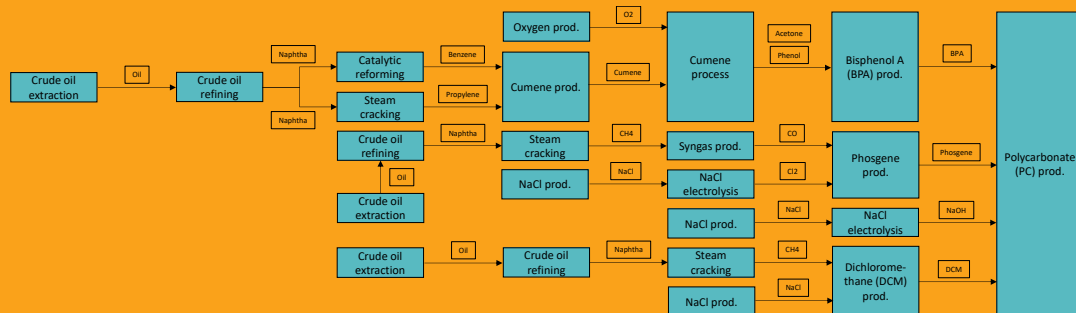


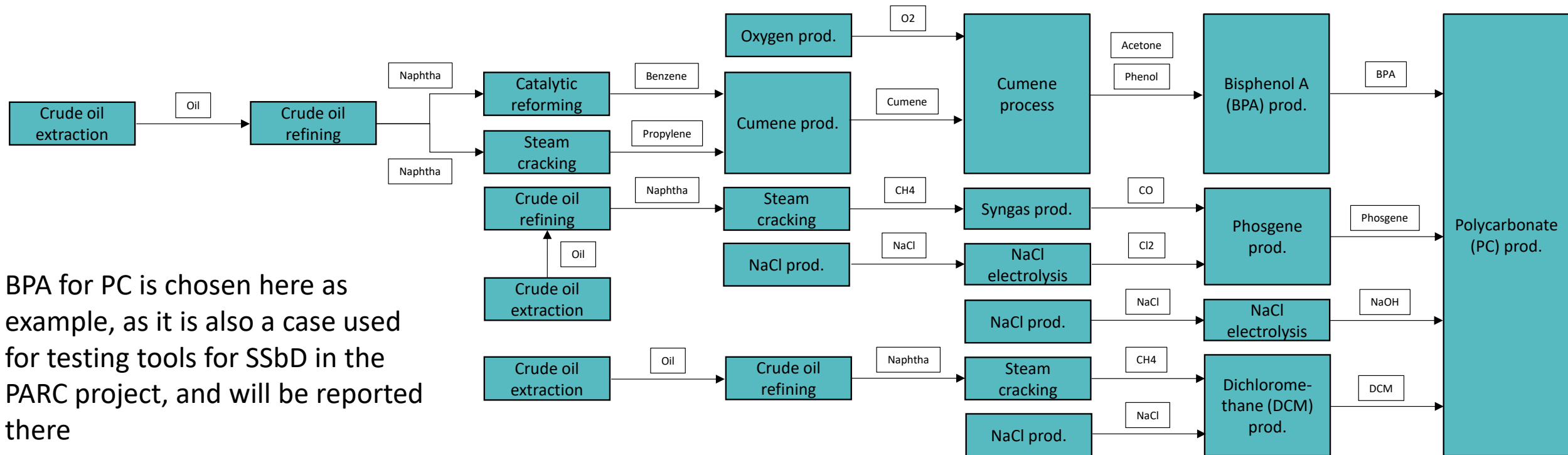
ProScale & ProScaleE case study example

Rosella Telaretti Leggieri, IVL, 2024-05-31



Purpose

Testing ProScale and ProScaleE on the life cycle (cradle-to-gate) of **polycarbonate (PC)** based on **bisphenol A (BPA)** and **phosgene**.

