

## Supplementary Information

**Table S1.** Organic carbon partition coefficient  $K_{oc}$  (L/kg) and aerobic degradation half-lives ( $T_{1/2}$ , days) of bronopol and two of its degradation products.

Transport Parameter	Measured or Calculated Value	Test Medium (soil/sediment/water)	Reference	
<i>Bronopol (BNP)</i>				
$K_{oc}$	0.93	Calculated with KOCWIN V2.00 estimation tool	EPI [1]	
	1.00	Calculated with KOCWIN V2.00 estimation tool	EPI [1]	
	2.64	Calculated with KOCWIN V2.00 estimation tool	EPI [1]	
	388	Batch equilibrium sorption, sand soil [96.8% sand, 1.4% silt, 1.8% clay]	ECHA [2]	
	1416	Batch equilibrium sorption, sand [96.8% sand, 1.4% silt, 1.8% clay]	ECHA [2]	
	46.7	Batch equilibrium sorption, loamy sand [86.3% sand, 3.6% silt, 10.1% clay]	ECHA [2]	
	62.0	Batch equilibrium sorption, loamy sand [86.3% sand, 3.6% silt, 10.1% clay]	ECHA [2]	
	171	Batch equilibrium sorption, loam [45.6% sand, 29.5% silt, 24.8% clay]	ECHA [2]	
	306	Batch equilibrium sorption, loam [45.6% sand, 29.5% silt, 24.8% clay]	ECHA [2]	
	36.8	Batch equilibrium sorption, clay loam [38.9% sand, 28.8% silt, 32.2% clay]	ECHA [2]	
$T_{1/2}$	41.3	Batch equilibrium sorption, clay loam [38.9% sand, 28.8% silt, 32.2% clay]	ECHA [2]	
	0.094	Hydrolysis tests in natural surface water: pH = 7.68, $E_h$ = 45 mV	Cui et al. [3]	
	0.108	Hydrolysis tests in natural surface water: pH = 7.53, $E_h$ = 37 mV	Cui et al. [3]	
	0.117	Hydrolysis tests in natural surface water: pH = 7.40, $E_h$ = 2–8 mV	Cui et al. [3]	
	0.131	Hydrolysis tests in natural surface water: pH = 7.75, $E_h$ = 49 mV	Cui et al. [3]	
	0.144	Hydrolysis tests in natural surface water: pH = 7.37, $E_h$ = 2–7 mV	Cui et al. [3]	
	60	Ambient natural conditions (20 °C), pH 8	US EPA [4]	
	548	Ambient natural conditions (20 °C), pH 6	US EPA [4]	
<i>2-bromo-2-nitroethanol (BNE)</i>				
$K_{oc}$	1.46	Calculated with KOCWIN estimation v1.66 tool	RSC [5]	
	24.7	Hydrolysis tests in natural surface water: pH = 7.68, $E_h$ = 45 mV	Cui et al. [3]	
$T_{1/2}$	12.8	Hydrolysis tests in natural surface water: pH = 7.53, $E_h$ = 37 mV	Cui et al. [3]	
	11.1	Hydrolysis tests in natural surface water: pH = 7.40, $E_h$ = 2–8 mV	Cui et al. [3]	
	51.5	Hydrolysis tests in natural surface water: pH = 7.75, $E_h$ = 49 mV	Cui et al. [3]	
$T_{1/2}$	37.8	Hydrolysis tests in natural surface water: pH = 7.37, $E_h$ = 2–7 mV	Cui et al. [3]	
	<i>Bromonitromethane (BNM)</i>			
	$K_{oc}$	19.7	Calculated with KOCWIN V2.00 estimation tool (based on Molecular Connectivity Index)	EPI [1]
		20.7	Calculated with KOCWIN V2.00 estimation tool (based on log $K_{ow}$ = 0.31)	EPI [1]
		15.8	Calculated with KOCWIN estimation v1.66 tool	RSC [5]
	$T_{1/2}$	8.6	Calculated with BIOWIN V2.00 estimation tool (BIOWIN4), aquatic environment	EPI [1]
15		Calculated with BIOWIN V2.00 estimation tool (BIOWIN3), aquatic environment	EPI [1]	
30		Half-life in soil calculated as twice the value in water	PBT [6]	

**Table S2.** van Genuchten soil hydraulic parameters and the bulk density of Vertosols (averages across the Cox's Creak Catchment area, NSW, Australia) (source: Bennett [7]).

