

Implementing AnIML 1.0:

The AnIML Technique Definition Document for Chromatography

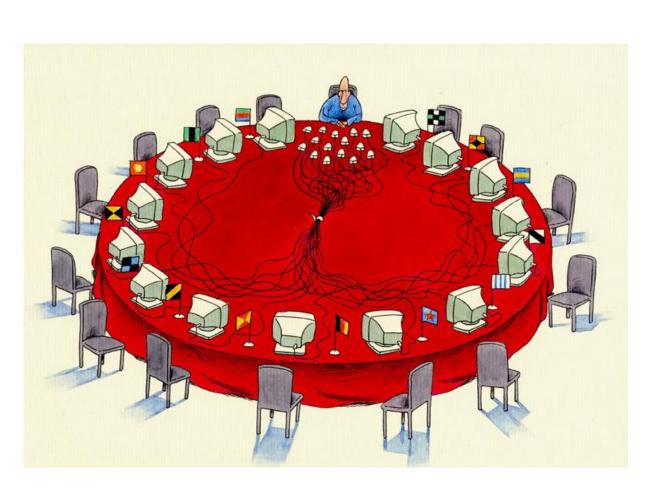
Dr. Maren Fiege Waters GmbH

March 13, 2011 PittCon 2011, Atlanta, GA, USA

Overview



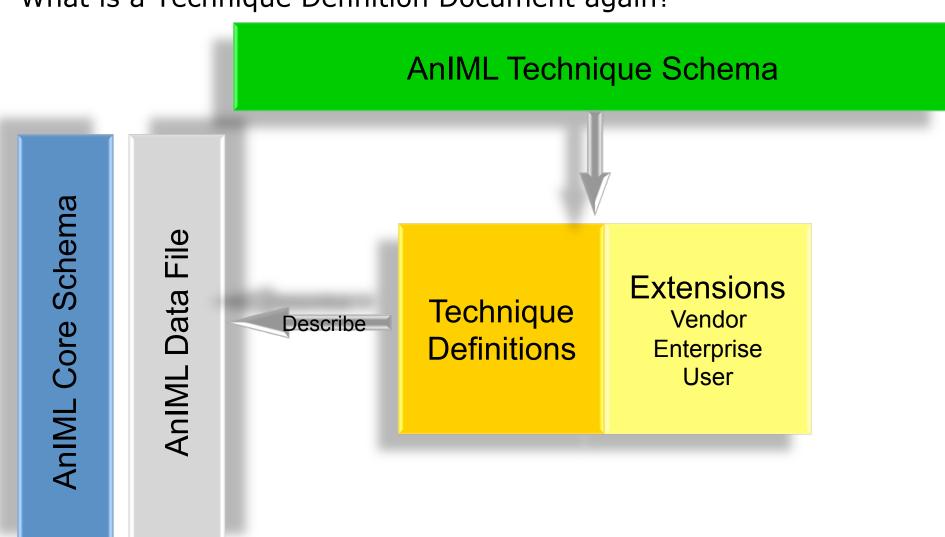
- Quick recap
- Development
- Applicability
- Lessons learned
- Q&A



Recap



What is a Technique Definition Document again?

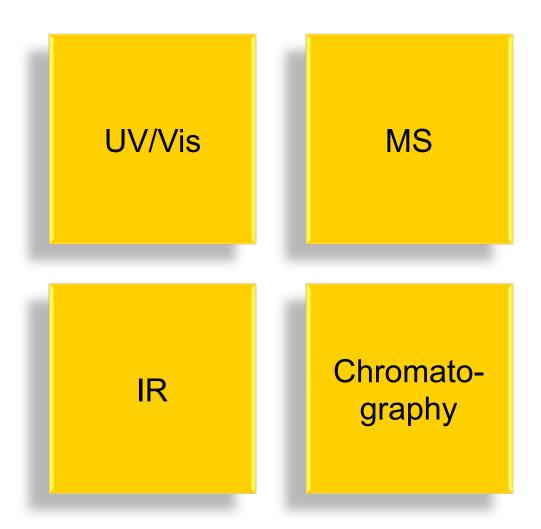


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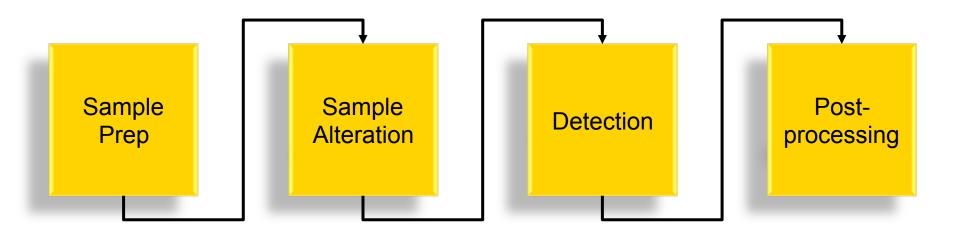
Which one is not like the others?





