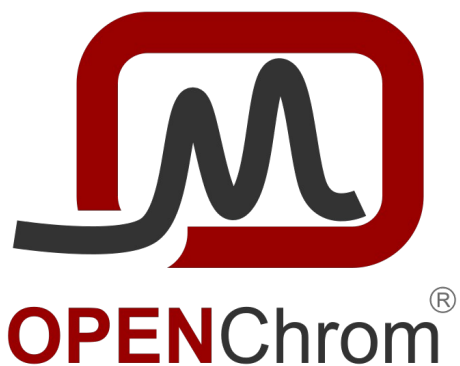
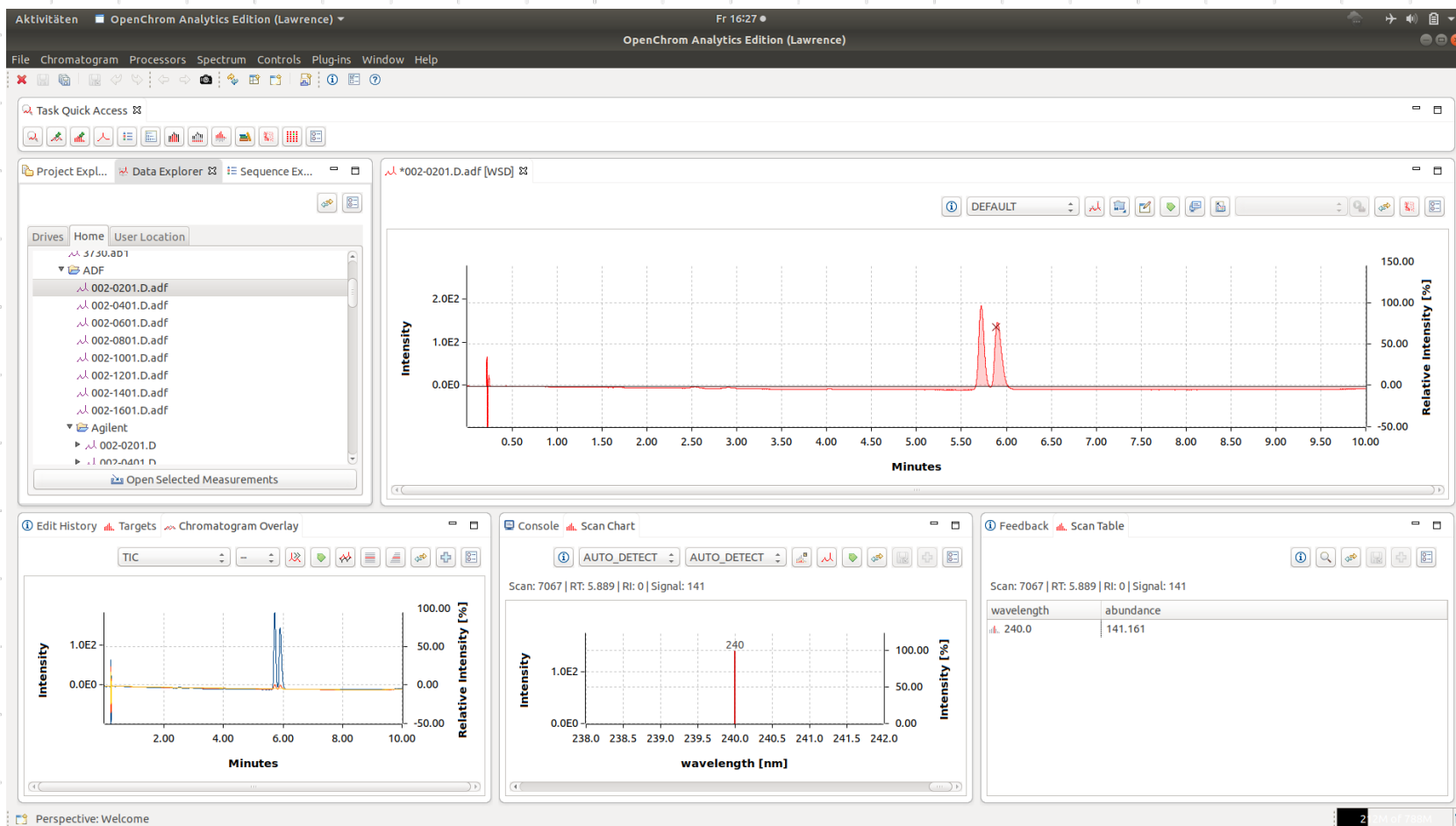
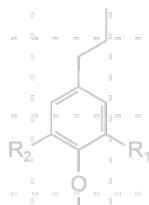




