Development of the ‘Cocktail Effect Calculator’

A tool for risk assessment of cocktail effects

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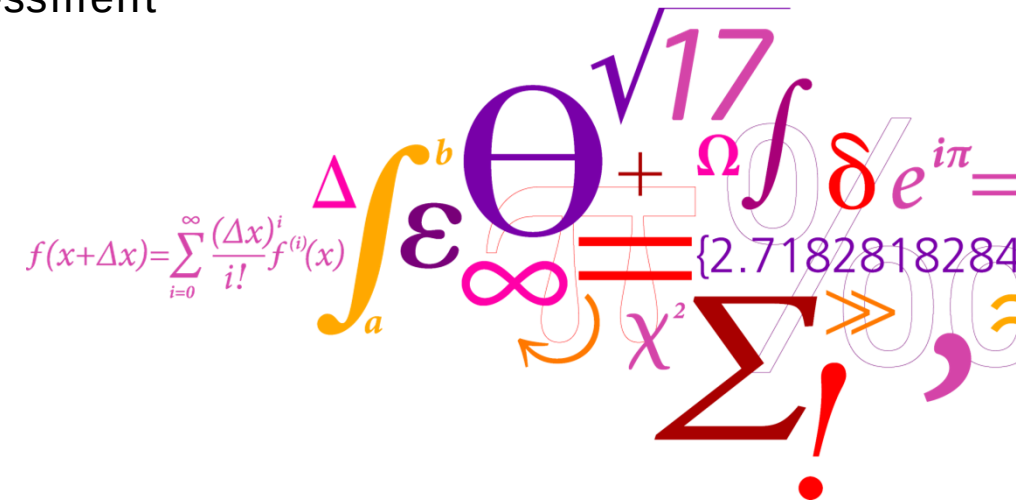
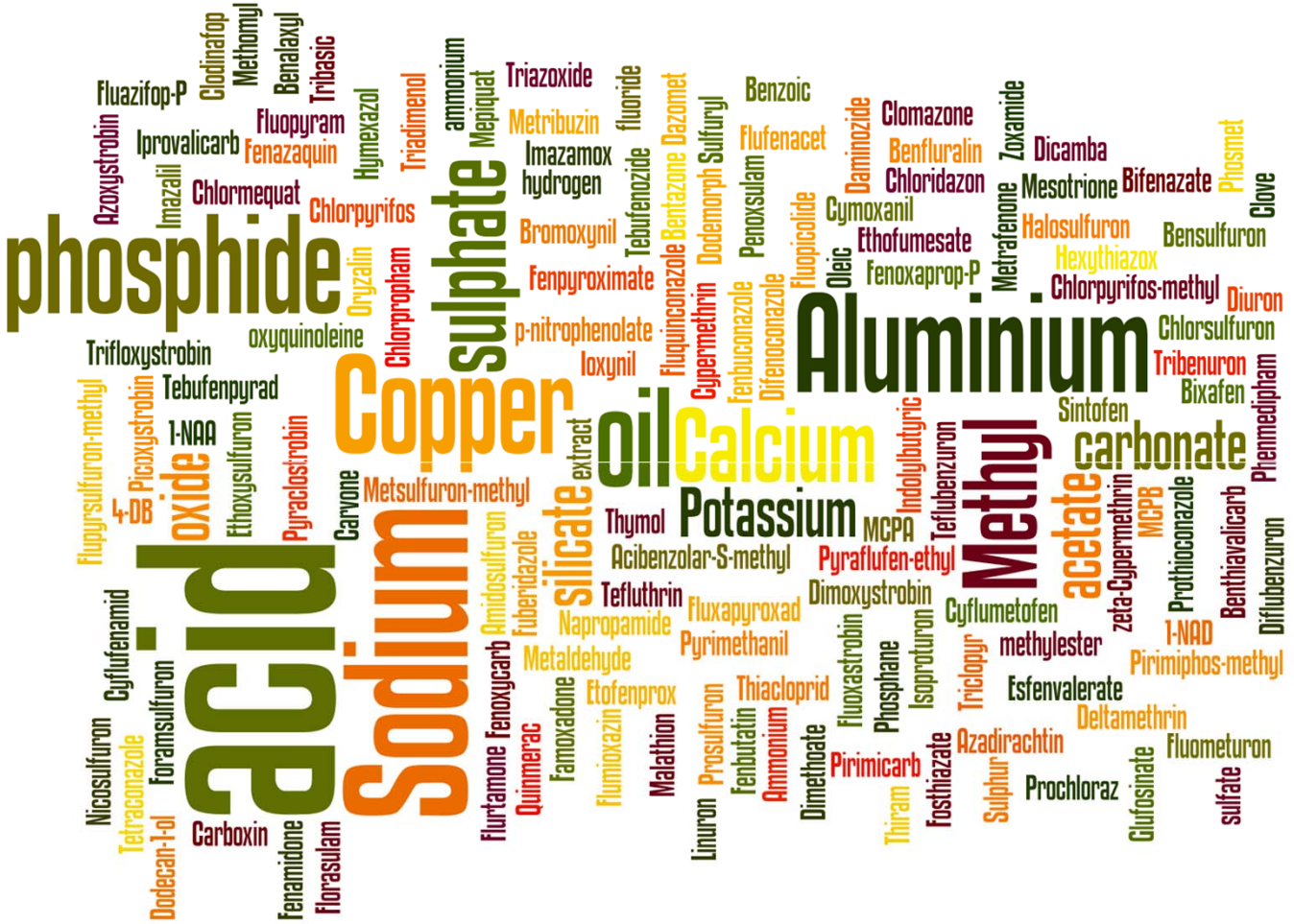


