



Exploring spectroscopic and morphological data as new signatures for uranium ore concentrates

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**IAEA Nuclear forensics
conference (7-10 July 2014)**

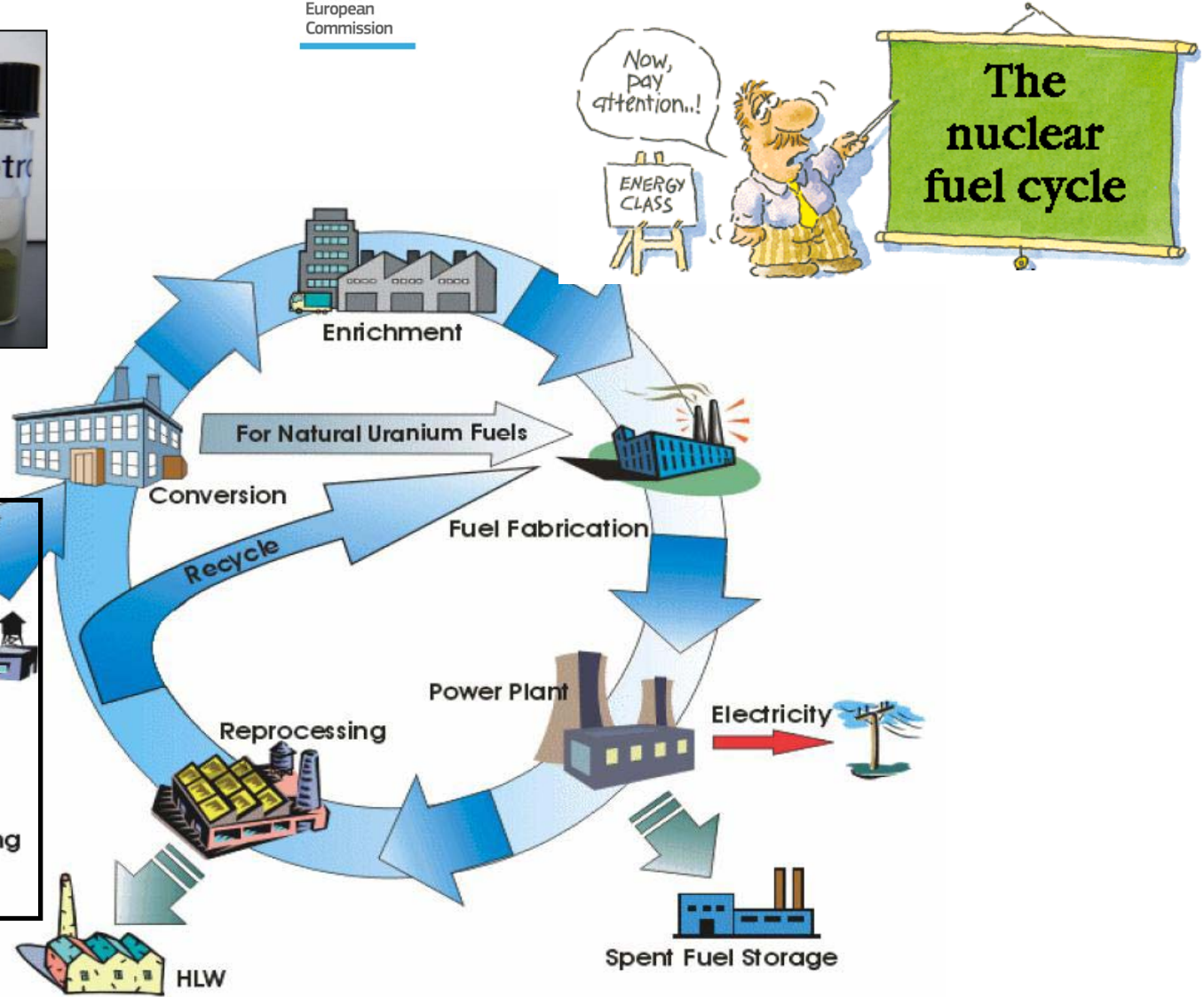
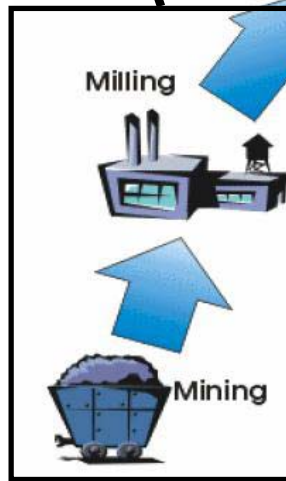
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Stimulating innovation
Supporting legislation*