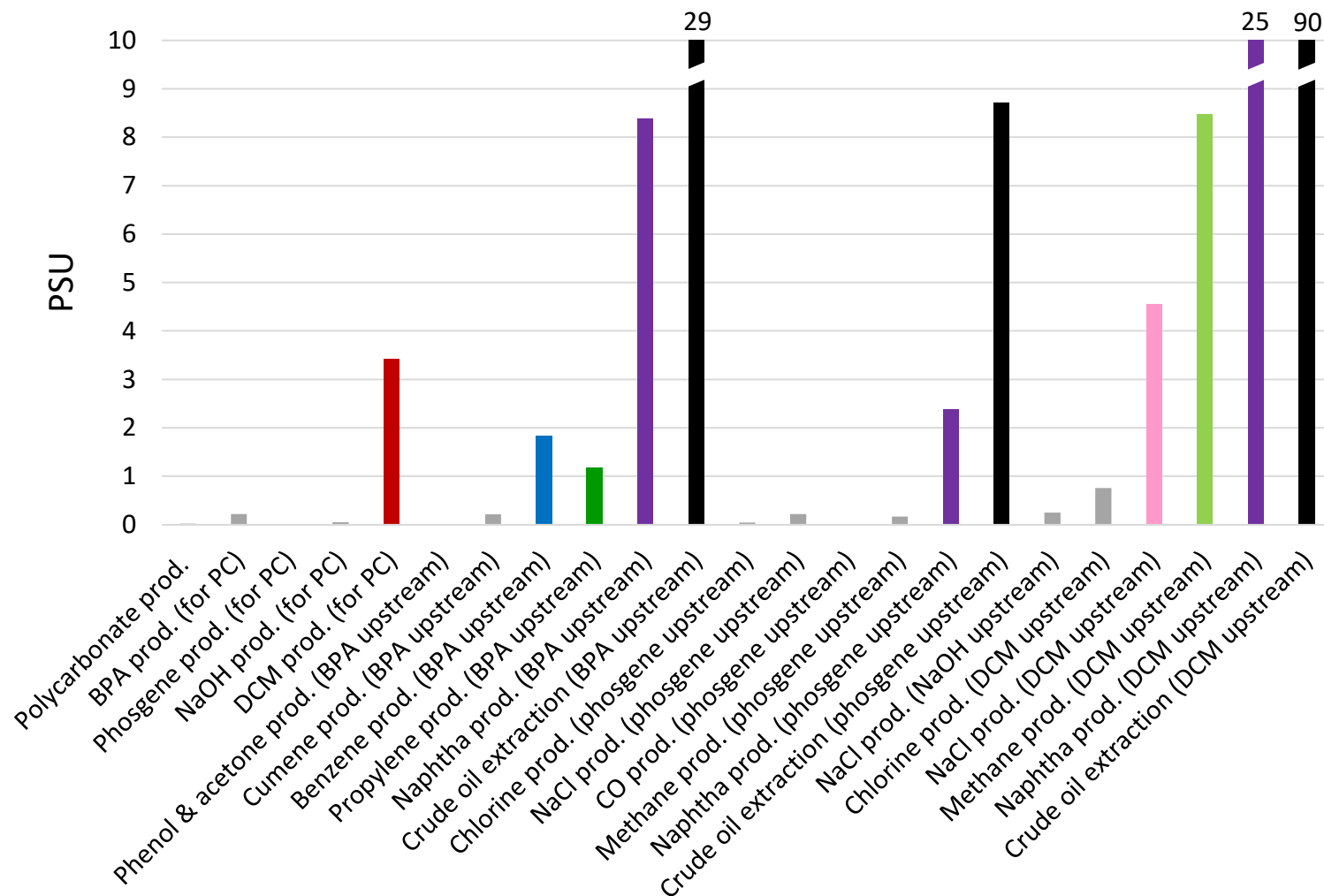


ProScale – Key results

Unit processes

- Crude oil extraction
- Naphtha prod. (crude oil refining)
- Methane prod. (steam cracking)
- NaCl prod. (brine purification)
- Dichloromethane (DCM) prod.
- Benzene prod. (catalytic reforming)
- Propylene prod. (steam cracking)

