Identification of potential risk drivers in weathered plastic leachates

Frank Menger, Helen Sepman, Stefan Lips, Annika Jahnke,
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frank.menger@su.se

Stockholm University

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https://www.ufz.de/p-leach/

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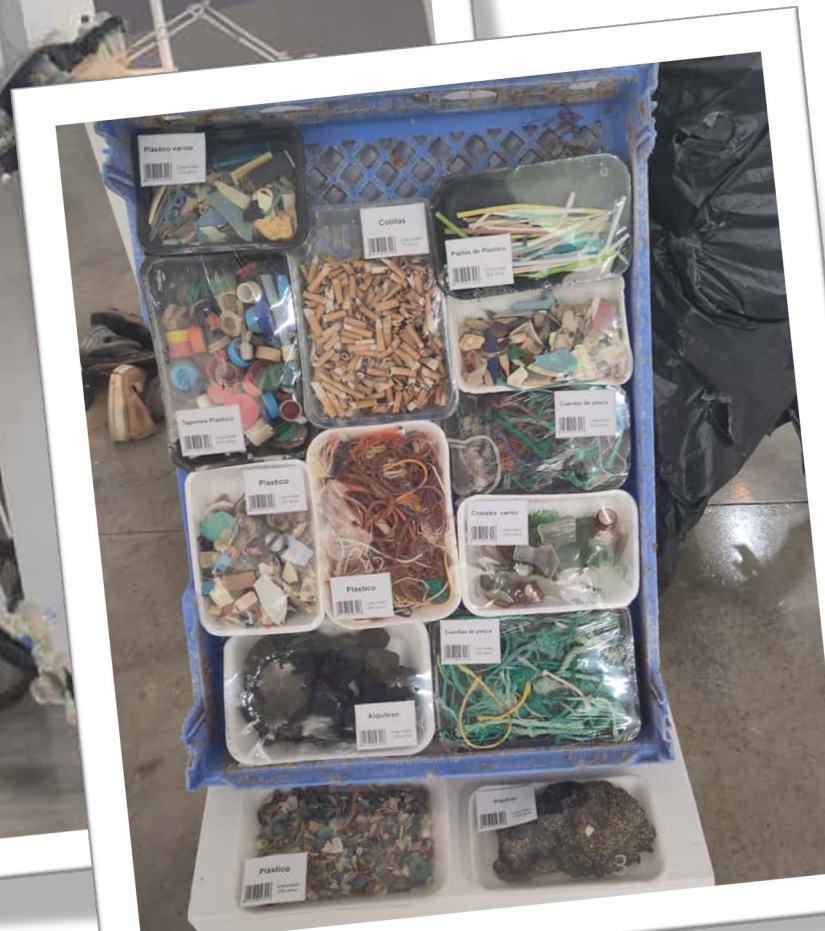
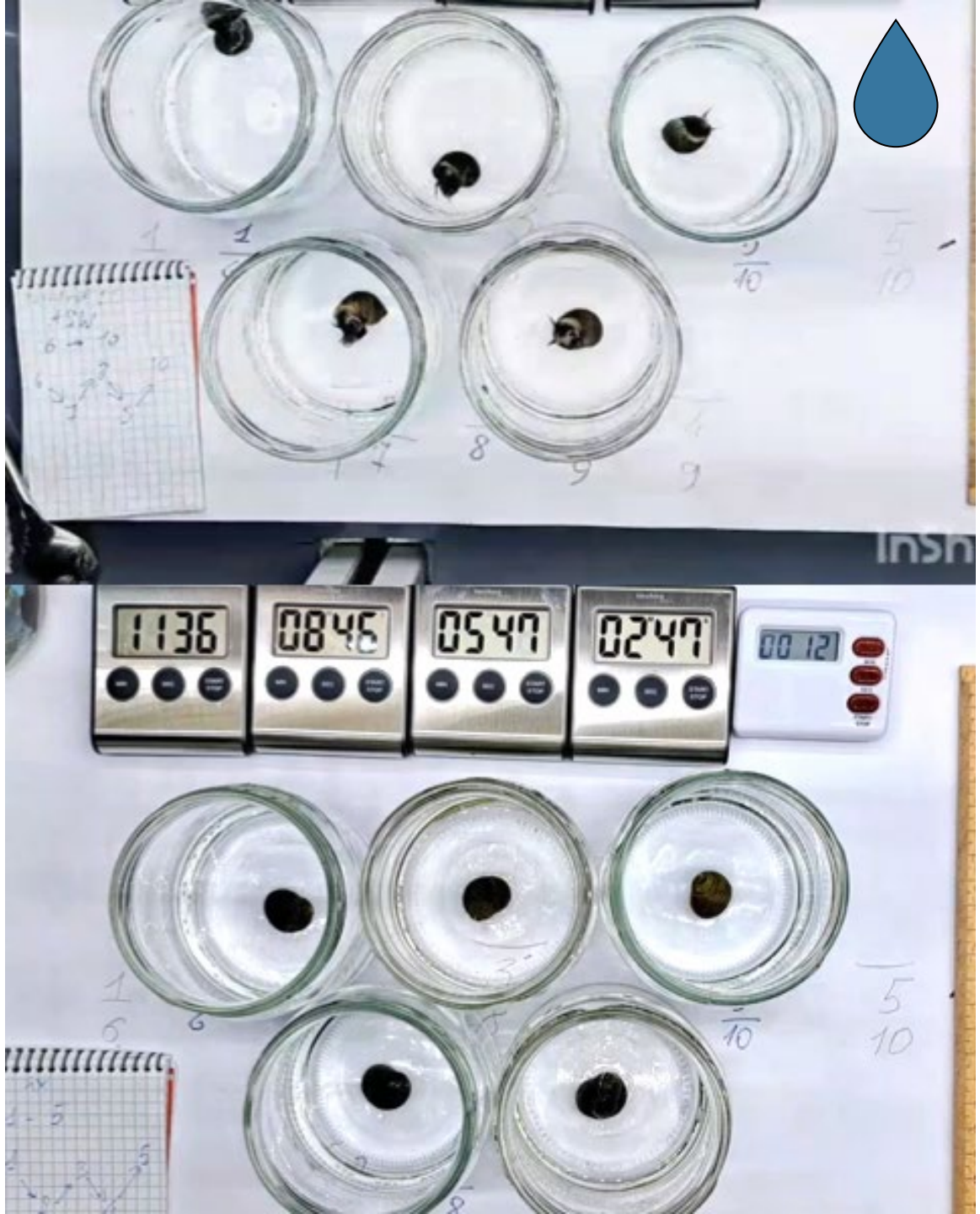
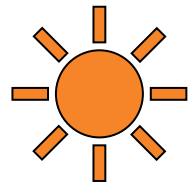


