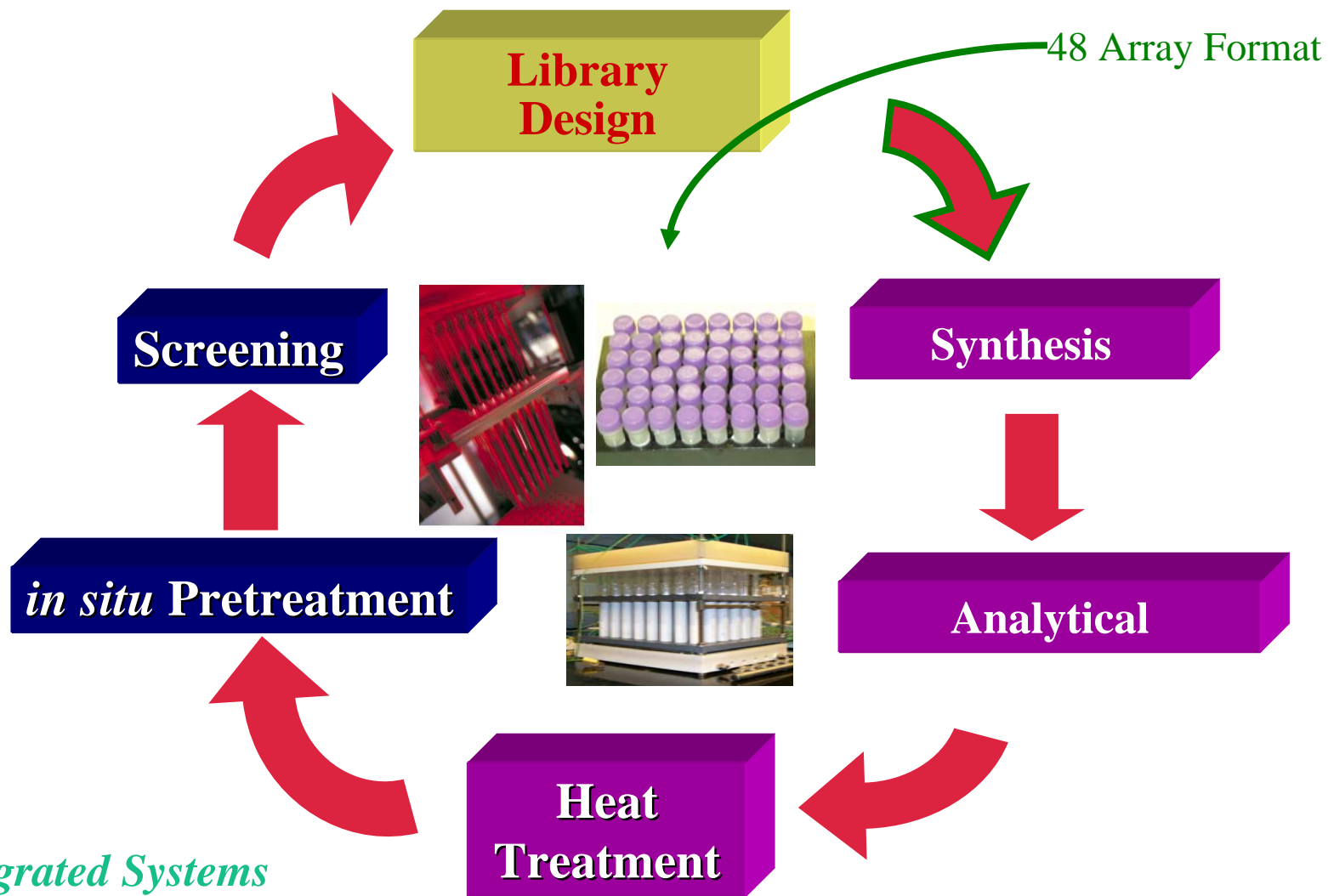


Parallel-kjemi mot katalyse og adsorbenter

Hva er eller *Hvorfor* "Combi"?

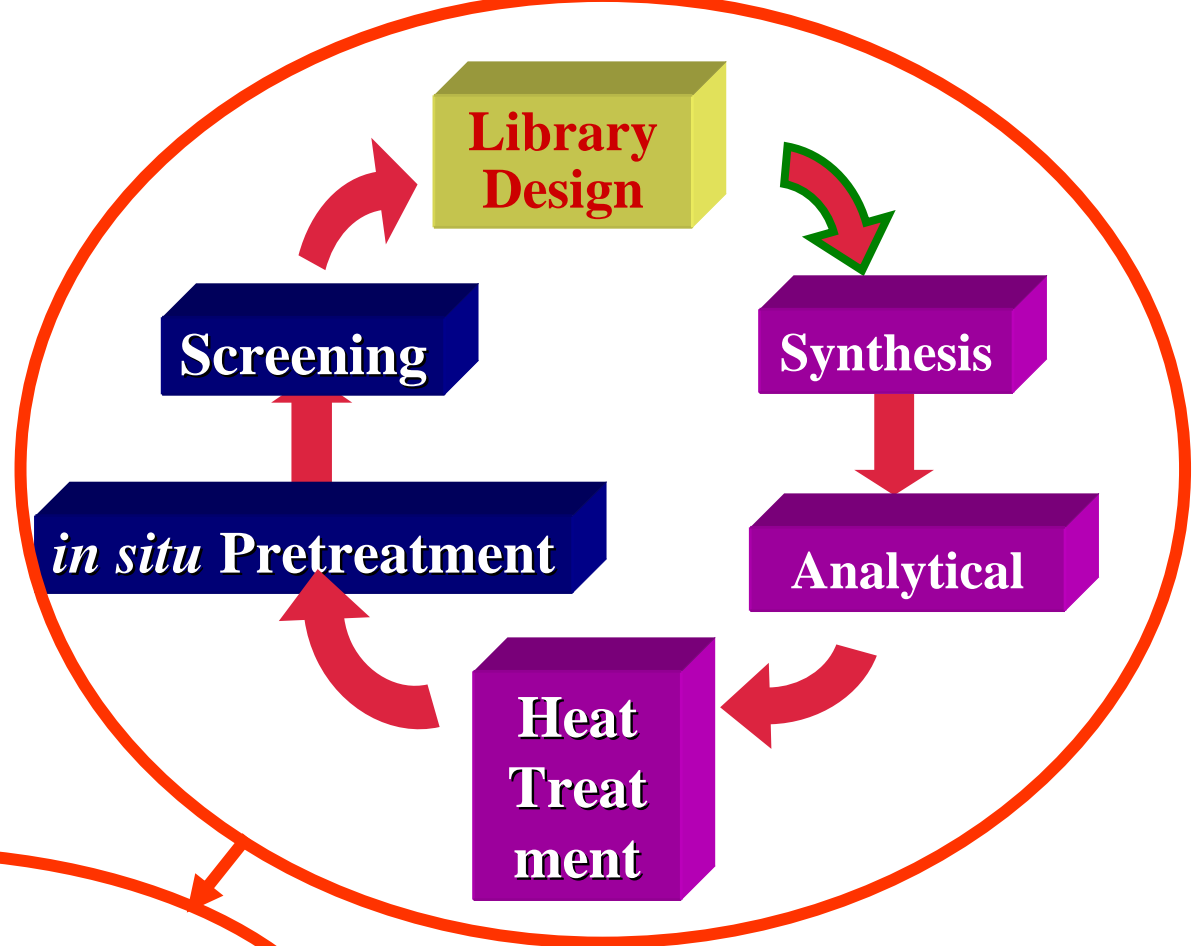


*Fully Integrated Systems
Not Just Moving Bottlenecks Around*

Case Study Drug development Cost

	Conventional	Combinatorial
Total Time	5 years	<3.5 months
No. of Scientists	15	4
No. of Compounds	3750	9000
Cost of Analysis	\$10000	\$10000
Manpower Costs	\$18.75 Million	\$167000
Cost per Compound	\$5000	\$19

¹Pharmacopeia



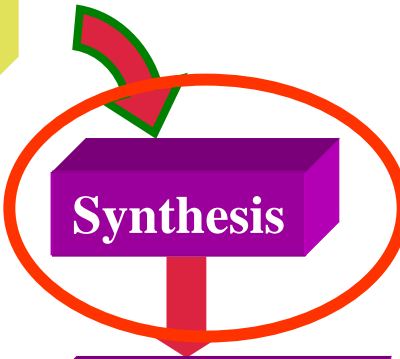
Key points: - Miniaturisation
- Parallelisation
- Automation

Synthesis

in situ Pretreatment

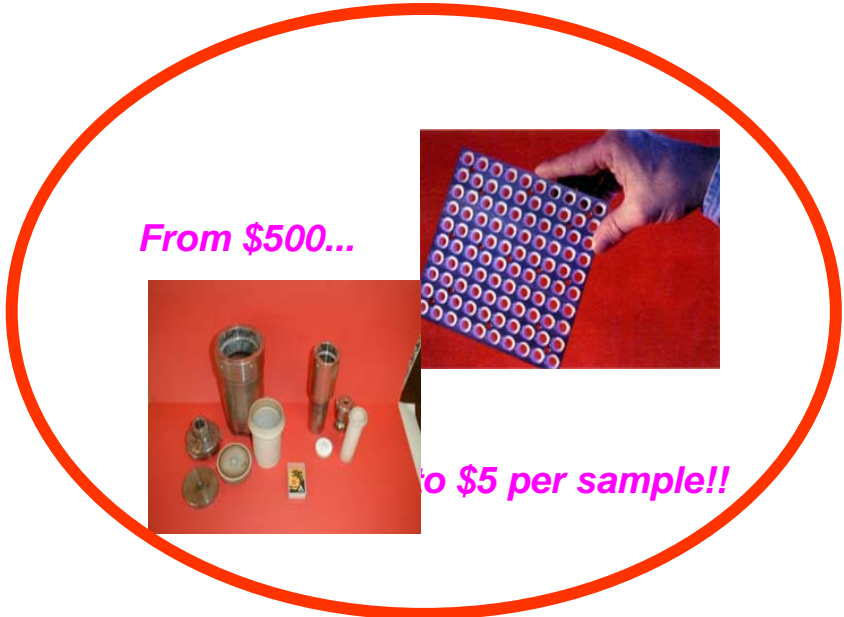
Screening

Library Design

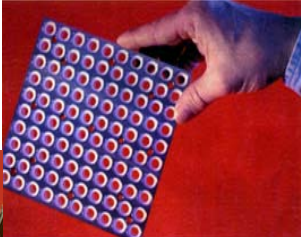


Analytical

Heat Treatment



From \$500...



to \$5 per sample!!

