

Incorporating **market data and use pattern** in Non-Target screening

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Outline of presentation

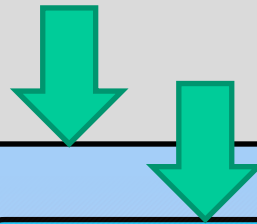
- Usefulness of chemical market data
- Data sources
- High-throughput screening
- Transformation products

What to do with market data

- Help in the identification of "unknowns" by focus on candidates with critical use patterns:
- Triggering factors:
 - High production quantity
 - Increasing production volumes
 - Opened use system
 - Use near sensitive environment

Will market data help the identifications?

Current substance libraries
for the interpretation of mass spectra
(e.g. cited substances in the opened literature)



Substances
on the market

Substances with critical uses

CONFIDENTIAL

Confidentiality can, however, be circumvented by aggregating and/or categorisation into general exposure index.

Data sources – (substances ”on the market”)

- Regulatory Inventory lists - Lists of traded chemicals
 - Official lists managed by national authorities
 - Available data: Chemical identity (CAS No, EC No., Trade name)
- Sources: US, Canada, China, Nordic countries, New Zealand, The Philipines (60 000 org.subst.;11 000 polymers; 4000 org. salts)
- Confidential parts (use pattern, volumes, impurities...)

Use data

- Chemical identity:
 - CAS No., EC No.
 - **Structure**
 - Molecular weight
 - Molecular formula
 - **Impurities**
- Volumes:
 - High volume chemicals
 - Low volume chemicals
 - **Tonnage** bands (e.g. 10-100 tonnes per annum)
 - **Time trends**
- Use pattern:
 - **Sector of use** (e.g. plastic industry, cosmetic industry)
 - **Product Category** (e.g. detergent, intermediate, antioxidants)

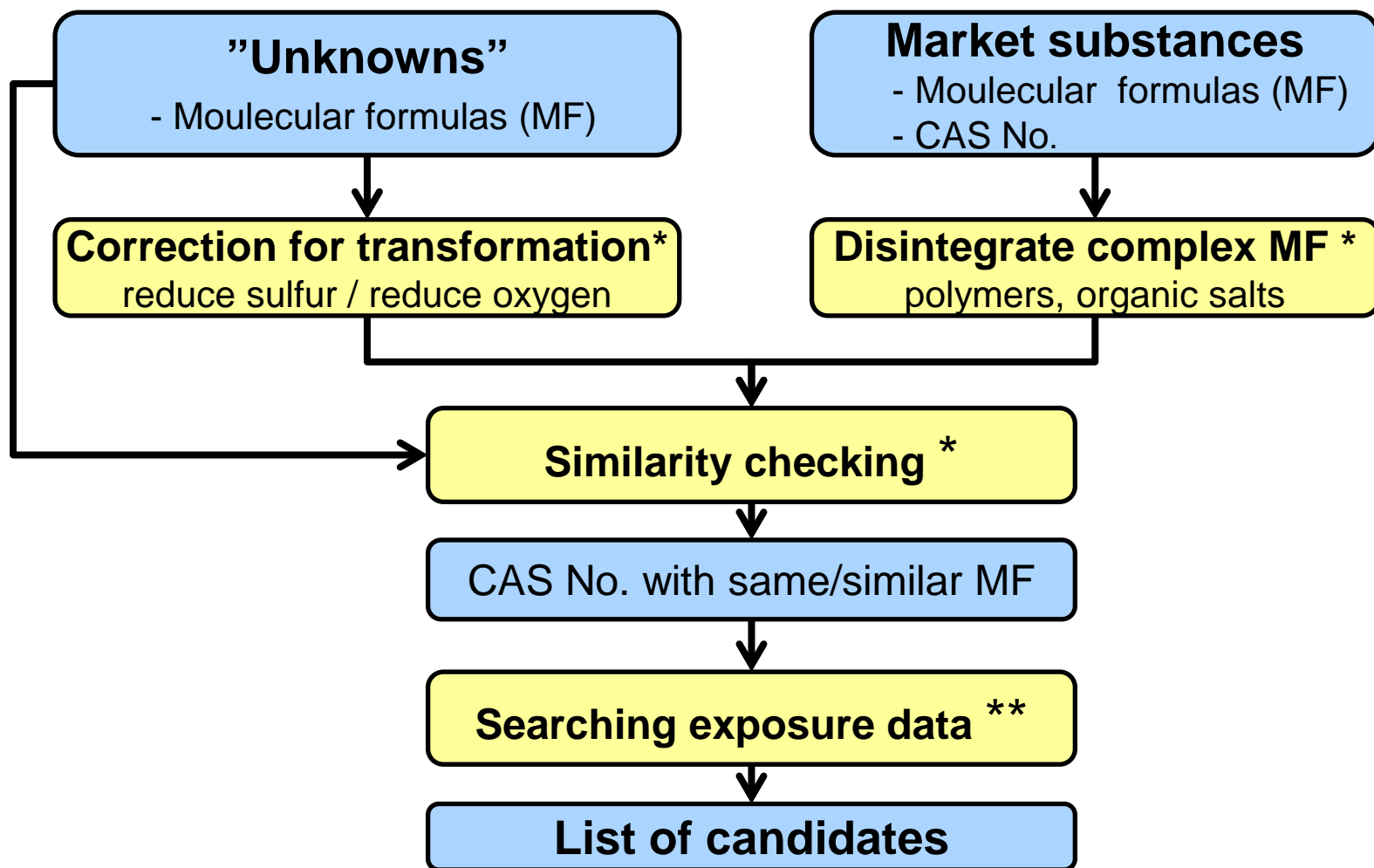
Data sources – (use data)

