



Mestrelab Research

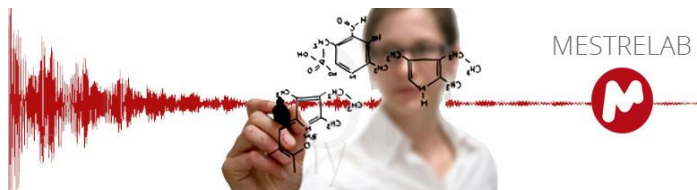
chemistry software solutions

Mbook

**10 reasons why synthetic chemists
should look no further**

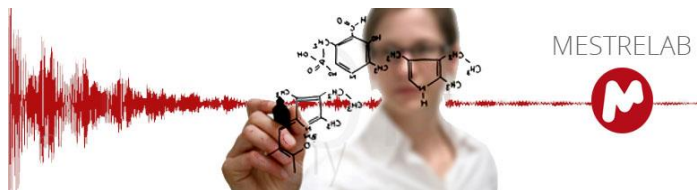
Wednesday, May 10, 2017

- A little bit about Mestrelab
- Introduction to Mbook
- How does Mbook use ChemAxon tools
- Other integration opportunities



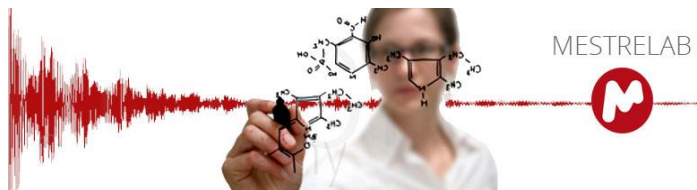
About Mestrelab

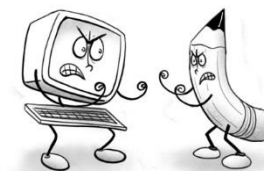
- Spanish software developer focused on processing and analysis of analytical data (NMR, LCMS, GCMS, UVIR, VIS, RAMAN, etc)
- Founded in 2004, sales offices in US, UK and Switzerland
- Areas of work include signal processing, mathematical analysis, artificial intelligence, etc.
- 120,000 users globally, mainly for NMR
- 35 people headcount, 25 developers, 35 people in the development and applications team
- Evolution from analytical data processing to management and storage, to ELN



About Mbook

So, what is Mbook?





#1 Designed for synthetic chemists

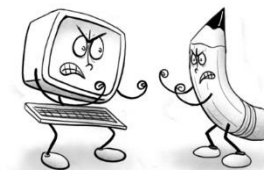
- If you are recording synthesis, Mbook is ready to use off-the-shelf
- No time consuming customization or complex set up
- Replicate your paper workflow on a digital environment
- No learning curve



Reaction scheme showing the synthesis of **P1** from **R1** and **R2** using **NH₄(R3)** and **DCC (R4)** in **DMF (R5)** at **0 to 25 °C**.

MF (Label)	MW	W (mg)	Moles (mmol)	Equiv	Conc (mol/L)	Vol (mL)	Density (g/mL)	Pur (%)	Yield (%)	Limiting Reagent
C₁₀H₁₁N₃O₂S (R1)	258.284	500.0	1.936	1.000				100.0		
C₁₀H₁₁N₃O₂S (R2)	135.124	261.6	1.936	1.000	2.000	0.968		100.0		
NH₄(R3)	17.031	33.0	1.936	1.000				100.0		
DCC (R4)	206.328	599.1	2.904	1.500				100.0		
DMF (R5)	73.094						0.943	100.0		
C₁₀H₁₁N₃O₂S (P1)	257.309	256.0	0.995					100.0	51.4	

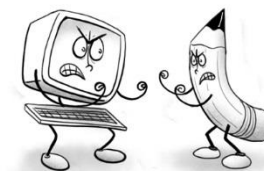
To a solution of 2-(tert-butylcarbamoyl)isomannoside(3)-thiazole-4-carboxylic acid in DMF were added and NEt₃. After cooling down to 0 °C, DCC was added and the mixture was stirred at room temperature for 12 h. The reaction mixture was filtered, and the solids were washed with EtOAc. A saturated aqueous NaHCO₃ solution was added, and after separating the layers, the aqueous layer was extracted with EtOAc (x3). The combined organic layers were washed with water (x2), dried (Na₂SO₄), and the solvent was evaporated. The residue was purified by column chromatography (silica gel, 95:5 DCE/DCU/MeOH) to afford a white solid identified as 2-(tert-butylcarbamoyl)isomannoside(3)-thiazole-4-carboxamide.