Introduction



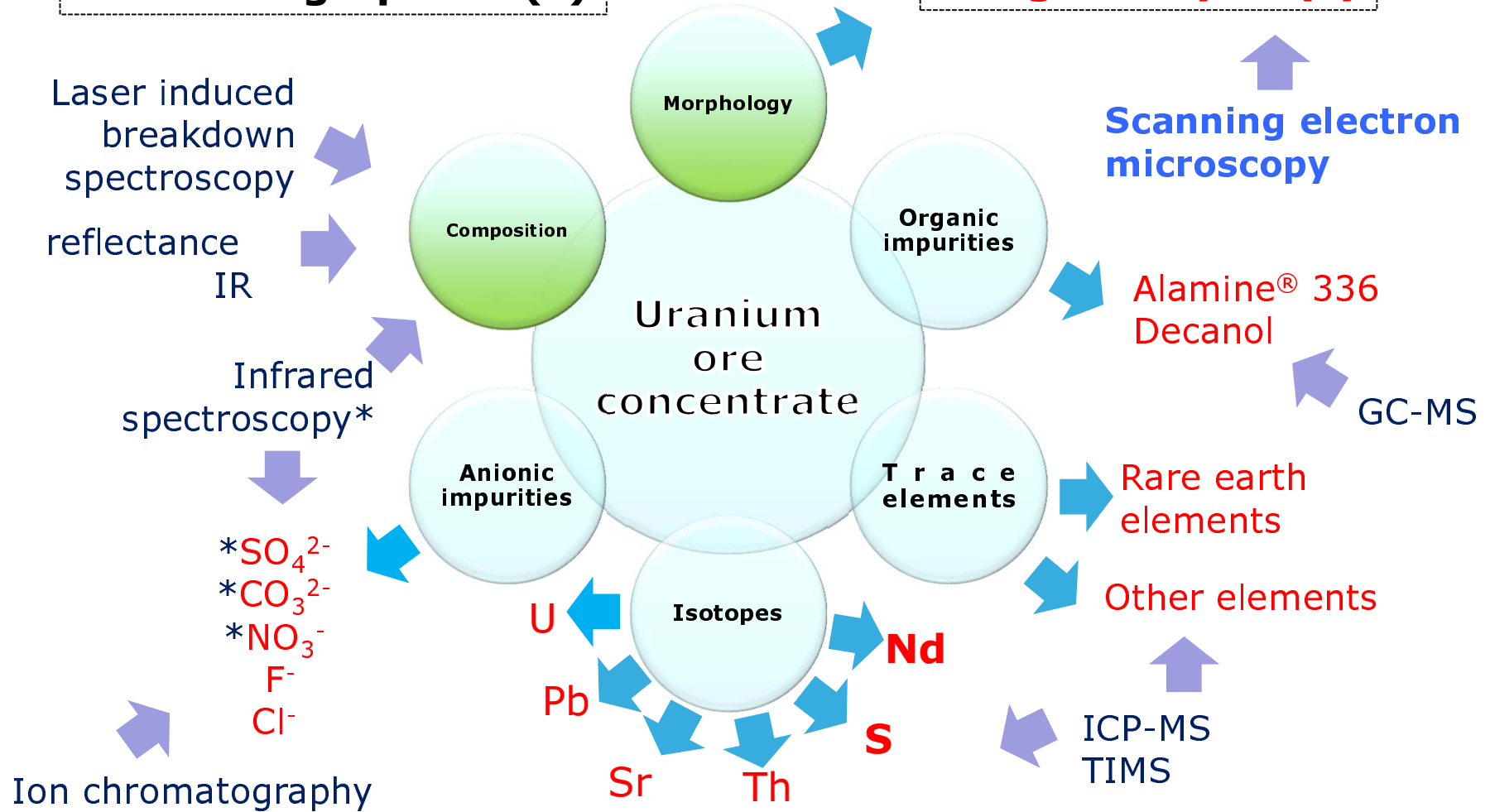
Uranium ore concentrates





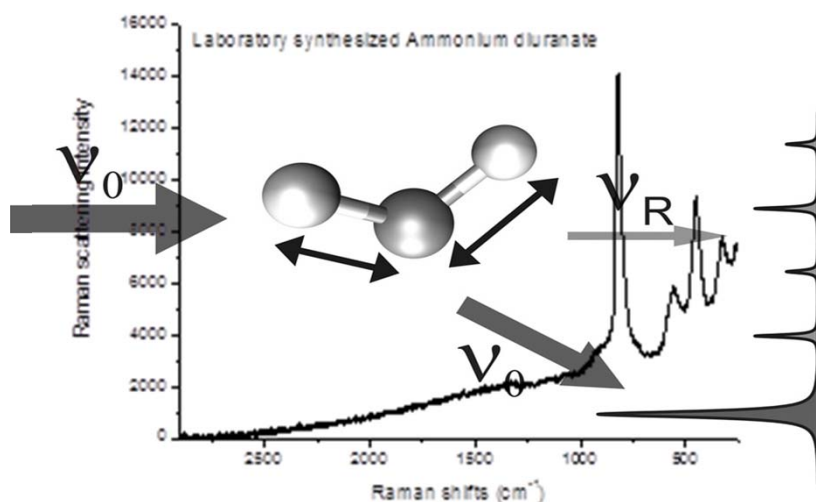
Raman fingerprints (?)

Image Analysis (?)



1. Raman spectroscopy

Raman spectroscopy (Bulk analysis)



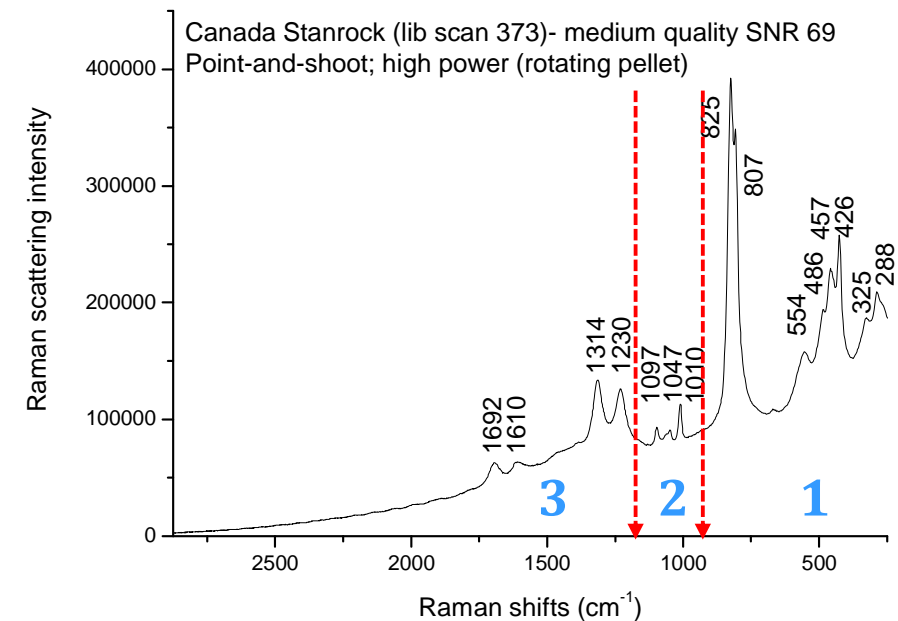
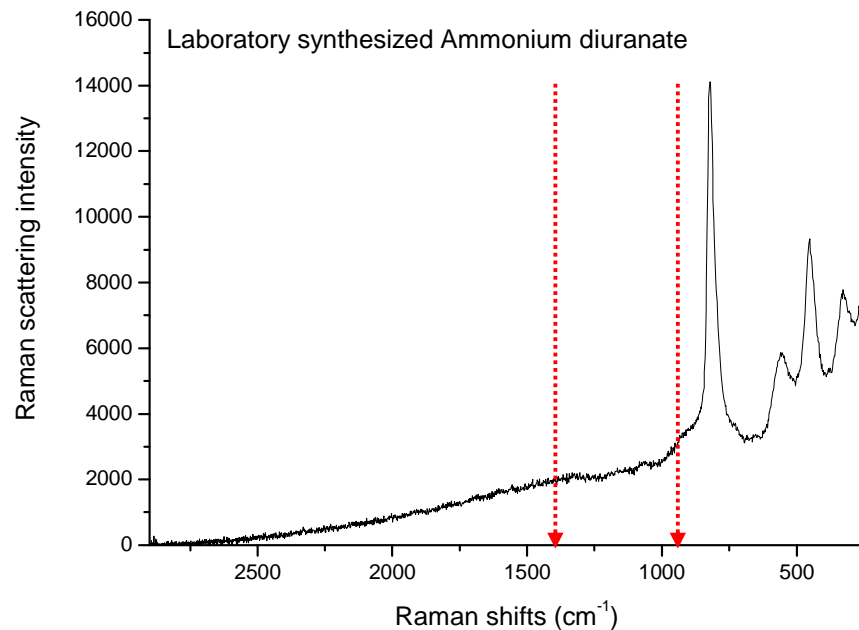
A laser (ν_0) is used to excite the molecules to virtual states. As a result of the interaction with molecules, incident photons are scattered *inelastically* (only 1 out of 10^8 photons) → Raman effect (ν_R)

