



# Mestrelab Research

chemistry software solutions

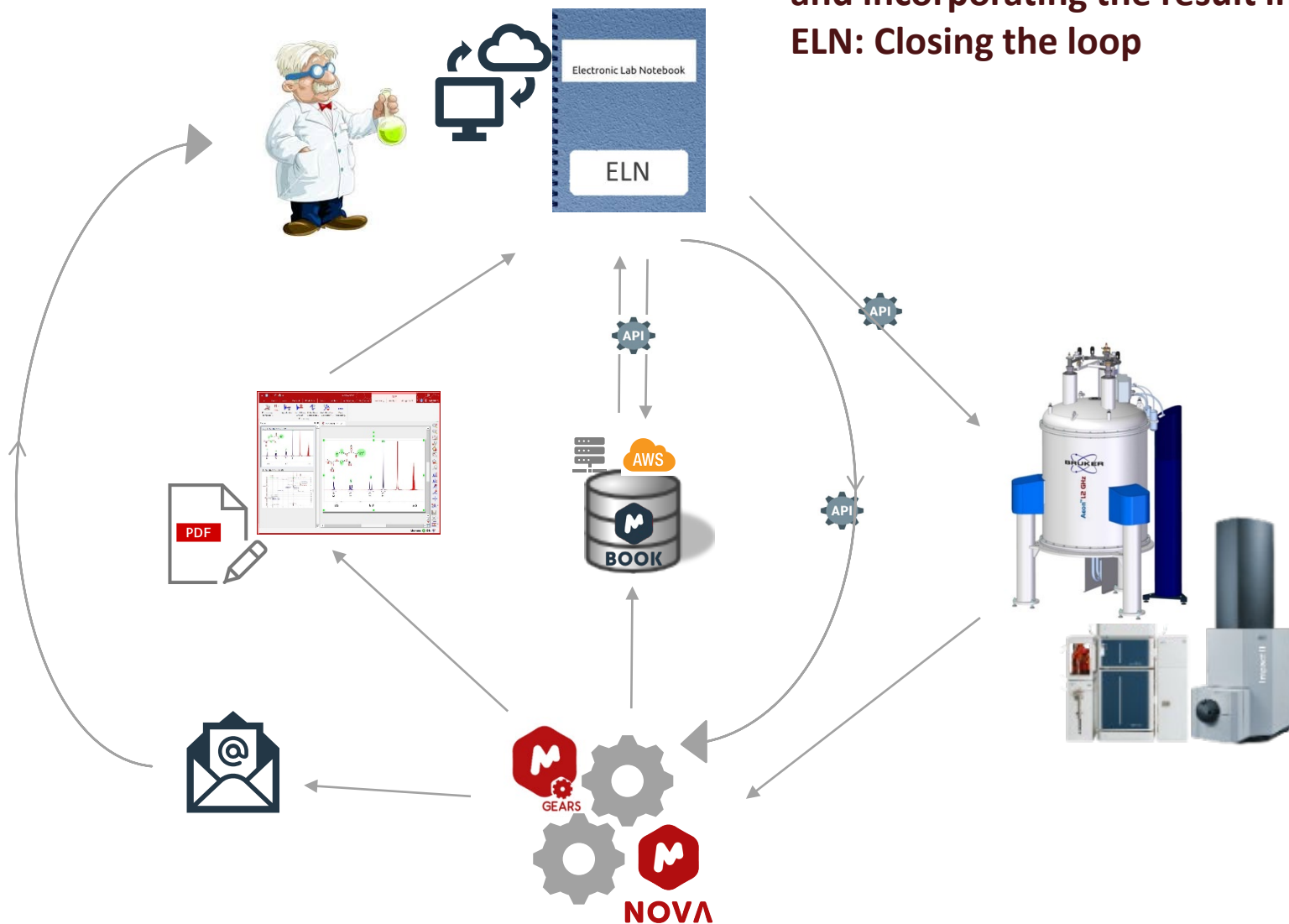
## Connecting Analytical Chemistry Software Tools To Web-based Laboratory Informatic Solutions

Guy Desmarquets

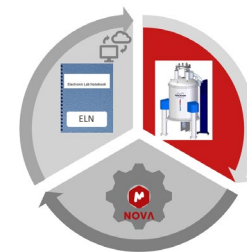
[Guy.desmarquets@mestrelab.com](mailto:Guy.desmarquets@mestrelab.com)

