



**“Att hitta vad som helst i  
vad som helst”**

Non-target screening  
Förutsättningslös analys

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Inget nytt under solen...

# THE PCB STORY

BY SÖREN JENSEN

*The accumulation of PCB in nature and thus in the food chains was unknown to scientists until 1966, although the substance had been used industrially since 1929. It was the Swedish chemist Sören Jensen who, when analyzing DDT accumulations in nature, accidentally found enormous quantities of unknown substances that were later on identified as PCB compounds. PCB constitutes perhaps the most stable group of organic substances in existence. It poses, therefore, a severe threat to life-forms.*

*In Sweden this discovery has led to a law prohibiting the use, import, manufacture and sale of PCB without permission from the authorities.*

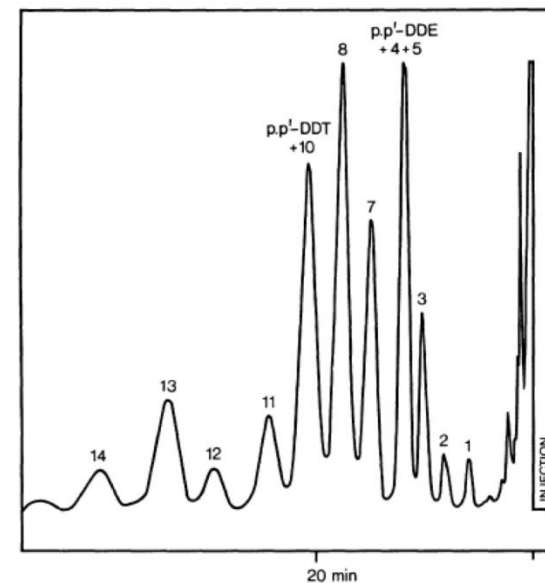
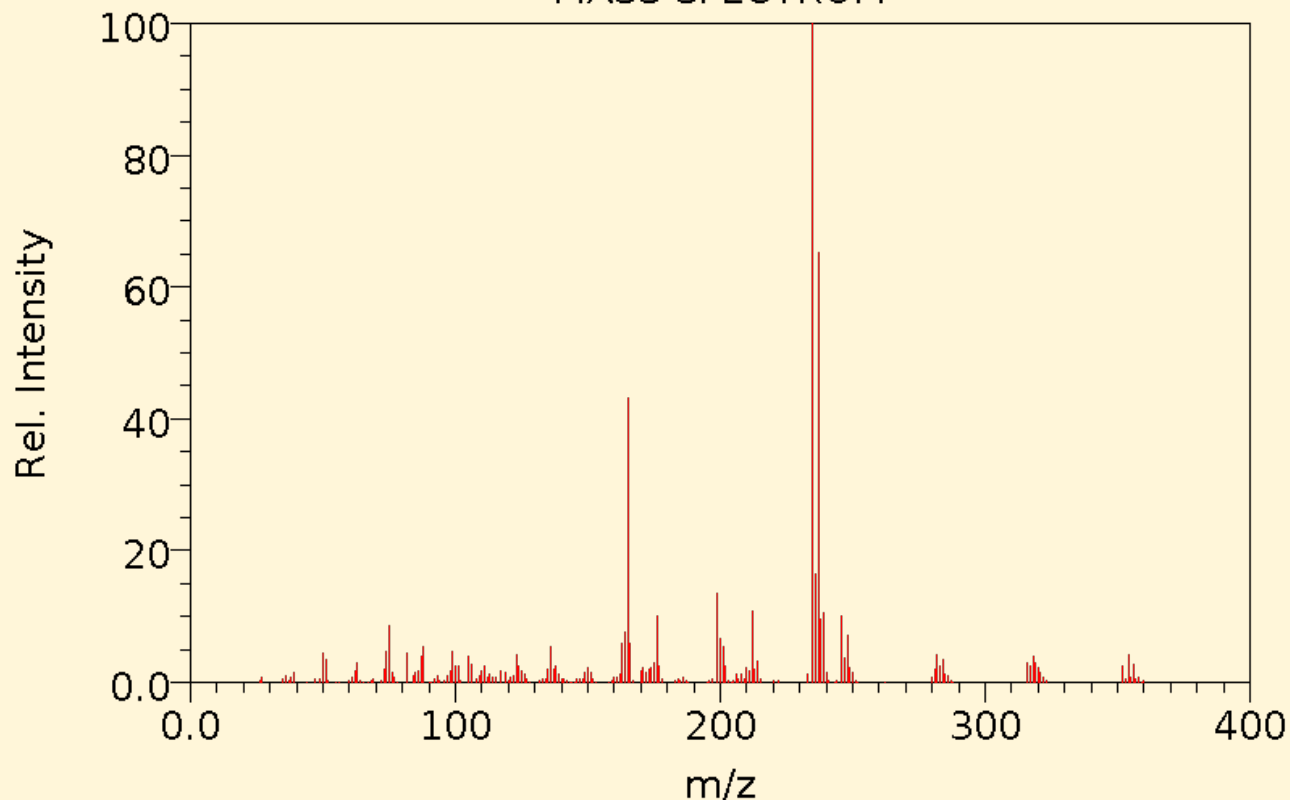