http://www.wiley-vch.de/books/sample/3527405062_c01.pdf
<http://www.nomenrl.com>
<http://www.bruker.com>
<http://www.physik.fu-berlin.de>

Results: Raman spectroscopy



Applicability of Raman spectroscopy to nuclear forensics



Raman bands relating to:

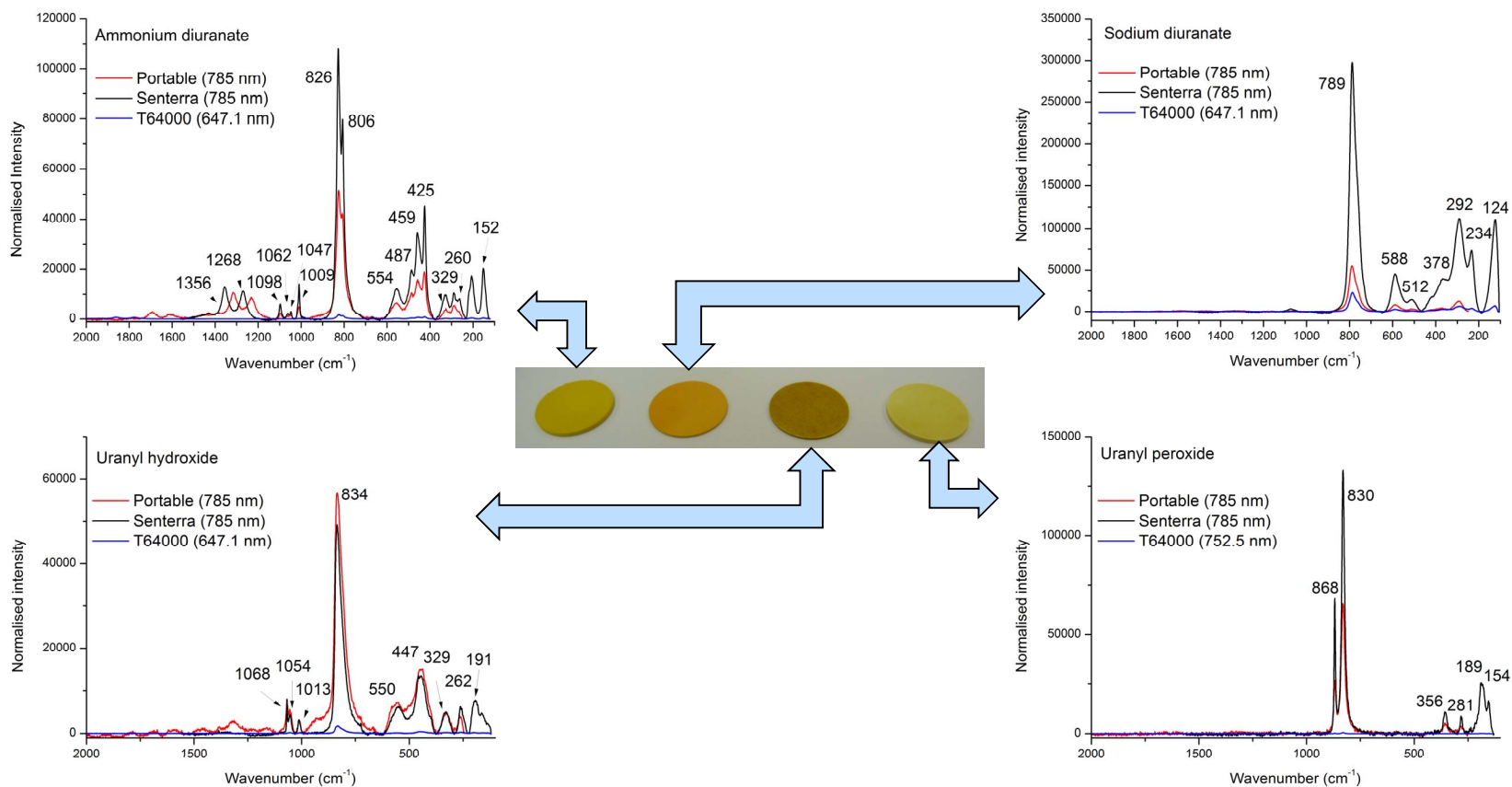
1. Uranium compound
2. Process related impurities
3. Electronic transitions (non-Raman effects)

D.M.L. Ho, D. Manara, Zs Varga, A. Berlizov, Th. Fanghänel and K. Mayer, *Radiochimica Acta* 12 (2013) 779-784.