Analytical

Screening

Library Design

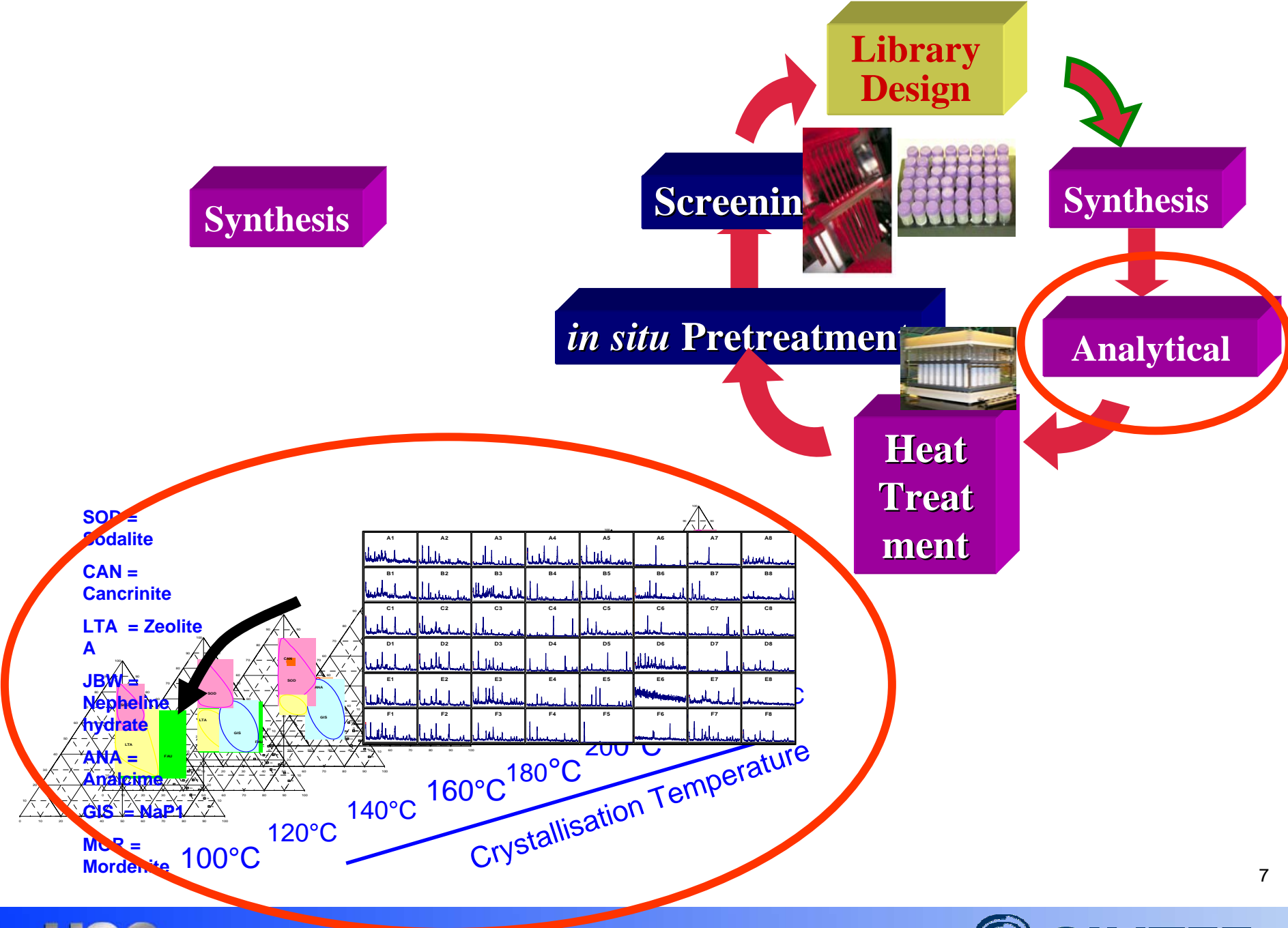
Synthesis

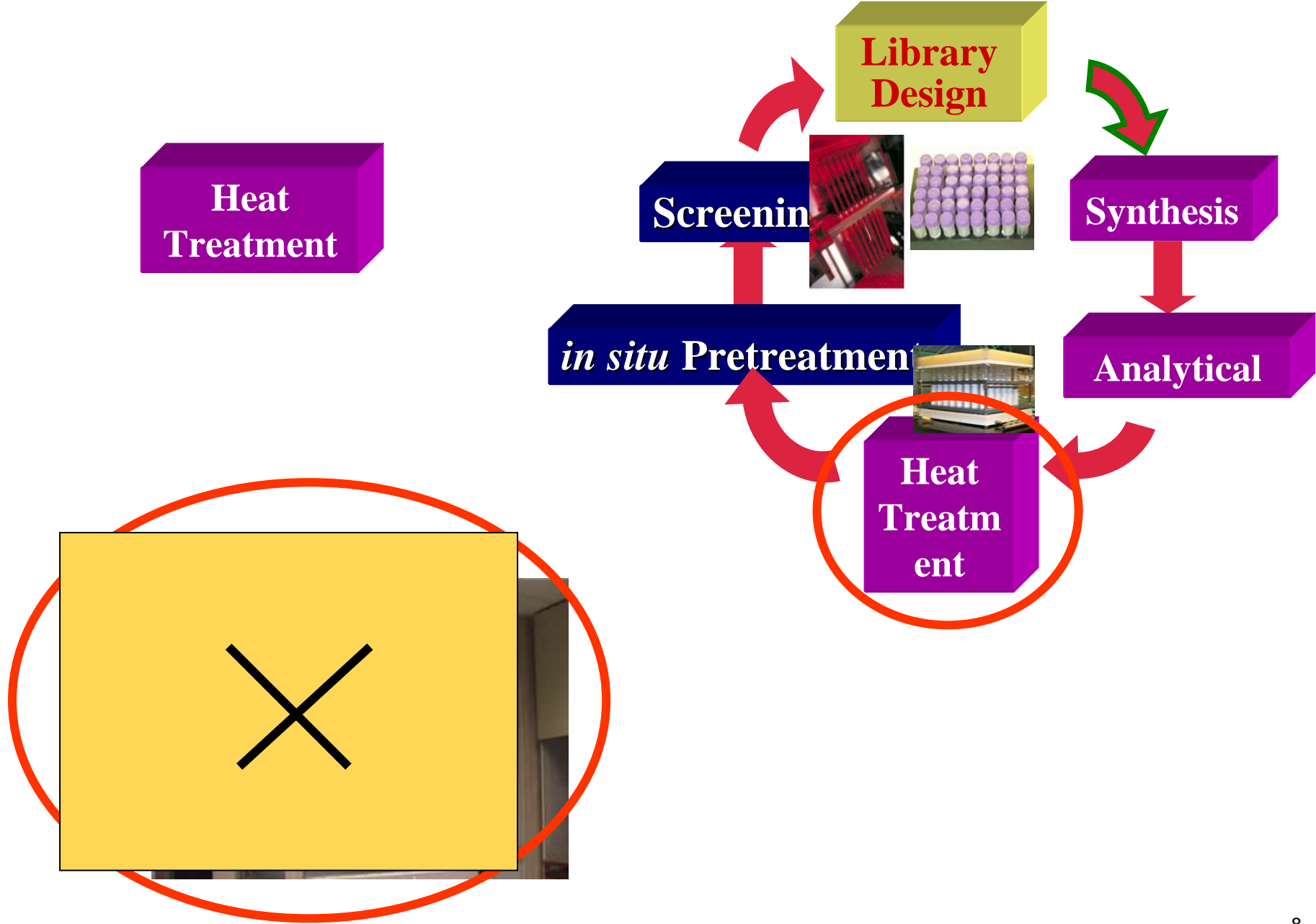
in situ Pretreatment

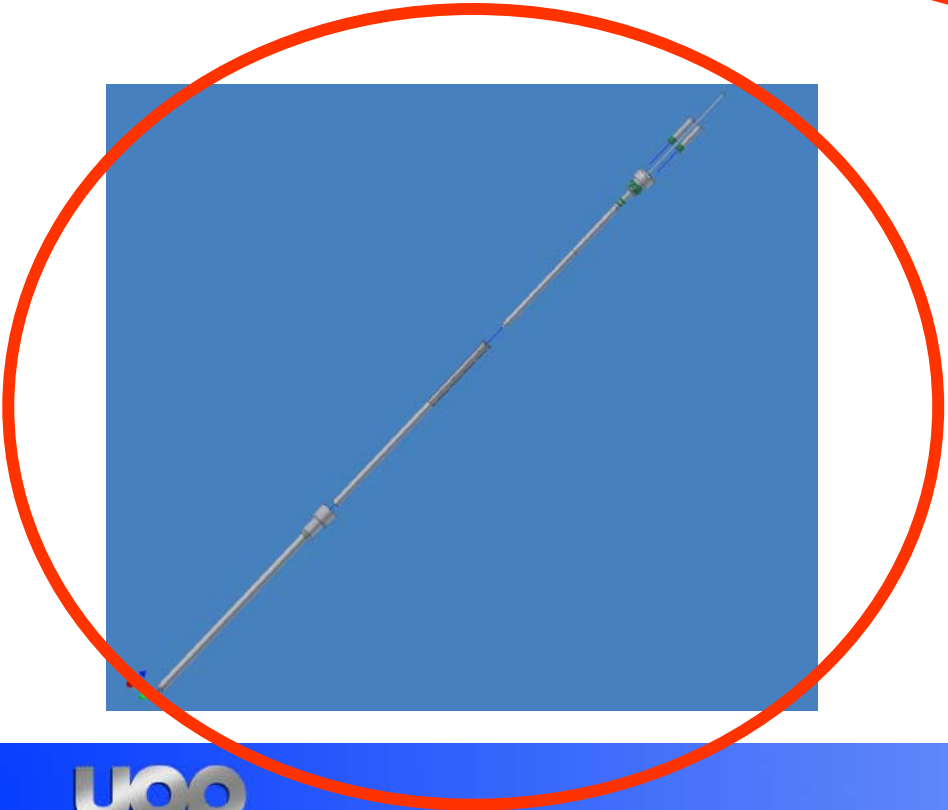
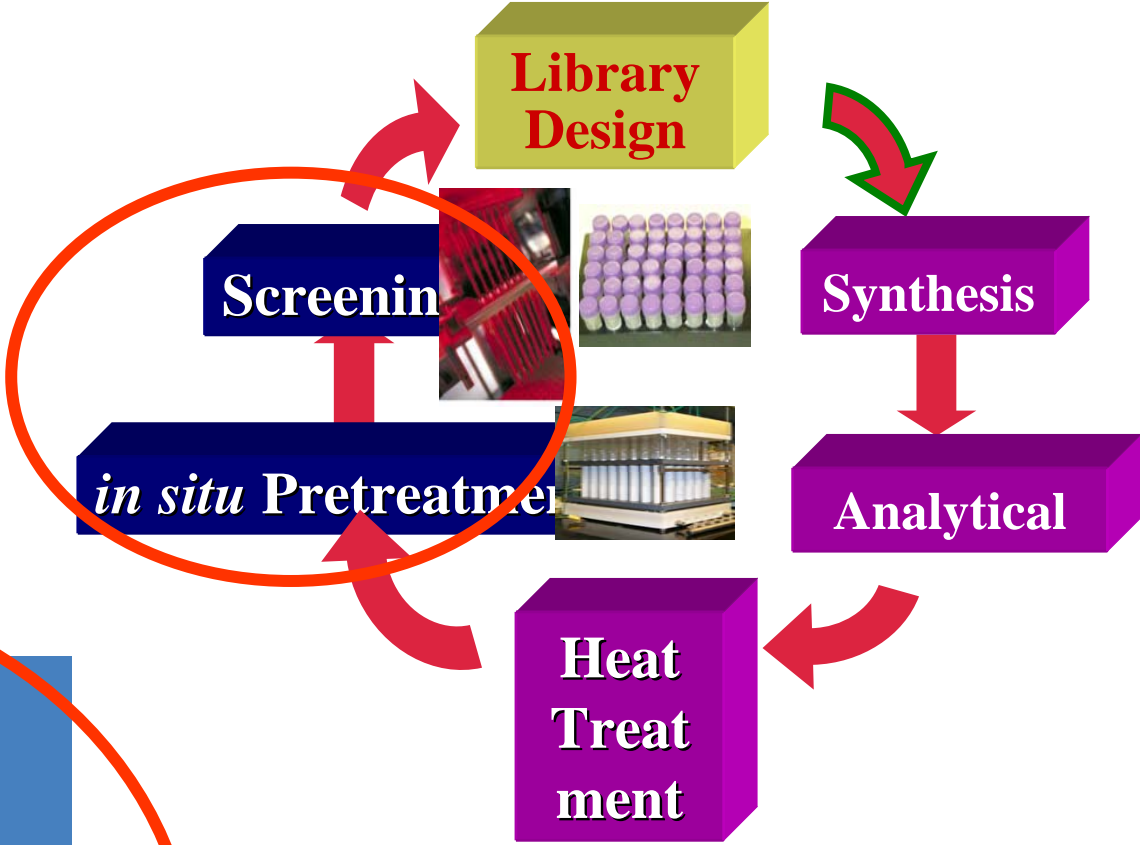
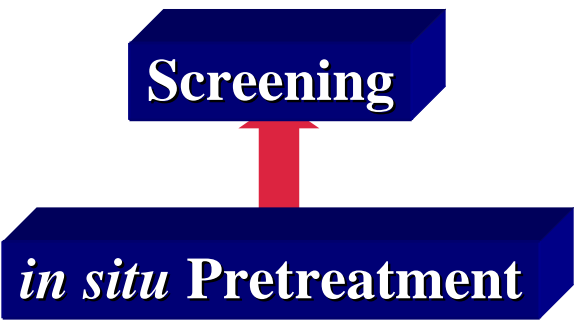
Analytical