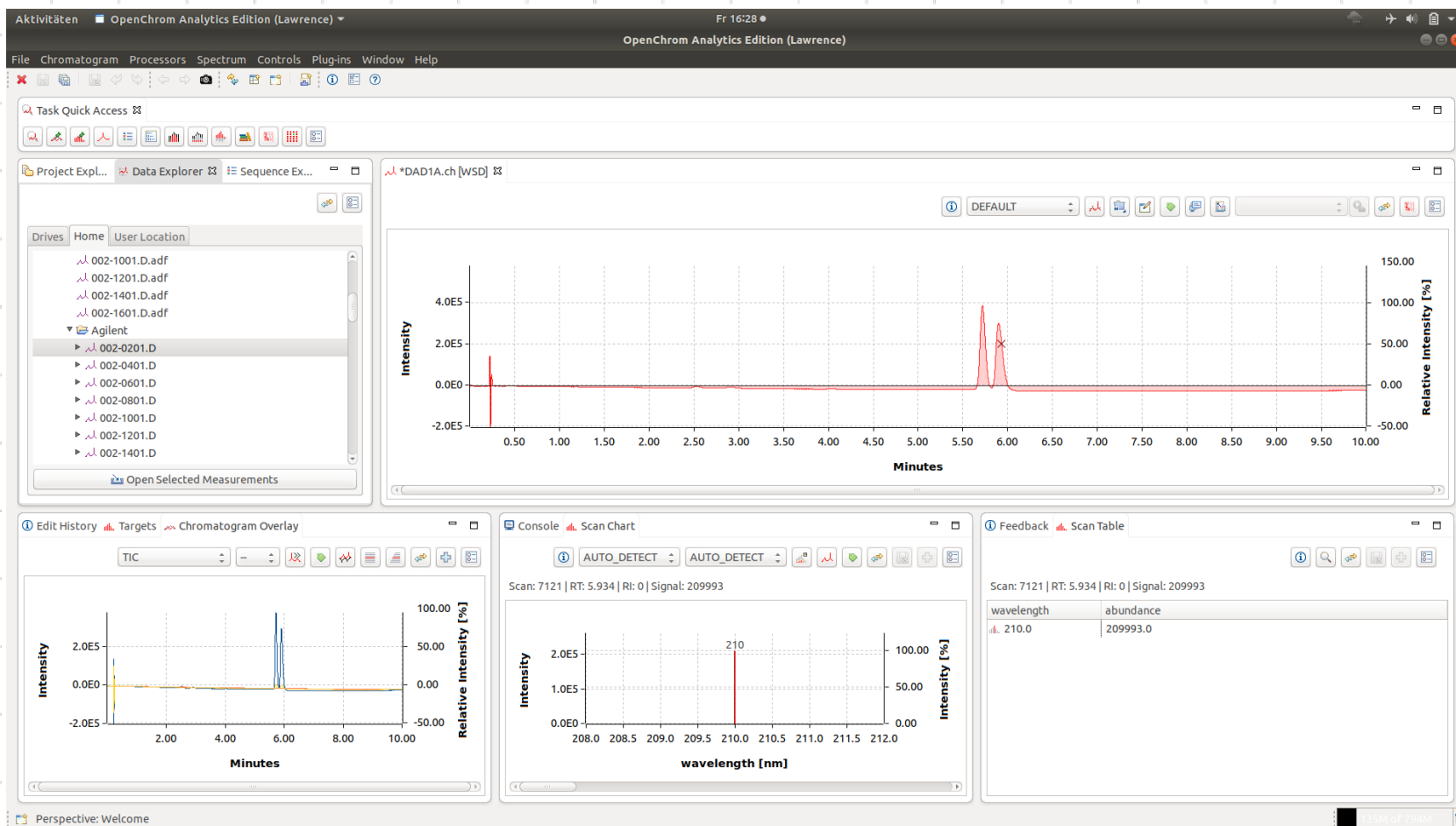
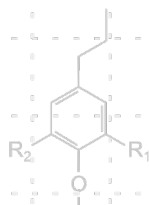
Desktop analysis of ADF files