art displayed at
MICRO 2024

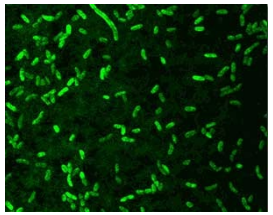


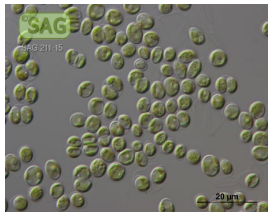


culprit(s)

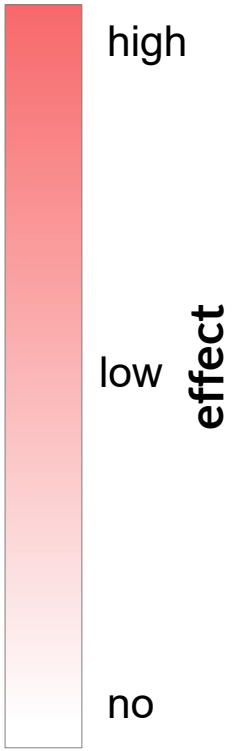
greenhouse foil

video by
Daria B.





	fish cell lines		green algae		*D. magna*
PVC0 DC	53		<EC50	<EC50	
PVC0 UV	60		<EC50		
PVC0.1 DC					
PVC0.1 UV	57				
PVC1 DC			<EC50		
PVC1 UV	44	stimulation	80	84	118
PVC2 DC	12		<EC50	<EC50	68
PVC2 UV	12		58	121	47
PVC3 DC	33	87			
PVC3 UV	53		44	<EC50	
PE0 DC		84		50	74
PE0 UV	<EC50				
PE1 DC			<EC50		
PE1 UV				126	18
PE2 DC			101	25	9
PE2 UV	4	3	107	44	NA
PET0 DC	<EC50			<EC50	
PET0 UV	44			73	
PET1 DC					
PET1 UV	<EC50		<EC50		
PET2 DC	<EC50		97	<EC50	8
PET2 UV	3	5	5	8	1

