



# Toxicological relevance of emerging contaminants for drinking water quality

Merijn Schriks, KWR Watercycle Research Institute (Nieuwegein, NL)

## Intro

- 100.000 chemicals registered in EINECS inventory;
- 30.000-70.000 in daily use;
- New and more sensitive analytical techniques lead to detection of new “emerging” contaminants in the water cycle;
- US EPA and WHO have derived approx. 125 statutory drinking water guideline values (GLVs);
- The toxicological relevance of many other unknown compounds for humans is often unknown;
- Presently, for unknown compounds in drinking water a threshold of toxicological concern (TTC) is applied (0.1 ug/L for nongenotoxic compounds; 0.01 ug/L for genotoxic compounds).

# Acknows

## Snyder et al., 2008

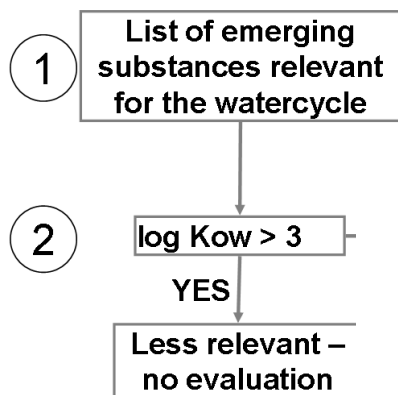
TABLE 6. Risk Assessment for Selected Pharmaceuticals

Drug	Toxic effect	ADI (mg/kg-d)	DWEL (µg/L)	Max Finished Water Conc. (µg/L)	Margin of Exposure (Finished Water)
Atenolol	Developmental, human	0.0027	81	0.020	0.00025
Atorvastatin	Cancer, rat	0.00054	16	<0.00025	0.000015
o-hydroxy atorvastatin				<0.00050	0.000031
o-hydroxy atorvastatin				<0.00050	0.000031
Carbamazepine	Cancer, rat	0.00034	10	0.018	0.0018
Diazepam	Developmental, rat	0.00016	4.8	<0.00025	0.000052
Diclofenac	Developmental, mouse	0.0016	48	<0.00025	0.0000052
Enalapril	Developmental, human	0.00023	6.9	<0.00025	0.000036
Fluoxetine	Developmental, human	0.0010	30	<0.00050	0.000017
Gemfibrozil	Cancer, rat	0.00056	39	0.0021	0.000054
Meprobamate	Systemic, mouse	0.0061	180	0.043	0.00024
Naproxen	Reproductive/ Developmental, mouse	0.046	1,400	<0.00050	0.00000036
Phenytoin	Cancer, mouse	0.000083	5.8	0.015	0.0026
Risperidone	Cancer, mouse & rat	0.000014	0.41	0.00034	0.00084
Simvastatin	Cancer, rat	0.00054	16	<0.00025	0.000015
Simvastatin hydroxy acid				<0.00025	0.000015
Sulfamethoxazole	Developmental, rat	0.28	8,400	0.0030	0.00000036
Triclosan	Systemic, hamster	0.012	360	0.0012	0.0000033
Trimethoprim	Developmental, rat	0.10	3,000	<0.00025	0.000000083

## Aim of the present study

- Obtain existing drinking water GLVs OR derive provisional GLVs with the aid of human relevant toxicological data for a selection of 110 emerging contaminants.
- Inclusion criteria:
  - A) Questions related to toxicity posed by drinking water companies;
  - B) Potential low removal during drinking water treatment;
  - C) Appearance in recent literature;
  - D) Occurrence in surface waters, ground water, and or drinking water.
- Compare the results to:
  - (i) max concentrations in surface water and/or ground water (RIWA, AWR, else);
  - (ii) max concentration found in drinking water (REWAB database, else);
  - (iii) the TTC.
- Prioritize compounds that may deserve additional attention (monitoring etc).