Results: Raman spectroscopy



Comparison of 3 different dispersive Raman spectrometers

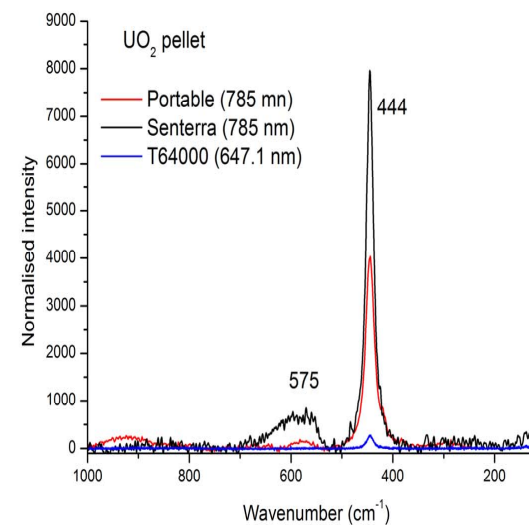
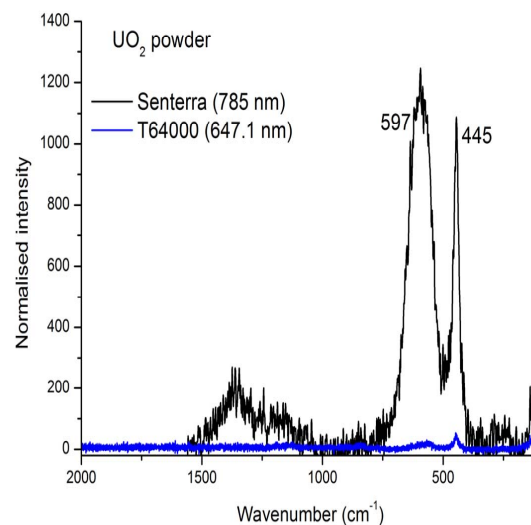
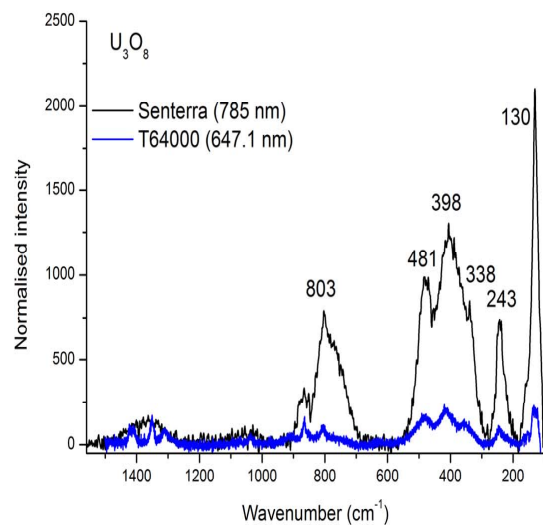


D.M.L. Ho, D. Manara, P. Lindqvist-Reis, Th. Fanghänel and K. Mayer, *Vibrational Spectroscopy* 73 (2014) 102-110.

Results: Raman spectroscopy



Comparison of 3 different dispersive Raman spectrometers



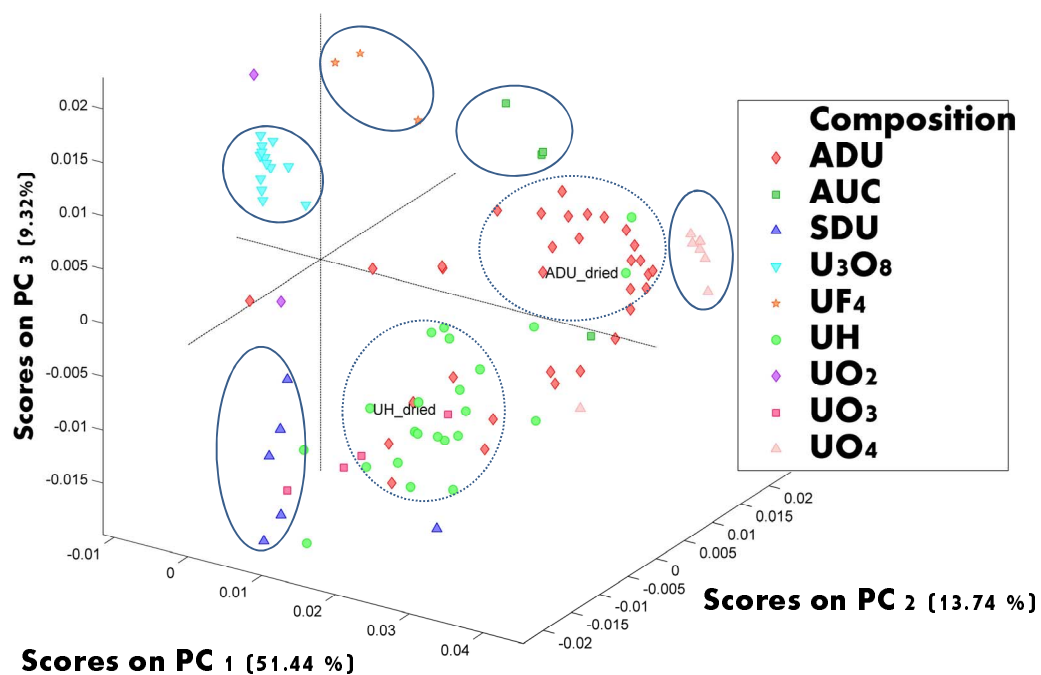
D.M.L. Ho, D. Manara, P. Lindqvist-Reis, Th. Fanghänel and K. Mayer, *Vibrational Spectroscopy* 73 (2014) 102-110.

Results: Raman spectroscopy

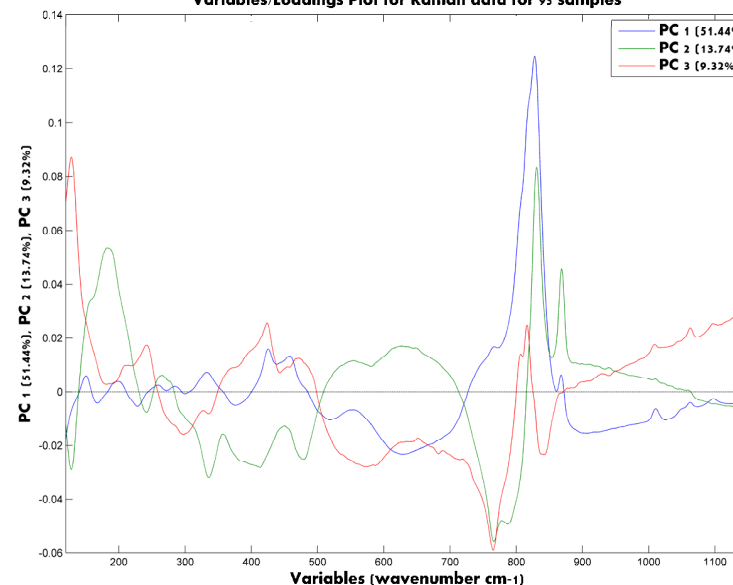


Unsupervised classifications of UOCs + other uranium compounds using principal component analysis (PCA)