DTU Food
National Food Institute

So many chemicals....



Challenge in risk assessment of cocktails

- Information on toxicity and exposure of chemicals is spread out in many databases and reports
- Time consuming to collect data for calculation of combination effects

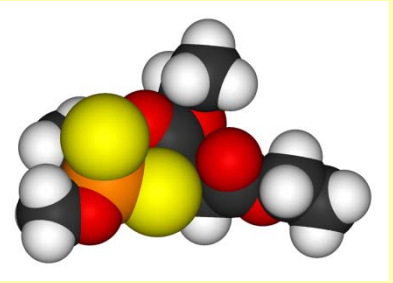
The ‘Cocktail Effect Calculator’

A user interface for:

- Finding information on **toxicity** and **exposure** data for chemicals
  - The toxicity information is limited to the critical toxicity on which the present EU regulation is based

- Calculating a **hazard index** for the actual cocktail

Chemical classes



- Selected chemicals with available information:
  - Phthalates
  - Perfluorinated compounds
  - Brominated flame retardants
  - Pesticides
  - Metals
  - Mycotoxins
  - PAHs
  - Dioxins and PCBs
  - Bisphenol A
  - Acrylamide

The collection of information

- Phthalates
- Perfluorinated compounds
- Brominated flame retardants
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- Metals
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- Acrylamide

Tox data

- critical adverse effect
- point of departure (e.g. NOAEL)
- reference dose (e.g. TDI/ADI)

Exposure data

- intake values for defined consumer groups
- exposure via food; does not cover the exposure from other sources such as cosmetics products

- **Hazard quotients** for the individual chemicals are, if possible, calculated based on the collected information
- Contains **links** to reports containing the collected toxicity and exposure information