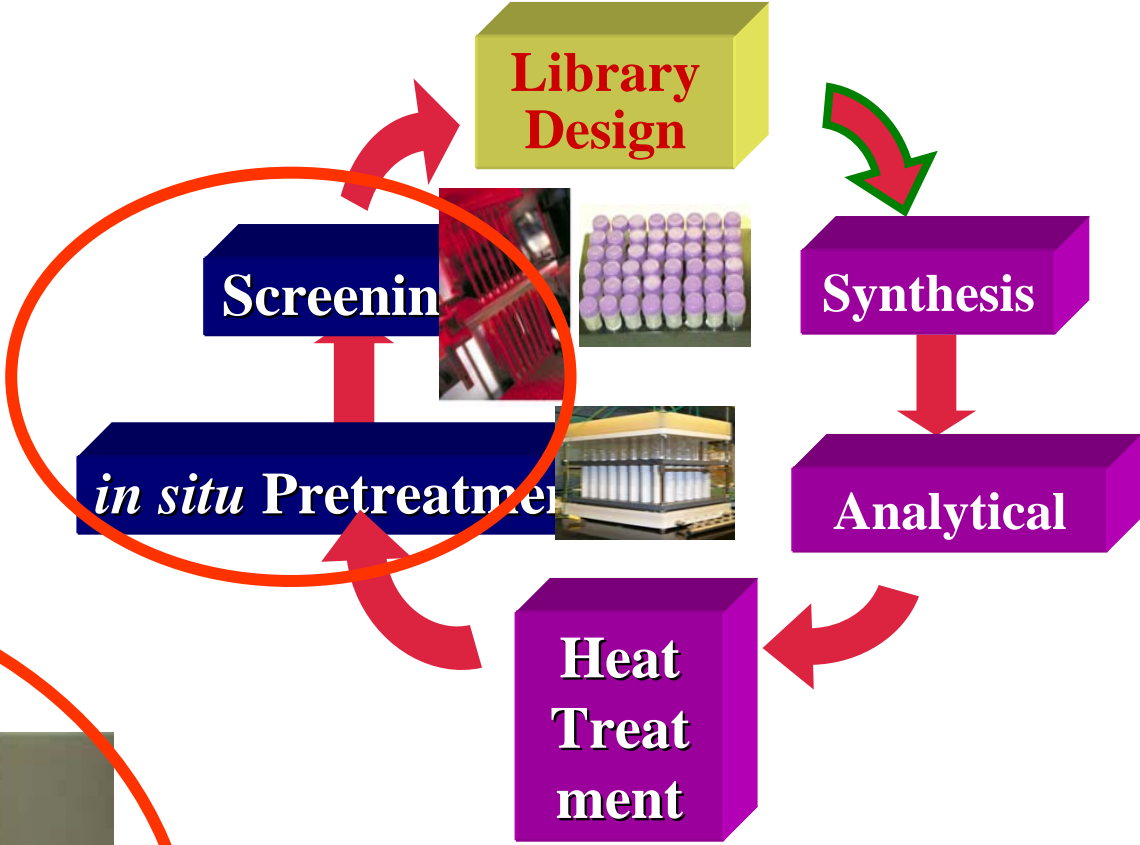
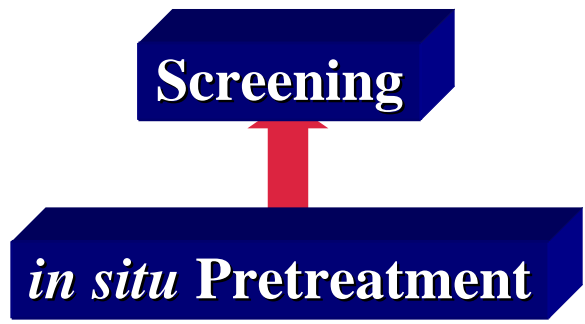
Heat Treatment