Scores Plot of Raman data for 95 samples



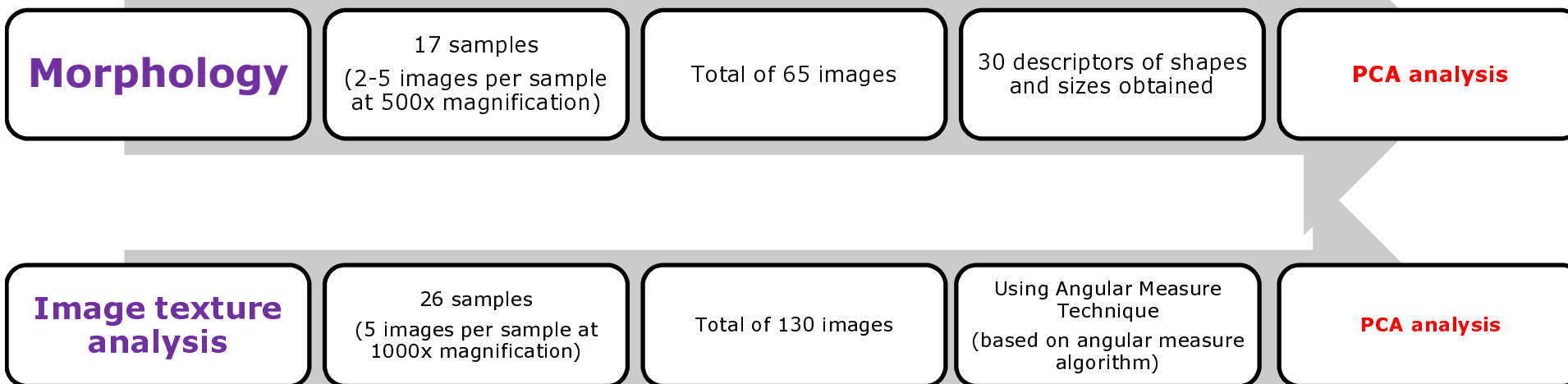
Variables/Loadings Plot for Raman data for 95 samples



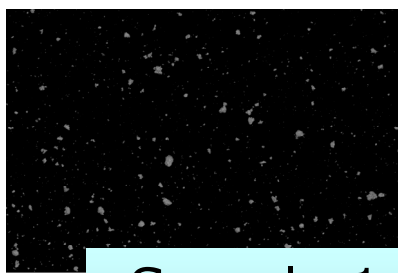
D.M.L. Ho, Z. Varga, L. Fongaro, P. Lindqvist-Reis, Th. Fanghänel and K. Mayer, Forensic Science International, -to be submitted for publication (together with AWE/Liverpool)



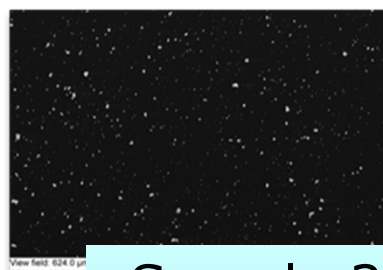
2. Image analysis of UOC



Sizes & shapes

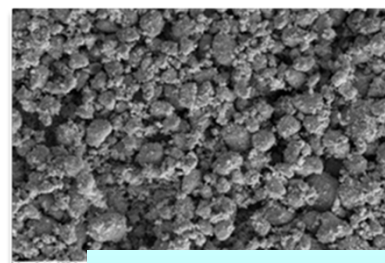


Sample 1

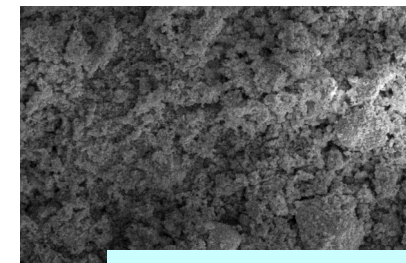


Sample 2

Image texture analysis



Sample 1



Sample 2

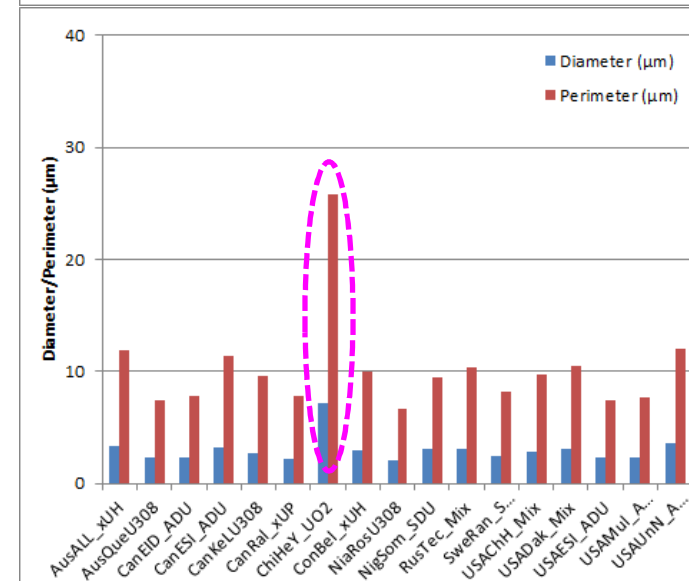
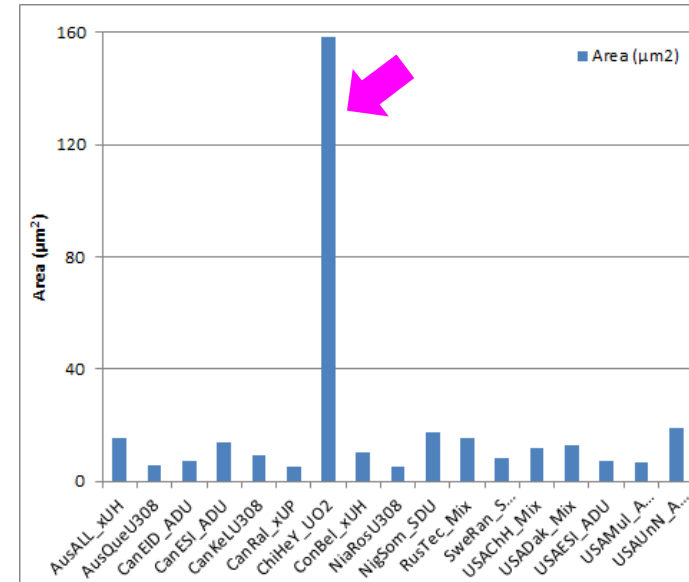
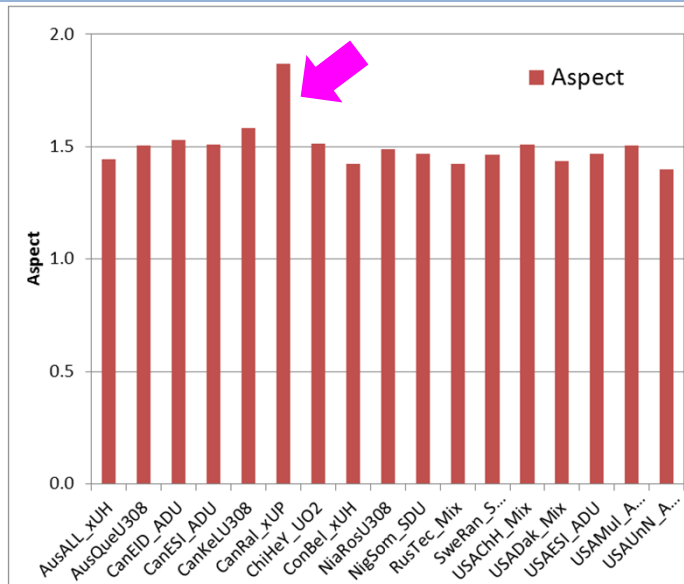
Results: Image Analysis

