Interpretation of results from Nordic Non-target screening

The CityLeaks semiarium
Malmö, 8-9 September 2018

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KEMI
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- Non-target screening
- Study design
- Data management
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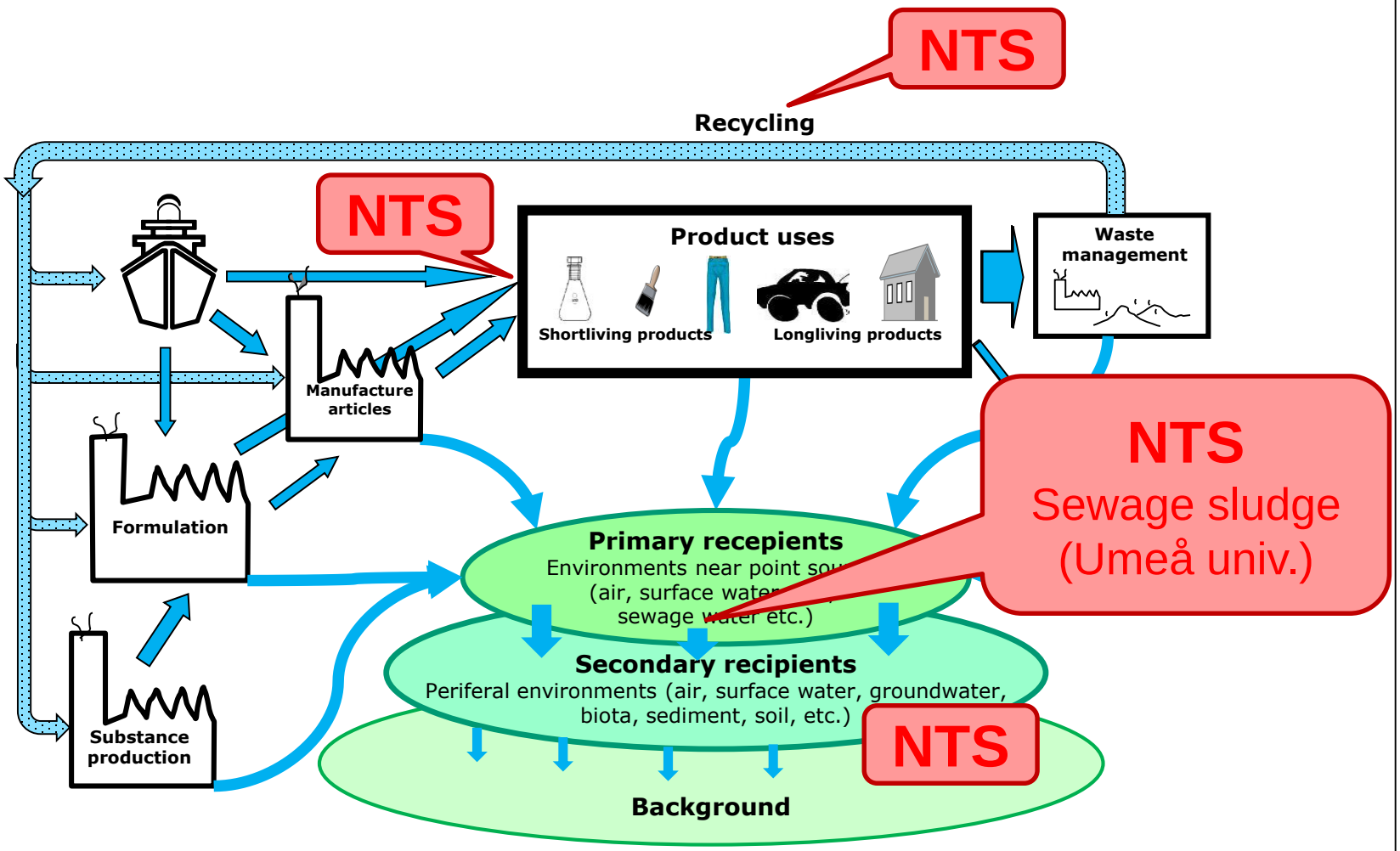
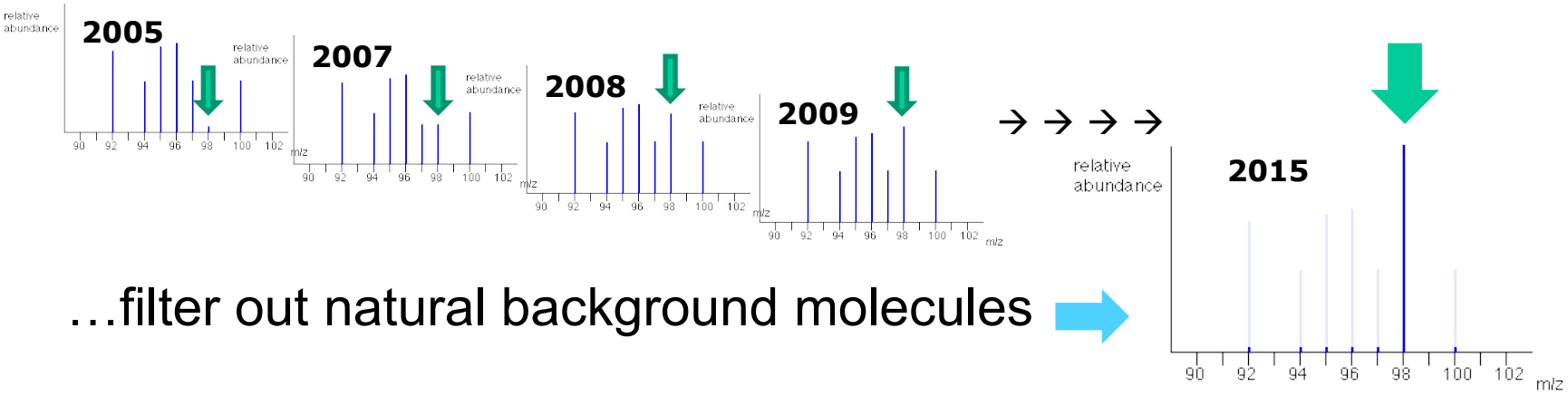
- Conclusions