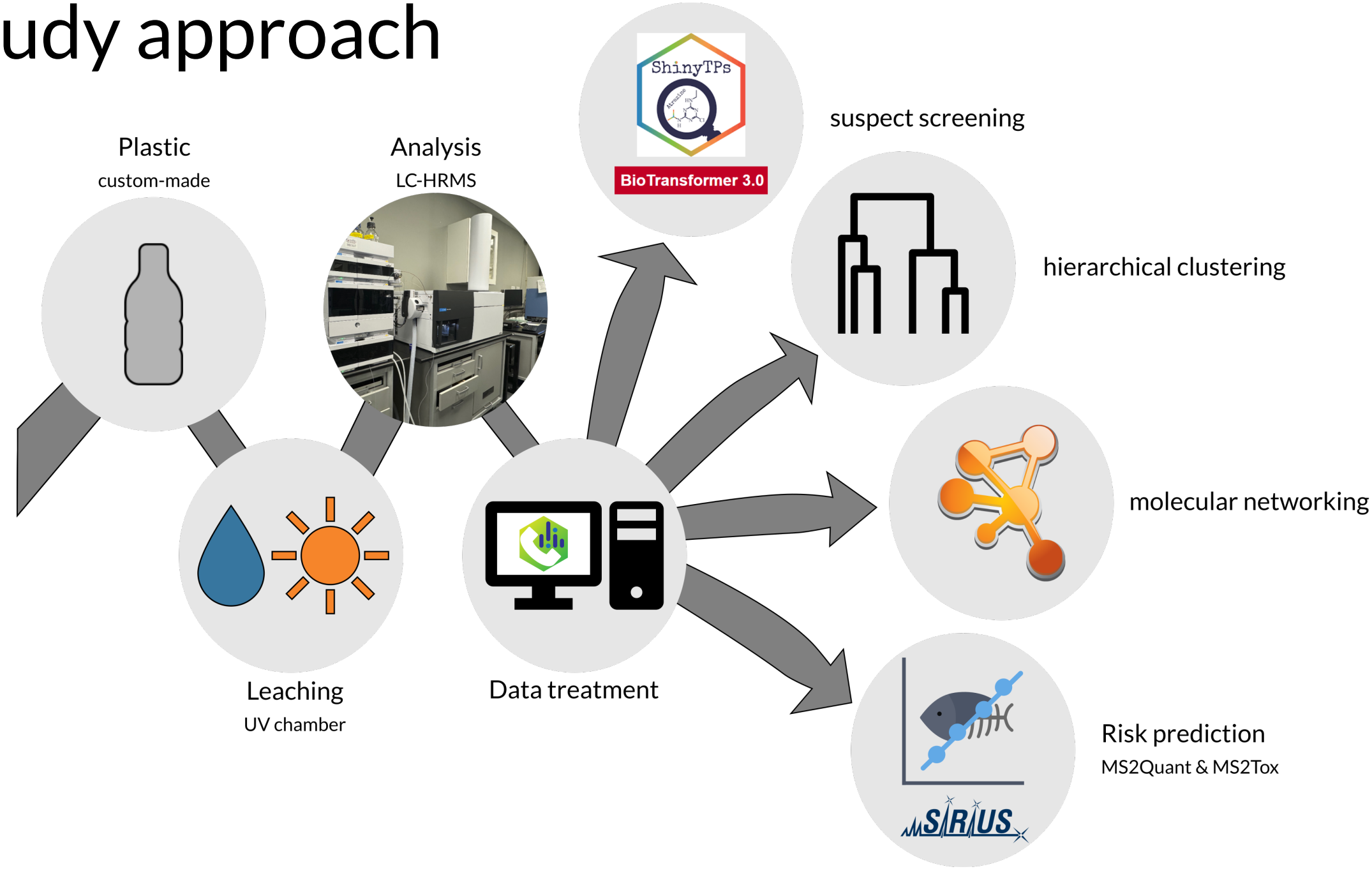


Plastic leachates can be toxic.