# Materials and Methods



## Compound categories:

Compound with established GLV	A
Compounds with established TDI, ADI, RfD	B
Compounds with established LO(A)EL or NO(A)EL	C
Compounds with miscellaneous toxicological information	D

# Materials and Methods

4

Compare surface-, ground- and/or drinking water concentrations to (provisional) GLV

5

Calculate Benchmark Quotient (BQ) value

$$BQvalue = \frac{\text{max concentrationwater}}{(p)GLV}$$

	BQ threshold for Surfacewater and/or groundwater	BQ threshold for Drinking water
<b>P(GLV) = max concentration in water</b>	<b>1</b>	<b>1</b>
<b>Potential human health concern</b>	<b>≥ 1</b>	<b>≥ 1</b>
<b>Further investigation may be necessary</b>	<b>≥ 0.2</b>	<b>≥ 0.1</b>
<b>No appreciable concern to human health</b>	<b>≤ 0.2</b>	<b>≤ 0.1</b>

# Results

~105 compounds of interest;

~30 compounds with a log Kow > 3;

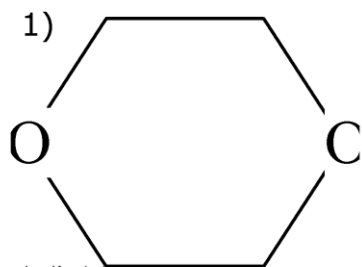
~20 compounds without useful toxicological data;

~5 compounds without a concentration in surface water or ground water;

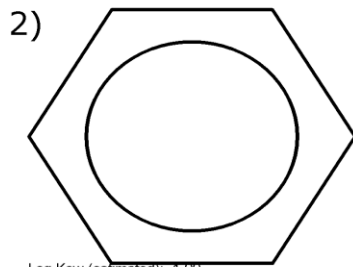
Final list contains 50 compounds (15 without drinking water concentrations).

Iodinated contrast media	5
Miscellaneous organic compounds	21
Miscellaneous pesticides	14
Oxygenated gasoline additives	2
Perfluorinated organic compounds	2
Pharmaceuticals	6

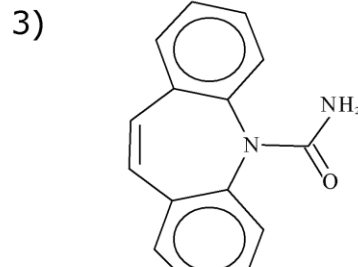
# Results



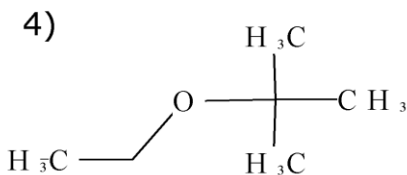
Log Kow (estimated): -0.32  
1,4-Dioxane



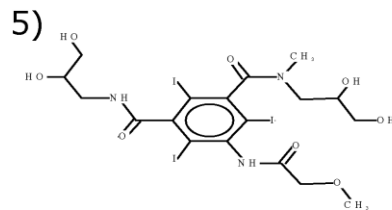
Log Kow (estimated): 1.99  
Benzene



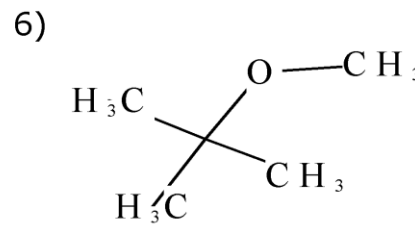
Log Kow (estimated): 2.25  
5H-Dibenz[b,f]azepine-5-carboxamide



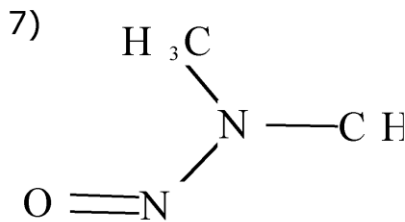
Log Kow (estimated): 1.92  
Propane, 2-ethoxy-2-methyl-



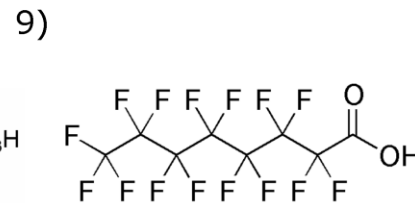
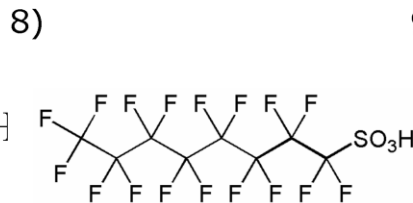
Log Kow (estimated): -2.49  
Iopromide



Log Kow (estimated): 1.43  
Propane, 2-methoxy-2-methyl-



Log Kow (estimated): -0.64  
Methanamine, N-methyl-N-nitroso-



- 1) 1,4-dioxane (MOC)
- 2) Benzene (MOC)
- 3) DEET (MP)
- 4) ETBE (OGA)
- 5) Iopromide (ICM)
- 6) MTBE (OGA)
- 7) NDMA (MOC)
- 8) PFOS (PFC)
- 9) PFOA (PFC)