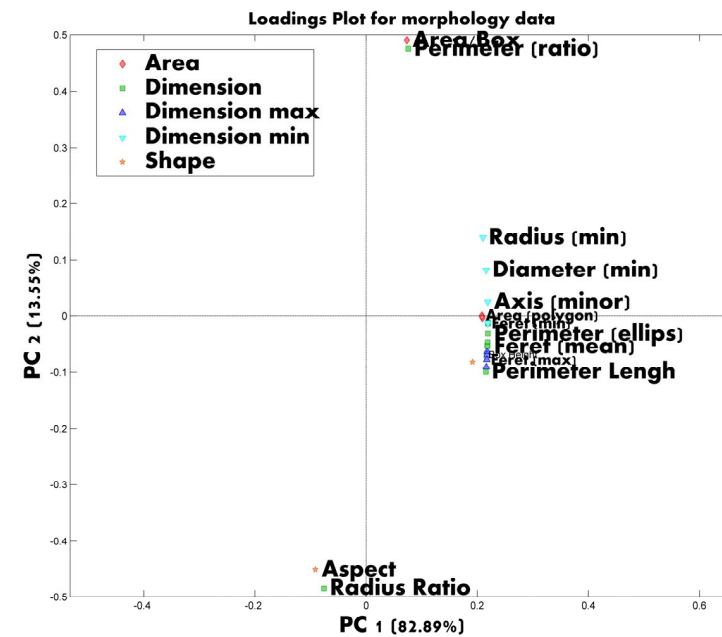
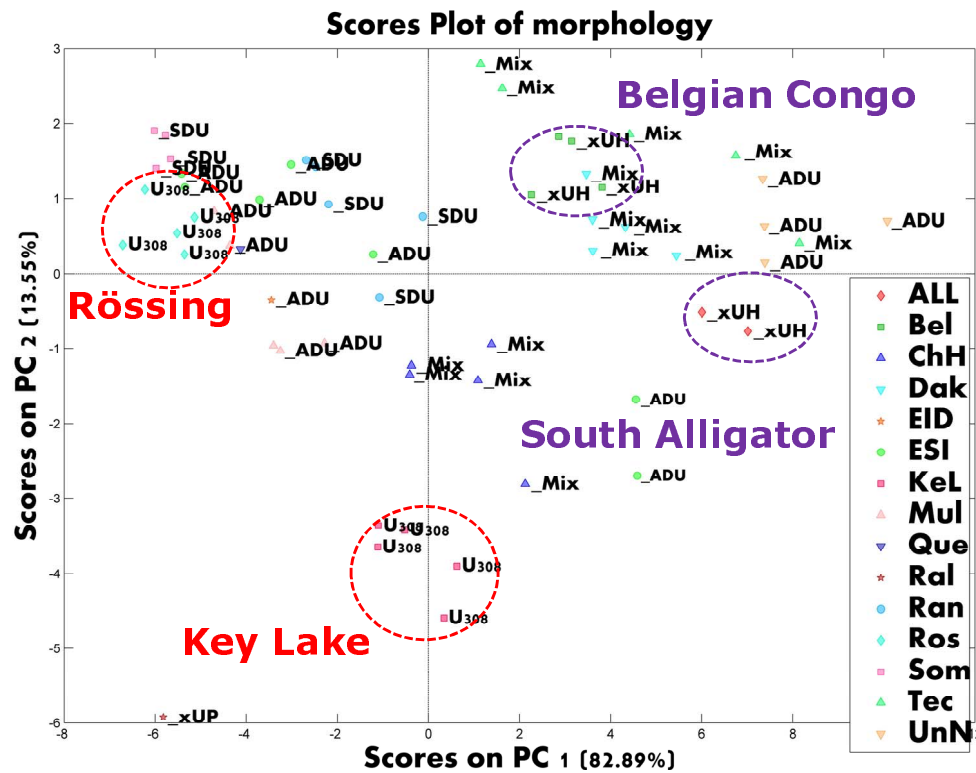


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Morphology

Sample name	Area (µm ²)	Diameter (µm)	Perimeter (µm)	Aspect
AusALL_xUH	15.16±0.53	3.38±0.08	11.88±0.32	1.44±0
AusQueU308	5.56±0	2.25±0	7.48±0	1.5±0
CanEID_ADU	7.15±0	2.32±0	7.85±0	1.53±0
CanESI_ADU	13.82±0.06	3.16±0.02	11.35±0.08	1.51±0.03
CanKeLU308	9.35±0.67	2.67±0.09	9.54±0.4	1.58±0.02
CanRal_xUP	5.21±0	2.13±0	7.83±0	1.87±0
ChiHeY_UO2	158.4±84.86	7.22±1.86	25.75±6.92	1.51±0.06
ConBel_xUH	10.23±0.48	3.01±0.07	9.93±0.23	1.42±0.02
NiaRosU308	5.36±0.59	2.08±0.07	6.63±0.26	1.49±0.02
NigSom_SDU	17.4±26.55	3.01±2.13	9.44±6.26	1.47±0.01
RusTec_Mix	15.37±4.89	3.13±0.32	10.4±1.32	1.42±0.02
SweRan_SDU	8.17±0.77	2.49±0.12	8.22±0.51	1.46±0.02
USACHH_Mix	11.91±1.22	2.76±0.12	9.69±0.55	1.51±0.02
USADak_Mix	12.98±2.03	3.12±0.09	10.48±0.42	1.44±0.01
USAESI_ADU	7.32±2.27	2.29±0.18	7.36±0.73	1.47±0.01
USAMul_ADU	6.91±0.96	2.31±0.1	7.67±0.5	1.51±0.03
USAUnN_ADU	18.97±1.66	3.54±0.15	12.02±0.5	1.4±0.03

