

Supplementary material

Table 1. Expected total degradation time

Expected total degradation time	
Calculated rating	Words assigned
>4.75 - 5	hours
>4.25 - 4.75	hours to days
>3.75 - 4.25	days
>3.25 - 3.75	days to weeks
>2.75 - 3.25	weeks
>2.25 - 2.75	weeks to months
>1.75 - 2.25	months
<1.75	recalcitrant

Calculated rating represents the numerical value from model and words assigned, representing expected total degradation time, it is ultimate/primary rating in time units, as reported by Boethling et al. (1994).

Table 2. Bioaccumulation rate classification.

Bioaccumulation			
Rating	Description	Criteria for Log Kow	Criteria for BCF
0	No potential to bioaccumulate	< 1 or >ca.7 or MW>1000	Not measurable
1	Very low potential to bioaccumulate	≥ 1 - <2	≥ 1- < 10
2	Low potential to bioaccumulate	≥ 2 - < 3	≥ 10 - < 100
3	Moderate potential to bioaccumulate	≥ 3 - < 4	≥ 100 - < 500
4	High potential to bioaccumulate	≥ 4 - < 5	≥ 500 - < 4000
5	Very high potential to bioaccumulate	≥ 5 - < ca. 7	≥ 4000

Adapted from GESAMP rating scheme for Bioaccumulation (GESAMP, 2014).

Log Kow = Log Pow; BFC – Bioconcentration factor; MW – Molecular weight.

Table 3. Aquatic toxicity classification.

Aquatic Toxicity				
Acute Toxicity			Chronic Toxicity	
Rating	Description	LC ₅₀ , EC ₅₀ , IC ₅₀ (mg/L)	Description	NOEC (mg/L)
0	Non-toxic	> 1000	Negligible	> 1
1	Practically non-toxic	> 100 - ≤ 1000	Low Toxicity	> 0.1 - ≤ 1
2	Slightly toxic	> 10 - ≤ 100	Moderate toxicity	> 0.01 - ≤ 0.1
3	Moderately toxic	> 1 - ≤ 10	High toxicity	> 0.001 - ≤ 0.01
4	Highly toxic	> 0.1 - ≤ 1	Very high toxicity	≤ 0.001
5	Very highly toxic	> 0.01 - ≤ 0.1		
6	Extremely toxic	≤ 0.01		

Adapted from Revised GESAMP rating scheme for aquatic toxicity (GESAMP, 2014).

LC₅₀ – lethal concentration 50%; EC₅₀ – median effective concentration; IC₅₀ – inhibition concentration 50%; NOEC – no observed effect concentration.

Table 4. Human health (Toxic effects to mammals).

Human Health (Toxic Effects to Mammals)							
Rating	Description	Acute Mammalian Toxicity			Irritation, Corrosion & Long term health effects		
		Oral Toxicity LD50/ATE (mg/Kg)	Dermal Toxicity LD50/ATE (mg/Kg)	Inhalation Toxicity LC50/ATE (mg/l)	Skin irritation & corrosion	Eye irritation & corrosion	Long term health effects
0	Negligible	>2000	>2000	>20	Not irritating	Not irritating	M - Mutagenicity
1	Slight	>300 - ≤2000	>1000 - ≤2000	>10 - ≤20	Mildly irritating	Mildly irritating	R - Reprotoxicity
2	Moderate	>50 - ≤300	>200 - ≤1000	>2 - ≤10	Irritating	Irritating	Ss - Sensitizing to skin
3	Moderately high	>5 - ≤50	>50 - ≤200	>0.5 - ≤2	Severely irritating or corrosive 3A Corr. (≤ 4h) 3B Corr. (≤ 1h) 3C Corr. (≤ 3 min)	Severely irritating	Sr - Sensitizing to respiratory system A - Aspiration Hazard T - Target organ toxicity N – Neurotoxicity I - Immunotoxicity
4	High	≤5	≤50	≤0.5			

Adapted from Revised GESAMP rating scheme for Human Health (Toxic Effects to Mammals) (GESAMP, 2014).

LD50 – lethal dose 50%; LC50 - lethal concentration 50%; ATE – acute toxicity estimate (dose range/extrapolated dose leading to lethal effects in mammals, equivalent to LD50/LC50 values).

Table 5. Carcinogenicity classification.

Score	IARC group	Description
0	4	Probably not carcinogenic to humans
1	3	Not classifiable as to its carcinogenicity to humans
2	2B	Possibly carcinogenic to humans
3	2A	Probably carcinogenic to humans
4	1	Carcinogenic to humans

Relation of the scores used to classify the 24 HNS relative to IARC classification (<http://monographs.iarc.fr/ENG/Classification/index.php>).