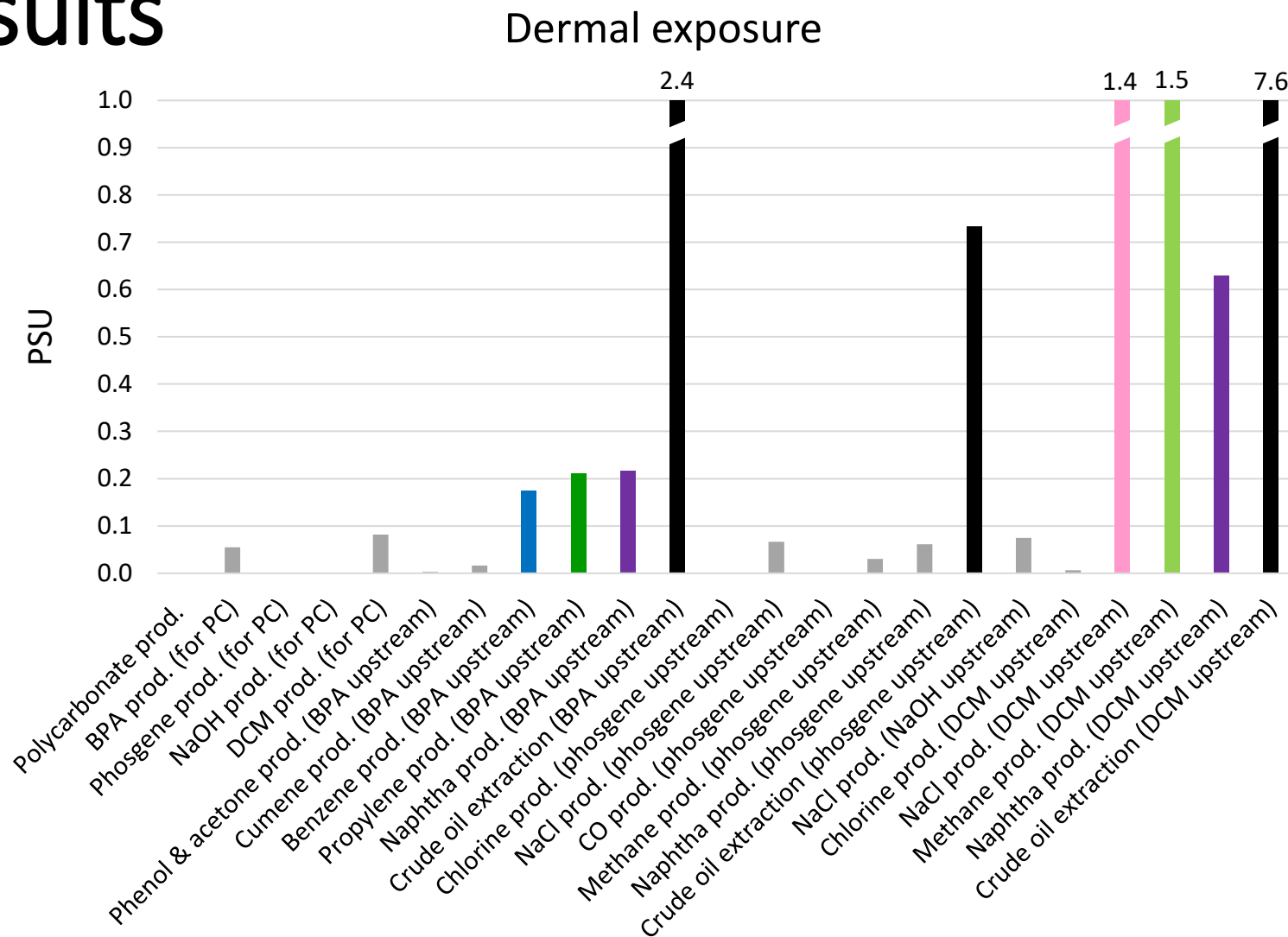
Inhalation exposure




ProScale – Key results

Unit processes

- Crude oil extraction
- Naphtha prod. (crude oil refining)
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- NaCl prod. (brine purification)
- Benzene prod. (catalytic reforming)
- Propylene prod. (steam cracking)





ProScaleE – Method

- Hazard Factor (HF_e):
 - Data from REACH dossiers
 - Data gaps filled with prediction tools
- Degradation Factor (DF):
 - Data from REACH dossiers
 - Data gaps filled with prediction tools
- Environmental Release Factor (ERF):
 - Environmental Release Categories (ERCs) from ECHA
 - SPERCs for solvents from European Solvents Industry Group
- Allocation of impacts conducted on mass basis