#2 Web based and native on iOS and Android

- Use Mbook on your web browser of choice
- No initial or updates installations, no maintenance
- Take your chemistry with you everywhere, with the only ELN with native iOS and Android versions.

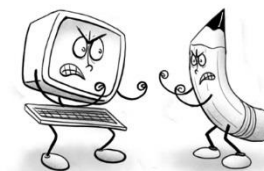




Don't let the deployment mode
define the tool you are going to use

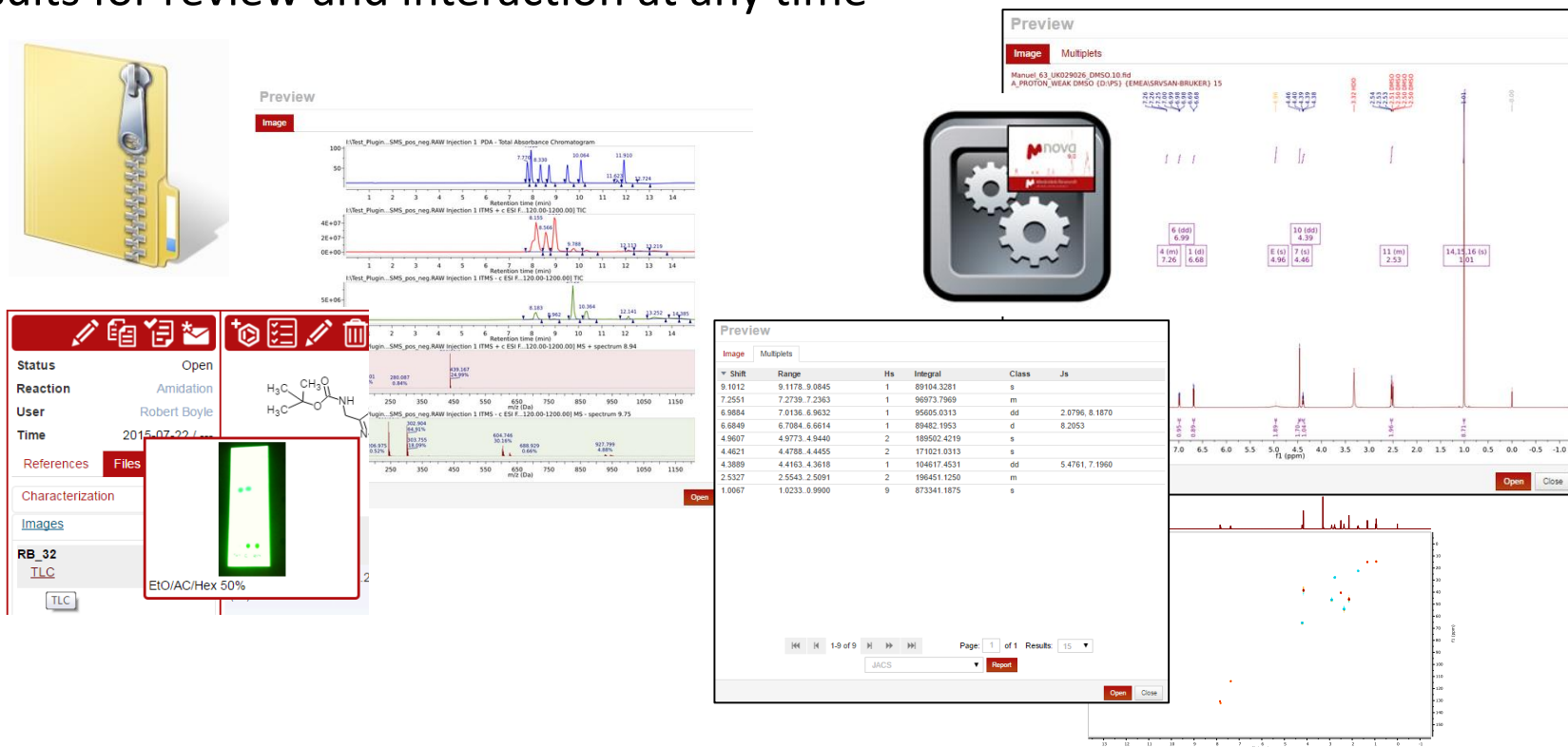
Choose the convenience of cloud
or the further control of in-house