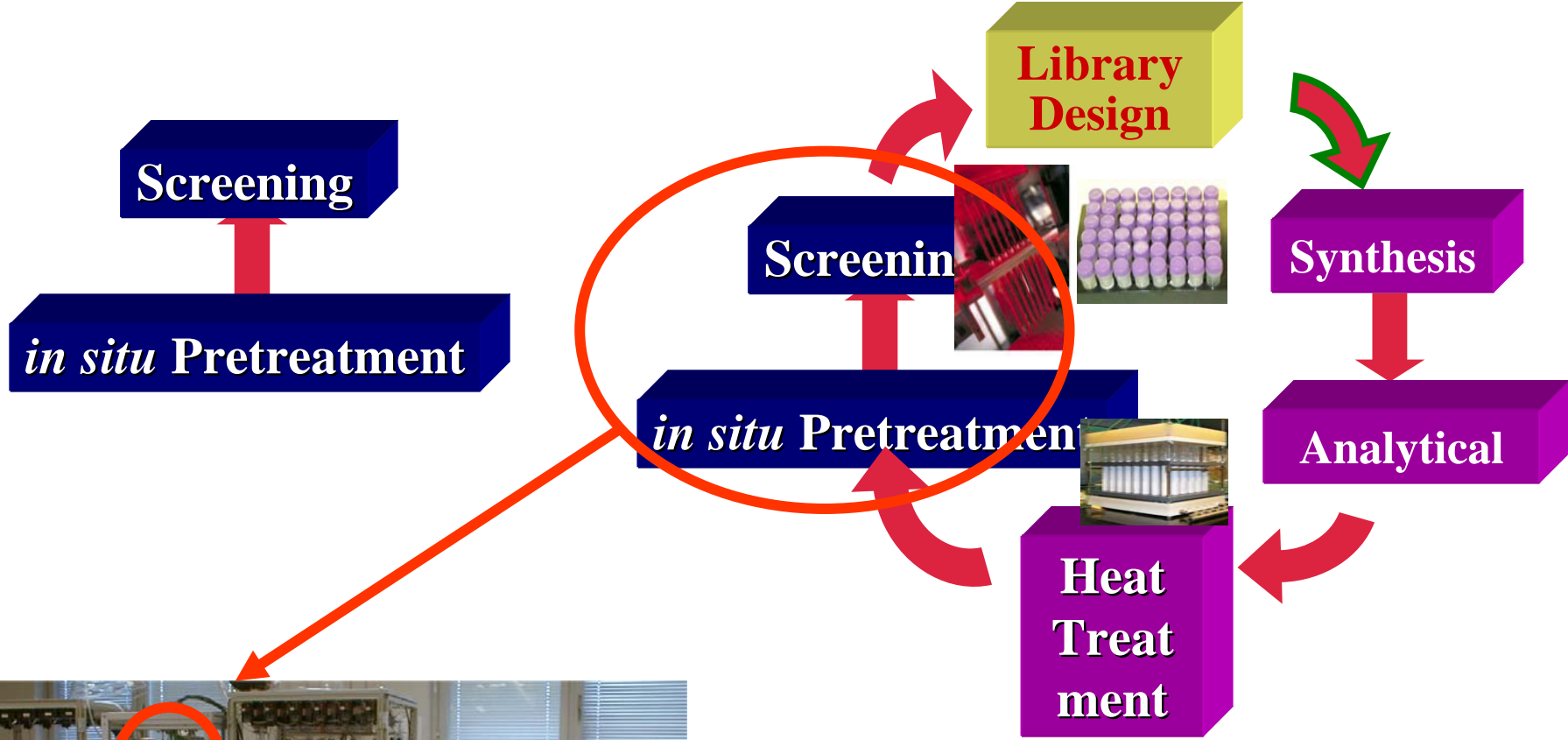


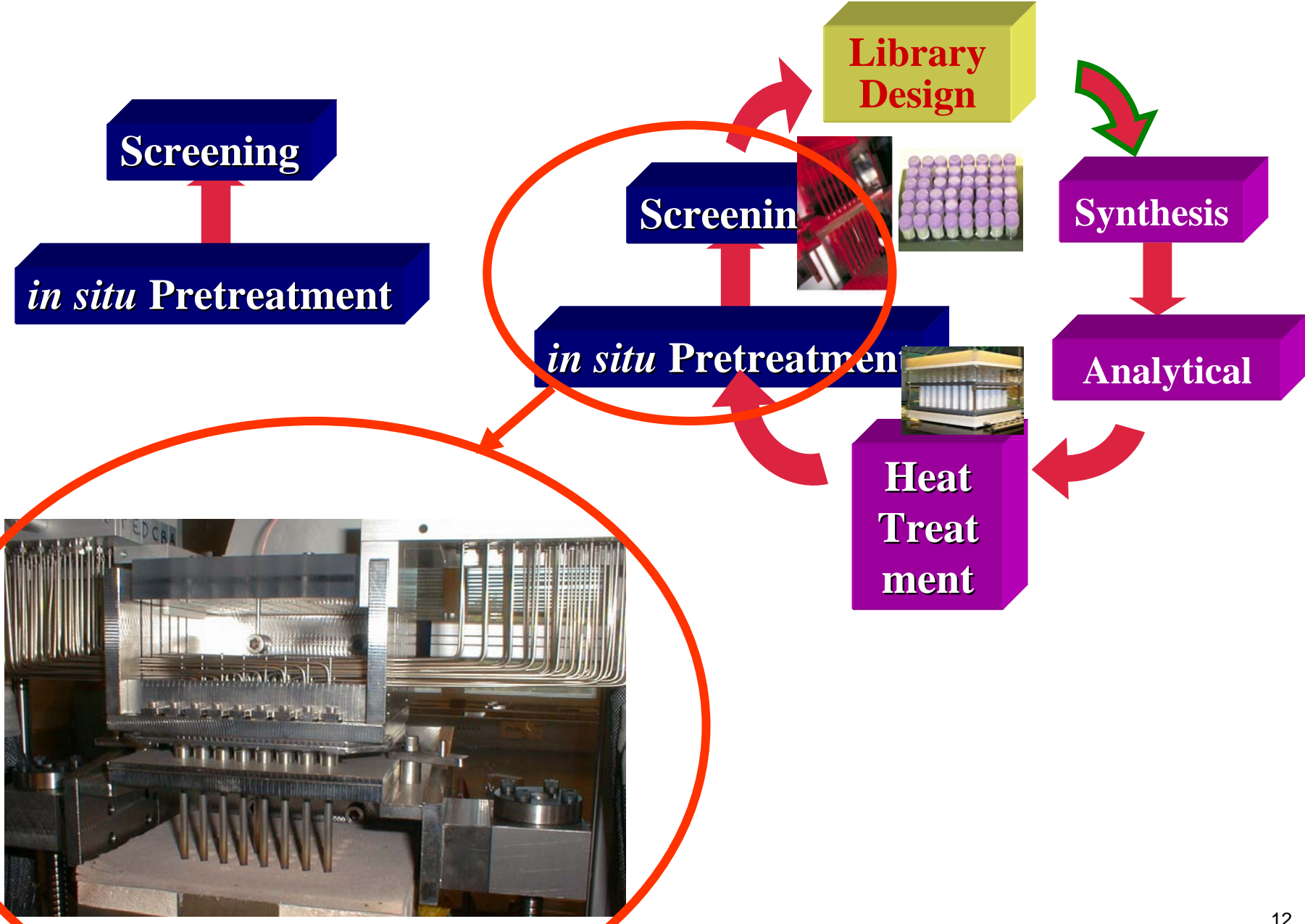


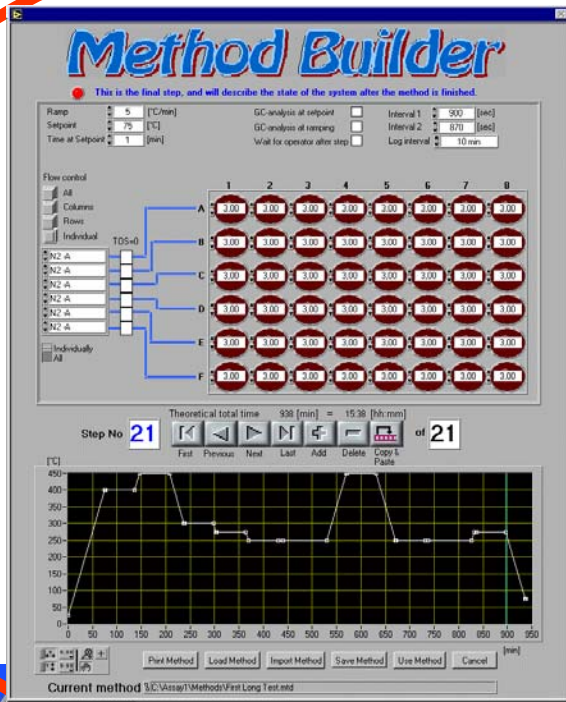
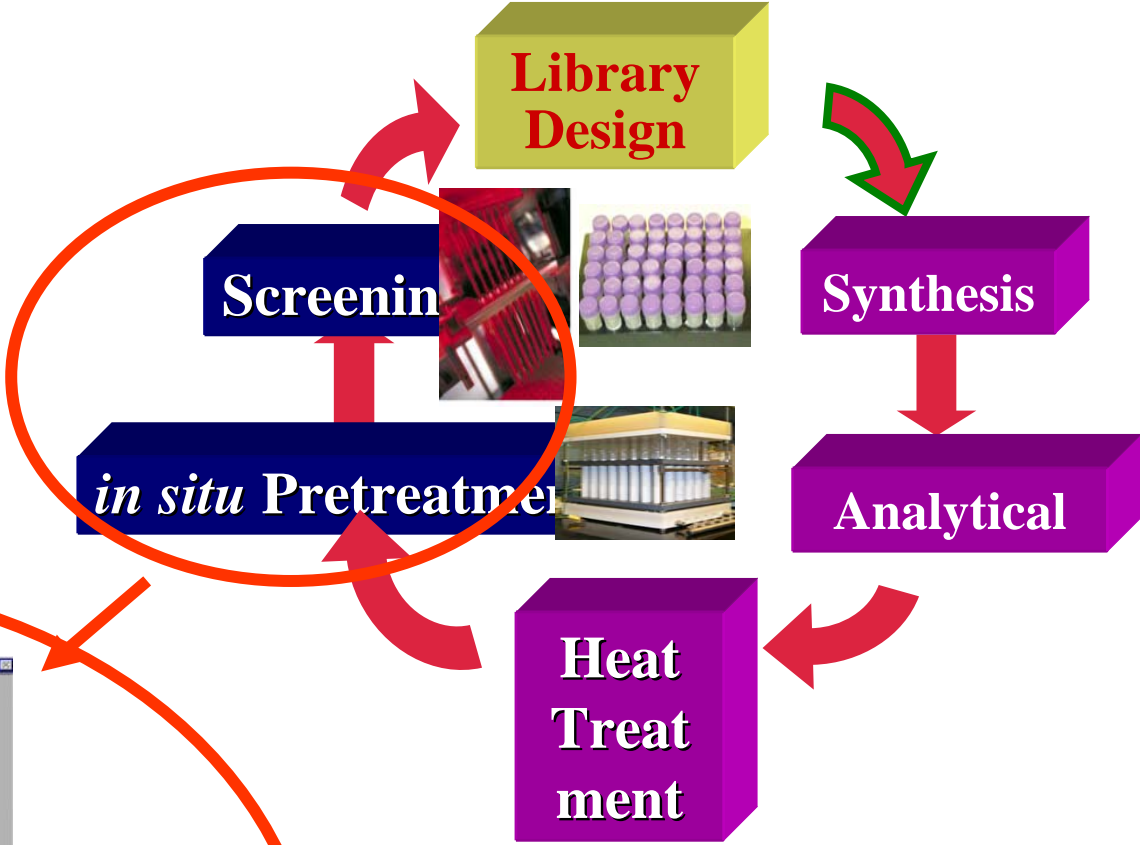
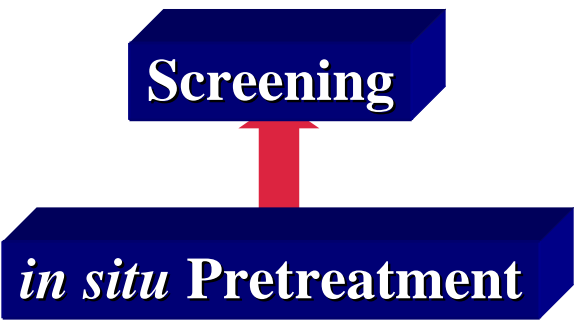




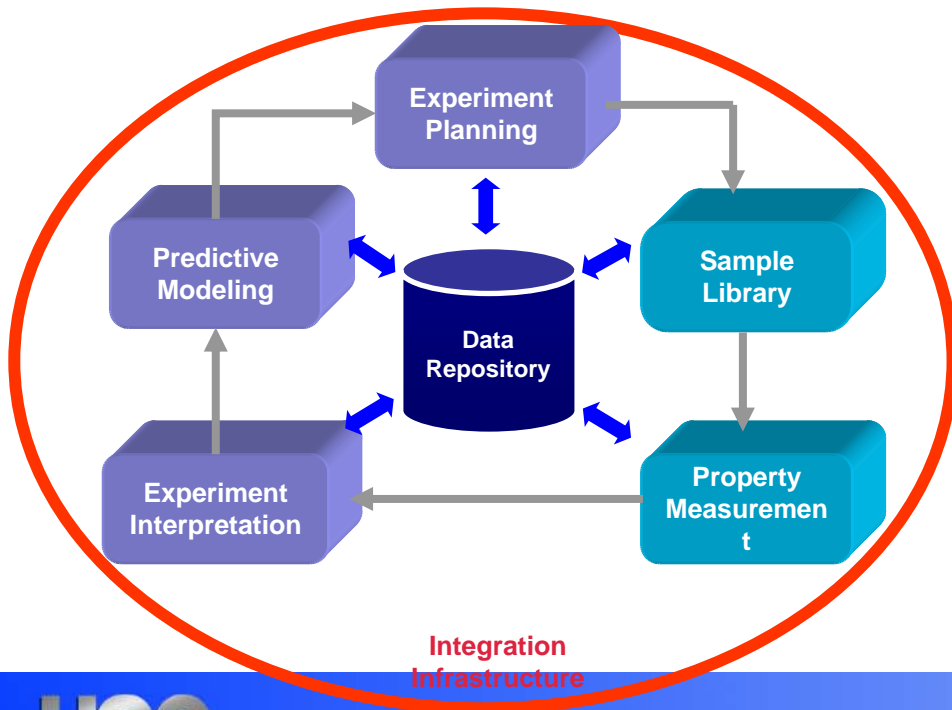
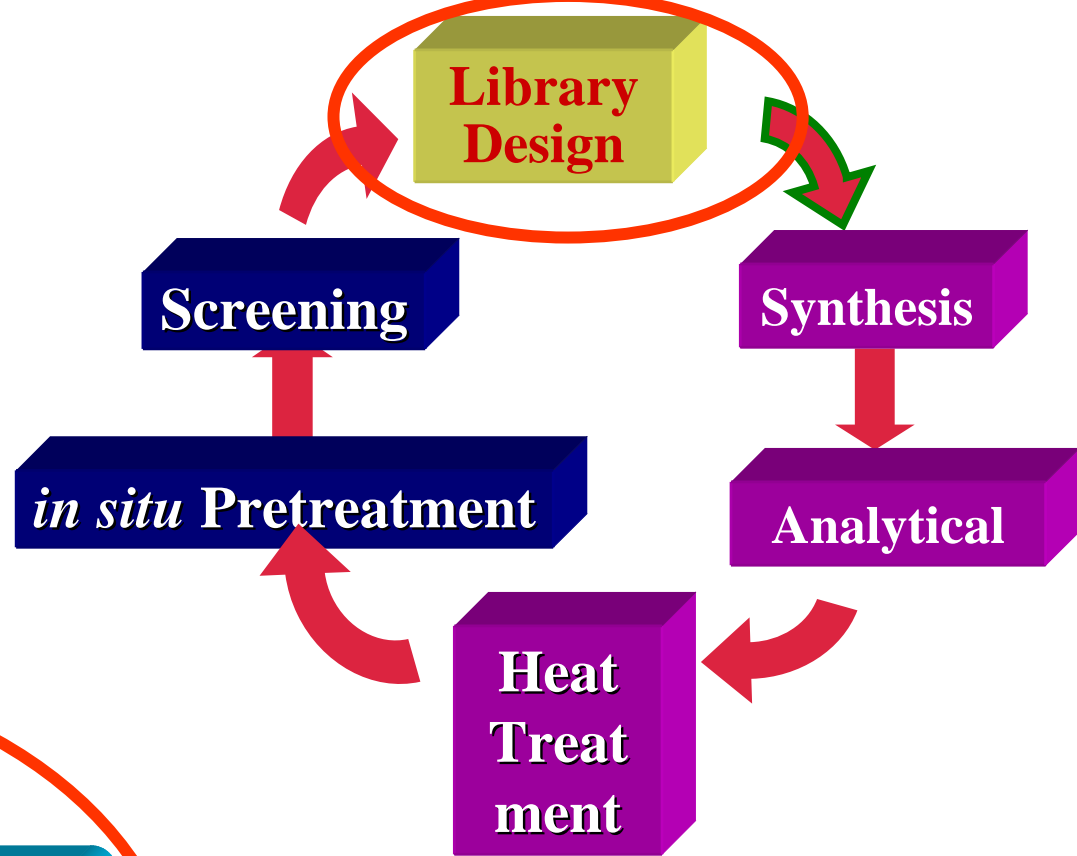








Library Design



Integration Infrastructure

UOP LLC - World's Largest Process Technology Licensing Organization



- ▶ 70 licensed processes
- ▶ 30,000+ patents, 90% licensable
- ▶ 70 catalysts
- ▶ Molecular sieves adsorbents
- ▶ 30 Engineered products
 - Packaged process units and systems
 - Proprietary equipment
 - Control systems and instrumentation