Figure 1. Gas chromatogram from purified extract from white-tailed eagle. All peaks but DDT and DDE were unknown. Column: SF 96 4 % on Gas Chrom P (HMDS-treated).

# GC har bra bibliotek

p,p'-DDT  
MASS SPECTRUM



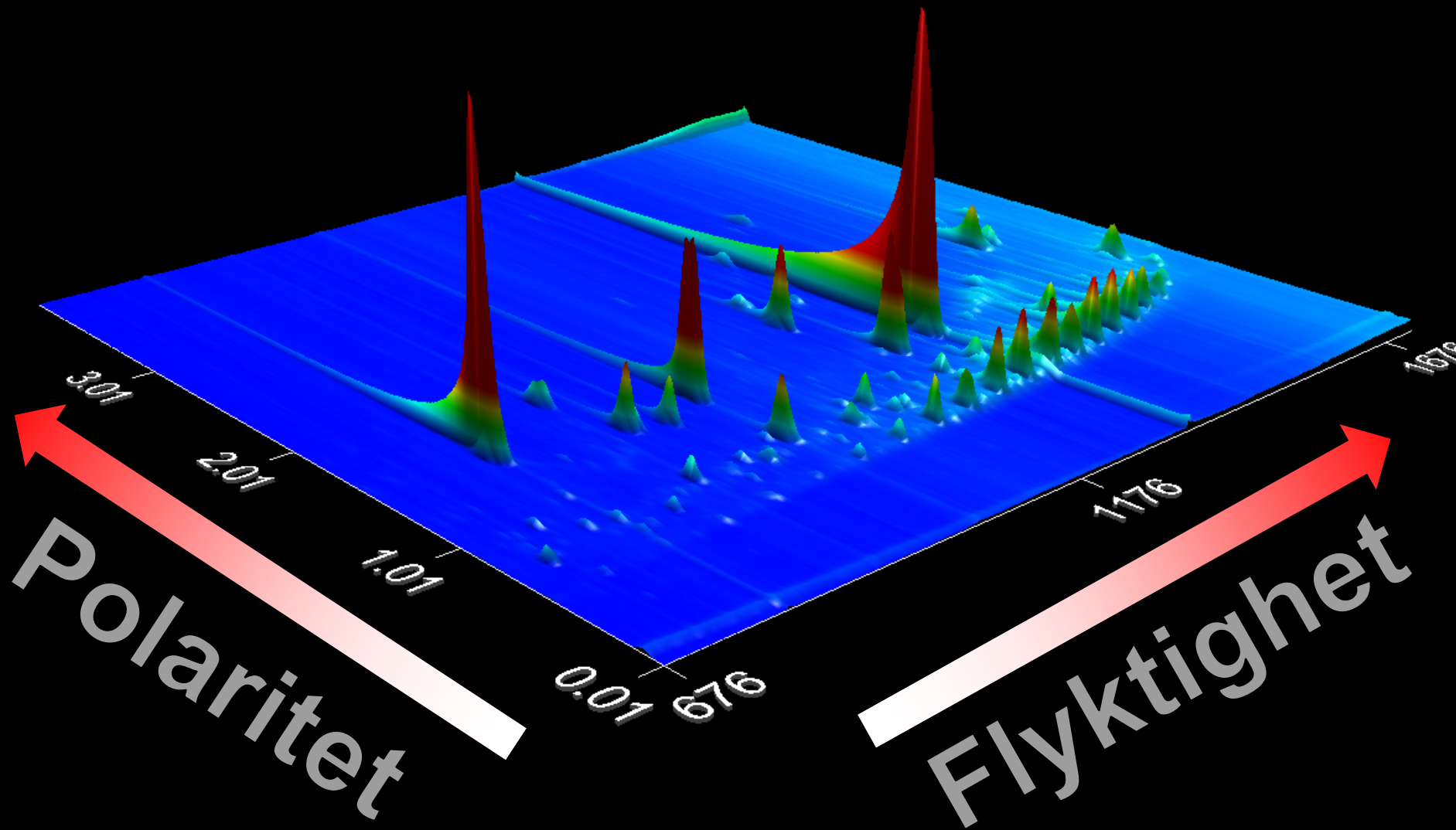
NIST Chemistry WebBook (<http://webbook.nist.gov/chemistry>)