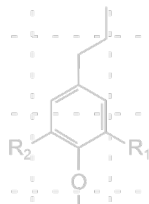
Allotrope Connect Workshop, Cambridge, USA, 2018/11/06

Load ADF and raw data



Load ADF and raw data





Automation of **Py-GC/MS** data analysis

2004: VB6 and ChemStation macros

2007: **Java** and **Eclipse RCP**

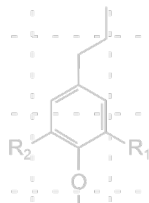
2010: First Release

2012: Finish PhD

2013: Founding a company (Lablicate GmbH)

2013: **Eclipse Foundation** membership

2018: **Allotrope Foundation** membership



GC/MS – nominal, tandem, high resolution

GC/FID – and other detectors

LC/DAD – and UV-Vis detectors

PCR and other analytical data

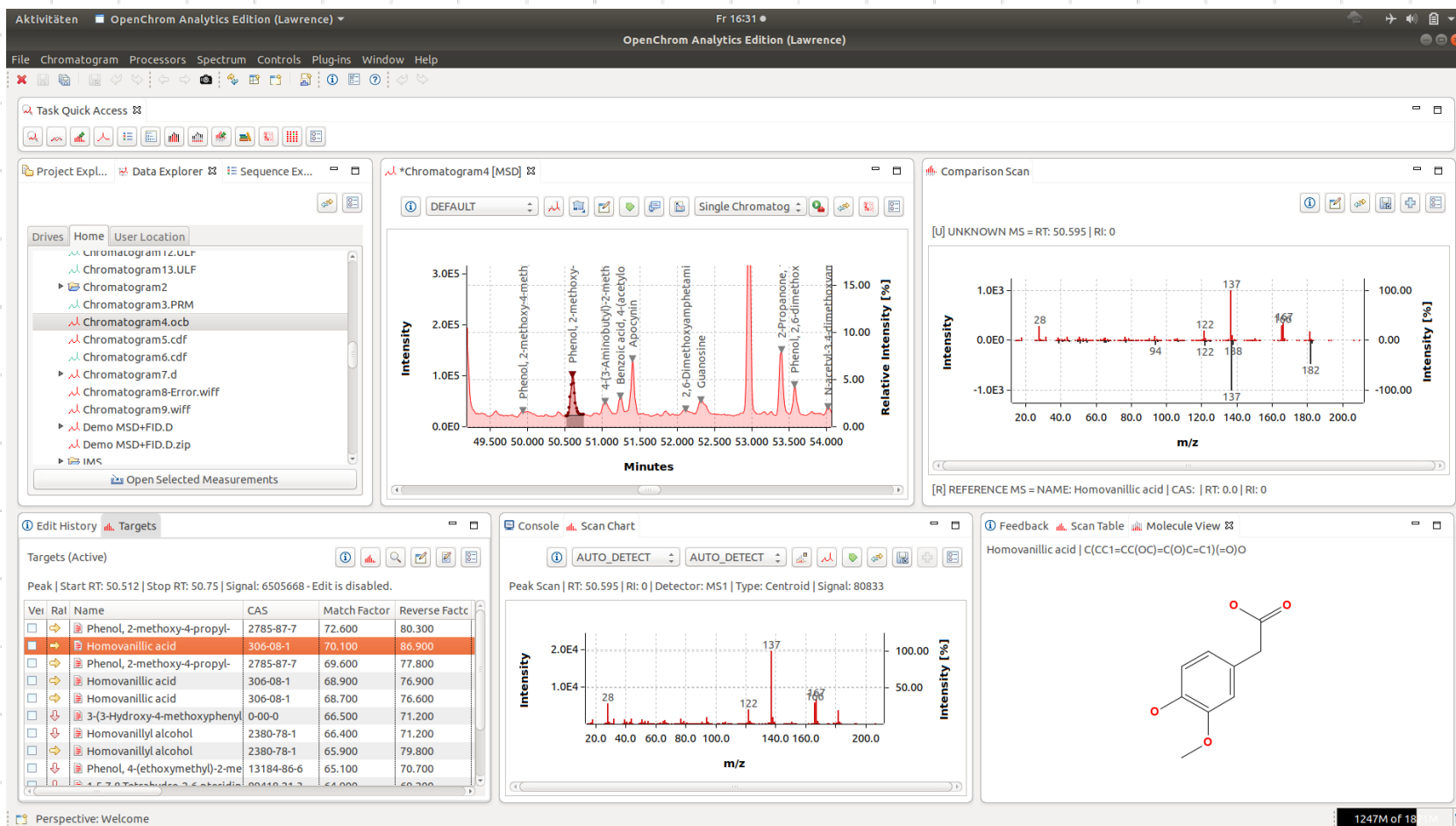
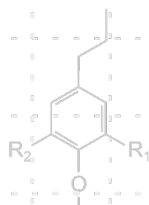
MALDI-TOF – spectrum analysis

