



SUPPLEMENTARY MATERIAL TO

**Validation and uncertainty estimation of an analytical method
for the determination of phenolic compounds in concrete**

BRANISLAVA G. SAVIĆ^{1*}, IVANA J. MIHAJLOVIĆ², SLOBODAN M.
MILUTINOVIĆ¹, MINA M. SEOVIĆ¹, ŽELJKA M. NIKOLIĆ¹, MILOŠ S. TOŠIĆ¹
and TANJA P. BRDARIĆ¹

¹Vinča Institute of Nuclear Sciences, University of Belgrade, Department of Physical Chemistry,
Mike Petrovića Alasa 12–14, 11351 Vinča, Belgrade, Serbia and ²University of Novi Sad,
Faculty of Technical Sciences, Department of Environmental Engineering, Trg Dositeja
Obradovića 6, 21000 Novi Sad, Serbia

J. Serb. Chem. Soc. 84 (1) (2019) 55–68

The needed information for uncertainty calculations for both methods (GUM and Monte Carlo) for the other 8 phenolic compounds (2-chlorophenol, 2,4-dimethylphenol, 2,4-dichlorophenol, 2,6-dichlorophenol, 4-chloro-3-methylphenol, 2,4,6-trichlorophenol, 2,3,4,6-tetrahalorophenol, pentachlorophenol) are summarized in Tables S-I, S-III, S-V, S-VII, S-IX, S-XI, S-XIII, S-XV.

The results obtained by processing the set of available information by GUM uncertainty approach and corresponding statistical parameters obtained by Monte Carlo simulation for the other 8 phenolic compounds (2-chlorophenol, 2,4-dimethylphenol, 2,4-dichlorophenol, 2,6-dichlorophenol, 4-chloro-3-methylphenol, 2,4,6-trichlorophenol, 2,3,4,6-tetrahalorophenol, pentachlorophenol) are presented in Tables S-II, S-IV, S-VI, S-VIII, S-X, S-XII, S-XIV, S-XVI.

2-Chlorophenol

TABLE S-I. Uncertainty sources and associated distributions with their respective parameters for the estimation of uncertainty for the 2-chlorophenol compound

Uncertainty source	Distribution	Parameters of a distribution
Volume (V)	Normal	Mean: 75 ml; SD : 2.55 ml
Mass (m)	Normal	Mean: 10 g; SD : 0.22g
Recovery (R)	Student's t location-scale	Mean: 87.02 %; SD : 5.67 %; DF : 3
The area of peak (y)	Student's t location-scale	Mean: 177131; SD : 9000; DF : 3
Intercept (a)	Student's t location-scale	Mean: -9888; SD : 4938; DF : 3
Slope (b)	Student's t location-scale	Mean: 416101 l/mg; SD : 9593 l/mg; DF : 3
Purity of standard	Uniform	Min: -0.0201 mg/kg; Max: 0.0201mg/kg

*Corresponding author E-mail: branislava@vin.bg.ac.rs

TABLE S-II. Results obtained using the GUM and Monte Carlo uncertainty approach for uncertainty estimation for the 2-chlorophenol compound

Parameter (GUM)	Value	Parameter (MC)	Value
Mean	3.87 mg/kg	Median	3.87 mg/kg
Combined standard uncertainty	0.38 mg/kg	Low endpoint for 95%	2.79 mg/kg
Expanded uncertainty for 95%	0.83 mg/kg	High endpoint for 95%	5.13 mg/kg

2,4-Dimethylphenol

TABLE S-III. Uncertainty sources and associated distributions with their respective parameters for the estimation of uncertainty for the 2,4-dimethylphenol compound

Uncertainty source	Distribution	Parameters of a distribution
Volume (<i>V</i>)	Normal	Mean: 75 ml; <i>SD</i> : 2.55 ml
Mass (<i>m</i>)	Normal	Mean: 10 g; <i>SD</i> : 0.22g
Recovery (<i>R</i>)	Student's t location-scale	Mean: 33.71 %; <i>SD</i> : 3.47 %; <i>DF</i> : 3
The area of peak (<i>y</i>)	Student's t location-scale	Mean: 73259; <i>SD</i> : 4000; <i>DF</i> : 3
Intercept (<i>a</i>)	Student's t location-scale	Mean: -10495; <i>SD</i> : 7726; <i>DF</i> : 3
Slope (<i>b</i>)	Student's t location-scale	Mean: 500447 l/mg; <i>SD</i> : 15007 l/mg; <i>DF</i> : 3
Purity of standard	Uniform	Min: -0.0193 mg/kg; Max: 0.0193 mg/kg

TABLE S-IV. Results obtained using the GUM and Monte Carlo uncertainty approach for uncertainty estimation for the 2,4-dimethylphenol compound

Parameter (GUM)	Value	Parameter (MC)	Value
Mean	3.72 mg/kg	Median	3.72 mg/kg
Combined standard uncertainty	0.58 mg/kg	Low endpoint for 95%	1.99 mg/kg
Expanded uncertainty for 95%	1.30 mg/kg	High endpoint for 95%	5.83 mg/kg