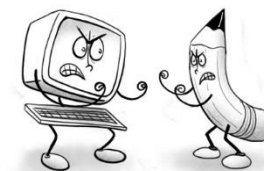




#4 Analytical data integration

Mbook can process and analyse your analytical data, and store the analysis results for review and interaction at any time

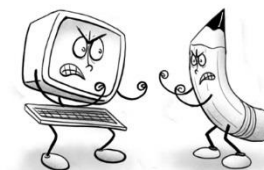




#5 Preloaded compound database

The screenshot shows the Mbook software interface. At the top, there's a navigation bar with 'mbook', 'Desk', 'People', 'Database', and 'Message'. Below this, a breadcrumb trail shows 'Organic Reactions / BOC 001 / RB_11'. A toolbar contains various icons, with the 'Add Participant' icon (a plus sign in a circle) highlighted by a blue circle. Below the toolbar, a form displays reaction details: Status (Open), Reaction (BOC protection), User (Robert Boyle), Time (2015-03-04 / ...), and Source. To the right, a chemical structure of a benzylamine derivative is shown. At the bottom left, a dropdown menu for 'Add Participant' is open, showing a list of preloaded compounds including Benzoyl Chloride, Benzoyl Peroxide, Benzoylacetone, Benzoylacetone nitrile, Benzoylaminoacetic Acid, Benzoyleneurea, Benzoylhydrazine, Dibenzylmethane, N-Benzoylaniline, N-Benzoylglycine, Hexahydrobenzoyl Chloride, N-(4-Aminobenzoyl)glycine, O-(4-Chlorobenzoyl)hydroquinidine, and 2,4,6-Trichlorobenzoyl Chloride. The main workspace shows a chemical structure of a benzyl ester derivative. On the right, a 'Material Safety Data Sheet' for 1-Hydroxybenzotriazole hydrate is displayed, showing sections for Identification, Composition, Hazards, and Precautions.

- Over 2,700 common reactants and solvents loaded and searchable from day one, including Health & Safety data sheets
- Huge time savings on compound loading



#6 Integrated inventory

Mbook implements an inventory function, allowing you to track the location and stock levels of all your reactants, solvents and products.

Make sure you don't have to buy an inventory solution after you buy your ELN

Desk
People
Search
Inventory ▾
Message

Tetrahydrofuran

Name

Tetrahydrofuran

Acronym

THF

MF

C₄H₈O

Health/Safety

109-99-9

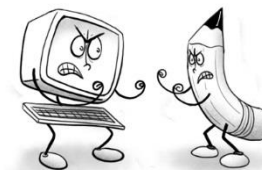
MSDS

Inventory

Experiment

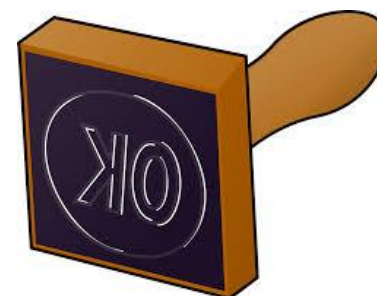
Supplier	Status	Batch number	Remaining (Initial)
Sigma-Aldrich	Available	asdfgh	3.253 L (10.000 L)
Test Supplier	Available	BA123	150.000 mL (200.000 mL)
Test Supplier	Available	BA234	400.000 mL (500.000 mL)
Acros	Available	Batch245u	2.416 L (2.500 L)
Acros	Finished	Batch250d	0.010 L (1.000 L)

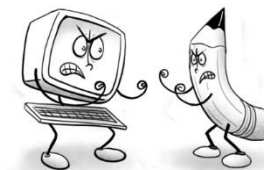
#7 CFR21 Part 11 compliant



Gives you the peace of mind that your Intellectual Property is safe, readily searchable and will stand up if challenged.

