

# Mnova SMA 3.1

## **USER MANUAL**



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## 1. Introduction

The Simple Mixture Analysis (SMA) plugin is a simple and versatile tool for the quantitation of mixtures of components via NMR. It allows the development and storage of methods for the rapid and consistent analysis of samples. SMA also includes advanced reporting options, result visualization and reviewing capabilities, and a system of alerts to automatically highlight potential errors.

In this manual, we describe all the features provided by the Mnova SMA plugin.

## 2. SMA dialog

The SMA plugin is found under the **Quantitation** tab in the Mnova software's upper ribbon.

When opened, the SMA dialog presents the main buttons used to **Analyze** and **Update** results, generate **Quick Reports** and **Advanced Reports**, and configure the general analysis **Settings** at the top of the screen. Below, the two associated tabs are shown:

- The Analysis Data tab, where you will define the experiment to use, your sample and spectrum parameters, and certain other metadata related to the current analysis
- The **Results** tab, in which you will review your analysis results and receive appropriate alerts about errors (should they occur) and tests (when configured).

💌 📇 선 🔆 🚔 구 🛛 Mes	Nova BETA	
File Home View Molecule Prediction Tools Data Analysis Database Verification Elucidation	Chemometrics Binding A	utomation Quantitation 🗸 🚺 🐼 🕲 Options 🗸
Concentration Purity qNMR		
Pages Simple Mixture Analysis	Simple Mixture Analysis	
Andryce Update     Quark Report AdvancReport Setting     Andryck Data     Resoilt	Expe Analyze Update	Quick Report AdvancReport Settings Expert
Mixture		
Stature: SNA Libraries See Mixture: Descriptor		Compound Result SNR C. C. 0.00
Parameters		
Standard Custom	ā ā	<u> </u>
Sample D: Number of Scans (N5): Receiver Gain (R6):		<u>k</u>
Reference Concentration (RC): 1.0 Pulse Width (PW):	©_0	
Sample Weight (SW) [mg]: Temperature (T):		
Reference Weight (RW) [mg]: Spectral Width (SpecW):		
Dilution Factor (DF): Spectrometer Frequency (SF):		
Metadata	•	•
✓ Alerts —	✓ Alerts	
Dates Mr	C	<b>e</b>
rojes ry		<u> </u>

All the available action buttons are described below:

Button	Description	Results Ta	ab
Analyze	Analyze sample	Button	Description
(D) Update	Update result		Zoom on first compound to view detailed resu
Settings	Configure SMA analysis settings		Zoom on previous compound
Quick Report	Create a quick report with result		Zoom on next compound
Advanced Report	Create an advanced report with result		Zoom on last compound
Expert	Lock Expert mode		Uncheck all displayed results
Expert	Activate Expert mode		Check all displayed results
Analysis Da	ata Tab	Ref	Show/hide Reference results
Button	Description	•	Show/hide results with no valid multiplets
	Open Library manager	0.00	Change number of decimals
5	Create a new mixture	₫¢	Modify zoom factor on the spectrum
٢	Edit mixture	24 <u>0</u>	Smart cuts of areas between the multiplets
<b></b>	Read Sample's parameters	<u>i</u>	Stack compound spectra from DB
	Clear parameters and metadata	L	
-	Load results saved in the active document		
🕒 📈	Group alerts by time or compound		
	Clear alerts		
	Open custom parameters manager		

## Simple Mixture Analysis dialog

The Expert mode gives access to all of the SMA plugin's features. It allows expert chemists to set up an experiment's SOPs and define analysis settings. Locking the Expert mode will hide these functionalities, as can be seen in the image below.

Simple Mixture Analysis	Expert mode 🔮 🔹	Simple Mixture Analysis	Non-Expert mode • *
Analyze Update	Quick Report Valvanced Report Settings	Analyze Update	Quick Report
Analysis Data Result Mixture Library: Brucine	Mixture:	Analysis Data Result Mixture Library: Brucine Mixture	: escription:







## 3. SMA analysis setup

SMA analysis requires a valid mixture/experiment (".exp" file). Developed and validated methods can be stored in libraries for future use and can easily be shared with other users. It is possible to create an unlimited number of different experiments and save them to either pre-existing or new libraries.

## 3.1. Creating a new library

In the Simple Mixture Analysis dialog, click on <sup>Sel</sup> to open the Library Manager.

- 1. Click on New Library
- 2. Choose a name for the library
- 3. Click on OK
- 4. Select the folder in which you want to save the library
- 5. Hit OK

Your new library is created in the location specified.

Library Manager	rary /Usuario/Desktop/Datasets/By plugin	/SMA/Brucine		]		
Mixture 1 brucine_solvent	Choose a name for the L New Library	ibrary	? × Cancel	New Mixture		
		Select a folder to save the li	brary			×
		← → 👻 ↑ 🖡 « SMA	» #15591 Aspirin	ٽ ~		n
		Organize  • New folder				?
		<ul> <li>Desktop</li> <li>Downloads</li> <li>Documents</li> <li>Pictures</li> <li>4_Course Certificates</li> <li>7_Software_Mnova_Mb</li> <li>Mixture</li> <li>Results</li> <li>SMA</li> <li>ownCloud</li> <li>OneDrive</li> <li>This PC</li> </ul>	*     Name       *     Image: Mixture       *     *       *     *       *     *		Date mo	vdified 21 10:02 A
		Folder:	v < #15591 Aspirin	[	Select Folder Can	> cel

You can now click on **New Mixture** <sup>6</sup> to create a new experiment (refer to section 3.4).



## 3.2. Selecting a previously created Library

In the Simple Mixture Analysis dialog, click on 🋸 to open the Library Manager.

- 1. Click on Select Library
- 2. Choose the location of the library you have already saved, or where you want to save your new experiment
- 3. Select Folder.

	Library Manager				
	New Library Select Library				
Coad library	$\vee$			× —	
← → • ↑ 🖡 «	> Data > SMA > Aspirine dataset	ٽ ~		aset	
Organize • New folder				- 0	
<ul> <li>Documentos</li> <li>Imágenes</li> <li>This PC</li> <li>3 D Objects</li> <li>Desktop</li> <li>Documents</li> <li>Documents</li> <li>Dounloads</li> <li>Music</li> <li>Pictures</li> <li>Videos</li> <li>Windows (C)</li> </ul>	Name  #15591 Aspirin Aspirine sample Mixture components New Library  Components	Date modified 7/15/2021 12:20 PM 7/15/2021 12:20 PM 7/21/2021 12:20 PM 7/21/2021 12:49 PM 7/21/2021 7:02 PM 8/19/2021 3:08 PM	Type File folder File folder File folder File folder File folder	Size	New Mixture Delete Mixture
Folder: Exp	• <	<b>3</b> -	elect Folder Ca	> incel	OK Cancel

You can now select an experiment from the open library and hit **OK** to use it for your analysis, or even delete a previously added mixture by clicking on **Delete Mixture**.

ibrary Manager		
New Library Select Library		
Current Library: X:/Data/SMA/Aspin	ine dataset/Experiments	
Mixture	Description	New Mixture
1 Aspirin Exp 1 2 Aspirin Exp 2	Determination of the levels of: Acetylsalicylic acid, Ascorbic aci	Delete Mixture
		Import AssureNMR Method
		OR
	OK	Cancel

Otherwise, you can **Import an AssureNMR Method**, as explained in <u>section 3.3</u>, or create a **New Mixture** steps described in <u>section 3.4</u>.

## 3.3. Importing an AssureNMR Method

To import an AssureNMR method, press the **Import AssureNMR Method** button and select the "\*.quantMethod" file from your directory. Click on **Open**.

	Library Manager			
	New Library Select Library	Desktop/SMA Libraries		
	File File C:/Users/Usuario/Desktop/	Mixture Aspirin Ci	Description Quantifying Aspirin components	New Mixture
Select Method File $\leftrightarrow \rightarrow \sim \uparrow$	4	~ C	Search AssureNMR experime	Delete Mixture
Organize • New folder			≣ • 💷 💡	
<ul> <li>NO.</li> </ul>	Name	Date modified	Туре	OK Cancel
- Netter Reads	TestMethod.quantMethod	4/11/2022 6:20	PM QUANTMETHOD File	Cancer
Fiename Fiename Fiename Fiename	quantificationMethod	 3	.quantMethod ~ Open Cancel	

SMA will convert the AssureNMR Method into and ".exp" file that can be correctly read and run using Mnova SMA. A message will appear when the conversion is complete. Click on **OK**. The AssureNMR mixture will appear in the library table as seen below.

File       Information         Image: C:/Users/Usuario/Desktop/SMA Libraries/       Image: C:/Users/Usuario/Desktop/SMA Libraries/         Image: Italian in the second	File C:/Users/Usuario/Deskt	ition ixture has been successfully cre /Users/Usuario/Desktop/SM istMethod.exp	× eated: A Libraries/	New Mixture	
Library Manager				¥ 1	
	Library Manager	vesktop/SMA Libraries			



You can now select the mixture and press **OK** to open the **Mixture Creation/Edition** dialog and edit it, or to otherwise simply use it for your analysis.

	y: C:/Users/Usuario/Deskto	p/SMA Libraries				
	File			Mixture	Description	65
1 C:/Users/	'Usuario/Desktop/SMA Lib	oraries/Aspirin Ci.exp	A A	spirin Ci	Quantifying Aspirin components	New Mixture
			//P			Delete Mixture
ixture Cri	eation/Edition			Compound		2 ок Са
ame:	New Method	Units: %	¥	Save Compou	ind Add From Document	DB Assistant
escriptio	Imported from Assure	) NMR	-			
<b>I</b> #	Compound	Туре	+			
Ø <u>√</u> 3	TSP	Reference	/			
<b>– –</b> 4	Aspartic acid	Compound				
⊻ 5	Citric acid	Compound	▼	Click on 👕 to add	d a new Compound	_
☑ 6	Salycilic acid	Compound		Click on 🔆 to add	d a new Compound from the current	t Document
				Click on 💕 DB A	ssitant to start the Wizard	

#### Notes about imported AssureNMR experiments:

- The generated ".exp" file name matches the original AssureNMR method file name.
- The Mixture name is set to "New Method" and the Description to "Imported from Assure NMR".
- The Calculations, PCA, and Processing options are all unchecked by default.

- The "Std. Concentration Eq." is set as the default **Formula** for 1D NMR methods and generated automatically for each compound; for 2D methods, the default **Formula** would be the "User Eq" and must be manually entered by the user.

- The "Sum" integration method is set by default for all the compounds.



## 3.4. Creating a new mixture/experiments

To add a new mixture/experiment to your library, use the **New Mixture** button <sup>©</sup> in the **Library Manager** or in the **Simple Mixture Analysis** panel.