NMR* – currently under development

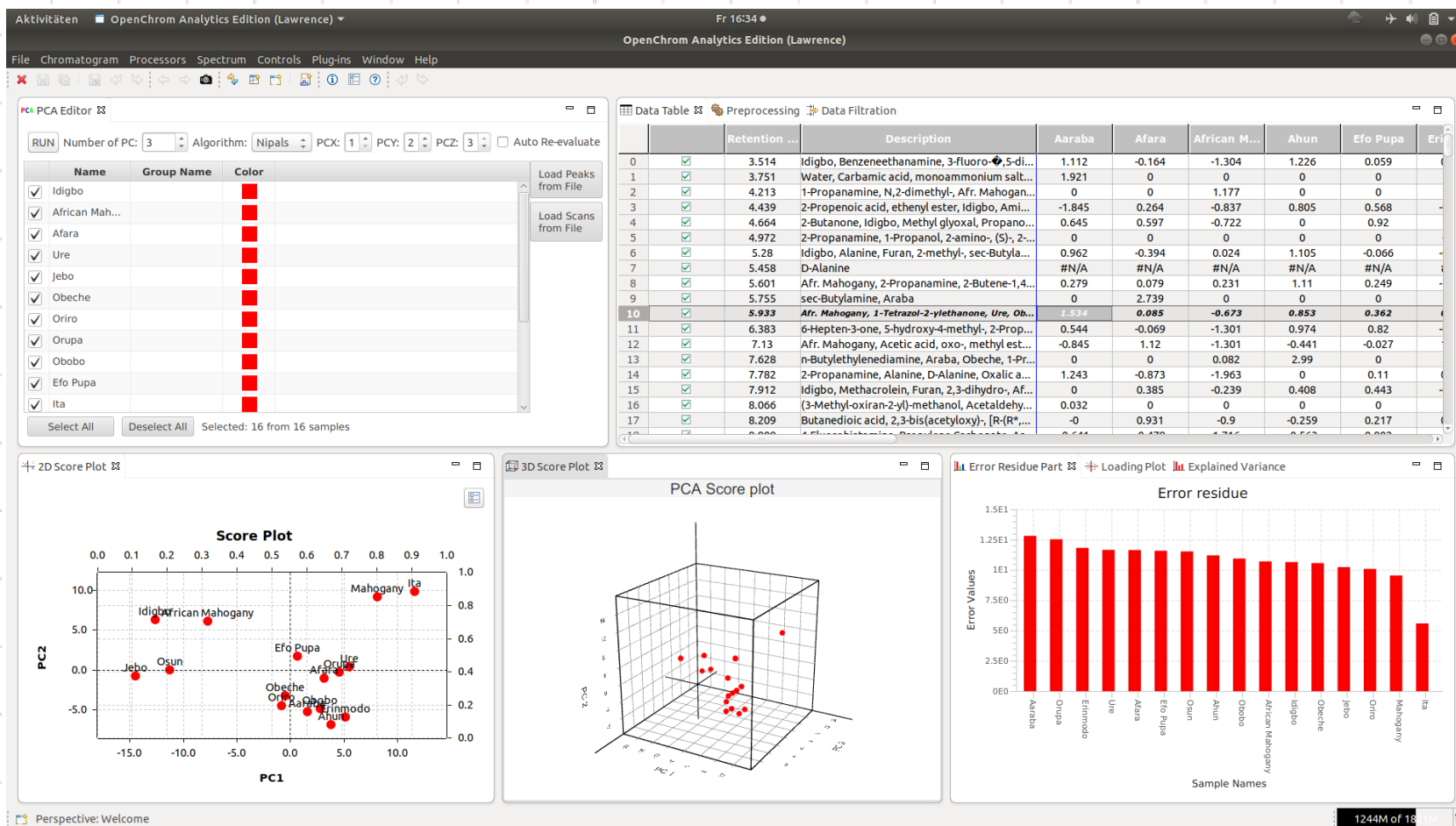
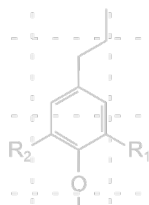
FTIR* – currently under development

