Campus:

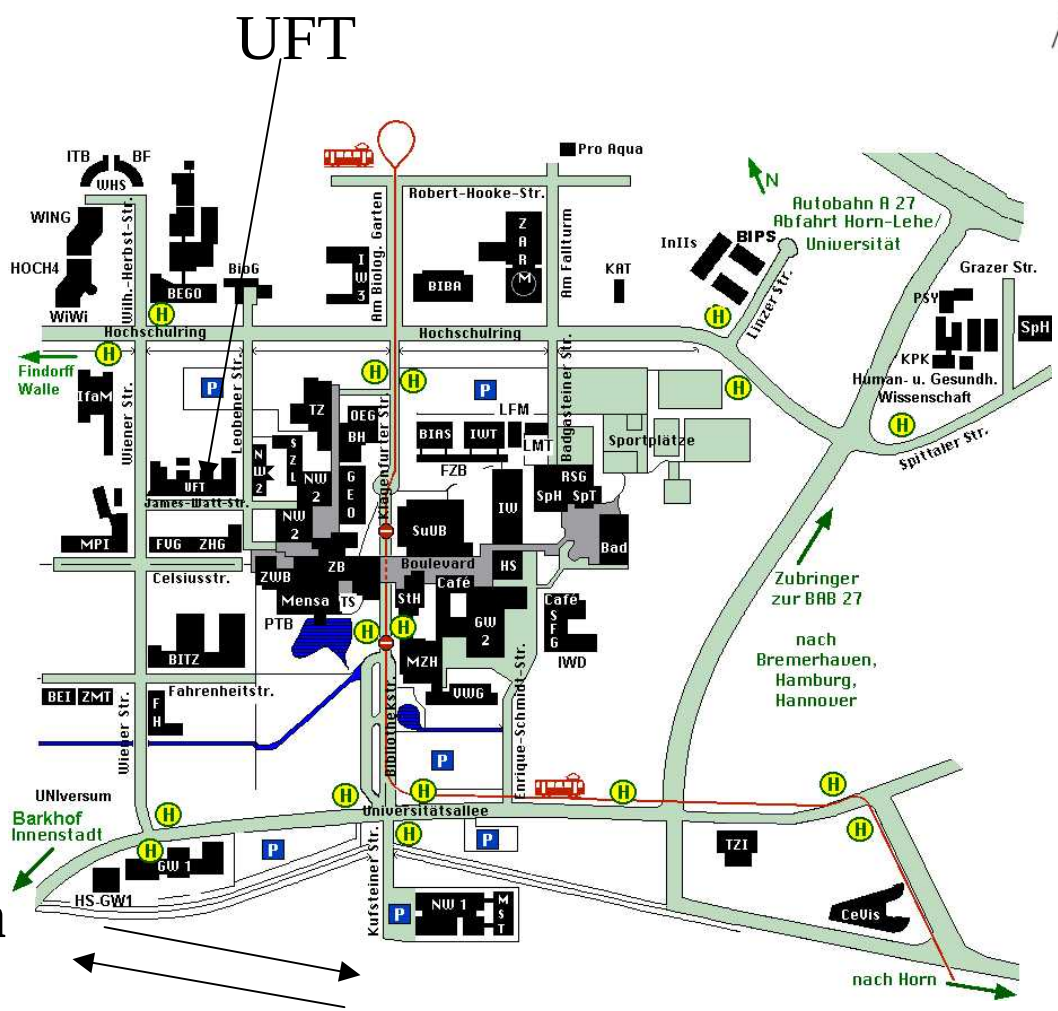
63.000 m², 10.800 m² buildings 180.000 m² used aera

12 Faculties

ca. 21.500 students

ca. 1.700 scientists

ca. 1.100 employiers



University of Bremen

Surrounded by an
Industrialpark: 170 ha
320 companies
7000 working places

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Strategien zum Design nachhaltiger Industriechemikalien am Beispiel Ionischer Flüssigkeiten

Bernd Jastorff

Strategische Partnerschaften
mit
Prof. Ondruschka, Annegret Stark,
Universität Jena

Merck, IoLiTec und
Solvent Innovation

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Design of
sustainable industrial chemicals -

an interdisciplinary challenge

?!

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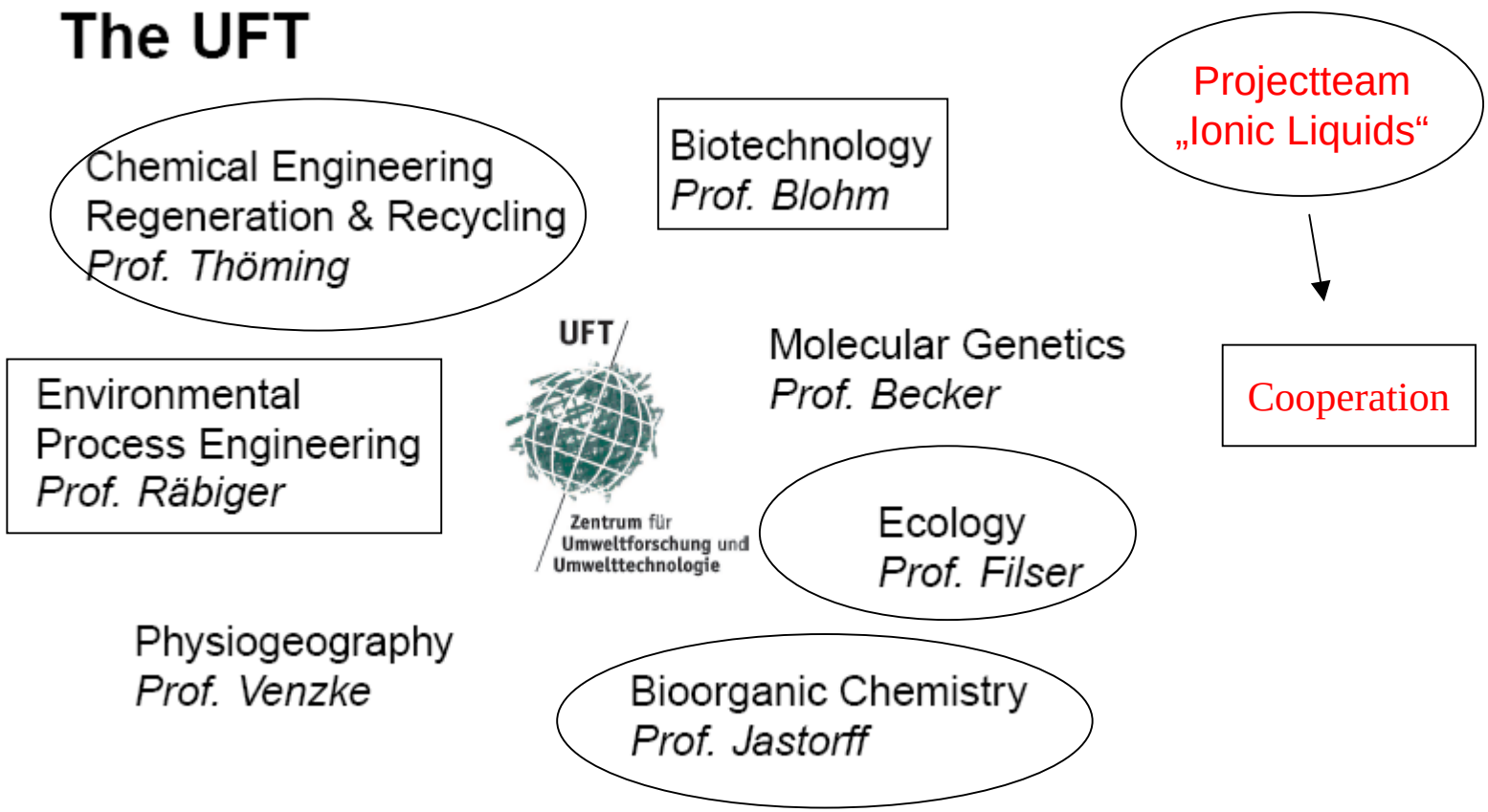
THE CENTRE OF ENVIRONMENTAL SCIENCE AND TECHOLOGY: **UFT**

THE BUILDING


The UFT
Chemical Engineering
Regeneration & Recycling
Prof. Thöming
Biotechnology
Prof. Blohm
Projectteam
„Ionic Liquids“
Environmental
Process Engineering
Prof. Räbiger
UFT
Zentrum für Umweltforschung und Umwelttechnologie
Molecular Genetics
Prof. Becker
Cooperation
Ecology
Prof. Filser
Physiogeography
Prof. Venzke
Bioorganic Chemistry
Prof. Jastorff

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Zentrum für Umweltforschung und Umwelttechnologie

Projektteam „Ionic Liquids“

UFT

MERCK

Strategic Partnerships

U. Welz-Biermann, N. Ignatiev , W. Pittner and T. Colnot
Merck KGaA, New Business Chemicals and
Institute of Toxicology,

IoLiTec, Freiburg
Solvent Innovation

Roman Herzog, former German President
in his Berlin speech, November 1997:

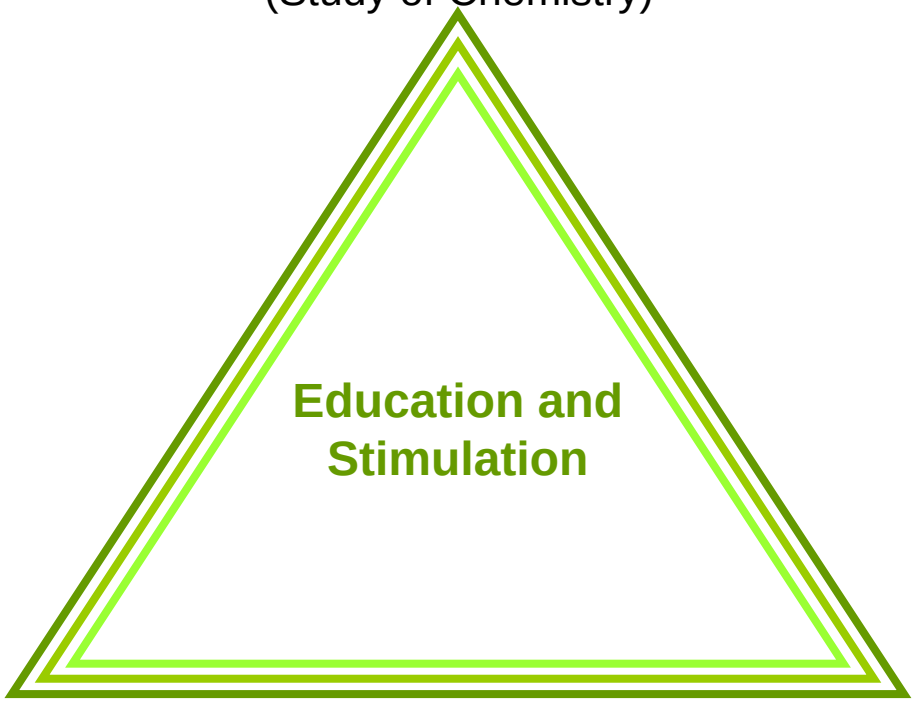
A new
project-oriented and interdisciplinary
form of learning is required,
one which - for example - combines
specialist knowledge of chemistry
with that of
biology and ethics".