	Library Manager				
	New Library				
	Current Library: X:/Data/SMA/Aspin	rine dataset/Experiments			
	Mixture		Description		<b>\$</b>
Simple Mixture Analysis					New Mixture
				id, Ascorbic aci	Delete Mixture
Analyze Update			0	R	Import AssureNMR Method
Analysis Data Result					
Mixture 🛛 🔊		😂 🇐 Mixture:			
Parameters				OK	Cancel

The **Mixture Creation/Edition** dialog will open. Add a name and short description for your experiment.

Mixture Creation/Edition							
Mixture					1		
Name:	Aspirin Exp	Units:	mg/L	-			
Description:	Determination of the levels of: Acetvlsalicvlic acid, Ascorbic acid, Citric acid, Salicvlic acid, Acetic acid			<b></b>			



Mixture compounds can be added in one of three ways:

- A. Manually, by entering compound details piecemeal
- B. Automatically, from an open Mnova document
- C. Using the DB assistant

Mixture Cr	eation/Edition				-		
Mixture				Compound	<u>B</u>		
Name:	Aspirin Exp	Units: mg	ı/L ▼	E Course Compound		t DRA	Sistant
Descriptio	Determination of the lev	els of:		Save Compound	Add From Documen	UB AS	ssistant
Compoun	d List		A				
Ø	Compound	Туре		Click on to add a new Con Click on to add a new Con	mpound mpound from the curr tart the Wizard Is in the list to see its a	rent Document details.	
						OK	Cancel



#### A. Manual addition of mixture compounds

Click on the 🕈 button to add a new compound, then fill in the compound's information.

#### A.1. Compound details

In the **Compound details** section, enter the compound **Name**, **Type** (Reference, Compound, Impurity, or solvent), **Molecular weight**, and NMR **dimension**. Then, choose a **Color** from the available color palette to use in the display of the results.

-	소: 🛋			
Save Compound	Add From Document DB Assistant			
Compound Details				
Name:	Acetylsalicylic_acid			
Color:	Orange 👻			
Spec. Nº:	1 ~			
Type:	Compnd			
Mol. Weight:	180.16			
Dimensions:	1D ~			
	Pick Screen Color			
	Pick Screen Color	Hue:	0 🗘 Red:	255 \$
	Pick Screen Color	Hue: Sat:	0       Red: 255       Green:	255 0
	Pick Screen Color	Hue: Sat: Val:	0   Red: 255  Green: 255  Blue:	
ompound Formula	Pick Screen Color  Custom colors  Add to Custom Colors	Hue: Sat: Val: HTML:	0	



When adding a Reference to a mixture, a new bloc of fields appears to allow you to choose the Reference

type and fill in the Reference Spectrum Acquisition Parameters.

When using an Internal Reference, these parameter fields can be completed manually.

Compound		Compound	
E Save Compound	Add From Document DB Assistant	Save Compound A	dd From Document DB Assistant
Compound Details		Compound Details	
Name:	TMSP	Name:	TMSP
Color:	Black 👻	Color:	Black 👻
Type:	Reference 👻	Туре:	Reference
Reference Type:	Reference	Reference Type:	
Mol. Weight:	Compound	Mol. Weight:	116.07
Dimensions:	Solvent	Dimensions:	1D
Spec. Nº:	1 ~	Spec. Nº:	1
		Reference Spectrum Acquisition	Parameters
		Number of Scans (NSR):	
		Receiver Gain (RGR):	
		Pulse Width (PWR):	
		Temperature (TR):	
		Spectral Size (SpecSR):	
		Spectral Width (SpecWR):	
		Dilution Factor (DFR):	
		Shadon (Brity)	

When using an **External PULCON** reference, you must define the path in which your reference spectrum can be found. The **Reference Spectrum Acquisition Parameters** are then automatically completed with the information available in the spectrum file.

Reference Type:	External PULCON 👻
Mol. Weight:	116.07
Dimensions:	1D 🔹
Spectrum File: Jsuario/Desktop/Datase	ts/Mnova docs/ExternalRef.mnova
Reference Spectrum Acquisition Param	eters
Number of Scans (NSR):	8
Receiver Gain (RGR):	38
Pulse Width (PWR):	6
Temperature (TR):	29
Spectral Size (SpecSR):	16384
Spectral Width (SpecWR):	4801.34437643
Dilution Factor (DFR):	

When using an **External Bruker PULCON automatic** reference, the **Reference Spectrum Acquisition Parameters** are automatically parsed from the eretic file.



#### A.2. Compound formula

In the **Compound Formula** section, you should add your compound's multiplet(s) chemical shift range(s) and the Number of Nuclides (NN) required for the calculation. These ranges can either be added manually or imported from an active spectrum or a document. Follow the steps in the images below in each case.



8.0 7.5

7.0 6.5

6.0 5.5 5.0

3.0 2.5

4.5 4.0 3.5 1H (ppm) 2.0 1.5 1.0 0.5 0.0



Another possibility is to run a **Peak Pattern Recognition** to find a multiplet pattern in your 1D spectrum when peaks overlap. In this case, a spectrum of the pure compound and a set of parameters must be provided to be used as a reference for the Pattern Recognition.

Pattern Recognition												
Select Pattern File				×								
← → × ↑ 🖡 « Data > SMA :	> Aspirine dataset > Mixture components	ٽ ~		mponents						2		
Organize • New folder						attern Re	cognitior	n Settings		f	×	
🤞 Testing and Validation Data 🔨	Name	Date modified	Туре	Size	Ар	ply To All	Compoun	ds				
OneDrive	• AspirinC-1	12/22/2015 1:22 AM	MNOVA File		Multi	iplet Searc	h Window	Amplitud	e: 0.100 ppm		÷	
Documentos	AspirinC-2	1/27/2018 3:27 PM	MNOVA File		Inter	wation Th	achold:		10.96			
Imágenes	<ul> <li>AspirinC-3</li> </ul>	1/27/2018 2:39 PM	MNOVA File		Integ	grauon in	esnoid:		10 %		*	
	AspirinC-4 2	1/27/2018 2:39 PM	MNOVA File		Cent	roid Toler	ance:		0.100 ppm		-	
S This PC	AspirinC-5	1/27/2018 4:33 PM	MNOVA File						G OK		Cancol	
3D Objects	<ul> <li>AspirinC-Ref</li> </ul>	1/27/2018 2:43 PM	MNOVA File						U UK		Callee	
Desktop				(					$\overline{}$			
Documents												 
Downloads					⊢ Add ran	aes fron	n curren	t Spectru	um – – Patte	rn Recor	nition ——	
Music						A				-		
Pictures						<b>~</b>	-/	6			<b>Y</b> Q	
Videos					3	_		_			_	4
Windows (C)					Active	From	То	Mult.	J's	NN	Pattern	1.1
- minuona (c.)												
· · · · · · · · · · · · · · · · · · ·	<				$\checkmark$	8.00	7.95	dd	10.8,1.7	1		1.
												L F
File name: AspirinC	-4	~	*.mnova	~	$\checkmark$	7.72	7.65	ddd	8.1,7.8,1.7	1		1
			Open	Cancel								

The Pattern Recognition Settings include:

- The Multiplet Search Window Amplitude: to determine the amplitude, in ppm, of the peak search window for the mixture multiplet. The search window will be the range of the Pattern Multiplet extended by the amplitude: (from\_pattern+amplitude, to\_pattern-amplitude). For example, the search window for the first multiplet in the example above, where amplitude is set to 0.1000 ppm, would be [8.022 + 0.1, 7.935 0.1].
- **The Integration Threshold:** to define the limiting percentage of the total area of the peaks within a scale of search window.
- **The Centroid Tolerance:** to determine the distance between the centroid of the reference pattern multiplet and the multiplet to be considered by the tool. The higher the tolerance, the greater the number of matches that might occur.

Once you have configured these parameters, you can apply them to all the compounds in the mixture.



Next, you must determine the equation to use for quantification. You can either choose one of the three hardcoded formulae available for Concentration, Mass % and Purity, add your own formula, or select an External PULCON equation to be applied. In any case, by clicking **Apply to all** you can apply the formula you choose to all the mixture components. Otherwise, you must add a formula for each compound separately.

Compound	l Formula	
Formula	]	
Mode:	Std. Concentration Eq.	🙆 Apply To All 🔛 🛃
	Std. Concentration Eq.	
((NN1/	Std. Mass Eq.	$\sim$
	Std. Purity Eq.	
	User Eq.	
	External PULCON Eq.	
	External Bruker PULCON Automatic Eq.	

#### A.2.1. Std. Concentration, Std. Mass, or Std. Purity equations

When applying one of the hard-coded concentration, mass, or purity formulae, the equation is automatically generated with the multiplets and retrieved spectrum parameters, as shown below.

Formula Mode: Std. Concentration Eq.  Apply To All	
(((I1/NN1)+(I2/NN2)+(I3/NN3)+(I4/NN4)+(I5/NN5))/5)*CCF Formula Mode: Std. Mass Eq. (((I1/NN1)+(I2/NN2)+(I3/NN3)+(	Apply To All     All     Formula
	Mode: Std. Purity Eq.  Apply To All  (((([1/NN1)+(I2/NN2)+(I3/NN3)+(I4/NN4)+(I5/NN5))/5) *(CCF*MW)/ SW)*100

#### A.2.2. External PULCON equation

When using an **External PULCON equation** for quantitation, PULCON parameters must be provided (via an "eretic" file or manually) to correctly apply the equation.

Click on this button is to open the **PULCON Parameters Manager**:

 Enable and import the "eretic" file included in the raw data folder. The parameters are retrieved and displayed in the table, as seen in the image below.

Compound Formula				
Formula Mode: External PULCON Eq. CCF * [ ECORR * CAL ] / [ / NS ] * [RGR / RG] * [Spect NN2)+(I3/NN3)+(I4/NN4)+	ESCAL * INTSCL ] SR / SpecS] * [Spe (I5/NN5))/5 PULCON Param	Apply 1     [T / TR] * [PW cW / SpecWR] *(r eters Manager	To All [] [] [] [] [] [] [] [] [] [] [] [] []	?
	✓ Import Paramete	rs File: C:/L	/pdata/1/eretic	
	Name	Identifier	Value	
	TITLE	TITLE	Parameterfile,TopSpin3.5pl5	
	CALDATE	CALDATE		<b>E%</b>
	ECONC	ECONC	15	
	ECONCU	ECONCU	mmol/l	
	ECORR	ECORR	1	
	EINT	EINT	8613174.015625	
	ELW	ELW	1	
	EPOS	EPOS	0	•
			ОК	Cancel

– Otherwise, press the Add button 📫 and type the parameters Name and Value manually.

