

Mnova Gears 2.5

USER MANUAL



Document Number

P/N 236 R3



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Mnova Gears is a software suite that can be used to build automation workflows for your analytical data analyses (NMR, MS, IR, etc.). It is built around the concept of plugins called "bricks" that execute specific tasks in a fully automatic mode from data pickup and processing to results reporting, saving, and databasing. In addition to full automation, Mnova Gears allows for the customization of every step in your workflow to adapt it to your specific needs.

Mnova Gears comes in two flavors:

- The **Mnova Gears** product, suitable for the processing large datasets in batches or in real time.
- The **Mnova MyGears** product, that allows you to build and run workflows based on single samples. MyGears is best suited to small-scale analyses, where the overhead of manually opening data is not significant but the benefits of automating processing and reporting are hugely so.

Several **Mnova Gears bricks** are currently available that can be used as standalone components or in combination in a workflow.

Please check our website page for more details about available bricks and don't hesitate to contact us to discuss your custom automations!





Apart from running automated workflows, Mnova Gears allows you to operate in a machine-to-machine mode* which means that you can run one or several workflows on your datasets with minimal human intervention. In this case, datafiles and workflow parameters must be provided by the user or an external program so that Mgears can operate on them.



*Requires Machine-to-machine license



2. Installation

Once you receive your software or plugin license, open Mnova and drag-and-drop your license file into the application. Then, go to the **File** tab > **Advanced Plug-ins.** A new window will open. In the **Available** tab, select the **Mnova Gears plugin** and click on **Install**.



A window will open to prompt you to restart the application. Click on **OK**.



Close Mnova and open it again.



Check that the plugin has been installed correctly. All installed plugins will be listed in the **Installed** tab (File > Advanced Plug-ins).

| vailable Updates I | installed | | | |
|---|-----------------------|-------------------|---------|--|
| Name ^ | Default Version | Installed Version | <u></u> | |
| 🗌 Mnova Batch qNMR | 3.0.0.6161 | 3.0.0.6161 | 0 | |
| Mnova Gears | 2.1.0.6269 | 2.1.0.6269 | | |
| Mnova QC Profiling | 1.1.0.6088 | 1.1.0.6088 | | |
| Mnova SMA | 2.0.7.5698 | 2.0.7.5698 | | |
| Mnova Screen | 1.3.3.5178 | 1.3.3.5178 | | |
| Mnova qNMR | 3.0.0.6273 | 3.0.0.6273 | | |
| | Mnova QC I | Profiling | | |
| Description: QC | Profiling for Mgears | | | |
| Installed Version: 1.1 | .0.6088 | | | |
| Release Date: Fri | day, 17 July 2020 | | | |
| Requires: MestReNova (>=14.2.0-24628) Mnova Gears (>=2.1.0.6044) | | | | |
| <i>Requires:</i> Me Mr | iova Gears (>=2.1.0.6 | 6044) | | |

If installation has been successful, you will find Mgears, Mgears Viewer, MyGears and MyGears Workflows in the Mnova ribbon under the **Automation** section.





Note. If the **Automation** tab is not visible in the Mnova Ribbon, go to **Options>Customize**..., and manually add **Automation** to the ribbon.

| Mes Elucidation $\underline{U} \mid \mathbf{X}_2 \mid \mathbf{X}^2$ | tReNova Chemometrics | Binding Automation AX AX Insert Add Object Signature Insert Digital Signature | Quantitation | Style Customize Customize | Options |
|---|--|---|--|---|---------|
| b.com | Options Quick Access Toolba Customize Ribbon | r Customize the Ribl Choose commands from: All Commands | bon Customize the Ribl Customize | bon: ass] [Mass] g [El gg [C ion tion v u kename Reset | |
| | Reset | | O | K Cancel | |

3. Mgears dialog

The Mgears dialog has a simple and straightforward design that includes:

- six tabs, each allowing the setup of a single part of the workflow
- a set of commands to control analysis

| Tab | Description | Command | Description |
|--------------|---|-----------------|--|
| 🛃 Input | Choose analysis input | Resume | Load resume file and restart data processing |
| 💝 Processing | Customize processing or enable advised processing | Load Settings | Load all mgears settings from OS registry |
| Plugins | Select analysis plugins and configure plugin settings | Save Settings | Save all mgears settings to the OS registry |
| 🔀 Design | Apply layout template to your Mnova analysis result | import Settings | Load all mgears settings from file |
| 📑 Output | Choose repository to save your data and output files | Export Settings | Save all mgears settings into a file |
| Settings | Configure Mgears general settings | Cancel | Close mgears |
| | | Run | Start the automation |

As represented by the dialog sections, a full Mgears workflow will start with the selection of the input data and then go to the rest of the processing, analysis, and reporting configuration. Alternatively, when using MyGears, the workflow starts a step further on, at the processing tab, since the user should already have the relevant data file opened in Mnova.



In the following sections, we will detail each tab of the Mgears dialog and the many configuration options each tab offers.



3.1. Input

Mgears can handle input data saved on **Disk** directories, in a database (**DB**), or acquired in **Real Time** from a disk or from a network drive. These three modes are visible on the left-hand side of the Mgears dialog.

| ♥ Mnova Gears | | | | | |
|---------------|---|--|--|--|--|
| ÷ | Input 😵 Processing 🚱 Plugins 🔀 Design 💽 Output 🔅 Settings | | | | |
| Disk | 2 Using Automatic Detection | | | | |
| Ô | Main Directory: | | | | |
| | Optional Directory: | | | | |
| a a | | | | | |
| <i></i> | IH I3C I9F HSQC HMBC | | | | |
| ime | NOESY TOCSY ROESY H2BC COSY | | | | |
| ्रे Real T | GC/LC/MS Chromatography UV/IR/Raman/Fluorescence Mnova Documents Or | | | | |

Each mode has a specific configuration that will allow you to adapt Mgears to your data and handle your analysis appropriately.

3.1.1. Data from disk

To analyze input data from your **Disk**, click on ... and select the **Main directory** in which your data files are saved. If part of your input data is saved in another folder, you can additionally select and add that folder in the **Optional directory**.





3.1.1.1. Mask manager

Click on this button to open the **Mask Manager** where you can edit and add new masks for your experiment files to be automatically detected by Mgears. The following default masks are available:

- NMR (FID): fid,ser,*.jdf
- NMR (Spectrum): 1r, 2rr
- LC/GC/MS: _FUNC001.DAT, MSD1.MS, analysis.baf, _FUNC001.IDX, *.cdf, *.sms, *.ch, *.lcd, *.mcds
- Chromatography: *.cdf, *.asc
- UV/IR/Raman/Fluorescence: *.jdx, *.spa, *.spc
- Structures: *.mol, *.sdf

If your data mask is not in the list above, type it in the corresponding box for the experiment type then click **OK** to save your changes. See example in the image below.

| Input | | | | |
|---------------------------|---------------------------------------|--------------------------------------|--|-------------------|
| Name | Туре | | | |
| Compound1 | MOL File | | | |
| Compound2.smi | SMI File | | | |
| Compound3.sdf | SDF File | | | |
| Defaults masks | | | | |
| | | 🐑 Using Automatic | | - |
| NMR(FID): | fid.ser.*.idf | Main Directory: | C:/Lisers/Lisuario/Desktop/Datasets/Masks/Input | |
| NMR(Spectrum): | 1r. 2rr | Optional Directory: | | |
| GC/LC/MS: | X * cdf * sms * ch * lcd * mcds | | Experiments Found: 2 ? X | |
| Chromatography: | * cdf * asc | | List of detected experiments: | |
| LIV/IR/Raman/Fluorescence | * idv * spa * spc | | Structure: C:/Users/Usuario/Desktop/Datasets/Masks/Input/Compound1.mol | |
| Structures: | * mol * cdf | Advanced Options | Structure: C:/Users/Usuario/Desktop/Datasets/Masks/Input/Compound3.sdf | |
| | | Allow More than Experiment Selection | One Experi | Regular E |
| Edited masks | | | | |
| Standard Formats | | Using Automatic | Detection Experiments Selection | |
| NMR(FID): | fid,ser,*.jdf | Main Directory: | C:/Lisers/Lisuario/Deskton/Datasets/Masks/Input | |
| NMR(Spectrum): | 1r, 2rr | Optional Directory: | | |
| GC/LC/MS: | DX, *.cdf, *.sms, *.ch, *.lcd, *.mcds | | Construction Const | |
| Chromatography: | *.cdf, *.asc | > | List of detected experiments: Experiment: COMPOUND1 | |
| UV/IR/Raman/Fluorescence | : *.jdx, *.spa, *.spc | | Structure: C:/Users/Usuario/Desktop/Datasets/Masks/Input/Compound1.mol Experiment: COMPOUND3 | |
| Structures: | *.mol, *.sdf, *.smi | Advanced Options | Structure: C:/Users/Usuario/Desktop/Datasets/Masks/Input/Compound3.sdf Experiment: COMPOUND2 | |
| | √≷ Type ー | Master File: | Structure: C:/Users/Usuario/Desktop/Datasets/Masks/Input/Compound2.smi | Tag with |
| | | Allow More than (| One 1000 | Regular E |
| | | Experiment Selection | Mo 30 Dec | 1969 • To: |
| | | | OK | |