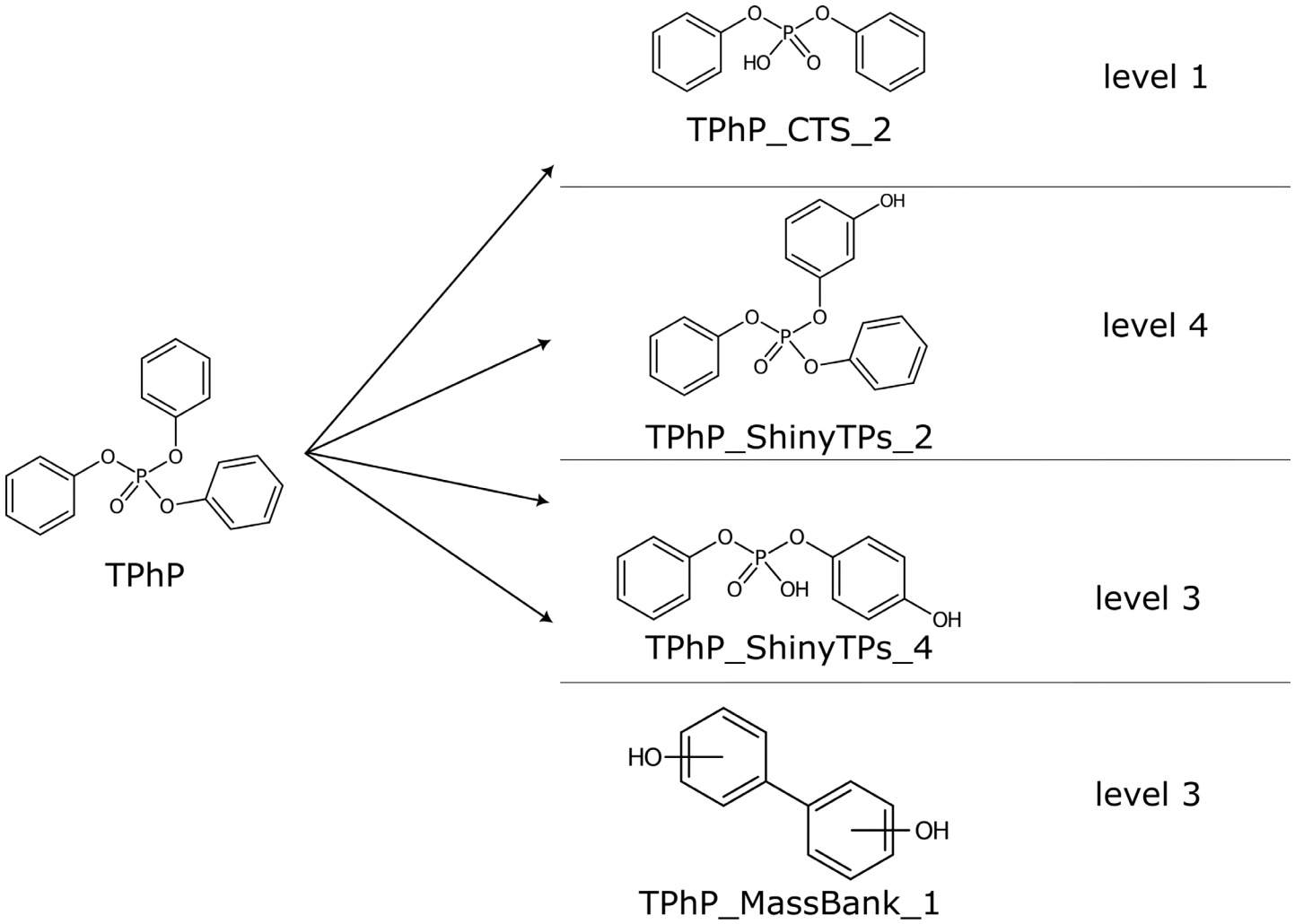
Aims

- Investigate chemical changes caused by UV-radiation
- Risk-based prioritization using Toxic Units (TUs)
- Identify potential chemical risk drivers

