» Forschung in Wildau – innovativ und praxisnah «

Establishment of a digitalized workflow for the analysis of polycyclic aromatic compounds (PACs)

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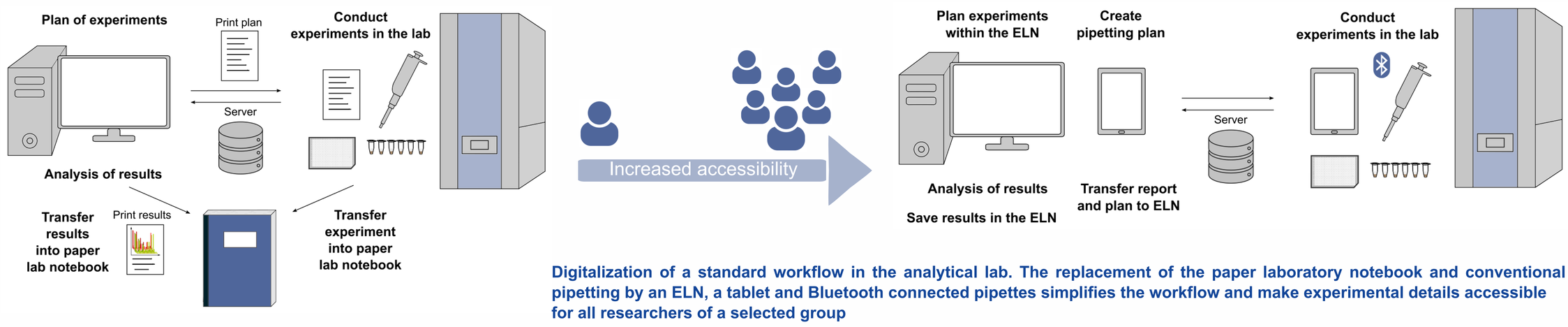
One-month project

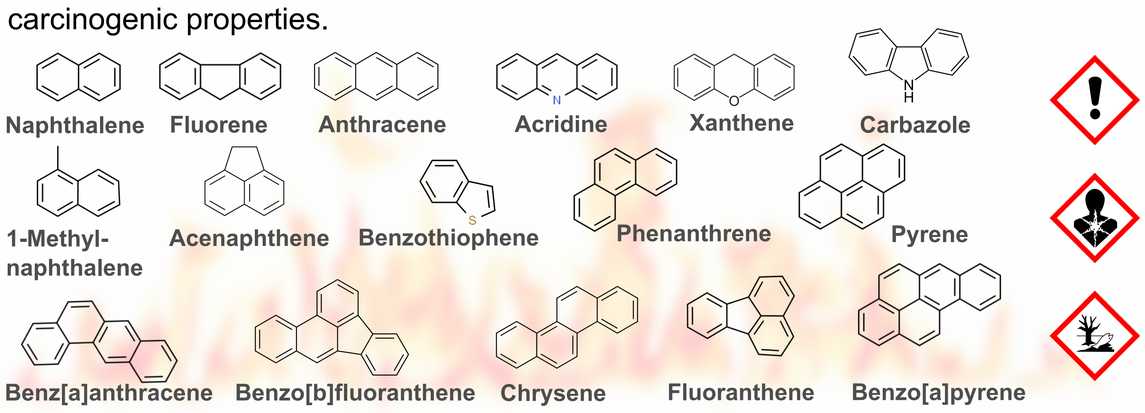
The project between SciNote, Gilson pipettes and the department of Molecular Biotechnology and Functional Genomics was initialized to drive the establishment of digitalization in the analytical laboratory. For this purpose, MALDI-TOF MS and LC-MS/MS experiments were planned with the Electronic Laboratory Notebook (ELN) of SciNote and conducted with the Bluetooth pipetting system Gilson TRACKMAN Connected. Results and all related experimental data were saved within the ELN.



Digitalization of a standard workflow in the analytical lab. The replacement of the paper laboratory notebook and conventional pipetting by an ELN, a tablet and Bluetooth connected pipettes simplifies the workflow and make experimental details accessible for all researchers of a selected group

Research objective

The focus of research was the establishment of analytical methods for the detection and quantification of polycyclic aromatic compounds (PACs) within the project agruPhysics PAK[1]. PACs is a collective term for polycyclic aromatic hydrocarbons (PAH) and heterocyclic aromatic compounds (NSO-HET). PAH are fused aromatic rings with C and H atoms only, whereas NSO-HET include N, S or O heteroatoms also. The ubiquitous and persistent environmental pollutants are released through incomplete combustion of organic material and exhibit toxic, mutagenic and carcinogenic properties.