Compound Formula					
Formula Mode: External PULCON CCF * [ ECORR * CAL ] / NS ] * [RGR / RG] * [S	I Eq.  / [ ESCAL * INTSCL ] pecSR / SpecS] * [Spe	<ul> <li>Apply To A</li> <li>* [T / TR] * [PW / P</li> <li>cW / SpecWR] *((I1/</li> </ul>	WR] * [NSR NN1)+(I2/		
NN2)+(13/NN3)+(14/NF	PULCON Parame	eters Manager		?	×
		s File:			2
	Name	Identifier	Va	alue	+
	ECORR		1 3	Туре	-
			<b>4</b>	K Ca	incel

You can remove parameters from this table using the **Remove** — button.

Click **OK** to save your changes. The **External PULCON equation** is now correctly defined.

#### A.2.3. External Bruker PULCON automatic equation

When using an **External Bruker PULCON automatic equation** for quantitation, PULCON parameters are automatically read from the raw data files and no further configuration is needed.



#### A.2.4. User equation

To add your own formula, choose the **User Equation** mode; the **Formula Editor** will open. Use the available buttons to type and check your formula for errors. You can read more about the <u>formula editor</u> in our associated blog post.

Formula Editor	? ×
(((NN1/I1)+(NN2/I2))/2)*RC	
Concentration Purity Statistics	Check Formul
Legend	
Compounds CCF : Concentration Factor of Reference C_Salicylic_acid: Concentration of: Salicylic_acid C_Ascorbic_acid: Concentration of: Ascorbic_acid C_Acetic_acid: Concentration of: Acetic_acid C_Citric_acid: Concentration of: Citric_acid Number of Nuclides Integrals	×
Custom Parameters	
ERETIC Parameters	
Others	
ОК	Cancel



Note that you can also define custom or PULCON parameters to be used in the equation for the concentration calculation.

#### **Custom Parameters**

Defining custom parameters can either be achieved from the **SMA** main dialog in the **Custom** tab, or from the **Mixture Creation/Edition** tab in the **Compound Formula** section. Click on this button, M, to open the **Custom Parameters Manager**, then on P to add a new row in the table. Select the cell and type a name and an identifier (a nomenclature to use in the formula) for your custom parameter, then click **OK**.

Save Compound Add From Document DB Assistant Compound Details Compound Formula Formula Mode: Std. Concentration Eq.   Apply To All  ((((1/NN1)+(12/NN2)+(13/NN3)+(14/NN4)+(15/NN5))/5)*CCF Add ranges from current SpectrumPattern Recognition
Add ranges from current Spectrum _ Partern Recognition
Formula Mode: Std. Concentration Eq.  Apply To All  ((((11/NN1)+(12/NN2)+(13/NN3)+(14/NN4)+(15/NN5))/5)*CCF Add ranges from current Spectrum  Pattern Recognition
Mode: Std. Concentration Eq.  Apply To All  ((((11/NN1)+(12/NN2)+(13/NN3)+(14/NN4)+(15/NN5))/5)*CCF Add ranges from current Spectrum
Add ranges from current Spectrum
Add ranges from current Spectrum
Add ranges from current Spectrum
Add ranges from current Spectrum Pattern Recognition
M M 📂 📩
? 🗙 luit. J's NN Pattern 📤 🕇
tifier 🕇
-
ame
Cancel
t

The custom parameters are now added to the **Custom** table and to the **Formula editor** and can be used in the equation. **Values** for custom parameters can be added manually or read from the **Parameters** table of the sample, as shown in the image below.

Formula Editor     ?     X  (((NN1/I1)+(NN2/I2))/2)*(CLJ/CP)*CCF			Par Re	rameters	up Customize	
			1	Parameter Data File Name	Value X:/2014/20140701/Aspirin_A2_neu Aspirin_A2_neu_NOESY_01.fid/fid	u_01/
Concentration Purity Statistics			2	Title	Aspirin_A2_neu_NOESY_01	
Legend			3	Comment	RC:10.0 EXP:Aspirin_Ci.exp CP:20 CU:10	
Compounds Number of Nuclides	Parameters			Page	navamatara	
Integrals	Standard Custom Name	Identifier			Value	
Custom Parameters	Custom parameter 1	CP1 2	:0			•
Custom parameter 2: CU	Custom parameter 2	CU 1	0			
ERETIC Parameters						
Others						
OK Cancel						



#### **PUCLON Parameters**

How one defines PULCON parameters is described <u>above</u>. The PULCON parameters are added to the **Formula editor**, as seen in the image below, and can be used to complete the user custom equation.

egend		
Compounds		
Number of Nuclides		
Integrals		
Custom Parameters		
PULCON Parameters		
ECONC: ECONC ECONCU: ECONCU ECORR: ECORR EINT: EINT ELW: ELW EPOS: EPOS ESCAL: ESCAL EUNIT: EUNIT INTSCL: INTSCL Others		
	OK Cancel	

#### A.3. Compound options

In this section, you can configure the following calculations and analysis options:

• Not Show in results: if checked, the results of the analysis will not be displayed in the **Results** tab. This is particularly useful when you want to use the integrals of a certain *compound* A to calculate the concentration of another *compound* B of the mixture, but you are not interested in the quantification of *compound* A itself.

Compound Options	
General	
✓ Not Show in Results	

• Force compound creation: if checked, a compound will be created, even if no peaks were found in the defined ranges. This "fake" compound will be visible in the results table, and alert messages about the creation of peaks will be displayed so that you can review the spectrum and fix the problem manually.

Calculations			
✓ Force Comp	ound Creation		
Use Absolut	e Integrals Values		
Integration Me	ethod		
O Peaks	Sum	O Edited Sum	Apply To All



• Enable/disable the **Use of absolute values** for integrals.



• Integration method: choose the integration method and apply it to all compounds, if needed.



• Once all the required information is entered, press this button, 🗎, to save the compound to the **Compound List**, as shown below.



#### B. Adding mixture compounds from an Mnova document

Open your mixture component files in Mnova. You can either have them saved in separate files or grouped on several pages in a single Mnova file.



Select the Mnova document or Mnova document pages with the compounds you wish to add, then click on

to import the compound's details into the SMA Mixture Creation/Edition panel.

Asp	rin_components* X				Pages
Units: mg/L V	Compound Save Compound	E DB Assistant		-160 -150 -140	4. (1) Apprin plus C. Test NOESY 02 Test Historical Control of the second seco
'pe 🕇				-120	
	Click on 🕈 to add a new Compound			-90 -90 -80 - -80 -90 -00-	5. (1) Aspirin_plus_C_Test_NOESY_02
•	Click on 🔆 to add a new Compound from the current Docum	ent		-60 -50 -40	аранана и калана и к Самана и и калана и к Самана и и калана и к Самана и и калана и к Самана и и калана и к Самана и и калана и к
	Click on B DB Assitant to start the Wizard			-30 -20 -10	
	Click on any of the Compounds in the list to see their details.		•	10 2 2.0	a de se
		OK	Cancel		



The added compounds will appear in the **Compound List**, as shown below.

Mixtu	ture Creation/Edition									
Mixtur	e —									
Name	e:	As	pirin Exp	Units: mg/L	•					
Descr	iptio	De	termination of the lev	els of:	<b>A</b>					
Com	pound	l Lis	st							
	#	^	Compound	Туре	+					
	⊻ 1		TMSP	Reference	2					
	<b>-</b> 2		Acetylsalicylic_acid	Compnd.						
	✓ 3		Salicylic_acid	Compnd.						
	✓ 4		Ascorbic_acid	Compnd.						
	✓ 5		Acetic_acid	Compnd.						
	✓ 6		Citric_acid	Compnd.						

You can now select any compound from the list and Edit  $\checkmark$  its details, as detailed in sections <u>A.1.-A.3</u>.

C. Using the DB assistant to add mixture compounds

Launch the **DB assistant** by clicking on <sup>SI</sup>. Enter the server connection details, then click on **Connect**.

Compound				1	
Save Co	mpound	Add From Doo	ument	S DB Assistant	
Connection	8				(
Server:	alhost		Port:	5504	
User:	Test		Password:	•••••	
	Keep Ope	en the Connection		✓ Save Password	

Check the Keep Open the connection or the Save Password options, if needed.

Choose the DB you want to search, then type the text and click on The to search. You can also search your database by multiplets/peaks. To do so, open a spectrum in Mnova, then click on the the button.



A search can be performed for a specific database field and/or by substrings. Results can be filtered by dimension (1D or 2D).

Search		
Database:	TestDB	~
Search for text:	Aspirin	T
Field:	NMR Spectrum -> Modified	✓ 人
✓ Substring	Molecule -> Atoms Molecule -> Aliases	
Results	Molecule -> Name	
#	NMR Spectrum -> Mnova Version NMR Spectrum -> Modified	ico 📑
	NMR Spectrum -> Created NMR Spectrum -> PageWidth NMR Spectrum -> PageHeight	
	NMR Spectrum -> PageID	
neidi.	L	
✓ Substring	Filter By Dimension:	1D 🔻

The search hits will appear in the **Results** section. You can double click on a database record to open and view it, or you can select more than one record and click on the zoom button  $\frac{N_{\odot}}{N_{\odot}}$  to open them all at once.

To help you select the hit spectrum that best fits your analysis, you can stack database hits with the analyte spectrum (open with Mnova or select in the **Current Mixture Spectrum File** box).

Current Mixture Spectrum File: plugin/SMA/Aspirine sample/Aspirin_C.mnova							
1ode:  ● Single ○ Multiple  (注) Stack Selection							



This option is available in the **Advanced View** panel (hidden by default) and offers two stacking modes:

• The **Single** mode: stacks spectra one by one with the base analyte spectrum. A new Mnova document is generated with the stacked spectra for every selected record.



• The Multiple mode: stacks all spectra together.