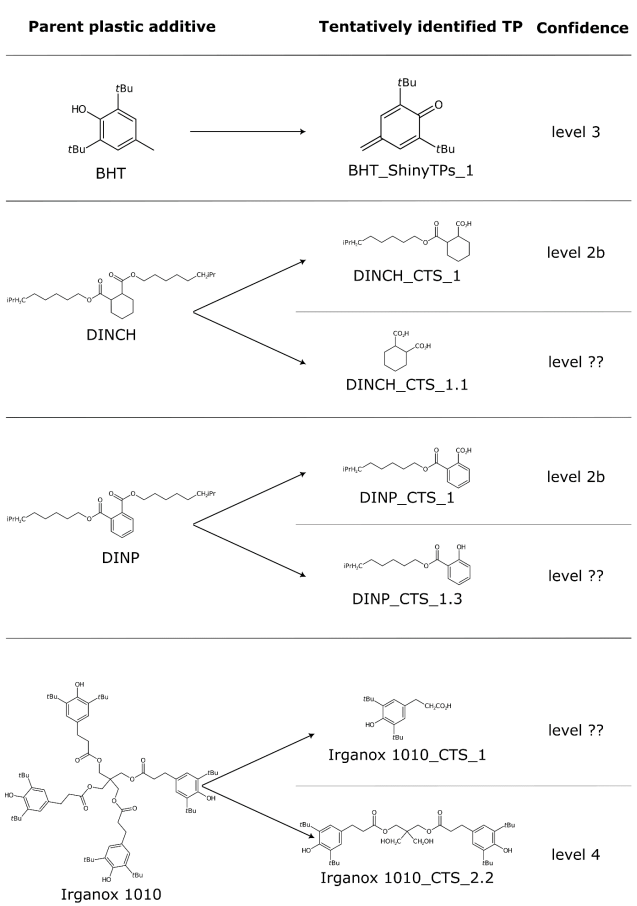
Study approach

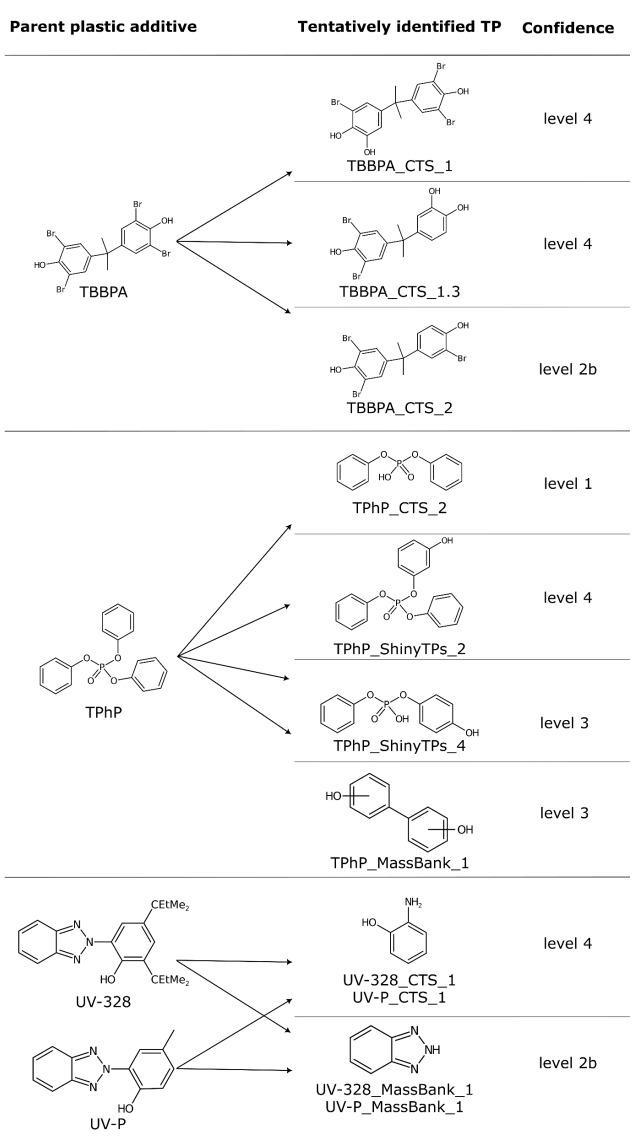


Influence of UV-radiation I



Influence of UV-radiation I

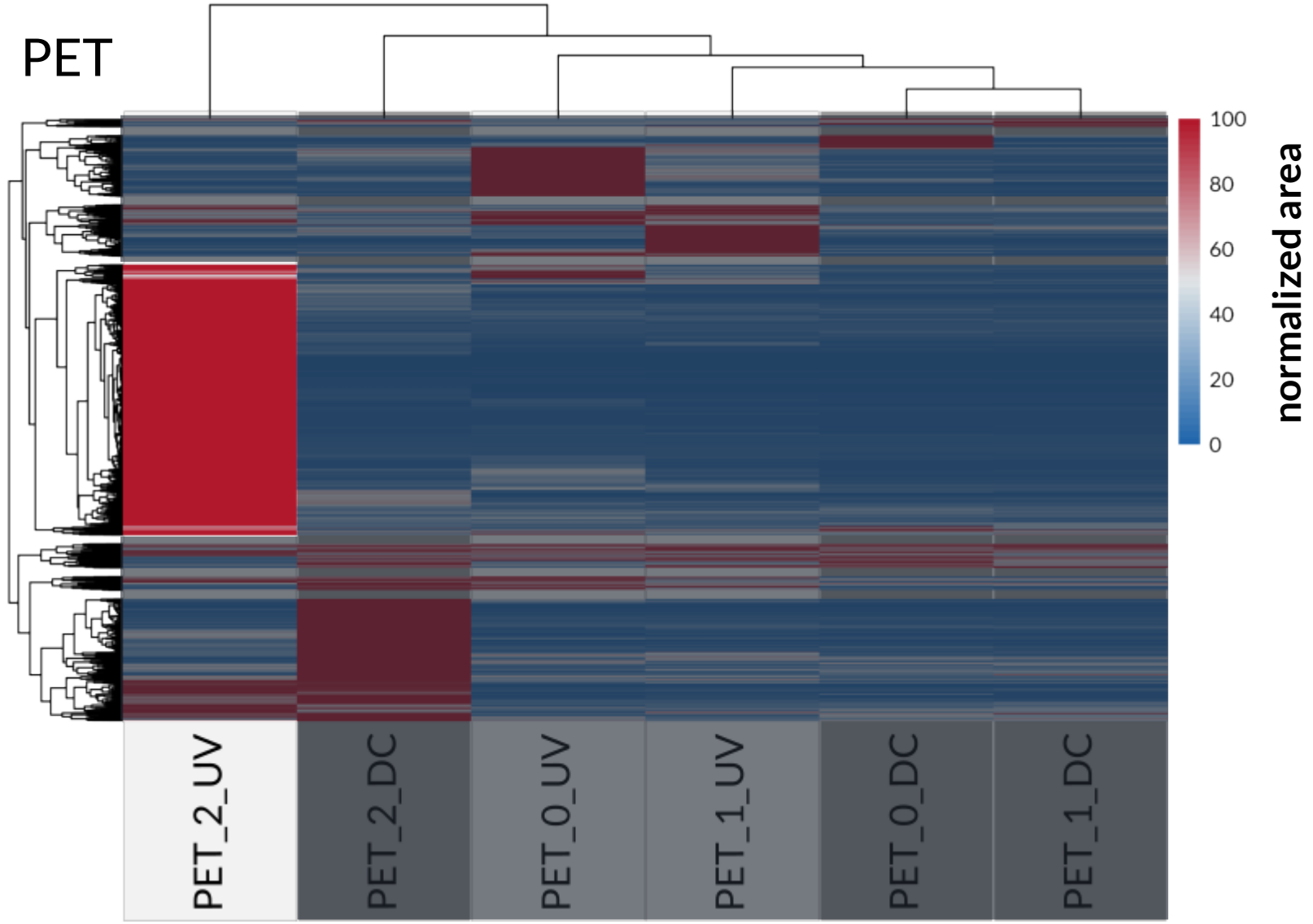




16 TPs identified from 8 targets

TPs = transformation products