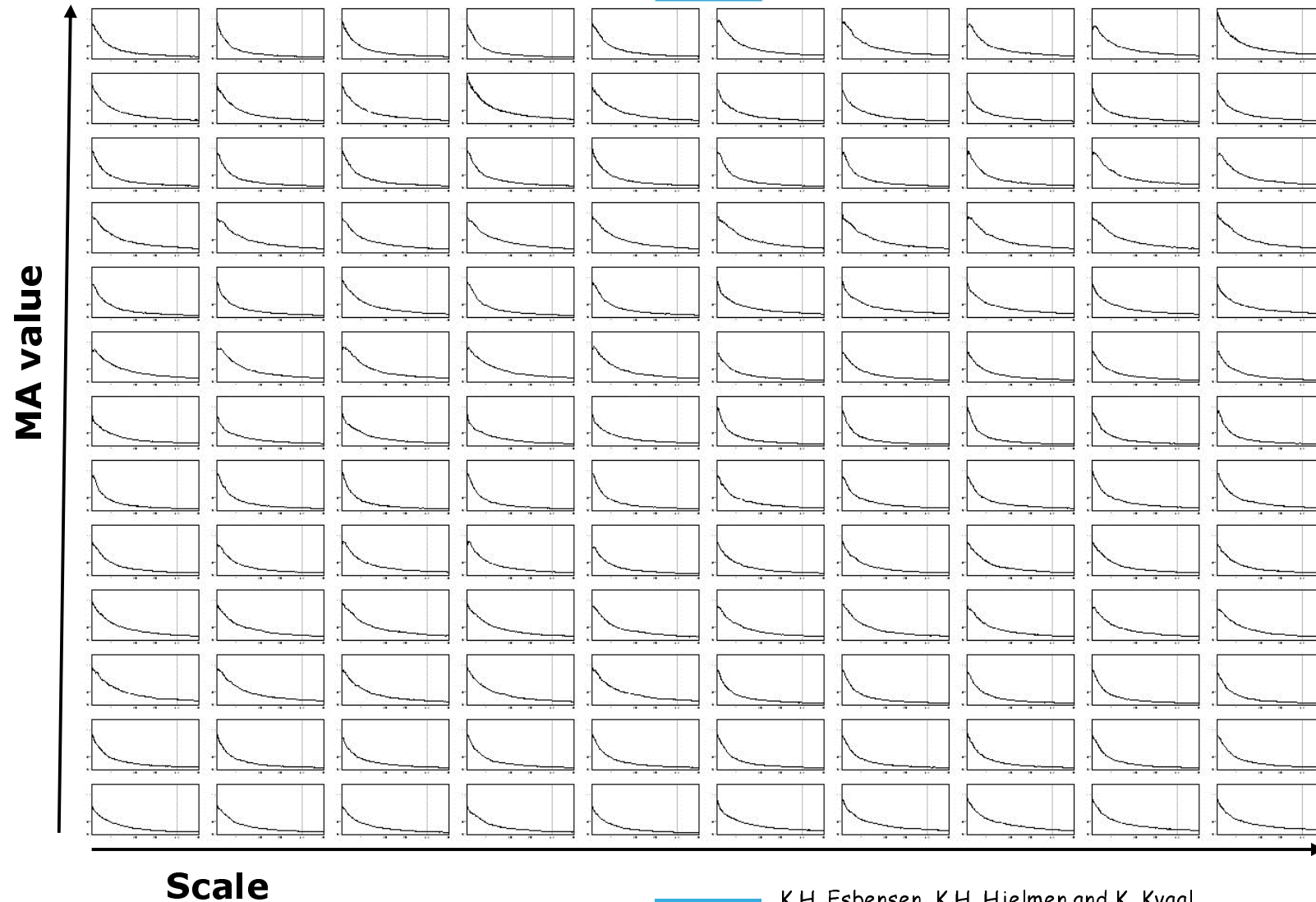




Results: Image texture analysis



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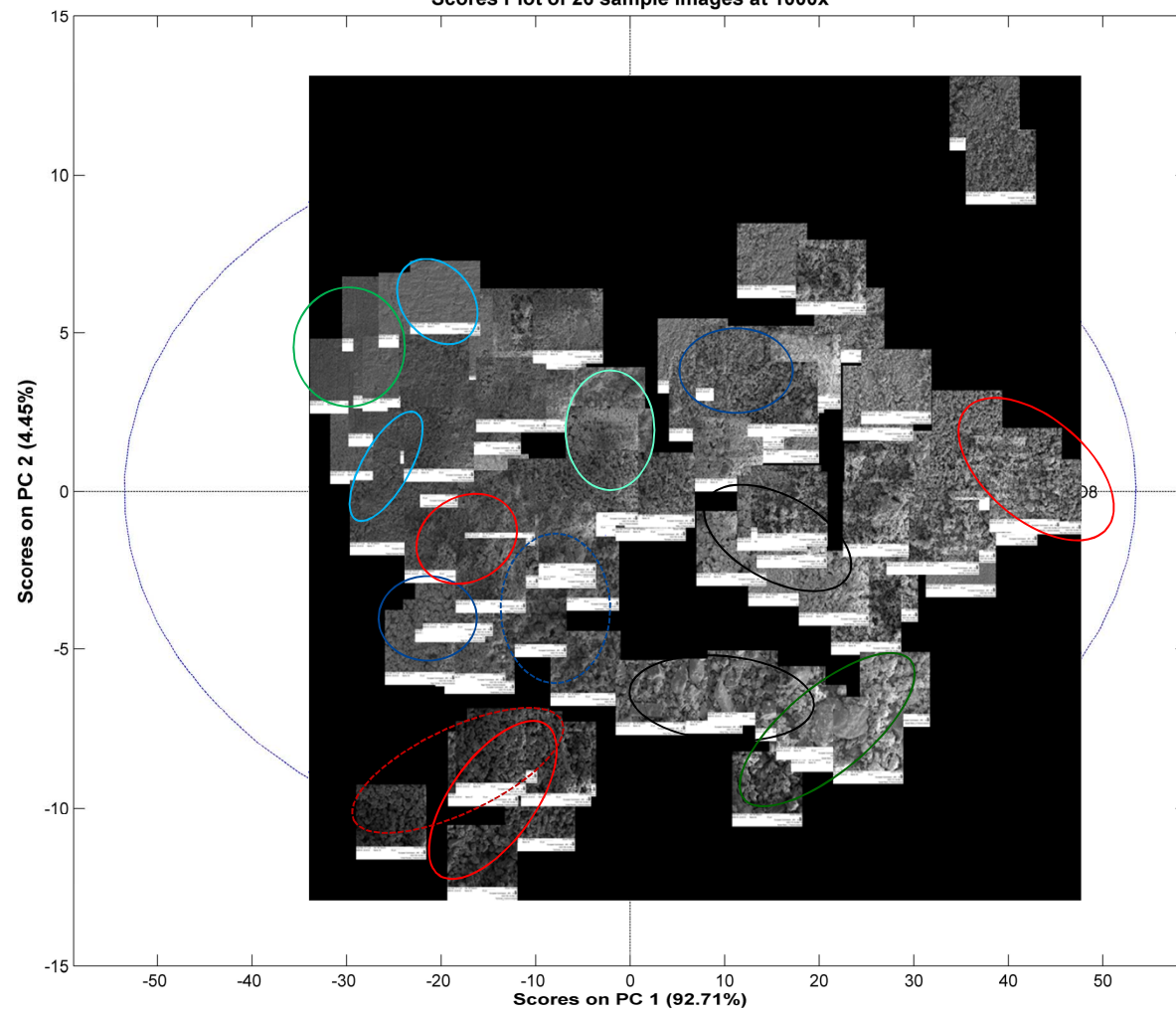
Joint
Research
Centre