Now select the compound(s) you want to add to your mixture and click on it (them) to the **Compound List**.

ixtur	<u>.</u>					Compou	und									
lame	. [	Aspirin Exp		Units: m	g/L 👻					썆		5				
Descri	ptio	Determination of the lev	els of:				Save C	ompound	A	dd From Docume	nt	DB Ass	istant			
Com	ound	List				Conne	ction									
Image: Sector A and a sector A an	# ^ Compound Type			+	Server:	connect	lo	calhost		Port:	5504					
	√ 1	TMSP	Referer	nce		User:		Т	est		Password:		,			
		A	6		-				Keep Oper	the Connection		Save Pa	assword			
	Part 2 Acetylsalicylic_acid Compnd.				Search	) ———										
	✓ 3	Salicylic_acid	Compr	nd.		Datab	ase:	TestDB					*			
	✓ 4	Ascorbic_acid	Compr	nd.		Searc	h for text:	Aspirin						Ţ	2	
	✓ 5	Acetic_acid	Comp	Compr	nd.		Field:						*	¥	▲	
	✓ 6	Citric_acid	Compr	nd.	<b>B</b>	Pocult	ubstring	Filter By	Dimension:				1D +			
						#	Record	Nam	ne	Title		Item	Score	•		
						⊻ 4	86	citric acid	As	pirin_plus_C_Tes	t_NOESY_	)2 1	1000		<u>ار</u>	
						5	81	salicylic ac	id As	pirin_plus_C_Tes	t_NOESY_	02 1	1000			
						•							Þ	•		
Optio	ns					Ad	vanced View	w								

You can select any compound from the list and Edit  $\checkmark$  its details, as detailed in sections <u>A.1.-A.3</u>.

Once all your mixture compounds are added, you can save your mixture/experiment by clicking **OK**.

✓ 3	Salicylic_acid	Compnd.		Dimensions:	10	
✓ 4	Ascorbic_acid	Compnd.				
5	Acetic_acid	Compnd.				
✓ 6	Citric_acid	Compnd.				
			-			
				Compound Formula		
					OK	Cancel



## 3.5. Configuring experiment options

In the **Calculations** tab, you can enable the option to **Calculate SNR**. When enabled, the SNR value will be calculated and included in the results table.



In the **PCA** tab, check the **Suitable for PCA** option if you want to retrieve the SMA results in a format suitable for a subsequent **principal component analysis** (PCA).

Options		
Calculations	PCA	Processing
<ul><li>✓ Suitable for I</li><li>☐ Read Parame</li></ul>	PCA	Each Spectrum on the Stack



When performing a PCA analysis with a stack of spectra, the option to **Read parameters for each spectrum on the stack** is also available. If enabled, SMA will update the parameters for each spectrum calculation from the comments field in the parameters table of the sample. The updated parameters can include the Reference Weight (RW), Sample Weight (SW), Reference Concentration (RC), Dilution Factor (DF), Number of Scans (NS), Pulse Width (PW), and Receiver Gain (RG).

Options			
Calculations PCA Processing			
✓ Suitable for PCA			
✓ Read Parameters for Each Spectrum on the sector of t	ne Stack		
Simple Mixture Analysis		Example_dient_weights* ×	
Analyze Update Quick Report Qui	AdvancReport Settings Expert	\$7.7%S*	
Mixture		Experiment: 31P SampleID: test	
<ul> <li>Library: SMA Libraries</li> <li>Workin:</li> <li>C:/Users/Usuario/Desktop/SMA Librarie</li> <li>Aspirin C</li> <li>Description</li> <li>Quantifying Aspirin components</li> </ul>	s/Aspirin CI.exp *	RW: 150 RC: 0.999	-3
Parameters	<b>1</b>		
Standard Custom Sample Spectrum			
Number of Scans (NS):	128	Experiment: 31P SampleID: test	
Receiver Gain (RG):	201.74	SW: 122 RW: 150	-2
Reference Concentration (RC): 0.999 Pulse Width (PW):	1.45	C: 0.999	
Sample Weight (SW) [mg]: 120 Temperature (T):			
Reference Weight (RW) [mg]: 150 Spectrol-Madth (SpecW):		ACC MARKED	
Dilution Factor (DF): Construction (DF):		Experiment: 31P	
Spectrometer Prequency (Sr).		Sample1D: test	Active spectrum
Metadata		RC: 0.999	
✓ Alerts			
	<b>2</b>	30 25 20 15 10	5 0 -5 -10 -15 -20 -25 f1 (ppm)

In the **Processing** tab, check the option **Apply a Processing Template** if you wish to add one or more processing templates for use in the current experiment. When you click on the blue cross button, +, a new dialog will open. Select and add the **Processing template** from your directories then hit **OK**. The added template will be listed in the table, as seen in the image below, and will be applied to the spectrum number 2.

Name:	Aspirin Ci Units: g/L -	
Descriptio	Ouantifying Aspirin components	Save Compound
Compour	d Liet	Compound Details
Options Calcula	tions PCA Processing	Name: Color:
Appl	Processing Template Processing Template	Type: Mol. Weight:
	1 C:/Users/Usuario/	Dimensions:
	Select Processing Template Spec. Nº: 2	< X
	OK	Cancel

When a mixture includes components with different types of nuclei and/or dimensions, it is possible to add a processing template for each. In such cases, a different spectrum number (**SpecNo**) must be attributed to each processing templates. In the example below, the 2D processing template will be applied to spectrum number 2 - of the Mnova document in hand - which includes the Salicylic acid 2D spectrum, whereas the 1D processing template will be applied to the other mixture components with a 1D spectrum.

Options	5							
Calc	ulations	PCA Processi	ng					
✓ Ap	oply Processi	ing Template						
	SpecNo		Processing	Template		+		
	C:/Users/Usuario/Desktop/Datasets/Proccessing templates/1D.mnp							
	✓ 2	C:/Users/Usuar	io/Desktop/Datasets/	Proccessing tem	plates/2D.mnp			
		[	Compound Details					
			Name:				Acetylsalicylic_acid	
			Color:				Orange	·
			Type:				Compnd.	~
			Mol. Weight:				180.16	
			Dimensions:				2D	-
			Spec. Nº:				2	-

Finally, you can check or uncheck table rows to delete processing templates 💻.



## 3.6. Reviewing/editing the mixture details

Your library and selected mixture are now displayed in the SMA panel. You can open your experiment to edit **Mixture** and **Compound** details by clicking on this button <sup>69</sup>.

Simple Mixture Analysis				
Analyze Update Analysis Data Result Mixture		Quick Report Advan	CReport Settings	Expert
📚 Library: SMA Libraries	Section Mixture: Name: Descriptior	C:/Users/Usuario/Desktop/SMA Libraries/Aspirin Ci.exp Aspirin Exp Determination of the levels of: Acetylsalysilic acid, Salycilic acid, Ascorb	pic acid, Acetic acid,	← Citric acid

Select a compound and hit the **Edit** button  $\checkmark$ . The **Compound** details section is accordingly activated and becomes editable. Make any modifications you want, then save them by clicking on this button:

Mixture Creation/Edition											
Mixture			Compound								
Name: Aspirin Exp	Units: mg/L	•	4				挫		1		
Descriptio Ascorbic acid,	Acetic acid, Citric acid		Save	e Compo	und	Ado	d From Docu	ment	DB Ass	istant	
Compound List			Compound	Details							
🕑 # 🗠 Compo	ound Type 👩	<b>;</b> .	Compound	Formula	3						
1 TMSP	Reference		Mode	Std. Co	ncontrat	ion Fa	~	4.0			
P 2 Acetylsalic	ylic_acid Compnd.		(((T1/N	N(1)+(12		(12/NN2	)+(TA/NNA)			<u>×</u> t	
✓ 3 Salicylic_ac	id Compnd.		(((1)))	<b>B</b> Ir	ntrod	ucen	nodificat	tions	<i>5)][5]</i> CG		
✓ 4 Ascorbic_a	cid Compnd.			•							
✓ 5 Acetic_acid	l Compnd.		Add ran	ges from	n curren	t Spectru	Im Patter	n Recog	nition		
G Citric_acid	Compnd.			<b>₩</b>		6			-O-		
			Active	From	То	Mult.	J's	NN	Pattern		+
			~	8.00	7.95	dd	10.8,1.7	1			-
			~	7.72	7.65	ddd	8.1,7.8,1.7	1			■
			~	7.48	7.42	td	7.6,1.2	1			
			<b>~</b>	7.26	7.20	dd	8.2,1.2	1		-	
		. 11							OK		Cancel

You can also select and delete a previously added compound, or select and change priority with . The analysis will be performed in the order you define.

						.omp	ound Lis	t	
							# ^	Compound	Туре
							<b>√</b> 1	Acetylsalicylic_acid	Compnd.
							<mark>√</mark> 2	Salicylic_acid	Compnd.
							<b>✓</b> 3	Ascorbic_acid	Compnd.
							✓ 4	Acetic_acid	Compnd.
					>		✓ 5	Citric_acid	Compnd.
t									
	Compound	Туре	+						
TM	SP	Reference							
Ace	tylsalicylic_acid	Compnd.	5						
Salicy	/lic_acid	Compnd.							
Asco	rbic_acid	Compnd.			1				
Aceti	c_acid	Compnd.							
					Co	ompo	ound Lis	t	
Ci	itric_acid	Compnd.							_
Citri	ic_acid	Compnd.		_			# ^	Compound	Туре
Citrie	c_acid	Compnd.		•			# ^ ✓ 1	Compound Acetylsalicylic_acid	<b>Type</b> Compnd.
Citr	ic_acid	Compnd.		•			# ^ ✓ 1 ✓ 2	Compound Acetylsalicylic_acid Salicylic_acid	<b>Type</b> Compnd. Compnd.
Citr	ric_acid	Compnd.		•			# ^ ✓ 1 ✓ 2 ✓ 3	Compound Acetylsalicylic_acid Salicylic_acid Ascorbic_acid	Type Compnd. Compnd. Compnd.
Cit	ric_acid	Compnd.		•			# ^ ✓ 1 ✓ 2 ✓ 3 ✓ 4	Compound Acetylsalicylic_acid Salicylic_acid Ascorbic_acid Acetic_acid	Type Compnd. Compnd. Compnd.
Citri	c_acid	Compnd.					# ^ ✓ 1 ✓ 2 ✓ 3 ✓ 4 ✓ 5	Compound Acetylsalicylic_acid Salicylic_acid Ascorbic_acid Acetic_acid Citric_acid	Type Compnd. Compnd. Compnd. Compnd.

Click on **OK** to save your modifications.



## 4. SMA general settings

Before proceeding with the analysis of the samples, you might want to configure some general calculations and reporting settings. To do so, click on the **Settings** icon in the **Simple Mixture Analysis** window. A new dialog will open with two tabs: **Calculations** and **Report**.



## 4.1. The Calculations tab

In this tab, you can indicate whether the Reference Concentration (RC) or the Reference Weight (RW) and Molecular Weight (MW) (RW/MW) will be used for calculation. RC and RW values can either be present in the parameters table of the sample or manually entered by the user in the SMA panel.