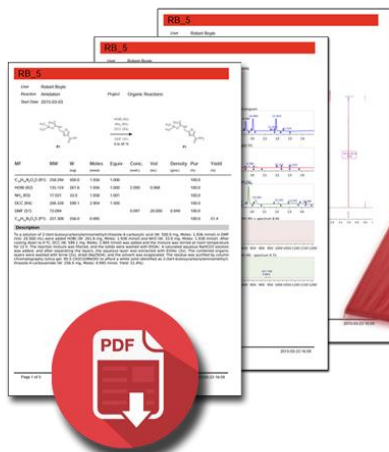
Currently undergoing certification

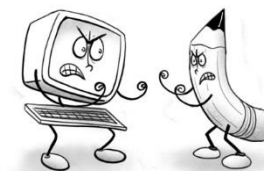




#8 Open data export

You can export your Mbook data to an easily parsable, JSON based format. Do not allow your data to be kidnapped in an application which does not allow you to export (in development).

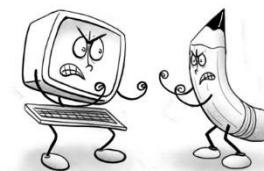




#9 Open application

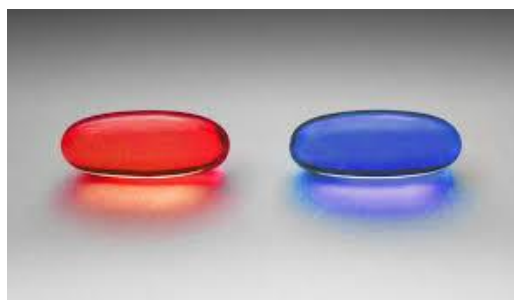
Mbook can be easily interfaced to and from third party applications for interrogation and data loading or retrieval (in development).

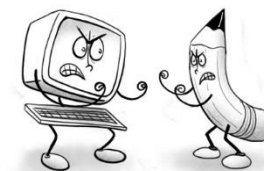




#10 Suitable for Research or manufacturing

Mbook supports the transfer of research results into manufacturing SOPs, therefore supporting knowledge transfer from R&D to manufacturing.





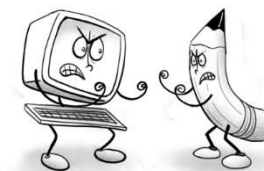
Responsive Web Interface

- Besides a great new appearance, Mbook can now adjust to your screen size optimising the available display space

The screenshot displays the Mbook software interface. At the top, there's a navigation bar with 'MBOOK', 'Desk', 'Search', 'Inventory', and 'Message'. Below this, a breadcrumb trail shows 'Mbook100 / Alkylation100 / VAL1_1'. The main area features a chemical reaction scheme: 3,4-dimethoxybenzoic acid (R1) reacts with n-BuLi (R2) and Dimethyl Sulfate (R3) in THF (S1) at -5 to 25 °C for 16h overnight to form 3,4-dimethoxybenzoic acid (P1). Below the reaction, a table lists the compounds and their quantities.

Compound	MW	W g	Moles mmol	Equiv	Conc (mol/L)	Vol mL
C ₉ H ₁₂ O ₃ (R1)	168.190	10.641	62.000	1.000		
n-BuLi (R2)	64.054	4.805	75.020	1.210	2.500	30.008
Dimethyl Sulfate (R3)	126.133	10.088	79.980	1.290		7.568
THF (S1)	72.106					
C ₁₀ H ₁₄ O ₃ (P1)	182.217	11.280	61.904	1.240		50.000

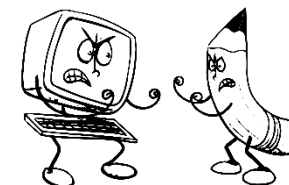
NEW LOOK!



Analytical Viewer

- Visualization tools are now integrated within Mbook. Spectral zooming and panning for review can be done directly from the ELN.