| Input | Defaults masks | | |
|---------------------|---|--|---|
| CHRO001.DAT | Standard Formats | | |
| | NMR(FID): | fid,ser,*.jdf | |
| J_CHROMS | NMR(Spectrum): | 1r, 2rr | |
| 🕤 _extern | GC/LC/MS: | _FUNC001.DAT, MSD1.MS, analysis.baf, _FUNC001.IDX, *.cdf, *.sms, *.ch, *.lcd, *.mcds | |
| FUNC001.DAT | Chromatography: | *.cdf, *.asc | |
| FUNC001.IDX | UV/IR/Raman/Fluorescence: | *.jdx, *.spa, *.spc | |
| | Structures: | *.mol, *.sdf, *.smi | |
| FUNC001.STS | | | |
| L _FUNC002.DAT | | | |
| LETTER FUNC002.IDX | eriments Selection | | |
| LETTER _FUNC002.STS | ktop/Datasets/By Plugin/Chrom RO/Dataset/I | Input | |
| LFUNC003.DAT | Sector Experiments Found: 10 | ? × | |
| L FUNC003.IDX | List of detected experiments | s: | |
| FUNCTNS | MS: C:/Users/Usuario/Desktop/Datase Experiment: REACTION-02 | ets/By Plugin/Chrom RO/Dataset/Input/Reaction-01.raw/_FUNC001.DAT | |
| | MS: C:/Users/Usuario/Desktop/Datase Experiment: REACTION-03 | ets/By Plugin/Chrom RO/Dataset/Input/Reaction-02.raw/_FUNC001.DAT | V |
| HEALLER | MS: C:/Users/Usuario/Desktop/Datase | ets/By Plugin/Chrom RO/Dataset/Input/Reaction-03.raw/_FUNC001.DAT | |
| | MS: C:/Users/Usuario/Desktop/Datase | ets/By Plugin/Chrom RO/Dataset/Input/Reaction-04.raw/_FUNC001.DAT | |
| | th S: C:/Users/Usuario/Desktop/Datase Experiment: REACTION-06 | ets/By Plugin/Chrom RO/Dataset/Input/Reaction-05.raw/_FUNC001.DAT | |
| | | Creation Date 🔻 | |
| | | UK | |

If the data file or folder incorporates both the experiment name and the extension (e.g., files named "C923m3.raw" or a folder named "A8723.D"), Mgears is capable of identifying the extension and excluding it from the experiment name. This functionality is facilitated by the list of masks accessible in the expert settings section. You have the flexibility to modify the default list and include your specific extensions, as illustrated in the image below.

| Input | Defaults masks | Edited masks |
|--|---|---|
| A8723.D B2332.D C1197.D | Expert > Masks for Special Extensions: ol,sdf.jdf.als.jcamp,dx.jdx.jcm,rpt.d.sms,xms,xmff,raw,lcd,cdf,mcds] Back to Default | Expert Special Extensions: [tjdf,als,jcamp,dx,jdx,jcm,rpt,d,sms,xms,wiff,raw,lcd,cdf,mcds,eqp] Back to Defaul Type |
| D3892.D | /Desktop/Datasets/Masks/Expert | /Desktop/Datasets/Masks/Expert |
| E7351.D | Separate Second: 11 ? X | Contract Experiments Found: 11 ? X |
| F7900.expl G1826.expl G8278.expl H8663.expl I5211.expl J6232.expl | Ekst of detected experiments: Type:Lent: 17990-LENE Experiment: 8329-LENE Experiment: 8339 E | List of detected experiments: Laperiaent: 17900 MS: C:/Very (Usuario)Deixtop/Datasets/Masks/Expert/F7900.expl/_FUNC001.DAT Taperiaent: 6826 MS: C:/Very (Usuario)Deixtop/Datasets/Masks/Expert/68278.expl/_FUNC001.DAT Terrer: Usuario/Deixtop/Datasets/Masks/Expert/68278.expl/_FUNC001.DAT Terrer: Usuario/Deixtop/Datasets/Masks/Expert/68278.expl/_FUNC001.DAT Terrer: Usuario/Deixtop/Datasets/Masks/Expert/19221.expl/_FUNC001.DAT MS: C:/Users/Usuario/Deixtop/Datasets/Masks/Expert/19232.oxpl/_FUNC001.DAT MS: C:/Users/Usuario/Deixtop/Datasets/Masks/Expert/19232.0/_FUNC001.DAT MS: C:/Users/Usuario/Deixtop/Datasets/Masks/Expert/19232.0/_FUNC001.DAT MS: C:/Users/Usuario/Deixtop/Datasets/Masks/Expert/19232.0/_FUNC001.DAT MS: C:/Users/Usuario/Deixtop/Datasets/Masks/Expert/19232.0/_FUNC001.DAT MS: C:/Users/Usuario/Deixtop/Datasets/Masks/Expert/19232.0/_FUNC001.DAT MS: C:/Users/Usuario/Deixtop/Datasets/Masks/Expert/19232.0/_FUNC001.DAT MS: C:/Users/Usuario/Deixtop/Datasets/Masks/Expert/19352.0/_FUNC001.DAT MS: C:/Users/Usuario/Deixtop/Datasets/Masks/Expert/19352.0/_FUNC001.DAT MS: C:/Users/Usuario/Deixtop/Datasets/Masks/Expert/E7351.0/_FUNC001.DAT MS: C:/Users/Usuario/Deixtop/Datasets/Masks/Expert/E7351.0/_FUNC001.DAT MS: C:/Users/Usuario/Deixtop/Datasets/Masks/Expert/E7351.0/_FUNC001.DAT |

To undo any changes you introduce, you can click on **Back to Default** and then on **OK**.



| *.new, *.ext | |
|---------------------------------|---|
| Jsuario/Desktop/Datasets/Custom | Script.qs |
| ОК | Cancel |
| | *.new, *.ext Jsuario/Desktop/Datasets/Custom OK |

Top Tip! Whenever you select your input data you can use the **Automatic inspection** button \mathbb{E} to preview the detected data in your directories that will be used by Mgears to execute the analysis.



3.1.1.2. Advanced options

Several advanced options are available to give you more flexibility at the time of selecting your input data:

Master file: If datasets are saved at different locations on the disk, it is possible to use a Master file with the list of paths to the directories with spectra and molecule files. A master file can be a .<u>txt</u> or a .<u>csv</u> file with an absolute path on each row.

| 1 | C:\Users\Downloads\16089\subset_1\SDH-0001_1_04_12_18_DMSO_1.raw |
|---|--|
| 2 | C:\Users\Downloads\16089\subset_1\SDH-0001_1_04_12_18_PBS_2.raw |
| 3 | C:\Users\Downloads\16089\subset_1\SDH-0001_1_04_12_18_PBS_3.raw |
| 4 | C:\Users\Downloads\16089\subset_1\SDH-0001_1_04_12_18_PBS_4.raw |
| 5 | C:\Users\Downloads\16089\subset_1\SDH-0002_1_04_12_18_DMSO_1.raw |
| 6 | C:\Users\Downloads\16089\subset_1\SDH-0002_1_04_12_18_PBS_2.raw |
| 7 | C:\Users\Downloads\16089\subset_1\SDH-0002_1_04_12_18_PBS_3.raw |
| 8 | C:\Users\Downloads\16089\subset_1\SDH-0002_1_04_12_18_PBS_4.raw |



Tick the **Master file** option then click on ... to add your master file.

| Advanced Options | | | |
|-------------------|--|--------------------------------|----------|
| | | | V |
| ✓ Master File: | C:/Users/Usuario/Desktop/Datasets/MasterFile.csv | | |
| Main SDF File: | | Tag with ID: | |
| ✓ Allow More than | One Experiment of Each Type | Join Folders with Similar Name | |

In the **Master file options** dialog, you can configure a set of basic features to give some flexibility to the input. You can indicate which column contains the path and set the starting and end row to read the data in the master file.