♥ Settings				
Load Settings	💾 Save Se	ttings		
Calculations	Alerts	目 Report		
-Reference Conce	ntration			
Use RW/MW	ind dd off		Use RC	

## 4.2.The Alerts tab

When running an analysis, SMA can run various tests and report on possible associated errors via the <u>alerts</u> window. In this tab, you can configure the tests you want to perform on your compounds. You can enable the following:

- Check Relative Areas ratio: to calculate the relative area (Integral\_i/NN\_i) / (Integral\_j/NN\_j) and compare it to the expected values (between 1-tolerance/100 and 1+tolerance/100). You can set the tolerance value in the dedicated box.
- **Check Js:** to calculate the Js value for a certain multiplet and compare it to that defined by the user. You can set the tolerance in the dedicated box.
- **Check Multiplicity:** to compare multiplicities found to those defined by the user in the Mixture.



• Verbose Pattern Recognition Algorithm: to display information about the search and search results when using the pattern recognition tool.

Load Settings	Save Settings		
Calculations	Alerts 🔠 Re	port	
Check Relative Are	as Ratio Tolerance	: 90% 🗘	
Check Js	Tolerance	: ± 0.05 Hz ‡	
Check Multiplicity			
Verbose Pattern Re	cognition Algorithm	ı	



#### 4.3.The Report tab

In this tab, quick and advanced reports can be customized.

#### A. Quick Reports

**Quick reports** are concise text reports that can be quickly pasted into the Mnova document or copied to the clipboard.

Report sections can include data (Mixture info, Sample parameters, Metadata, Spectrum acquisition parameters) and results (SNR, Ranges, Annotations), and are fully customizable.

When **Spectrum Acquisition Parameters** is checked, make sure you have an open Mnova document to retrieve and display the available parameters for selection.

The number of decimals to be used in the reported results can also be chosen in this section.

		🕑 Sele	ct the information from the Mixtu	re to report	?	×
Settings	? ×	ſ✔ Ge	neral Info			
		✓ L	ibrary Name			
Load Settings Eave Settings			lixture Name Inits			
Calculations			Description			
Quick Advanced		[ ✓ Co	mpound List			
			hecked			
Copy to Clinboard Z Paste in Current Document			ype			
			lol. Weight			
- Sections		✓ S	pectrum			
✓ Mixture Info		✓ F	ormula			
Sample Parameters		V (	Dimension			
✓ Metadata		✓ I	ntegration Method			
Spectrum Acquisition Parameters			options			
Results	\ \	1		OK	Can	cel
SNR Ranges Annotation	\	🕑 Select	the parameters to export	? ×		
		Active Sp	ectrum:			
Number of decimals		Aspirin_ RC:10.0;	A2_neu_NOESY_01 EXP:Aspirin Ci.exp			
esuits. Z -			Parameter	<b></b>		
ОК	Cancel	1	✓ Data File Name			
		2	✓ Title			
		3	✓ Comment			
		4	✓ Origin			
		5	✓ Owner			
		6	✓ Site			
		7	✓ Instrument	-		
		-				

See an example of a Quick Report in section 6.4.



#### **B. Advanced Reports**

On the other hand, **Advanced reports** are extent reports with complete information about the experiment's parameters and results. Various types of advanced reports are available and customizable (PDF, Mnova, HTML, XML, CSV). Advanced reports can be saved in the directory of your choice.

#### Mnova and PDF reports configuration:

Both Mnova and PDF reports can be generated, and PDF reports can be protected from editing.

General information about File names, Time stamp and Software version can be included along with data (Mixture info, Samples parameters, Metadata, Spectrum acquisition parameters) and results (SNR, Ranges, Annotations).

Default (**Continuous** or **One Section per Page**) or custom (**Layout Template** or **Configuration File**) layouts and designs can be applied to both Mnova and PDF reports.

😢 Settings		? ×		
Evad Settings				
Calculations				
Quick   Advanced				
Destination				
Directory: C:/Users/Usuario/Desktop/Results/SMA				
Save Results in Subfolders with Timestamp				
Туре	🕑 Document Settings			? ×
🗹 🧕 Document 🏼 🂭	-Format			
	✓ Mnova	✓ PDF	(	
		Prot	tect PDF from Editing	
🗆 🛶 XML 🔅	-Sections			
	Information			
	File names			
	Coffeense comien			
Number of decimals	Software version			
Results: 2 0	Data			
	✓ Spectrum			
· · · · · · · · · · · · · · · · · · ·	Sample Parameters			
	<ul> <li>Metadata</li> </ul>			
	Spectrum Acquisition Pa	rameters		
	Posults			
	SNR	✓ Ranges	✓ Annotation	
	-Layout and Design			
	Ontinuous			
	One Section per Page			
	Apply Layout Template			
	Apply Configuration File:			
			ОК	Cancel



Layout templates (".mnova") can be easily generated with Mnova itself and loaded for use in SMA.

Layout and Design		
Continuous		
One Section per Page		
Apply Layout Template	ers/Usuario/Desktop/Datasets/Layout templates/Layout template.mnova	
Apply Configuration File:		
L	OK Car	ncel

**Configuration files** (".json") can be customized based on a default file available for download, then saved and loaded for use.

1      Apply Configuration File:
Default      Download      Download
Name
ConfigurationFile.json
Template_CompoundList_FirstPage.mnova
Template_CompoundList_OtherPages.mnova
Template_Logo_SMA.mnova
Template_Metadata.mnova
Template_Results.mnova
Template_SampleParameters.mnova
Template_Signatures.mnova
Template_Spectrum.mnova
Template_SpectrumAcquisitionParameters.n
Template_TitleInfo.mnova
<pre>"apply":"true", @BB "applyToPage":"Cohers"@BB "applyToPage":"Cohers"@BB "applyToPage":"Cohers"@BB "applyToPage":"Cohers"@BB "footer":{@BB "footer":{@BB "alignment":"66",@BB "alignment":"66",@BB "alignment":"66",@BB "alignment":"60",@BB</pre>
One Section per Page
Apply Layout Template
Apply Configuration File:
O Default O Download
4 Custom /Usuario/Desktop/Datasets/By Plugin/SMA/MyConfigurationFile.json
Use Custom Configuration file OK Cancel



#### HTML, XML, and CSV report configuration

Report sections can include data (Mixture info, Sample parameters, Metadata, Spectrum acquisition parameters) and results (SNR, Ranges, Annotations) and are fully customizable.

Settings		?	$\times$	
Coad Settings 🔚 Save Settings				
Calculations				
Quick Advanced				
Destination Directory: C:/Users/Usuario/Desktop/Results/SMA				
Save Results in Subfolders with Timestamp				
Туре				
Document				
🗆 🐼 HTML 🔅				
CSV Settings			? ×	
- Sections				
Data Data Viscure Info				-
Results: 2 Sample Paramete	ers			_
✓ Metadata ✓ Spectrum Acquisi	ition Parameters			
Results				
SNR .	Ranges	✓ Ar	notation	
	OK		Cancel	

See examples of Advanced Reports in section 6.4.

Note that you can <b>Save</b> your settings	and easily <b>Load</b> them for future analyses.
😢 Settings	
🔚 Load Settings 🛛 💾 Save Settings	

When you have finished the configuration, click on **OK** to confirm your choices.



## 5. SMA sample analysis

Once you have selected a mixture (experiment) and configured your analysis preferences, running an SMA analysis becomes very easy. You first need to open your sample spectrum in Mnova, then click on the magnifying glass button is to read your sample parameters. The sample's parameters table will be automatically completed. If the dataset does not include this metadata (in the comment field of the parameters table), the user will be required to fill the table fields manually.

You can now analyze your sample by clicking on this button known.

ple Mixture Analysis				× .			
nalyze			Quick Report AdvancReport Settings	Expert	San	nple´s para	meters table
Analysis Data Result					Para	meters	
Mixture					Pen	nt Conv Sel	aun Customize
📚 Library: SMA Libraries 🛛 📢	Mixture:	C:/Users/Usuario/Desktop/SMA Libraries/Aspirin Ci	.exp	Ŧ	Kep	Parameter	Value
-	Name: Descriptior	Aspirin Exp Determination of the levels of: Acetylsalysilic acid, S	alycilic acid, Ascorbic acid, Acetic acid, Ci	ric acid	1	Data File Name	X:/2014/20140701/Aspirin_A2_neu_01 Aspirin_A2_neu_NOESY_01.fid/fid
Parameters					2	Fitle	Aspirin_A2_neu_NOESY_01
Standard Custom	Read from s	Spectrum	lied automatically		3	Comment	RC:10.0; SW:500; RW:2.4
Sample ID:		Number of Scans (NS):	128	+	4	Solvent	d2o_10
		Receiver Gain (RG):	0		5	Temperature	25.0
Reference Concentration (RC): 10	0.0	Pulse Width (PW):	7.2		6	Converse	NOECY
Sample Weight (SW) [mg]: 50	00	Temperature (T):	25		0	Puise Sequence	NUESY
Poforance Weight (DW) [mg]: 2	A	Spectral Width (SpecW):	9615.38461539		7	Experiment	1D
Kelerence weight (Kw) [hig]. 2.	4	Spectral Size (SpecS):	65536		8	Number of Scans	128
Dilution Factor (DF):		Spectrometer Frequency (SF):	599.9281593		9	Receiver Gain	0
Metadata					10	Relaxation Delay	3.5000
					11	Dulco Midth	7 2000

Note that you can also specify the mixture name on the comments field of the parameters table of your sample. The corresponding mixture is then loaded when the Read parameters button is used. The string to indicate the mixture name is case-insensitive and can start with "Experiment", "Exp", "Mix", or "Mixture", followed by the name of the experiment/mixture to be used.

Par	ameters		
Re	port Copy	Setup	Second Se
	Paramet	er	Value
1	Data File Na	me X:/	2014/20140701/Aspirin_A2_neu_01/ pirin_A2_neu_NOESY_01.fid/fid
2	Title	As	pirin_A2_neu_NOESY_01
3	Comment	RC	:10.0; SW:500; RW:2.4; EXP:Aspirin Exp



## 6. SMA results

Once the analysis is complete, results are automatically displayed in the **Results** tab.

SMA results can also be loaded from an active document by clicking on this button –. The results and related information (Mixture Information, Calculation Settings, Standard Parameters, Metadata) are accordingly pasted into the SMA panel and a library is generated in the default directory that facilitates the sharing of results for review and repetition of the analysis using the same mixture.

Note that when running an automated Batch or RT SMA analysis with Gears SMA, individual sample results can also be loaded into the SMA results tab for revision.

## 6.1. The results table

Your results will be displayed in the **Results** tab as follows. Mixture components will be colored in the results table and in the spectrum as specified in the experiment options.





A compound that is recolored "red" in the results table might be causing errors to occur, so remember to check the warning messages appearing in the Alerts section.