Information sources

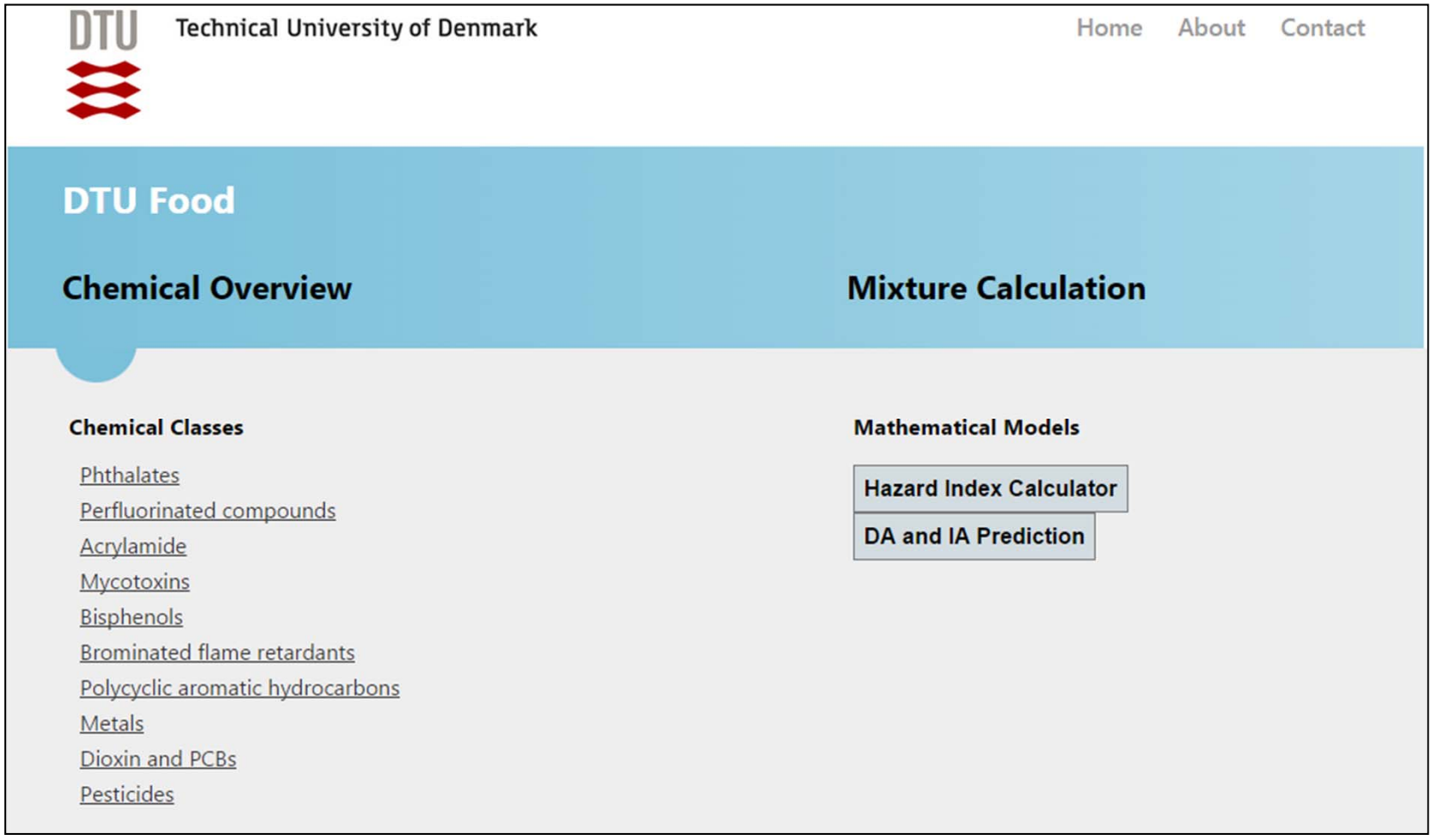
The toxicity information is limited to the critical toxicity on which the present EU regulation is based