Marvin JS used as drawing package

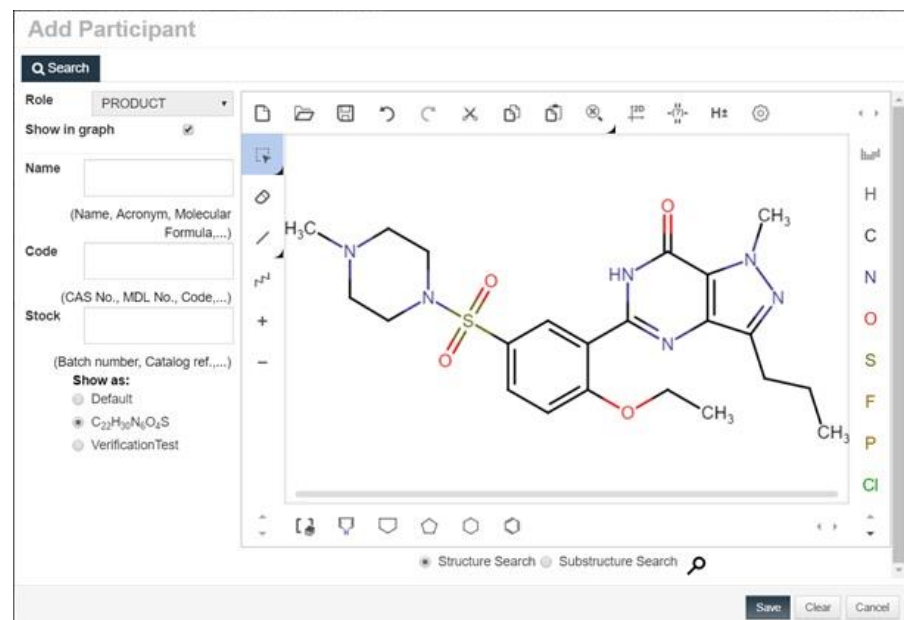
Marvin JS works as a widget and provides functionality to:

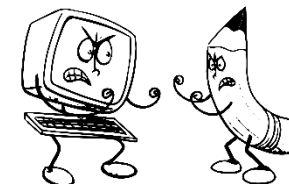
Draw structures

Import structures from 3rd party tools

Open structure files (.mol, .sdf, etc.)

Support for salts, metallic complexes, etc





Marvin JS for naming

Marvin JS generates IUPAC name from molecular structure, which can be used automatically for experimental write up, etc.

Chemical reaction scheme showing the synthesis of compound **P1** ($C_{22}H_{30}N_6O_4S$) from reactants **R1** ($C_{15}H_{23}N_3O_4S$) and **R2** ($C_9H_{15}N_3O$), with reagents **R3** (Imidazole) and **S1** ($C_3H_6O_2$).

Compound	MW	W [g]	Moles [mol]	Equiv	Conc (mol/L)	Vol [mL]	Density (g/mL)	Pur (%)	Yield (%)
C₁₅H₂₃N₃O₄S (R1)	341.430	1.000	0.003	1.000		0.082	12.200	100.0	
C₉H₁₅N₃O (R2)	181.239	0.557	0.003	1.050				100.0	
Imidazole (R3)	68.077	0.239	0.004	1.200		5.000		100.0	
C₃H₆O₂ (S1)	88.105						0.901	100.0	
C₂₂H₃₀N₆O₄S (P1)	474.576	1.319	0.003					100.0	94.9

The carboxylic function of compound **R1** (Vol: 0.082 mL, Moles: 0.003 mol, 2-ethoxy-N-methyl-5-[(4-methylpiperam)] can be activated using a 5% excess of carbonyldiimidazole (W: 0.239 g, Moles: 0.004 mol) in ethyl acetate (W: 0.239 g, Moles: 0.004 mol).

This intermediate can then be reacted with imidazole (W: 0.239 g, Moles: 3.515 mmol) and compound **R2** (W: 0.557 g, Moles: 3.075 mmol). The resulting compound is then cyclised to complete the reaction scheme and give sildenafil (W: 1.319 g, Moles: 2.779 mmol, Yield: 94.9%) by heating at 80°C during 3h with a 95% yield.

Add Participant

Search:

Role: **REACTANT**

Show in graph: ☒

Arrow section: ☐

Limiting Reagent: ☒

Name:

(Name, Acronym, Molecular Formula,...)

Code:

(CAS No., MDL No., Code,...)