Wiley/NIST

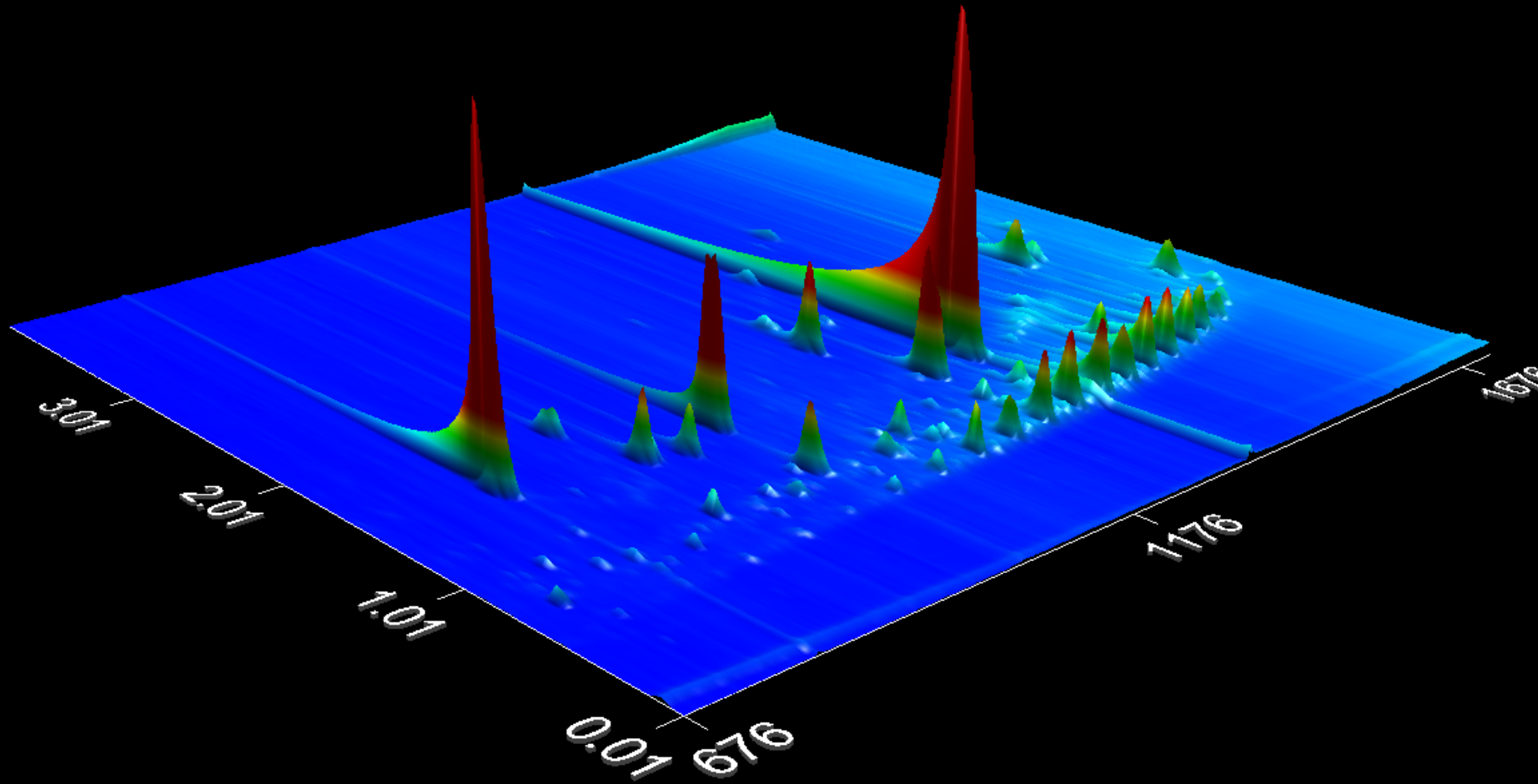
870,000 spektra + kemiska formler  
och exakta massor