Classifier, Filter, Baseline-, Peakdetection, Integration, RI
Calculation, Identification, Quantitation, PCA, Reporting, LIMS
Connectors, ... * in progress

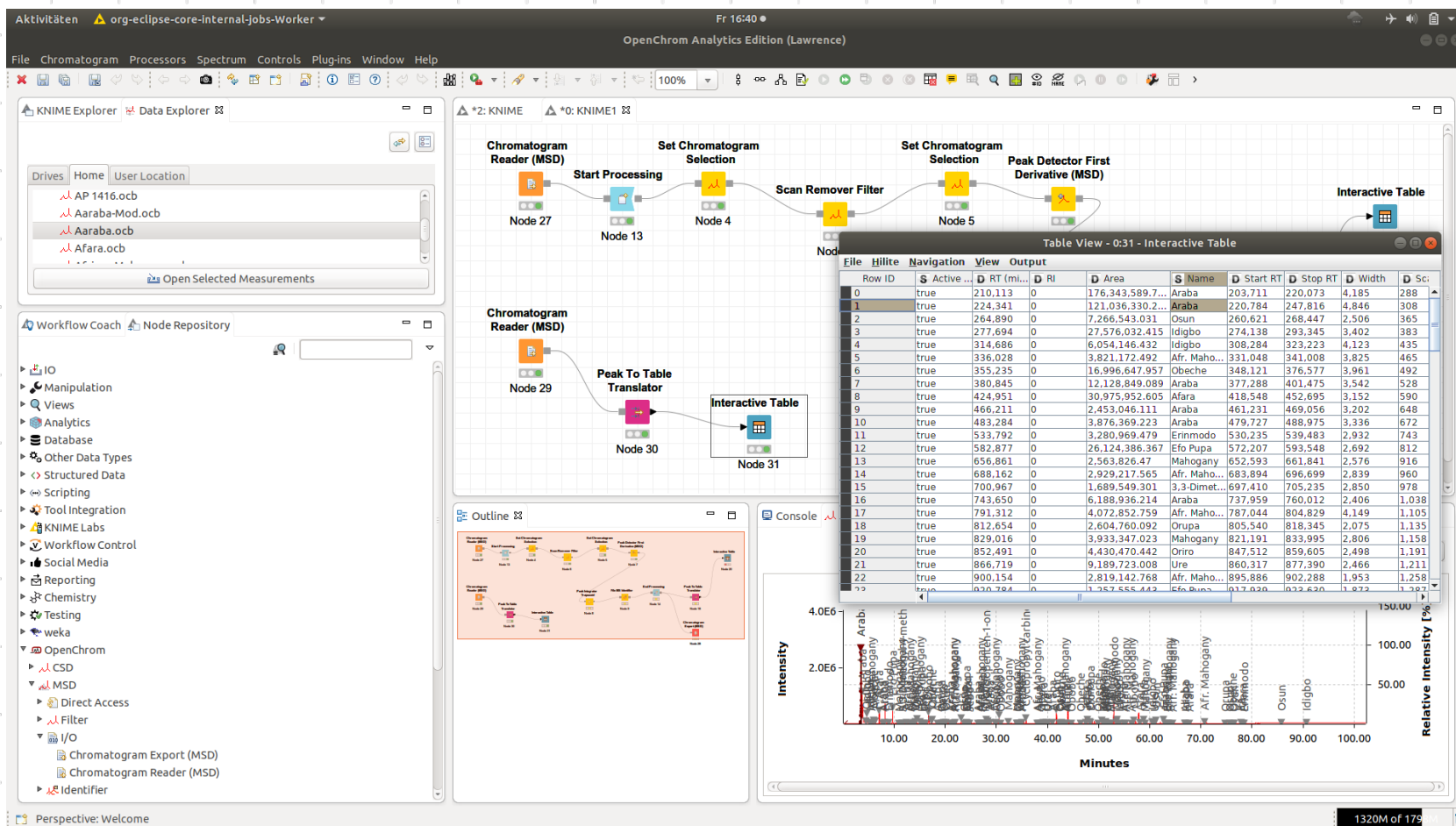
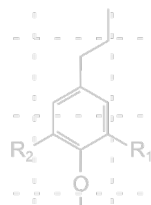
Peak identification via NIST-DB