Industrial chemicals:

- The SPIN Exposure Toolbox (worst case exposure estimates) *
 - 26 000 substances (until 2012)
- Exposure Index from the Swedish Product register
 - 22 000 substances (until 2012)
- Total annual tonnage bands for EU (REACH) *
 - 10 000 substances (until 2013)

* Data lists available on request to Stellan Fischer
(stellan.fischer@kemi.se)

High-throughput similarity matching - testing



* VBA program in EXCEL; ** Database queries with VB ACCESS

Testing set - (High-throughput similarity matching)


List of 2986 molecular formulas identified for "unknowns" (LC-MS) from environmental samples in Norway *

- Air remote, urban 466 samples
 - STP influent, effluent, sludge 1177 samples
 - Sediment marine 238 samples
 - Biota prawn, cod liver, bird egg 1105 samples
-
- The spectra was compared to the NIST 2011 library

Questions ?

Use information in the **SPIN** database

Main use information in the Nordic Products Registers

Subst. name	Volume	Function of the preparation	Sector of use	Number of products	Consumer availability
 26 000 CAS No.					

Exposure Toolbox
Non-confidential indications
of release & exposure
based on
registered use information

- Based on registered national use of chemical product.
- Annually updated (from year 2000).
- Support analytical chemists in the identification of "unknowns"

Data output example from *SPIN* *

Help

SPIN SUBSTANCES IN PREPARATIONS IN NORDIC COUNTRIES

Search mode
List
Guide
Reports
Exit

Cas no: 100-06-1 Name: Ethanone, 1-(4-methoxyphenyl)-

Tonnes/year

Consumer use

Sector of Use

Use Category

Nr. 1 of 1

Names/Exposure	Total use	Industr. NACE	Industr. Nation	Use Cat. UC62	Use Cat. Nation	References	Technical
Names/Exposure							
Name							
CAS							
PRD							
PRN							

Tonnage bands
release during 2014

Release
from use

Broadness
on the market

Article
use

SPIN Exposure Toolbox

Exposure information based on data from the Nordic product registers

Country	Latest year	Use Index (UI)						Range of Use (RoU)	Article Index (AI)
		Surface water	Air	Soil	Waste water	Consumer	Occu-pational		
DK	2011	x	xxx	xx	xxx	xxx	xxx	***	++
NO	2011	xx	x	xx	xxx	xxx	xx	*	+
SE	2011	-	x	-	xx	x	xx	*	+

* Web address: www.SPIN2000.NET

Possible output from the SPIN Exposure Toolbox *

The screenshot shows a Microsoft Excel spreadsheet with the following data:

	A	B	C	D	E	F	G	H	I	J	K	L	M
1	Annum	Country	CASno	CASnr	AI	RoU	QI	UI_Wat	UI_Air	UI_Soil	UI_Stp	UI_Cons	UI_Work
2	2012	SE	100-00-5	100005	1	1	1	1	2	1	4	3	3
3	2012	SE	1000172-11-1	1000172111	1	1	3	4	4	4	3	4	5
4	2012	SE	10004-44-1	10004441	1	1	2	0	0	2	0	1	1
5	2012	SE	1000-56-2	1000562	2	1	2	1	2	1	2	1	4
6	2012	SE	100-06-1	100061	1	1	1	2	3	1	4	3	4
7	2012	SE	10006-28-7	10006287	2	2	3	2	2	3	3	4	4
8	2012	SE	100084-96-6	100084966	1	1	1	2	3	1	4	3	4
9	2012	SE	100085-28-7	100085287	1	1	2	1	2	1	3	2	4
10	2012	SE	100085-39-0	100085390	1	1	2	1	1	1	4	2	2
11	2012	SE	100085-40-3	100085403	3	1	3	1	2	3	3	4	4
12	2012	SE	100-15-2	100152	1	1	1	1	2	1	3	2	4
13	2012	SE	10016-20-3	10016203	3	1	3	3	3	2	3	1	4
14	2012	SE	10017-56-8	10017568	3	2	2	2	2	3	3	4	4
15	2012	SE	100188-06-5	100188065	2	1	1	3	2	1	2	2	3
16	2012	SE	100188-12-3	100188123	1	1	1	1	2	1	4	3	3
17	2012	SE	100199-62-0	100199620	3	1	2	2	2	1	2	1	4
18	2012	SE	10020-43-6	10020436	1	1	1	1	2	1	3	2	4
19	2012	SE	100208-62-6	100208626	1	1	1	1	1	1	2	4	3

* Only on direct request to Stellan Fischer (stellan.fischer@kemi.se)

EU tonnage bands* (REACH) → Excel sheet

EC / List No.	CAS No.	Name	Total Tonnage Band	Registration Type	Submission Type
200-001-8	50-00-0	formaldehyde	1,000,000 + tonnes per annum	Full	Joint Submission
200-001-8	50-00-0	formaldehyde	Intermediate Use Only	Intermediate	Individual Submission
200-002-3	50-01-1	guanidinium chloride	100 - 1,000 tonnes per annum	Full	Joint Submission
200-004-4	50-03-3	hydrocortisone 21-acetate	Intermediate Use Only	Intermediate	Joint Submission
200-018-0	50-21-5	lactic acid	100 - 1,000 tonnes per annum	Full	Joint Submission
200-020-1	50-23-7	hydrocortisone	Intermediate Use Only	Intermediate	Joint Submission
200-021-7	50-24-8	prednisolone	1 - 10 tonnes per annum	Full	Joint Submission
200-023-8	50-28-2	estradiol	Intermediate Use Only	Intermediate	Joint Submission



EC_No	CAS_No	CAS_Nr	RegTpa_Score(0-10)	Intermediate	Full	RegTpa_Uncertainty(1-7)	#registrants
203-234-3	104-76-7	104767	5,5		x	1	1
203-236-4	104-78-9	104789	3,5		x	1	1
203-242-7	104-83-6	104836	2,5	x		3	1
203-247-4	104-88-1	104881	2,8	x		3,3	2
203-250-0			3,5			5	1
203-252-1	104-92-7	104927	2,5	x		3	1
203-253-7	104-93-8	104938	4,5		x	1	1
203-265-2	105-05-5	105055	2,5		x	1	1
203-268-9	105-08-8	105088	4,5		x	1	1
203-273-6	105-13-5	105135	0,5		x	1	1
203-288-8	105-34-0	105340	2,8	x		3,3	2
203-294-0	105-39-5	105395	3,5		x	1	1
203-299-8	105-45-3	105453	3,2	x	x	4	2
203-305-9	105-53-3	105533	2,5	x		3	1
203-309-0			2,5	x	x	3	1
203-309-0	105-56-6	105566	3,5	x	x	1	1
203-311-1	105-58-8	105588	2,5		x	1	1
203-312-7	105-59-9	105599	5		x	4	1
203-313-2	105-60-2	105602	6,5		x	1	1