ProScaleE – Characterization factors

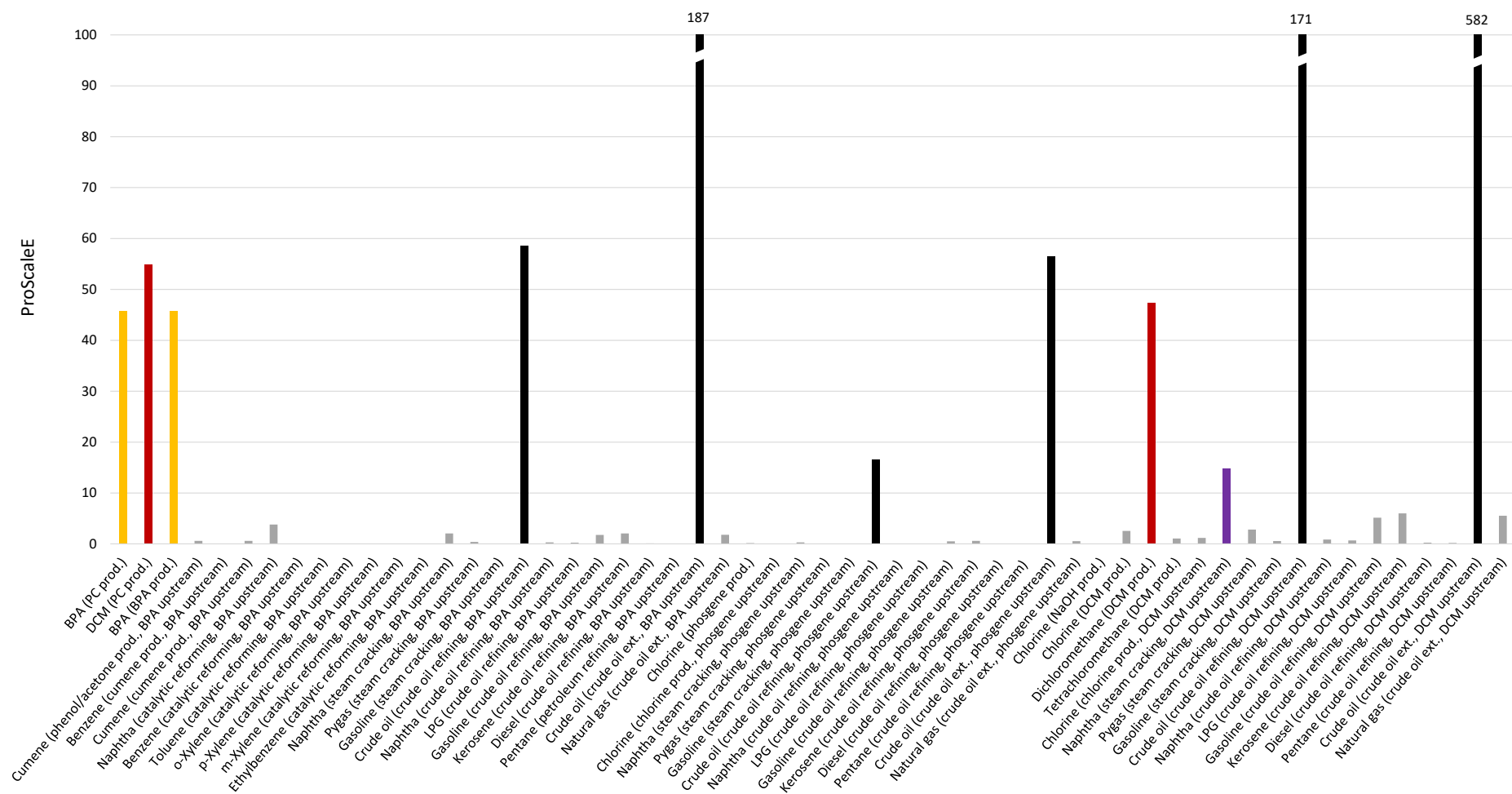
Substance	Class-determining H-phrase	Hazard class	Hazard Factor (HF _e)	Biodegradability/persistence class	Degradation factor (DF)	ProScale-E characterization factor
Bisphenol A (BPA)	ED 1	E	100 000	Readily biodeg.	0.01	1000
Crude oil	H410*	D	1000	Persistent*	1	1000
Dichloromethane	ED 2	D	10 000	Readily biodeg.	0.01	100
Naphtha	H411	C	1000	Inherently biodeg.*	0.1	100
Gasoline	H411	C	1000	Inherently biodeg.*	0.1	100
Kerosene	H411	C	1000	Inherently biodeg.*	0.1	100
Liquefied petroleum gas	H410*	D	1000	Inherently biodeg.*	0.1	100
Cumene	H411	C	1000	Readily biodeg.	0.01	10
Pentane	H411	C	1000	Readily biodeg.	0.01	10
Benzene	H412	B	100	Readily biodeg.	0.01	1
Toluene	H412	B	100	Readily biodeg.	0.01	1
Ethylbenzene	H412	B	100	Readily biodeg.	0.01	1

*Data from *in silico* prediction tools.