May 21, 2019

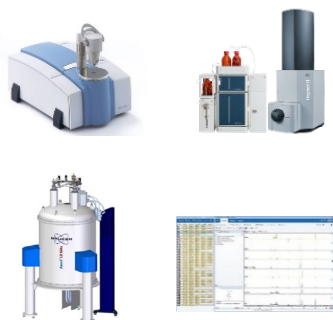
Connecting ELN to instrument, automatically processing the data and incorporating the result in the ELN: Closing the loop



**Improving efficiency by Working exclusively with your ELN**



## Partnership with Bruker

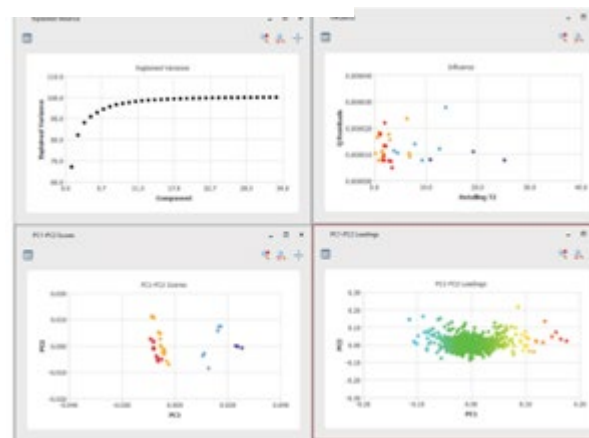


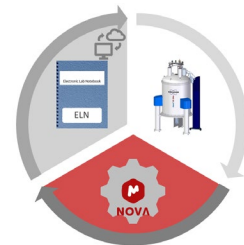
<http://resources.mestrelab.com/bruker-and-mestrelab-announce-strategic-collaboration-and-partnership-for-chemistry-and-pharma-software-applications/>

1. Vendor-agnostic lab-automation software solutions
2. Consolidation of common post-acquisition software
3. Co-development of innovative solutions and workflows

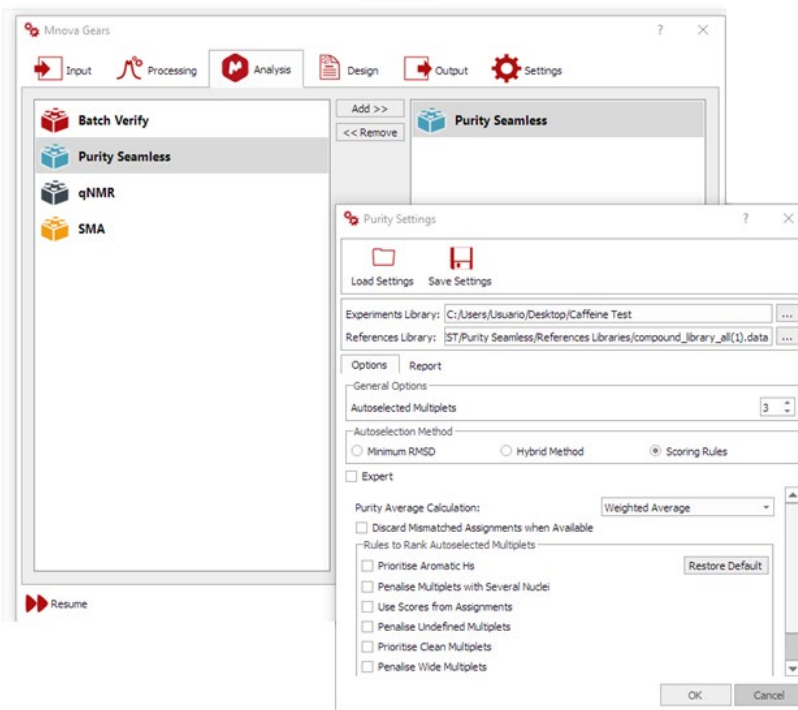
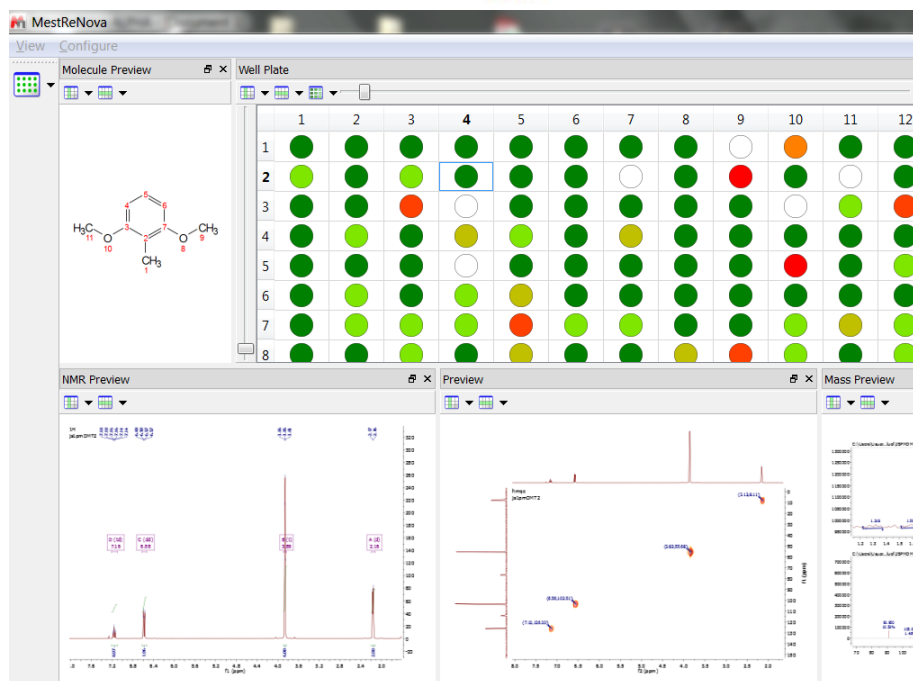
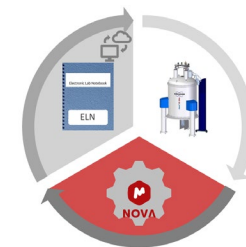
### Common Development: Analysis of Higher Order Structure in Biologics

