Emerging and future environmental contaminants: What should we be testing and monitoring?

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Outline

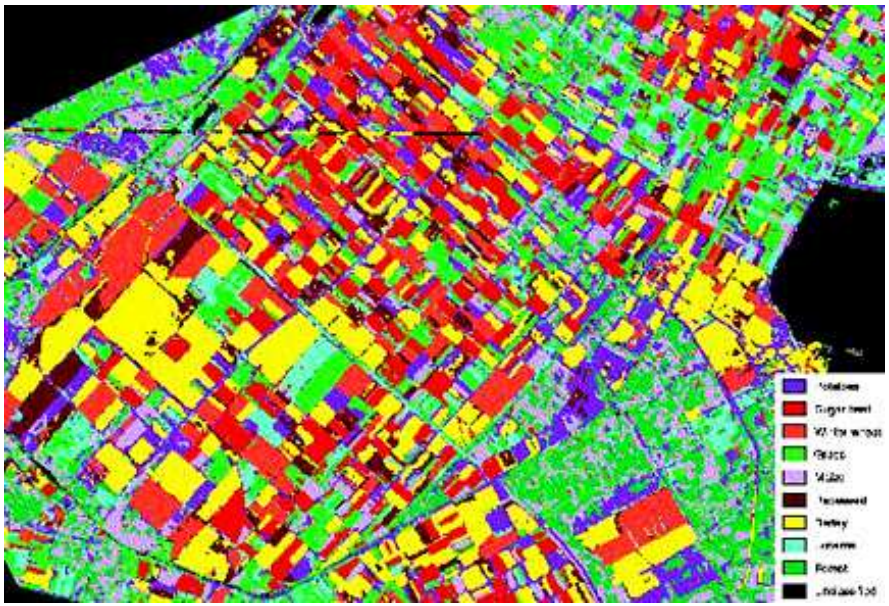
- Information needs to prioritisation
- Identifying the inputs
- Assessing exposure
- Assessing effects
- Risk-based prioritisation
- Future environmental drivers

Likely information needs

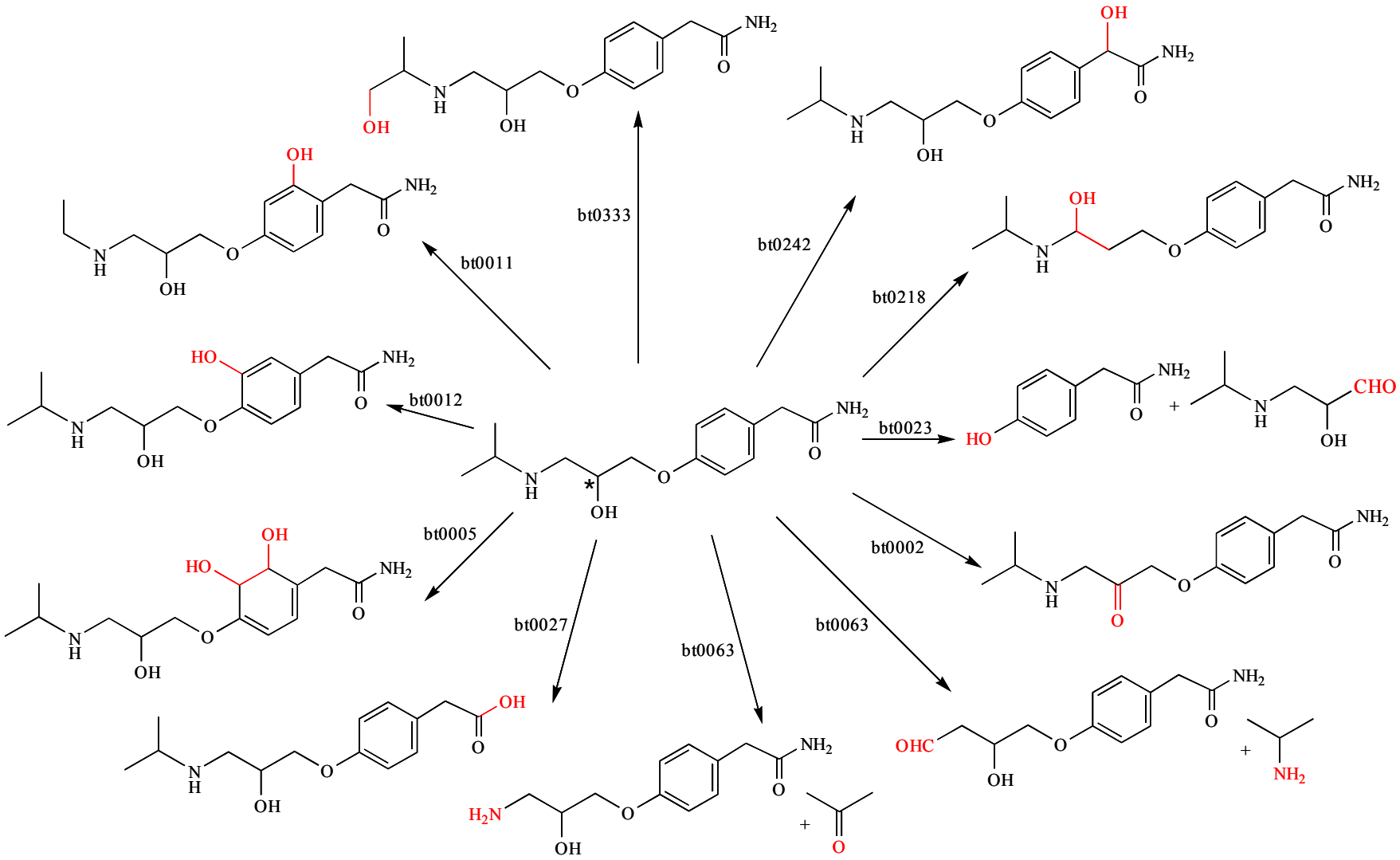
- Inputs
- Exposure
- Effects
- We can’t test everything so need to be predictive

Identifying the inputs

- Usage data
- Sales data
- Export/productivity data
- Remote sensing
- Patents
- Other sources (e.g. police seizures)