Non-target screening of the chemical flow



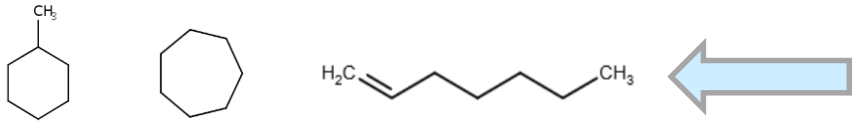
Non-target screening of sewage sludge

- Waste water treatment sludge collected in Stockholm
- Time trend study (2005 →→→ 2015)
- Liquid Chromatography → High Resolution Mass spectrometry ((HR LC-MS)
- Identify molecular peaks with significant time trends…

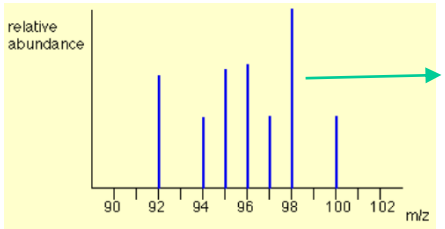


…filter out natural background molecules

Challenge in LCMS-identification of molecular peaks



One mass peek often matches to several molecules



98.10955 → 44 substances

Exposure Score	Chemical namne	Hazard Score
22	Methylcyclohexane	7
8	Cycloheptane	4
7	Heptene	6
4	1-Heptene	4
4	Dimethylcyclopentane	4
4	trans-1,2-dimethylcyclopentane	3
4	1,1-Diethylcyclopropane	3
4	Ethylcyclopentane	3
4	cis-1,3-dimethylcyclopentane	2
2	2-Heptene	4
2	2,3,3-Trimethylbut-1-ene	4
2	2-Methylpent-1-ene	4
2	3-Ethylpent-2-ene	4
2	cis-1,2-dimethylcyclopentane	4
2	trans-1,3-dimethylcyclopentane	4
2	3-Ethyl-1-pentene	4
2	(Z)-hept-2-ene	4
2	trans-hept-2-ene	4
2	(E)-hept-3-ene	4
2	Alkenes, C6-8, C7-rich	4
2	Hept-3-ene	3
2	2,4-Dimethylpent-2-ene	3
2	(E)-4,4-dimethylpent-2-ene	3
2	2-methylhept-1-ene	3
2	4-methylhept-1-ene	3
2	(Z)-4,4-dimethylpent-2-ene	3
2	2,4-Dimethylpent-1-ene	3
2	2,3-dimethylpentane	3
2	1,3-dimethylpentane	3
2	4-methylhex-2-ene	3
2	3-methylhex-1-ene	3
2	2,3-dimethylpent-1-ene	3
2	3,3-Dimethylpent-1-ene	3
2	5-Methylhex-1-ene	3
2	4-methylhex-1-ene	3
2	1-Hexene, 2-methyl-	3
2	2-Ethyl-3-methylbut-1-ene	3
2	3,4-dimethylpent-2-ene	3
2	Isoheptene	3
2	1,1-Dimethylcyclopentane	2
2	1,1,2,2-Tetramethylcyclopropane	2
2	Hydrocarbons, aliph.-arom.-C4-5-c	0
0	2-Hexene, 5-methyl-	3
0	cis-3-Heptene	3