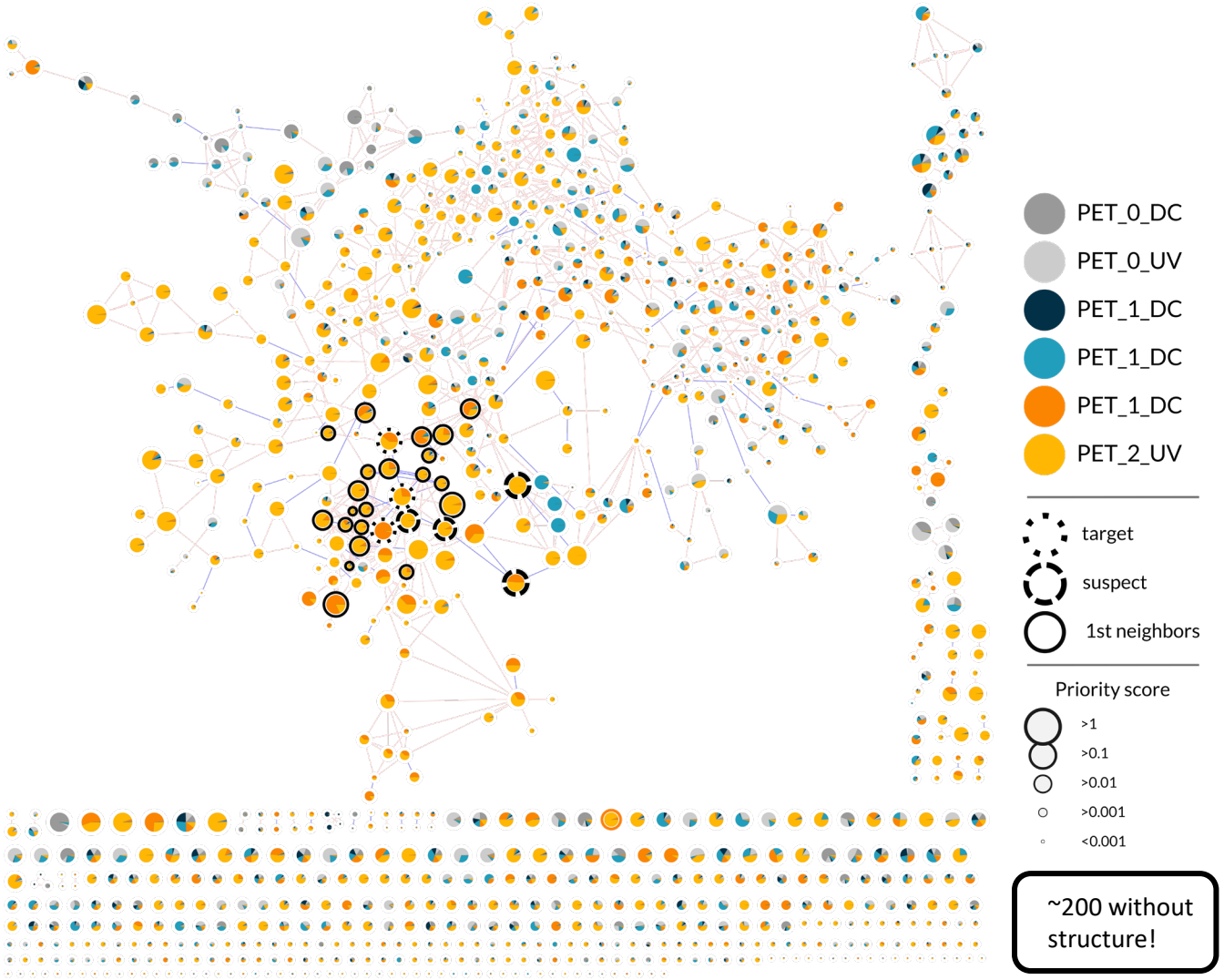
Influence of UV-radiation II



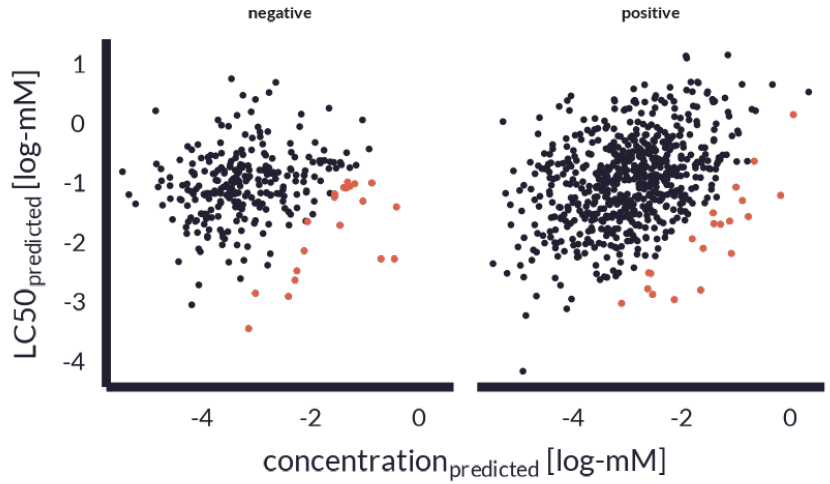
UV drastically shifted the chemical composition.

Risk-based prioritization

network parameters:
cosine score >0.6
matched peak(s) = 1



~200 without structure!