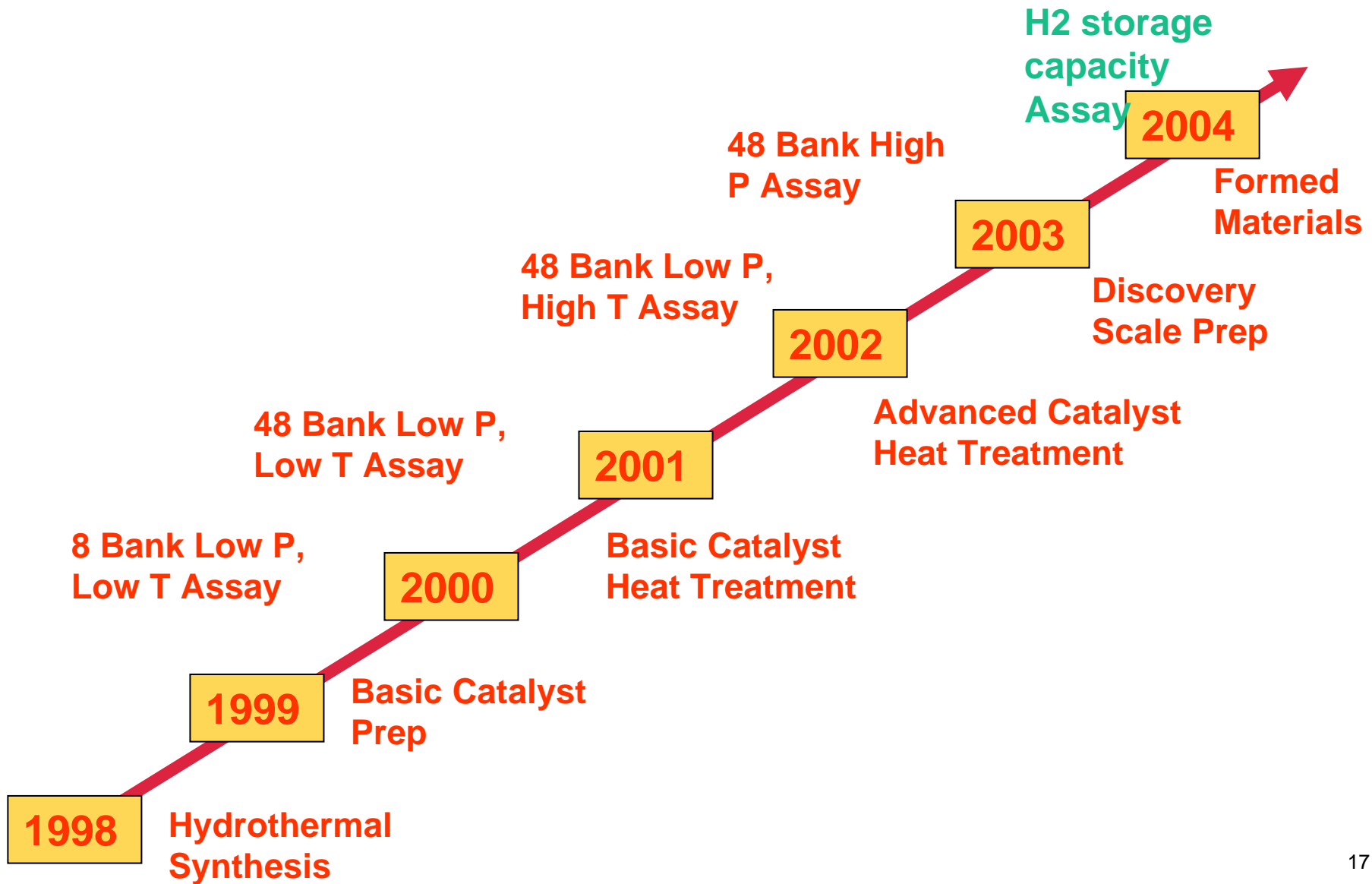


SINTEF

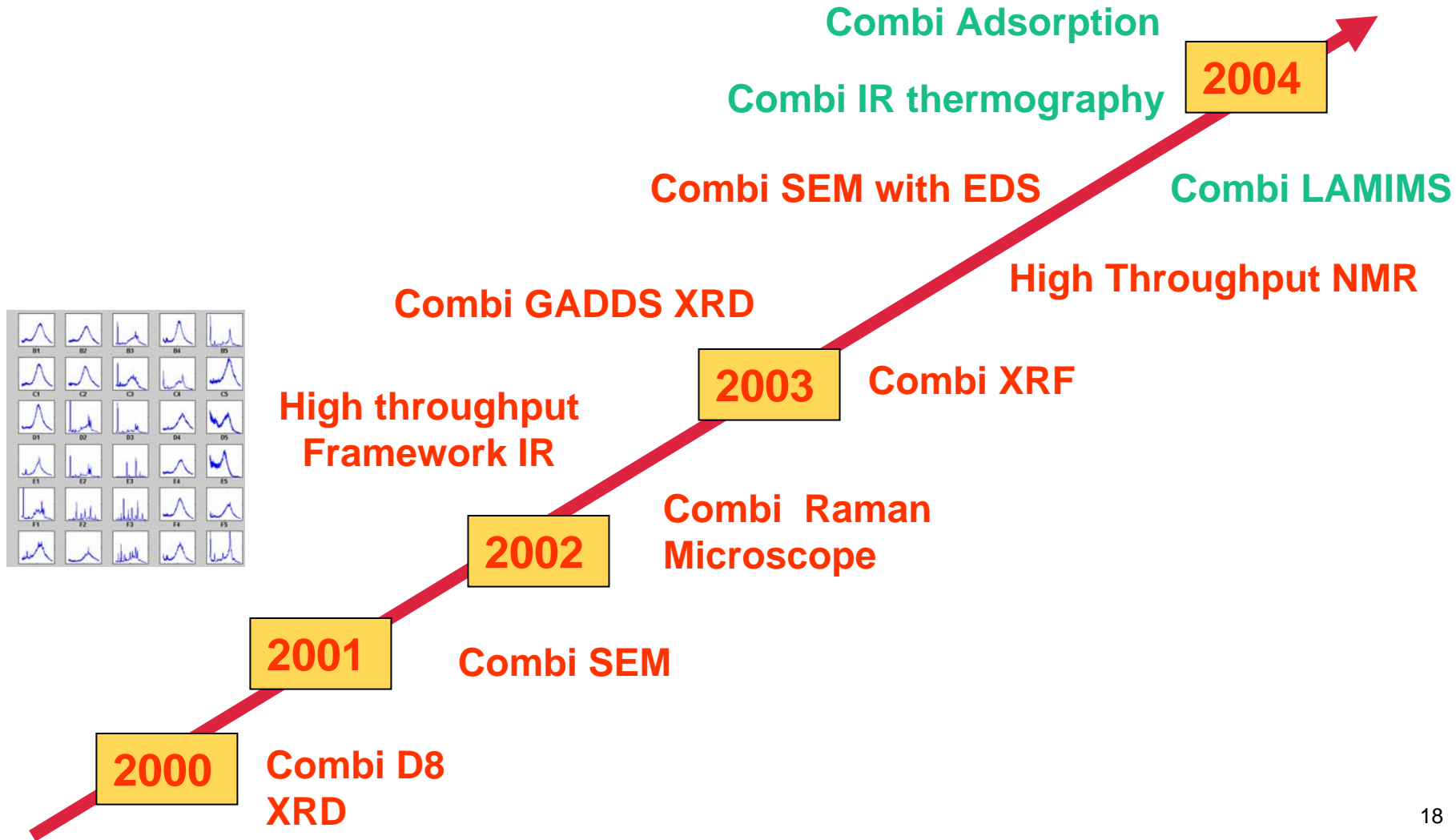
UOP



UOP Combi Capability Development

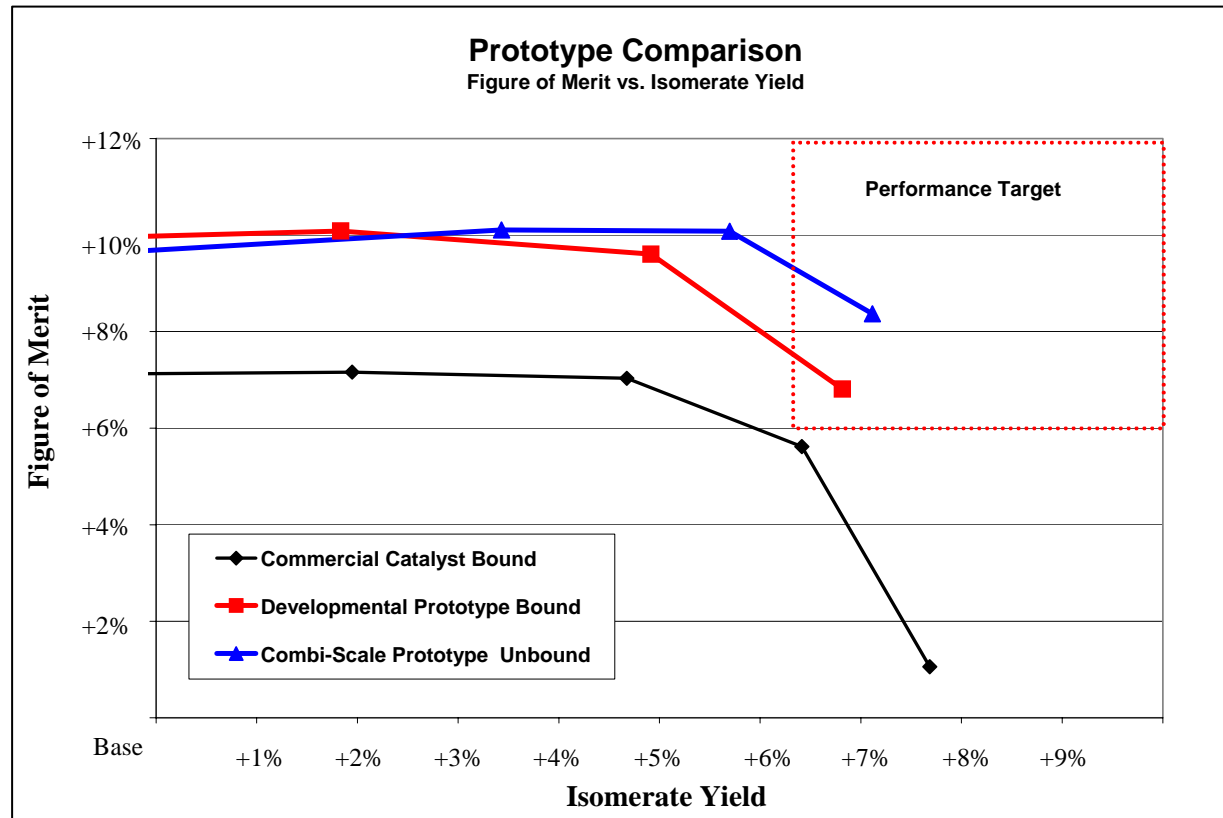


Combi Characterization Capability Development



Success of Combi in Discovery Program

- ✔ Synthesis of Relevant Materials
- ✔ Identification of Leads
- ✔ Verification of Leads
- ✔ Accelerate Fundamental Understanding
- ✔ Commercialize New Technology



New Catalyst Formulation for Commercialization

First commercial catalyst developed through combinatorial/parallel approach

Big West Oil LLC's Refinery Selects UOP's PI-242 Catalyst for Par-Isom Unit Reload

306 words

20 January 2004

13:13

Business Wire

English

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DES PLAINES, Ill. **Big West Oil LLC's refinery, located in North Salt Lake City, Utah, successfully reloaded its Par-Isom(TM) unit with newly developed PI-242(TM) catalyst. This marks the first commercial operation of the high activity PI-242 catalyst which is currently meeting all expectations.**

Big West Oil's Senior Vice President of Refining Operations Jeff Utley said, "Using PI-242 catalyst enables Big West Oil to increase production of low sulfur, high octane gasoline without any additional capital investment in our existing Par-Isom unit. This was a big plus for us because it directly ties into our on-going goal to be a primary supplier of high octane gasoline to the Rocky Mountain region."