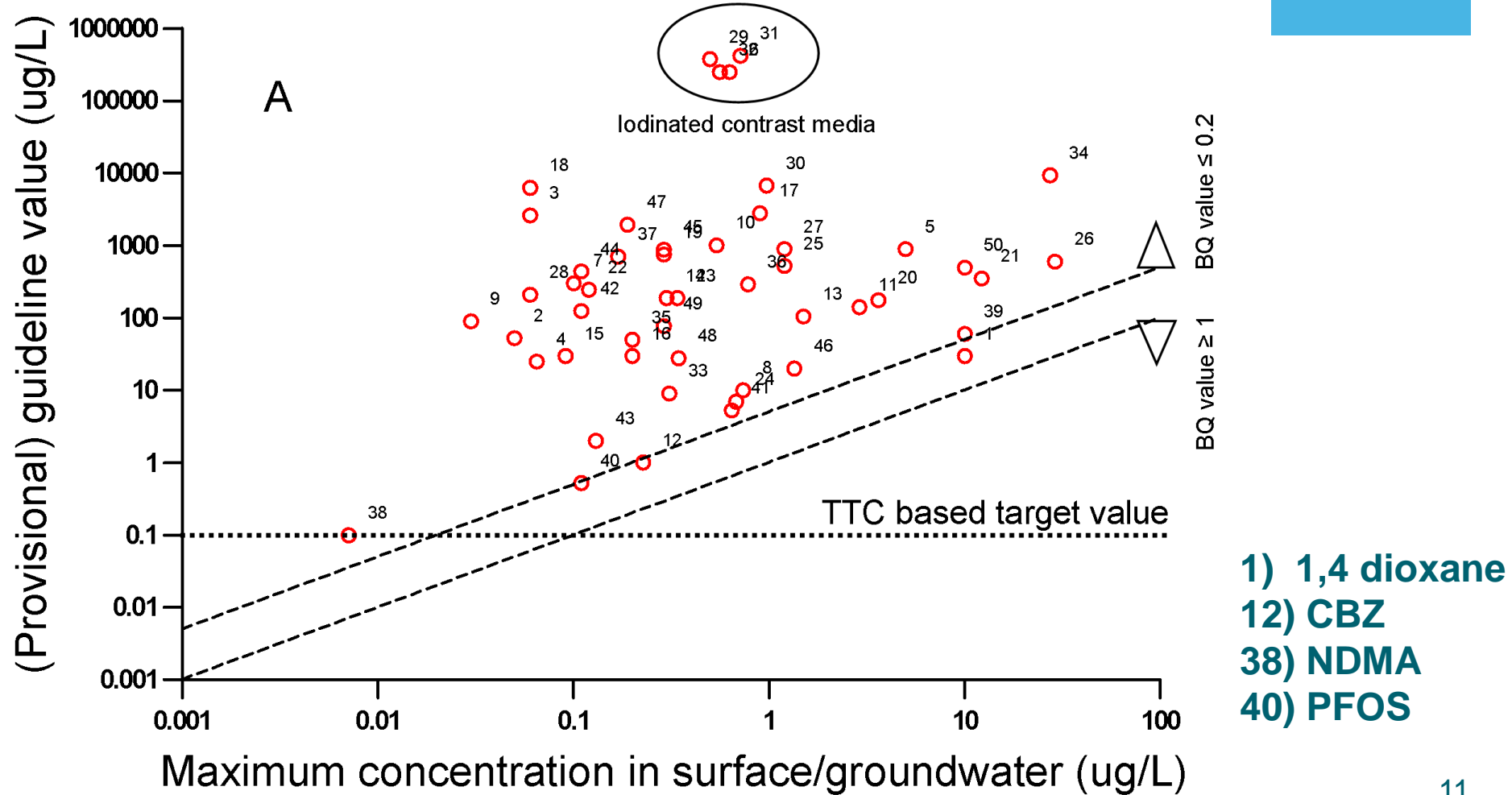
# Results

Compound category	Number	Examples
Cat A	10	AMPA, bentazone, benzene
Cat B	22	1,4-dioxane, acetylsalicylate, BCIPE
Cat C	7	Benzothiazole, benzotriazole, DEET
Cat D	11	Chloridazon, DTPA, iomeprol

