Digitalisierung im Metabolismus-Labor

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2. Lab organisation
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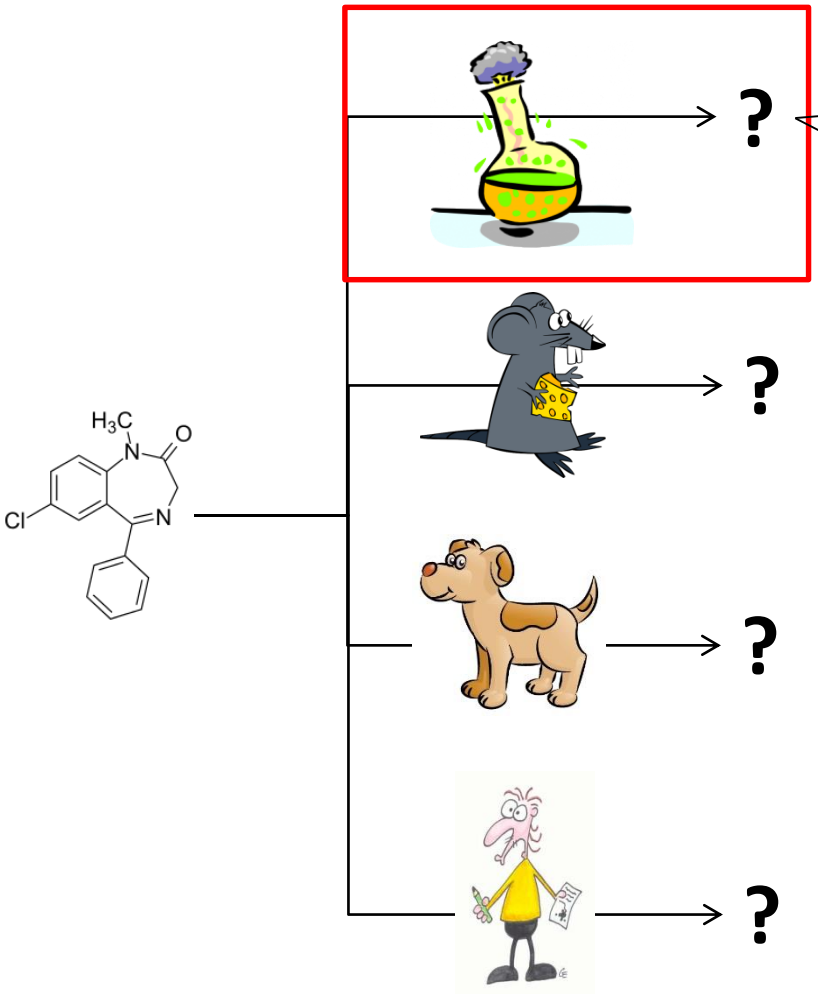
Xenobiotics

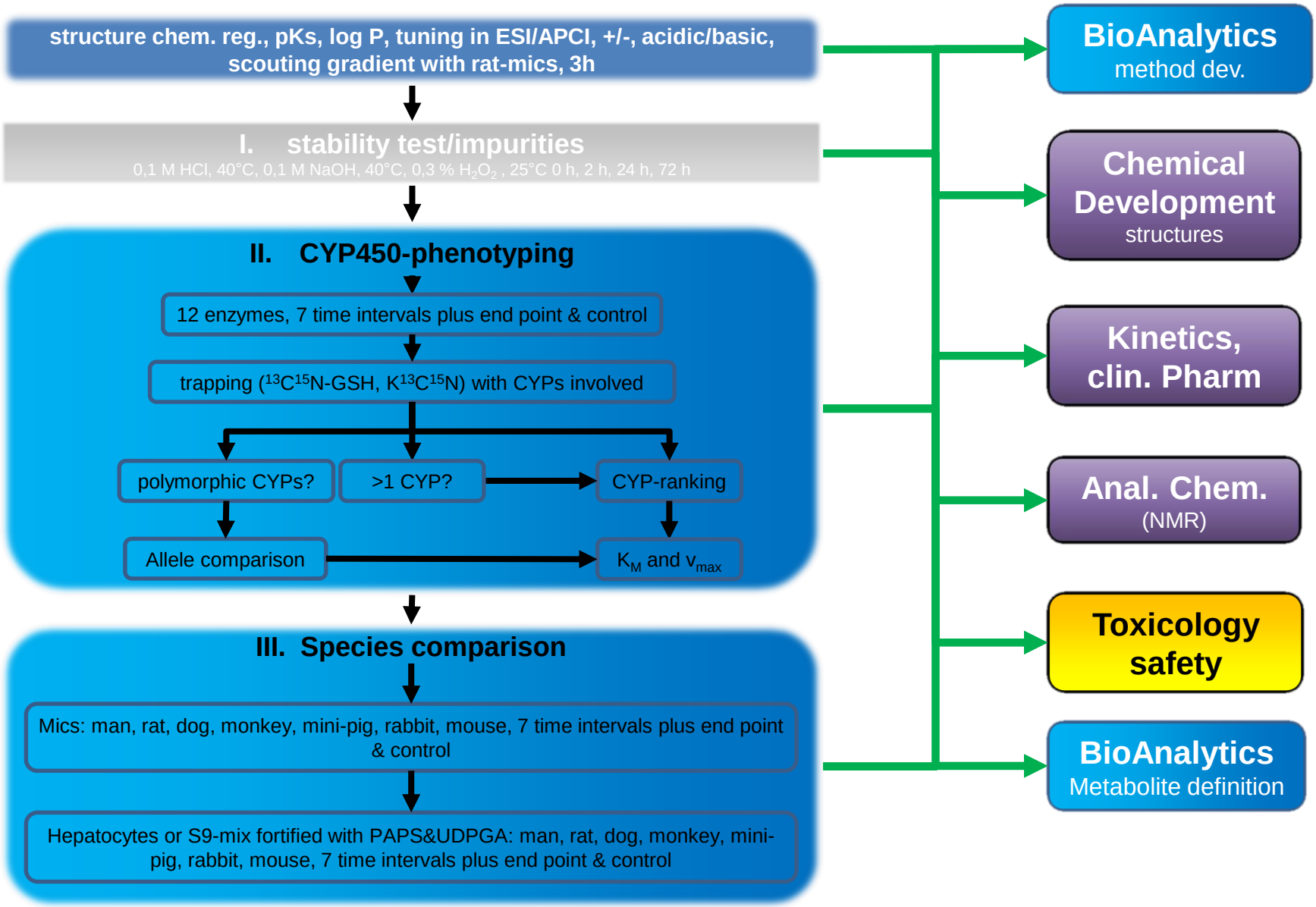
Metabolism

(gr: μεταβολή, "change")