The BiologicsHOS application is a tool for NMR researchers to analyze protein higher order structure (HOS) differences by 2D HSQC in order to evaluate this information as a QC criterion for Biologics – e.g. in the field of biologics productions. The application serves as a “one stop shop” for all the NMR analysis needs in this area.





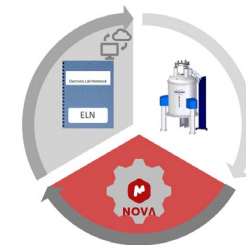
**NMR, MS, IR, RAMAN,..Post-Acquisition (Automated) Applications**



Information Stored Can Be Mined and Displayed In  
Various Layout  
(Decision Making Dashboards)

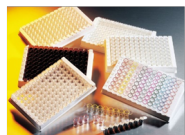
Mgears: A Brick-based System to Build your Analytical  
Workflow Pipes

**Easy to Create Automation and Databasing With Flexible Data Model**

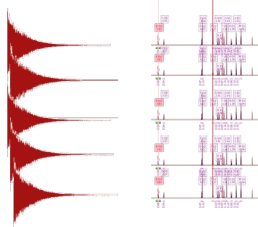


## Automated Data Processing & Reporting (MERCK)

- As samples are acquired report is produced (Merck)



Open  
Access  
HTS



Reprocessing



Report



Email - ELN

It has to contain meaningful and correct analysis of the spectra

## Display of NMR Structure Verification Results (GRÜNENTHAL)

Complex data made accessible to non-expert customers



### Non-expert User can quick-check results:

- read off ASV-score and relative purity
- compare  $^1\text{H}$  integral count with  $^1\text{H}$  atom count in  $^1\text{H-NMR}$
- compare  $\text{CH}_2\text{CH}_3\text{CH}_3$  signal count with count of respective atom groups in  $^{13}\text{C-}^1\text{H-NMR}$
- view outliers w.r.t chemical shift, integral, multiplet

GRÜNENTHAL

Seite 9

## Real Time Knowledge Extraction and Storage (ELI-LILLY & VERNALIS)

Compound registration gateway (Eli-Lilly), Report generator (Vernalis)