Anal	ysis Data	Result			
	# ^	Compound	Result (mg/L)	SNR	Annotatio
	2	Acetylsalicylic_acid	0	NC	
	3	Salicylic_acid	8.897	613.92 (422.89, 746.74)	
	4	Ascorbic_acid	15.340	1672.10 (740.89, 2313.00)	
	5	Acetic_acid	16.136	17751.11 (17751.11, 17751.11)	
•	6	Citric_acid	93.840	28745.88 (28143.49, 29348.27)	
Ref	to				
Ale	1.5				
Aler	ts General a	larts			
1		nd Acetylsalicylic acid			
> <	Compou	Id_AcetyIsalicylic_acid			

The alerts can be displayed by **Compound**  $\boxed{\mathbb{M}}$  or by **Time**  $\bigcirc$ .

Alerts	Вус	ompound	
Alerts			
<ul> <li>Compound_Acetyl</li> <li>Compound_Ascorl Relative areas r Relative areas r</li> <li>Compound_Citric_i</li> </ul>	ialicylic_acid ic_acid atio 2.78 between multiplet Ascorbic_acid_2 and multiplet Ascorbic_acid_1 is not the expected: Expected value in range [0.10-1.90] atio 2.67 between multiplet Ascorbic_acid_3 and multiplet Ascorbic_acid_1 is not the expected: Expected value in range [0.10-1.90] cid	2	By time
> General alerts	✓ Alerts           [12:17:57]: Error evaluating Custom Parameter           [12:17:57]: The Vultiplicity of the multiplet Citric_add_1 [3.06, 2.92] is d and it was expected to be m           [12:17:57]: The Multiplicity of the multiplet Citric_add_1 [3.06, 2.92] is d and it was expected to be m           [12:17:57]: Relative areas ratio 2.67 between multiplet Ascorbic_add_3 and multiplet Ascorbic_add_1 is not the expected: Expected value in rat           [12:17:57]: Relative areas ratio 2.78 between multiplet Ascorbic_add_2 and multiplet Ascorbic_add_1 is not the expected: Expected value in rat           [12:17:57]: The list of Js of the multiplet Acety/salicylic_add_2 [7.26, 7.20] is not the expected           [12:17:57]: The list of Js of the multiplet Acety/salicylic_add_2 [7.27, 7.65] is not the expected           [12:17:57]: The list of Js of the multiplet Acety/salicylic_add_1 [8.00, 7.95] is not the expected           [12:17:57]: The list of Js of the multiplet Acety/salicylic_add_1 [8.00, 7.95] is not the expected	nge [0.10-1.90] nge [0.10-1.90]	•



By default, compounds are displayed in the same order they have been assigned in the mixture panel. You can change this order to alphabetical or by increasing concentration, etc., by clicking on the headers of the results table.

Analy	sis Data	Result							
	# ^	Compound	Result (mM) 16.13 24.38			SNR	2		
	1	Acetic_acid			3296	51.71 (32961.71, 32 o	.00		
	2	Acetylsalicylic_acid			1175	52.85 (3049.81, 454	₫ <sup>‡</sup>		
	3	Ascorbic_acid	15.33	Analysi	s Data	Result			
	4	Citric_acid	93.79		#	Compound	Result (mM)	SNR	
• Ref	5	Salicylic_acid	8.89		5	Salicylic acid	8.89	1134.38 (783.87, 1373.1	
•0	Defa	ault order		▼ 3	3	Ascorbic_acid	15.33	3100.76 (1373.47, 4288	0.00
	•				I	Acetic_acid	16.13	32961.71 (32961.71, 32	0.00
					2	Acetylsalicylic_acid	24.38	11752.85 (3049.81, 454	1
					ţ	Citric_acid	93.79	53133.59 (52202.16, 54	
				•0		Ву	concentra	ation	
					•			•	

When the **Calculate SNR** option is enabled for the SMA experiment, a column with the SNR value and range is added to the results table. If the compound involves several multiplets, the SNR is the average of the individual values of such for each multiplet. The SNR is automatically recalculated if changes are made in the multiplets selection.

yze	(O) Update			Quick Report Advanced F	Report Settings	Expe
naly:	sis Data	Result				
Ζ	# ^	Compound	Result (mg/L)	SNR	Annotation	
	1	TMSP	6.35e-2	3571.18 (3571.18, 3571.18)		0.
	2	Acetylsalicylic_acid	24.26	2098.84 (1924.01, 2345.80)		0
	3	Salicylic_acid	8.90	718.02 (494.60, 873.36)		٩
	4	Ascorbic_acid	15.34	1955.63 (866.52, 2705.21)		
2	5	Acetic_acid	16.14	20761.11 (20761.11, 20761.11)		30
0	6	Citric_acid	93.85	33620.22 (32915.69, 34324.75)		

You can also show/hide the results with no valid multiplet  $\bullet$  or the results of the reference compound  $\blacksquare$ , as shown in the image below.

sis Data	Result							
# ^	Compound	Result (mg	g/L)		SNR	Annotat		
1	TMSP	6.355e-2		3571.18 (3	3571.18, 3571.18)			
2	Acetylsalicylic_ac	id 24.257						
3	✓ Salicylic_acid	8.898	Anal	lyze Update				
4	Ascorbic_acid	15.341	Ar	nalysis Data	Result			
5	Acetic_acid	16.137	. 7	<b>*</b> * ^	Compound	Result (mg/L)	SNR	Annotation
>	Citric acid	93.848		2	Acetylsalicylic_acid	24.257	2098.84 (1924.01, 2345.80)	
u 🗸				3	Salicylic_acid	8.898	718.02 (494.60, 873.36)	
				4	Ascorbic_acid	15.341	1955.63 (866.52, 2705.21)	
				5	Acetic_acid	16.137	20761.11 (20761.11, 20761.11)	

With the <sup>000</sup> button you can change the number of decimals used in the results table.

Simple	Mixture	Analysis						×
Analyze	() Update						Quick Report Vdvanced Report	Settings
Analy	sis Data	Result						
	# ^	Compound	Result (mg/	L) SN	R	Annotation		
	1	Imsp	6.35e-2	3571.18 (3571.18	8, 3571.18)			0.00
	2	Acetylsalicylic_acid	24.26	Result (mg/L)	2345.80)			
	3	Salicylic_acid	8.90	6.355e-2	3 <sup>.36)</sup>			<u>م</u>
	4	Ascorbic_acid	15.34	24.257	2705.21)			10
٢	5	Acetic_acid	16.14	8.898	1, 20761.11)			
•0	6	Citric_acid	93.85	15.341	9, 34324.75)	🕑 Ch	oose the number of de	? ×
				16.137	2	Result	s: 3 🌲	
				93.848			OK	Cancel



Use the **Smart cuts** tool <sup>SR</sup> to perform cuts in the areas between the multiplets. All cuts are restored when pressing the same button again.





The blue arrows  $\blacktriangle$   $\diamond$   $\checkmark$   $\checkmark$  allow you to navigate between the compounds. A view of the first multiplet in each compound can thus be obtained. To change the zoom factor on the viewed spectra you can click on the  $\overset{\circ}{}$  button to change the zoom value.



When mixture components come from a database (mixture created with database assistant), it is possible to stack analyte spectra with database records to review the spectral profile by clicking on the <sup>le</sup> icon.

## 6.2. Experiment suitable for PCA

When running an experiment that is "Suitable for PCA", the SMA dialog will present two buttons that will allow you to run the PCA and export the associated data to a CSV file. *A license for the Chemometrics plugin must be obtained to perform a PCA.* 

Simple M	xtı	ire Analysis							5 ×
Analyze	( Up	odate		Run PO	CA	Export as CSV	<b>O</b> Settings	Expert	
Analy	sis	Data Result							
		Result (mg/L)		1					
	1	Acetylsalicylic_acid	24.38						0.00
Ref	2	Salicylic_acid	8.89						<b>₫</b> ₽
•0	3	Ascorbic_acid	15.33						o (o
	4	Acetic_acid	16.13						
	5	Citric_acid	93.79						



If you click on **Run PCA**, a dialog with the original SMA data will open. *Please refer to the <u>Mnova manual</u> for more details about the PCA study.* 

When you click on **Export as CSV**, a new dialog with a set of parameters to choose from is opened. Select the rows you want to include in the CSV, then hit **OK** and save your report to the directory of your choice.

Simple M	lixture Analysis		e x			
Analyze	Update	Run PCA	1 Export as CSV Settings			
Analy	ysis Data Result					
	Result (mg/L)	1	2			
$\checkmark$	1 Acetylsalicylic_acid	24.38		2	<b>• r</b> = 1 = <b>r</b>	
Ref	2 Salicylic_acid	8.89	Select the parameters to export Active Spectrum:	Υ X	← → · ↑ I « By plugin > SMA > Results	→ ひ P Search Results
•0	3 Ascorbic_acid	15.33	Aspirin_A2_neu_NOESY_01 Aspirin_A2		Organize • New folder	III - 🕜
	4 Acetic_acid	16.13	SW: 500 RW: 2.4 NS: 128		Riesgos Laborales - For A Name Sales Materials	^ Date modified
	5 🗹 Citric_acid	93.79	Parameter		ø test	No items match your search.
			1     Image: Data File Name       2     Image: Title		<ul> <li>dest2</li> <li>desting and Validation E</li> <li>OneDrive</li> </ul>	
			3 Comment		Documentos	
			4 Origin		Imagenes	
			5 Owner		3D Objects	
			6 Site		Desktop	
			7 🗹 Instrument		File name: SMAReport Aspirin C	
			8 Author		Save as type: *.csv	
			9 Solvent			
			10 Temperature	•		
			ок	Cancel	▲ Hide Folders	3 Save Cancel
						s > By plugin > SMA > Results ame



#### 6.3. Revision and update

SMA results can be easily revised and updated. For instance, you can adjust the multiplet ranges on the spectrum and click on the **Update** button Storedo the analysis. This can be very useful if peak positions vary slightly from sample to sample.

You can also update the multiplet ranges used for the calculation. To do so, double-click on the compound of interest in the results table. The SMA Compound detail dialog will open. Check/uncheck the ranges you want to include/exclude, respectively, then **Apply changes**. The mixture will therefore be reanalyzed and the results updated in the results table.