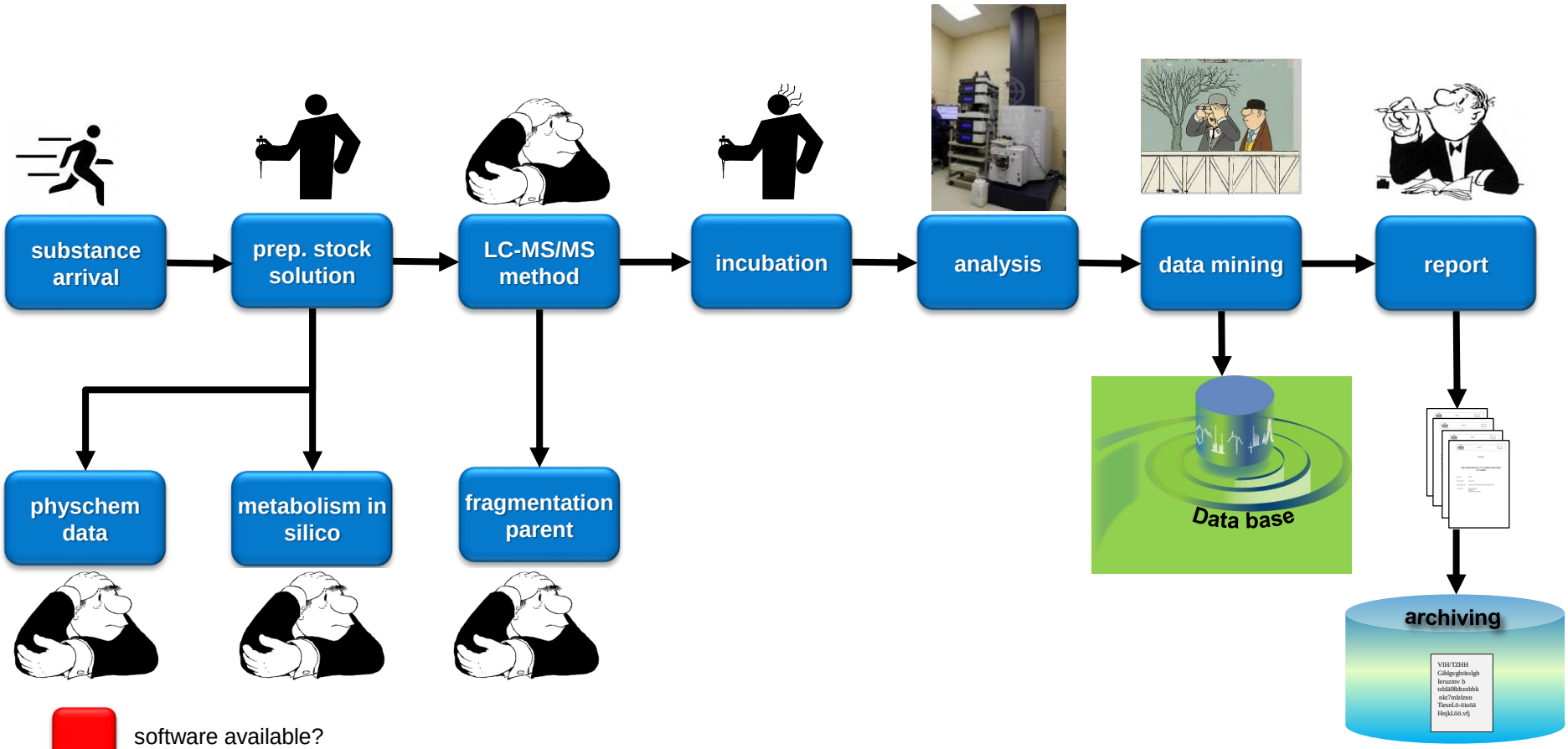


- Identification of an unknown number of unknown metabolites in complex matrices
- Determination of involved enzymes
- Establishing species dependent biotransformation pathways