PI-242 catalyst is the first commercial catalyst developed utilizing a new catalyst research methodology, combinatorial chemistry (combi chem). Combi chem incorporates traditional elements of sample preparation and testing using very small sample sizes. This allows for much faster screening and lower development costs for new catalysts. More than 500 catalyst formulations were screened in just five weeks using combi chem during the PI-242 catalyst development program.

Big West Oil LLC is a wholly owned subsidiary of Flying J Inc. Big West Oil is involved in crude oil purchasing and transportation in Utah, Wyoming, and Colorado. Oil refining is conducted at its 25,000 barrel per day refinery located in North Salt Lake, Utah. The refinery produces a full range of petroleum products.

UOP LLC, headquartered in Des Plaines, Ill., USA, is a leading international supplier and licensor of process technology, catalysts, process plants and consulting services to the petroleum refining, petrochemical, and gas processing industries.

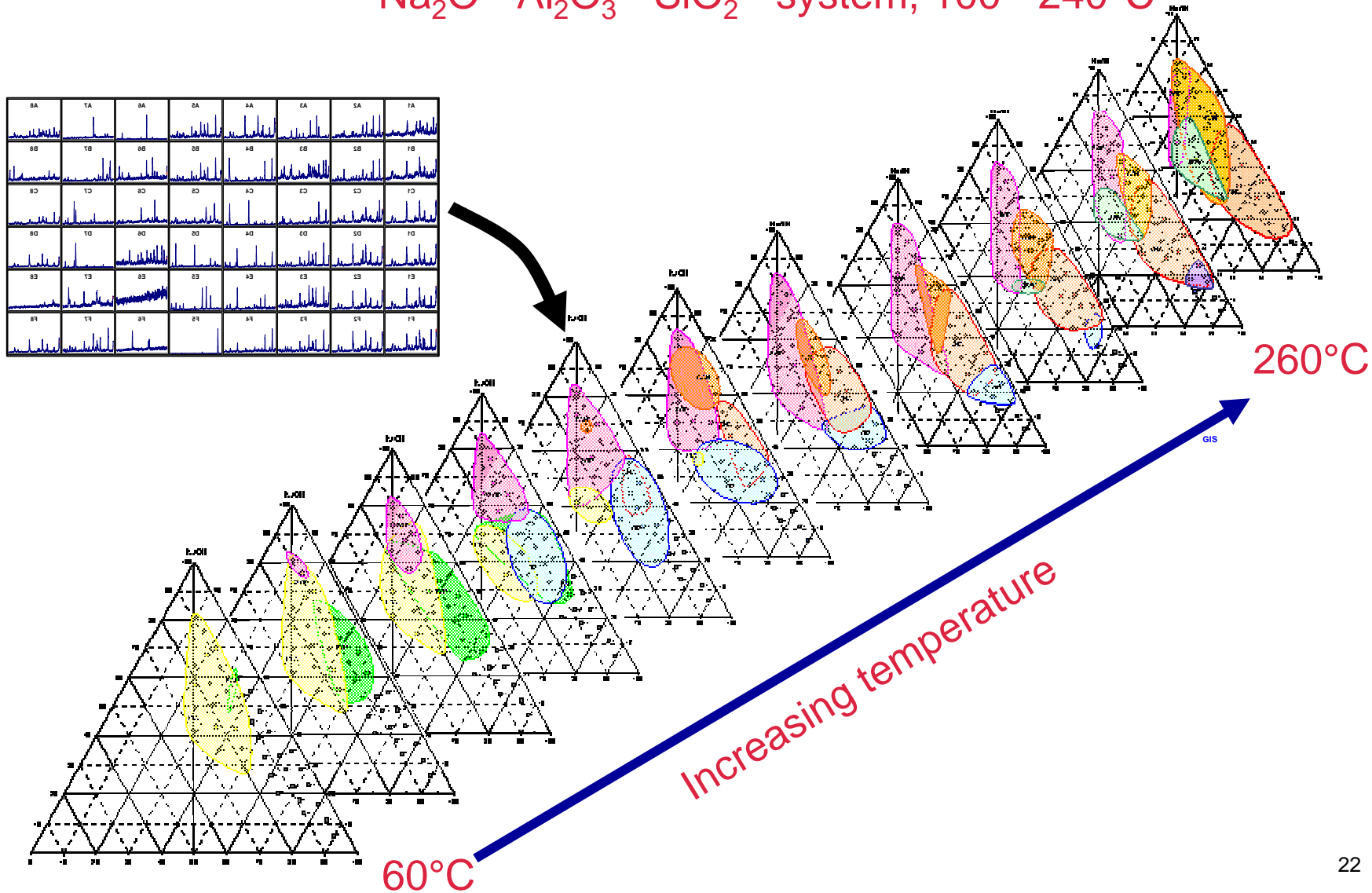
UOP LLC Anita Black, 847-375-7801 Anita.Black@uop.com

G. J. Davidson

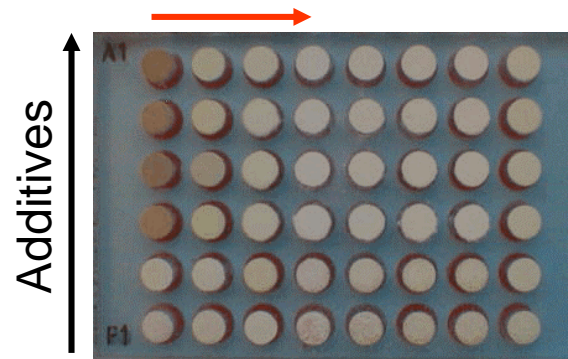
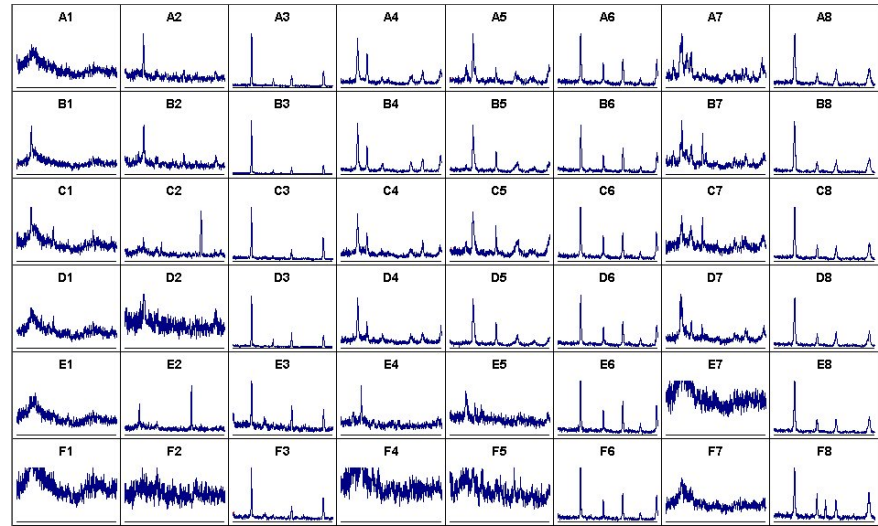
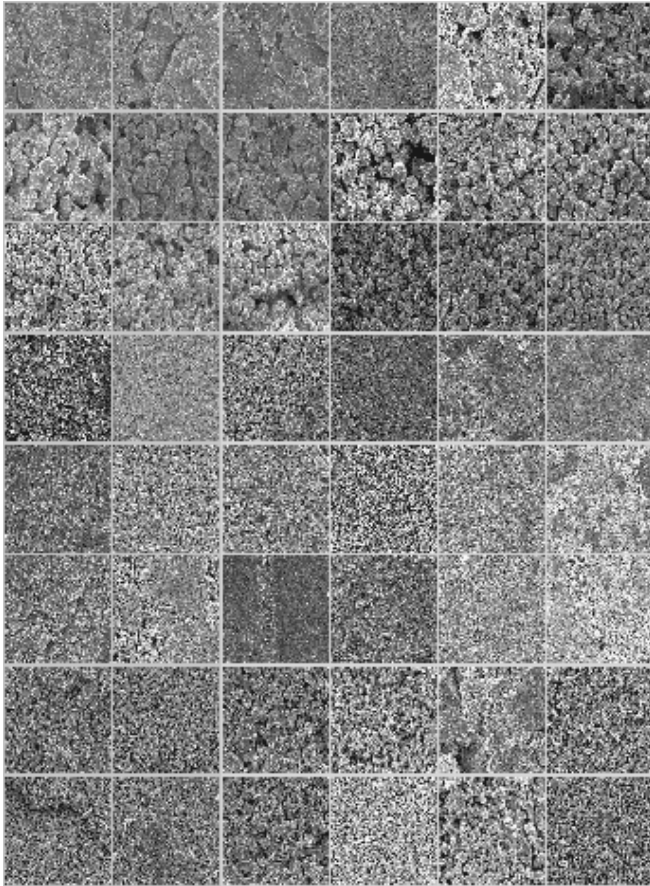
Parallel Technology Examples

Parallel Hydrothermal Synthesis

$\text{Na}_2\text{O} - \text{Al}_2\text{O}_3 - \text{SiO}_2$ - system, 100 - 240°C



Perovskites - (Pb, Ba, Sr)(Ti, Zr)O₃

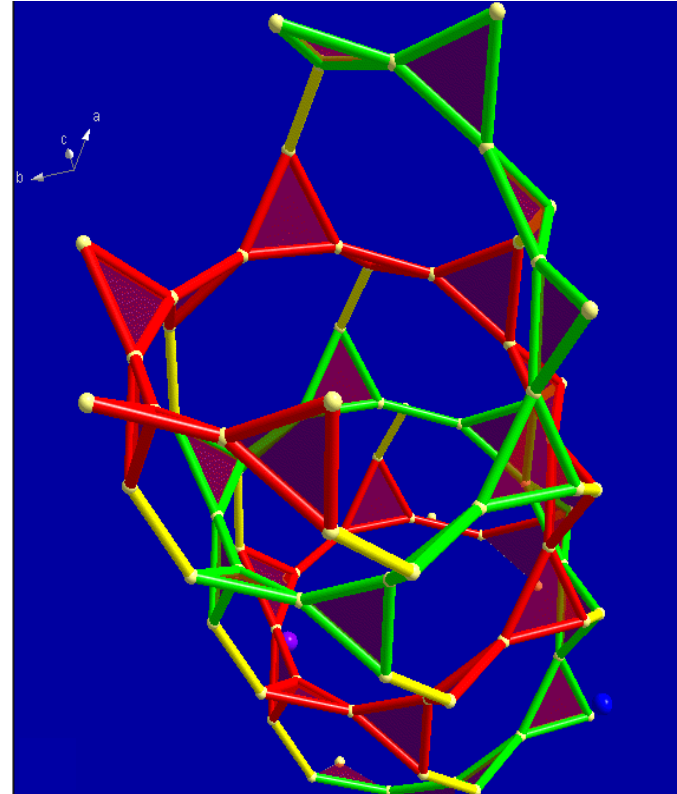


SEM AND
XRD ANALYSIS

HF Mediated Hydrothermal Synthesis

- **OSB-1 – the first zeotype structure formed only of 3-rings**

- ◆ Large pore volume
- ◆ 14-ring pore openings
- ◆ Chiral around the 14-ring channel
- ◆ Double helix of 3-rings form the walls of the chiral channels
- ◆ Si/Be = 2
- ◆ A major drawback – Beryllium ☠