Only chemical exposure via the food has been taken into account

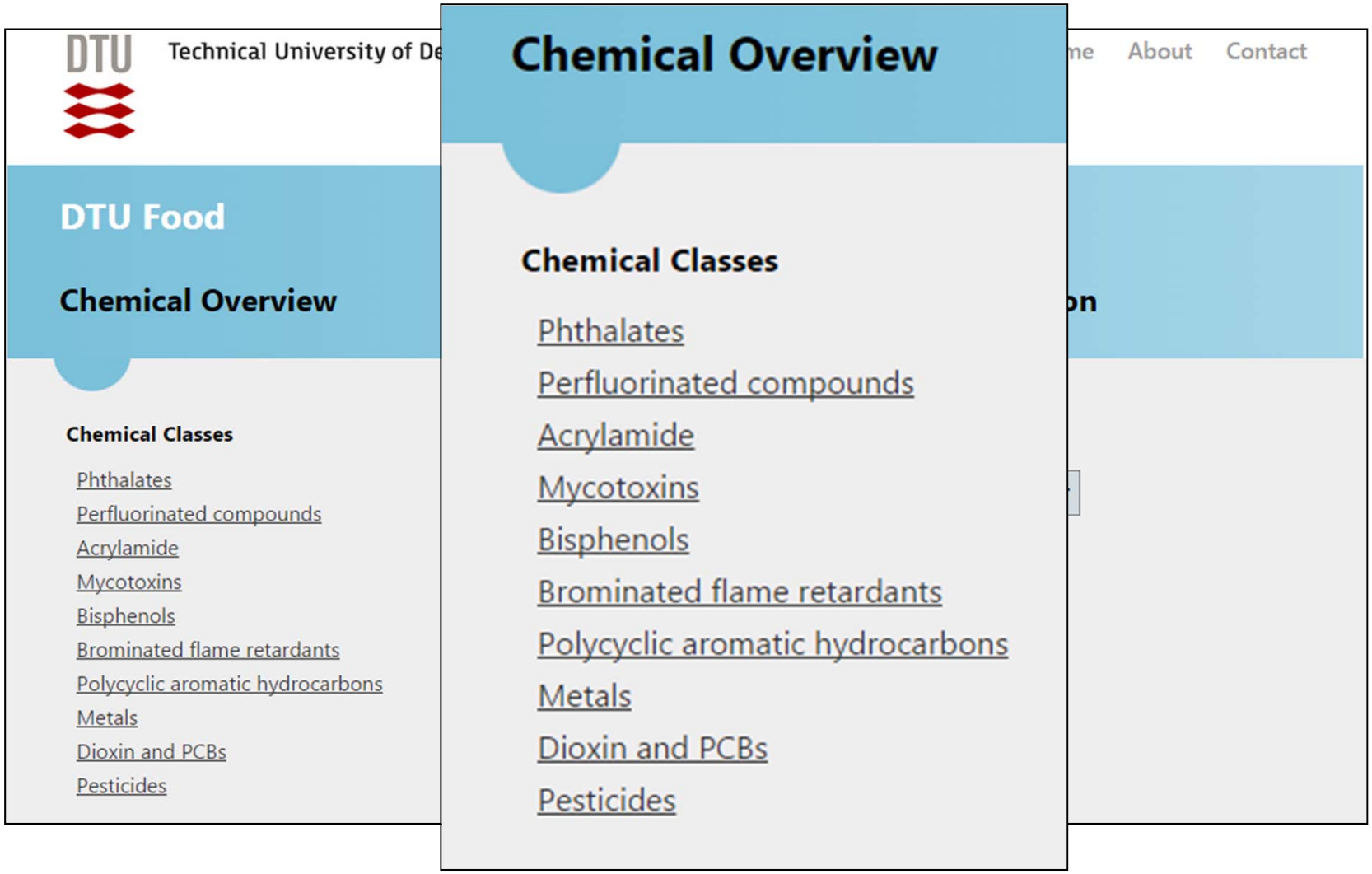
If no reference value such as TDI or ADI has been established, a reference dose was calculated using the formula: *point of departure / safety factor*

Data from EFSA and Danish reports are primarily used for the calculations; in some cases JECFA or ECHA data are used