Predicting transformation pathways



Fenner, unpublished

Projected Applications of Nanotechnologies

Cosmetics
Paints & coatings
Catalysts & lubricants
Water treatment
Security printing
Textiles & sports items
Medical & healthcare
Food/ food packaging
Plant protection products
Veterinary medicines
Construction materials
Electrical & electronics
Fuel cells & batteries
Paper manufacturing
Weapons & explosives

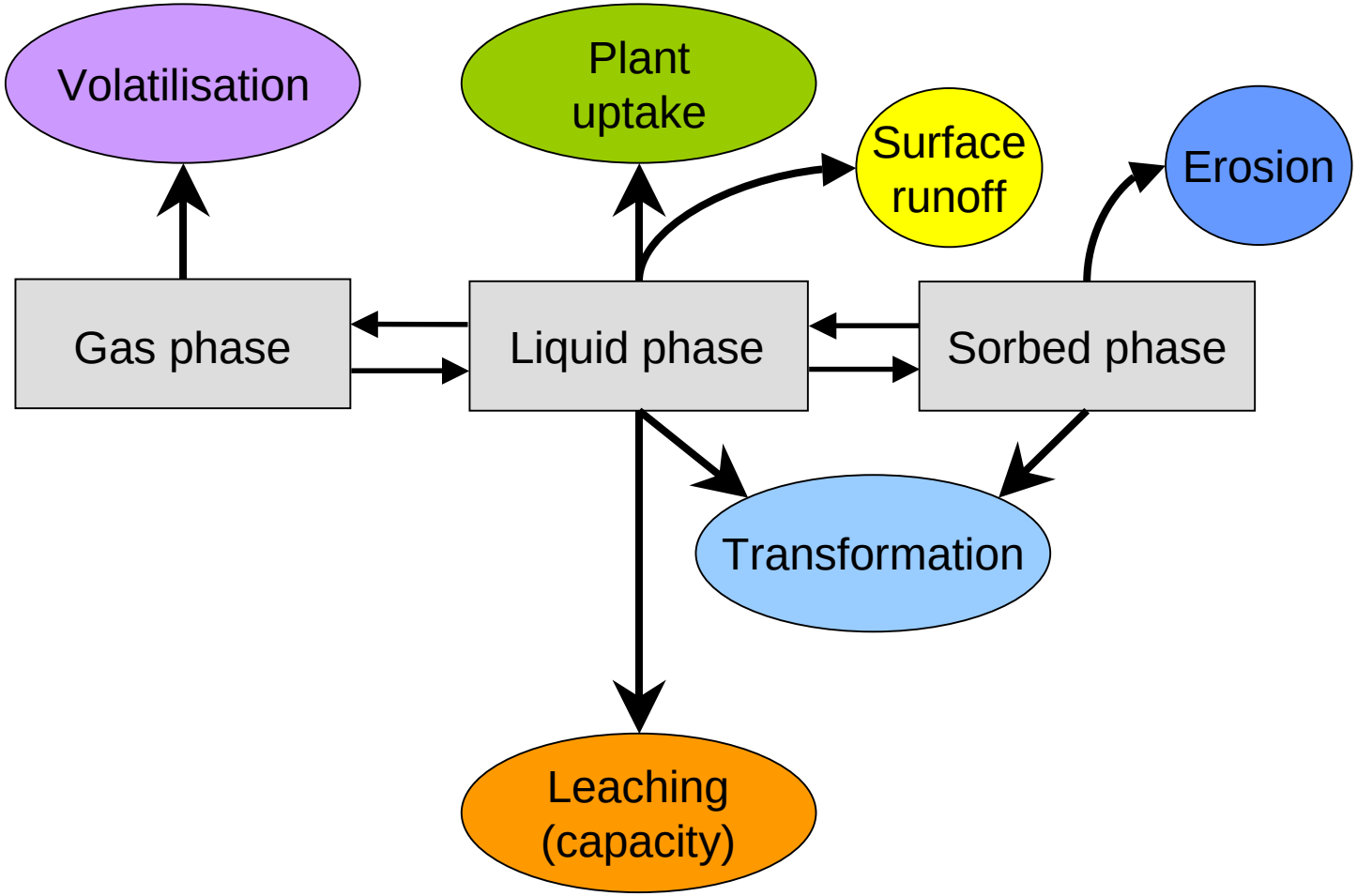
Cosmetics
Paints & coatings
Catalysts & lubricants
Water treatment
Food & food packaging
Plant protection products
Agrochemicals
Veterinary medicines

Aitken *et al* (2005) Occupational Medicine 56: 300 – 306

Concentrations of NPs

Application	Nanomaterial	Concentration (%)
Personal care products (sunscreens, toothpaste, soap, shampoo, face creams	TiO_2 Hydroxyapetite Ag Fullerene C_{60}	5 15 0.02 0.05 – 0.25
Paints and coatings	TiO_2 SiO_2 ZnO Alumina Silica/Alumina	5 15 1-10 0.5-5 7-10
Medical	Ag API	5 1-20
Food and packaging	nanoclay	5
Fuel catalysts	CeO2	5-10