University of Kiel

(Study of Chemistry)

Dr. Hans Hettler

Prof.Dr. Friedrich Cramer



Max Planck Institute for Experimental Medicine, Göttingen

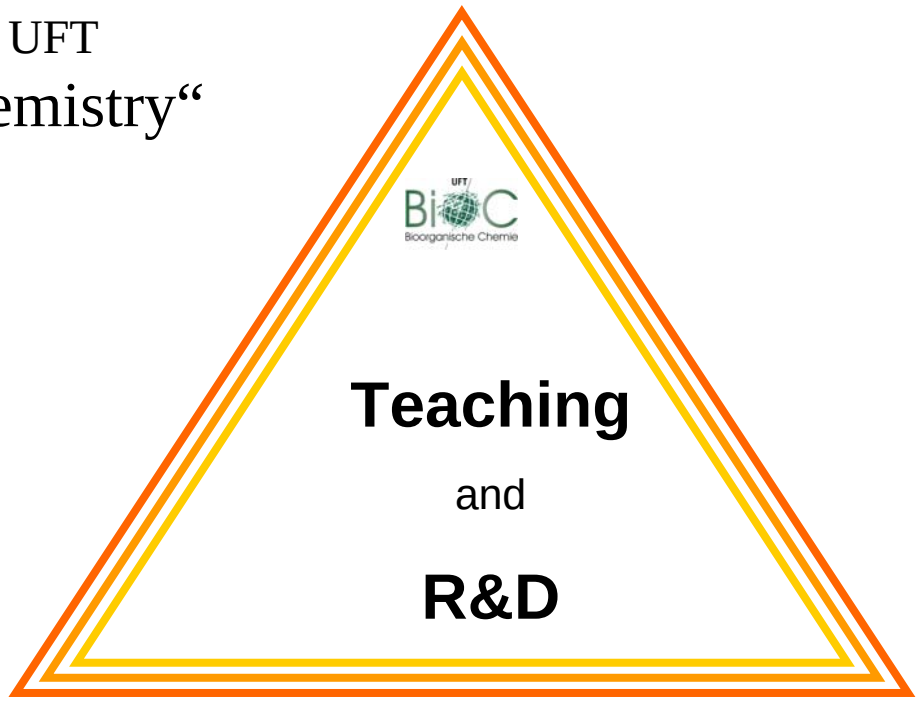
(Transdisciplinary thesis: networking chemistry with biology)

Reformuniversity of Bremen

Interdisciplinary Department of Bioorganic Chemistry

Department 3 at UFT

„Bioorganic Chemistry“



www.uft.uni-bremen.de/chemie

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Dept. of Bioorganic Chemistry

Students/ coworkers from chemistry, biology, environmental sciences and engineering are educated together to be trained disciplinarily and interdisciplinarily

Chemist`s Vision and Mission

Design
of
safer (sustainable)
Chemicals

(chemicals with inherent safety for man and the environment,
(which can be marketed)

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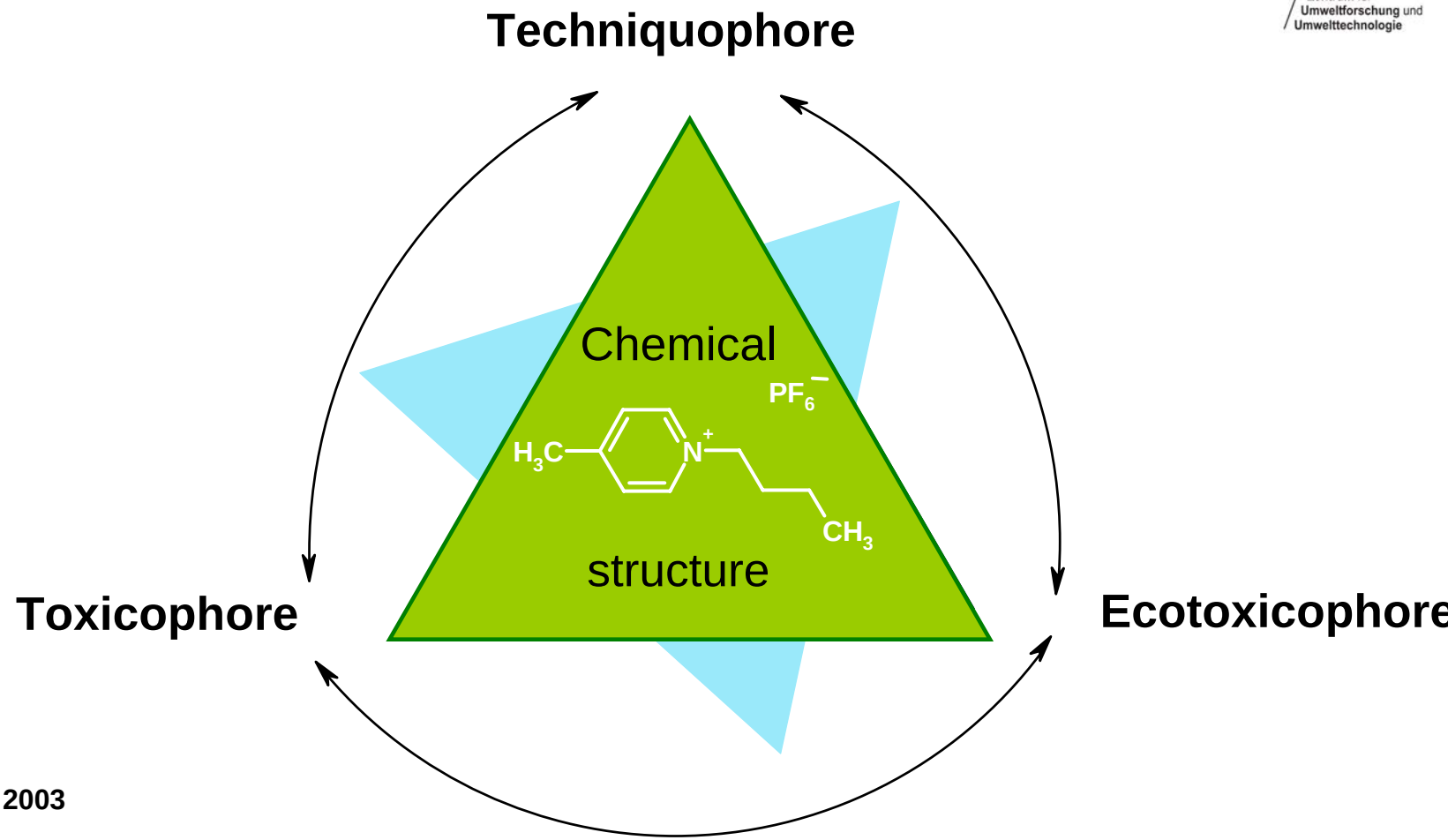
Chemical products should be designed to preserve efficacy of function while reducing toxicity.

Paul Anastas and John Warner
4.principle of Green Chemistry



Jastorff et al. 2003
and 2005
Green Chemistry

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Interdisciplinary teamwork

Our tools for the design of sustainable chemicals

Cooperation with companies

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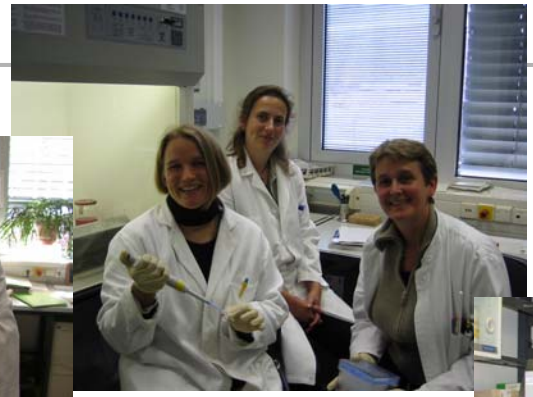
T. Juffernholz[2]

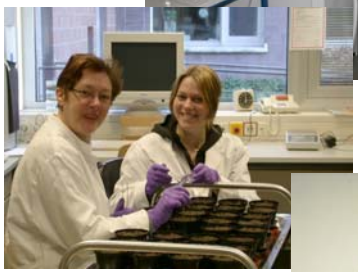


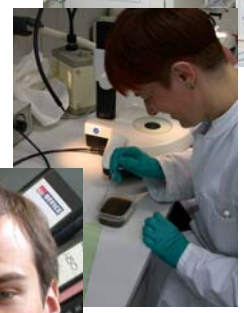
F. Stock[1]

U. Bottin-Weber[1]

A. Müller[1]

[1] Bioorganic Chemistry
[2] Ecology





P. Behrend[1]

M. Schaefer[2]

U. Uebers[2]

. Burfeindt [2]

S. Stolte[1]

J. Ranke[1]

R. Störmann[1]

j.Arning[1]

Universität Bremen

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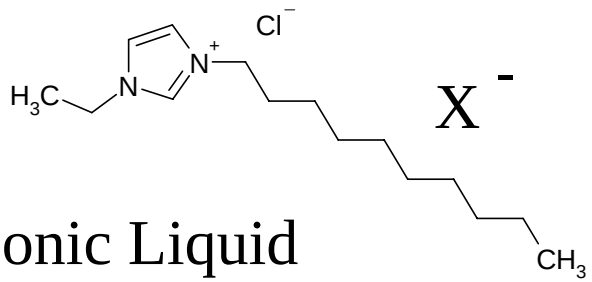
Interdisciplinary teamwork

Our tools for the design of sustainable chemicals

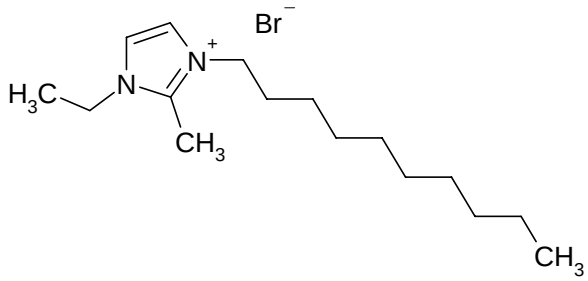
T-SAR/ QSAR

Cooperation with companies



X -

Ionic Liquid

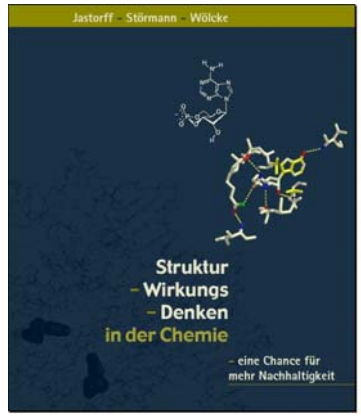


Patented plant growth regulator

„Struktur-Wirkungs-Denken“

Thinking in terms of **S**tructure-**A**ctivity-**R**elations

T-SAR



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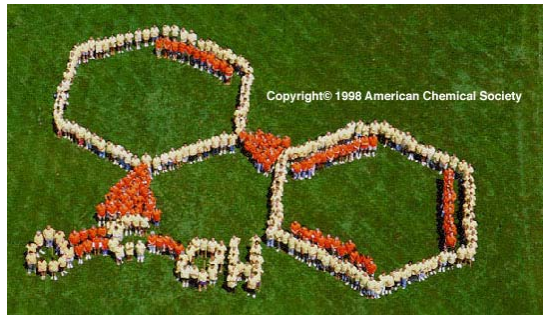
Quantitative Struktur-Wirkungs-Beziehungen

Quantitative **S**tructure-**A**ctivity-**R**elations

Q-SAR

One of the key problems in chemistry is the number of existing chemicals



18 Mill. Chemical entity in CAS, 1998

A problem of uncertainty !

