

Selvestrel et al.:

# SpheraCosmolife: A New Tool for the Risk Assessment of Cosmetic Products

## Supplementary Data

Tab. S1: Threshold of Toxicological Concern (TTC) according to the Cramer classes

Cramer class	TTC (µg/person/day)	TTC (µg/kg bw/day)
I	1800	30
II	540	9.0
III	90	1.5

Input Molecule	
SMILES	[Na+].[O-]C(=O)c1ccccc1
SMILES (neutralized)	O=C(O)c1ccccc1
CAS no.	532-32-1
INCI	SODIUM BENZOATE
Product Type	Liquid foundation
C (Product concentration) as percentage	0.3 %
C <sub>x</sub> (Product concentration)	3 mg/g

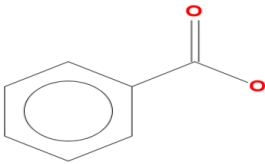


Fig. S1: Example of the first part of the specific report (e.g., sodium benzoate)

Retrieved parameters for the product type	
Values retrieved from: The SCCS notes of guidance for the testing of cosmetic ingredients and their safety evaluation - 10th revision	
E <sub>product ref</sub> (Relative daily exposure)	7.9 mg/kg bw/day
A (Surface area involved)	565 cm <sup>2</sup>
Type of exposure	Leave-on
T <sub>exp</sub> (Time of exposure)	24 h

1. Annex lists	
Data are based on the annexes list updated on November, 27th 2019.	
Molecules found in the annex lists: 1	
Found molecule no. 1	
CAS	532-32-1
INCI	SODIUM BENZOATE
Found in annex	ANNEX V: LIST OF PRESERVATIVES ALLOWED IN COSMETIC PRODUCTS
Annex details	ANNEX V: Reference Number: 1 ANNEX V: Product type, body part: a) Rinse-off products, except oral products b) Oral products c) Leave-on products ANNEX V: MAX Concentration in ready for use preparation: a) 2.5 % (acid) b) 1.7 % (acid) c) 0.5 % (acid) ANNEX V: NOTES: >0532/01 - Opinion on Benzoic Acid and Sodium Benzoate >0891/05 - Opinion on Benzoic Acid and Sodium Benzoate >0125/99 - Opinion concerning Restrictions on Materials listed in annex VI of Directive 76/768/EEC on Cosmetic Products
Found Safer Chemicals classification	Green [Circle]
Safer Chemicals details	Safer functional use: Preservatives-antioxidants
Found in CLP list	No

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## 2. External exposure assessment

E <sub>dermal</sub> (External exposure for dermal uptake)	0.02 mg/kg bw/d
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## 3. Internal exposure assessment

Kp (Skin permeation, VEGA prediction - Ten and Berge formula)	0.02 cm/h	EXPERIMENTAL value	✓
Kp (Skin permeation, VEGA prediction - Potts and Guy formula)	0.02 cm/h	EXPERIMENTAL value	✓
Kp (Skin permeation, worst case used for calculations)	0.02 cm/h		
Water solubility (VEGA prediction)	3.39 mg/cm <sup>3</sup>	EXPERIMENTAL value	✓
J <sub>max</sub> (Maximum flux)	0.05 mg/cm <sup>2</sup> h		

Systemic Exposure Dose calculated with three different absorption scenarios:

100% (oral absorption)

50% (dermal absorption)

80% (estimated absorption with the Kroes approach)

SED - Systemic Exposure Dose with 100% absorption	0.02 mg/kg bw/d
SED - Systemic Exposure Dose with 50% absorption	0.01 mg/kg bw/d
SED - Systemic Exposure Dose with 80% absorption (from Kroes thresholds)	0.02 mg/kg bw/d

**Fig. S2: Information about exposure (e.g., sodium benzoate)**

## 4. Hazard identification

Mutagenicity - Ames test (Janus workflow prediction)	NON-Mutagen (EXPERIMENTAL value)
In vitro micronucleus assay (IRFMN model prediction)	Inactive (EXPERIMENTAL value)
Chromosomal aberration test (Coral model prediction)	Inactive (good reliability)
Skin sensitization (Consensus of Caesar and JRC models)	NON-Sensitizer (EXPERIMENTAL value)
Skin sensitization (Caesar model prediction)	NON-Sensitizer (good reliability)
Skin sensitization (IRFMN/JRC model prediction)	NON-Sensitizer (EXPERIMENTAL value)

## 5. NOAEL

NOAEL (Experimental value, from internal database)	not found	
NOAEL (IRFMN/Coral model prediction)	27.66 mg/kg bw/d	moderate reliability ⚠
NOAEL used for calculations	27.66 mg/kg bw/d	

**Fig. S3: Information about hazard (e.g., sodium benzoate)**