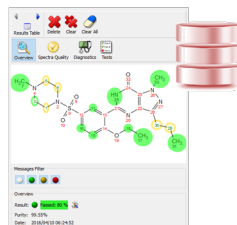
OA and  
Autopurification  
Acquisition



Reprocessing  
and analysis

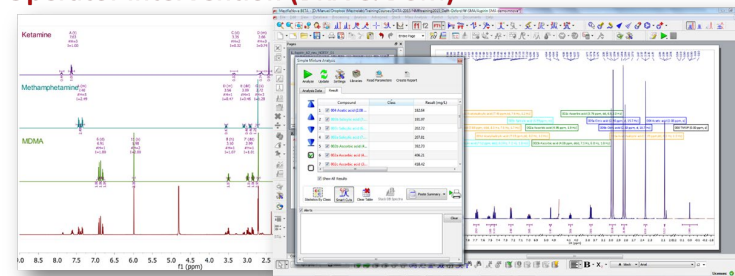


$^1\text{H-NMR}$  (499 MHz,  $\text{DMSO-}d_6$ )  $\delta$  12.19 (s, OH), 7.92 – 7.77 (m, OH), 7.37 (d,  $J = 8.7$  Hz, OH), 4.22 (q,  $J = 6.9$  Hz, OH), 4.16 (s, OH), 3.27 (s, OH), 3.11 – 2.81 (m, OH), 2.78 (t,  $J = 7.5$  Hz, OH), 2.36 (t,  $J = 4.9$  Hz, OH), 2.14 (s, OH), 1.74 (t,  $J = 7.4$  Hz, OH), 1.33 (t,  $J = 6.9$  Hz, OH), 0.94 (t,  $J = 7.3$  Hz, OH).



Email to specialist  
Report to ELN

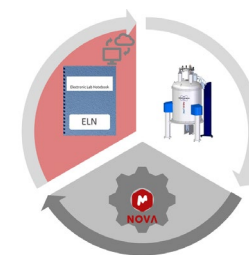
## Mixture Analysis and Reporting Without Operator intervention (BKA & DSM)



Mixture

Analysis

Results Report



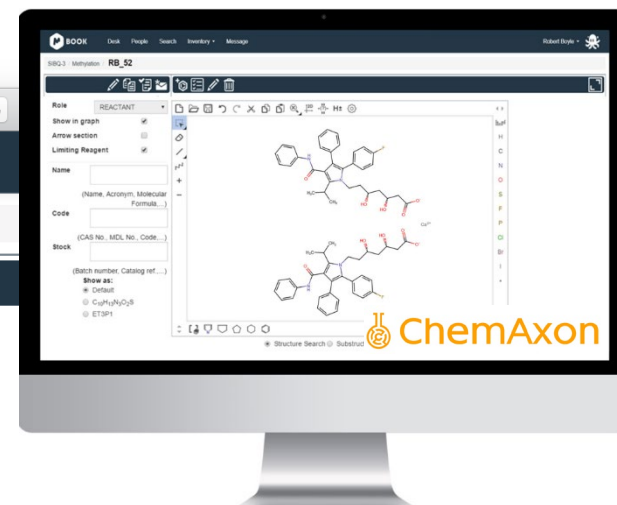
## Mbook Chemistry: Experiment Page

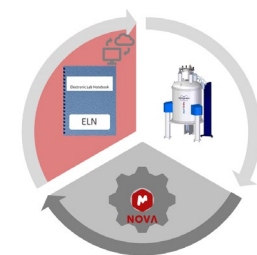
Mark's Ph.D. / Synthesis of 4-t..yran / 2-Ethoxy-5,6-dih..yran / **Halfway there**

Reaction scheme: CCOC1CC(Br)CCO1 (R1) + EtONa (R2) + EtOH (S1) → CCOC1CCOC1 (P1)

Compound	MW	W g	Moles mol	Equiv	Conc (mol/L)	Vol mL	Density (g/mL)	Pur (%)	Yield (%)
C <sub>7</sub> H <sub>13</sub> BrO <sub>2</sub> (R1)	209.083	19.690	0.094	1.000				100.0	
EtONa (R2)	68.050	7.000	0.103	1.096				100.0	
EtOH (S1)	46.069				1.343	70.0	0.789	100.0	
C <sub>7</sub> H <sub>12</sub> O <sub>2</sub> (P1)	128.171	3.750	0.029					100.0	30.9

Procedure: R1 (19.690 g, 0.094 mol, 1.000 eq, 3-bromo-2-ethoxyxane) was added to a stirred ethanolic solution of R2 (7.000 g, 0.103 mol, 1.096 eq). A white precipitate formed immediately. The suspension was refluxed for a further four hours, and then allowed to cool. The suspension was filtered with suction, and the precipitate washed with ether to yield P1 (3.750 g, 0.029 mol, 30.9%, 6-ethoxy-3,6-dihydro-2H-pyran) as a pale yellow oil.