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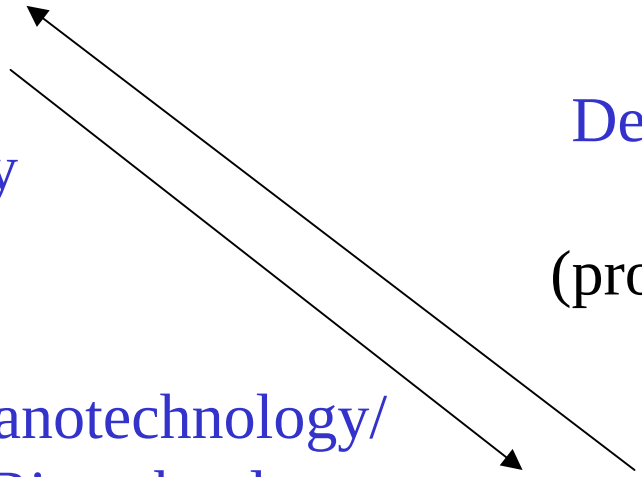
QSAR and T-SAR
both try to overcome this problem

T-SAR and QSAR
can be used on
existing chemicals
and on those
designed theoretically
to be (eventually)
synthezised

T-SAR

Design of drugs and pesticides
„biological effects“



Chromatography
„Retention“

Design of sustainable Chemicals
(properties and effects)

Nanotechnology/
Biotechnology
„properties“

QSAR

Structural formular(s)

Assessment of
stereochemical features

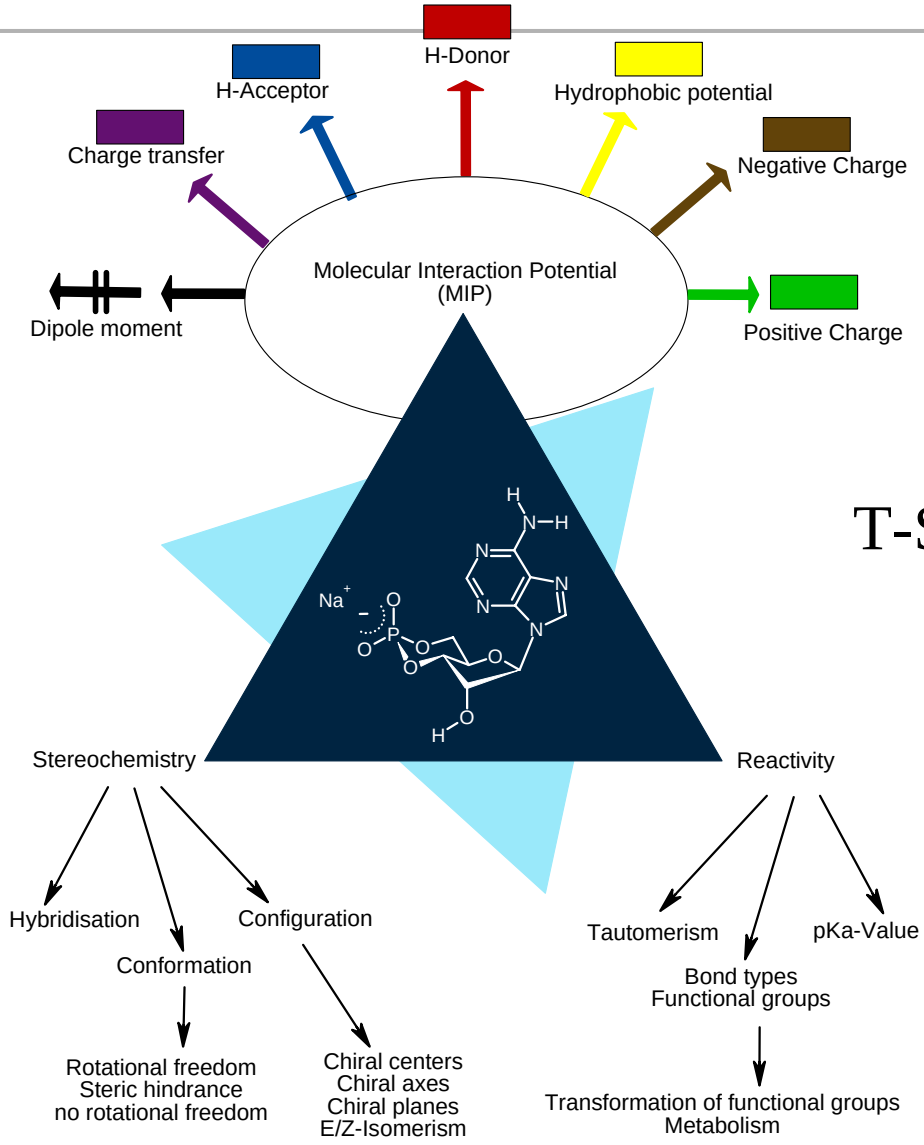
Tools of T-SAR

Chemical (biochemical) reactivity

Colour coding of
molecular interaction potential

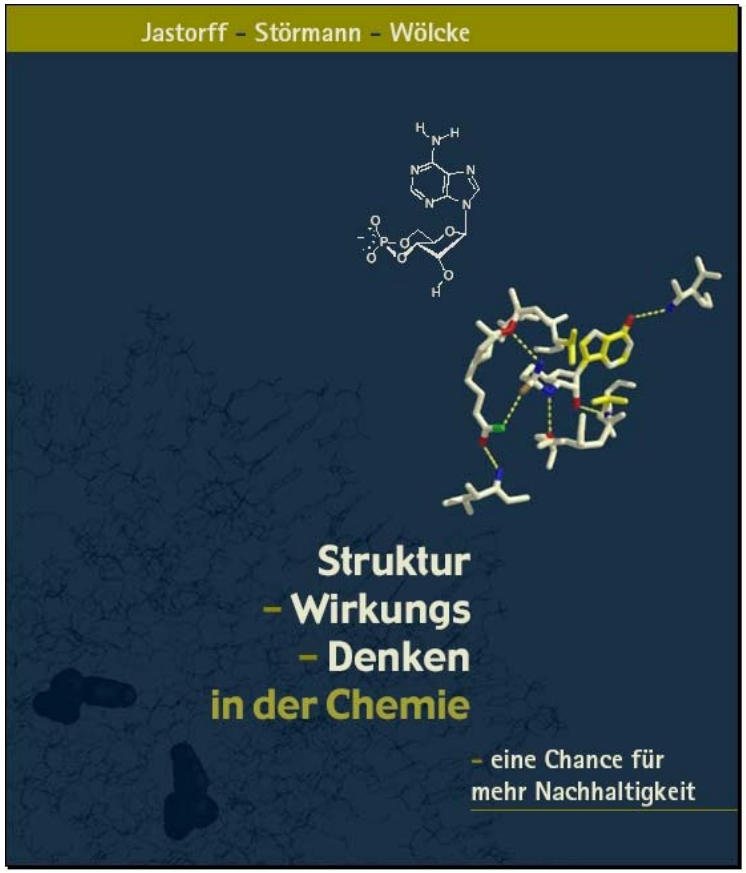
19 lead questions!