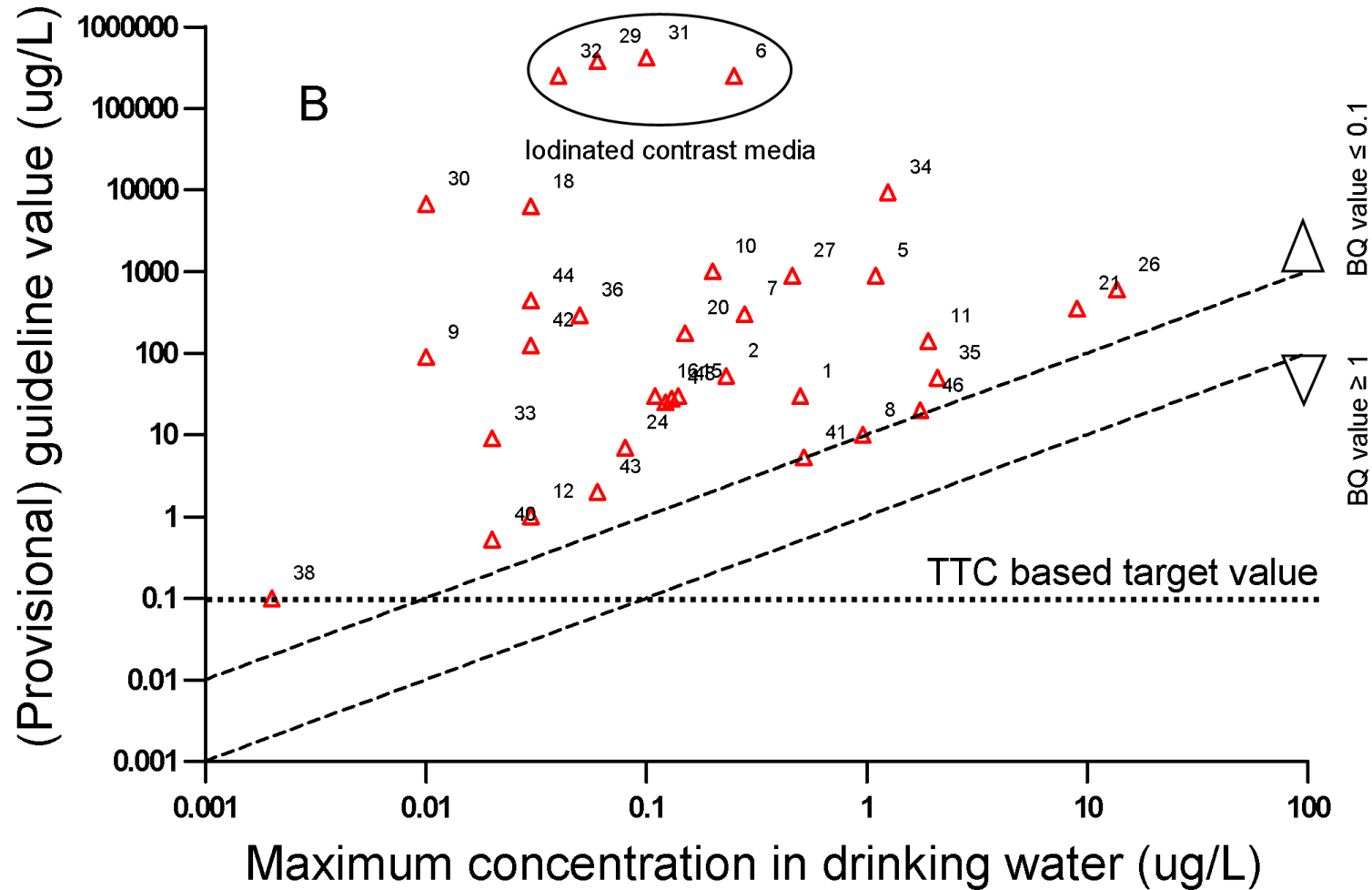
# Results

Highest concentration in ground-/ surface water	EDTA (29 ug/L) SW MTBE (27.3 ug/L) GW
Highest concentration in drinking water	EDTA (13.6 ug/L)

# Results – ground-/surface water



# Results – drinking water



**8) benzene**  
**41) PFOA**

## Discussion / conclusions

- For most compounds evaluated there is large margin of safety between the p(GLV and the max concentration in various waters;
- PFOA and PFOS are becoming a global problem and environmental concentrations (may) increase. More research should be devoted to removal during drinking water treatment (Christian Eschauzier/Pim de Voogt PERFOOD project);
- Compounds with a low (p)GLV deserve attention since seasonal factors may influence concentrations, resulting in temporarily higher BQ values;
- The toxicological assessment of the studied compounds shows that the TTC concept may be very conservative → safe to use in absence of any tox-data;
- Obtain better understanding of mixture toxicity effects.