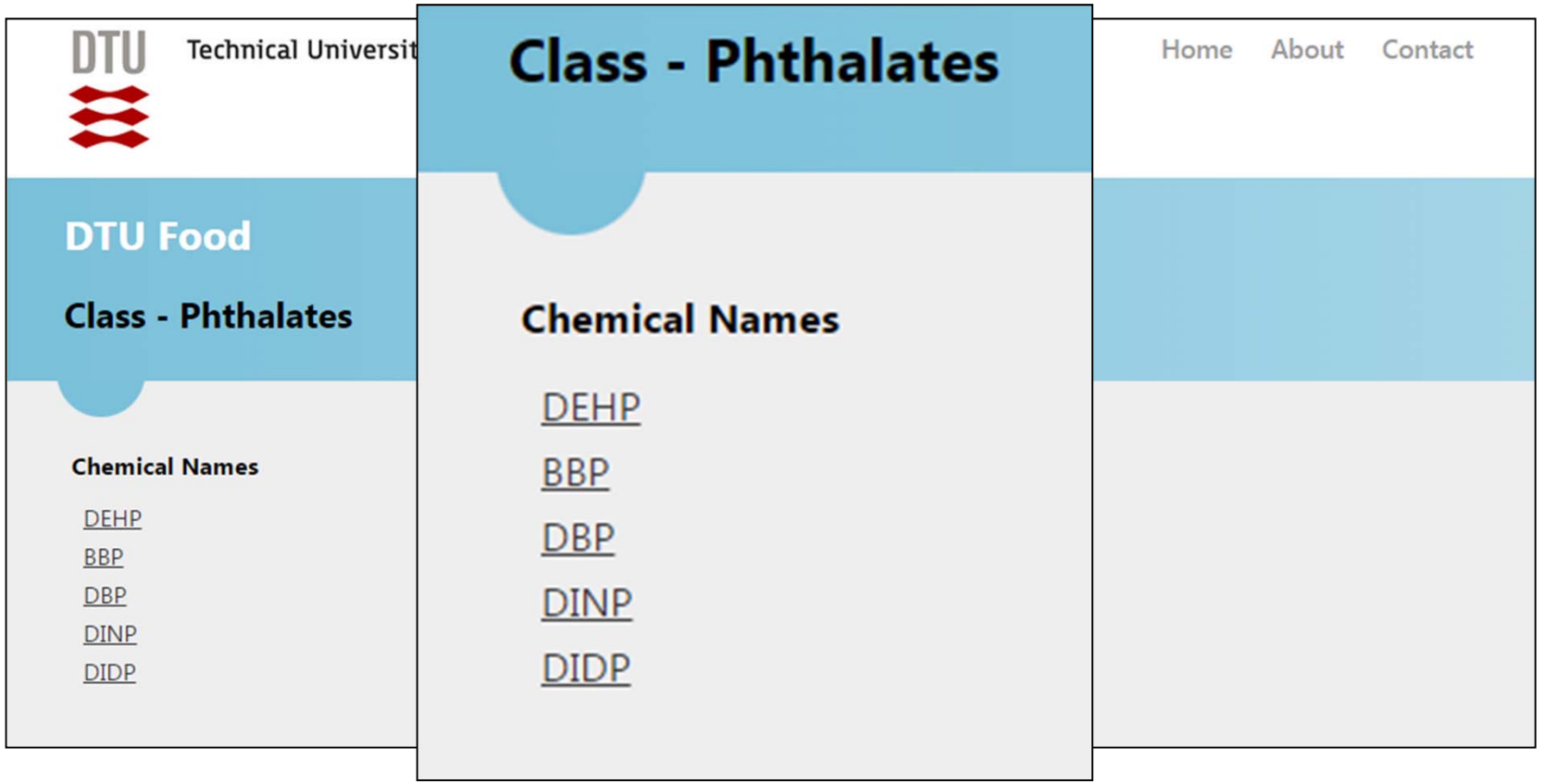
Front page of the user interface – overview of entries