¹ Cheetham, T., Fjellvåg, H., Gies, T.E., Kongshaug, K.O., Lillerud, K.P., Stucky, G.D., Proc 13th IZC, Montpellier, France, (2001), 05-O-05

DOE and Work-flow

i-iii) Design Of Experiment (DOE)

i) Input - defining gel ratios

ZnO K ₆ ZnO ₄	H ₂ O H ₂ O	KOH KOH _(aq)
1	100	1.5
		2
		2.5
		3
		4
		5
		6
		8
		11
		15
		25

iii)

ii) Molecular ratio of the gel

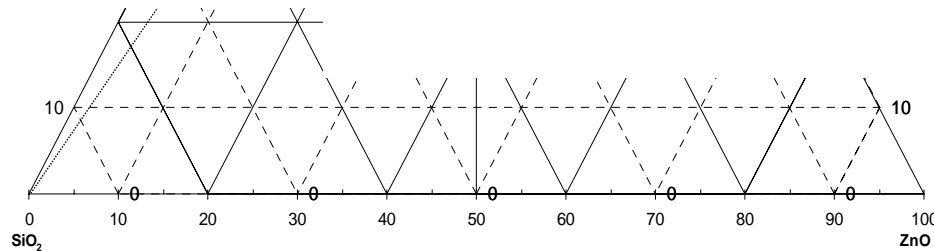
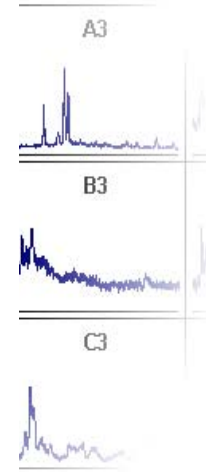
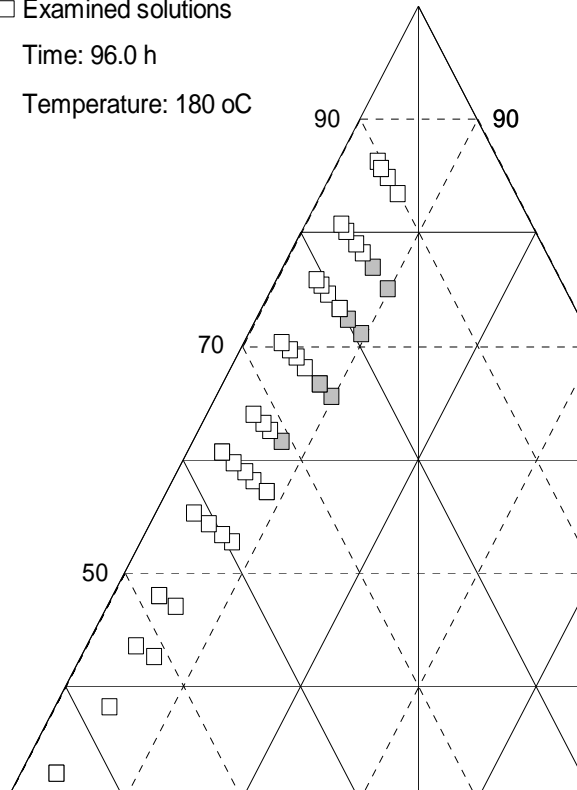
Gel #	ZnO
1	1
2	1
3	1
4	1
⋮	
120	1
121	1

v)

□ Examined solutions

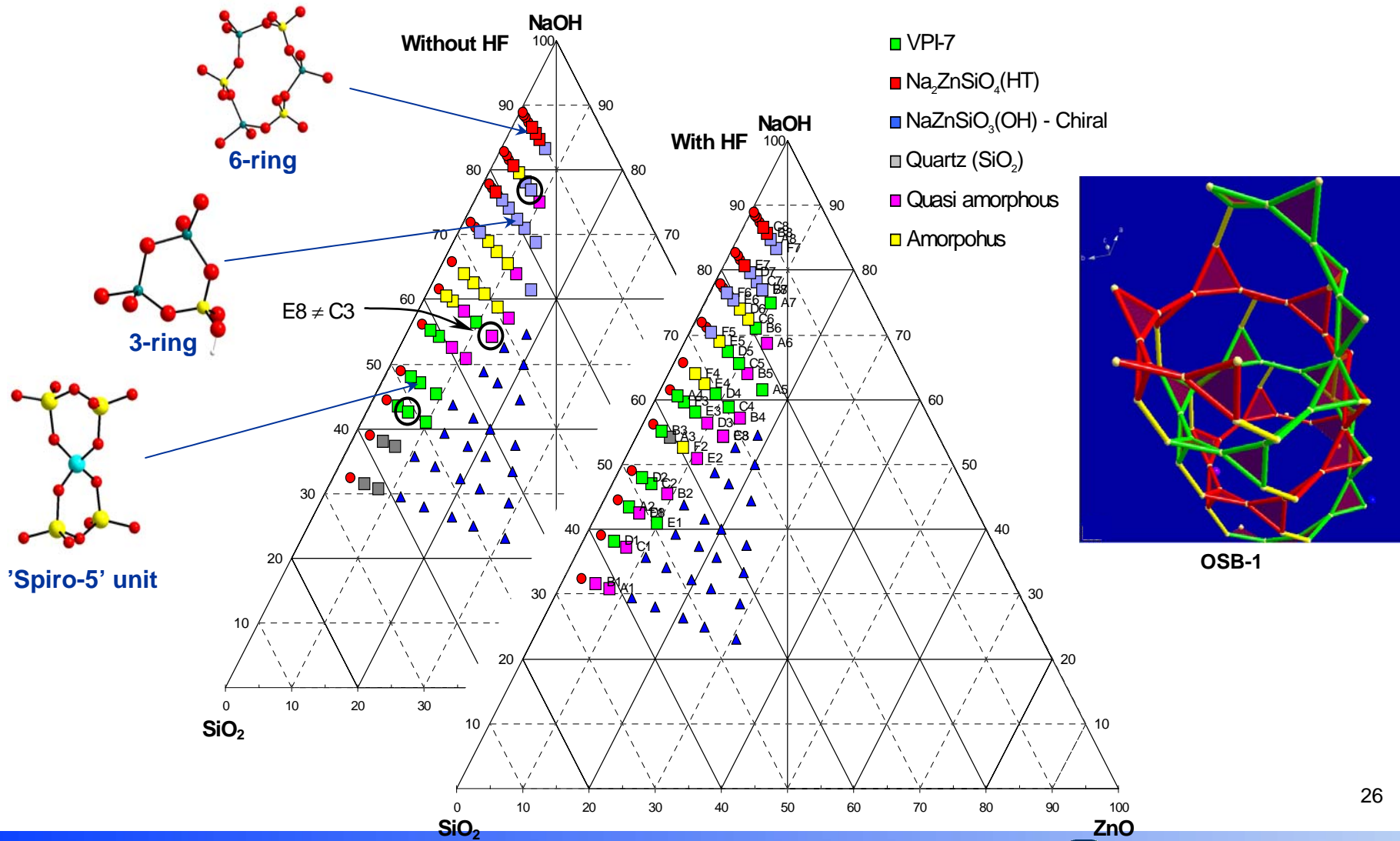
Time: 96.0 h

Temperature: 180 oC

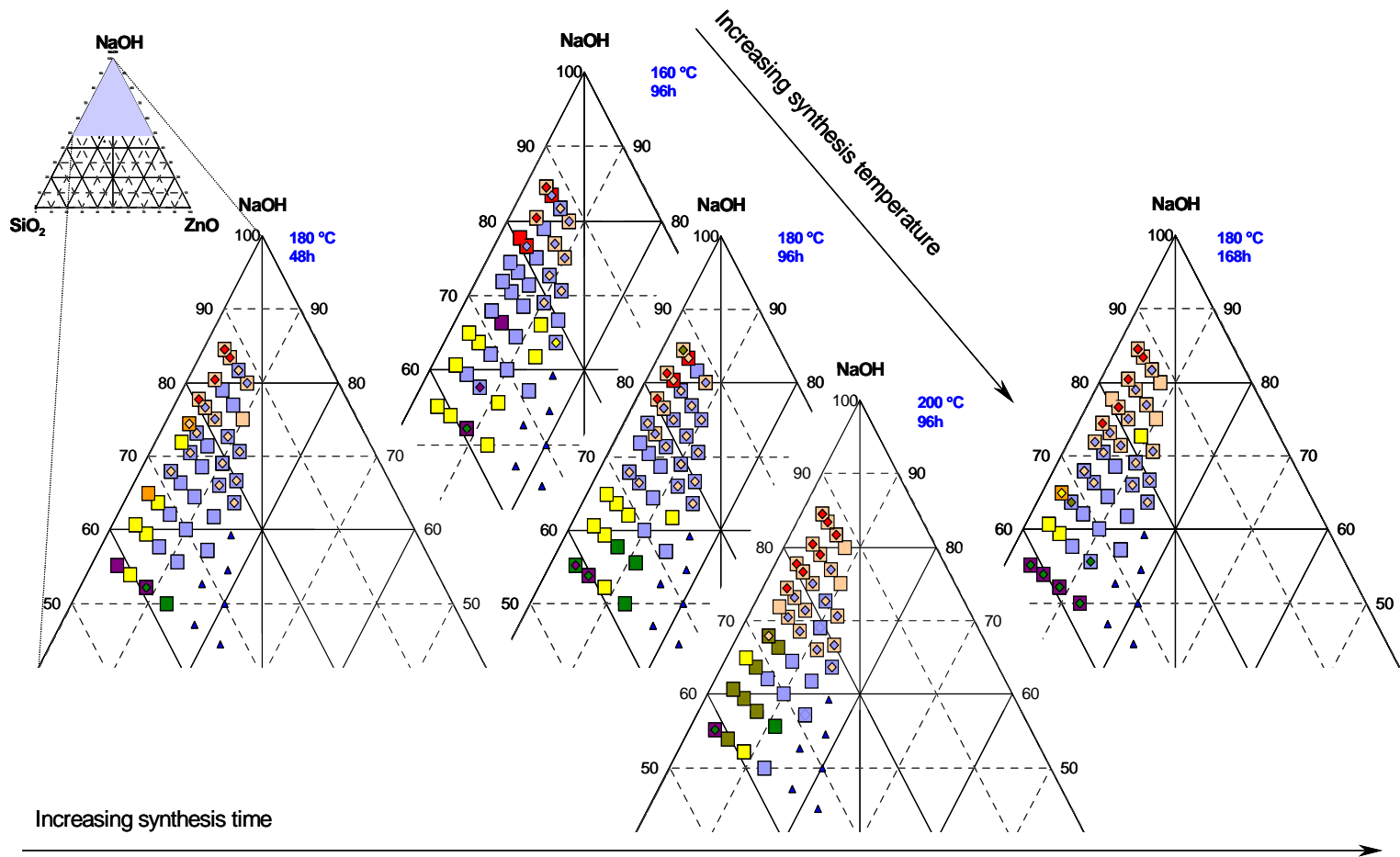


ZnO – SiO₂ – NaOH – HF

(96h and 180 °C, Zn/F = 0.25)



ZnO – SiO₂ – NaOH – TiO₂ f(time, temperature) & Zn/Ti=1

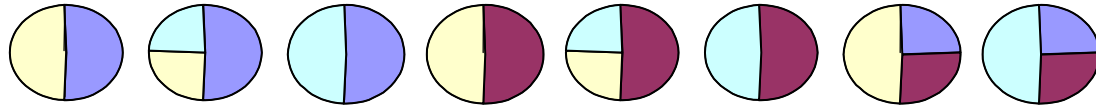


- ETS-4
- Na₇ZnSiO₄ (HT)
- Quartz
- Impurity (mainly in ETS-4)
- NaZnSiO₃(OH) - chiral
- Unknown
- Natisite
- Quasi amorphous
- Amorphous