ChEmitEcs

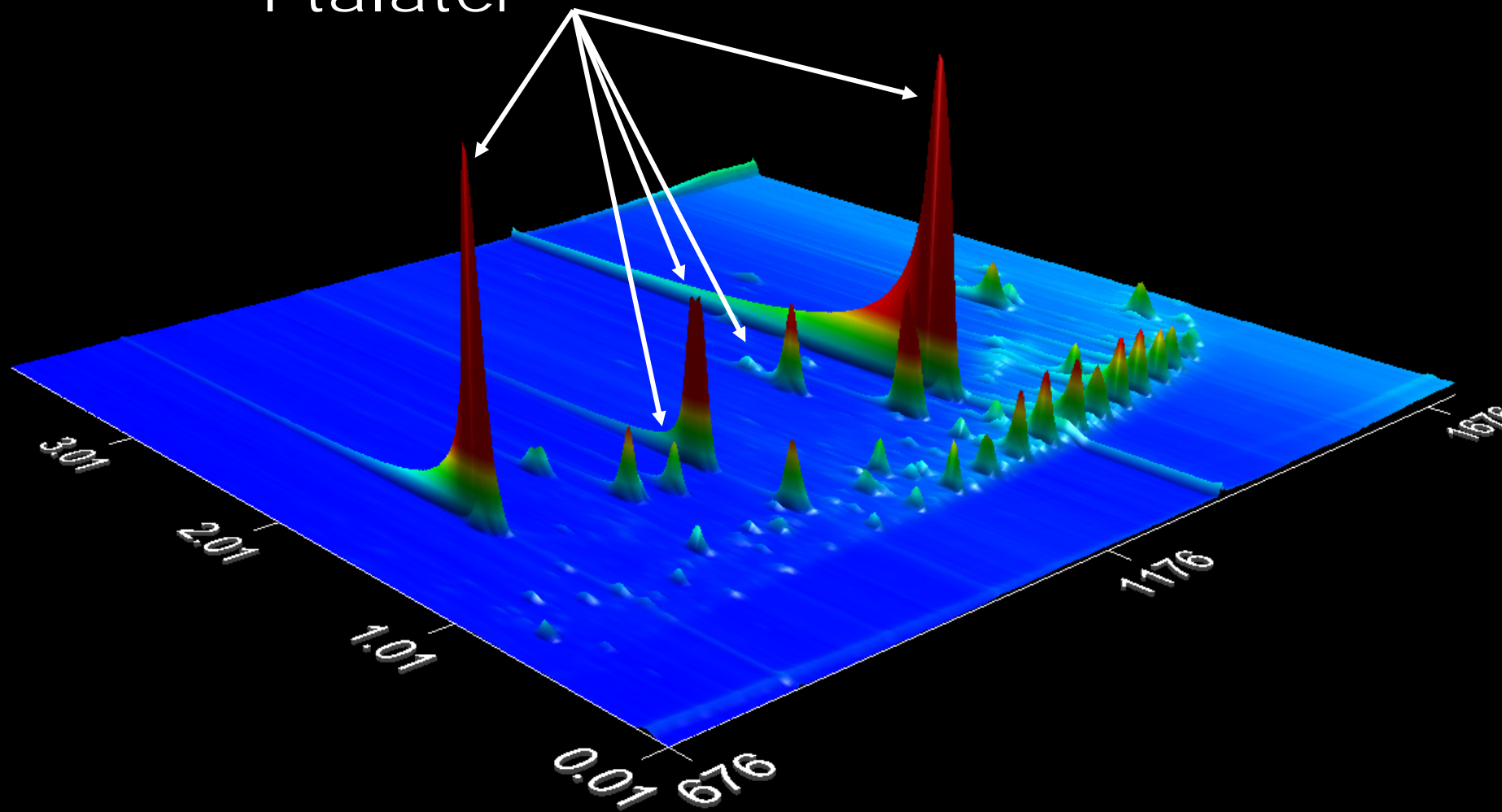
# GCxGC



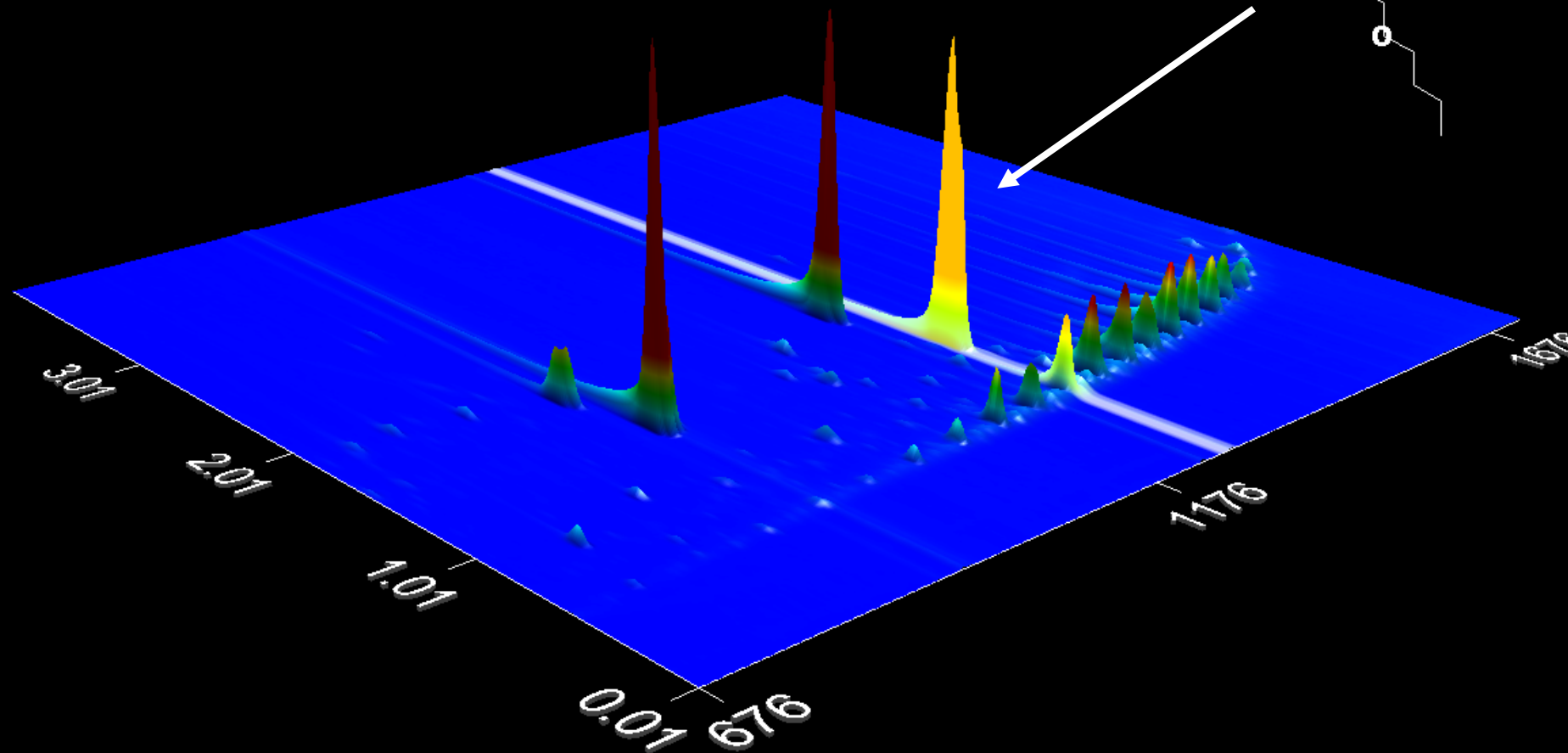
# Damm från Umeå kommunhus



Ftalater