## Verification Driven by Mbook Chemistry or Third Party ELN

✎ 📄 ✓ ✉
⊕ ☰ ✎ 🗑

**Status** Open

**User** Robert Boyle

**Start** 2017-07-13 10:33

**End**

References **Files**

Characterization

Images

Text

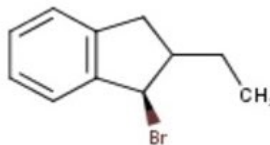
Other 📄

Verification

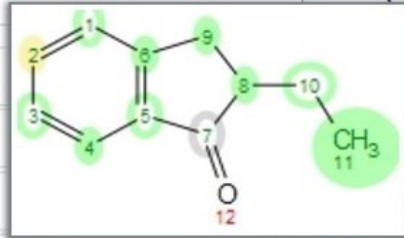
**2-ethyl-2,3-dihy...-one (P1)**

High 0.510

2017-09-14 13:18

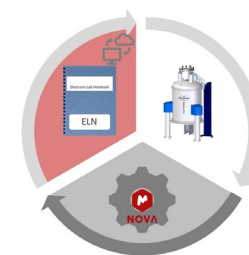


**(1R)-1-brom...dene (R1)**



Compound	MW
bromo-2-e...dene (R1)	225.129
NaOAc (R2)	82.034
H <sub>2</sub> O <sub>2</sub> (R3)	34.015
KMnO <sub>4</sub> (R4)	158.034
CH <sub>2</sub> Cl <sub>2</sub> (S1)	84.932
C <sub>7</sub> H <sub>8</sub> (S2)	92.139
2-ethyl-2,3-dihy...-one (P1)	160.216





# Analysis Request and Management with MBook

M BOOK
Desk Team Search Inventory Message
Analysis Manager


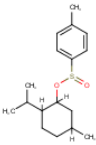
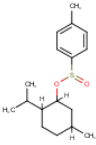
Desk

Home Add Filter Mail


Open Projects

- AnalysisPro..ect1
- AnalysisPro..ect2
- AnalysisPro..ect3
- AnalysisPro..ect4
- AnalysisPro..ect5

Closed Projects

Date	Code	Status	Completeness	User	Project	Reference	Batch Number	Structure
2018-12-12 13:12	3195	Assigned	3 / 5	Requester 1	AnalysisProject1	ref-1	batch-1	
2018-12-03 13:33	3194	Completed	1 / 1	Requester 2	AnalysisProject1	ref-0312-2		
2018-11-30 12:12	3193	Approved	1 / 1	Requester 1	AnalysisProject1	ref-2		
2018-11-28 15:20	3192	Approved	1 / 1	Requester 2	AnalysisProject1	req2-2811-2-RS		
2018-11-28 15:19	3191	Completed	1 / 1	Requester 2	AnalysisProject1	req2-2811-1-RS		
2018-11-27 13:29	3190	Approved	1 / 1	Requester 1	AnalysisProject1	rq1-2711-2		
2018-11-27 13:29	3189	Completed	1 / 1	Requester 1	AnalysisProject1	rq1-2711-1		
2018-11-27 09:41	3188	Open	0 / 1	Requester 4	AnalysisProject2	req4-2711-1		
2018-11-27 09:38		New	0 / 1	Requester 2	AnalysisProject1	req2-2711-1		
2018-11-22 11:19	3183	Approved	2 / 2	Requester 1	AnalysisProject1	2211-2	AN-12736	
2018-11-22 11:14	3182	Cancelled	0 / 0	Requester 1	AnalysisProject1	2211-1	AN-12735	
2018-11-21 13:51	3184		0 / 1	Requester Sun1	AnalysisProject1	sun-2111-1		