		,,								×							
e	(O) Update					Quick R	] eport \dv	anced Report	Ö: Settings	1 Expert							
al	sis Data	Result															
Z	# ^	Compo	und	Re	sult (mg,	/L)		SNR		2							
	1	TMSP		6.35e-	2		5616.89	(5616.89, 5	5616.89)	0.00							
	2	Acetylsalia	ylic_acid	24.24			3334.97	(3049.81, 3	3680.88)	<b>G</b> ₽							
	3	Salicylic_a	da 1	Dou	ıble-	clic	1134.38	(783.87, 13	373.12)	410							
	4	Ascorbic_	Ascorbic_acid 15.33 3100						4288.80)	l							
	5	SMA Cor	SMA Compound Details										1	2 X			
0	6							6	Apply (	Thanges	Q Lindate Mixture						
	4		<i>~</i>						Apply	andinges	oputernixture	Ana	lyzing	Mixture			
		Name:		Ace	tylsalicyli	ic_acid		Spec. Nº:		1		4		83%			
		Valid Lin	nit From:		nige			To:		100.10				Cancel			
		Type:		Con	npnd.			Formula									
		Type: Integrati	on Metho	Con d: Sun	npnd. n			Formula (((I1/NN1)	+(I2/NN2)	+(I3/NN3)+(I	4/NN4))/4)*CCF						
		Type: Integrati Dimensio	on Metho ons:	Con d: Sun 1D	npnd. n			Formula (((I1/NN1)	+(I2/NN2)·	+(I3/NN3)+(I	4/NN4))/4)*CCF	Simple 1	/lixture /	Analysis			
		Type: Integrati Dimensio	on Metho ons:	Con d: Sun 1D	npnd.			Formula (((I1/NN1)	+(I2/NN2)	+(I3/NN3)+(I	4/NN4))/4)*CCF	Simple N	Aixture a	Analysis			¢
		Type: Integrati Dimensio	on Metho ons:	Con d: Sun 1D	npnd.			Formula (((I1/NN1)	+(I2/NN2)·	+(I3/NN3)+(I	4/NN4))/4)*CCF	Simple N	Vixture V Update	Analysis	Quic	Ck Report Vdvanced Report	<b>O</b> Settings
		Type: Integrati Dimensio - Ranges - Active	on Metho ons: From	d: Sun 1D	Mult.	J's	NN	Formula (((I1/NN1))	+(I2/NN2)·	+(I3/NN3)+(I [conc]	4/NN4))/4)*CCF Pattern	Simple I Analyze Analyze	Vixture v Update ils Data	Analysis	Quit	Ch Report I dvanced Report	Settings
		Type: Integrati Dimension - Ranges Active	From 7.950	Con Sun 1D To 8.000	npnd. n Mult. dd	J's	NN 1	Formula (((I1/NN1))	+(I2/NN2) SNR 3423.35	+(I3/NN3)+(I [conc] 23.49	4/NN4))/4)*CCF	Simple I Analyze	Mixture d Update ils Data # ^	Result Compound	Quid Result (mg/L) 6 35-2	ck Report Vdvanced Report	Settings
		Type: Integrati Dimension Ranges – Active V	From 7.950	Con Sun 1D To 8.000 7.720	Mult. dd	J's	NN 1	Formula (((11/NN1)) Integral 369.80 402.18	+(I2/NN2)- SNR 3423.35 3049.81	+(I3/NN3)+(I [conc] 23.49 25.54	4/NN4))/4)*CCF	Simple I Analyze Analyze	Mixture Update is Data # ^ 1	Analysis       Result       Compound       TMSP	Que Result (mg/L) 6.35e-2	(1) (1) (1) (1) (1) (1) (1) (1)	Settings
		Type: Integrati Dimension	From 7.950 7.420	Con Sun 1D To 8.000 7.720 7.480	Mult. dd td	J's	NN 1 1 1	Formula ((((11/NN1)) Integral 369.80 402.18 404.14	+(I2/NN2)- <b>SNR</b> 3423.35 3049.81 3680.88	(I3/NN3)+(I [conc] 23.49 25.54 25.67	4/NN4))/4)*CCF	Simple I Analyse	Mixture d Update is Data # ^ 1 2	Result Compound I TMSP	Quit Result (mg/L) 6.35e-2 10 24.38 5	(Constant)      (Constant)	Settings 616.89) 45424.33
		Type: Integrati Dimension - Ranges Active V V	From 7.950 7.420 7.200	Con Sun 1D To 8.000 7.720 7.480 7.260	Mult. dd td	J's	NN 1 1 1 1 1	Formula ((((11/NN1)) Integral 369.80 402.18 404.14 350.60	+(I2/NN2)- <b>SNR</b> 3423.35 3049.81 3680.88 3185.82	( <b>I</b> CONC) ( 23.49 25.54 25.67 22.27	4/NN4))/4)*CCF Pattern	Simple N Analyse Analyse	Vixture V Update iis Data # ^ 1 2 3	Result Compound I TMSP Salicylic,acid	Qui Result (mg/L) 6.35e-2 24.38 <b>5</b> 8.89 15.22	Image: Signal and Sig	Settings 516.89) 45424.37 73.12)
		Type: Integrati Dimension Ranges Active V V V	From 7.950 7.420 2.340	Con Sun 1D To 8.000 7.720 7.480 7.260 2.380	Mult. dd td td dd s	J's	NN 1 1 1 1 3	Formula ((((11/NN1)))) Integral 369.80 402.18 404.14 350.60 1177.48	+(I2/NN2)- SNR 3423.35 3049.81 3680.88 3185.82 45424.37	(conc) ( 23.49 ( 25.54 ( 22.27 ( 24.93 (	4/NN4))/4)*CCF Pattern	Simple 1 Analyse Analyse	Mixture A Update is Data # ^ 1 2 3 4	Result Compound TMSP Salicylic,acid Ascorbic,acid	Que Result (mg/L) 6.35e-2 24.38 8.89 15.33 16.13	SNR           5616.89 (5616.89, 56           11752.85 (3049.81, 4           1134.38 (783.87, 137           3100.76 (1373.47, 42           236617 (1373.47, 42	Settings 616.89) 45424.31 73.12) 288.80) 32961
		Type: Integrati Dimension Ranges Active V V V V Results	From 7.950 7.420 7.200 2.340	Corror Sunna To 8.000 7.720 7.480 7.260 2.380	Mult. dd td td dd s	J's	NN 1 1 1 1 3	Formula (((11/NN1) 369.80 402.18 404.14 350.60 1177.48	+(I2/NN2)- <b>SNR</b> 3423.35 3049.81 3680.88 3185.82 45424.37	( <b>conc)</b> 23.49 25.54 22.67 22.27 24.93	4/NN4))/4)*CCF Pattern	Simple I Analys Analys	Vixture J Update iis Data # ^ 1 2 3 4 5 6	Analysis       Result       Compound       Image: TMSP       Acetylsalkcylic,acid       Salicylic,acid       Ascorbic,acid       Cacid,acid	Que Result (mg/L) 6.35e-2 424.38 8.89 15.33 16.13 0.2 70	SNR           5616.89 (5616.89, 56           11752.85 (3049.81, 4           1134.38 (783.87, 137           3100.76 (1373.47, 42           32961.71 (32961.71, 32961.71)	Settings 516.89) 45424.31 73.12) 288.80) .32961.1 54065
		Type: Integrati Dimension Ranges Active V V V Results Averag	From 7.950 7.420 2.340	Corr d: Sun 1D To 8.000 7.720 7.480 7.260 2.380	Mult. dd td dd s	J's	NN 1 1 1 1 3 SNR A	Formula (((11/NN1)))	+(I2/NN2)- SNR 3423.35 3049.81 3680.88 3185.82 45424.37 334.97	(I3/NN3)+(I [conc] 23.49 25.54 25.57 22.27 24.93 SNR Range	Pattern : [81, 3680.88]	Simple N Analyze Analyze	Viixture Vii	Result Compound TMSP Salicylic,acid Acetylsakcylic,ac Salicylic,acid Acetic,acid Citric_acid	Que Result (mg/L) 6.35e-2 24.38 8.89 15.33 16.13 9.79	SNR           5616.89 (5616.89, 56           11752.85 (3049.81, 4           1134.38 (783.87, 137           3100.76 (1373.47, 42           32961.71 (32961.71, 32961	Settings 616.89) 45424.31 73.12) 288.80) . 32961.1 . 54065.0



Once you have applied changed to a compound, the **Update Mixture** button will become active and will allow you to save those changes to the mixture used for the analysis.

ls			Mixt	ure Crea	tion/Edition											
			-Mixt	ure				Compou	nd							
	V Apply	Changes 💱 Update Mixture	Nar	ne: A	Aspirin Exp	Units: mg/L	<b>•</b>		ave Con	pound		Add From	<mark>샷</mark> n Docum	ent DB	Sistan Assistan	t
etylsalicylic_acid	Spec. Nº:	1	Co	mpound	List			Compo	und Deta	ils						
ange	Mol. Weight:	180.16			Compound	Type	+	Compo	und Forn	nula						
	To:			] ⊿ 1	TMSP	Reference	/	Forr	nula —			_				
mpnd.	Formula (((I1/NN1)+(I2/NN2	)+(I3/NN3)+(I4/NN4)+(I5/	6	✓ 2	Acetylsalicylic_ac	id Compnd.		Moi	1/NN1)+	Concent	2)+(13/	±q. ▼ NN3)+(I4	 /NN4)+()	Apply To Al	U 🕺   DF	<b>***</b>
m	NN5))/5)*CCF	, (,, (-,, (,		⊻ 3	Salicylic_acid	Compnd.	▼		-,,-	(,	.,		,,			
				⊻ 4	Ascorbic_acid	Compnd.										
				⊻ 5	Acetic_acid	Compnd.		Add	ranges f	rom curi	ent Spe	ectrum – r	Pattern	Recognition		
				⊻ 6	Citric_acid	Compnd.			<b>₩</b>		NS.		/	Ö		
								Activ	e From	То	Mult.	J's	NN	Pattern		+
									7.420	7.480	td	7.6,1.2	1		- 1	-
					A				7.200	7.260	dd	8.2,1.2	1			
				N	nuitiplet ra	ange inc	iude		2.340	2.380	s		3		-	

## 6.4.Reporting

Click on **Quick Report** to generate the report type you configured in the **Settings** > **Report** > **Quick** menu item. An example of a quick report pasted into an Mnova document is provided below.