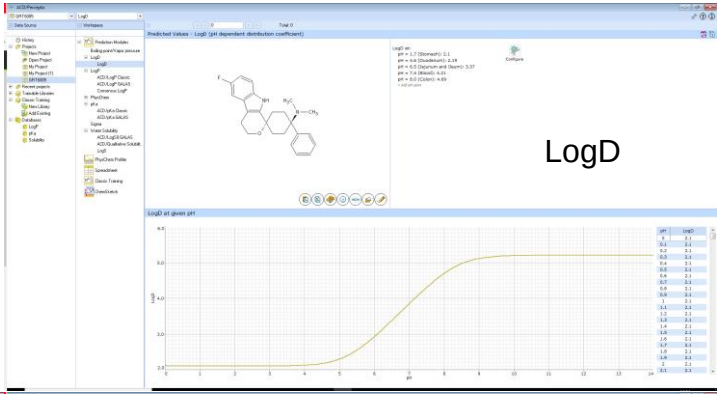
Work-flow, cross-links



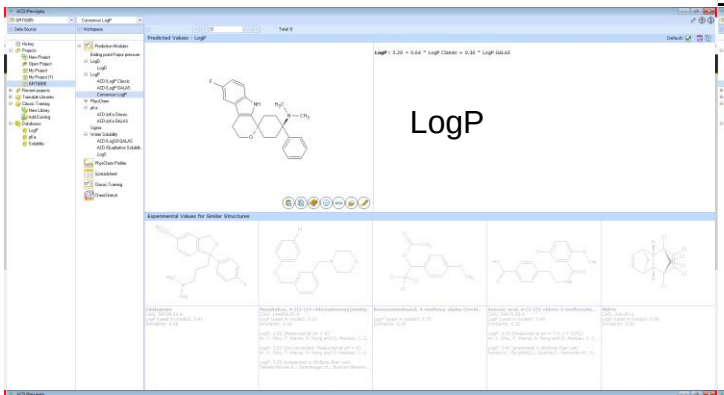
Lab organisation, work-flow



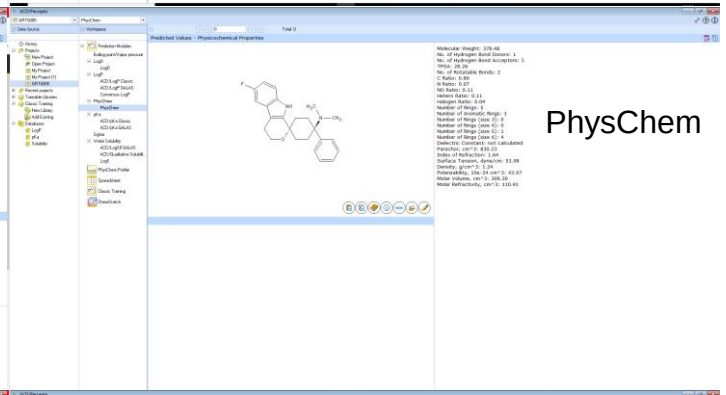
Calculation of PhysChem data



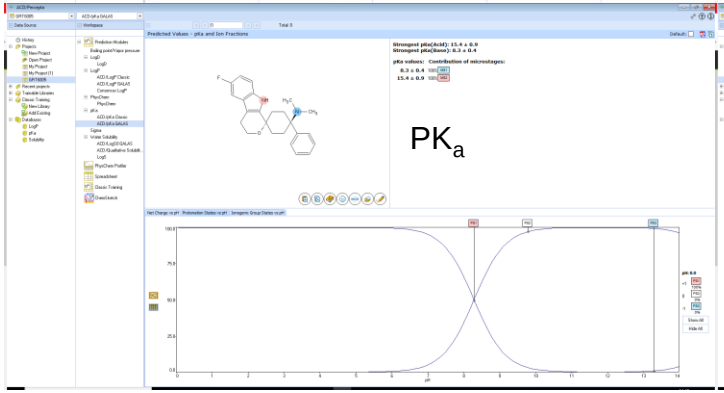
LogD



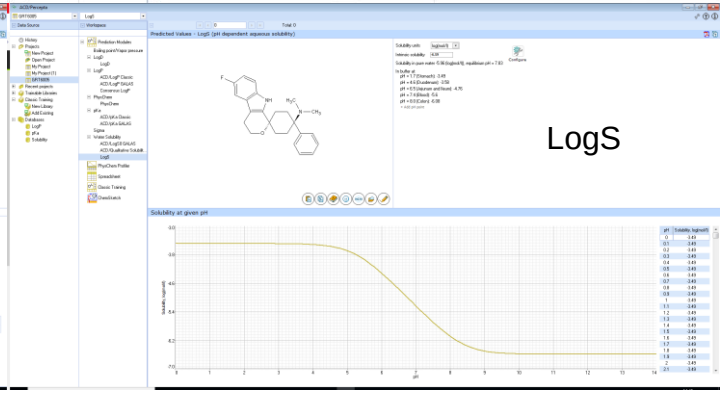
LogP



PhysChem