Structures of investigated polycyclic aromatic hydrocarbons and NSO heterocyclic compounds

Automated pipetting system

The pipetting system Gilson TRACKMAN Connected integrates a tablet and Bluetooth connected pipettes to facilitate the pipetting of 96 and 384 well microtiter plates. All pipetting plans are first created on the tablet. After initiating the program the pipettes are connected. The predefined volumes are automatically transferred to the pipettes and the user can follow the instructions shown on the tablet.

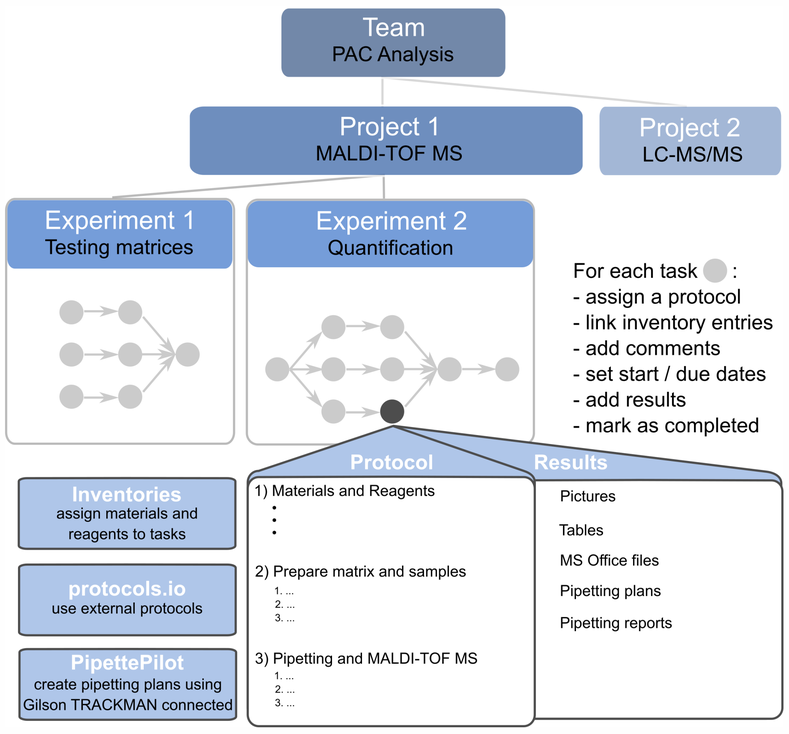
Further features:

- multi-pipetting and automated mixing
- visual and acoustical assistance of pipetting
- environmental sensor (temp., humidity, pressure)
- detailed report generation with experimental data
- direct connection to SciNote to export pipetting plans and reports

Experimental setup with the Gilson TRACKMAN connected for the MALDI-TOF MS of PACs

Electronic laboratory notebook (ELN)

An Electronic Laboratory Notebook is an online platform, on which a group of scientists (team) can work together on projects, write and share protocols, plan experiments and store all data in one place.



Overview of the project organization within SciNote for the analysis of PACs

Integrated functionalities of the SciNote ELN:

- inventories to organize material
- MS Office Online for protocols and results
- accessibility of external protocols (protocols.io)
- activity lists to track all changes
- experiment reports
- Manuscript Writer add-on

Lab experiences of the digitalization

The integration of the ELN and the connected pipetting system was started with remote trainings which were accomplished quickly through the intuitive handling of the SciNote and Gilson PipettePilot software, respectively. It took some time to get familiar with the new workflow which includes the programming of the pipetting plans that increased the time necessary for the experimental setup. Finally, significant advantages of the digitalized workflow could be shown:

- data accessibility for every team member, anywhere, anytime
- data organisation: results are directly linked to the protocols
- faster and easier pipetting with standardized protocols
- accessibility for academia: free version of SciNote with 1 GB storage capacity
- increased sustainability: less consumables and paper sheets used

Comparison of the standard and the digitalized workflow for a selected protocol

Parameter	Standard workflow	Digitalized workflow
Writing the protocol	17 min	33 min (ELN: 13 min, Pip. plan: 20 min)
Experimental setup	14 min	9 min
Pipetting	27 min	19 min
Analysis of results	1 h	1 h
Laboratory notebook (LN)	37 min (exp. execution, some results)	5 min (comments, all results)
Consumables	24 tubes, 53 tips	3 tubes, 28 tips, 21/384 wells of a MTP
Paper (A4)	3.5 (2 printed, 1.5 LN)	/

The outcome of using an ELN in numbers:

1 Team · 3 Inventories · 6 Projects · 18 Experiments · 34 Tasks · 17 Protocols · 755 A4 sheets saved

Homepage:
www.th-wildau.de/molekularbiologie

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[1]The project agruPhysics PAK is funded within the NEMO network agruPhysics (www.agru-physics.de) by the BMWi in the program "Zentrales Innovationsprogramm Mittelstand (ZIM)" managed by VDI/VDE/IT under Reg. No. 16KN073440.