Stock:

(Batch number, Catalog ref,...)

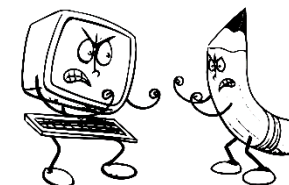
Show as:

- ☒ Default
- ☐ 2-ethoxy-N-methyl-5-[(4-methylpiperam)]
- ☐ 2-ethoxy-N-methyl-5-[(4-methylpiperam)]
- ☐ SP1

Chemical structure: CCOC(=O)Nc1ccc(cc1)S(=O)(=O)N2CCN(C)CC2

Structure Search | Substructure Search

Save | Clear | Cancel



Migration from 3rd party tools

ChemAxon tools allow us to support migration from existing ELNs to Mbook (Marvin, JChem, Structure to Name and Name to Structure)

Mbook Importer

Indicate the path for importing:

4 experiments loaded.
 Loaded Experiments:

☐ View all ☐ View incorrects one ☐ Select project:

☐	Project	Reaction	Experiment	Status
☐	Helio	HF11	HF11-005	Molecules not assigned
☐	Helio	HF11	HF11-057	Incorrect file load
☒	Ronald	RN1	RN1-001	Correct
☐	Ronald	RN1	RN1-004	Molecules not assigned

4 experiments, 1 marked.

Result revision:

PHASE VALIDATION
Molecules list to solve (use Manage molecules button):

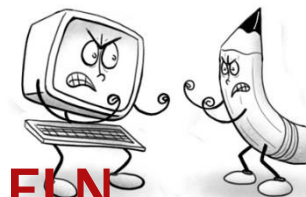
- C49H68AuClNO3P-F6Sb
- A - mixture of products, among them the minor diastereoisomer of (2+2+2) and the (2+2) products
- CH2Cl2
- DCM
- tris(2,4-di-tert-butylphenyl) phosphite (P3L3-CAJA SECA)
- (Dimethyl sulfide) gold (I) Chloride (P3L3-CAJA SECA)
- C42H63AuClO3P
- Toluene

Manage compounds

Found compounds: Filter by:

Name	Formula	MW	Mol File	Coincidents	Modified
BENZALDEHYDE	 C ₇ H ₆ O	106.124	☒	1	☐
4-methyl-1,2-dihydronaphthalene	C ₁₁ H ₁₂	144.217	☒	0	☐
3-(propa-1,2-dienyl)oxazolidin-2-one	C ₆ H ₇ NO ₂	125.127	☒	0	☐
C49H68AuClNO3P-F6Sb	C ₄₉ H ₆₉ AuClF ₆ NO ₃ PSb	1218.213	☐	0	☐
(Z)-3-((8b-methyl-2,2a,3,4-tetrahydrocyclobuta[a...	C ₁₇ H ₁₉ NO ₂	269.344	☒	0	☐
(Z)-3-((10b-methyl-2-phenyl-4,4a,5,6-tetrahydro...	C ₂₄ H ₂₅ NO ₃	375.468	☒	0	☐
3-((Z)-((2S,4aR,10bS)-10b-methyl-2-phenyl-4,4a,...	C ₂₄ H ₂₅ NO ₃	375.468	☒	0	☐
A - mixture of products, among them the minor ...	A - mixture of produ...		☐	0	☐
CH2Cl2	CH2Cl2		☐	3	☐
DCM	DCM		☐	1	☐
tris(2,4-di-tert-butylphenyl) phosphite (P3L3-CAJ...	tris(2,4-di-tert-butyl...		☐	0	☐

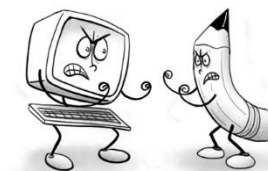
Note: Compounds with 0 coincidents are created in Mbook