T-SAR Triangle



Detailierte Informationen

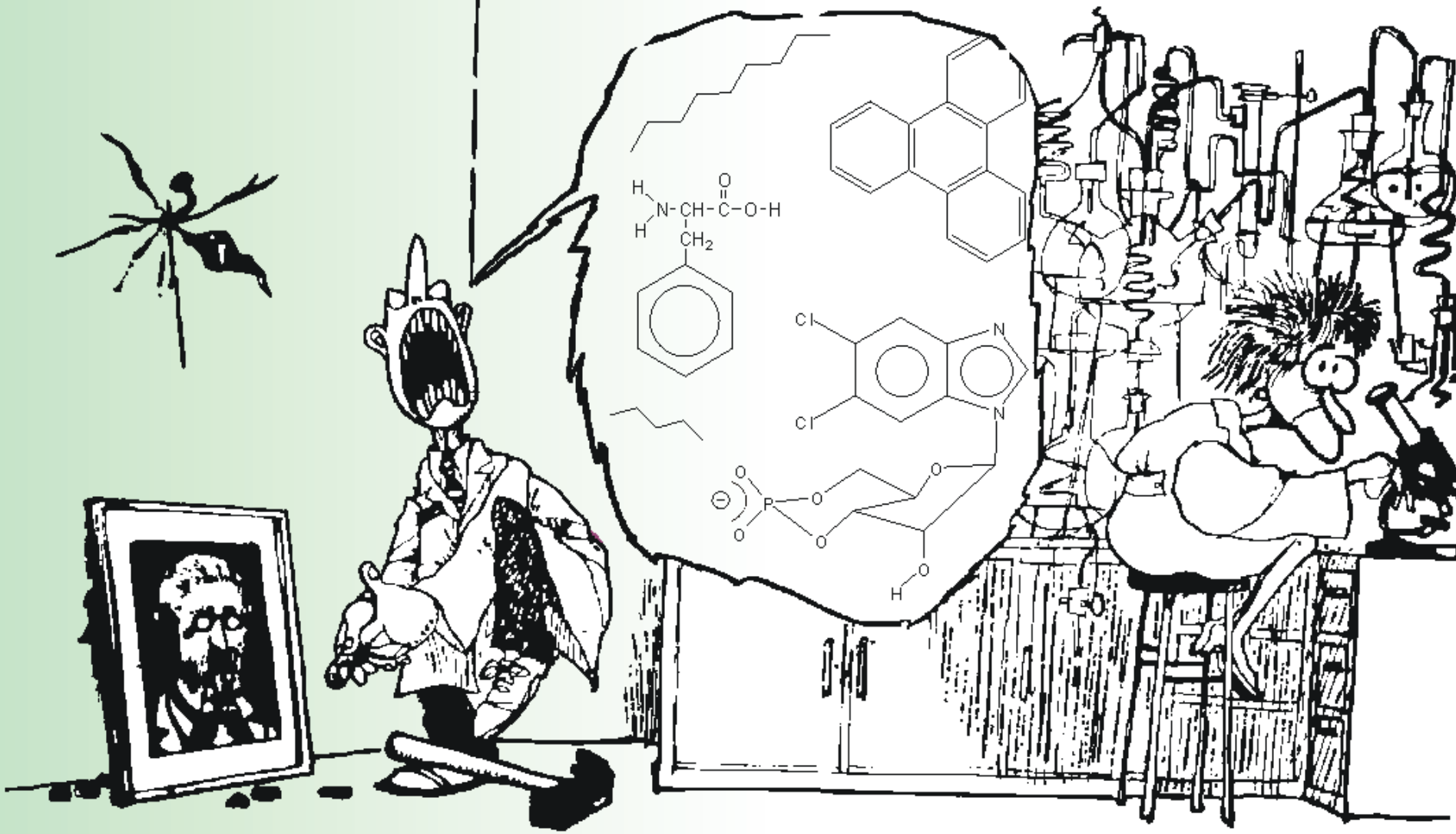
www.uft.uni-bremen.de/chemie



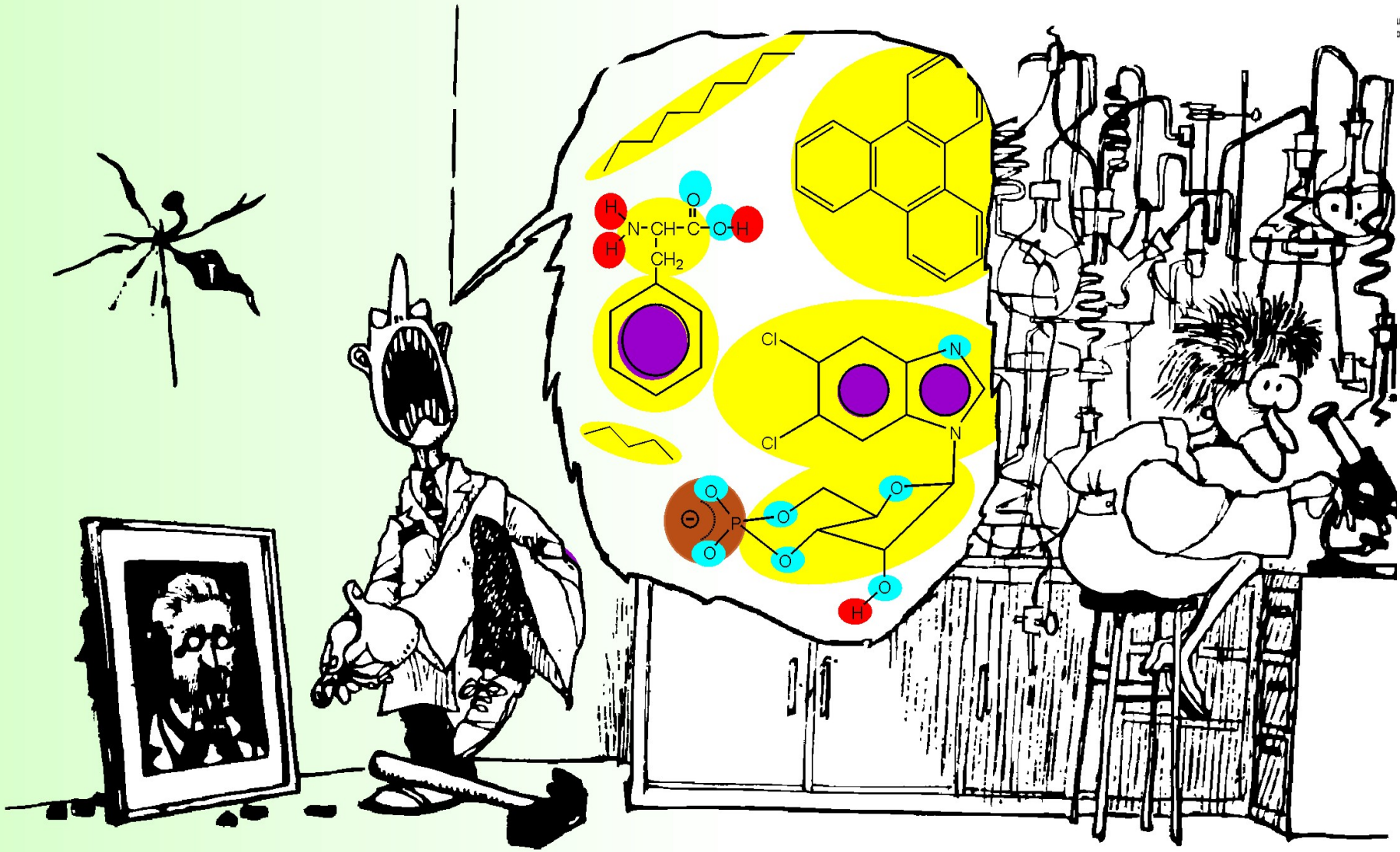
Publisher:
Aschenbeck and Isensee
Universitätsverlag Oldenburg-Bremen, 2003
(Internet Bestellung:
www.Isensee.com)

300 pages, 4 colours
42 Euro

A chemist swears!



A chemist swears after having heard Jastorff´s lecture on T-SAR



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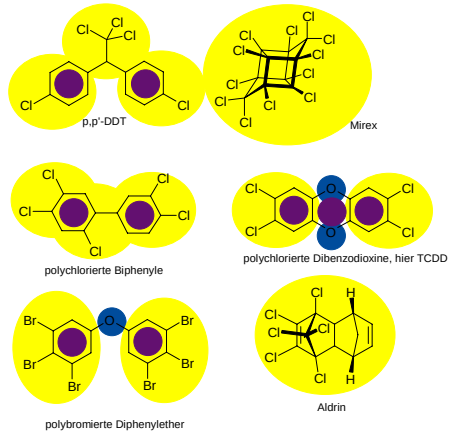
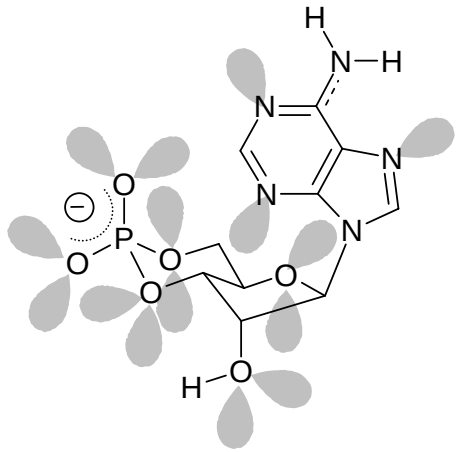
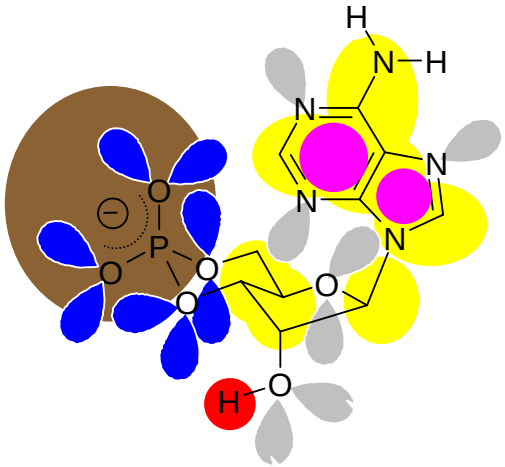
Coding of the molecular interaction potentials of a chemical within the structural formular by means of characterising colours

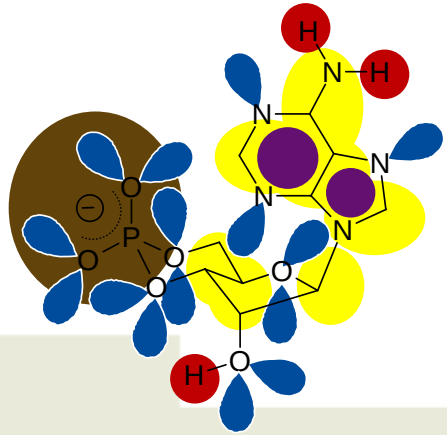
- Cation (ionic Interaction)
- Anion (ionic Interaction)
- H-Bonding-donor
- H-Bonding-akceptor
- π-π-Bonding-Potential
- hydrophobic interaction potential