Soil layer	$\theta_r$ [cm <sup>3</sup> /cm <sup>3</sup> ]	$\theta_s$ [cm <sup>3</sup> /cm <sup>3</sup> ]	$\alpha$ [1/m]	$n$ [-]	$K_s$ [m/day]	$l$ [-]	Bulk density (g/cm <sup>3</sup> )
1 (0–0.3 m)	0.059	0.515	8.3	1.217	6.04	0.5	1.32
2 (0.3–0.7 m)	0.066	0.538	7.4	1.190	4.51	0.5	1.42
3 (0.7–1.0 m)	0.07	0.515	7.9	1.150	3.35	0.5	1.45

The cation exchange capacity in mol/dm<sup>3</sup> soil was calculated from the following equations (using data from Table 3):

$$\begin{aligned} & ((\text{conc}(\text{Ca}) + \text{conc}(\text{Mg})) \times 2 + \text{conc}(\text{Na}) + \text{conc}(\text{K})) \times \text{bulk density} = \\ & ((0.044 + 0.022) \times 2 + 0.0013 + 0.0065) \left[ \frac{\text{mol}}{\text{kg}} \right] \times 1.32 \left[ \frac{\text{kg}}{\text{dm}^3} \right] = 0.184 [\text{mol}(+)/\text{dm}^3] \end{aligned} \quad (\text{S1})$$

**Table S3.** Conversion of the concentrations [ppm] measured by de Caritat and Lech [9] to the initial concentrations [mol/kg] on the cation exchanger.

Chemical compound	Molar Mass [g/mol]	Concentration measured by de Caritat and Lech [9] [ppm]	Calculated concentration [mol/kg]
UO <sub>2</sub> <sup>2+</sup>	270	0.025	9.27 × 10 <sup>-8</sup>
Cd <sup>2+</sup>	112	0.004	3.57 × 10 <sup>-8</sup>
Pb <sup>2+</sup>	207	0.06	2.90 × 10 <sup>-7</sup>
Zn <sup>2+</sup>	65	0.05	7.70 × 10 <sup>-7</sup>
Cu <sup>2+</sup>	64	0.99	1.57 × 10 <sup>-5</sup>

**Table S4.** Aqueous phase species of the heavy metals included in the model (phreeqcU.dat database used).

Aqueous Phase Solution Species		
Element	Reaction	logk
Cd	Cd <sup>2+</sup> + H <sub>2</sub> O = CdOH <sup>+</sup> + H <sup>+</sup>	-10.08
	Cd <sup>2+</sup> + 2 H <sub>2</sub> O = Cd(OH) <sub>2</sub> + 2 H <sup>+</sup>	2-0.35
	Cd <sup>2+</sup> + 3 H <sub>2</sub> O = Cd(OH) <sub>3</sub> <sup>-</sup> + 3 H <sup>+</sup>	-33.3
	Cd <sup>2+</sup> + 4 H <sub>2</sub> O = Cd(OH) <sub>4</sub> <sup>2-</sup> + 4 H <sup>+</sup>	-47.35
	Cd <sup>2+</sup> + Cl <sup>-</sup> = CdCl <sup>+</sup>	1.98
	Cd <sup>2+</sup> + 2 Cl <sup>-</sup> = CdCl <sub>2</sub>	2.6
	Cd <sup>2+</sup> + 3 Cl <sup>-</sup> = CdCl <sub>3</sub> <sup>-</sup>	2.4
	Cd <sup>2+</sup> + CO <sub>3</sub> <sup>2-</sup> = CdCO <sub>3</sub>	2.9
	Cd <sup>2+</sup> + 2 CO <sub>3</sub> <sup>2-</sup> = Cd(CO <sub>3</sub> ) <sub>2</sub> <sup>2-</sup>	6.4
	Cd <sup>2+</sup> + HCO <sub>3</sub> <sup>-</sup> = CdHCO <sub>3</sub> <sup>+</sup>	1.5
	Cd <sup>2+</sup> + SO <sub>4</sub> <sup>2-</sup> = CdSO <sub>4</sub>	2.46
	Cd <sup>2+</sup> + 2 SO <sub>4</sub> <sup>2-</sup> = Cd(SO <sub>4</sub> ) <sub>2</sub> <sup>2-</sup>	3.5
	Cd <sup>2+</sup> + F <sup>-</sup> = CdF <sup>+</sup>	1.2
	Cd <sup>2+</sup> + 2 F <sup>-</sup> = CdF <sub>2</sub>	1.5
Cu	Cu <sup>2+</sup> + H <sub>2</sub> O = CuOH <sup>+</sup> + H <sup>+</sup>	-8
	Cu <sup>2+</sup> + 2 H <sub>2</sub> O = Cu(OH) <sub>2</sub> + 2 H <sup>+</sup>	-13.68
	Cu <sup>2+</sup> + 3 H <sub>2</sub> O = Cu(OH) <sub>3</sub> <sup>-</sup> + 3 H <sup>+</sup>	2-6.9
	Cu <sup>2+</sup> + 4 H <sub>2</sub> O = Cu(OH) <sub>4</sub> <sup>2-</sup> + 4 H <sup>+</sup>	-39.6
	Cu <sup>2+</sup> + SO <sub>4</sub> <sup>2-</sup> = CuSO <sub>4</sub>	2.31
	Cu <sup>2+</sup> + F <sup>-</sup> = CuF <sup>+</sup>	1.26
U	U <sup>+4</sup> + H <sub>2</sub> O = UOH <sup>3+</sup> + H <sup>+</sup>	-0.65
	U <sup>+4</sup> + 4 H <sub>2</sub> O = U(OH) <sub>4</sub> + 4 H <sup>+</sup>	-12
	U <sup>+4</sup> + F <sup>-</sup> = UF <sup>3+</sup>	9.3
	U <sup>+4</sup> + 2 F <sup>-</sup> = UF <sub>2</sub> <sup>2+</sup>	16.22
	U <sup>+4</sup> + 3 F <sup>-</sup> = UF <sub>3</sub> <sup>+</sup>	21.6
	U <sup>+4</sup> + 4 F <sup>-</sup> = UF <sub>4</sub>	25.5
	U <sup>+4</sup> + 5 F <sup>-</sup> = UF <sub>5</sub> <sup>-</sup>	27.01
	U <sup>+4</sup> + 6 F <sup>-</sup> = UF <sub>6</sub> <sup>2-</sup>	29.1
	U <sup>+4</sup> + Cl <sup>-</sup> = UCl <sup>3+</sup>	1.72
	U <sup>+4</sup> + SO <sub>4</sub> <sup>2-</sup> = USO <sub>4</sub> <sup>2+</sup>	6.58
U <sup>+4</sup> + 5CO <sub>3</sub> <sup>2-</sup> = U(CO <sub>3</sub> ) <sub>5</sub> <sup>-6</sup>	33.9	