Predicting exposure



Reliant on good predictive models or input data

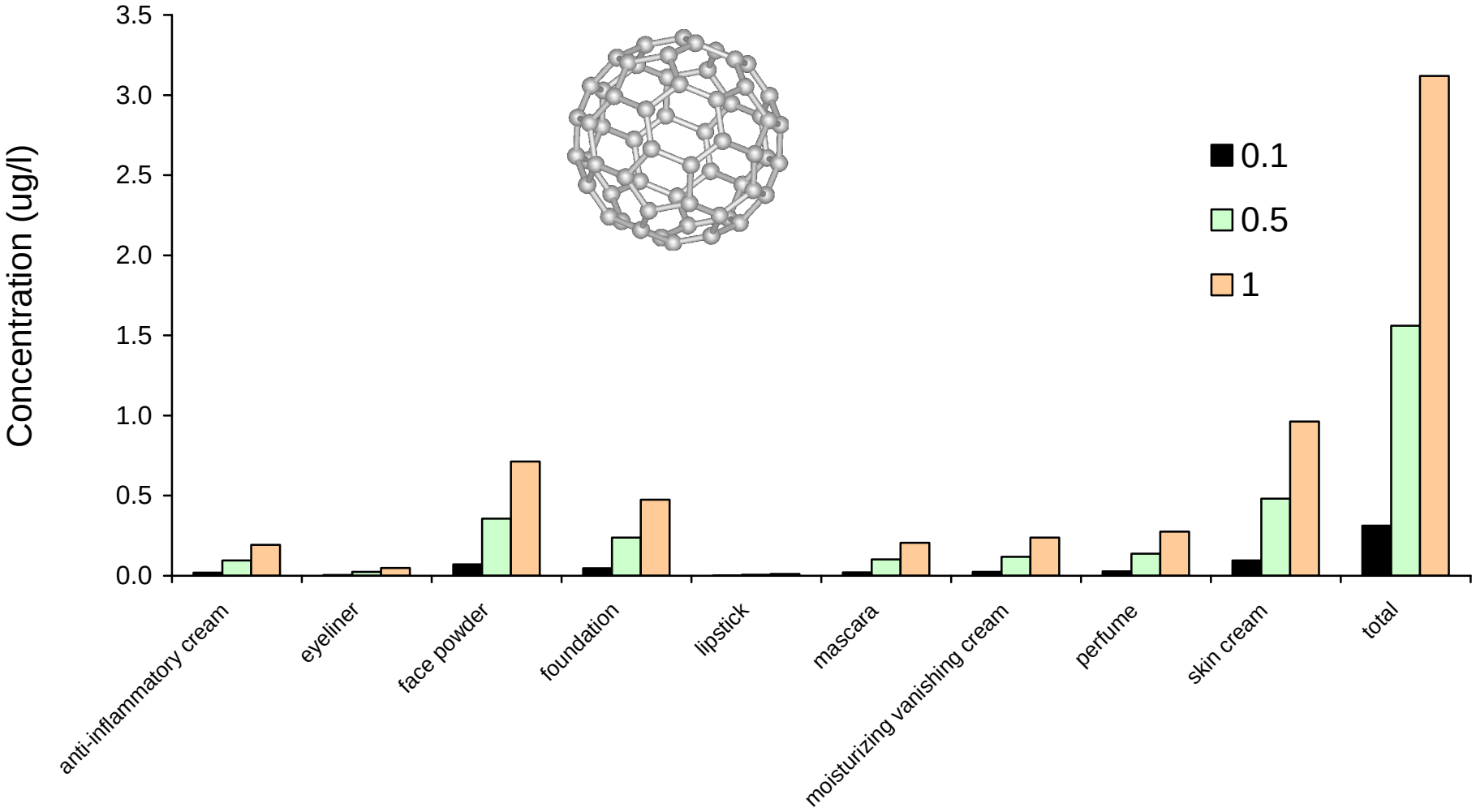
High exposure degradates

E = A.F.P

Transformation product	Pesticide	*E*
metazachlor sulfonic acid	metazachlor	0.0229
cyanazine acid	cyanazine	0.0214
metazachlor oxalic acid	metazachlor	0.0167
reference compound 2	azoxystrobin	0.01
3-carbamyl-2,4,5-trichlorobenzoic acid	chlorothalonil	0.009
propachlor oxanilic acid	propachlor	0.0071
R419492	chlorothalonil	0.0066
3-(3-chloro-p-tolyl)-1-methylurea	chlorotoluron	0.0063
TCPSA	tri-allate	0.006
R417811	chlorothalonil	0.0059
thiomethylol terbutryn	terbutryn	0.0054
2-hydroxy ethyl phosphonic acid	ethephon	0.0052
ethylenebisisothiocyanide sulfide	mancozeb	0.0049
2-hydroxy terbutryn	terbutryn	0.0046
CGA-321113	trifloxystrobin	0.0043
2,6-dinitro-3,4-xylidine	pendimethalin	0.0042
propachlor ethane sulfonic acid	propachlor	0.0041