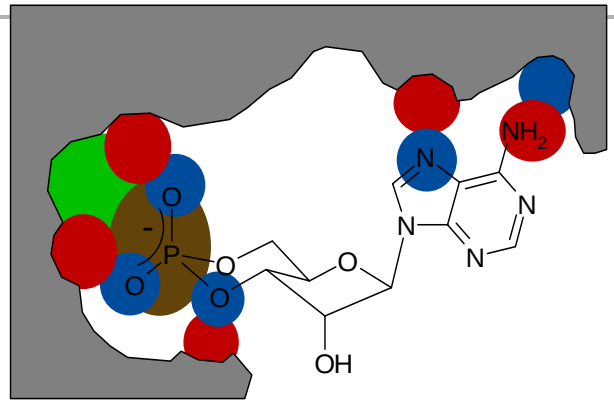
„POPs“



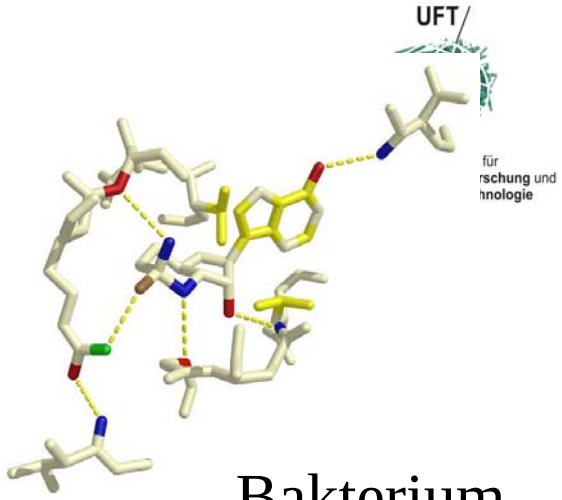




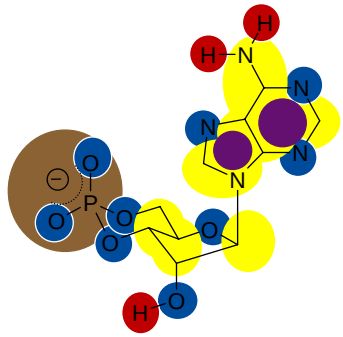
Second messenger cAMP



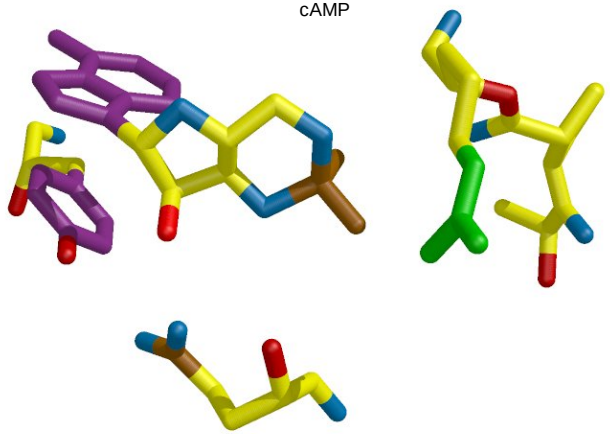
Pilz



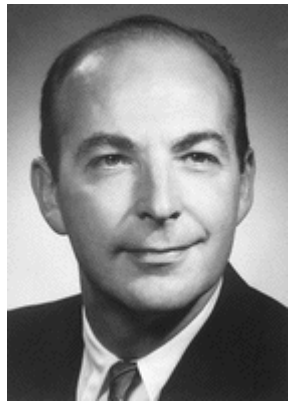
Bakterium



cAMP

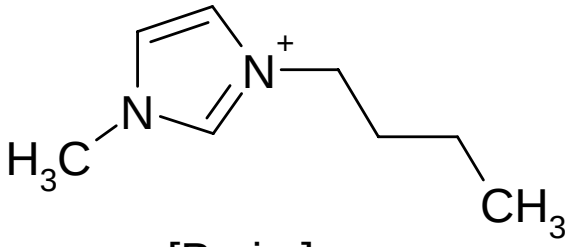


Säuger



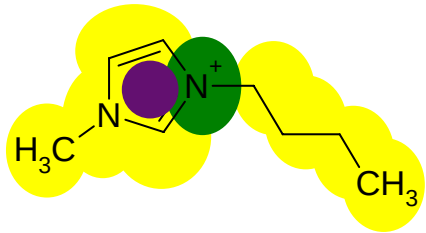
Much of life can be understood in rational terms, if expressed in the language of chemistry

Arthur Kornberg was born 1918, Nobel Prize Winner for medicine/physiology 1959
Keynote speech at the 17th International Congress of Biochemistry and Molecular Biology
San Francisco 1997

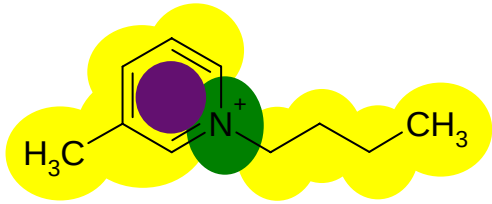


[Bmim]

T-SAR



Imidazoliumverbindungen



Pyridiniumverbindungen

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Interdisciplinary teamwork

Our tools for the design of sustainable chemicals

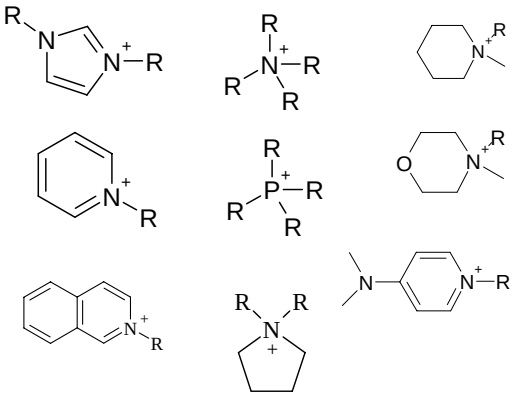
T-SAR/ QSAR

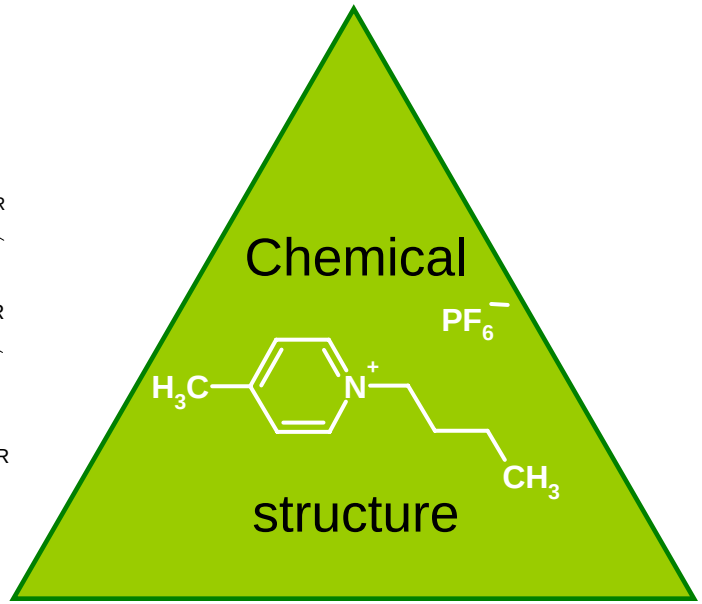
Cooperation with companies

Testkit-Concept

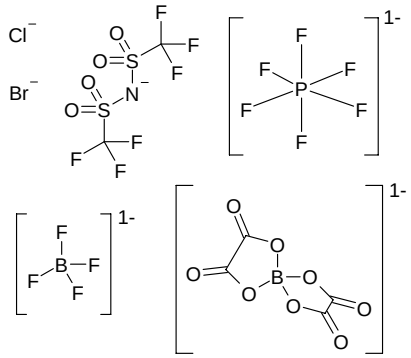
Testkit of Ionic Liquids

Headgroup

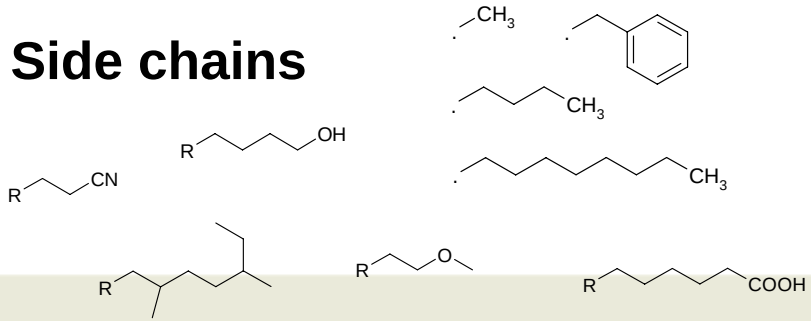




Anions



Side chains



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Interdisciplinary teamwork

Cooperation with companies

Our tools for the design of sustainable chemicals

Hazard/ risk assessment

T-SAR/ QSAR

Testkit-Concept

RISK ASSESSMENT

exposition

$$\frac{\text{PEC (predicted environmental concentration)}}{\text{PNEC (predicted no effect concentration)}} = \text{risk ratio}$$

effects

EU-Approach

Indicators:

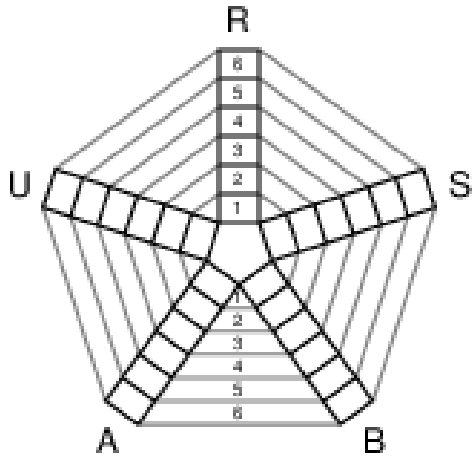
R = Release

S = Spatiotemporal range

B = Bioaccumulation

A = Biological Activity

U = Uncertainty

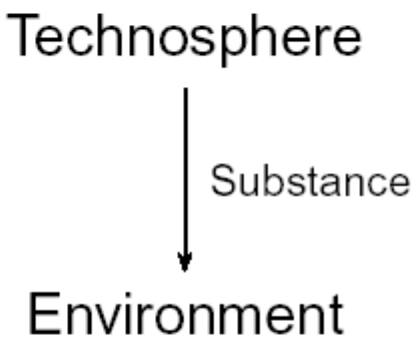


Multidimensional risk analysis

Developed by Dr. Johannes Ranke,
University of Bremen, 2001

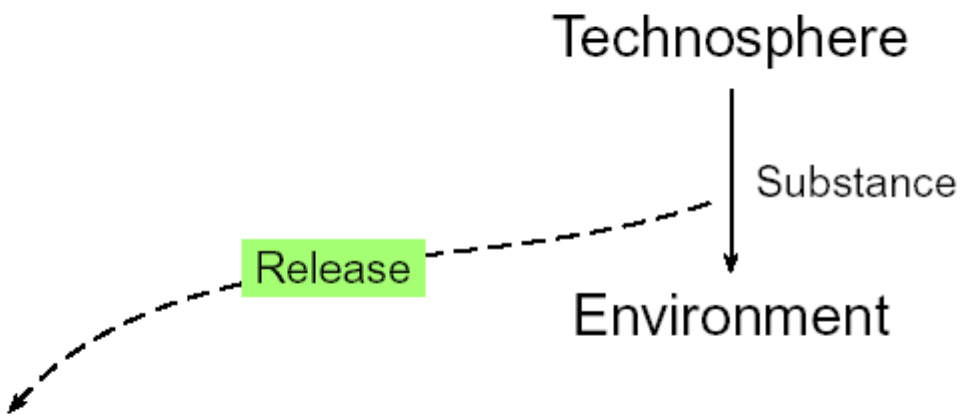
Ranke J (2001) PhD Dissertation

Five risk indicators



Ranke J (2001) PhD Dissertation

Five risk indicators



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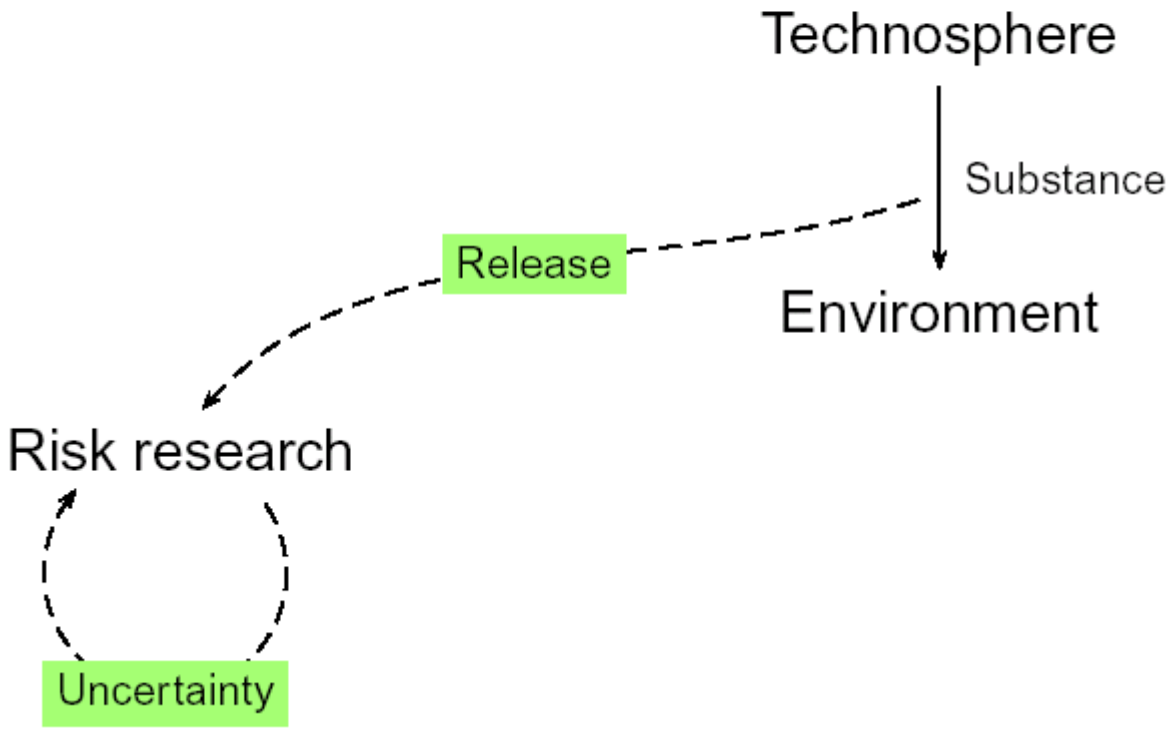
Five risk indicators



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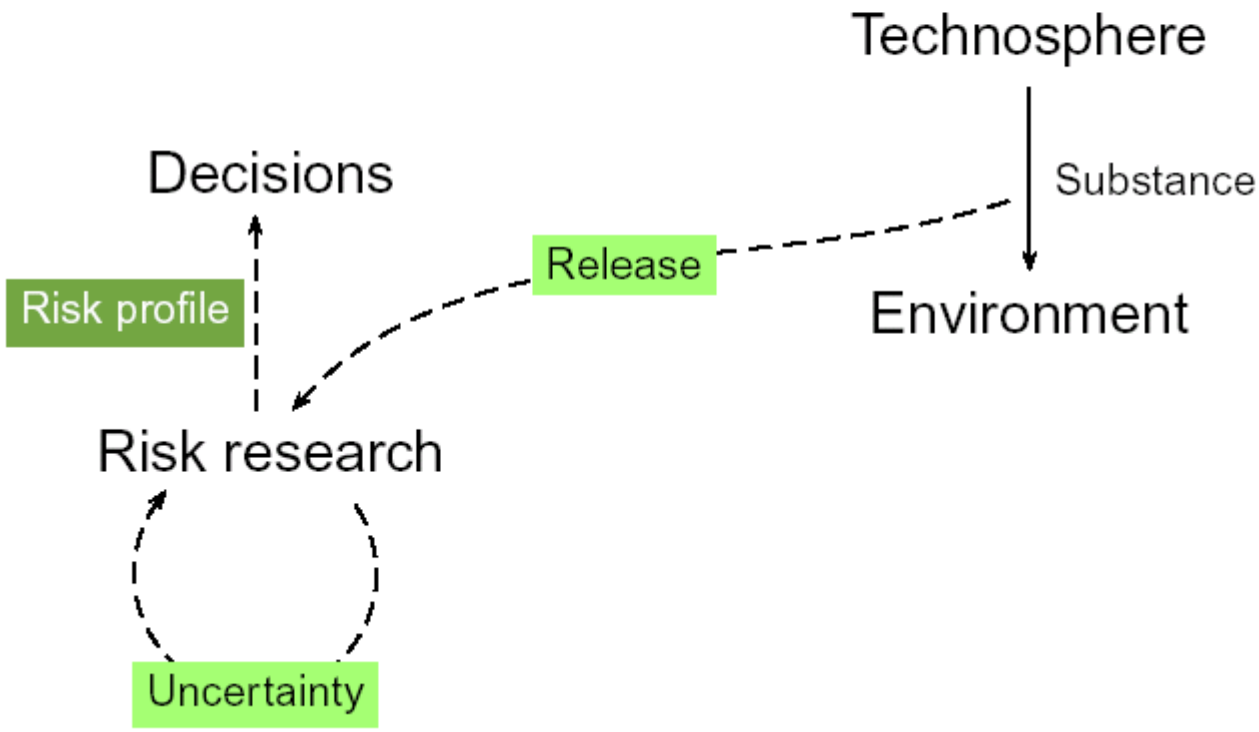
Five risk indicators



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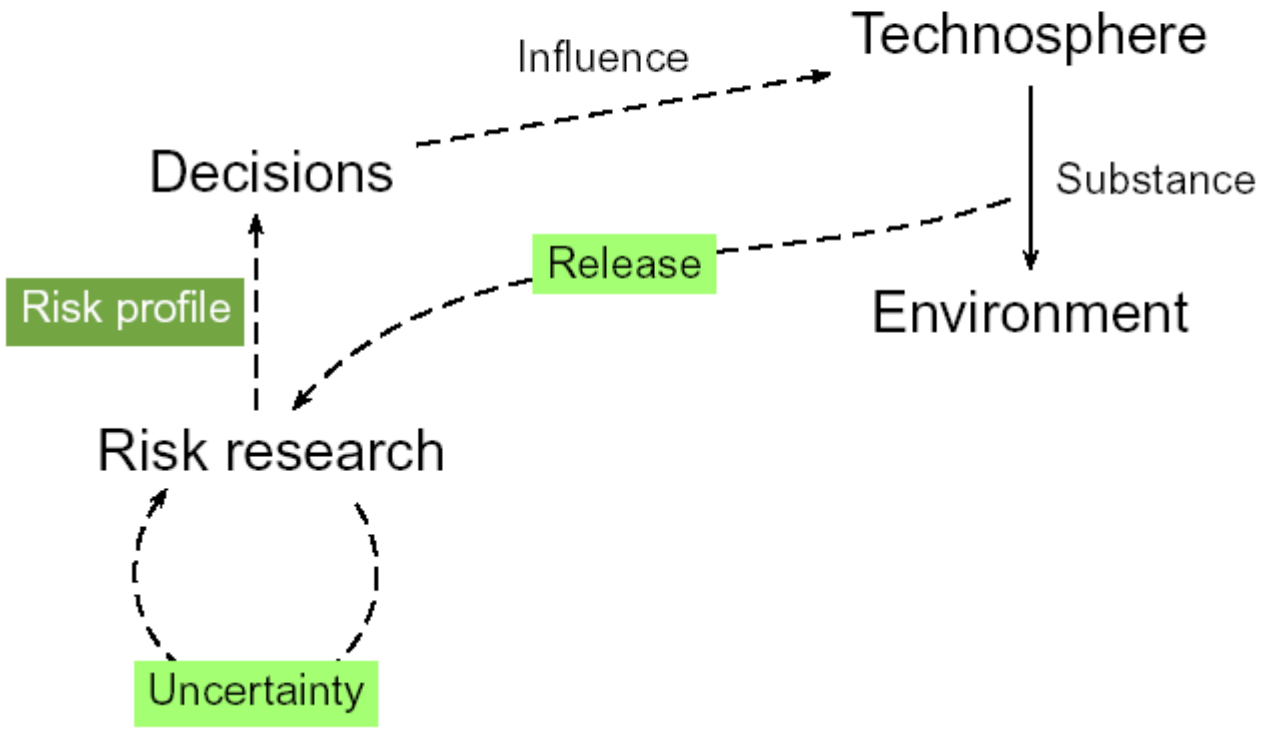
Five risk indicators



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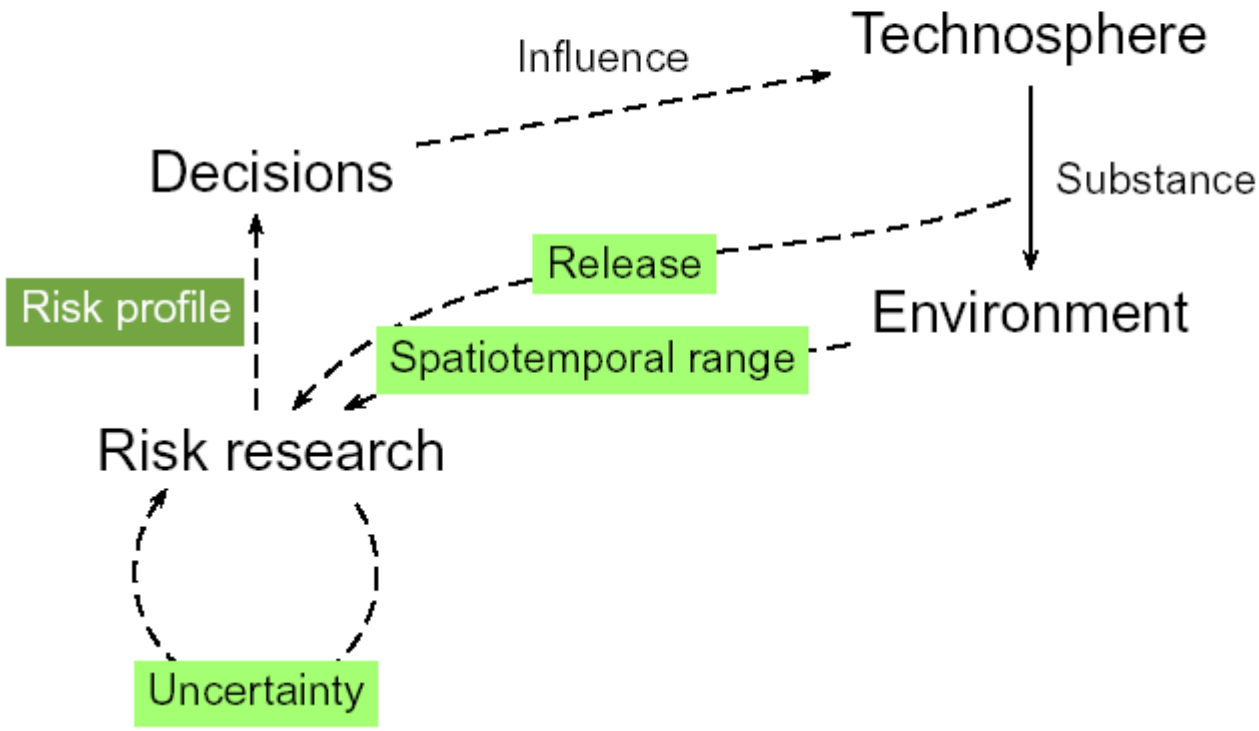
Five risk indicators