ProScaleE – Key results

Emissions to air

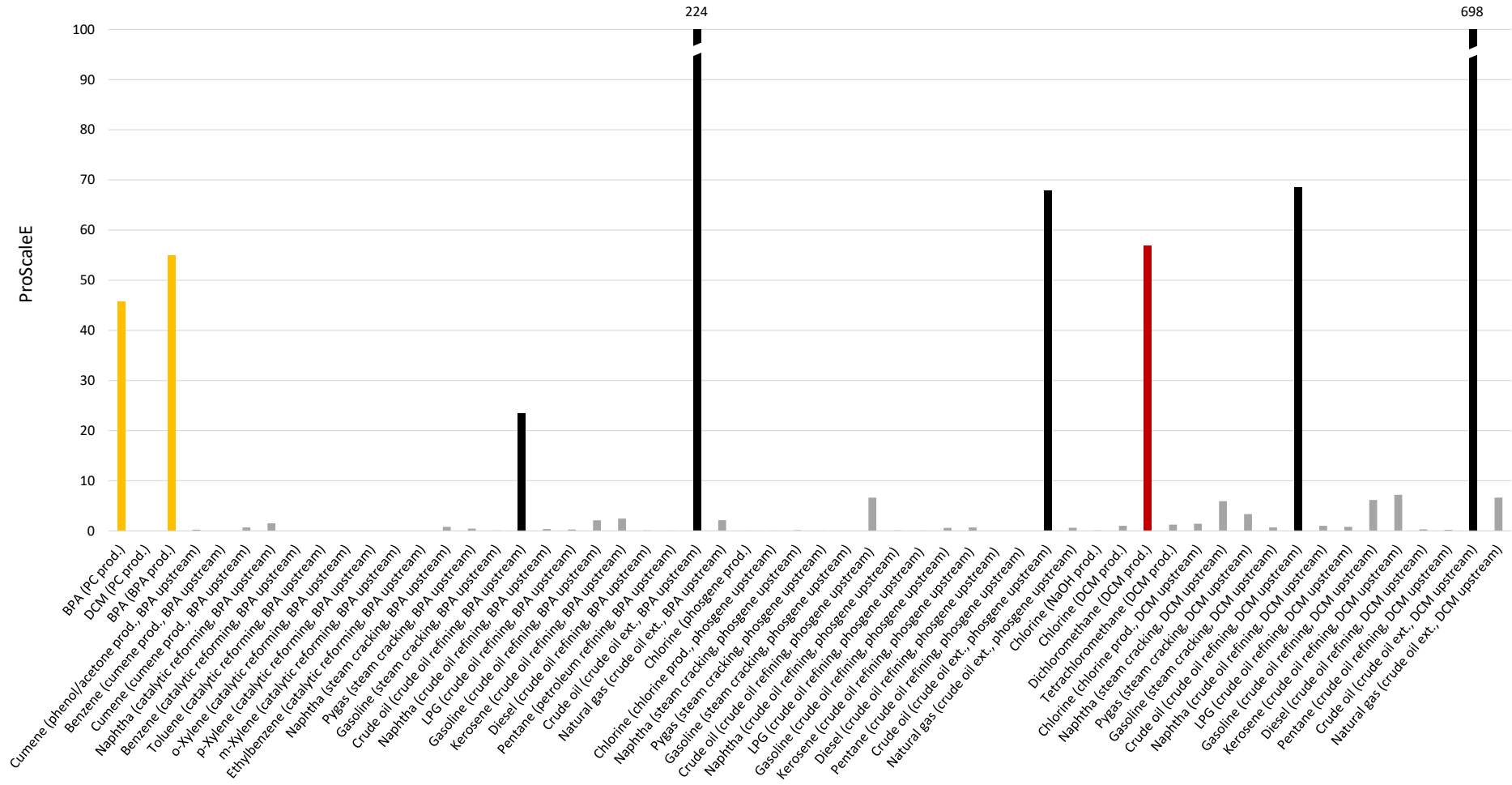
- Crude oil
- Bisphenol A (BPA)
- Dichloromethane (DCM)
- Naphtha