| Advanced Options | 🕑 Master File Options | ? × | |
|---|-----------------------|--------|---|
| ✓ Master File: C:/Users/Usuario/Desktop/Datasets/MasterFile.csv | 1 . | | 🜣 |
| Main SDF File: | Column with the Path: | 1 🗘 | |
| Allow More than One Experiment of Each Type | Charting Down | | |
| | Starting Row: | 1 - | |
| | ✓ Read until Row: | 6 🗘 | |
| | ОК | Cancel | |

Main SDF File: If you have all the molecular structures saved in a single SDF file, you can unable this option to automatically match each molecule to the corresponding datafile analyzed in a batch. Matching is done using a tag that is added to each molecule (*"mixture_id"* in the example below). Enable the Main SDF File option and upload your SDF file, then type the Tag with ID to be used.

| Advanced Options | |
|---|--|
| Master File: | |
| Main SDF File: C:/Users/Usuario/Desktop/Datasets/ | Tag with ID: mixture_id |
| Allow More than One Experiment of Each Type | Jon Folders with Similar Name |
| | |
| | Compounds 🗗 |
| | |
| | Molecule Properties |
| | Molecular Formula: Monosotopic Mass: Monosotopic Mass: Label: Color: Assignments: mixture_idi: |
| | 2 Color: Assignments: Color: C |

Mgears detects and matches each structure with the corresponding datafile.

| Speriments Found: 4 | ? | \times |
|---|--------|----------|
| List of detected experiments: Experiment: 1 MS: C:/Users/Usuario/Desktop/Datasets/i Structure: Found in Main SDF File with ID: 1 | 01.DAT | A |
| Experiment: 2 MS: C:/Users/Usuario/Desktop/Datasets/i Structure: Found in Main SDF File with ID: 2 | 01.DAT | • |



Allow more than one experiment of each type: Activate this option when you want Mgears to detect several experiments of the same type in a document. In the example below, two MS raw datafiles are detected in each group.



Allow More than One Experiment of Each Type

| 1 | 😓 Experiments Found: 18 (Preview using a subset of 1000 files) | ? | \times | |
|---|--|-----------|----------|--|
| | List of detected experiments: Experiment: 1.20-1 MS(2): C:/Users/Usuario/Desktop/Datasets/By plugin/MSRO/Data/L20-1.raw/_FUNC001.DAT,C:/Users/Usuario/Desktop/Datasets/By plugin/MSRO/Data/L20-1.raw/_FU | NC001.IDX | | |
| | Experiment: L26-1 MS(2): C:/Users/Usuario/Desktop/Datasets/By plugin/MSRO/Data/L26-1.raw/_FUNC001.DAT,C:/Users/Usuario/Desktop/Datasets/By plugin/MSRO/Data/L26-1.raw/_FU | NC001.IDX | | |
| | Experiment: L27-1 MS(2): C:/Users/Usuario/Desktop/Datasets/By plugin/MSRO/Data/L27-1.raw/_FUNC001.DAT,C:/Users/Usuario/Desktop/Datasets/By plugin/MSRO/Data/L27-1.raw/_FU | NC001.IDX | | |
| | Experiment: L28-1 MS(2): C:/Users/Usuario/Desktop/Datasets/By plugin/MSRO/Data/L28-1.raw/_FUNC001.DAT,C:/Users/Usuario/Desktop/Datasets/By plugin/MSRO/Data/L28-1.raw/_FU | NC001.IDX | | |

Join folders with similar name: This option is used to join spectra with similar starting names within the same group. If enabled, Mgears will detect repetitions or small variations in the data folder names. For instance, if there is a group "ABC" and a new spectrum is found named "ABC_raw", it will be included in the "ABC" group because the start of the new file's name, "ABC", matches the previous group name.





Experiment Selection Mode: Choose this option if you want to detect raw data files only (FID) or both raw and processed data files (FID/Spectrum). When the FID/Spectrum mode is enabled, it is possible to manually select which data files to use for each type of experiment, as seen below:

| ° _@ № | ၀ Mnova Gears | | | | | | | |
|---|---|--|--|--|--|--|--|--|
| ÷ | Input 😵 Processing 🚱 Plugins 🔀 Design 📑 Output 🔅 Se | | | | | | | |
| s S Disk | Using Automatic Detection Experiments Selection Main Directory: C:/Users/Usuario/Desktop/Datasets/Raw data Optional Directory: | | | | | | | |
| al Time | NMR ✓ 1H FID ✓ 13C FID ✓ NOESY Spectrum TOCSY FID ✓ Change All FID ✓ | | | | | | | |
| GC/LC/MS Chromatography U/IR/Raman/Fluorescence Mnova I Advanced Options | | | | | | | | |
| | Master File: Main SDF File: Allow More than One Experiment of Each Type | | | | | | | |
| | Preview Subset Only 1000 | | | | | | | |

□ Select data files dates: Activate this option to detect data files created or modified between two specific dates. You can choose to filter by file Creation or Modification date.

| Join Folders with Similar Name | | |
|--|------------------------------------|---|
| ✓ Filter by Date From: 1 Jan 2022 ▼ To: 31 Mar 2022 ▼ Filter by: | Creation Date | Ŧ |
| Regular Expression to Adapt Match / | Creation Date Modification Date | |
| | | M |

Preview Subset Only: Activating this feature allows you to choose the number of files you want to visualize in the Automatic inspection dialog . This option is checked by default and uses 1000 as its default value. When unchecked, all detected files are visualized.

| Advanced Options | 🐅 Experiments Found: 123 (Preview using a subset of 100 files) | ? | Х |
|---|---|---|---|
| Master File: Main SDF File: Allow More than One Experiment of Each Type Experiment Selection Mode: FID/Spectrum | List of detected experiments: "Result filtered using expression: "/"/".fid Experiment: 01-AZ092 1H: C:/Users/Documents/3-DATA/1Hs/01-AZ092/1H/fid Experiment: 02-AZ117 1H: C:/Users/Documents/3-DATA/1Hs/02-AZ117/1H/fid | | |
| ✓ Preview Subset Only 100 ↓ | Experiment: 03-CATECHIN 1H: C:/Users/Documents/3-DATA/1Hs/03-Catechin/1H/FID | | |
| | Experiment: 04-MOL 12 1H: C:/Users/Documents/3-DATA/1Hs/04-mol 12/1H/fid | | |
| | Experiment: 05-MOL22 1H: C:/Users/Documents/3-DATA/1Hs/05-mol22/1H/fid | | |
| | Experiment: 06-NAPROXENE 1H: C:/Users/Documents/3-DATA/1Hs/06-Naproxene/1H/fid | | |





Use the Automatic inspection button $\overline{\blacksquare}$ to check how Mgears has grouped the detected data.

| Separate Providence 2 | ? | × |
|--|--------|---------|
| List of detected experiments: | | |
| Experiment: C031- MS(3): C:/Users/ | FUNC00 | 1.DAT, |
| Experiment: D047- MS(3): C:/Users/EmgGlamman/Documents/test data/webinaregs/BM/d047-m1.raw/ | FUNCO | 01.DAT, |
| | | |
| | | |
| 4 | | • |
| | OK | |

Use Custom function: Check this option and upload a custom script to replace the default grouping algorithm used by Mgears. This is particularly useful when your data files names are not easy to group (for instance, when the file name is an ID generated automatically by the instrument). You can contact our team for advice and support.



A simple script of about ~20 lines long can allow Mgears to:

- Find all the header files in the specified directory from settings
- Read the "sample description"
- Create a group for each unique sample ID
- Add relevant samples to this ID



Use the **Automatic inspection** button **a** to check how Mgears has grouped the detected data.