	$\text{UO}_2^{2+} + 4\text{H}^+ + 2\text{e}^- = \text{U}^{+4} + 2\text{H}_2\text{O}$	8.89	
	$\text{UO}_2^{2+} + \text{e}^- = \text{UO}_2^+$	2.97	
	$\text{UO}_2^{2+} + \text{H}_2\text{O} = \text{UO}_2\text{OH}^+ + \text{H}^+$	-5.2	
	$\text{UO}_2^{2+} + 2\text{H}_2\text{O} = \text{UO}_2(\text{OH})_2 + 2\text{H}^+$	-12	
	$2\text{UO}_2^{2+} + 2\text{H}_2\text{O} = (\text{UO}_2)_2(\text{OH})_2^{2+} + 2\text{H}^+$	-5.62	
	$3\text{UO}_2^{2+} + 5\text{H}_2\text{O} = (\text{UO}_2)_3(\text{OH})_5^+ + 5\text{H}^+$	-15.55	
	$\text{U}\text{UO}_2^{2+} + 3\text{H}_2\text{O} = \text{UO}_2(\text{OH})_3^- + 3\text{H}^+$	-19.2	
	$3\text{UO}_2^{2+} + 7\text{H}_2\text{O} = (\text{UO}_2)_3(\text{OH})_7^- + 7\text{H}^+$	-31	
	$4\text{UO}_2^{2+} + 7\text{H}_2\text{O} = (\text{UO}_2)_4(\text{OH})_7^+ + 7\text{H}^+$	2-1.9	
	$\text{UO}_2^{2+} + \text{CO}_3^{2-} = \text{UO}_2\text{CO}_3$	9.67	
	$\text{UO}_2^{2+} + 2\text{CO}_3^{2-} = \text{UO}_2(\text{CO}_3)_2^{2-}$	17	
UO <sub>2</sub>	$\text{UO}_2^{2+} + 3\text{CO}_3^{2-} = \text{UO}_2(\text{CO}_3)_3^{4-}$	21.63	
	$\text{UO}_2^{2+} + \text{F}^- = \text{UO}_2\text{F}^+$	5.09	
	$\text{UO}_2^{2+} + 2\text{F}^- = \text{UO}_2\text{F}_2$	8.62	
	$\text{UO}_2^{2+} + 3\text{F}^- = \text{UO}_2\text{F}_3^-$	10.9	
	$\text{UO}_2^{2+} + 4\text{F}^- = \text{UO}_2\text{F}_4^{2-}$	11.7	
	$\text{UO}_2^{2+} + \text{Cl}^- = \text{UO}_2\text{Cl}^+$	0.17	
	$\text{UO}_2^{2+} + 2\text{Cl}^- = \text{UO}_2\text{Cl}_2$	-1.1	
	$\text{UO}_2^{2+} + \text{SO}_4^{2-} = \text{UO}_2\text{SO}_4$	3.15	
	$\text{UO}_2^{2+} + 2\text{SO}_4^{2-} = \text{UO}_2(\text{SO}_4)_2^{2-}$	4.14	
	$\text{UO}_2^{2+} + \text{HPO}_4^{2-} = \text{UO}_2\text{HPO}_4$	7.71	
	$\text{UO}_2^{2+} + \text{H}_3\text{PO}_4 = \text{UO}_2\text{H}_2\text{PO}_4^+ + \text{H}^+$	1.12	
	$\text{UO}_2^{2+} + \text{H}_3\text{PO}_4 = \text{UO}_2\text{H}_3\text{PO}_4^{2+}$	0.76	
	$\text{UO}_2^{2+} + \text{PO}_4^{3-} = \text{UO}_2\text{PO}_4^-$	13.69	
		$\text{Zn}^{2+} + \text{H}_2\text{O} = \text{ZnOH}^+ + \text{H}^+$	-8.96
		$\text{Zn}^{2+} + 2\text{H}_2\text{O} = \text{Zn}(\text{OH})_2 + 2\text{H}^+$	-16.9
	$\text{Zn}^{2+} + 3\text{H}_2\text{O} = \text{Zn}(\text{OH})_3^- + 3\text{H}^+$	2-8.4	
	$\text{Zn}^{2+} + 4\text{H}_2\text{O} = \text{Zn}(\text{OH})_4^{2-} + 4\text{H}^+$	-41.2	
	$\text{Zn}^{2+} + \text{Cl}^- = \text{ZnCl}^+$	0.43	
	$\text{Zn}^{2+} + 2\text{Cl}^- = \text{ZnCl}_2$	0.45	
Zn	$\text{Zn}^{2+} + 3\text{Cl}^- = \text{ZnCl}_3^-$	0.5	
	$\text{Zn}^{2+} + 4\text{Cl}^- = \text{ZnCl}_4^{2-}$	0.2	
	$\text{Zn}^{2+} + \text{CO}_3^{2-} = \text{ZnCO}_3$	5.3	
	$\text{Zn}^{2+} + 2\text{CO}_3^{2-} = \text{Zn}(\text{CO}_3)_2^{2-}$	9.63	
	$\text{Zn}^{2+} + \text{HCO}_3^- = \text{ZnHCO}_3^+$	2.1	
	$\text{Zn}^{2+} + \text{SO}_4^{2-} = \text{ZnSO}_4$	2.37	
	$\text{Zn}^{2+} + 2\text{SO}_4^{2-} = \text{Zn}(\text{SO}_4)_2^{2-}$	3.28	
	$\text{Zn}^{2+} + \text{F}^- = \text{ZnF}^+$	1.15	