1-25 of 30
Page: 1 of 2
Results: 25



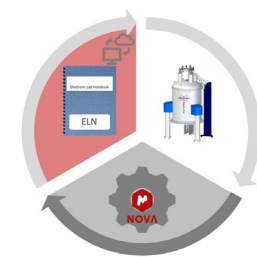
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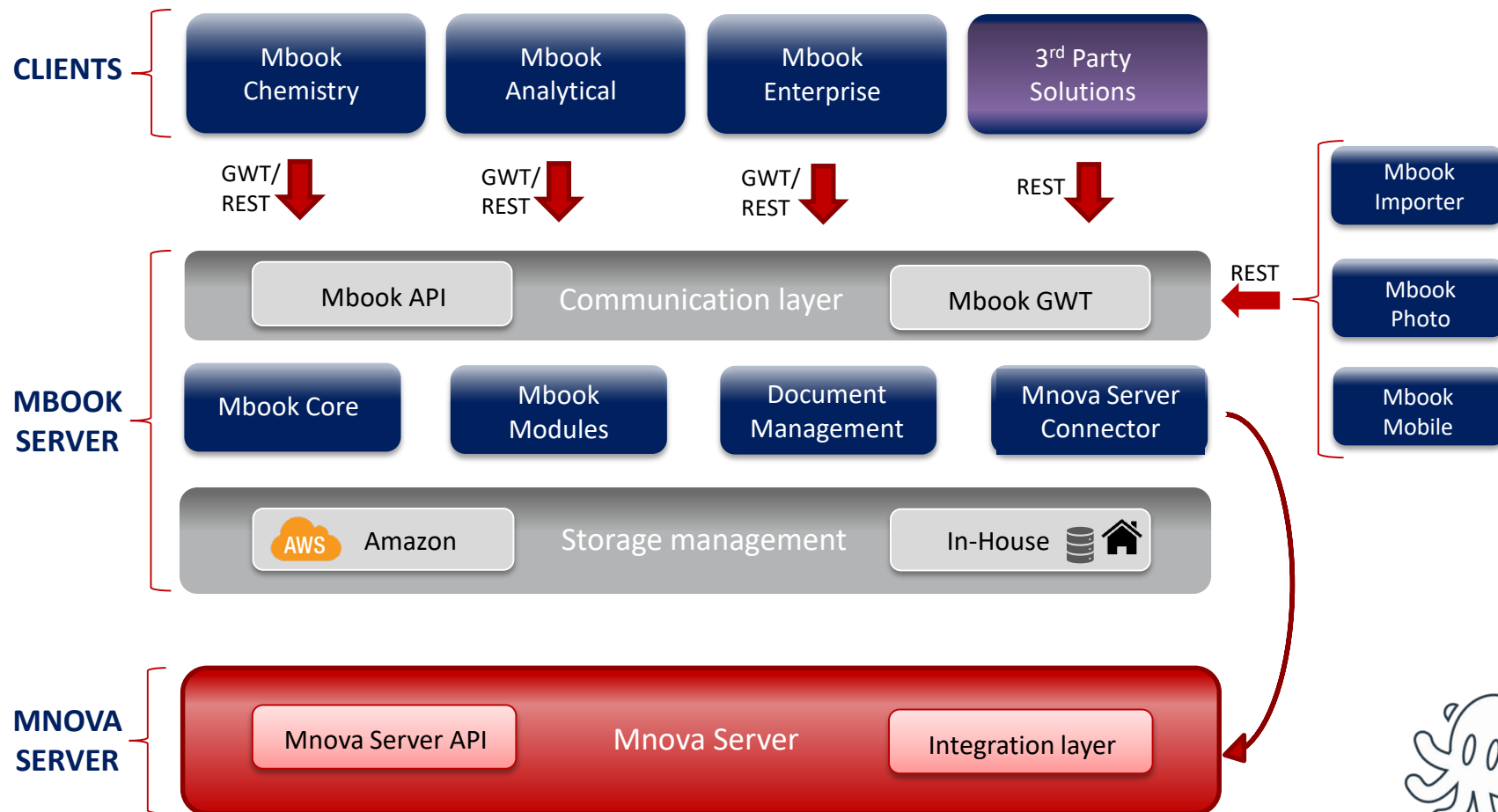
JBILITY

X

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# Mbook: Analytical Chemistry-Based Web Ecosystem



I am available the rest of the day, this evening and tomorrow at anytime, please feel free to connect with me if you are interested to discuss any aspect of our offer or send me an email to book an appointment: [guy.desmarquets@mestrelab.com](mailto:guy.desmarquets@mestrelab.com) or [guy@mestrelab.com](mailto:guy@mestrelab.com)



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chemistry software solutions

*thank  
you*