| <pre>function PWDatasetGrouper(aSettings) {</pre> | |
|---|--|
| <pre>//basedir for search of datasets</pre> | |
| <pre>var basedir = aSettings.path;</pre> | |
| <pre>var dir = Dir(basedir);</pre> | |
| <pre>//find all _header.txt files</pre> | |
| <pre>var datasets = dir.entryListAdv("*.raw/_HEADER</pre> | .TXT"); |
| <pre>var results = {};</pre> | |
| var names = []; | |
| <pre>for (var i = 0; i < datasets.length; i++) {</pre> | |
| <pre>var f = new File(datasets[i]);</pre> | |
| <pre>f.open(File.ReadOnly);</pre> | |
| <pre>var s = new TextStream(f);</pre> | |
| var line; | |
| do { | |
| <pre>line = s.readLine();</pre> | |
| //read sample description field | |
| if (line.indexOf("\$\$ Sample Description | n:") != -1) { |
| <pre>var sname = line.substring(22).trig</pre> | (); |
| <pre>if (!includes(names, sname)) {</pre> | |
| names.push(sname); | |
| var a = {}; | |
| a.MS = []; | |
| results[sname] = a; | |
| results[sname].MS.push(dataset | <pre>s[i].replace("_HEADER.TXT", ""));</pre> |
| } else { | |
| results[sname].MS.push(dataset | s[i].replace("_HEADER.TXT", "")); |
| } | |
| } | |
| <pre>} while (!s.atEnd());</pre> | |
| try { | |
| f.close(); | |
| } catch (e) {} | |
| } | |
| return results; | |
| | |
| | |

| 😓 Experiments Found: 2 | | ? | × |
|---|--|----------|--------|
| Results obtainded using custom script: C:/U | sers; //////////////////////////////////// | ipts/PWD | ataset |
| List of detected experiments: | | | |
| MS(3): C /Users | Documents/test data/webinaregs/BM2/29c7-de87.raw/,C:/Users/ | Doc | uments |
| Experiment: NBRef-3456 MS(3): C /Users) | /Documents/test data/webinaregs/BM2/a123-45fd.raw/,C:/Users/Gu-,u-u. | , Doc | uments |
| | | | |
| | | | |
| | | | |
| 4 | | | Þ |
| | | OK | |

Watch out! When using a custom function, a **Warning** symbol \triangle appears next to the **Automatic inspection** button with a tooltip indicating that a custom scripting function is active.



-



3.1.1.3. Filtering options

A **Filtering string** or a **Mapping file** can be used to filter your input data from the disk. *Please refer to section* 3.1.4.

Watch out! Advanced filtering will be disabled (hidden) while working with a Master file.

3.1.2. Data from database

Input data can also be retrieved from one or more Mnova spectral **Databases** (DB). In this mode, a list of spectra can be retrieved via a number of search terms for database fields.

In the **DB** section, click on \clubsuit to add a DB.

| ° <mark>⊘</mark> № | Inova Gears | | | | | ? | × |
|--------------------|--------------------|-----------|----------|----------|------------|------------|-----------|
| ÷ | Input 😵 Processing | 🔗 Plugins | 🔀 Design | 📑 Output | 🔅 Settings | | |
| Disk | Name | | | | Server | | ŧ |
| 8 | | | | | | | |
| 8 | | | | | | | |
| Ö | | | | | | | |
| ле | Search for text: | | | | | Substrin | ng Search |
| eal Tir | Field: | | | | | ▼ 🗟 Search | Text |

A dialog will appear. Enter the **Server** name, **Port**, **User**, and **Password**, then click on **Connect**.

| 🕑 Select D | atabase | | ? | \times |
|------------|-----------|-----------|--------|----------|
| Connection | | | | |
| Server: | localhost | Port: | 5504 | |
| User: | Test | Password: | ••••• | • |
| Database: | | | 🥌 Conn | ect |
| | | ОК | Cano | el |

Once you have connected successfully to the server, select the **Database** containing your input data and click on **OK**.

| 🕑 Select D | atabase | | ? | \times |
|------------|----------------------|-----------|------------|-----------|
| Connection | | | | |
| Server: | localhost | Port: | 5504 | |
| User: | Test | Password: | ••••• | |
| | | | 🥑 Disconne | ct |
| Database: | TestDB Metabolite | S | | ¥ |
| | TestDB | S UK | Cance | , |

The selected database will appear in the table as seen in the image below. Click again on + to add another database if needed, or on + to delete a previously added database.

| Name | Server | ÷, |
|------------------|------------------|----|
| 🗹 TestDB | localhost | |
| | | |
| | | |
| Search for text: | Substring Search | h |
| Field: | Search Text | |

It is possible to **Search for text** in the database. Type the text in the dedicated box then click on **Search Text**. You can optionally select a specific **Field** in the database for your search. In this example, two databases are searched by **Molecule name**. You can disable the search in one of these two databases by unchecking the corresponding box.

| ° @ M | nova Gear | 'S | | | | | | | ? | \times |
|--------------|---------------------|--------------|-----------|---|--|----------|--------|---|---------------|----------|
| Ð | Input | 💖 Processing | 😚 Plugi | ns 🔣 Design | 📑 Output | Settings | | | | |
| Sid | | Name | | | | | Server | | | + |
| 8 | 🗹 Metab | olites | localhost | | | | | | | |
| 8 | ✓ TestD8 | 3 | localhost | | | | | | | |
| ٢ | | | | | | | | | | |
| Real Time | Search fo Field: | r text: | | quinine Molecule -> Aliases | | | | | Substring Sea | arch |
| ۲ | # | Structure | Record | Molecule -> Label Molecule -> Name | | | | | \sim | |
| | | | | NMR Spectrum -> M NMR Spectrum -> M NMR Spectrum -> C NMR Spectrum -> P NMR Spectrum -> P NMR Spectrum -> P NMR Spectrum -> P | nova Version odified reated ageWidth ageHeight ageID age | | | • | | |



| N | ame | | | Server | + |
|--------------|------------|-----------|----------|------------|-----------|
| 🗹 Metabo | lites | localhost | | | |
| ✓ TestDB | | localhost | | | |
| | | | | | |
| Search for t | text: | | quinine | Substrir | ng Search |
| Field: | | | | 👻 🗟 Search | Text |
| # | Structure | Record | Database | Score | |
| ☑ 1 | Untitled 2 | 75 | TestDB | 1000 | |
| | | | | | |
| | | | | | |
| | | | | | |
| | | | | | |

If your search results include many records, you can exclude the records you don't want to use in your analysis by unticking the corresponding checkbox.

| # | Structure | Record | Database |
|------------|------------|--------|-------------|
| ✓ 1 | Untitled 2 | 75 | TestDB |
| F.2 | Untitled 2 | 75 | Metabolites |

You can also use these buttons, \heartsuit , \square , and \square , to **Check all** and **Uncheck all**, or **Clear** the results table, respectively.

Enable the **Substring Search** option to perform a search using substrings.

3.1.2.1. Filtering options

A **Mapping file** can be used to filter input data from a DB. *Please refer to section* 3.1.4.

Watch out! When using the DB mode, the filtering options override the manual selection of data files, and therefore Mgears will disable the list of records if the Filter mode is selected.

3.1.3. Data acquired in real time

Input data can also be analyzed as soon as it is acquired. With the **Real time** (RT) mode, Mgears will watch (Listener) a set of folders for incoming data and operate on it as it arrives (or optionally when all expected parts of a set are ready). The RT input mode can help improve productivity by taking care of all the routine analysis before the user even interacts with the data.



| Q | Mnova Gears | ? | \times | ٦ |
|---|---|---|----------|---|
| ł | 🕨 Input 🛛 Processing 🚱 Plugins 🐹 Design 📑 Output 🏟 Settings | | | |
| ł | S Using Automatic Detection 🗮 Experiments Selection | Ð | | |
| ľ | Path | | H | Ļ |
| | | | | ~ |
| | | | | |

You can add one or more paths. These will appear in the table as seen below. You can **Delete** a path or **Clear** the whole table by clicking on or or , respectively.

| 00 | Anova Gears | | | ? | \times |
|-------------|--|--------------------|------------------------------|---|----------|
| Ð | Input 😵 Proce | sing 🔗 Plugins | 🔀 Design 📑 Output 🄅 Settings | | |
| Disk | 2 Using Automatic | Detection 📒 Experi | nents Selection | | |
| °, | | | Path | | + |
| 8 | C:/Users/Usuario/Desktop/Datasets/DataAcquisition-Instr1 | | | | |
| | C:/Users/Usuario/Desktop/Datasets/DataAcquisition-Instr2 | | | | |
| ि Real Time | | | | | |
| | Online | | | | |

3.1.3.1. Options

Process old files: If checked, all files already present in the directory will be processed. In this case you can choose to Ignore Files and Directories older than a certain time.