Athority stategy: Focus on candidates of regulatory concern by **use pattern** (release) & **hazard** data

Chemical producers and importers → Regulatory registration databases → KEMI Market list*

* The ”KemI Market list” with Exposure & Hhazard scores can be downloaded at the NORMAN Suspect Lists wed site: https://www.norman-network.com/?q=node/236

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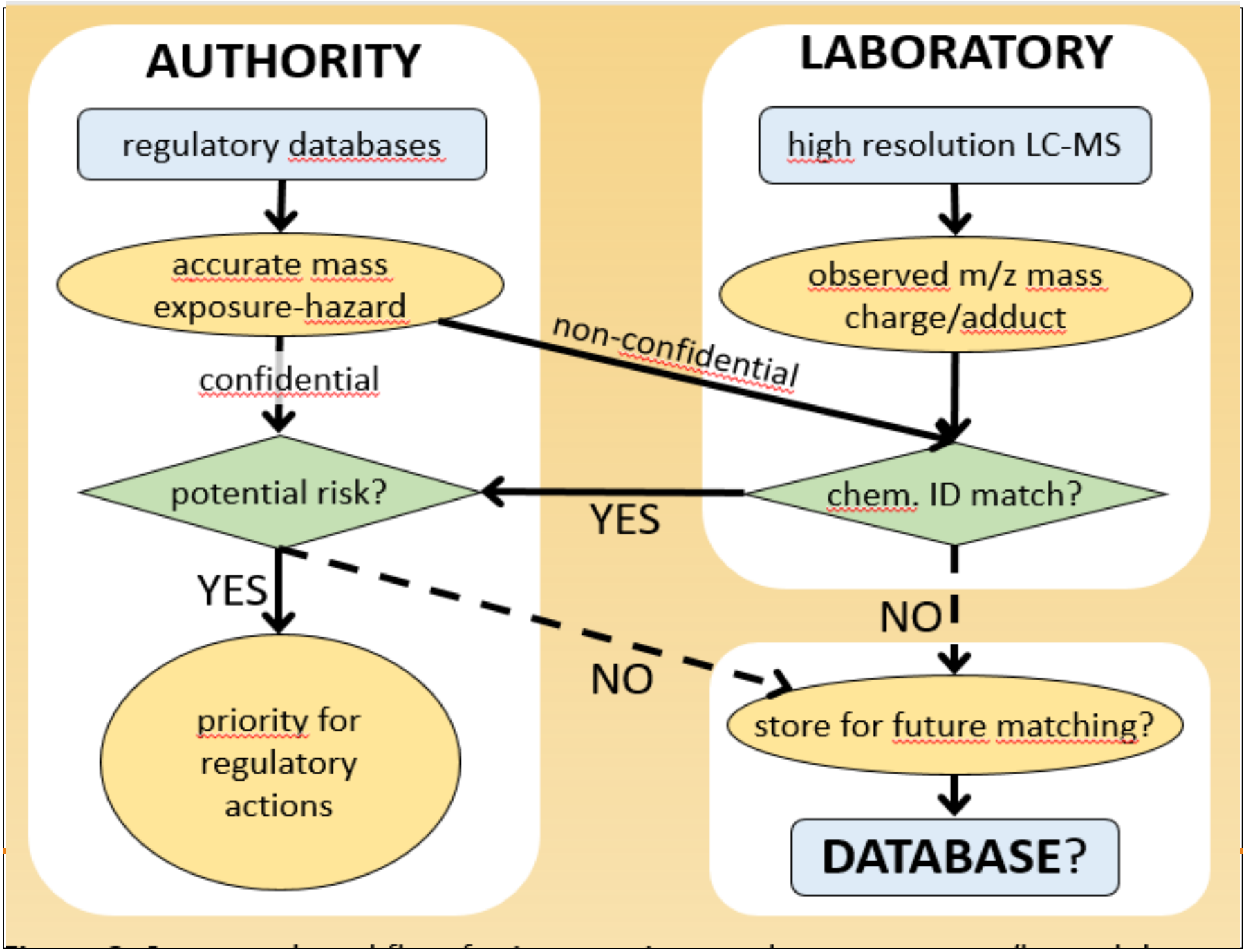
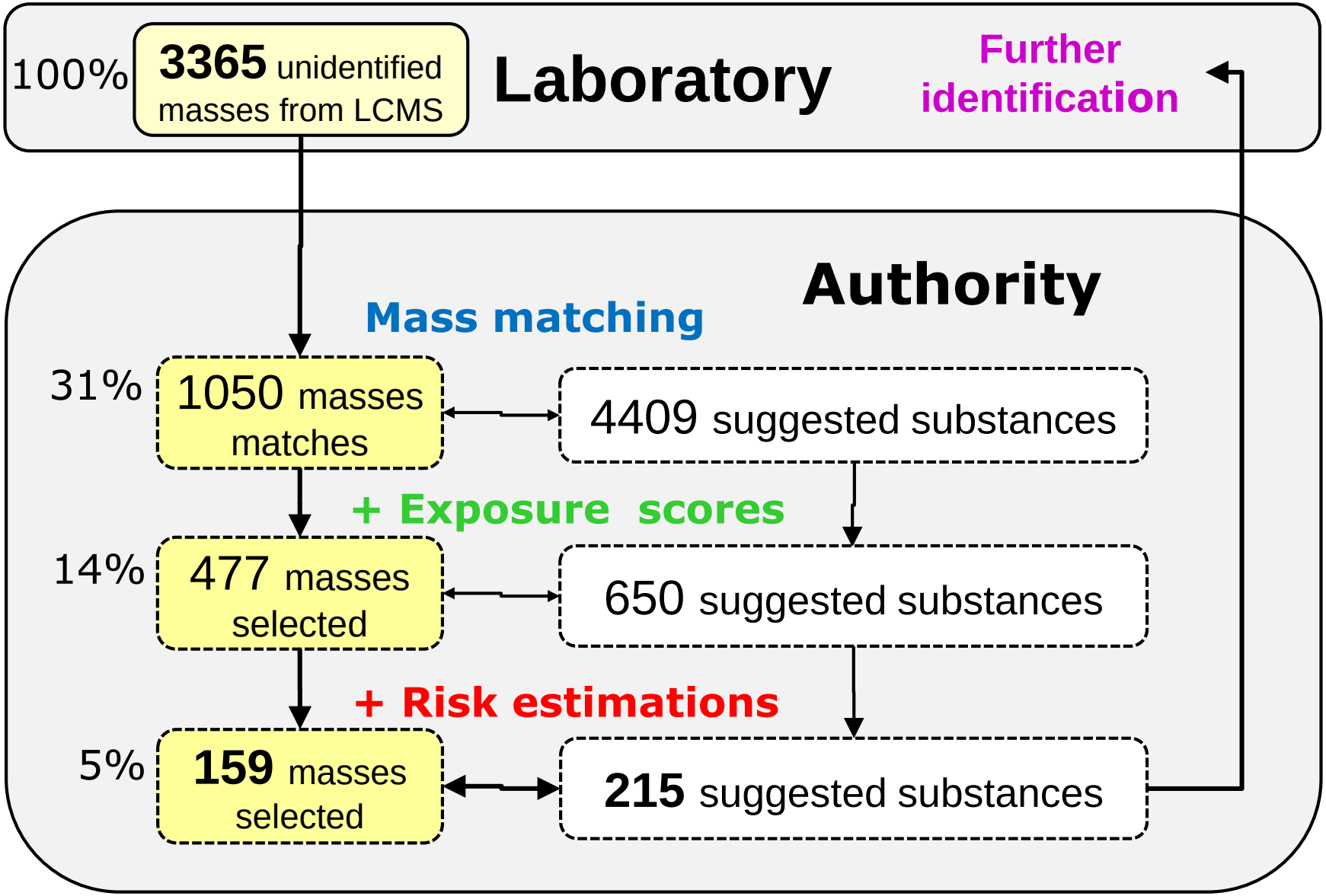

AUTHORITY
LABORATORY
regulatory databases
high resolution LC-MS
accurate mass
exposure-hazard
observed m/z mass
charge/adduct
non-confidential
confidential
potential risk?
chem. ID match?
YES
YES
NO
NO
priority for
regulatory
actions
store for future matching?
DATABASE?