Sinclair et al., (2006) 40(23): 7283-7289

Predicted Exposure to ENPs



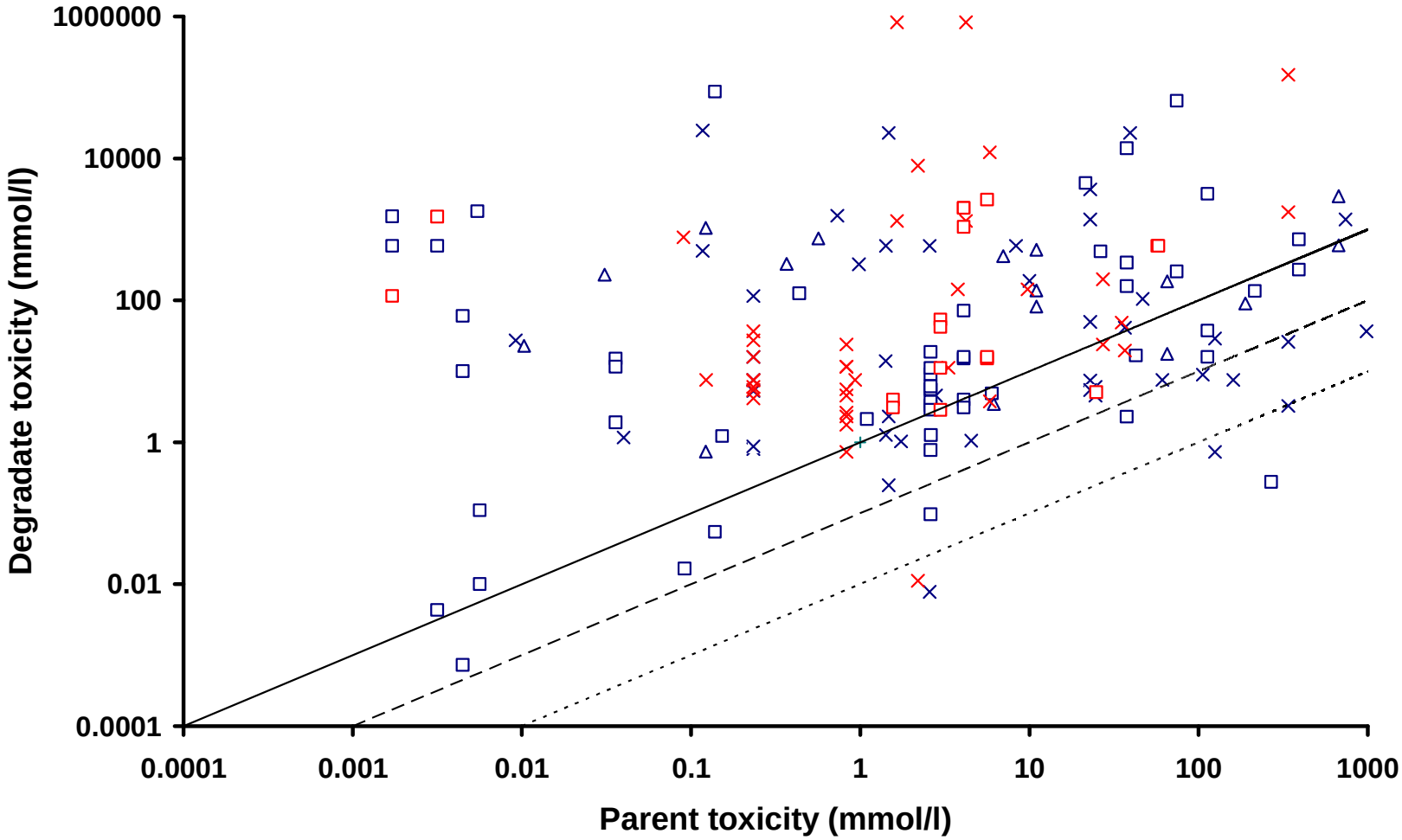
Boxall et al (submit) ES&T

Exposure predictions

	Water (μg/l)	Soil (μg/kg)	Air (mg/m^3)	Aggregate size (nm)
Ag	0.010	0.43	-	-
AlO_3	0.0002	0.01	-	-
Au	0.14	5.99	-	-
CeO_2	<0.0001	<0.01	6×10^{-7}	-
fullerenes	0.31	13.1	-	75 (25-500)
hydroxyapatite	10.1	422	-	-
latex	103	4307	-	-
organo-silica	0.0005	0.02	-	-
SiO_2	0.0007	0.03	-	205 (135-510)
TiO_2	24.5	1030	7	330 (175-810)
ZnO	76	3194	-	480 (420 – 640)

Boxall et al (submit) ES&T

Acute effects of degradates



Sinclair and Boxall (2003) ES&T 37: 4617-4625

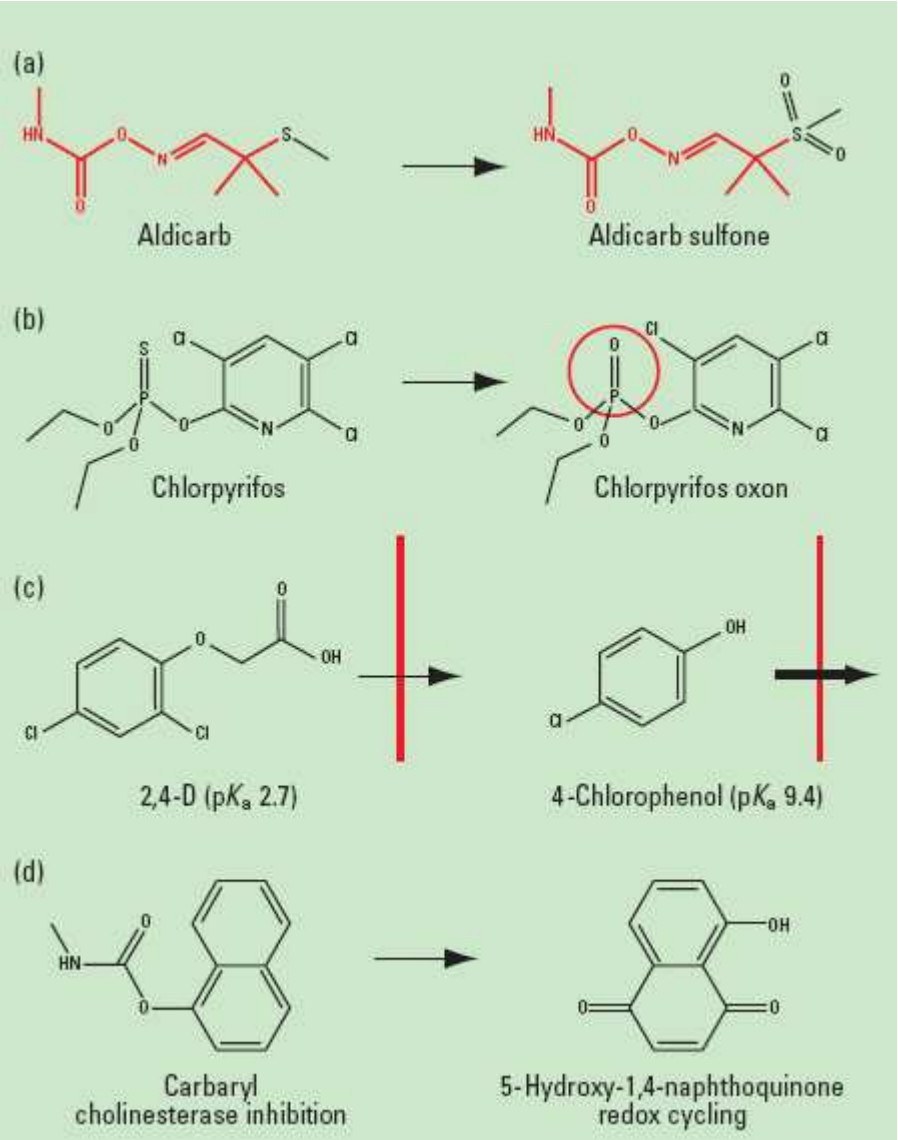
Structure and properties explain the increases