# BINNENLAND

## Onderzoek 'nieuwe' vervuilers water

UTRECHT - De Nederlandse drinkwaterbedrijven onderzoeken de gezondheidsrisico's van 'nieuwe' vervuillende stoffen die in het water zijn aangetroffen. Zij kijken of bepaalde stoffen zodanig op elkaar inwerken, dat ze samen een gezondheidsrisico vormen.

Dat meldt het KWR Watercycle Research Institute uit Utrecht dinsdag. Onderzoeker Merijn Schriks van dit instituut heeft vijftig nieuwe stoffen die in drinkwater zijn aangetroffen onderzocht op gevaar voor de volksgezondheid. Hij vond vijf chemische stoffen (benzeen, 1,4-dioxane, NDMA carbamezepine en twee perfluorverbindingen) die in de gaten gehouden moeten worden, omdat hun concentratie snel te hoog wordt.

De Wereldgezondheidsorganisatie WHO heeft voor veel vervuilers drinkwaternormen vastgesteld. Maar door verbetering van onderzoekstechnieken zijn er steeds meer stoffen op te sporen in een watermonster, terwijl er ook steeds nieuwe middelen ontstaan die in het water terechtkomen.

Schriks deed onderzoek in grondwater, drinkwater en oppervlaktewater in de Rijndelta. Hij zocht naar stoffen als geneesmiddelen, resten van benzine, gewasbestrijdingsmiddelen en resten van medische contraststoffen. Alle vervuilers werden aangetroffen, maar de meeste in zo'n lage concentratie dat ze geen effect op de gezondheid hebben.

Voor een deel van de 'nieuwe' stoffen bestaat nog geen drinkwaternorm. Schriks heeft voor de door hem onderzochte stoffen indicaties vastgesteld, die de drinkwaterbedrijven als richtlijn kunnen gebruiken. Hij publiceert zijn onderzoek en de normen in het internationale vakblad Water Research.

*De Telegraaf, d.d. 13 oktober 2009*

lende  
erken,

chriks  
gevaar

it hun

teld.  
in

cht

e door  
search.