* Non-confidential data available for 10 047 registered substances (2013)

The Swedish Exposure Index

ExposureIndex Table on Product Register data for year 2011

Date for database output: 28.02.13; Contact address: stellan.fischer@kemi.se

Chemical identity (CAS Index nomenclature)			Use data (Grp.No.) "99" see explanation					Exposure Index (group No. 1-7)							First year in PR	Last year in PR	Summaformel	PPcheck(0-100)		
CAS No.	EC No.	Name	Range of Use (0-7)	#Prod grp (0-7)	Consumer availability (0-7)	Article prod (1-7)	Quantity (0-7)	Quantity red. >25%	Surface water	Air	Soil	STP	Human	Human (-2 - +2)					Environment (-2 - +2)	Use Change Index (-1-4)
68988-10-3	273-514-8	Zirconium, dipropylene glycol iso-Bu alc. neod	3	3	7	3	4		4	4	4	7	7				1996	2011		98
7699-43-6	231-717-9	Zirconium, dichlorooxo-	1	1	1	7	1		1	1	1	1	1	-1	-1		1996	2011	Cl2O2r	100
1291-32-3	215-066-8	Zirconium, dichlorobis(.eta.5-2,4-cyclopentadie			1	7											1995	1995	C10H10Cl2Zr	1
100163-29-9		Zirconium, dichloro[rel-(7aR,7'aR)-1,2-ethanediy	1	1	1	6	1		1	1	1	1	1	-2	-2		2008	2011	C20H24Cl2Zr	100
90604-80-1	292-375-4	Zirconium, chloro glycine hydroxy aluminum c	1	1	1	1	5		1	1	1	5	3	1		1	1992	2011		100
90604-79-8	292-374-9	Zirconium, C8-10-branched fatty acids C9-11-ne	1	1	1	7	1		1	1	1	1	1				1992	2011		100
84067-14-1	281-951-0	Zirconium, C5-23-branched carboxylate octano	1	2	6	6	4		2	1	1	1	6	1		1	1992	2011		100
83711-55-1	280-552-9	Zirconium, C5-23-branched carboxylate naphth	1	1	7	1	3		1	1	1	6	7				2010	2011		100
84067-12-9	281-948-4	Zirconium, C5-23-branched carboxylate C4-10-f	1	1	7	1	3		1	1	2	4	4	-1		1	1998	2011		100
73364-10-0		Zirconium, bis[(1,2,3,4,5-.eta.)-1-butyl-2,4-cyclop	1	1	1	6	1		1	1	1	1	1				2000	2011	C18H26Cl2Zr	100
13826-66-9	237-529-3	Zirconium, bis(nitrato-O)oxo-	1	1	1	5	3		1	1	1	1	1				2004	2011	N2O7Zr	100
5153-24-2	225-924-3	Zirconium, bis(acetato-O)oxo-	3	1	5	6	4		5	5	5	7	7	2	1	1	2002	2011	C4H6O5Zr	100
226996-19-6		Zirconium, aqua 3,5-bis(1,1-dimethylethyl)-2-hy	1	2	1	1	4		1	1	1	1	4				2011	2011		100
97375-39-8	306-696-5	Zirconium, 4,5-dihydro-5-oxo-1-(4-sulfophenyl)	1	1	7	1	2		1	1	1	3	3				1996	2011		100
117101-65-2		Zirconium, [2,2-bis[(2-propenyloxy)methyl]-1-bu			1	7											2004	2007	C60H123O15I	100
12036-01-0	234-835-9	Zirconium oxide (ZrO)			1	7											1993	2008	O2r	100
1314-23-4	215-227-2	Zirconium oxide	7	6	1	7	6		5	6	7	7	7	1	1		1992	2011	O2Zr	100
14475-63-9	238-472-7	Zirconium hydroxide			1	6											2000	2009	H4O4Zr	100

21451 subst. (accumulated from 1992); 14609 subst. in active products (2011)

Time trend data for 6005 active subst. (changed use, change exposure index)

KEMI