Front page – Chemical Classes



Example of a chemical class – phthalates



Example of a phthalate – DEHP

DEHP

CAS RN: 117-81-7

Toxicity and Exposure Information

Critical Effect	Testes (rat)	**Intake (µg/kg/day)**	6.9	**Hazard quotient**	0,138
Point of departure (mg/kg/day)	NOAEL: 5	**Consumer Group**	Toddlers (2.5-3.5 y). UK 95% perc., LB		
ADI/TDI (mg/kg/day)	TDI: 0.05				

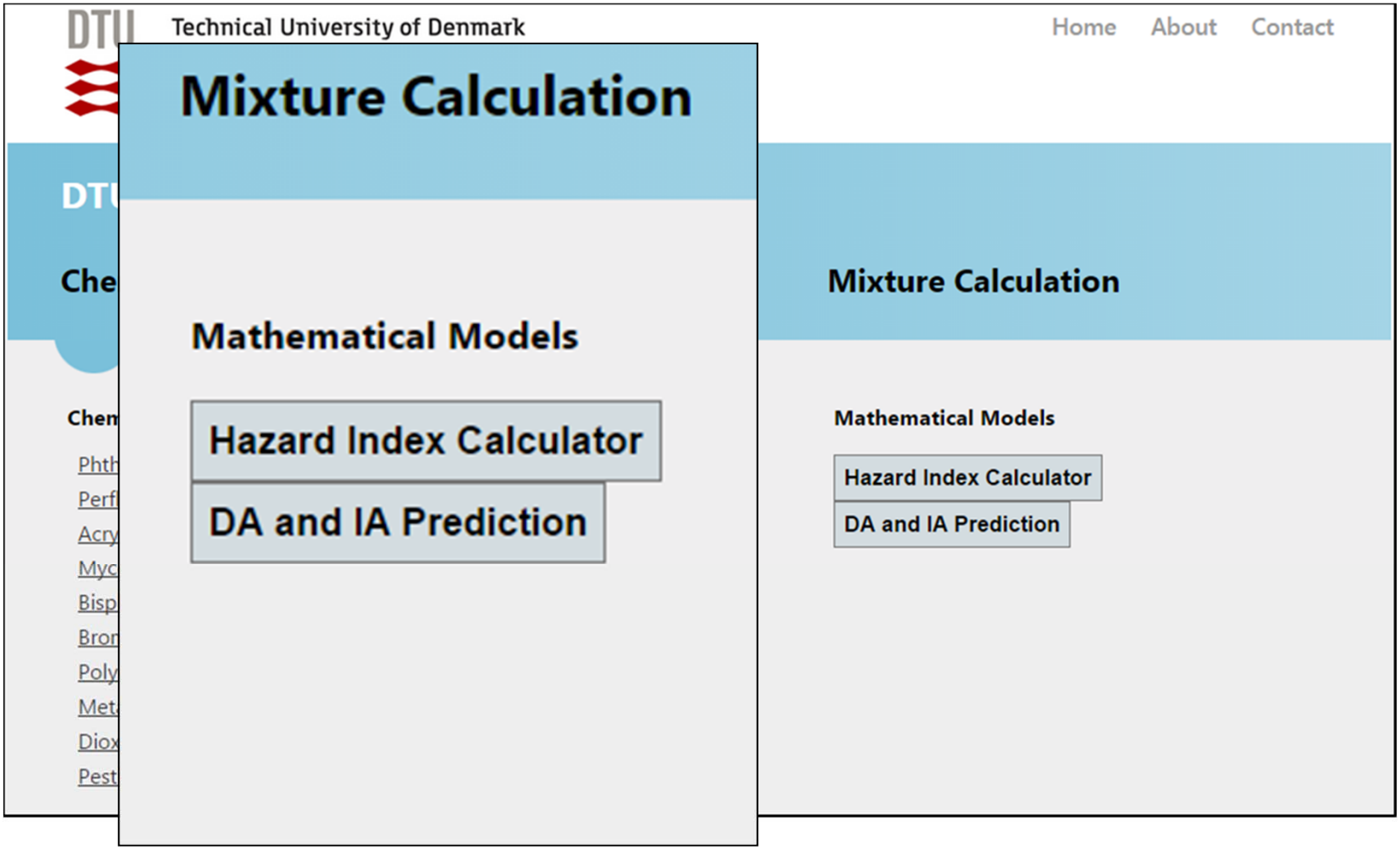
Comment

LB: Lower bound; all results <LOD/LOQ=0

Tox Link http://www.efsa.europa.eu/en/efsajournal/pub/243.htm
Description: - Scientific opinion on DEHP, EFSA 2005

Intake Link http://cot.food.gov.uk/cotstatements/cotstatementsyrs/cotstatements2011/cot201104
Description: - Committee of toxicology 2011

Back to front page – Mixture Calculation



Hazard Index Calculator

Hazard Index Calculation

Hazard Index Value: 0

Print

CAS-RN / Chemical Name	Critical Effect	POD	SF	RfD	Exposure	HQ
CAS-RN Chemical Name	Critical Effect	Type of Value POD Value Unit	SF	POD / SF Unit	Type of Value EXP Value Unit	HQ
CAS-RN Chemical Name	Critical Effect	Type of Value POD Value Unit	SF	POD / SF Unit	Type of Value EXP Value Unit	HQ