Pro-compounds

Toxicophore still present

Increased accumulation

New mode of action



Boxall *et al* (2004) ES&T 38(19): 369A-375A

Predicting effects

<u>Properties</u>

Hydrophobicity

Shape and Size

Electronic

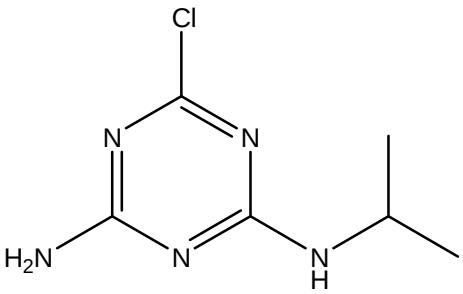
QSAR

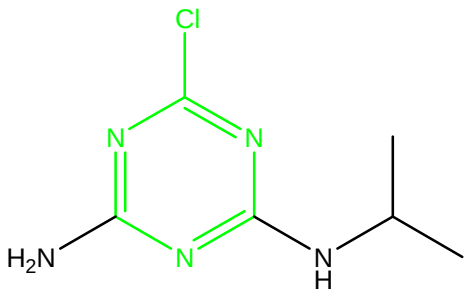
<u>Activity</u>

Toxicity to Fish

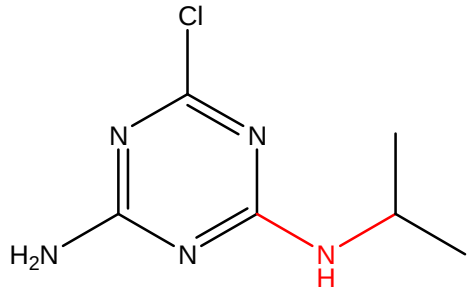
Toxicity to Algae

Toxicity to Daphnia



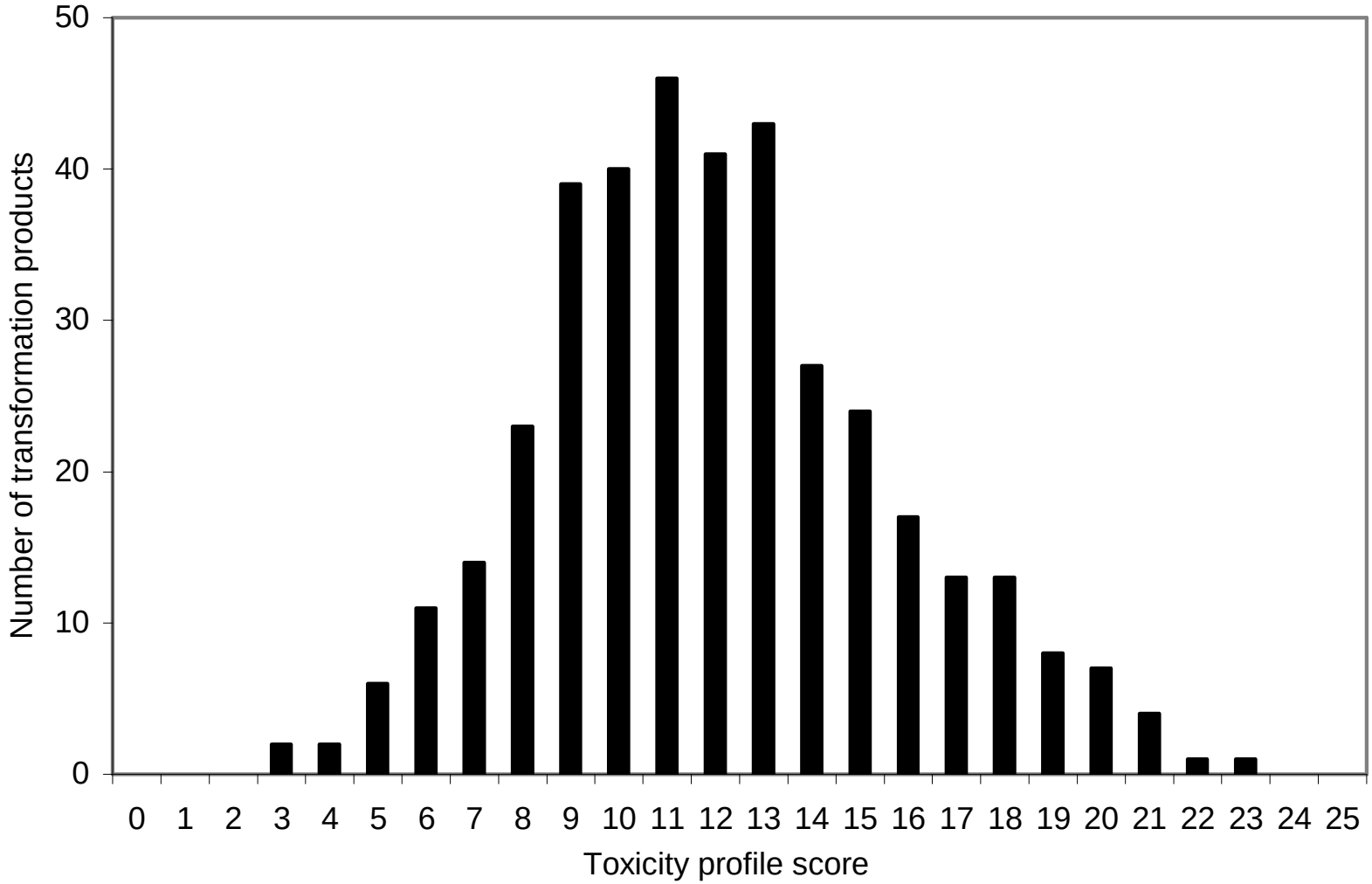


triazine - respiratory sensitization



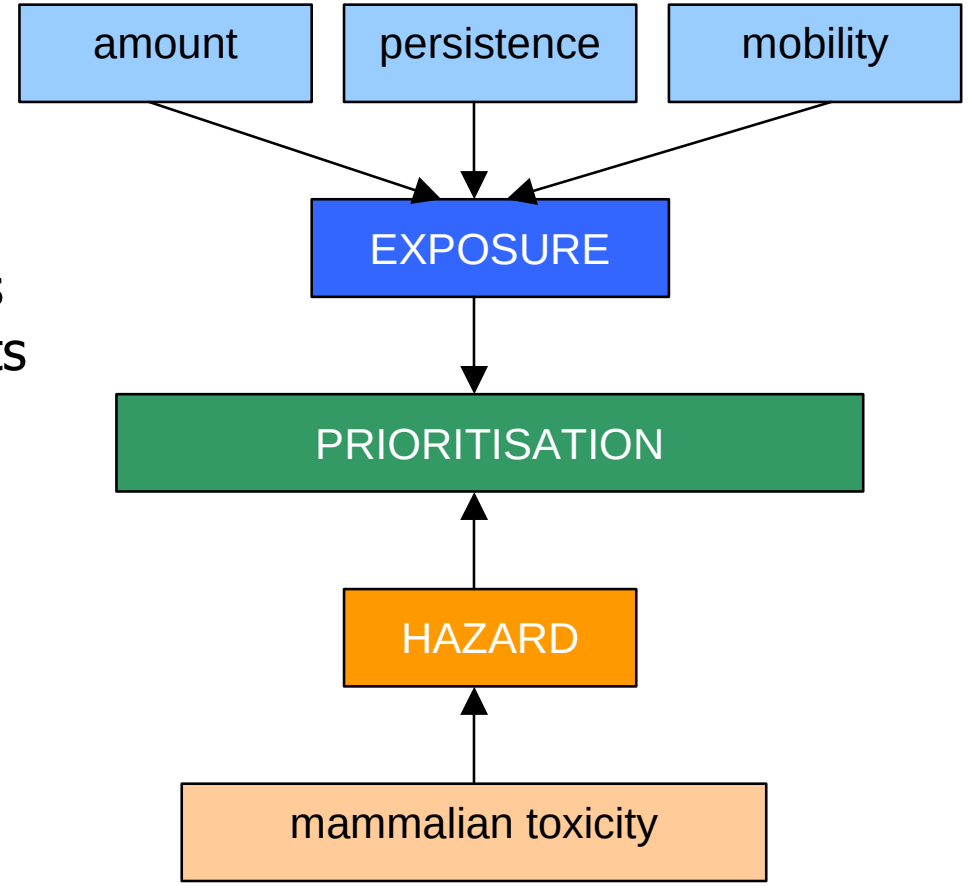
secondary amine - carcinogenicity

Expert system evaluation of degradate toxicity in a UK catchment



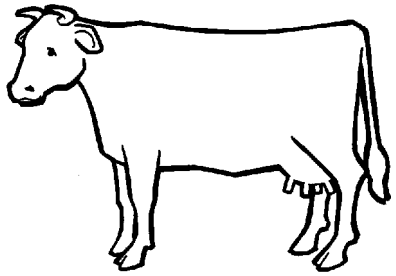
Risk-based prioritisation approaches

- Development of risk-based priority setting schemes
- Application to veterinary medicines, pharmaceuticals and transformation products
- Environmental and human health impacts considered



Boxall *et al* (2003) Toxicol. Lett.
Capleton *et al* (2006) Toxicol. Lett.
Sinclair *et al* (2006) Envir. Sci. Technol

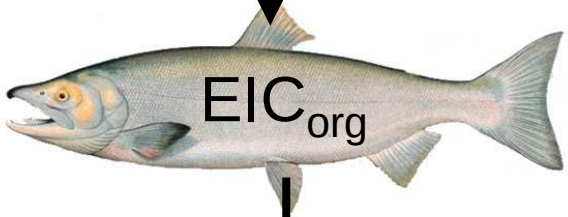
Risk-based ranking of vet meds



Environmental exposure assessment

$EIC_{aquatic}$

Uptake prediction



Dose

EIC_{org} : Dose

Fullerenes

100 mg/l

10

Daphnids – mortality (Zhu et al., 2006; Oberdorster et al., 2006)

1.0

Bacteria – respiration (Fortner et al., 2005)

Daphnids – molting and reproduction (Oberdorster et al., 2006)

Fish - biomarkers (Oberdorster et al., 2006)