□ **Group by folder:** Enable this option to group spectra with similar folder names into a unique Mnova results document. Two other options are configurable in this case: **Wait for all the Selected experiments** to process them together (otherwise experiment files are processed once available in the watched folder), and **Allow more than one experiment of Each type.** Also, in this case, **Filtering** options are made available.

| Process Old Files | Group By Folder | Ignore Files And Directories Older Than: | 6 days | Real Time Se | ettings |
|----------------------------------|----------------------------|--|----------------------------------|--------------|---------|
| ✓ Wait for Structure and Spectra | Wait for All The Selection | ted Experiments 📃 Join Folders with Similar Name | ✓ Allow More than One Experiment | of Each Type | |



- □ **Wait for Structure and Spectra:** This option will prompt Mgears to wait for at least one structure and one spectrum before processing an experiment.
- □ Join Folders with similar name: This option is used to join spectra with similar starting names within the same group. If enabled, Mgears will detect repetitions or small variations in the data folder names. For instance, if there is a group "ABC" and a new spectrum is found named "ABC-1" or "ABC_raw", it will be included in the "ABC" group, because the start of the new file name, "ABC", matches the previous group name. *Please refer to section 3.1.1.2*.
- Real Time settings: By clicking on this button, a dialog will open to allow you to set the folder listener's settings.

| 😢 Real Time Settings | | ? | × |
|-------------------------|-----------|------|------|
| Mode: | Real Time | | * |
| Listened Folder Levels: | | 2 🧘 | |
| Delay: | | 1 s | * |
| Time Between Checks: | | 0 m | in ‡ |
| ✓ Use Multithreading | | | |
| Fast Hash Mode | | | |
| Back to Default | ОК | Canc | el |

Real-time acquisition can be performed in two modes:

- The **Real Time** mode, in which the listener will rely on the operating system (OS) to determine when changes happen in the listened directories. Such changes in the file system are therefore immediately reported to the user. With this mode, the listened folders can also be periodically checked for modifications every X minutes (X is the time set in the **Time Between Checks** option). This is useful when working with network shared units because, depending on the configuration, the OS may not report the changes correctly/in time.
- The **Timer** mode, in which the listener will check the directories every "X" minutes to detect changes ("X" is the time set in the **Time Between Checks** option). With this option, the listener will generally consume fewer system resources.

Another configurable setting is the **Listened folder Levels** value, which corresponds to the directory tree level that the listener will reach to look for modified files. When set to zero (0), the listener will only look in the top directory. Note that your folders' architecture and size may affect the performance.

The **Delay** value corresponds to the number of seconds that the system will wait to check whether the modifications in a specific file have finished.

Finally, you can check the **Multithreading** option if you want the listener try to use several threads when creating the file cache, which will increase the performance of the system; and the **Fast Hash Mode** if you want the listener to only use the modification date of the file when looking for changes.



3.1.3.2. Advanced options

- Experiment Selection Mode: Choose this option if you want to detect raw data files only (FID) or both raw and processed data files (FID/Spectrum). When the FID/Spectrum mode is enabled, it is possible to manually select which data files to detect for each type of experiment.
- □ **Regular Expression to Adapt match:** This option will allow you to group samples when only part of the file name matches. The regular expression you type will be used to capture the common part of the string in the names of the files detected and group them in a single experiment. *Please refer to section* <u>3.1.1.2.</u>
- Allow Reprocessing Custom Format File: When working with custom format files, this option allows you to reprocess a custom file after making changes. If this option is disabled, Mgears will discard a previously processed file and won't reprocess it.
- □ **Ignore Problem Opening spectra:** Sometimes Mnova will return an error when opening a file even though the file has loaded correctly. By enabling this option, you can force Mgears to ignore problems detected by Mnova and use the file anyway, otherwise Mgears will not use the affected spectrum.

Experiment Selection Mode: FID/Spectrum 🗸 Ignore Problems Opening Spectra Regular Expression to Adapt Match /

3.1.3.3. Filtering options

A **Filtering string** or a **Mapping file** can only be used when the **Group by Folder** option has been enabled. *Please refer to section 3.1.4.*

3.1.4. Filtering options

Filtering options are available for all three sources of input data (from Disk, DB, or Real Time), which allows you to refine your data detection and better adapt it to your data configuration.

3.1.4.1. Filtering string

The Filtering string can be used to filter the detected files from Disk or Real time acquisition using a string with common wildcards (* and ?) or a regular expression.

Type your filtering string in the corresponding box. The **Automatic inspection** button $\overline{\blacksquare}$ is used to preview the detected data before and after filtering.

| Without filtering | | |
|--|------------------|----------|
| 🛠 Experiments Found: 1 (Preview using a subset of 1000 files) | ? | \times |
| List of detected experiments: | | |
| Experiment: TESTDATA 1H: C:/Users/Usuario/Desktop/Testdata/10/fid 13C(2): C:/Users/Usuario/Desktop/Testdata/100011/fid,C:/Users/Usuario/Desk Structure: C:/Users/Usuario/Desktop/Testdata/10/78554980.mol [] | top/Testdata/11/ | fid |
| | ОК | |

With filtering

| Optional Directory: | |
|--|--|
| Master File: | Separate Sep |
| dvanced Options | List of detected experiments: *Result filtered using expression: /^((?!\/10001[0-9]).)*\$/i |
| ✓ Allow More than One Experiment of Experiment Selection Mode: FID ✓ Preview Subset Only 1000 | Experiment: TESTDATA 1H: C:/Users/Usuario/Desktop/Testdata/10/fid 13C: C:/Users/Usuario/Desktop/Testdata/11/fid Structure: C:/Users/Usuario/Desktop/Testdata/10/78554980.mol |
| Filtering String:/ ^((?!\/10001[0-9]).)*s | \$ /i ✓ Regular Ex |
| Mapping File: | |

You can check the **Regular expression** option to force the use of a regular expression over the normal filtering string.

Check the option **Filter by name only** to only filter the name and not the full paths of the spectra.

| Y | Filtering String:/ ^((?!\/10001[0-9]).)*\$ | /i | ✓ Regular Expression ✓ Filter by Name Only |
|--------|--|----|--|
| Filter | Mapping File: | | Substring Matching |

3.1.4.2. Mapping file

Using a Mapping file is convenient when input files are listed in an .<u>txt</u> or <u>.csv</u> document along with other metadata. Mgears will map the information found in the file provided with the information found in the selected input directory (on Disk, DB, or RT folder).



Click on ... to choose your mapping file from your directory.

| Y | Filtering String: | Regular Expression Filter by Name Only | у |
|--------|---|--|---|
| Filter | Mapping File: C:/Users/Usuario/Desktop/Datasets/Mapping/Mapping file_Smiles.csv | Substring Matching 😫 | ¥ |

More filtering options are available when the input data is retrieved from Disk or through Real time acquisition.

To configure these **Advanced Filtering Options,** click on ¹. In the dialog that appears, indicate which column of the mapping file will be used to match information in your data directory. You can either type the column

number or click and open the assistant 🛄 to visualize the .csv and select the desired column. In the assistant, only the first 10 rows of the filtering file will be loaded.

| Advanced Filtering O | ptions | ? > | × |
|---------------------------|-------------------|--------------|----------|
| Column for Matching: | | 1 🗘 | 5 |
| Starting Row: | | 1 | 1 |
| Read until Row: | | 9999 | * |
| ✓ Allow Gaps in Results | | | |
| Read Column with the F | Position in the W | /ell Plate — | |
| Column: | | 5 ‡ | |
| Read Column with ID o | f Compound — | | |
| Column: | | 1 🔹 | |
| ┌ 🗸 Read Column with SMIL | ES Compound | | |
| Column: | | 6 🗘 | |
| | ОК | Cance | |

| lio | ck or Select co | olumn with value | s for: Nam | e for Matchin | g | |
|-----|-----------------|----------------------|------------|---------------|-----|---|
| | 1-A | 2-B | 3-C | 4-D | 5-E | 4 |
| 1 | ABC-1 | ^S 1125110 | | 7886.6 | A01 | • |
| 2 | ABC-2 | 1156569 | | 7885.7 | A02 | - |
| 3 | ABC-3 | 1099323 | | 7787.7 | A03 | |
| 4 | ARC-4 | 1099204 | | 7872 7 | A04 | • |

Choose the Starting row you want to read your .csv from and, optionally, enter the last row you want to read.



Enable the **Allow Gaps in Results** option if you want to include void results for the empty cells in the plate with the lines in the filtering files.