Sample Altering Technique





n/a

Chromatography UV/Vis

MS

NMR

IR

PeakFinding

Smoothing



Typical Detection Technique

Samples and their Roles

Parameters (Instrument...)

Measurement Data (Spectra...)

Chromatography

Samples and their Roles

Parameters (Instrument, Method...)

Measurement Data



Chromatography

Samples and their Roles

Parameters (Instrument, Method...)

Measurement Data

Test Sample

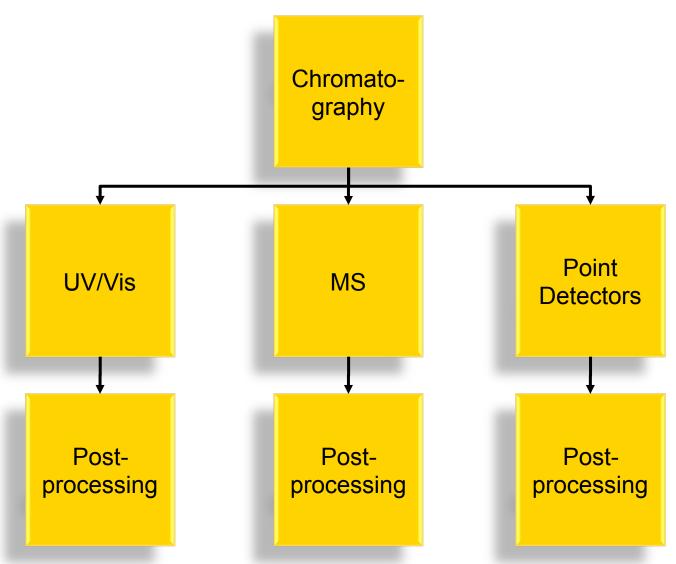
Mobile Phase

Wash Solvent Weak/Strong

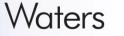
Instrument System Descr.
Sample Introduction
Inlet
Pump
Carrier Gas Control
Mixing
Separation Medium
Oven
Switch Valve
Fraction Collector
AD Converter Channel

Separation Monitoring Timeline!

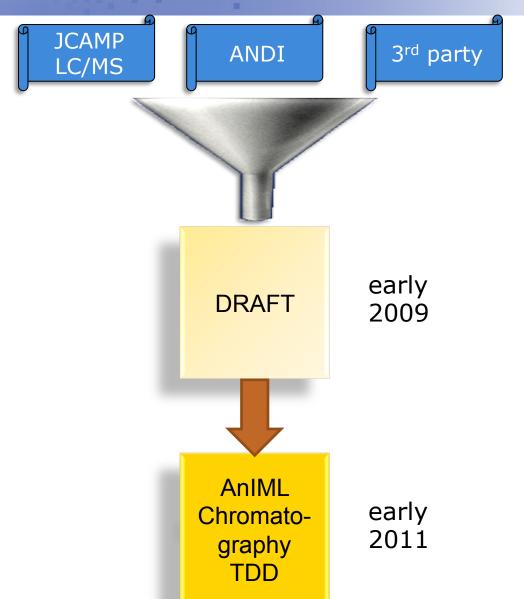




Development



THE SCIENCE OF WHAT'S POSSIBLE.™



2007

Who is involved?







Agilent Technologies

















and more...

Applicability



In:

- LC (incl. HPLC, U(H)PLC)
- GC
- TLC, prep. TLC
- Paper Chromatography
- Gel Permeation
- Ion Exchange
- Flash Chromatography
- Separation Monitoring (T, p, Flow rate)

Out:

- SFC (Extension)
- Electrophoresis (Extension)

- Any detectors
- Fraction Collection (Extension)

Lessons Learned



Chromatography is...

- Different
- Challenging
- A good test of the AnIML concepts

Keys to success:

- Frequent, regular meetings
- Subject matter experts
- Collaboration
- Participation!



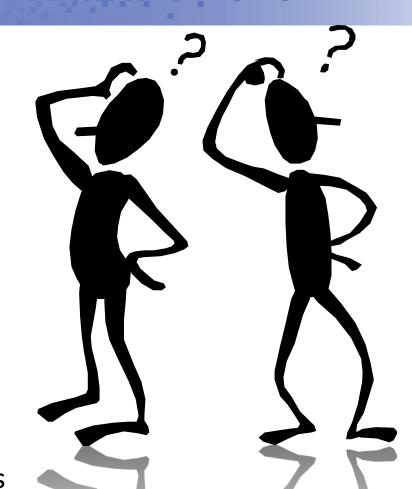
Sources of Information



- The AnIML Web Site
 - http://www.animl.org
- The SourceForge Analytical Information Markup Language Project: Summary Page
 - http://sourceforge.net/projects/animl

Thank you!





Next:

■ 2:20 PM - Recess

 2:35 PM - Crosswalking AnIML with Legacy Data Formats, Stuart Chalk