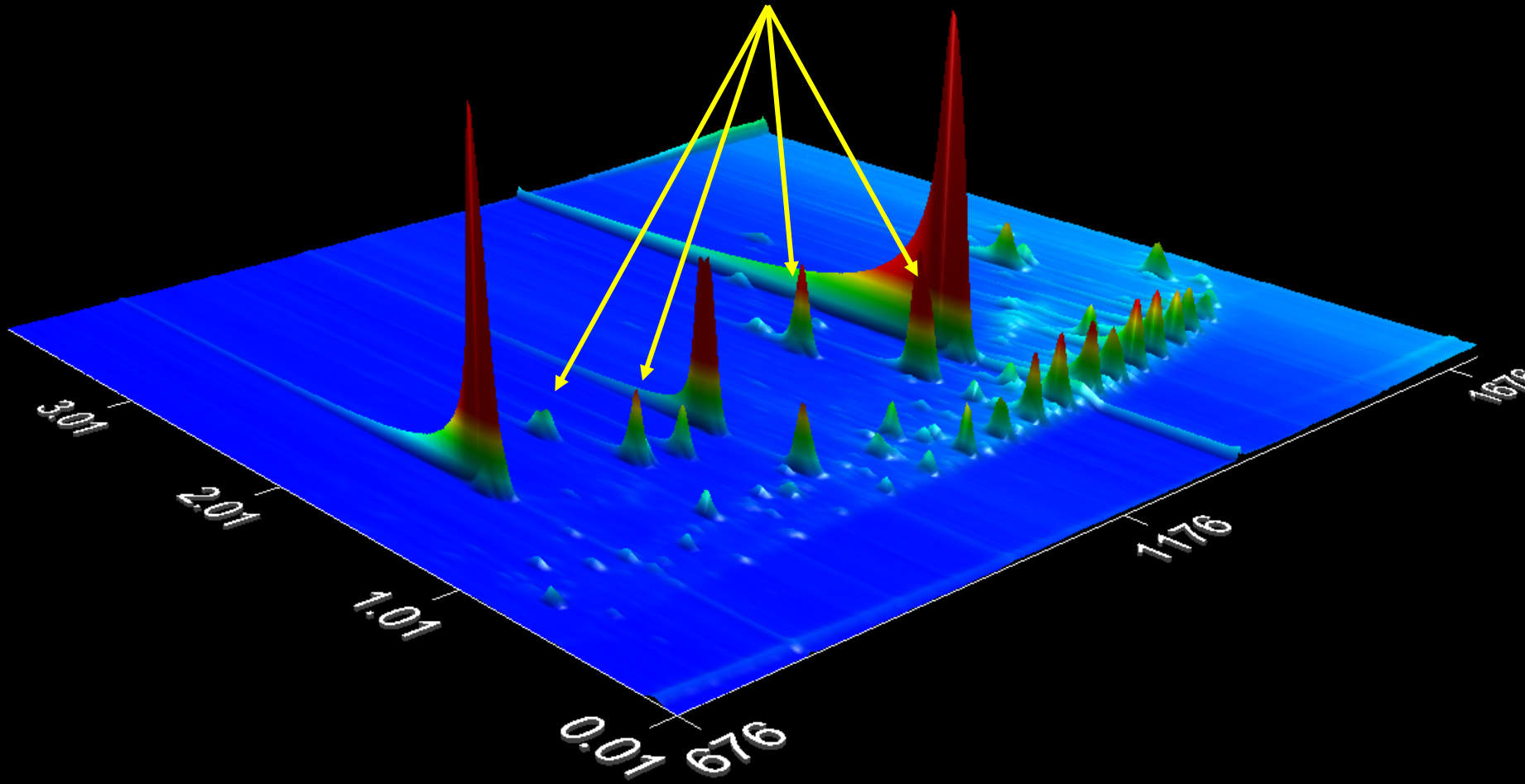


# Organofosfat screening/ identifierring (m/z = 99)



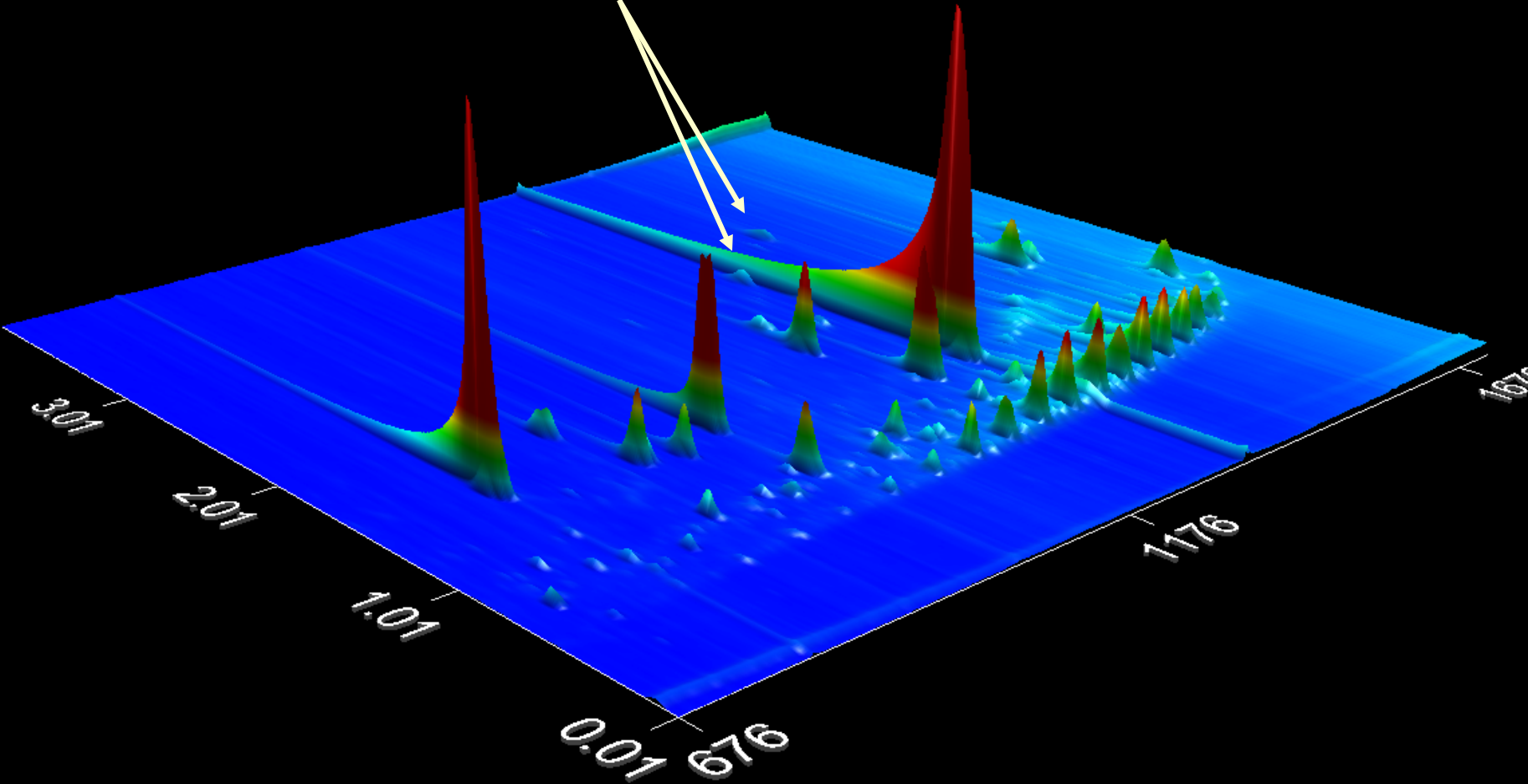
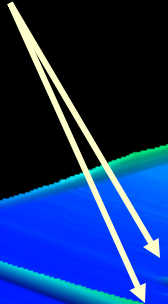
Name	Similarity	Reverse	Probability	CAS
Ethanol, 2-butoxy-, phosphate (3:1)	857	860	8680	78-51-3
Ethanol, 2-butoxy-, phosphate (3:1)	839	862	8520	78-51-3
7-Methyl-Z-tetradecen-1-ol acetate	524	537	85	0-00-0