- sample **Position in the well plate** (only available when the Allow Gaps in Results option is enabled)
- compound ID
- compounds **SMILES** string.

| Advanced Filtering Option | าร | ? | × | 8 | CSV Colur | nn Detection | | |
|--------------------------------|---------------|-----------|---|-----|--------------|-------------------|-------------|--------------|
| Column for Matching: | | 1 🗘 | | Cli | ck or Select | column with value | es for: Pos | ition in the |
| Starting Row: | | 1 | - | 1 | ABC-1 | 2-D | 3-0 | 7886.6 |
| Read until Row: | | 9999 | * | | | 1156560 | | 7005.7 |
| ✓ Allow Gaps in Results | | | | 2 | ABC-2 | 1150509 | | 7885.7 |
| ✓ Read Column with the Positio | on in the Wel | I Plate – | | 3 | ABC-3 | 1099323 | | 7787.7 |
| Column | | 5 | | 4 | ABC-4 | 1099204 | | 7872.7 |
| Column: | | 7 * | 5 | | | | | |
| Read Column with ID of Com | pound | | | | | | | |
| Column: | | 1 🗘 | | | | | | |
| ✓ Read Column with SMILES Co | ompound — | | | | | | | |
| Column: | | 6 ‡ | | | | | | |
| | OK | Can | | | | | | |

With this configuration, SMILES strings and well positions are read and recognized by Mgears, as you can see when using the **Automatic inspection** button $\overline{\blacksquare}$.

| | | | -0 |
|--|-----------------------------|-------|----|
| September 2015 - Septem | ? | × | |
| List of detected experiments: Result filtered using file: C:/Users/Usuar Experiment: ABC-1 Structure: OC(=O)C2=Cc1c(Br)cncc1S2 Position: A01 Experiment: ABC-2 Structure: OC(=O)CCC(=O)c1ccc(Br)cc1 Position: A02 | rio/Desktop/Datasets/Mappin | ng/Ma | |

Substring Matching: If this option is checked, the clustering algorithm will include spectra with small differences at the ends of their names. For example, if the requested group is "ABC", detected files "ABC_1" and "ABC_raw" will be included in the group ABC. If not checked, spectra that do not match the exact name in the file will be discarded.

Top tip! Sometimes the Mapping file can be used to generate final reports with input and output data. In these cases, a configuration of the columns reserved for output can be set in the plugin-specific settings dialog.

?

OC(=O)C2=Cc OC(=O)CCC(= OC(=O)c1cnc(OC(=O)c1cc(C

×

6-F 📤

► Cancel



3.1.5. Experiment detection modes

Detection of the experiment files to be used for the analysis can be achieved either automatically or manually. This can be selected at the top left-hand side of the **Input** tab when data files are retrieved from **Disk** or in **Real Time**.

In the Automatic detection mode, experiment files will be automatically recognized by the system.

| °o M | Autom | atic Detection | sign ection | Output | Settings |
|-------------|---------------------|----------------|----------------|--------|----------|
| 0 | Main Directory: | | | | |
| ω | Optional Directory: | | | | |
| | | | | | |
| чш) | | | | | |
| Real Time | | | | | |
| ((· | Advanced Options | | | | |

Given that Mgears can support various types of analyses (NMR (1H, 13C, 19F, HSQC...), LC/GC/MS, chromatography, UV/IR/Raman/Fluorescence) as well as any Mnova documents, it is possible to select the type of data files you wish to analyze, and restrict detection by Mgears to those.

To do so, click on **Experiment Selection**. A new section with all available experiment types will appear on your screen. Check the boxes of the experiments of interest.

| °⊚ Mr | nova Gears | | | | | | | | |
|--------------|--|--|--|--|--|--|--|--|--|
| • | input 😵 Processing 🚱 Plugins 🎉 Design 📑 Output 🏠 Settings | | | | | | | | |
| | Using Automatic Detection Experiments Selection | | | | | | | | |
| | Main Directory: | | | | | | | | |
| ŵ | Optional Directory: | | | | | | | | |
| e e | NMR ✓ 1H ✓ 15N 19F ✓ 31P HSQC COSY NOESY HMBC ROESY TOCSY H2BC | | | | | | | | |
| Tin | GC/LC/MS Chromatography UV/IR/Raman/Fluorescence Mnova Documents Orders Custom Format | | | | | | | | |
| e. | | | | | | | | | |
| | | | | | | | | | |

Watch out! You may need to configure the file masks to ensure the correct automatic detection of experiment files.



In the **Manual detection** mode, a **Path Mask** must be provided to define the experiments that should be considered in the analysis. All Operating System standard conventions apply (*, ?, !, etc.).

To do so, enter the **Path mask** for the experiments of interest. Use the **Inspection** option \bigcirc to inspect the detected files.

| Disk n | node | | 2 | | |
|--|------------------------------------|---|--|--|--|
| Input | Process | ing 🔗 Plugins 🔀 Design 📑 Output 🔅 Settings | : × | | |
| Main Direct | 1anua | l Detection | | | |
| NMR 1H Path Ma HSQC Path COSY Files | GC/LC/MS isk: Mask: Mask: | - Chromatography - UV/IR/Raman/Fluorescence Structures | | | |
| | NMR MS Path | GC/LC/MS - Chromatography - UV/IR/Raman/Fluorescence Structures Mask: | ······································ | | |
| | Chromatography Path Mask: | | | | |
| | | Main Directory: | · | | |
| | Amova Gears | Disk mode | Disk mode Nova Gears Input Procession Plucins Design Output Settings Manual Detection Main Directory: NMR GC/LC/MS - Chromatography - UV/IR/Raman/Fluorescence Structures IH Path Mask: COSY Files Mask: COS | | |



3.2. Processing

The processing tab allows you customize data processing:

□ **Solvent:** Tick this option to replace the default solvent with another one by simply typing your new solvent name.

| °⊚ Mnova G | ears | | | | | ? | × |
|-------------------|--------------|-----------|----------|----------|------------|---|---|
| 🛃 Input | 😵 Processing | 🚱 Plugins | 🔀 Design | 📑 Output | 🔅 Settings | | |
| ✓ Solvent | | | | | | | |
| Replace Defa | It With: THF | | | | | | |

Blind regions: can be added to NMR or LC/GC-MS spectra. You can either:



Processing Templates: To add templates, click on +, specify the type of spectra this template should apply to, then add the template path.

| Processing Templates | | | 6 |
|--|---------------------------------|---|---|
| Template | Туре | + | Ļ |
| Select Type ? Select the Type of the Spectrum: 1H 13C 1SN 13F 19F 10 10 10 < | OSY.mnp · .mnp 3 Open Cancel | | 5 |



Your added template will be displayed in the table as seen below:

| | ✓ Processing Templates |
|---|--------------------------|
| emplate Type + | |
| ts for testing/#19237 Processing templ COSY | 1 C:/Users/Usuario/Deskt |
| ts for testing/#19237 Processing templ 2D | 2 C:/Users/Usuario/Deskt |
| | |
| ts for testing/#19237 Processing templ 2D | 2 C:/Users/Usuario/Deskt |

You can add one more template and each will be applied to the corresponding spectra. When simultaneously applying a template for COSY and another for 2D, then the most specific template (in this case the COSY template) will be applied to the COSY spectra, whilst the 2D template will be applied to the 2D spectra in your analysis.

Click on 🗖 or 🗖 to **Delete** a row or **Clear** the whole table, respectively.

Apply NMR Advised Processing: If you enable this feature, the best processing options will be automatically applied to the data in hand. This includes automatic referencing by solvent and linear prediction for your spectra. You can check/uncheck the type of processing you want to apply in the advised processing setting dialog.

| NMR Advised Processing | Advised Processing ? × Advised Options Application 1D V 1H Auto Reference V Auto Reference V Aut | Advised Processing Settings |
|------------------------|--|-----------------------------|
| | OK Cancel | |



□ Script: Various custom Mnova scripts can be applied for processing. You can run a single script at the beginning of automation (Starting script), a separate script for each sample (Processing script), and a third script to automatically rename groups assigned by Mgears (Script for renaming groups). Click on and upload a script to use. Below is an example of a processing script that will run a multiplet analysis on each spectrum of a document:



In this other example, we will use a script to rename input data groups. The script used will add "_new extension" to our data groups.

| Scripting: | | | - |
|-----------------------------|---------------------------------------|---|---|
| Starting Script: | | | |
| Processing Script: | | | |
| Script for Renaming Groups: | C:/Users/Usuario/Desktop/Datasets/Cha | angingName/newName.qs | |
| | | | |
| | | <pre>function newName(aOldName) { return aOldName + "_new Extension"; }</pre> | |

After running the Mgears analysis, data files will be renamed as indicated in the script.

| # | Title | Document | |
|---|--------------|--------------------|--|
| 1 | CATECHIN | CATECHIN.mnova | |
| 2 | ETHYLBENZENE | ETHYLBENZENE.mnova | |
| 3 | FELODIPINE | FELODIPINE.mnova | |
| 4 | QUININE | QUININE.mnova | |

Without script for renaming groups

With script for renaming groups

| # | Title | Document |
|---|----------------------------|----------------------------------|
| 1 | CATECHIN_new Extension | CATECHIN_new Extension.mnova |
| 2 | ETHYLBENZENE_new Extension | ETHYLBENZENE_new Extension.mnova |
| 3 | FELODIPINE_new Extension | FELODIPINE_new Extension.mnova |
| 4 | QUININE_new Extension | QUININE_new Extension.mnova |



3.3. Plugins

The plugins tab is where you select and configure the analysis plugins you want to run. To include a brick in your workflow, select it and click the **Add** button.