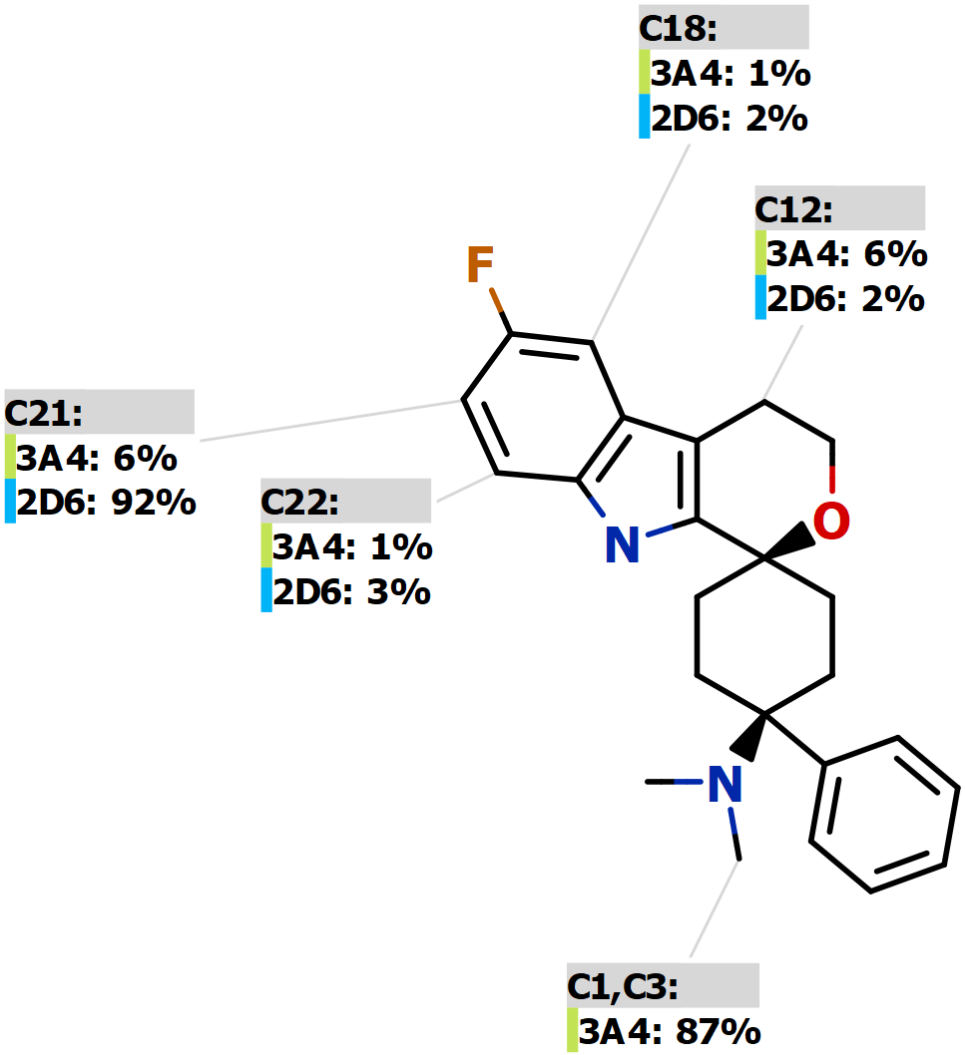


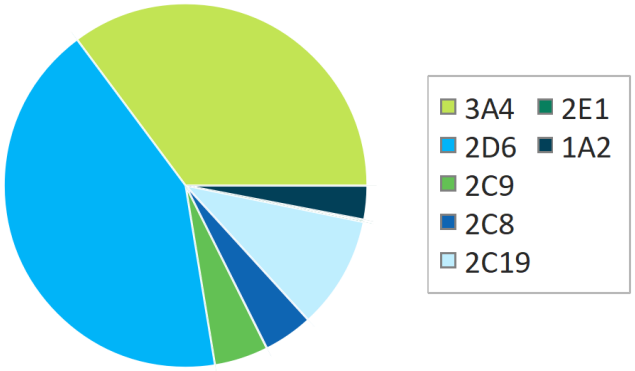
PK_a

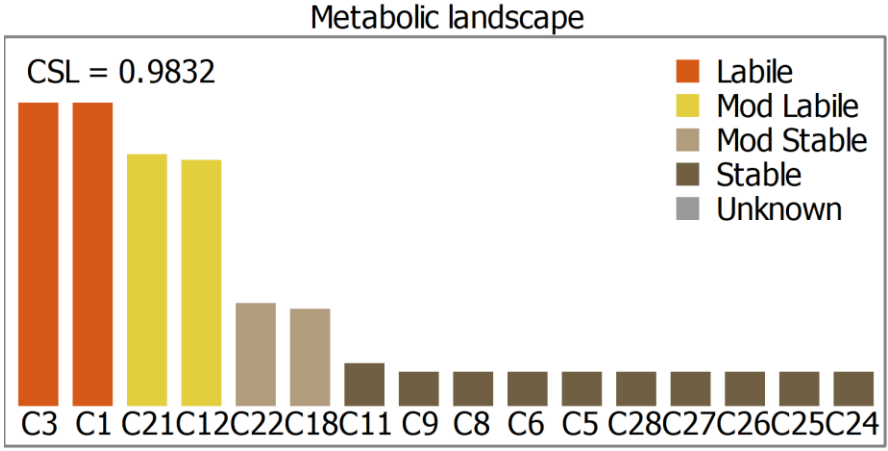


LogS

Metabolism in silico



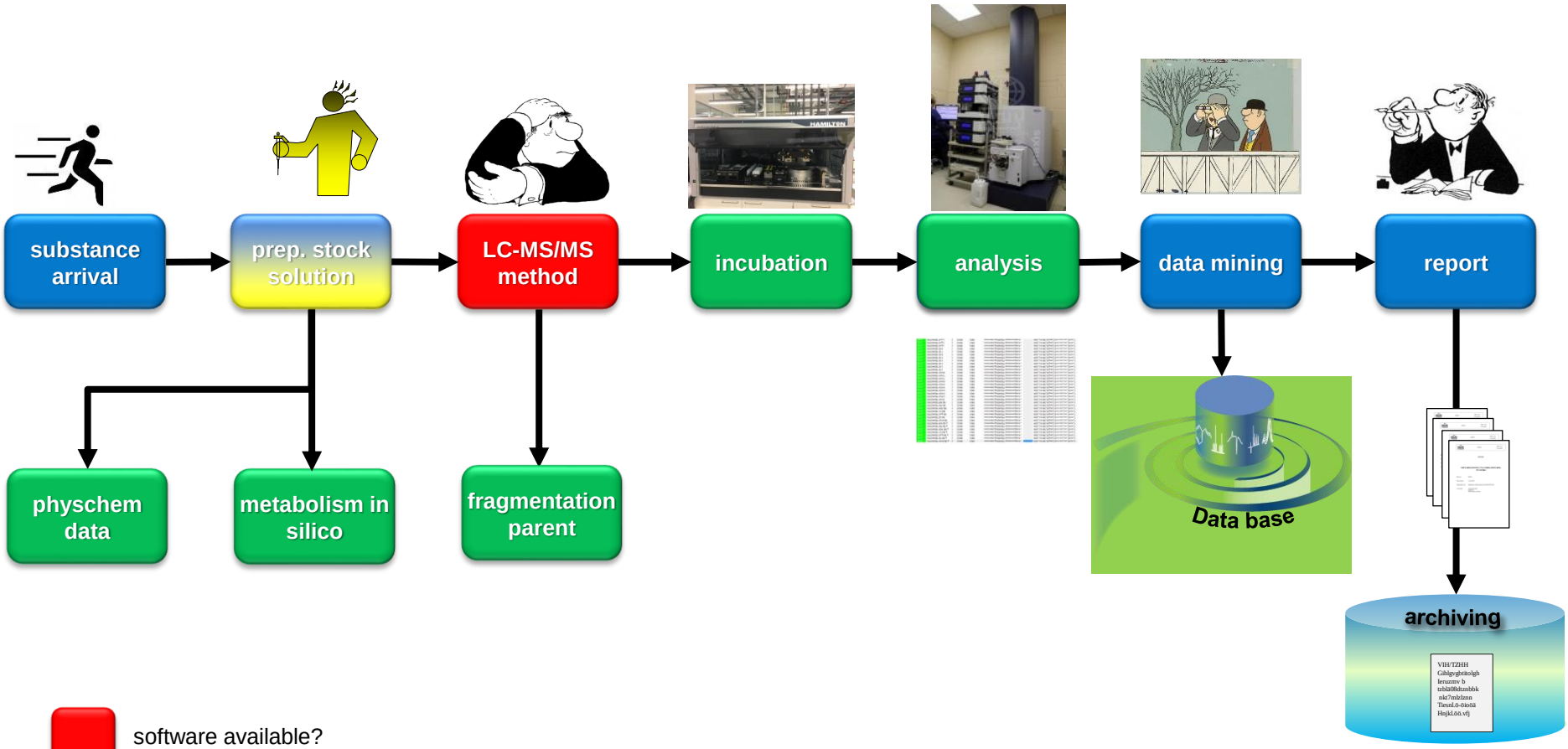




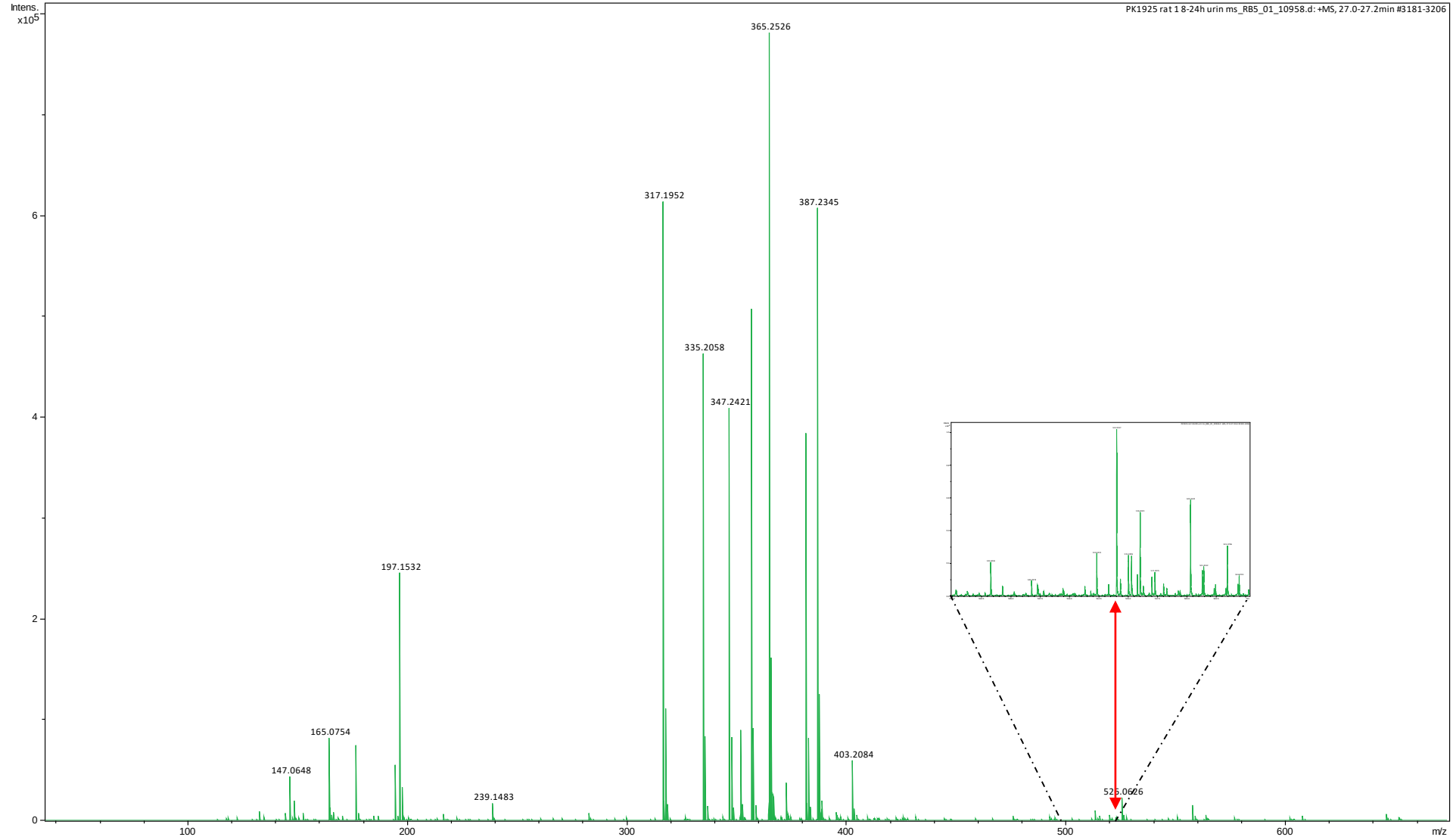
work-flow: incubations

Incubation vial	96 well plate
Mix buffer, microsomes, regenerating system	
Start of reaction by addition of substrate	
Incubation at 37°C on shaker for 60 min	Remove six aliquots at fixed time points
Incubation at 37°C on shaker for 120 min	Transfer into 96 well plates (stop with ACN)
Stop of reaction by addition of ACN	Protein precipitation centrifugation
	Evaporate to dryness Reconstitute with eluent