0.1

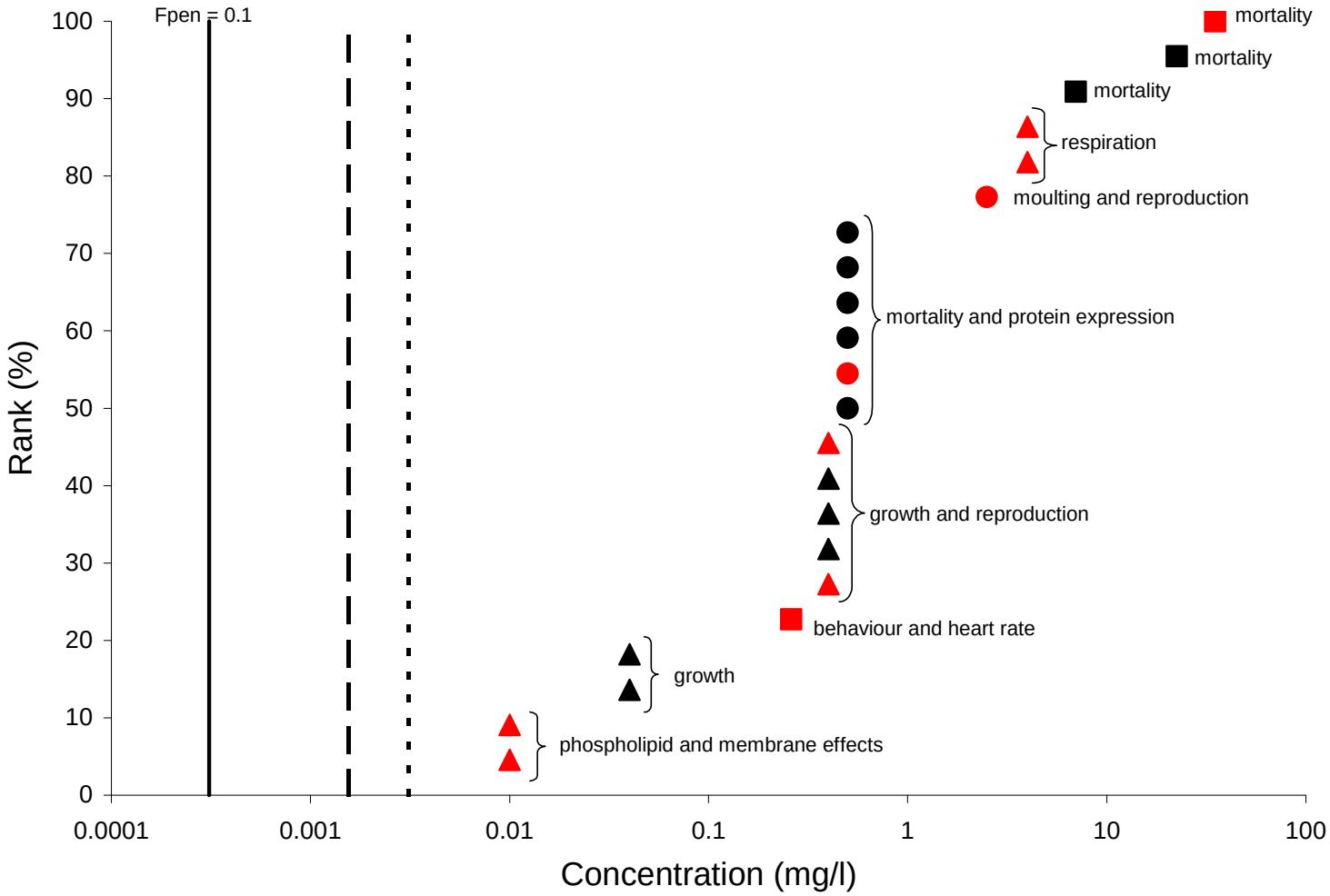
Bacteria - growth (Fortner et al., 2005)

Daphnids – hopping, heart rate, appendage movement (Lovern et al., 2007)

Bacteria - phospholipids & membrane phase behaviour (Fang et al., 2007)

0.01 mg/l

Fullerenes


Fpen = 0.1
mortality
mortality
mortality
respiration
moulting and reproduction
mortality and protein expression
growth and reproduction
behaviour and heart rate
growth
phospholipid and membrane effects
Rank (%)
100
90
80
70
60
50
40
30
20
10
0
0.0001
0.001
0.01
0.1
1
10
100
Concentration (mg/l)

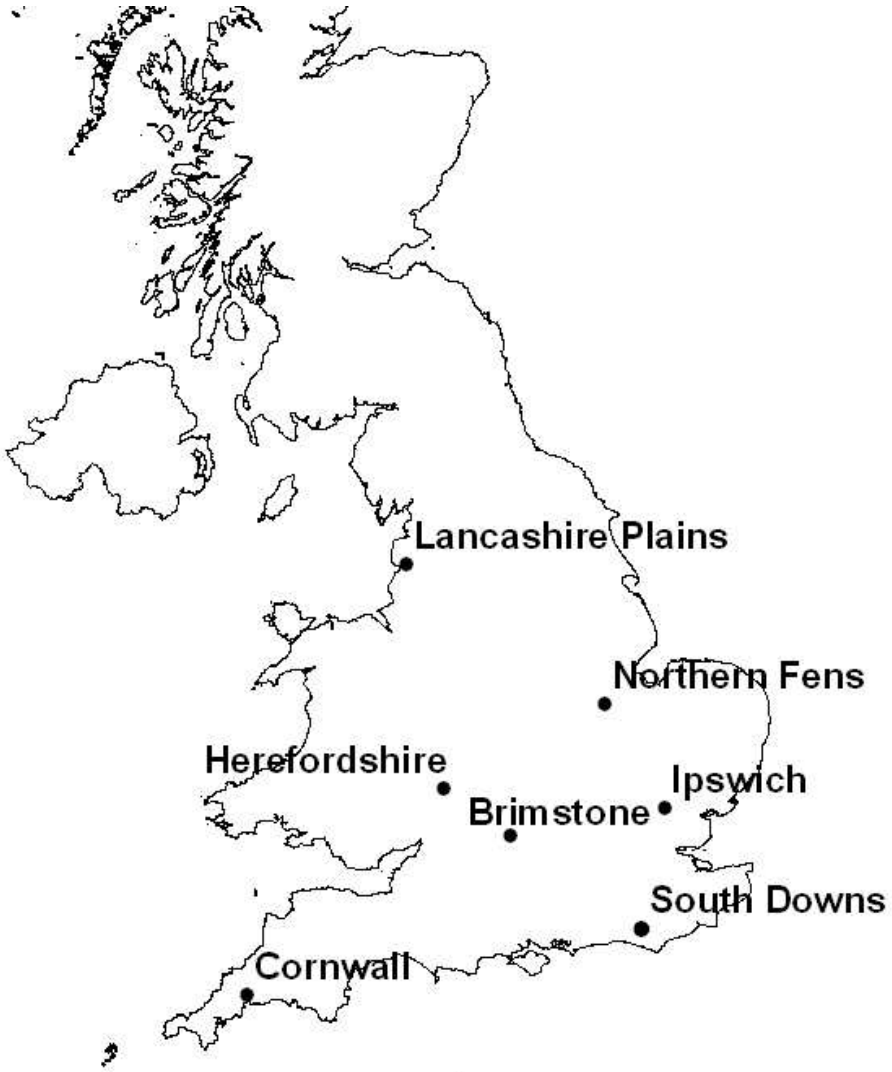
Risks are likely to change

- Temperatures will increase, winters will be wetter, summers drier and there will be an increase in intense rain events
- Climatic changes likely to affect inputs, fate and transport of pathogens and chemicals
- Risks could be very different from today