ProScaleE – Key results

Emissions to water

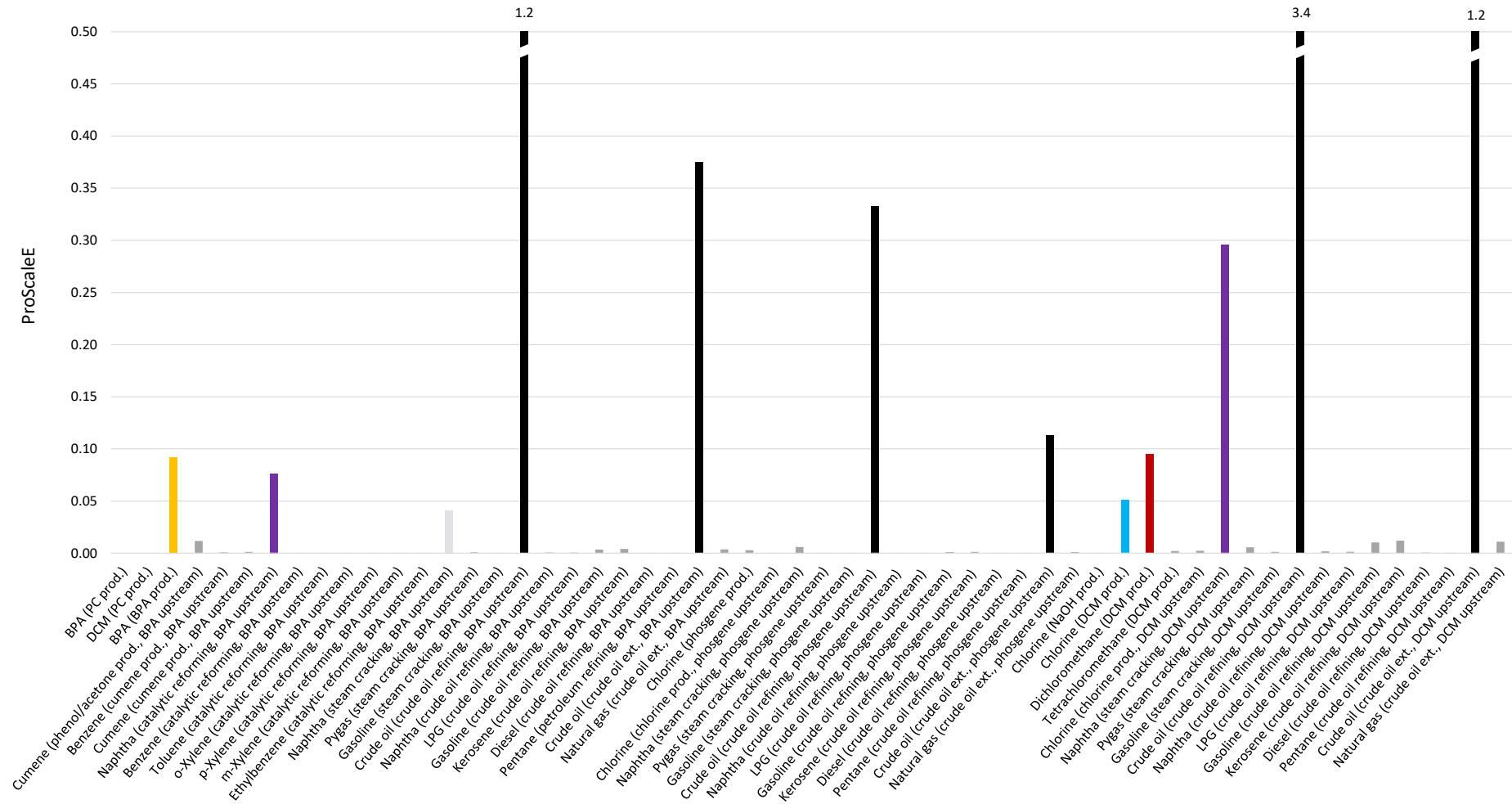
- Crude oil
- Bisphenol A (BPA)
- Dichloromethane (DCM)



ProScaleE – Key results

Emissions to soil

- Crude oil
- Bisphenol A (BPA)
- Dichloromethane (DCM)
- Naphtha
- Chlorine



Takeaways

- ProScaleE can successfully translate **REACH data** into ecotoxicity potential of modelled emissions throughout the life cycle of a product.
- **ERCs** and **SPERCs** allow for a rough modelling of substance release to air, water and soil.
- The ProScaleE practitioner can easily identify **ecotoxicity hotspots**.



Thank you !

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