2,4-Dichlorophenol

TABLE S-V. Uncertainty sources and associated distributions with their respective parameters for the estimation of uncertainty for the 2,4-dichlorophenol compound

Uncertainty source	Distribution	Parameters of a distribution
Volume (<i>V</i>)	Normal	Mean: 75 ml; <i>SD</i> : 2.55 ml
Mass (<i>m</i>)	Normal	Mean: 10 g; <i>SD</i> : 0.22g
Recovery (<i>R</i>)	Student's t location-scale	Mean: 86.61 %; <i>SD</i> : 7.84 %; <i>DF</i> : 3
The area of peak (<i>y</i>)	Student's t location-scale	Mean: 165832; <i>SD</i> : 8000; <i>DF</i> : 3
Intercept (<i>a</i>)	Student's t location-scale	Mean: -10262; <i>SD</i> : 5325; <i>DF</i> : 3
Slope (<i>b</i>)	Student's t location-scale	Mean: 394626 l/mg; <i>SD</i> : 10345 l/mg; <i>DF</i> : 3
Purity of standard	Uniform	Min: -0.0201 mg/kg; Max: 0.0201 mg/kg

TABLE S-VI. Results obtained using the GUM and Monte Carlo uncertainty approach for uncertainty estimation for the 2,4-dichlorophenol compound

Parameter (GUM)	Value	Parameter (MC)	Value
Mean	3.86 mg/kg	Median	3.87 mg/kg
Combined standard uncertainty	0.45 mg/kg	Low endpoint for 95%	2.59 mg/kg
Expanded uncertainty for 95%	1.06 mg/kg	High endpoint for 95%	5.46 mg/kg

2,6-Dichlorophenol

TABLE S-VII. Uncertainty sources and associated distributions with their respective parameters for the estimation of uncertainty for the 2,6-dichlorophenol compound

Uncertainty source	Distribution	Parameters of a distribution
Volume (<i>V</i>)	Normal	Mean: 75 ml; <i>SD</i> : 2.55 ml
Mass (<i>m</i>)	Normal	Mean: 10 g; <i>SD</i> : 0.22g
Recovery (<i>R</i>)	Student's <i>t</i> location-scale	Mean: 91.03 %; <i>SD</i> : 7.21 %; <i>DF</i> : 3
The area of peak (<i>y</i>)	Student's <i>t</i> location-scale	Mean: 154874; <i>SD</i> : 8000; <i>DF</i> : 3
Intercept (<i>a</i>)	Student's <i>t</i> location-scale	Mean: -6017; <i>SD</i> : 3182; <i>DF</i> : 3
Slope (<i>b</i>)	Student's <i>t</i> location-scale	Mean: 343841 l/mg; <i>SD</i> : 6181 l/mg; <i>DF</i> : 3
Purity of standard	Uniform	Min: -0.0200 mg/kg; Max: 0.0200 mg/kg

TABLE S-VIII. Results obtained using the GUM and Monte Carlo uncertainty approach for uncertainty estimation for the 2,6-dichlorophenol compound

Parameter (GUM)	Value	Parameter (MC)	Value
Mean	3.86 mg/kg	Median	3.86 mg/kg
Combined standard uncertainty	0.41 mg/kg	Low endpoint for 95%	2.63 mg/kg
Expanded uncertainty for 95%	0.94 mg/kg	High endpoint for 95%	5.19mg/kg

4-Chloro-3-methylphenol

TABLE S-IX. Uncertainty sources and associated distributions with their respective parameters for the estimation of uncertainty for the 4-chloro-3-methylphenol compound

Uncertainty source	Distribution	Parameters of a distribution
Volume (<i>V</i>)	Normal	Mean: 75 ml; <i>SD</i> : 2.55 ml
Mass (<i>m</i>)	Normal	Mean: 10 g; <i>SD</i> : 0.22g
Recovery (<i>R</i>)	Student's <i>t</i> location-scale	Mean: 83.88 %; <i>SD</i> : 7.79 %; <i>DF</i> : 3
The area of peak (<i>y</i>)	Student's <i>t</i> location-scale	Mean: 80524; <i>SD</i> : 4000; <i>DF</i> : 3
Intercept (<i>a</i>)	Student's <i>t</i> location-scale	Mean: -4857; <i>SD</i> : 2310; <i>DF</i> : 3
Slope (<i>b</i>)	Student's <i>t</i> location-scale	Mean: 201366 l/mg; <i>SD</i> : 4487 l/mg; <i>DF</i> : 3
Purity of standard	Uniform	Min: -0.0394 mg/kg; Max: 0.0394 mg/kg

TABLE S-X. Results obtained using the GUM and Monte Carlo uncertainty approach for uncertainty estimation for the 4-chloro-3-methylphenol compound

Parameter (GUM)	Value	Parameter (MC)	Value
Mean	3.79 mg/kg	Median	3.79 mg/kg
Combined standard uncertainty	0.44 mg/kg	Low endpoint for 95%	2.53 mg/kg
Expanded uncertainty for 95%	1.05 mg/kg	High endpoint for 95%	5.37 mg/kg