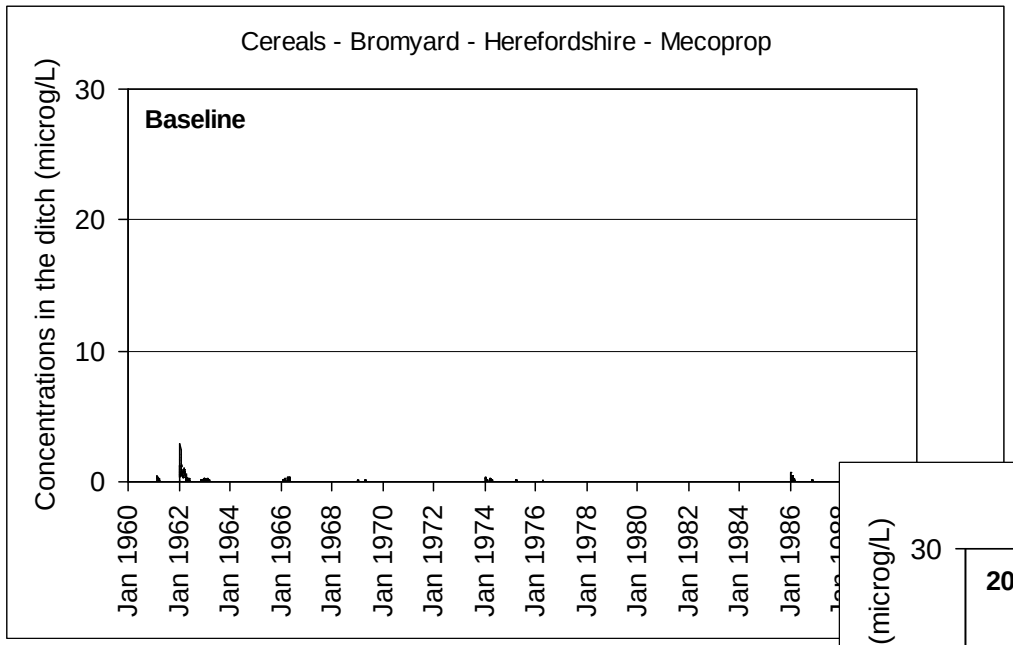
Baseline scenarios

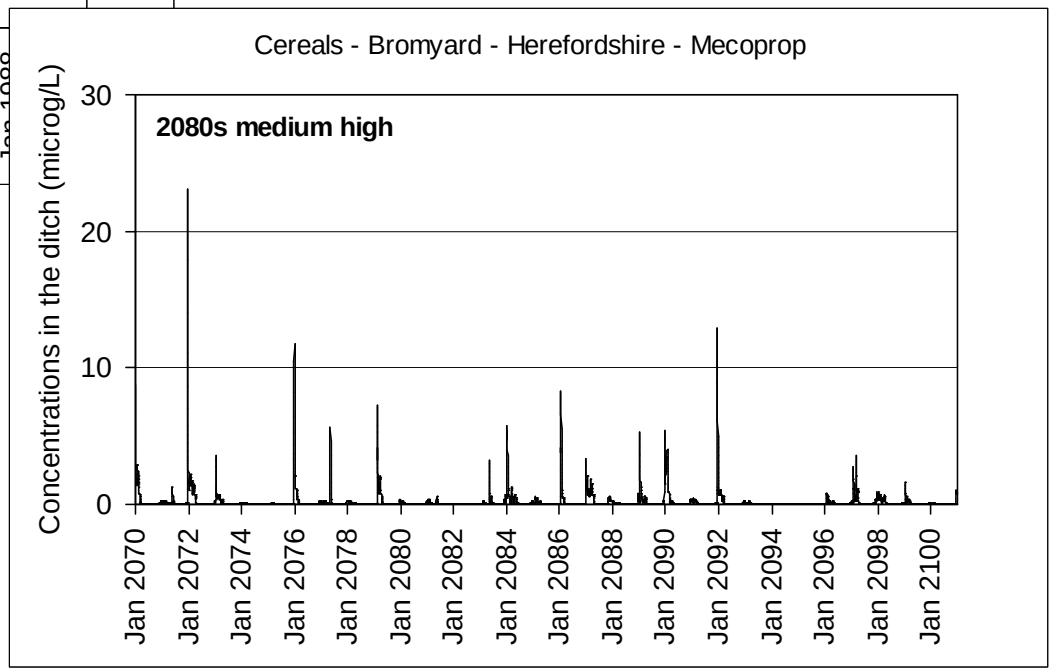
Crop	Location	Soil	Pesticide	Compartment
Vegetables	Lancashire Planes	Brockhurst	propachlor, chlorothalonil	SW (drainage), GW
Grass	Herefordshire	Bromyard	dicamba, MCPA, dichlorprop	SW (runoff, drainage)
Winter cereals	Herefordshire	Bromyard	isoproturon, mecoprop, metsulfuron-methyl, chlorothalonil	SW (runoff, drainage)
Winter cereals	Brimstone	Denchworth	isoproturon, mecoprop, metsulfuron-methyl, chlorothalonil	SW (drainage)
Winter cereals	Ipswich	Hanslope	isoproturon, mecoprop, metsulfuron-methyl, chlorothalonil	SW (drainage)
Flower bulbs	Cornwall	Denbigh or East Keswick	chlorpyrifos	SW (runoff)
Sugar beet	Northern Fens	Wisbech	ethofumesate, metamitron	SW (runoff)
Maize	South Downs	Curtisden	propachlor	GW
Maize	Northern location	Arrow	propachlor	GW
Winter oilseed rape	Brimstone	Denchworth	metazachlor, fungicide	SW (drainage)

Location of scenarios



Mecoprop simulations





Summary

- A combination of input data, models and expert systems can be very useful for prioritisation purposes
- Usage and input data often impossible to obtain
- Predictive models poorly developed for many variables and chemical classes – this could change as REACh develops
- Risks likely to change in the future
- It is probably impossible measure everything or to predict every possible impact

Thank you for listening

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