The sludge-time trend study



Possible risk candidates found* - 1

Nine from the REACH candidate list (ANNEX 17)

- 1 vPvB
- 3 Toxic for reproduction
- 2 Toxic for reproduction + Endocrine disrupting properties (human health)
- 2 Endocrine disrupting properties (environment)
- 1 Carcenogenic

Possible uses

- Odour agent in cosmetic
- Softener (paint, paint remover, adhesive, putties, plasters)
- Viscosity adjustor
- Process regulator
- Explosives
- Washing and Cleaning Products
- Solvent, flocculants, precipitants, neutralization agents

* among the selection of 215 substances

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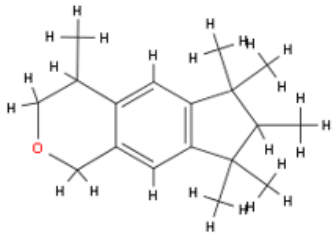
Possible risk candidates found - 2

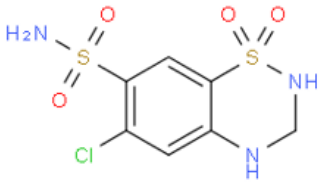
Four with restrictions (in Sweden)

Possible uses

- Adhesives, Sealants, coatings, paints
- Thinners, paint removers
- Fillers, putties, plasters.
- Softeners
- Pesticide
- Drug



Possible risk candidates found - 3



Twenty with high hazard classification (CLP)

Eleven CMR - harmonised (Cancer,Mutagen or Reprotox cat. 1)

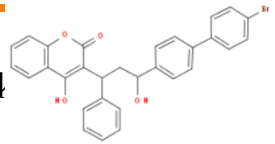
Possible uses: softeners, solvent, fluoro surfactant, pesticide, rodenticide, fungicide, cosmetic, textile.

Ten CMR – self classified (category 1)

Possible uses: fluoro surfactant, drug, process regulators (cosmetics, personal care products, plant protection products; pharmaceuticals), processing aid (adhesives, sealants ;coatings, paints), drug, stabilizer in textile.

Nine Aquatic chronic - harmonised (category 1)

Possible uses: odour agent (e.g. fabric softeners and detergents), fungicide (e.g. in wood), roenticide.



Conclusions & recommendations

- The chemical flows from the society can be documented
- More industrial chemicals can be identified
- Develop the laboratory - authority collaboration
- Establish routines for data sharing:
  - Lists of chemicals candidates
  - Digital banked mass spectra
- Future revisions of chemical regulation will be adapted to the improved monitoring capacity

Thanks to Peter Haglund and Christine Gallampois at the chemistry department at Umeå University for making their experimental data available.

Questions ?

Extra slides

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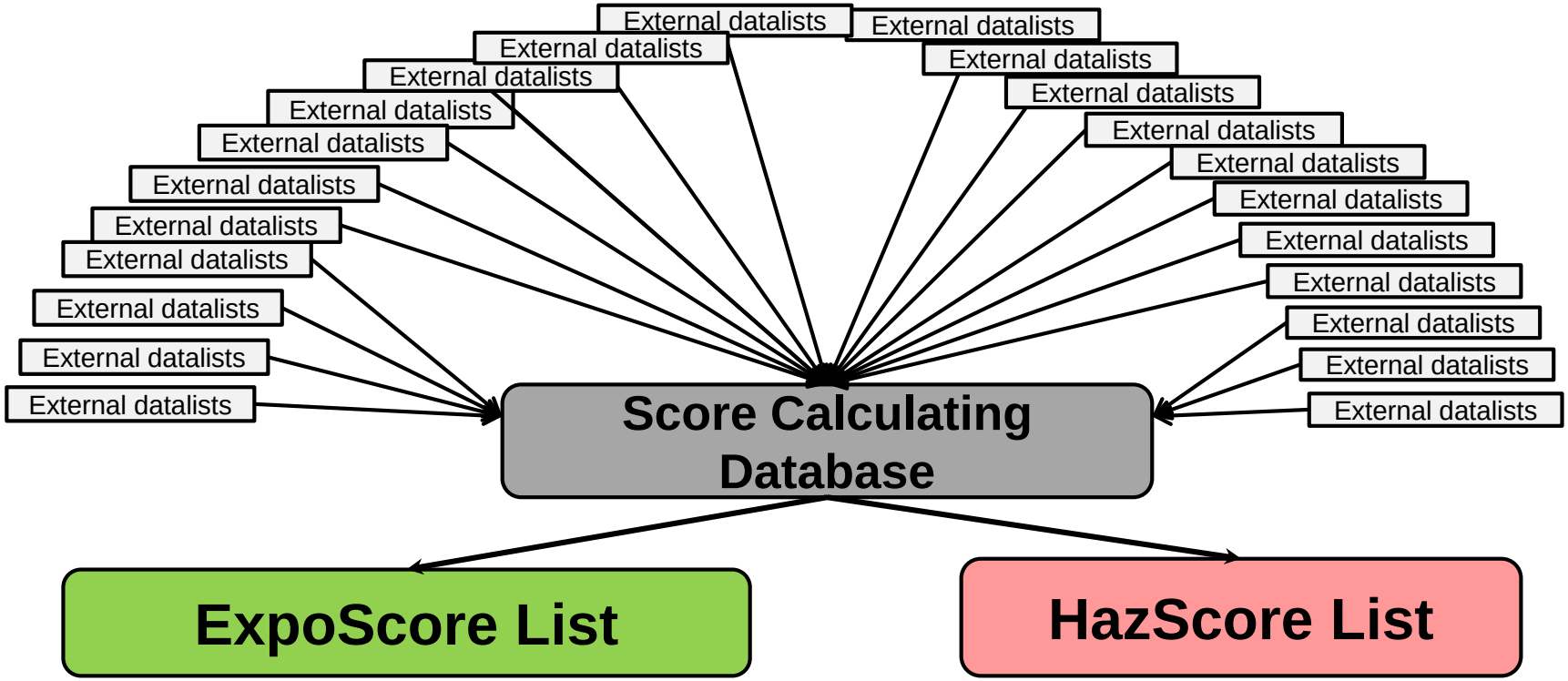
KemI output screening data