CAS-RN Chemical Name	Critical Effect	Type of Value POD Value Unit	SF	POD / SF Unit	Type of Value EXP Value Unit	HQ

Example with toddlers and phthalates

Hazard Index Calculation

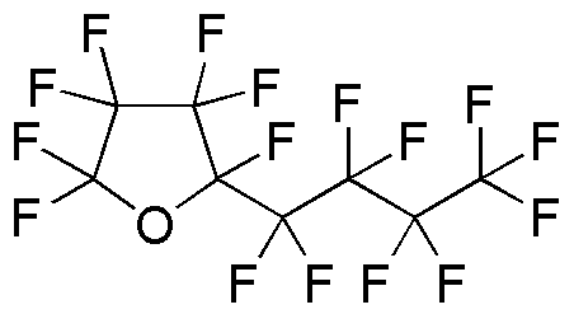
Hazard Index Value: 0.17800000000000002

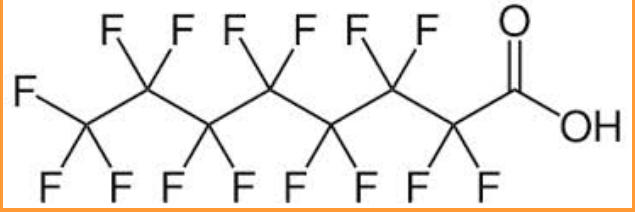
Print

CAS-RN / Chemical Name	Critical Effect	POD	SF	RfD	Exposure	HQ
117-81-7 DEHP	Testes (rat)	NOAEL 5 mg/kg/day	100	0.05 mg/kg/day	Intake 0.0069 mg/kg/day	0.138
84-74-2 DBP	Testes (rat)	LOAEL 2 mg/kg/day	200	0.01 mg/kg/day	Intake 0.0004 mg/kg/day	0.04
CAS-RN Chemical Name	Critical Effect	Type of Value POD Value Unit	SF	POD / SF Unit	Type of Value EXP Value Unit	HQ

Limitations in hazard index calculation

- The calculations are based on available data and regulations
- For some groups of chemicals (e.g. perfluorinated chemicals) this means that the risk may be underestimated due to lack of data





Expanding and updating the ‘Cocktail Effect Calculator’

- Other exposure sources

- New exposure/tox data

Acknowledgements

- Sina Hadi Sohi
- Annette Petersen
- Niels Hadrup
- Anne-Marie Vinggaard

- Pelle Thonning Olesen
- Julie Boberg
- Marta Axelstad Petersen
- Sofie Christiansen
- Ulla Hass
- Max Hansen

Thank you for listening