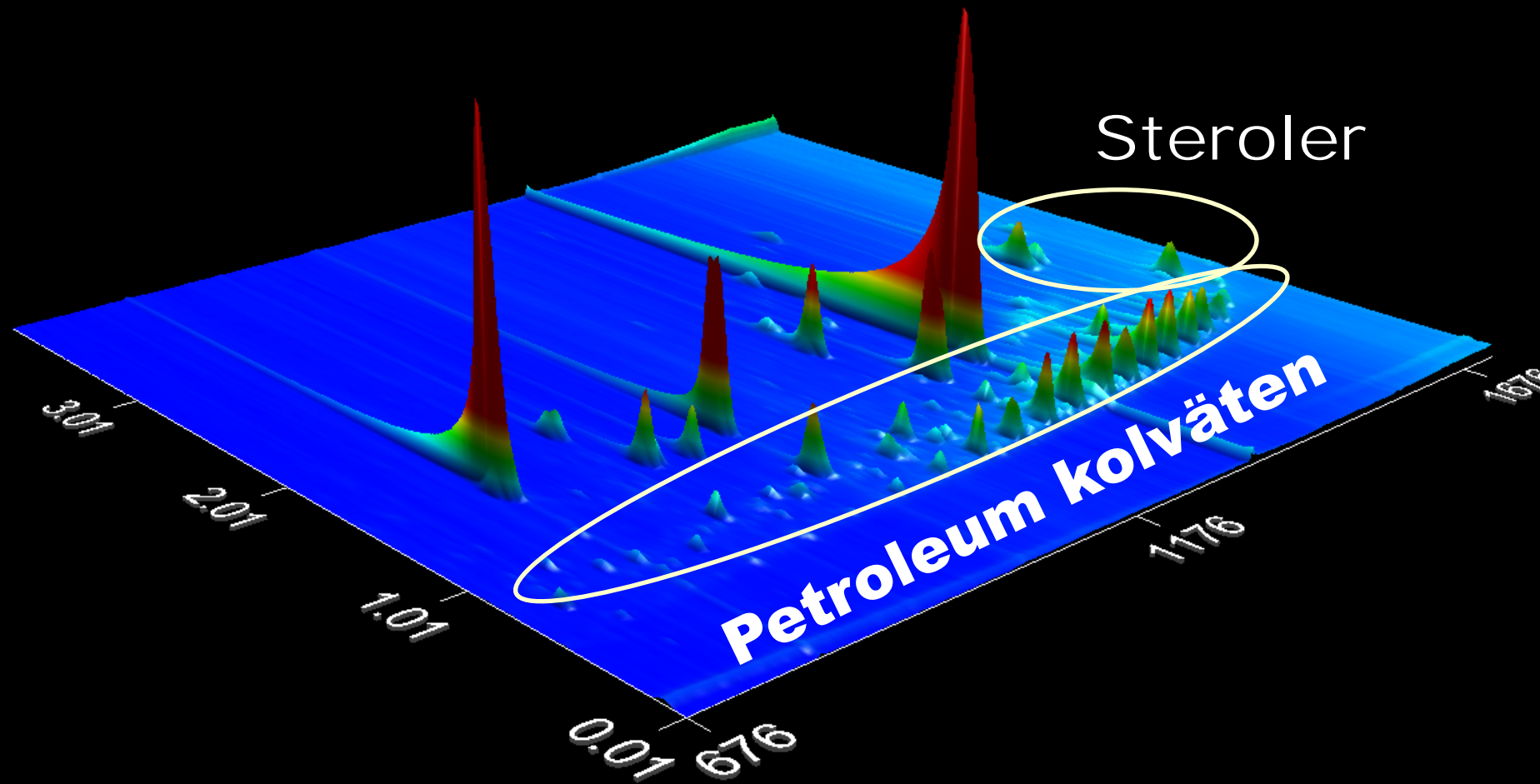
# Organofosfater





PBDE





Steroler

**Petroleum kolväten**

# Nytt NV projekt: Non-target screening av slam, vatten och luft

- Metodik för förutsättningslös karaktärisering
- Ny teknik för datautvärdering
- Protokoll för långtidslagring av data (digital provbankning)
- Karaktärisera slam-, vatten- och luftprover
- Potential för retrospektiv analys
- Internationell harmonisering