K.H. Esbensen, K.H. Hjelmén and K. Kvaal,
'The AMT Approach in Chemometrics-First Forays',
Journal of Chemometrics 10 (1996) 569-590.

Results: Image texture analysis

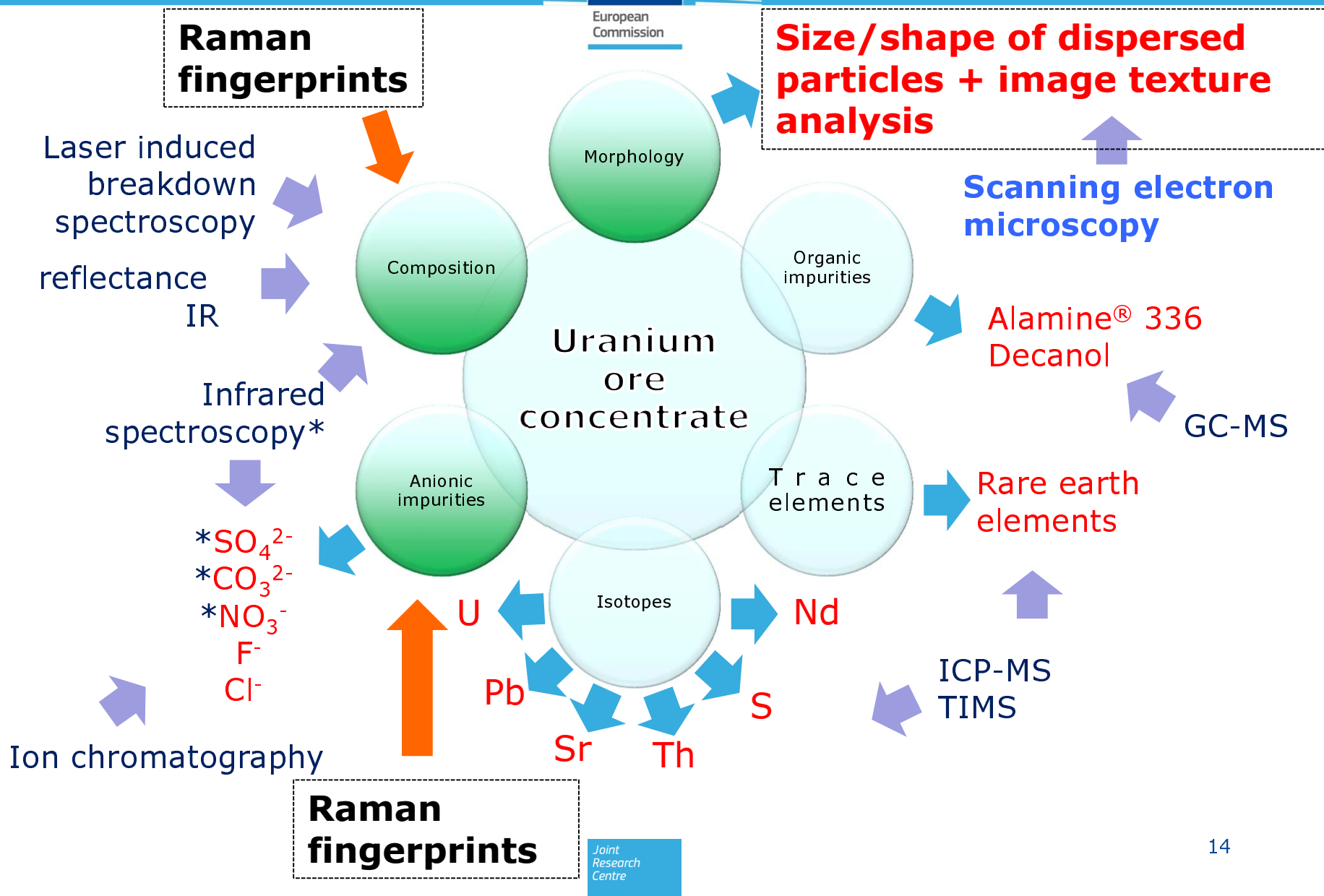


Scores Plot of 26 sample images at 1000x



- Scores on PC 2 (4.45%)
- ▼ All
 - * Atl
 - ChH
 - + Con
 - ◇ Dak
 - ▲ ES1
 - ★ ESI
 - EID
 - ▼ FAP
 - * HeY
 - KeL
 - + MaK
 - ◆ Mul
 - ▲ Nuf
 - ★ OID
 - Pal
 - ▽ Pet
 - * Que
 - RaL
 - + Ran
 - ◆ Ršs
 - ▲ SUP
 - ☆ Som
 - SpB
 - ▼ Tec
 - * UnN
 - 95% Confidence Level

Summary



Raman fingerprints

Size/shape of dispersed particles + image texture analysis

Laser induced breakdown spectroscopy
reflectance IR

Infrared spectroscopy*

- *SO₄²⁻
- *CO₃²⁻
- *NO₃⁻
- F⁻
- Cl⁻

Ion chromatography

Raman fingerprints



Acknowledgements



- Dieter Schild
(Institute for Nuclear Waste Disposal, Karlsruhe)
- International Atomic Energy Agency, Vienna
(for hand-held Raman and UOC samples)
- Springfields, UK for the UOC samples