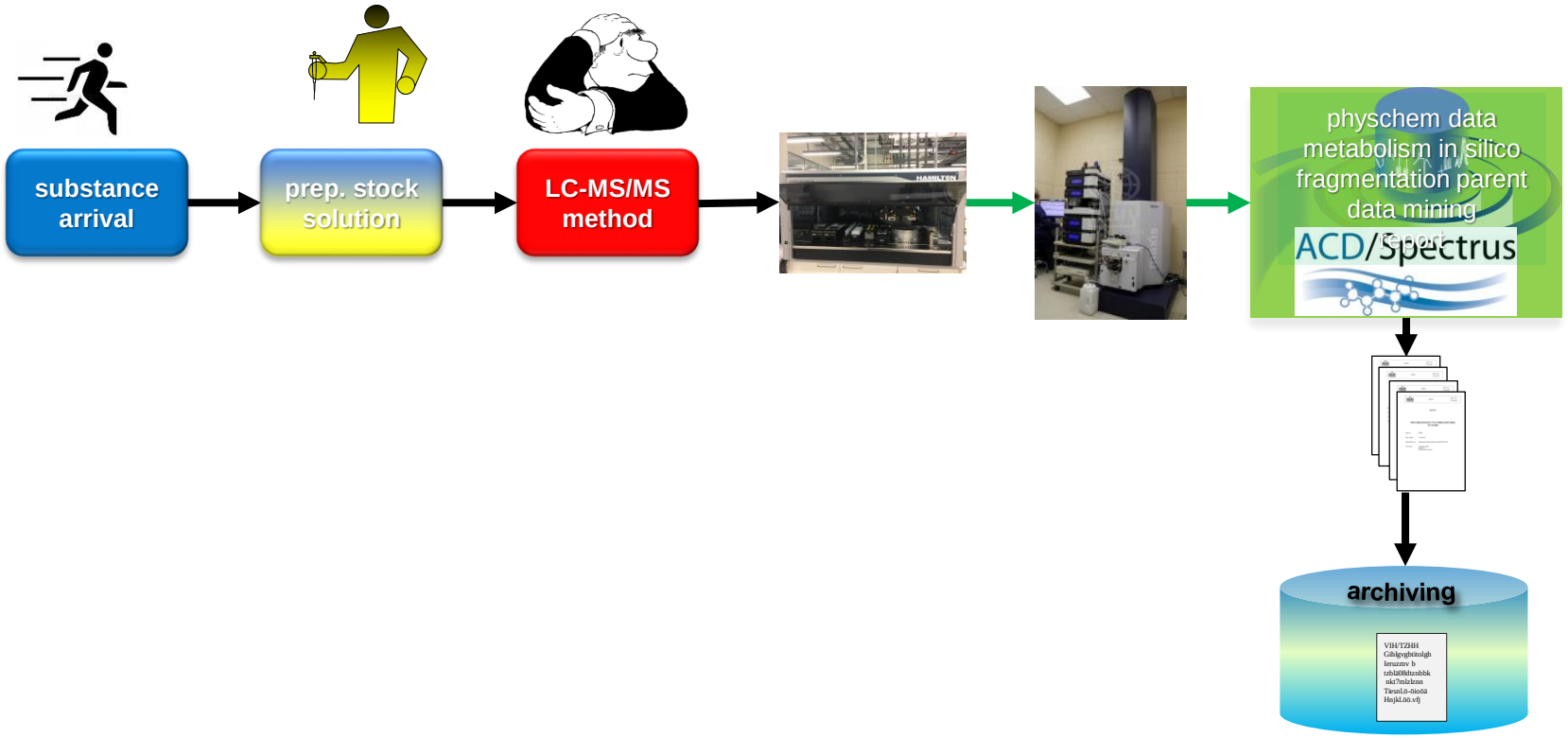
Lab organisation, work-flow



Lab organisation, data analysis

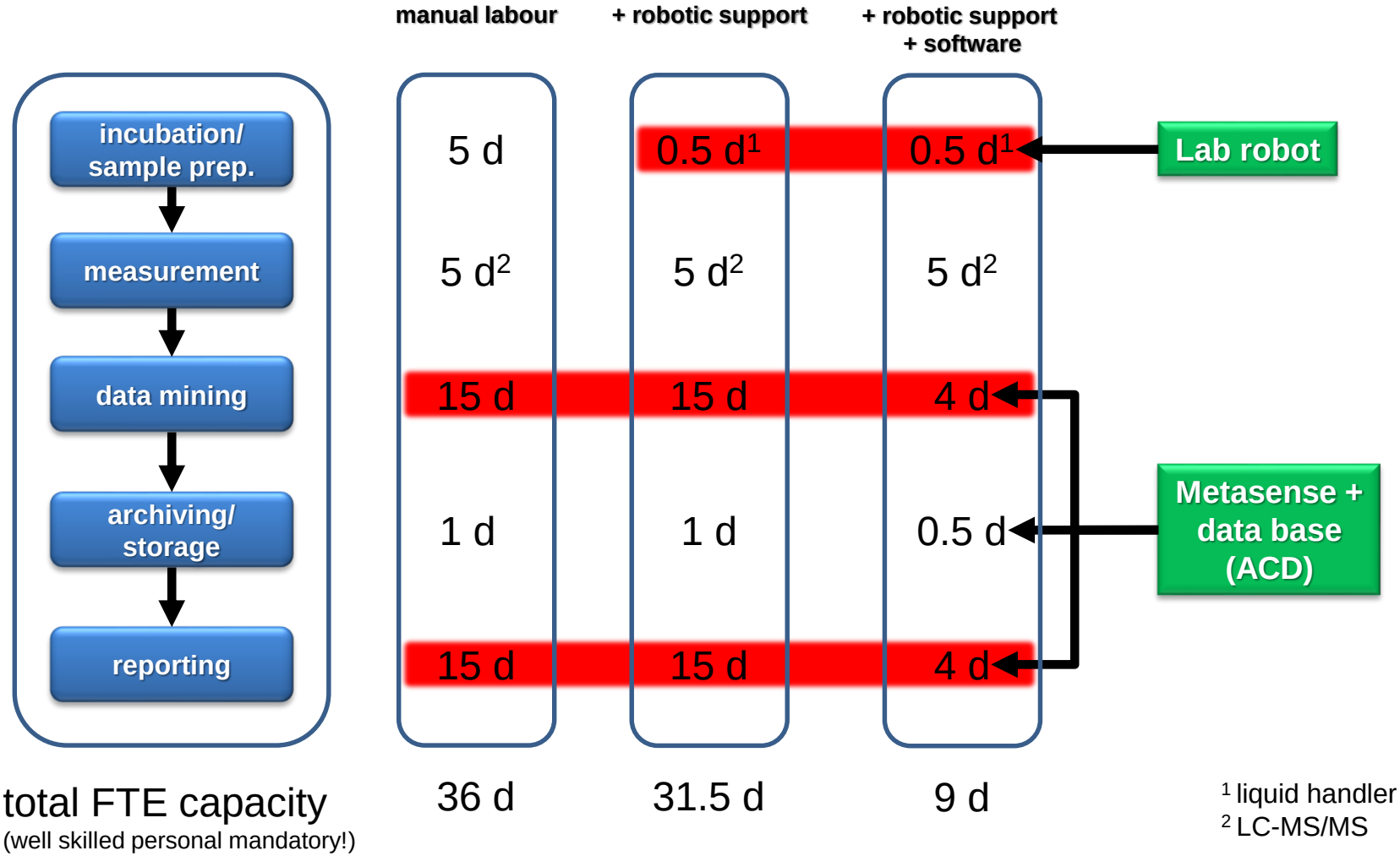


Lab organisation, work-flow



Capacities

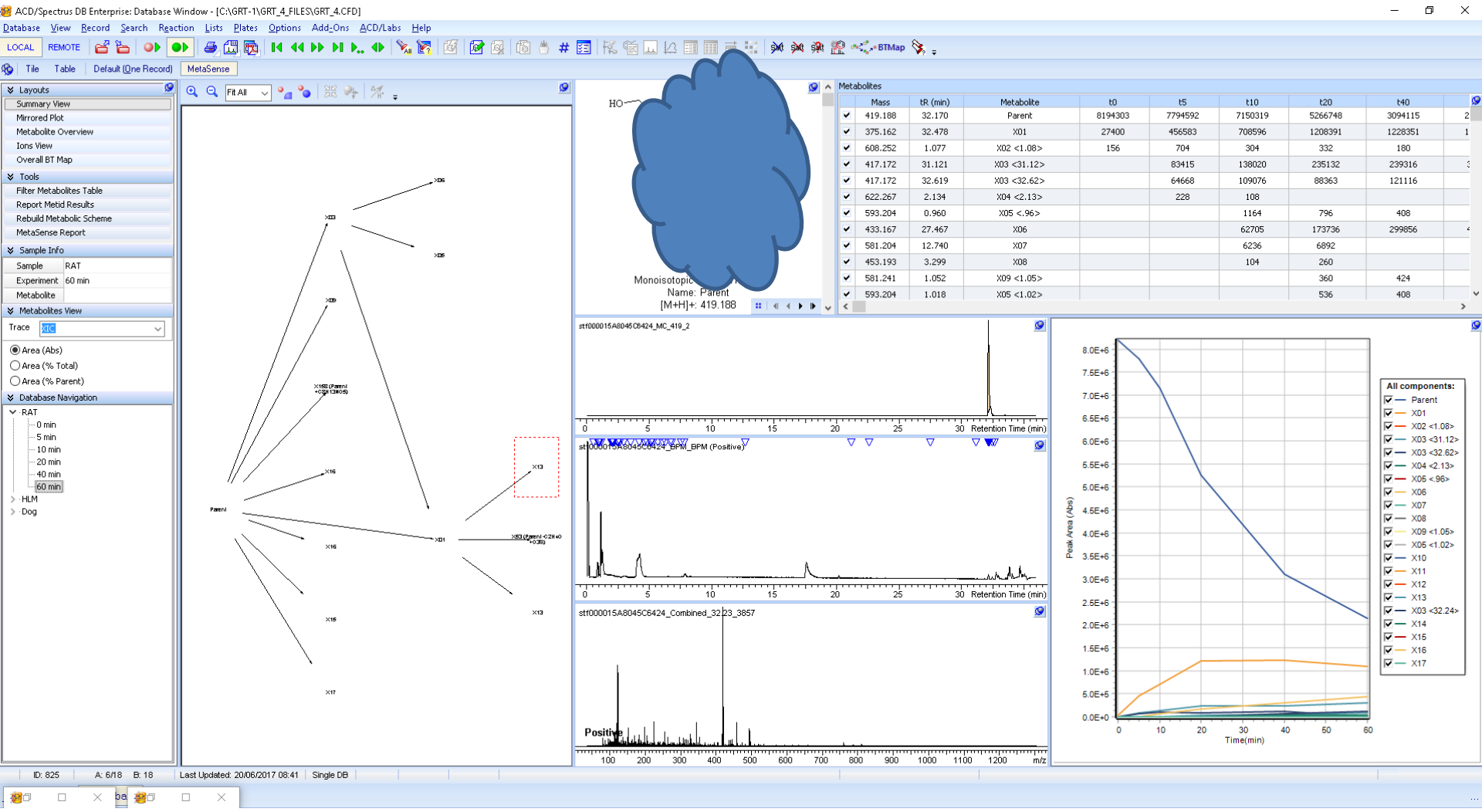
A typical pre-clin. work package contains app. 500 samples (per NCE)