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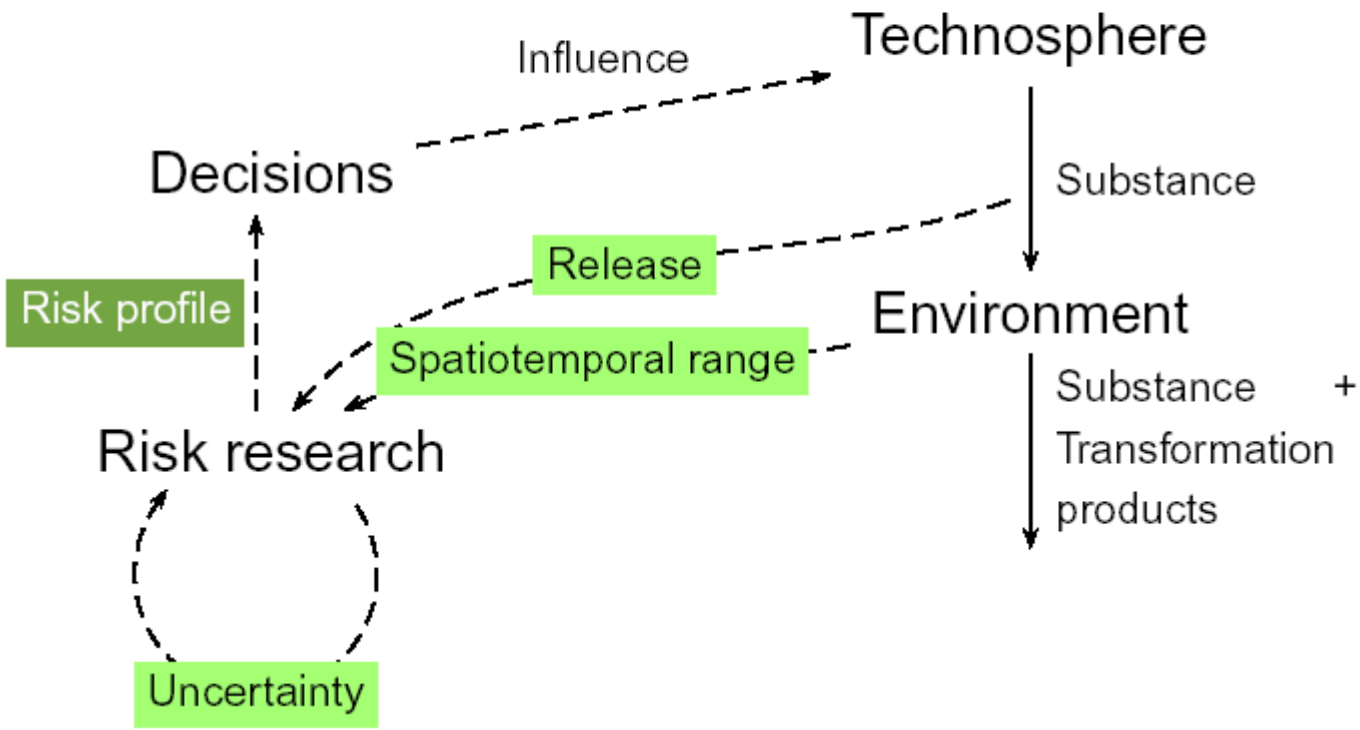
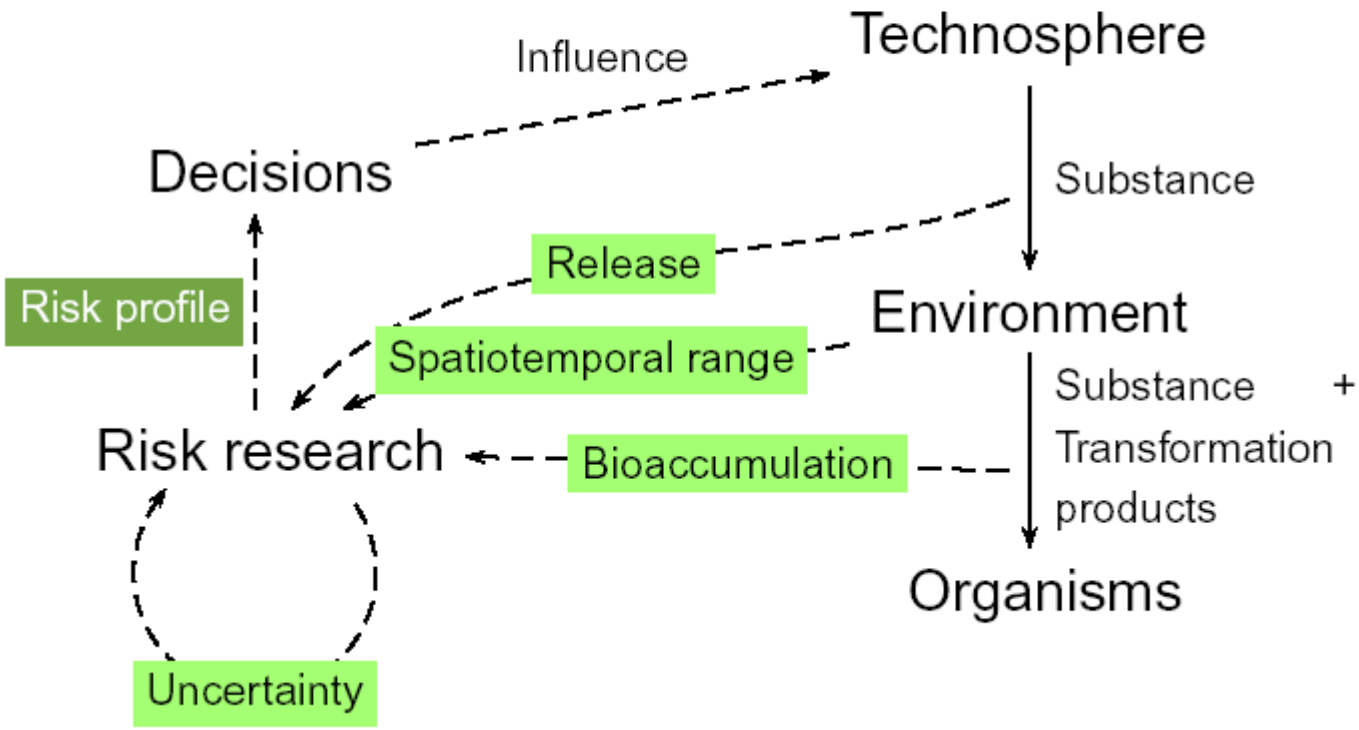
Five risk indicators



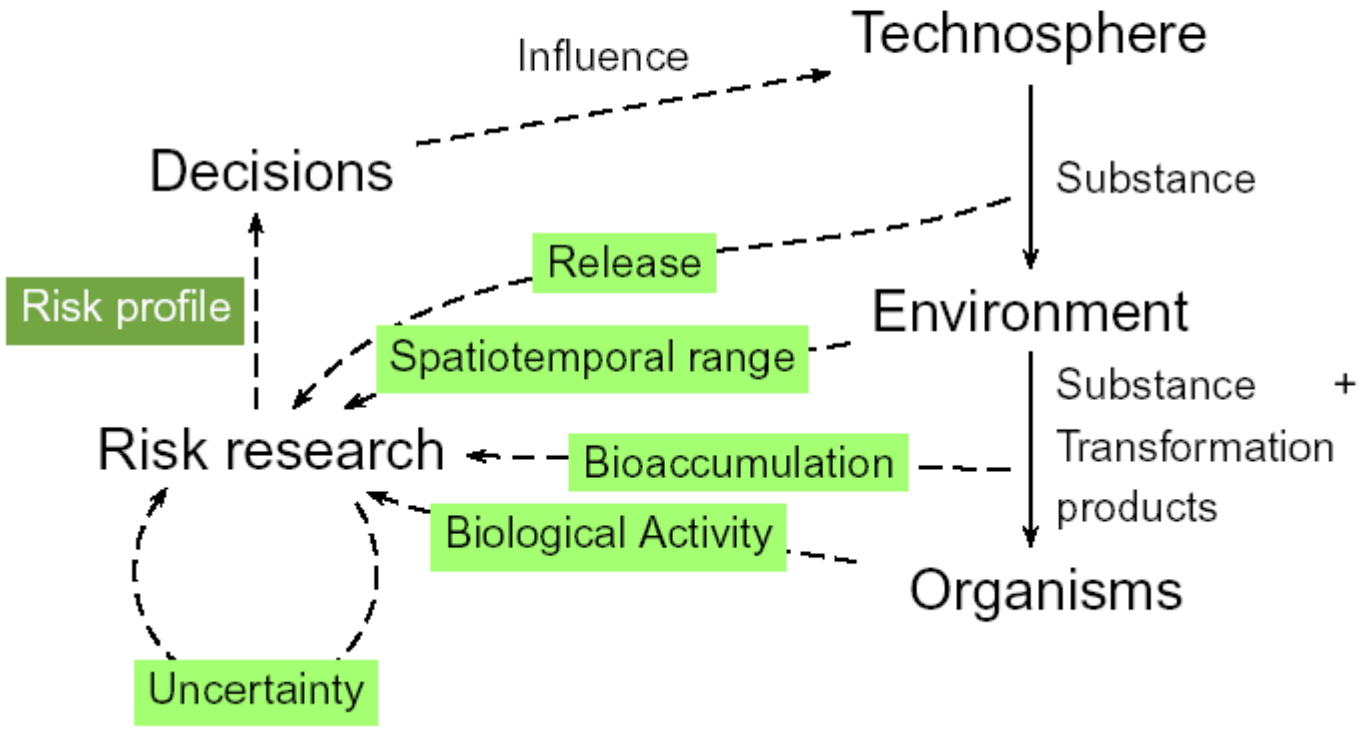
Ranke J (2001) PhD Dissertation

Five risk indicators



Ranke J (2001) PhD Dissertation

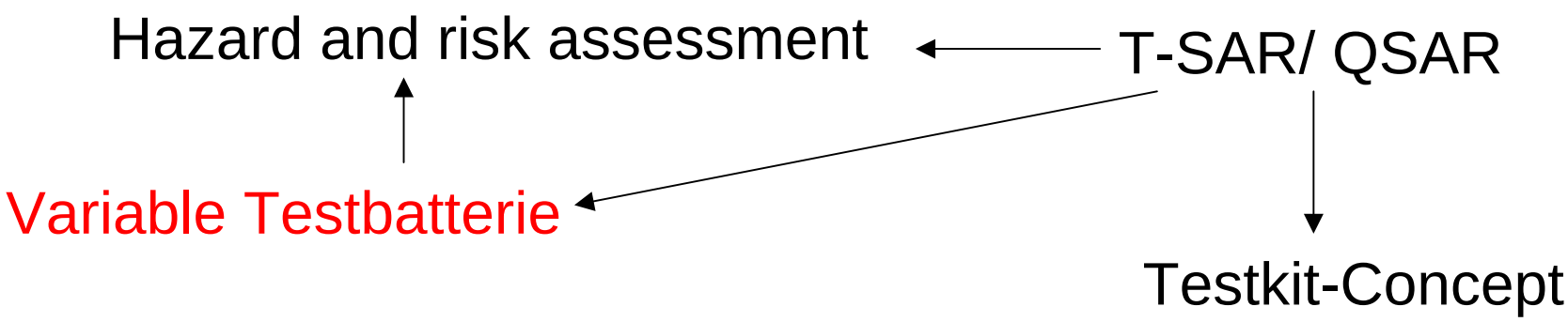
Five risk indicators



Interdisciplinary teamwork

Cooperation with companies

Our tools for the design of sustainable chemicals



TOXICOLOGY:

Effects of chemicals on an organism;

especially

biochemical, physiological or pathological effects

in man

ECOTOXICOLOGY:

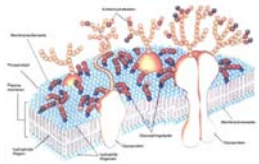
Effects of chemicals in the environment

on different levels

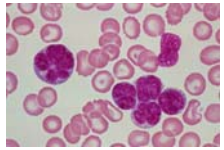
of biological omplexity

(Fent 1998)

Molecules of life



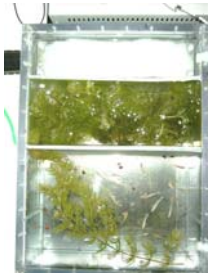
cell



organism

population

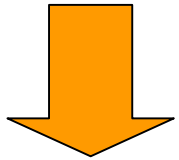
mesocosm



HIGH THROUGHPUT

SCREENING

rapid, simple, cost-effective

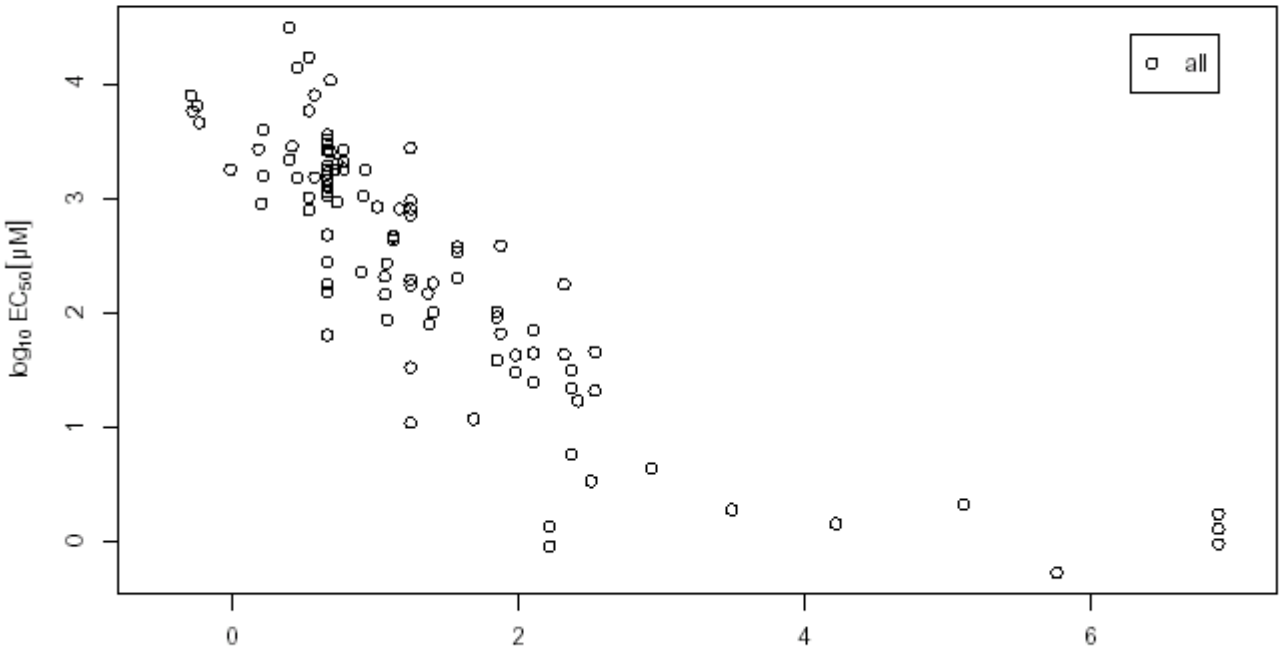


selected

SINGLE TESTS

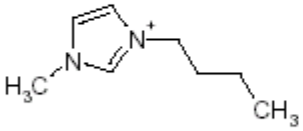
time-consuming, complex, expensive

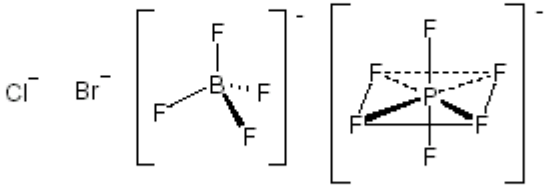
Cation lipophilicity and cytotoxicity



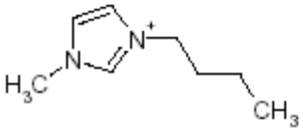
Ranke et al. *Ecotoxicol Environ Safety* **2006** in press
Stolte et al., in preparation

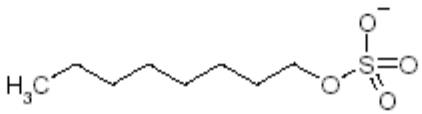
Are IL readily biodegradable?



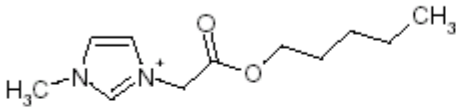


0 - 3 %



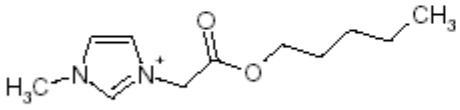


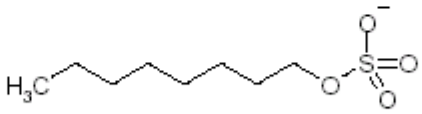
25 %



Br^-

32 / 41 %



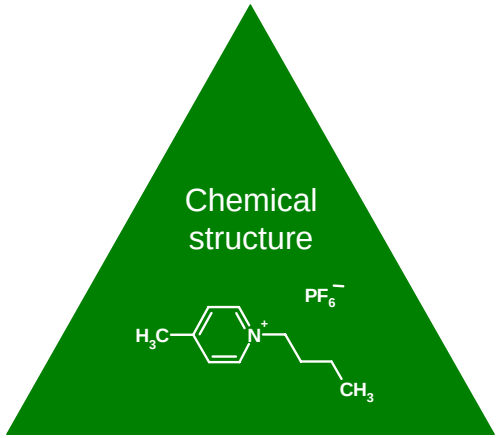


54 / 67 %

N. Gathergood, M. T. Garcia, and P. J. Scammells. *Green Chem* **2004**, **2005**, **2006**

Aim: „Sustainable Productdesign)

Technical needs

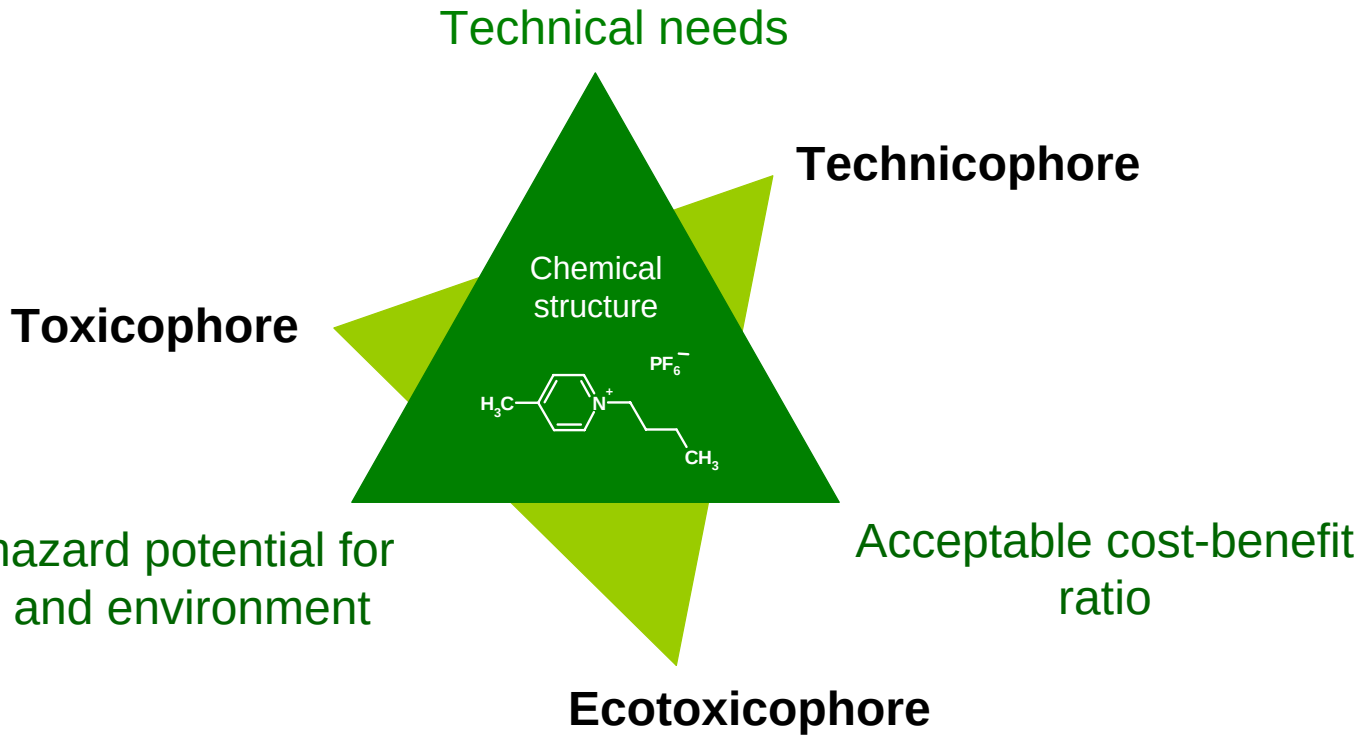


Low hazard potential for
Man and environment

Acceptable cost-benefit
ratio

Jastorff et al. 2003
Green Chemistry 5
136-142

Aim: „Sustainable Productdesign)



Jastorff et al. 2003
Green Chemistry 5
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**„The significant problems
we face
cannot be solved
at the same level of thinking
we were at
when we created them“**

Albert Einstein

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Sustainability

starts in the mind