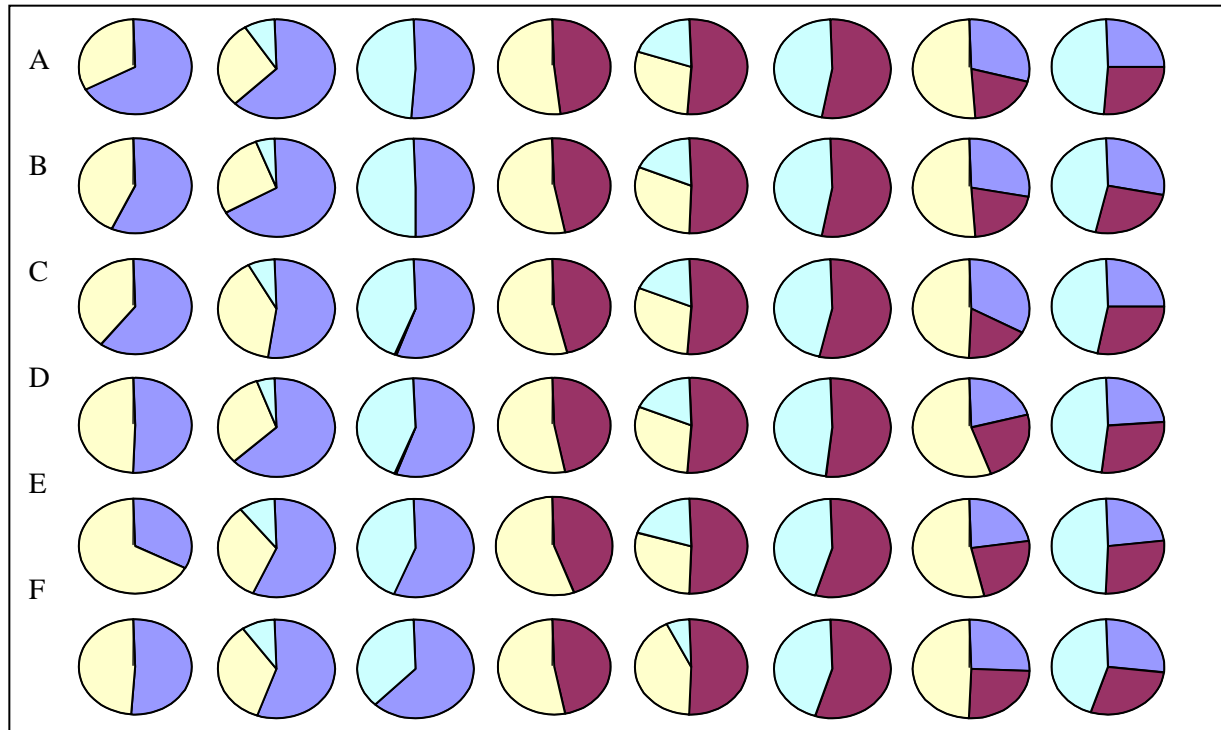
Impact of Synthesis on final Composition

Initial Composition

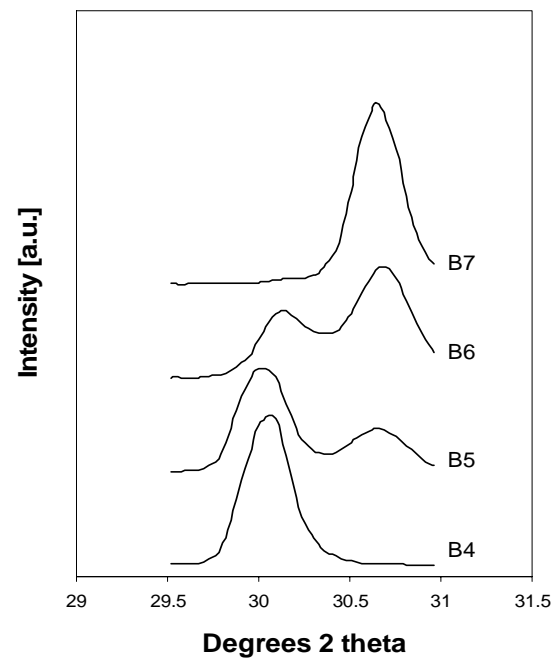
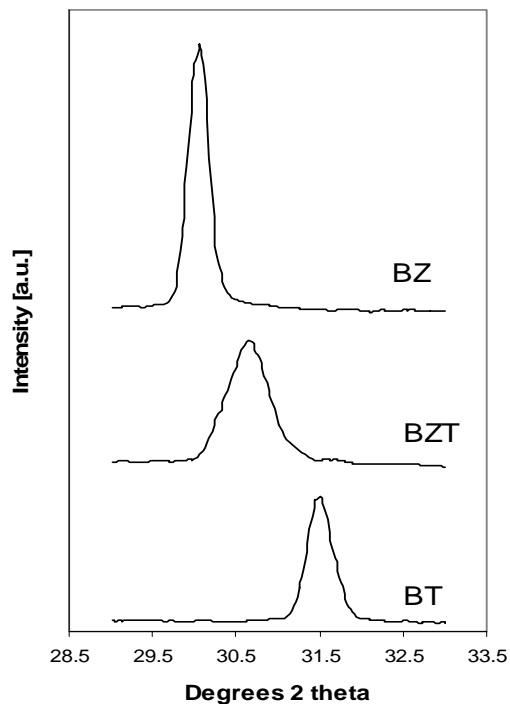
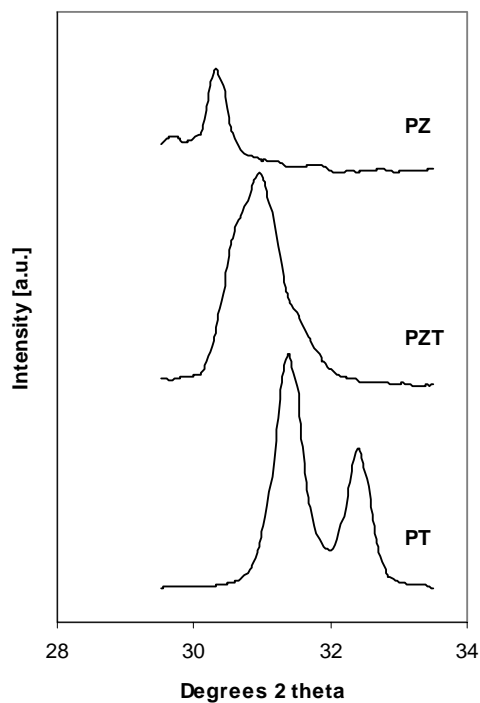
Pb Ba Zr Ti



pH + Additives



Following changes in phases by XRD



Novel Material Screening

<u>Zeolite</u>	<u>Modification #</u>					
	1	2	3	4	5	6
UZM-8	○	○	○	○	○	○
UZM-9	○	○	○	○	○	○
UZM-12	○	○	○	○	○	○
UZM-13	○	○	○	○	○	○
UZM-14	○	○	○	○	○	○
UZM-16	○	○	○	○	○	○
FER	○	○	○	○	○	○
Y-84	○	○	○	○	○	○

Andre ting vi jobber med

Oljefelt kjemikalier

Hydrogenlagring

MOF syntese

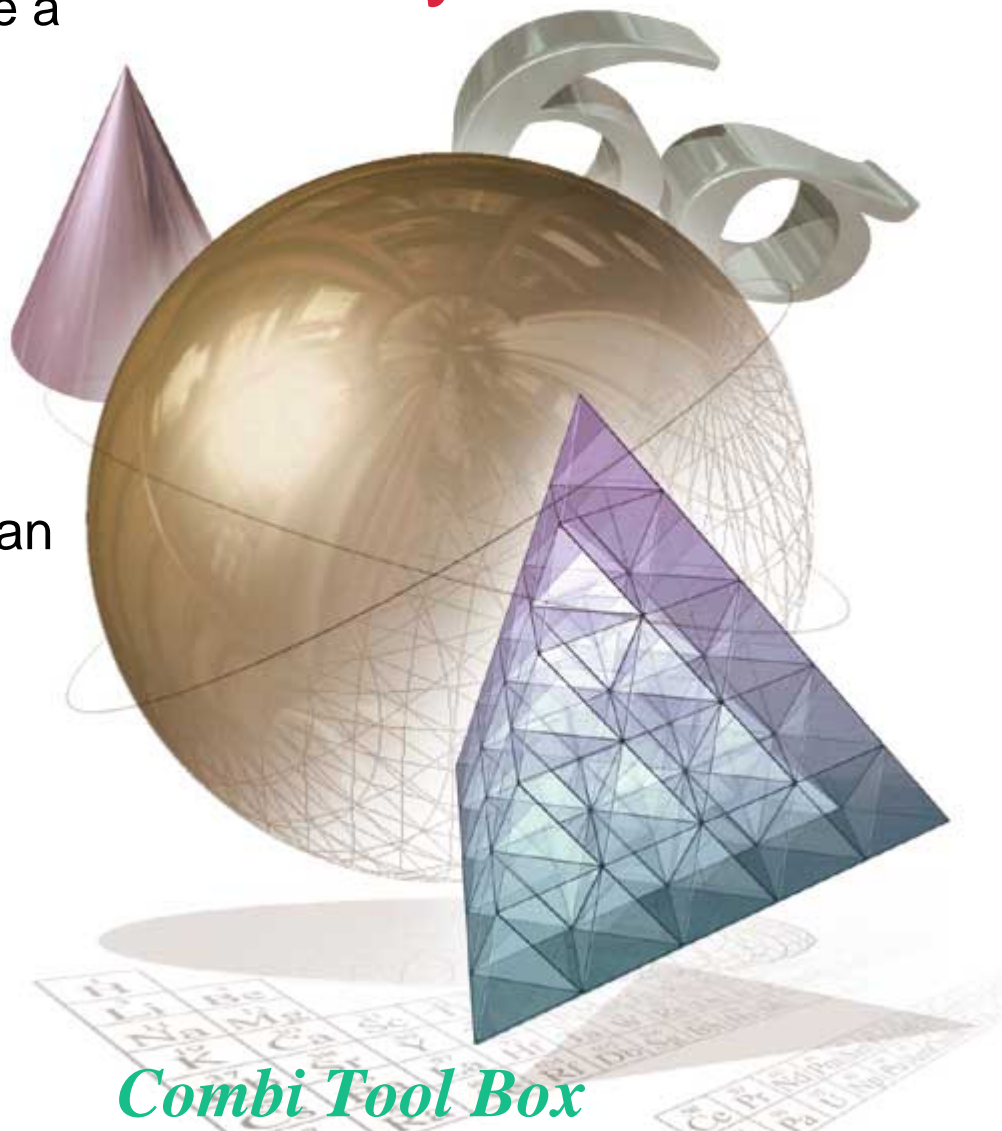
Perovskitter

Adsorpsjon

NO_x

Summary

- ▶ Combinatorial chemistry will create a step change in chemical R&D
 - Impact beyond discovery
- ▶ Success requires creation of a capability which is:
 - Realistic
 - Scalable
 - Combinatorial
- ▶ UOP and SINTEF have created an End-to-End™ combinatorial capability which has resulted in
 - New materials (structures/compositions)
 - Shortened scale-up times
 - New catalysts
- ▶ Demonstrated: fast track route from **Discovery** to **Optimization** through **Scale-up** and final **Commercialization**



Combi Tool Box

Key Component in Chemical R&D Tool Box