spirin* ×								Pa	ges	D now NOECY O		
AREPORT									L. ASpinin_A.			8
nple Parameters:									5 1 5 18	1111	1	
Sample Weight: 500									Salicylic_acid_3 7.52	1.000		
Reference Weight: 2.4										Salicylic_acid_3 (m) Asterbic_acid_ 6.00 4.08	t (640) Konstratovit (, acid, 5 (2) 2, 6	
tom Parameters:									Acitybalicylic 7.4	acid_3(u) Ascerbic_acid_1(d) As	cobic_acid_3(m) 0 mic_acid_2(d) 4 artic_acid 376 283 218	d (s) TMSP (s) 0:00
ults:									Salicylic_acid_1(dd) 7.87	haleyle, acid, 4 (dd) 7.23	28	
							- 11					
Compound	Result(mg/L)	SNR Mean (min, max)		Ranges		Annotations						
Acetyls alicylic_acid	24.394	7408.83 (1924.01, 28647.82)	From To Mult	NN Integral	SNR				1. 1. 1			
			7.9500 8.0000 dd	1 389.78	2158.89							
			7.4200 7.4800 td	1 404.18	2345.80				481 80 79 78 77 76 75 7	4 73 72 73 70 69 50 49 42 41 4	38 37 3 63 1 30 29 28 27 24 23 21 2	
			7.2000 7.2600 dd	1 350.67	1966.64					1H	(ggm)	
			2.3400 2.3800 s	3 1177.53	28647.82				2.			
Salicylic_acid	8.898	718.02 (494.60, 873.36)	From To Mult	NN Integral	SNR				LMAREPORT			
			7.8500 7.9000 dd	1 143.25	786.11				Reference Concentration 1.0 Secole Weight Titl			
			7.4900 7.5500 ddd	1 141.12	494.60				Reference Weight: 2.1 Seton Parameters			
			6.9500 7.0200 m	2 271.37	873.36				PIRO Results:			
As corbic_acid	15.341	1955.63 (866.52, 2705.21)	From To Mult	NN Integral	SNR				Compound Party and the party	Resulting QQ         SHR Mean (min, max)           24.334         7425430 (1907.01, 3004732)	Ranges	Amoteliane
			4.9300 4.9600 d	1 194.50	2295.17						7.600 6.000 66 1 26676 256.89 7.600 7.700 66 1 400.21 50.01	
			4.0500 4.1200 000	2 518 57	2705.21						7.4200 7.4800 M 1 404.16 2245.60 7.2000 7.2000 Ad 1 250.07 1666.64 3.300 3.2000 a 9 407.63 8447.63	
Acetic acid	16.137	20761.11							Sala ya ah	8.660 718.02 (194.60) 875.36)	Run         To         Mat         NN         Magai         SNR           7.600         7.600         6d         1         14325         36.11	
			2 0700 2 1000 s	NN Integral 3 761.81	20761.11						7.680 7.580 666 1 14112 64.60 6.6800 7.080 m 2 271.37 673.36	
Citric add	93.848	33820 22 (32915 69, 34324 75)							Austic, ald	153H 1855B (866.9, 20521)	Run         To         Muit         NN         Imageal         SNR           4.8200         4.0000         d         1         104.50         205.17	
0.0.0_000			2 9200 3 0600 d	2 2953.29	32915.69				-	10.17 Dama 44	12000 11200 add 11 27076 86032 37000 34000 m 2 01657 270521	
			2.7600 2.8800 d	2 2953.90	34324.75					2018.11	Run         To         Mult         NN         Imagest         DKR           2.0100         2.0200         a         3         161.81         20761.11	
										AND 27 (101140(19(37.73)	Hum         to         Hum         Hill         Hemgenial         DERR           2.6020         3.0620         d         2         2653.38         31915.68           2.7500         2.8620         d         2         2653.88         313015.63	
							V					



Click on **Advanced reports** to generate the output files you configured in the **Settings** > **Report** > **Advanced** menu item. All associated files will be saved in the directory you specified.

SMA > Results

Name

- SMAReport\_Aspirin\_C
- SMAReport\_Aspirin\_C
- SMAReport\_Aspirin\_C
- SMAReport\_Aspirin\_C
- SMAReport\_Aspirin\_C

You can find examples of such advanced reports below:

## Mnova report



## CSV report

	A	В	С	D	E	F	G	н	1	J	К	L	м	N	0	Р	0	R	S
1	Mixture Info:																-		
2		Library	Mixture name	Description	Units														
3		New Library	Aspirin Exp	Determination of	Ascorbic acid	Citric acid	Salicylic a	Acetic aci	d										
4	Intermediate analysis	mg/L																	
5		Compound List:																	
6			Checked	Compound	Туре	Mol.Weight	Spectrum	Formula	Dimensio	r Integratio	Options	Ranges Frc R	anges To	Ranges M	Ranges J	Ranges NN			
7			yes	TMSP	Reference	116.07	1 1	((NN1/I1))	1D	Sum		-0.1	0.1			9			
8			yes	Acetylsalicylic_a	Compnd.	180.16	5 1	(((I1/NN1)	1D	Sum	Verbose P	8	7.95	dd	10.8	1.7	1		
9												7.72	7.65	ddd	8.1	7.8	1.7	1	
10												7.48	7.42	td	7.6	1.2	1		
11												7.26	7.2	dd	8.2	1.2	1		
12												2.38	2.34	s		3			
13			yes	Salicylic_acid	Compnd.	138.12	2 1	(((I1/NN1)	1D	Sum	Verbose P	7.9	7.85	dd	7.9	1.85	1		
14												7.55	7.49	ddd	8.3	7.2	1.8	1	
15												7.02	6.95	m		2			
16			yes	Ascorbic_acid	Compnd.	176.13	1	(((I1/NN1)	1D	Sum	Verbose P	4.96	4.93	d	1.9	1			
17	•											4.12	4.05	ddd	7.1	6	1.8	1	
18												3.8	3.7	m		2			
19	1		yes	Acetic_acid	Compnd.	60.05	5 1	((I1/NN1))	1D	Sum	Verbose P	2.07	2.1	s		3			
20	1		yes	Citric_acid	Compnd.	192.13	3 1	(((I1/NN1)	1D	Sum	Verbose P	3.06	2.92	d	15.7	2			
21												2.88	2.76	d	15.7	2			
22	Sample Parameters:																		
23	i	Reference Concentration																	
24			1																
25	Custom Parameters:																		
26																			
27	·																		
28	Metadata:																		
29																			



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## **HTML report**

SMA RE

												<u> </u>	1
Mixture Info													
Library:	New Library												
Mixture	name : Aspirin Exp 1												
_													
Descrip	tion :												
Units : r	ngl.												
Compos	und List:												
Chec	ked Compound	Type			Ra	inges		Mol.Weight	Spectrum	Formula	Dimension	Integration	I
	THED	Defenses	From	50	Mult	3	NN	116.0700		00044100000	10	Sum.	
	I Imar	Poplarence	-0.1	0.1			9	110.0700		(()(()()))(()())	10	ourn	
			From	To	Mult	3	NN						
			7.950	8.000	66	108,57	1						
	Acetylsalicylic acid	Compost	7.650	7.720	666	81,78,17	1	180 1600	1	((()1/NN1)+(12/NN2)+(13/NN3)+	10	Sum	
		- Comprise	7.420	7,480	td	7.6,1.2	1	100.1000		(14/NN4))/4)*CCF	10	- Courte	
			7.200	7.250	66	82,12	1						
			2.340	2.360			3						
			From	To	Mult		NN						
		C	7.9	7.85	00	7.9,185	1	400 4000			40		
	Sancync_acid	Compria	7.55	7,49	686	8.3,7.2,1.8	1	138.1200	1	(((11/NN1)+(12/NN2)+(13/NN3))/3)/CCF	10	Sum	
			7.02	4.95			2						
			fine	To	Mult		-						
			4.95	493	4	1.0	1						
	Ascorbic_acid	Comprid.	4.12	4.05	000	7.16.0.18	1	176.1300	1	(((11NN1)+(12/NN2)+(13/NN3))/3)*CCF	1D	Sum	
			3.80	3.70			2						
		-											ł
	Acetic_acid	Comprid.	From	Ye	Mult	3	NN	60.0500	1	(((1/NN1))*CCF	1D	Sum	
	-		2.07	2.19	5		3						L
			From	50	Mult	3	NN						
	Citric_acid	Compnd.	3.05	2.92	6	15.7	2	192.1300	1	()()1/NN1)+((2/NN2))/2)*CCF	1D	Sum	
			2.88	2.76	d	15.7	2						

#### Sample Parameters:

Reference Concentration: 1.0

**Custom Parameters:** 

#### Metadata:

#### Spectrum Adquisition Parameters:

ectrum Adquisition Parameters: Data, Jila, Jtame: X.2014/20140/101/Asprin, A2\_neu\_01/Asprin,A2\_neu\_NOESY\_01.6.04 Tite: Asprin,A2\_neu\_NOESY\_01 Commet: Asprin,A2\_neu\_NOESY\_01 Commet: Asprin,A2\_neu\_NOESY\_01 She: Instrument: vinnes Author: She: Instrument: vinnes Author: Prote: C0 Prote:

#### Results:

Compound	Result(mg/L)	SNR Mean (min, max)				Ra	nges		Annotati
THEO	63514.3	6448.00	From	To	Mult	NN	Integral	SNR	
1MSP	0.3310-2	3010.09	-0.1000	0.1000	1	9	141.71	5616.09	
			From	To	Mult	NN	Integral	SNR	
			7.9500	8.0000	05	1	309.80	3423.35	
Acetylsalicylic_acid	24.240	240 3334.97 (3049.81, 3680.88)	7.6500	7.7200	м	1	402.18	3049.81	
			7.4200	7.4800	10	1	404.14	3680.88	
		7.2000	7.2500	05	1	350.60	3185.82		
							and and a second	110	
	cylic_acid 8.891 1134.38 (783.87, 1373.12)	Prom	10	Mult.	NN	Integral	SNOC		
Salicylic_acid		7.8500	7.9000	00	,	140.26	1245.15		
			7.4927	7.5500	000	1	141.01	783.87	
			6.9500	7.6200	-	2	271.42	1373.12	
			From	To	Mult	NN	Integral	SNR	
Annuality savid	46.333	2100 78 (1272 17 1208 80)	4.9300	4 9500	d	1	194.45	3640.00	
Ascoroic_acio	10.332	3100.70 (1373.47, 4200.00)	4.0500	4.1200	666	1	279.52	1373.47	
			3.7000	3 8000	85	2	518.59	4268.00	
Acate and	10.100	20064 74	From	To	Mult	NN	integral	SNR	
Acetoc_acid	10.128	32001.71	2.0790	2.1000	1	3	761.85	32961.71	
			From	To	Mult	NN	Integral	SNR	
Citric_acid	93.793	53133.59 (52202.16, 54065.02)	2.9200	3.0500	d	2	2953.41	52292.16	
CHINE_BOO			3 7455						1

Options

Verbose Pattern Recognition Algorithm

Verbose Pattern Recognition Algorithm

Verbose Pattern Recognition Algorithm

Verbose Pattern Recognition Algorithm Verbose Pattern Recognition Algorithm