| လူ Mnova Gears | | | | |
|---|--|--|--|--|
| Hugins Processing Plugins Design Output Output | | | | |
| SQA Verify Concentration Purity DB Search SMA CProfiling Multiplet Report IUPAC Name MS Scan Peak Report Peak Report Mpublish | Add Add New Custom Plugin Delete Custom Plugin Custom Plugin Custom Plugin Custom Plugin Custom Plugin Custom Plugin | | | |
| ▶ Resume 🔹 Load Settings 📩 Save Settings 🕴 Import Settings 👻 | Export Settings 👻 | | | |

You can add one or multiple plugins to run one after the other on the same dataset. The plugins are displayed in the order they will be executed.



| A number of plugins are | available with Mgears 2.5: |
|-------------------------|----------------------------|
|-------------------------|----------------------------|

| Plugin | Technique | Analysis | |
|-----------------------------------|------------------|---|--|
| <u>SQA</u> | NMR | Spectral quality assessment | |
| <u>Verify</u> | NMR, LC/GC-MS | Automatic structure verification on NMR and LC/GC-MS data | |
| <u>Purity</u> | NMR | Purity determination by quantitative NMR analysis | |
| Concentration | NMR | VIR Concentration determination by quantitative NMR analysis | |
| Peak Report | NMR | VIR Automated peak reporting | |
| <u>Multiplet</u> <u>Report</u> | NMR | Automated multiplet reporting | |
| <u>MPublish</u> | NMR | Automated preparation of supporting information for publications | |
| IUPAC Name | NMR | Automated and batch IUPAC naming of molecular structures | |
| DB Search | NMR | Automated search of spectral data in one or more databases | |
| <u>SMA</u> | NMR | Targeted mixture analyses by NMR for batch and real time workflows | |
| MANIQ | NMR | Automated identification and quantification of compounds in a mixture | |
| QC profiling | LC/GC-MS | Purity assessment of DNA encoded library compounds | |
| <u>MS Scan</u> | LC/GC-MS | Automated extraction of mass spectra and mass chromatograms for total ion chromatograms | |
| Chrom Reaction Optimization | LC/GC-MS | Automated analysis to determine the optimal chemical reaction conditions | |
| Chrom Cal | LC/GC-MS | Automated evaluation and generation of calibration curves for many compounds at the same time | |
| Affinity Screen | LC/GC-MS | Automated solution for affinity selection mass spectrometry data processing, interpretation, and hit identification | |
| Fraction Analysis | LC/GC-MS | Automated evaluation of fractions collected with preparative chromatography | |
| Chrom Best | LC/GC-MS | Automatic scoring tool for selection of chromatographic methods with optimal | |
| Method | | separation conditions | |

Each brick has its own settings that can be configured in just a few clicks (details about plugin configuration are provided in a separate starting guide for each application).

To open the plugin-specific settings, select the plugin and then click on the settings button, or simply doubleclick on the plugin.



M



If the analysis you want to perform is not covered by our plugins, it is possible to create a custom plugin by uploading your own script. To do so, click on the **New Custom Plugin** icon, **Name** your plugin, then upload the **Analysis Script** (which could be developed outside the automation on individual samples). Then, choose the **Reporting** preferences (optionally also using your own reporting script), and click on **OK**.



The new custom plugin will appear in the list of available plugins. You can delete a previously added custom plugin by selecting it and clicking on **Delete Custom plugin**.



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3.4. Design

In the design tab, Mnova layout templates can be applied to the output documents resulting from the analysis performed. You can easily create your own template with Mnova, laying out the pages as per your requirement and including any custom graphics or images, then save that document as a template that can be used with Mgears.

| 🙌 1H Report | | | |
|---------------------------------------|----------|------------------------|--|
| Text: Report Special, [Peaks,1H] | Molecule | NMR Spectrum: 1D, [1H] | |
| Text: Report Special, [Multiplets,1H] | | | |

Click on ... and select the template file you want to apply. You can check the **Apply Layout Template to All Pages** option to apply the layout on every page of the output document.

| ſ | ିତ୍ତ Mnova Gears | ? | \times |
|---|---|-------------|----------|
| | 🛨 Input 😵 Processing 🚱 Plugins 🔀 Design 💽 Output 🏠 Settings | | |
| | Layout Template: C:/Users/Usuario/Desktop/Datasets/Layout templates/Layout template.mnova | te to All P | Pages |
| | Advanced | | > |

A **Script** can also be applied to achieve highly complex layout needs.

| ¢ | 🗑 Mnova Gea | ars | ? | \times |
|---|---------------|---|-----------------------------|----------|
| | 🛃 Input | 😵 Processing 🔗 Plugins 🔀 Design 💽 Output 🔅 Settings | | |
| | Layout Templa | ate: | Apply Layout Template to Al | Pages |
| | Script: | C:/Users/Usuario/Desktop/Datasets/1H.qs | | |
| | Advanced | | | > |



Advanced design section and click on ^T to add your different templates. A dialog will open to allow you to choose the analysis type. You can then select the template path from the directory.

| Template | Туре | |
|----------|---|--|
| | Select Type ? X | |
| | Select the Type of the Spectrum: 1H OK 1H 1SN | |
| | 19F 31P 1D | |

Your added templates will be displayed in the table as seen below. You can click on 🗖 to delete a previously added template, or on 🗖 to clear the entire table.

| Ac | dvanced | | V |
|----|---|------|---|
| | Template | Туре | + |
| | C:/Users/Usuario/Desktop/Datasets/Layout HSQC.mnova | HSQC | |
| i | 2 C:/Users/Usuario/Desktop/Datasets/Layout 1H.mnova | 1H | |
| | | | |
| | | | |
| | | | |
| | | | |

When different templates can be applied to the same dataset, the most specific one will be used. For instance, if a template for COSY and another for 2D spectra are added, then the COSY template will be applied to COSY spectra.



3.5. Output

The output tab is where options for saving reports are configured. There are two main options: saving data in Disk directories and saving data in a Database. In addition, several advanced switches allow you to customize how the output is saved.

3.5.1. Saving output on Disk

To save output data on disk, click on and choose a directory in which to save your analysis results.

| ⁰⊗ Mnova Gears | ? | < |
|---|----------------------------------|----|
| 🛨 Input 😵 Processing 🔗 Plugins 🔀 Design 💽 Output 🔅 Settings | | |
| Disk | | |
| Directory: C:/Users/Usuario/Desktop/Results | Add Nickname to the Results Fold | er |

The result folder is by default named according to the date and time of your analysis, e.g., 2021-01-08T08.06.58. However, it is possible to either add a nickname to the result folder name or completely replace the result folder default name with a nickname of your choice.

Enable the Add Nickname to the Results Folder option and type the desired nickname.



Enable the **Only Nickname** option to remove the timestamp from the folder name and only use the indicated nickname.

| ✓ Add Nickname to the Results Folder | Test | Add Incremental Numbering | Only Nickname | Output | Test |
|--------------------------------------|------|---------------------------|---------------|--------|------|
| | | | | | |

Enable the **Add Incremental Numbering** option to add a number to the folder's name when another folder with the same nickname is detected in the output directory.

| ✓ Add Nickname to the Results Folder | Test | ✓ Add Incremental Numbering Only Nickname | Output | 2022-04-19T15.44.18_Test-2 2022-04-19T15.44.00_Test-1 |
|--|------|---|--------|--|
| \fbox Add Nickname to the Results Folder | Test | ✓ Add Incremental Numbering ✓ Only Nickname | Output | Test-2 |





When you activate the **Sort in Subfolders** option, you can also utilize the **Split Results in Subfolders** feature. Enabling this option allows you to save the Mnova and PDF outputs in subfolders named after the corresponding input subfolders.





Both an interactive Mnova file and a human readable PDF can be generated and saved along with your analysis results.

3.5.1.1. Saving an Mnova document

Check the **Mnova** options and configure the saving settings as needed:

• The Mnova document is saved by default in the output folder in a sub-folder named "documents".