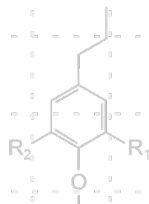
Principal Component Analysis (PCA)



Individual workflows via **KNIME**



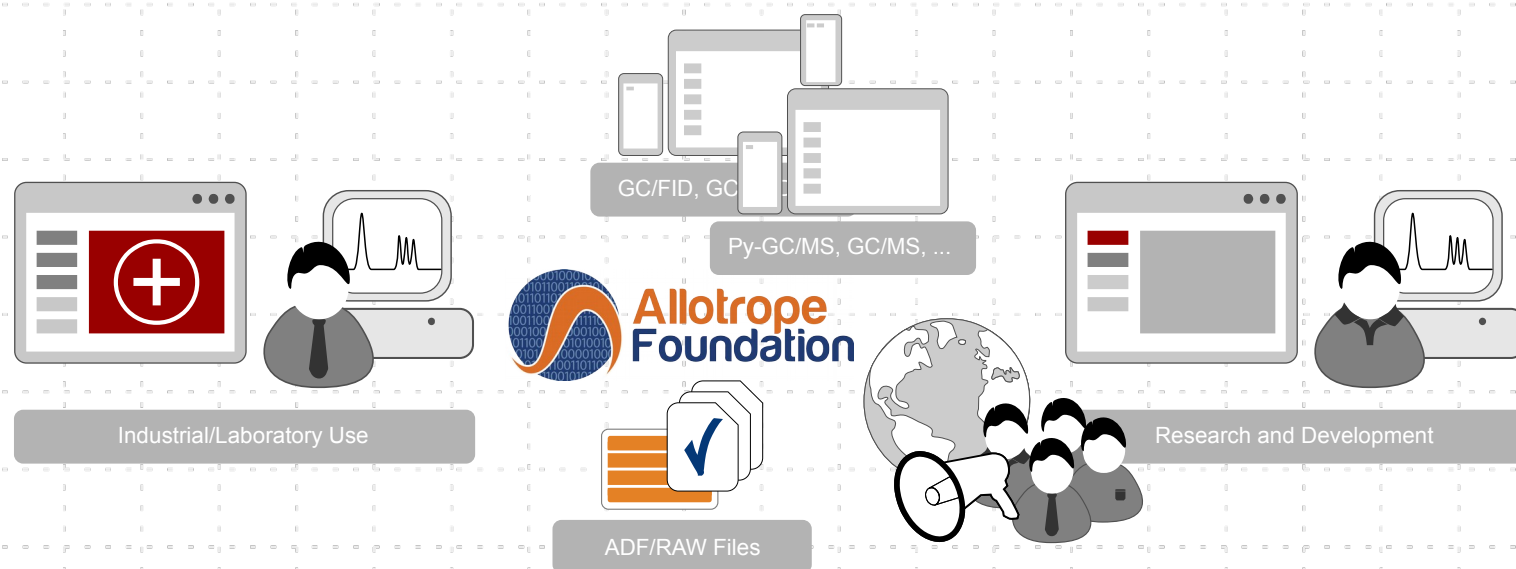
Modular approach via Eclipse



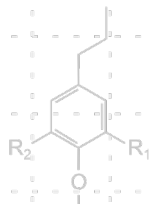
Suitable for **research** as well as **industrial** use

Combination of **open-source** and **proprietary** modules possible, **join the project**

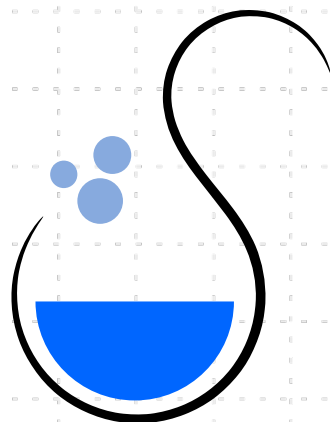
Available for Windows, macOS and Linux



Eclipse & Science Working Group

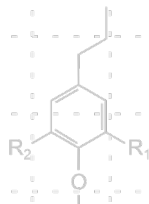


Bosch, **BMW**, Continental, IBM,
Mercedes, Microsoft, Red Hat,
SAP, **Telekom**, ...



SCIENCE
eclipse.org

AIRBUS, **Diamond Light Source**, Itema, Lablicate,
Oak Ridge National Laboratories, Soleil, ...



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