2,4,6-Trichlorophenol

TABLE S-XI. Uncertainty sources and associated distributions with their respective parameters for the estimation of uncertainty for the 2,4,6-trichlorophenol compound

Uncertainty source	Distribution	Parameters of a distribution
Volume (<i>V</i>)	Normal	Mean: 75 ml; <i>SD</i> : 2.55 ml
Mass (<i>m</i>)	Normal	Mean: 10 g; <i>SD</i> : 0.22g
Recovery (<i>R</i>)	Student's t location-scale	Mean: 88.41 %; <i>SD</i> : 8.80 %; <i>DF</i> : 3
The area of peak (<i>y</i>)	Student's t location-scale	Mean: 106234; <i>SD</i> : 5000; <i>DF</i> : 3
Intercept (<i>a</i>)	Student's t location-scale	Mean: -6070; <i>SD</i> : 3479; <i>DF</i> : 3
Slope (<i>b</i>)	Student's t location-scale	Mean: 246943 l/mg; <i>SD</i> : 6759 l/mg; <i>DF</i> : 3
Purity of standard	Uniform	Min: -0.0401 mg/kg; Max: 0.0401 mg/kg

TABLE S-XII. Results obtained using the GUM and Monte Carlo uncertainty approach for uncertainty estimation for the 2,4,6-trichlorophenol compound

Parameter (GUM)	Value	Parameter (MC)	Value
Mean	3.86 mg/kg	Median	3.86 mg/kg
Combined standard uncertainty	0.48 mg/kg	Low endpoint for 95%	2.48 mg/kg
Expanded uncertainty for 95%	1.17 mg/kg	High endpoint for 95%	5.56 mg/kg

2,3,4,6-Tetrahalorophenol

TABLE S-XIII. Uncertainty sources and associated distributions with their respective parameters for the estimation of uncertainty for the 2,3,4,6-tetrahalorophenol compound

Uncertainty source	Distribution	Parameters of a distribution
Volume (<i>V</i>)	Normal	Mean: 75 ml; <i>SD</i> : 2.55 ml
Mass (<i>m</i>)	Normal	Mean: 10 g; <i>SD</i> : 0.22g
Recovery (<i>R</i>)	Student's t location-scale	Mean: 89.03%; <i>SD</i> : 11.86%; <i>DF</i> : 3
The area of peak (<i>y</i>)	Student's t location-scale	Mean: 43749; <i>SD</i> : 2000; <i>DF</i> : 3
Intercept (<i>a</i>)	Student's t location-scale	Mean: -4218; <i>SD</i> : 2948; <i>DF</i> : 3
Slope (<i>b</i>)	Student's t location-scale	Mean: 109197 l/mg; <i>SD</i> : 5727 l/mg; <i>DF</i> : 3
Purity of standard	Uniform	Min: -0.0385 mg/kg; Max: 0.0385 mg/kg

TABLE S-XIV. Results obtained using the GUM and Monte Carlo uncertainty approach for uncertainty estimation for the 2,3,4,6-tetrahalorphenol compound

Parameter (GUM)	Value	Parameter (MC)	Value
Mean	3.70 mg/kg	Median	3.71 mg/kg
Combined standard uncertainty	0.62 mg/kg	Low endpoint for 95%	1.92 mg/kg
Expanded uncertainty for 95%	1.51 mg/kg	High endpoint for 95%	6.14 mg/kg

Pentachlorophenol

TABLE S-XV. Uncertainty sources and associated distributions with their respective parameters for the estimation of uncertainty for the pentachlorophenol compound

Uncertainty source	Distribution	Parameters of a distribution
Volume (<i>V</i>)	Normal	Mean: 75 ml; <i>SD</i> : 2.55 ml
Mass (<i>m</i>)	Normal	Mean: 10 g; <i>SD</i> : 0.22g
Recovery (<i>R</i>)	Student's t location-scale	Mean: 85.13 %; <i>SD</i> : 14.16%; <i>DF</i> : 3
The area of peak (<i>y</i>)	Student's t location-scale	Mean: 28669; <i>SD</i> : 1400; <i>DF</i> : 3
Intercept (<i>a</i>)	Student's t location-scale	Mean: -5042; <i>SD</i> : 3019; <i>DF</i> : 3
Slope (<i>b</i>)	Student's t location-scale	Mean: 82373 l/mg; <i>SD</i> : 5864 l/mg; <i>DF</i> : 3
Purity of standard	Uniform	Min: -0.0375 mg/kg; Max: 0.0375 mg/kg

TABLE S-XVI. Results obtained using the GUM and Monte Carlo uncertainty approach for uncertainty estimation for the pentachlorophenol compound

Parameter (GUM)	Value	Parameter (MC)	Value
Mean	3.61 mg/kg	Median	3.61 mg/kg
Combined standard uncertainty	0.76 mg/kg	Low endpoint for 95%	1.42 mg/kg
Expanded uncertainty for 95%	1.86 mg/kg	High endpoint for 95%	6.95 mg/kg