Suspected chemical	Charge	Adducts	Observed mass (m/z)	Exposure Score (4-24)	Quantity Index (1-9)	Wide Use Index (1-9)	Release Potential Index (1-9)	Hazard Score EcoAcute (0-1)	Hazard Score EcoChronic (0-1)	Hazard Score HumAcute (0-1)	Hazard Score HumChronic (0-1)
1,2-Benzenedicarboxylic acid, 1,2-dieth	pos	-H	223.0965	18	5.1	6.4	6.4	0.9	0.9	0.5	0.9
Propanoic acid, 2-methyl-, 4-formyl-2-m	pos	-H	223.0965	13	1	3.3	9	0.1	0.1	0.2	0.1
2-Propenoic acid, 2-hydroxy-3-phenoxy	pos	-H	223.0965	11	6.4	3.3	1.3	0.1	0.2	0.3	0.1
Oxirane, 2,2'-[1,3-phenylenebis(oxymet	pos	-H	223.0965	5	1.3	3.3	1.3	0.8	1	0.8	0.8
1,2-Benzenedicarboxylic acid, di-C4-13-(	pos	-H	223.0965	4	2	1	1	0.2	0.3	0.2	0.3
1,2-Benzenedicarboxylic acid, mono(2-r	pos	-H	223.0965	4	2	1	1	0.3	0.3	0.3	0.3
1,3-Benzenedicarboxylic acid, 1,3-dieth	pos	-H	223.0965	4	2	1	1				
1,4-Benzenedicarboxylic acid, 1,4-dieth	pos	-H	223.0965	4	1	1.8	1.8	0.1	0.1	0.2	0.1
Benzoic acid, 2-hydroxy-3-methoxy-5-(2	pos	-H	223.0965	4	2	1	1				

Figur?: Underhåll av *Prioriteringstabellen*



Main data sources

- Broad market databases
  - The Swedish Product register
  - SPIN database
  - Registration data – REACH
  - CPcat database (US market)
  - CLP database (Hazard classification)

- Sector specific databases
  - Textile inventories
  - Polymer inventories
  - Cosmetic inventories (world, EU)
  - Pharmaceutical inventories (SE, EU, US)
  - Printing agent inventory (EU)
  - PFAS inventory (world)
  - Pesticide inventory (SE)

Exposure Score

A probability of a substance to be released to the environment durings life-time in the society

A combination of three use pattern elements:

Exposure score = **Quantity index** + **Wide use index** + **Release index**

Score Range: 0 – 27 (max.)

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Hazard Score

- Source: EU Hazard Classification (CLP)
- Harmonised classification / Self classification / No classification
- Structure similarity
- Score range: Null*, 0 – 9 (max.)

** If the substance have no classification and is not structure similar to a classified substance*

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