



Mestrelab Research

METHODOLOGY			
General keyword	Details in topic	Researchers involved	Institute (Group Acronym)
Mnova NMR	*Visualization, processing, analysis, and reporting of 1D and 2D NMR data. Automatic data processing (for ¹ H, ¹³ C, DEPTs HSQC, HMBC, NOESY, COSY, TOCSY, etc.)	Identify researchers that could be involved in master thesis supervision	
Mnova MS	*Visualization, processing, analysis, and reporting of LC-MS and GC-MS data. Generation of EMC/EIC traces and UV spectra for a given mass range, a certain m/z ratio or wavelengths from DAD traces.	Identify researchers that could be involved in master thesis supervision	

Mnova ElViS	<p>*Visualization, processing, analysis, and reporting of various electronic and vibrational spectroscopic techniques. Supports the majority of data file formats for ultraviolet and visible (UV/Vis), near and mid infrared (NIR/MIR), Raman, and fluorescence methods. Basic processing methods such as baseline correction, spectral intensity normalization, signal smoothing, spectral derivative, peak picking, etc.</p>	Identify researchers that could be involved in master thesis supervision	
Mnova NMR Predict	<p>Prediction of 1D NMR data (¹H, ¹³C, ¹⁹F, ³¹P, ¹⁷O, ¹⁵N, ¹¹B, ²⁹Si) from a chemical structure.</p>	Identify researchers that could be involved in master thesis supervision	
Mnova Verify	<p>Confirmation of structure identity based on NMR (¹H, ¹³C and HSQC, HMBC and COSY) and/or LC/GC-MS data</p>	Identify researchers that could be involved in master thesis supervision	

Mnova Structure Elucidation	Computer-assisted 2D Structure Elucidation by NMR	Identify researchers that could be involved in master thesis supervision	Mestrelab Research S.L.
Mnova qNMR	Quantitative analysis via NMR for concentration and purity/potency determination	Identify researchers that could be involved in master thesis supervision	
Mnova SMA	Identification and quantification of components in mixtures via NMR	Identify researchers that could be involved in master thesis supervision	
Mnova Reaction Monitoring	Extraction of spectroscopy and chemical kinetic concentrations from arrayed NMR datasets	Identify researchers that could be involved in master thesis supervision	
Mnova SteroFitter	Automated or Computer- assisted 3D Structure Elucidation by NMR – 3D structure in solution	Identify researchers that could be involved in master thesis supervision	
Mnova BioHOS	Analysis of NMR spectra for the determination of biologic drugs' higher- order structures (HOSs)	Identify researchers that could be involved in master thesis supervision	
Mnova Screen	Batch fragment-based screening and hit identification via NMR	Identify researchers that could be involved in master thesis supervision	

Mnova Binding	Chemical shift perturbation analysis for fragment-based drug discovery	Identify researchers that could be involved in master thesis supervision		
Mnova PhysChem	Computation of extensive physico-chemical properties	Identify researchers that could be involved in master thesis supervision		
Mnova DB	Database environment for the storage and searching of analytical data (NMR, LC/GC-MS...)	Identify researchers that could be involved in master thesis supervision		
Mnova Gears	A full automation environment for unattended analysis workflows	Identify researchers that could be involved in master thesis supervision		
Mbook Chemistry (ELN)	Cloud-based electronic laboratory notebook with built-in tools for synthetic chemistry workflows	Identify researchers that could be involved in master thesis supervision		
APPLICATIONS				
Systems	Property	Methods	Researchers involved	Insitiute (Group Acronym)

Data processing, analysis and reporting	A multiplatform (Windows, Mac, Linux) and multivendor software suite designed to accept combined analytical data from NMR, LC/GC-MS, IR, UV-Vis, (FT)IR, and Raman techniques.	Mnova	Identify researchers that could be involved in master thesis supervision	Mestrelab Research S.L.
Databasing	A professional database with a flexible data model integrated within Mnova to allow for the efficient and shared storage of molecular structures, NMR, and LC/GC-MS analytical data, as well as other Mnova objects.	Mnova DB	Identify researchers that could be involved in master thesis supervision	Mestrelab Research S.L.
Automation	A modular and flexible software suite to build automation workflows for your analytical data. Mnova Gears makes automation simpler and faster by giving users full control over the design and testing of their workflows.	Mnova Gears	Identify researchers that could be involved in master thesis supervision	Mestrelab Research S.L.

Lab informatics	Professional web-based solutions developed and tested by scientists for synthetic and analytical chemistry workflows.	Mbook Chemistry (Electronic Laboratory Notebook (ELN))	Identify researchers that could be involved in master thesis supervision	Mestrelab Research S.L.B25: E26B16 C24:E26 B22:E26 A22C24: E26
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