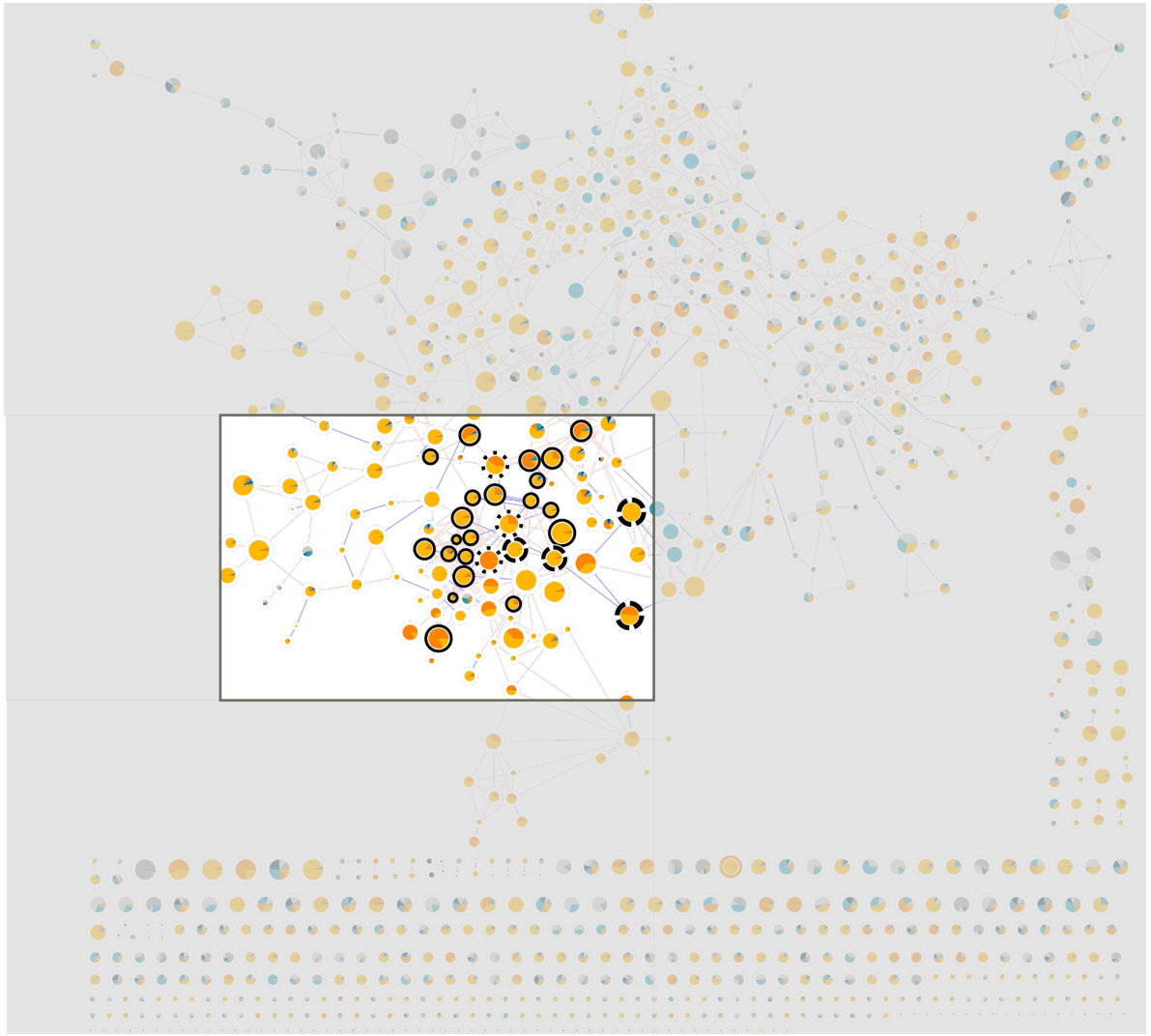


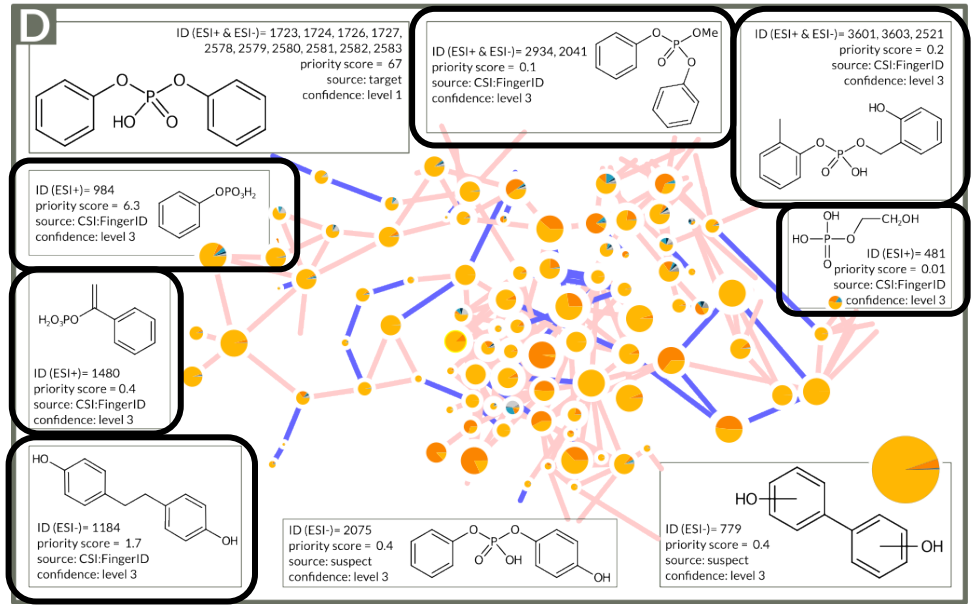
Conc. & tox. are both important

Potential risk drivers specific to leachates

Risk-based prioritization

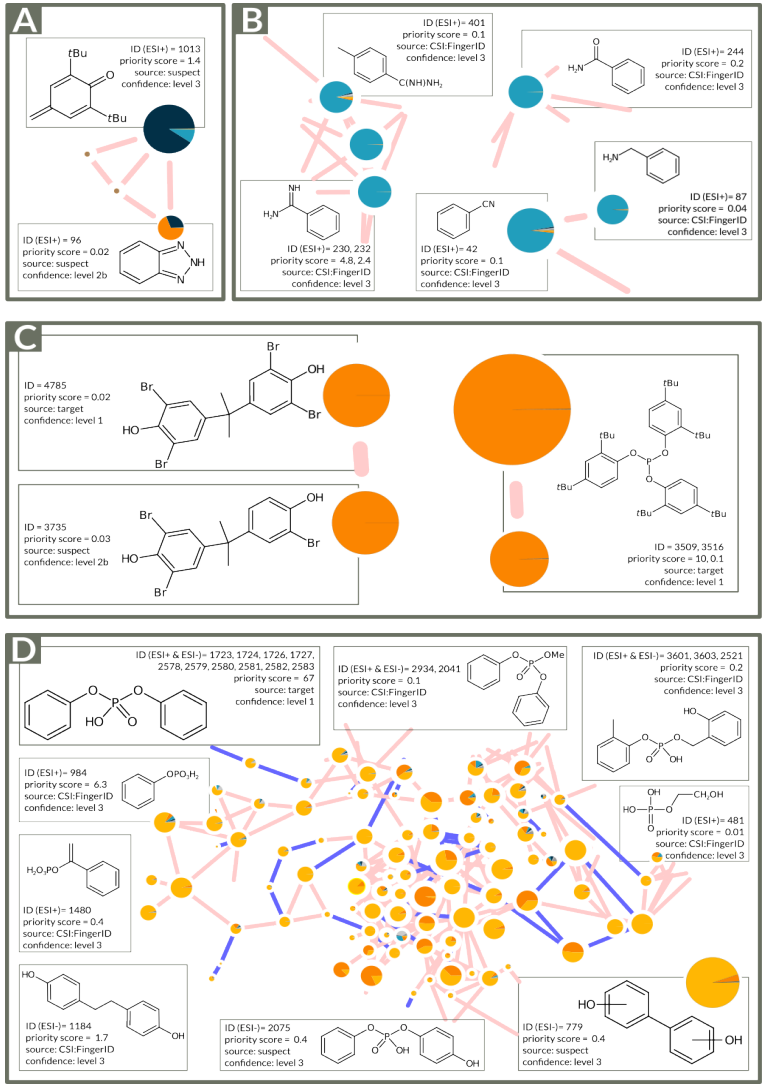
network parameters:
cosine score >0.6
matched peak(s) = 1

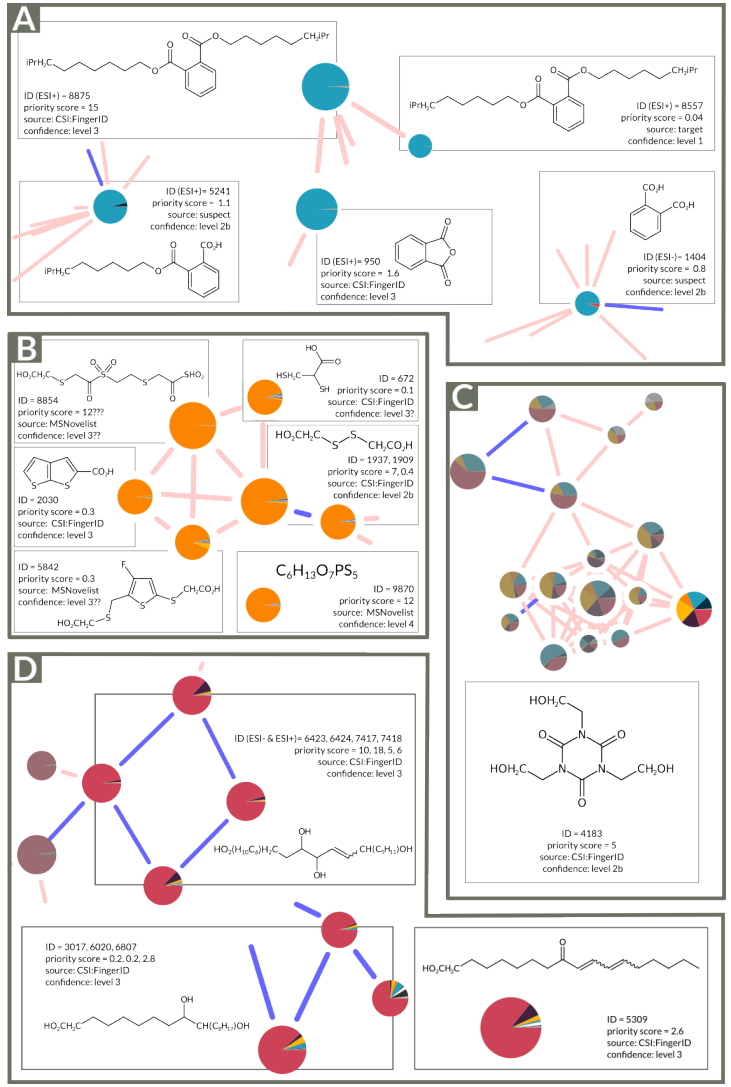




Potential risk drivers specific to leachates

Risk-based prioritization





Transformation reactions are complex

Conclusions

- Complementary analytical techniques
  - Target analysis: high confidence & model performance evaluation
  - Suspect screening: high(er) confidence, 'works' without MS^2
  - Risk-based prioritization: find emerging contaminants (risk!)
- No structure/MS^2 = big problem
- (Publication in the making)

Acknowledgements

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