Automated QC and spectral analysis integrated in ELN

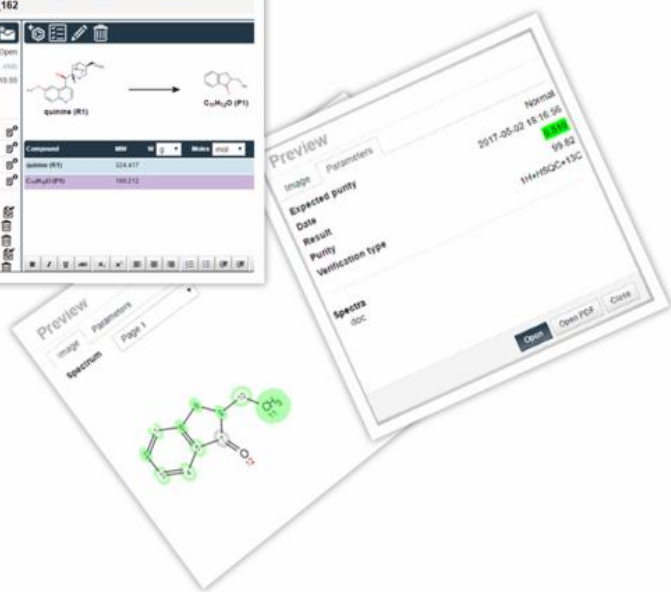
- We have implemented a structure verification tool which runs the powerful Mnova Verify module in the background as part of our ELN workflow

The image displays three overlapping screenshots of the Mbook software interface. The top-left screenshot shows a chemical reaction: c1ccc2c(c1)cnc2 (quinoline) reacting with Cu2O to form Cu2O (IP1). The bottom-left screenshot shows a 'Preview' window with a chemical structure of a quinoline derivative. The rightmost screenshot shows a 'Preview' window with verification results for 'Normal' (2017-05-02 15:16:36), 'Date' (2017-05-02 15:16:36), 'Result' (99.82), and 'Verification type' (1H/13C+13C).

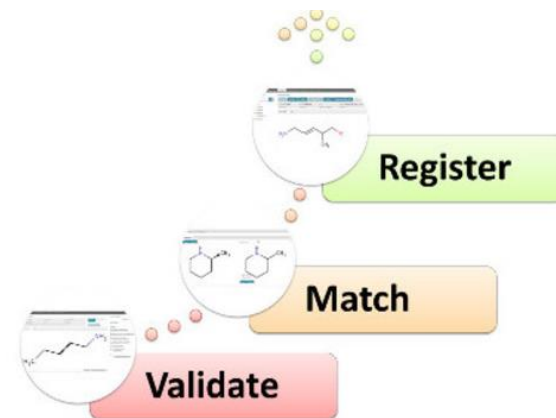


Next integration steps

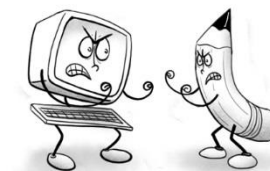
- The next step is to use ChemAxon tools to support one-click registration from our ELN (Communication from Mbook to ChemAxon CompReg)



One click

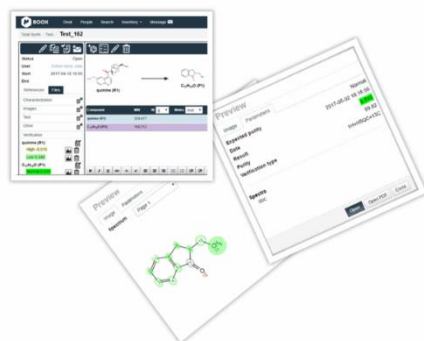


Registration
System

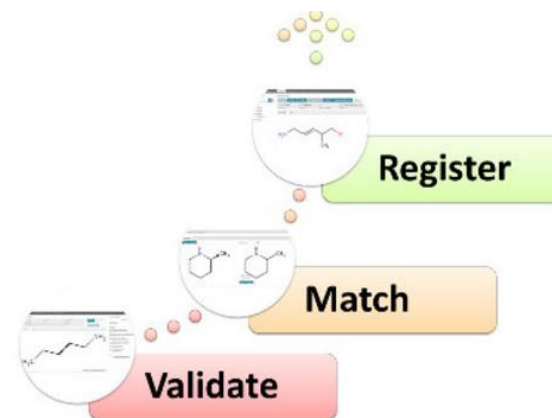


3rd party ELNs and registration systems?

- These tools are also potentially available as modules for integration in other 3rd party ELNs and registration systems



QC based on
analytical data



Web spectral
viewer

Mnova ELN
Connector





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