol	PNP	0.768 ± 0.071

[(a)] These values are expressed as $x \pm 2u(x)$, where x is a mean value and $u(x)$ is its associated standard uncertainty. While the best estimate of measurand mass fraction lies within the interval $x \pm 2u(x)$, neither the purity nor the identity of the calibrants used have been determined by NIST. For purposes of harmonization and process control, the imprecision and homogeneity components of uncertainty can be propagated as $u(x)/x$ relative standard deviations.

[(b)] CDC LC-MS/MS analysis; data were converted from ng/mL using the density of the materials which was measured to be 1.0074 ± 0.0001 g/mL.

[(c)] The non-certified value is the arithmetic mean from one procedure. The standard uncertainty of the mean is the standard deviation divided by the square root of the number of replications. The expanded uncertainty is estimated using the Student's t 0.95 confidence level for n–1 degrees of freedom as the coverage factor.

Period of Validity: The non-certified values delivered by **SRM 3673a** are valid within the measurement uncertainty specified until **01 March 2040**. The non-certified values are nullified if the material is stored or used improperly, damaged, contaminated, or otherwise modified.

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 Appendix. 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).

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APPENDIX B

Source and Preparation: The SRM is a pool of human urine from more than 10 donors, over 18 years old, who are non-smokers who also do not vape and are not exposed to second-hand smoke or second-hand vapor. Each urine donation was tested to ensure blood content was below five cells per microliter and protein content was less than 14 mg/dL to prevent potential transmission of bloodborne pathogens and the inclusion of pregnant or ill donors. Sterility testing was completed on the full lots post-filtration at 0.2 µm to test for the presence of infectious bacterial organisms. Urine was stored at 4 °C until homogenization in a 20 L carboy on top of a stirring plate. The pool was continually mixed with a stir bar and aliquoted into sterile amber glass vials with a cleaned and primed Hamilton diluter dispenser. Vials are capped with a butyl stopper and aluminum tear-away crimp cap and frozen at –20 °C until shipped to NIST.

Analysis: Value assignment of the mass fractions of analytes in SRM 3673a were based on single methods or the combination of measurements made by NIST using liquid chromatography with tandem mass spectrometry (LC-MS/MS) or gas chromatography tandem mass spectrometry (GC-MS/MS), and/or by CDC using LC-MS/MS. Methods are described in NIST.SP.260-256r1.

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