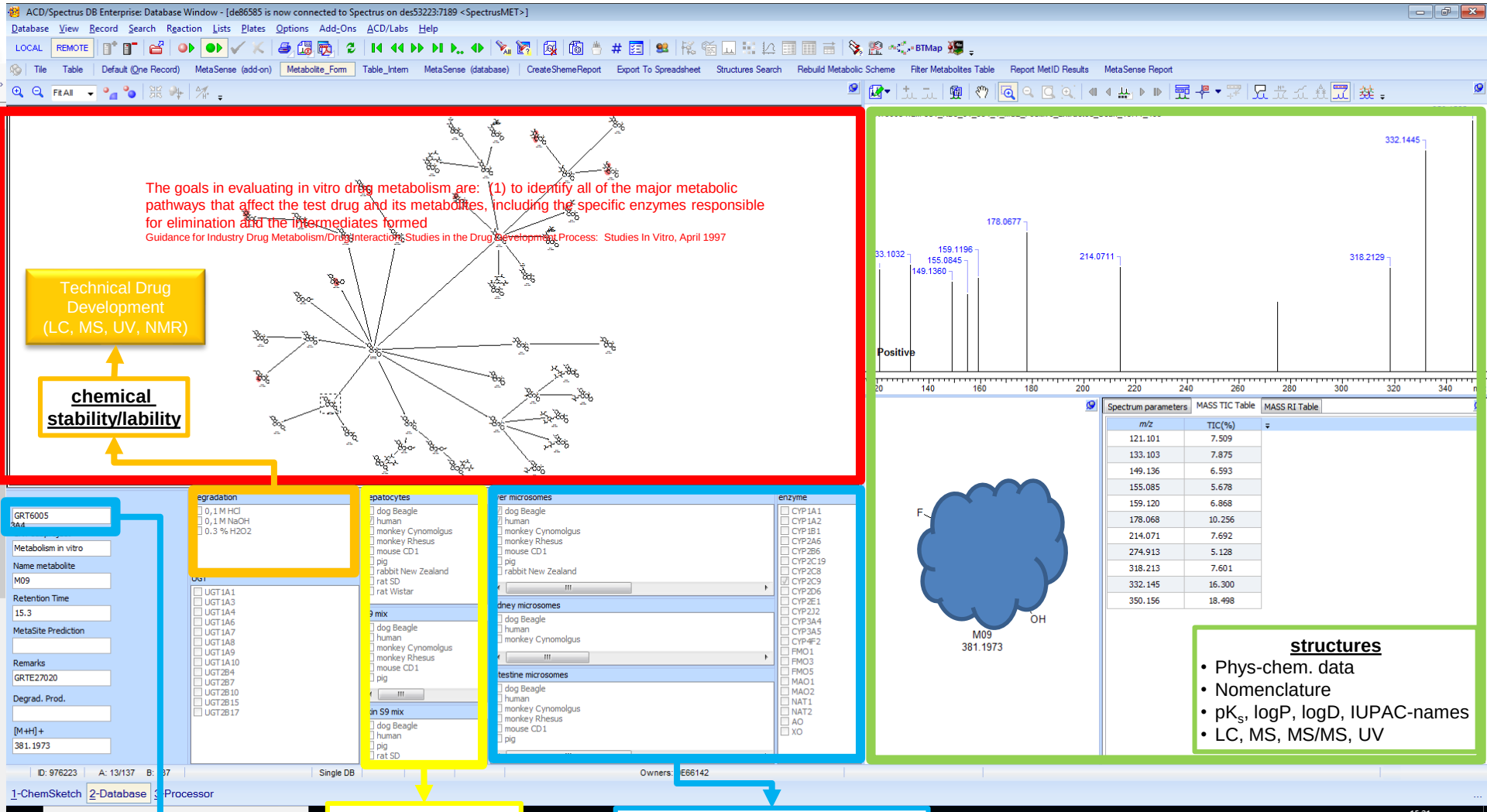
total FTE capacity
(well skilled personal mandatory!)

[1] liquid handler
[2] LC-MS/MS

Linking-up, ULI Result table



Linking-up, ULI Result table

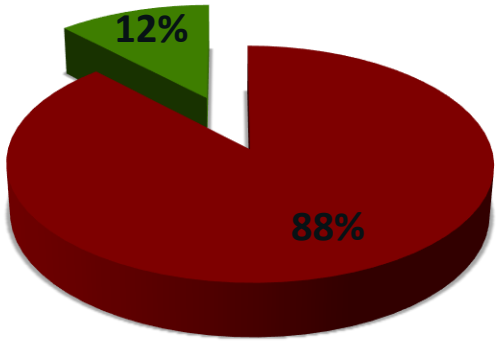


ULI (Unified Lab Information)

with courtesy from ACD-LABS

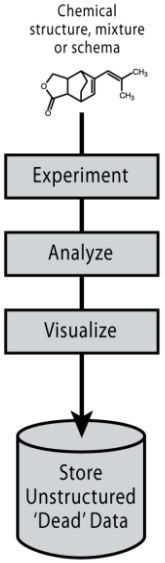
88% of R&D organizations lack adequate systems to automatically collect data for reporting, analysis, and decision-making[1]