**Table S5.** Rainfall data and chemical composition of rainwater at Wagga Wagga, Australia (Source: Crosbie et al. [9]). HP1 input data calculated for an infiltration flux of 40 mm/year.

Rainwater	mm/y	Alkalinity	Cl	SO <sub>4</sub>	Ca	K	Mg	Na	Units
Rainfall	700	0.06	0.65	0.33	0.24	0.11	0.08	0.48	[mg/L]
Infiltration flux	40	1.05	11.375	5.775	4.2	1.925	1.4	8.4	[mg/L]

## References

1. US EPA; EPI (Estimation Program Interface) Suite™ 2012.
2. ECHA; European Chemical Agency, Registration dossier bronopol (<https://echa.europa.eu>)
3. Cui, N.; Zhang, X.; Xie, Q.; Want, S.; Chen, J.; Huang, L.; Qiao, X.; Li, X.; Cai, X.; Toxicity profile of labile preservative bronopol in water: The role of more persistent and toxic transformation products. *Environmental Pollution* **2011**, 159, 609–615.

4. US EPA; Reregistration Eligibility Decision (RED) Bronopol. United States Environmental Protection Agency. Prevention, Pesticides And Toxic Substances (7508W), EPA738-R-95-029 October 1995.
5. RSC (Royal Society of Chemistry); Chemspider, [www.chemspider.com](http://www.chemspider.com).
6. PBT; PBT profiler, Environmental Health Analysis Center, [www.pbtprofiler.net](http://www.pbtprofiler.net) (Version 2.001).
7. Bennett, S.; Key Spatiotemporal Factors Determining Uncertainty of Deep Drainage in a Semi-Arid Area. PhD thesis 2012, The University of New South Wales.
8. de Caritat, P., and M.E. Lech. 2007. Thomson Region Geochemical Survey, Northwestern New South Wales. CRC LEME Open File Report 145.
9. Crosbie, R., Morrow, D., Cresswell, R., Leaney, F., Lamontagne, S., Lefournour, M., 2012. New insights to the chemical and isotopic composition of rainfall across Australia. Water for a Healthy Country Flagship Report series ISSN: 1835-095X. CSIRO.