### Nieuwsbrief 1

- Vroege Vogels
- Natuur in Beeld

Naam

E-mail \*

### Meldpunt Kappen!

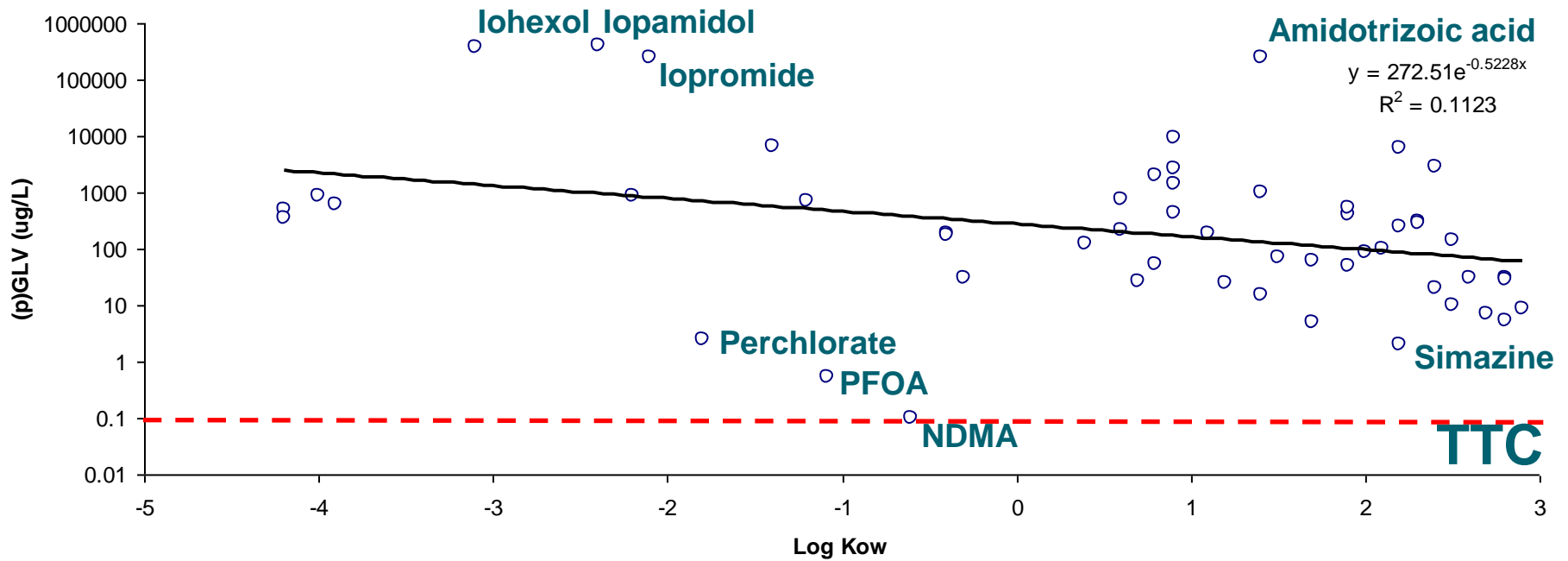


## Acknows

**Margo van der Kooi, Leo Puijker, Minne Heringa, Pim de Voogt,  
Annemarie van Wezel**

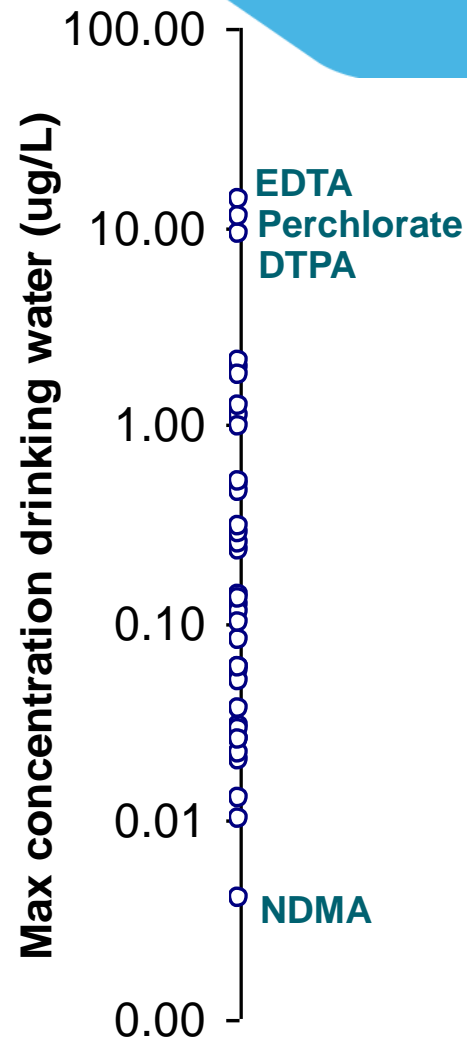
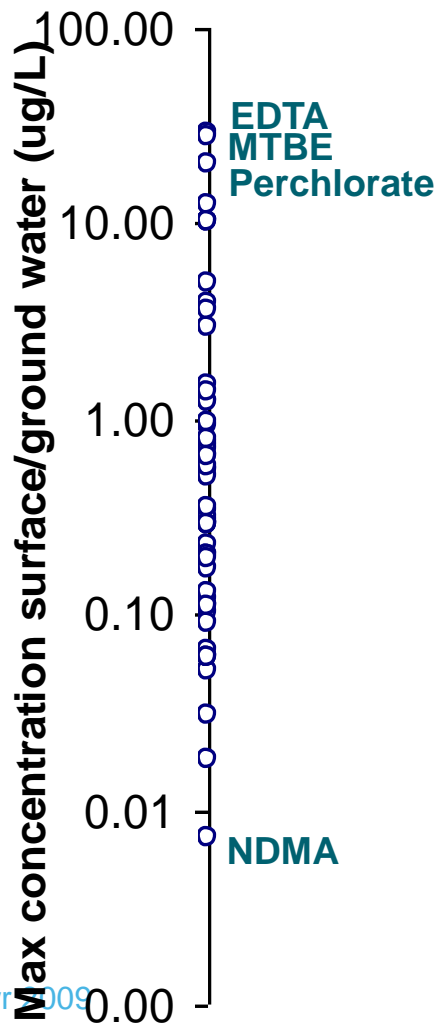
**This research was funded by the Joint Research Programme of the  
Dutch Water Utilities (BTO)**

# Results (relationship between (p)GLV and log Kow)





# Results max concentrations



# Results risk ratios (RR) for compounds in surface water, ground water, and drinking water