[1]*Scientific Computing Research Study 2011*

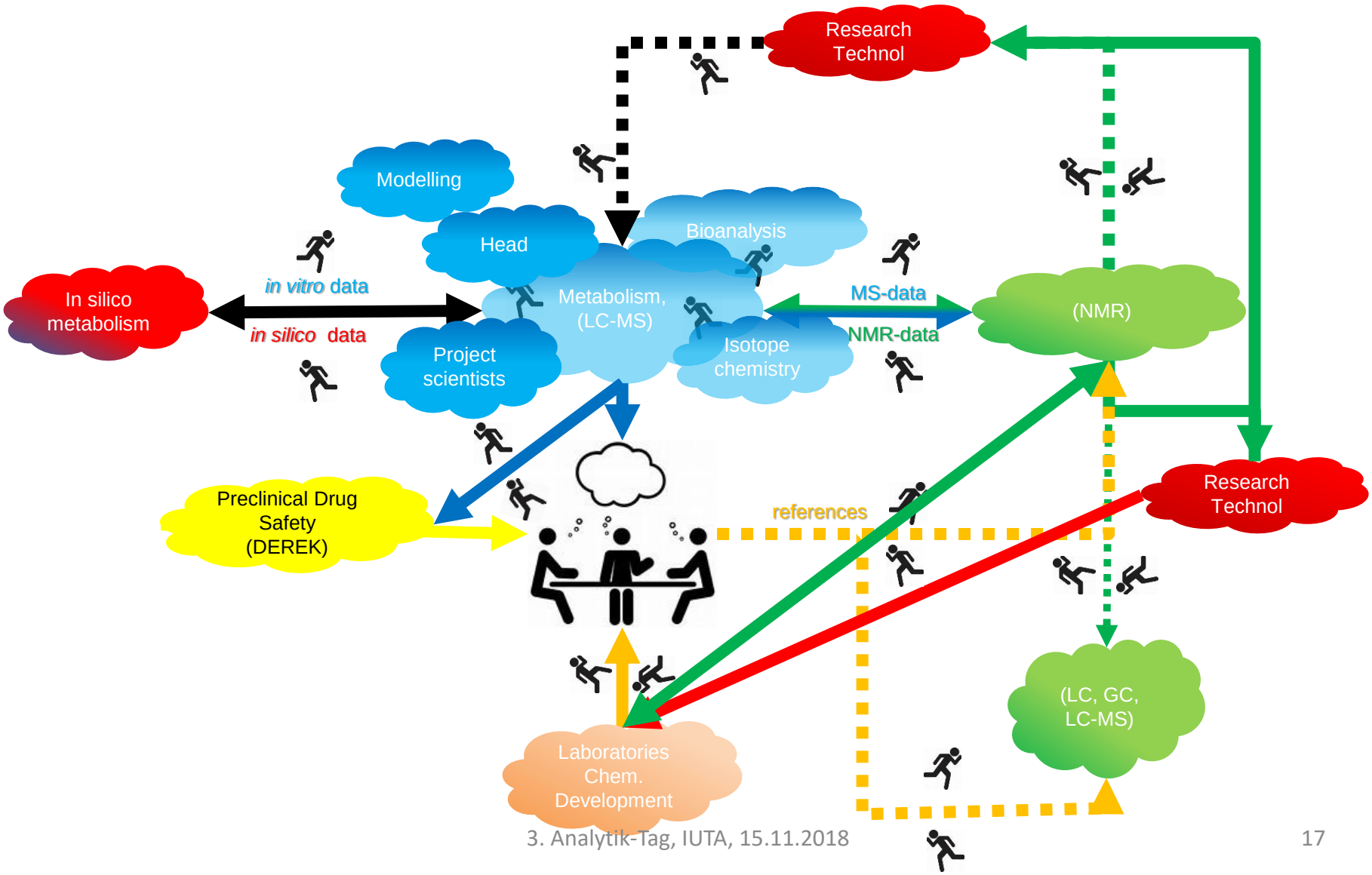


ACD/Spectrus

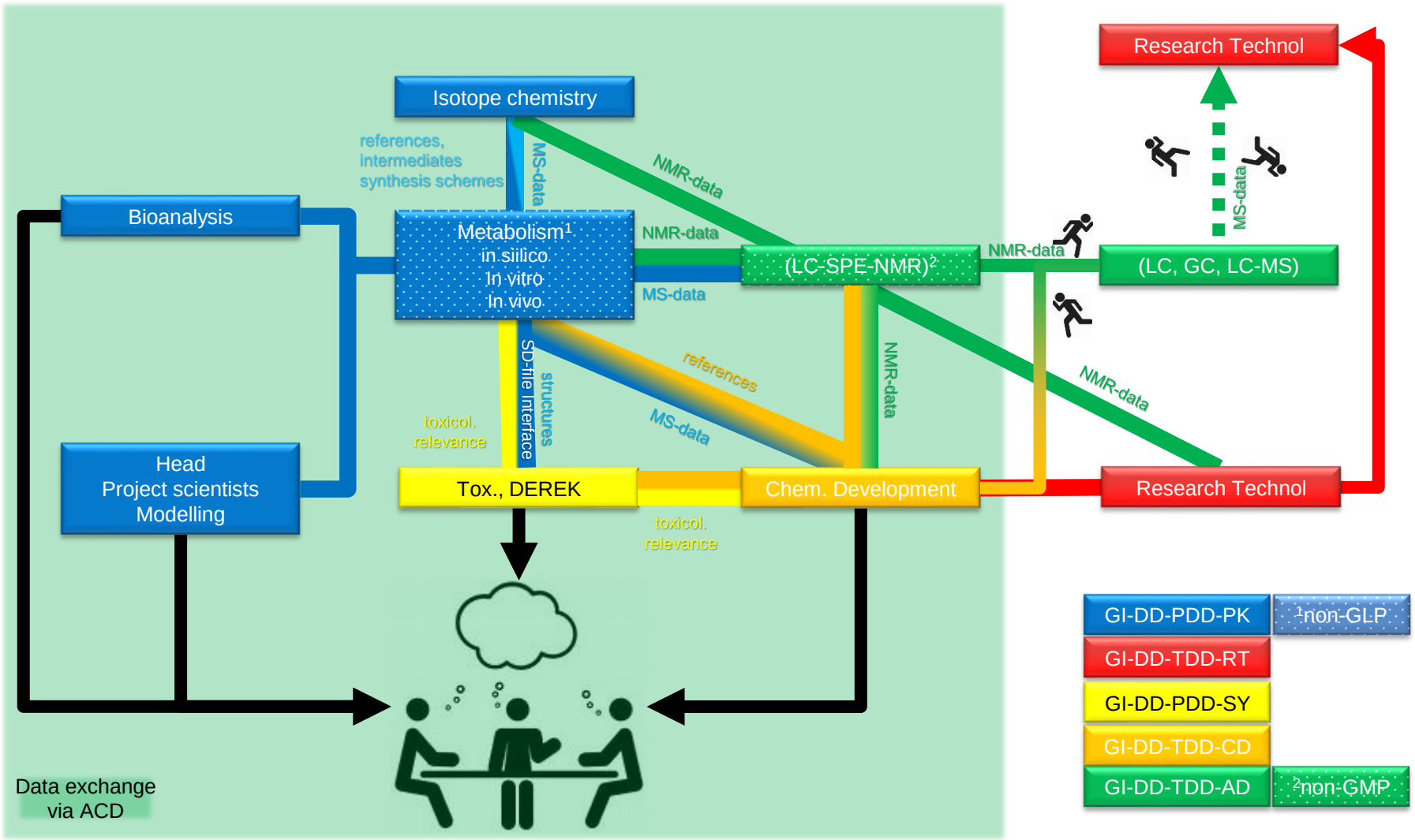
One-to-Many	One-and-Done
'Live' Data	**Dead Data**
Structured	Unstructured
Homogeneous	Heterogeneous
Unified Data	Siloed Data
Metadata for Search	Metadata for Search?
Analyze Repeatedly	Analyze Once
Accumulate Knowledge	Discrete Knowledge
Create Intelligence and Gain Insight	—



Data exchange



Data exchange



Conclusions

- Regulatory demands are constantly increasing
- Automation allows an efficiency increase at constant head count by replacing manual labour
- However: The full benefits of automation can **only** be obtained by implementing software solutions for data analysis
- A common data base allows fast and simple cross-functional data- and knowledge-transfer (ULI)

Hurdels

1. Time & money
2. Human factors: staff needs to
   - have or acquire skills in laboratory robotics, liquid handling, pipetting robots, analytical technologies, sample tracking/data base management, laboratory software
   - accept new work-flows
   - overcome fears
   - be stable

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