• You can save the Mnova document in the folder of your choice by ticking the option **Save Mnova Document in** and selecting the desired destination folder.

| Disk | | | |
|---|---|--------------------------------|---|
| Directory: | C:/Users/Usuario/Desktop/Resu | llts | |
| ✓ Mnova ✓ Save Mnova Docum Save a Copy of the | ent in: C:/Users/Usuario/Deskt Mnova Document with the Raw | op/Results/Mnova files Data | |
| | Output | Results > Mnova files | ^ |
| | | | |

• You can also Save a copy of the Mnova document with the input data by ticking the corresponding option.

| Disk | |
|--|-----------------------------------|
| Directory: C:/Users/Usuario/Deskt | op/Results |
| ✓ Mnova | |
| Save Mnova Document in: | |
| Save a Copy of the Mnova Document with t | he Raw Data |
| Output | Datasets > Report > Catechin > 1H |
| | PROCPAR TEXT |



3.5.1.2. Saving a PDF document

Check the **PDF** options and configure the saving settings as needed:

• You can save the PDF document in the **Results folder** (configured above as the Directory). It will be saved in a sub-folder named 'pdf'.

| ✓ PDF● Save in R | esults Folder |
|---|-------------------------------------|
| Output | Results > 2021-05-12T12.12.13 > pdf |

• The PDF can also be saved along with the input raw data.



• The PDF can alternatively be saved in a separate folder by ticking the **Save PDF in** option and selecting the desired destination folder.

| ✓ PDF | | |
|--------------|------------------------------|------------------|
| Save PDF in: | C:/Users/Usuario/Desktop/Res | ults/PDF results |
| | Results > PDF results | |
| Output | Name | ^ |

• You can **Protect PDF from Editing** by enabling the corresponding option:



• You can also Add Analysis type in the Name of the PDF;





• or Embed PDF in Mnova document.



• When results are saved to a database, it is also possible to **Save PDF in a New record**. If this option is unchecked, the PDF will be saved in the record along with the processed data.

| V PDF | | |
|---|--|--------------------------|
| Save in Results Folder Save with the second s | the Raw Data 🔿 Save PDF in: | |
| Protect PDF from Editing | Add Analysis Type in the Name of the PDF 📃 Embed in Mnova Document | Save PDF in a New Record |
| ✓ DB | | |



3.5.2. Saving output in a Database

Mgears results can be saved to an Mnova spectral database. To do so, you will need to check the **DB** option, indicate your **Server** address, **Port**, and your credentials (**User** and **Password**), then click on **Connect**.

| / DB | | | | |
|----------------------|-----------|-----------|--------------------|-----------------|
| Connection | | | | |
| Server: | localhost | Port: | 5504 | |
| User: | Test | Password: | ••••• | ✓ Save Password |
| Connect | | | Selected Database: | TestDB |
| Update Ssting Record | | | | |

Once connected to the server, you can select the database you want to save the results to.

| | | Metabolites |
|----|--------------------|---------------|
| | Selected Database: | |
| ł: | ••••• | Save Password |
| | 5504 | |

Check the **Update Existing Record** option if you want Mgears to search for and attempt to update an existing record in the DB before saving your results to a new one:

| ✓ DB | |
|------------------------|--|
| Connection | |
| Server: | |
| User: | |
| Disconnect | |
| Update Existing Record | |
| \sim | |

- When the input comes from Disk directories, Mgears will search for the name of the experiment in the DB. If the ID is found in one record, it will be updated, otherwise a new record will be created. If the ID is detected in more than one record, the log will show an error, and nothing will be saved to the DB.
- When the input comes from the DB, it will update the registry associated with the input.

Watch out! This feature will only work with DBs created with Mnova 14.0.0 or higher, and the Mnova DB Server version 1.8.3 or higher (with a field custom ID on each item).

3.5.3. Saving output in an ELN

Mgears can detect your ELN plugin and save the analysis output directly to it. <u>Contact us</u> for assistance.

3.5.4. Expert settings

Additional settings can be configured for analysis output under the **Expert** section:

An Output Script that gives complete control over the output generation and saving can be used, for example, to send details of the report to a web service and update an external database, or to write

results in a custom data folder structure, etc. Click on _____ to select your **Output Script**.

Expert
Output Script: C:/Users/Usuario/Desktop/Datasets/OutputScript.qs



□ A **Summary Script** that runs at the end of a batch analysis (in disk or DB modes) to evaluate all the results of the different bricks together and provide a global result (e.g. statistical estimators for all the

results). Click on to select your **Summary Script**. of running a Summary script to

| Expert | | ~ |
|-----------------|--|-----|
| Output Script: | | |
| Summary Script: | C:/Users/Usuario/Desktop/Datasets/SummaryScript.qs | |
| | | 1.5 |

□ **Zip and Save Raw Data:** If checked, Mgears will create a zip file with the raw data from the processed directory and save it in the output folder.



Zip and Attach Raw Data: If checked, Mgears will create a zip file with the raw data from the processed directory and embed it in the resulting Mnova document.



Attach Data from Input Folders: Enable this feature if you want to attach all Zip and PDF files from each processed input directory to the Mnova document.



Output

- □ Save Structure in a New Record: This option is available when output is saved into a database. If checked, the structure will be saved in a new separate record, otherwise it will be saved together with the processed spectra.
- □ **Avoid Saving Images:** You can enable this option to avoid saving images of the molecules and spectra in the output folder. Images will not be displayed in the html report either.
- □ **Create Reports on-the-fly:** If this option is checked, Mgears will create all reports after processing each experiment instead of waiting until the end of the whole task.
- Save Results in Subfolders Sorting by Parameter: With this option enabled, it is possible to distribute the results into different folders according to any of the available spectral parameters. Open an input spectrum by clicking on Open Parameters. Mgears will read the available parameters in your input data and list them so you can select one to sort your results. Click on OK.

| Save Results in Subfolders Sorting by Parameter: Instrument Open Parameters | | | | | | |
|---|---|--------|-----------------------|--|--|--|
| | Select One Parameter ? × | | VS | | | |
| | Title Comment Origin Instrument Solvent Temperature Pulse Sequence Experiment Probe Number of Scans Receiver Gain Relaxation Delay Pulse Width Acquisition Time Spectrometer Frequency Spectral Width Lowest Frequency Nucleus Acquired Size Spectral Size | Output |)).resume ults | | | |

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3.6. The Settings tab

The settings tab does not form part of Mgears workflow but allows the specification of various aspects of automation, and the configuration of the **Notifications** system for receiving automatic emails related to your Mgears analyses.

3.6.1. General settings

The general settings include the following:

- □ **Verbose log:** Check this option to include detailed information in the log.
- □ **Autoload Results in the Viewer when Finished:** If enabled, the Mgears Result Viewer will automatically load the results of a batch analysis once completed.
- □ **Autoload Results in the Viewer on-the-fly:** If enabled, the Mgears Result Viewer will automatically load the results in real time, as soon as they are obtained.
- Copy Files Only: If enabled, Mgears will exclusively copy data to the output folder without opening, processing, or analyzing it. This option hides processing and analysis related tabs and options and is functional only with automatic data detection in Batch and Real-time modes.

| 🗞 Mnova Gears | 🗞 Mnova Gears | |
|---|--|---------------|
| Tinput Output 🄅 Settings | 🔁 Input 💽 Output 🔅 Settings | |
| Image: Selection Main Directory: Optional Directory: Image: NMR IH FID IH FID COSY FID NOESY FID GC/LC/MS Chromatography UV/IR/Raman/Fluorescence Mr Advanced Options | General Verbose Log ✓ Copy Files Only Expert ✓ Debug Mode (Execute All Process in Foreground) Debug Log | |
| Master File: | | |
| ∞ Mnova Gears | | ? × |
| Finput Output Settings | | |
| Disk Directory: | Add Nickname to the Results Folder Sort in Subfolders Split Results | in Subfolders |
| | | |

3.6.2. Expert settings

More settings options are included in the **Expert** section:

Debug Mode (Execute all processes in Foreground): If enabled, the log will contain information about the internal state of the objects inside Mgears. This option is mainly used for debugging and development purposes.





Debug Log: If checked, the Mgears log file will give information about Mgears, the available plugins, and the current analysis, and will be saved in the results folder.

| [2021-03-12T14.34.56] | Running Mgears 2.2.0.7037 |
|-----------------------|-------------------------------------|
| [2021-03-12T14.34.38] | Plugins available: |
| [2021-03-12T14.34.38] | SQA 14.2.0-26256 |
| [2021-03-12T14.34.38] | Verify 3.0.0.6085 |
| [2021-03-12T14.34.38] | Concentration 3.0.0.6161 |
| [2021-03-12T14.34.38] | Purity 3.0.0.6161 |
| [2021-03-12T14.34.38] | DB Search 1.0.0.6640 |
| [2021-03-12T14.34.38] | SMA 3.0.0.7013 |
| [2021-03-12T14.34.38] | QC Profiling 1.1.0.6088 |
| [2021-03-12T14.34.38] | Multiplet Report 1.0.0.6703 |
| [2021-03-12T14.34.38] | IUPAC Name 1.0.0.6908 |
| [2021-03-12T14.34.38] | MS Scan 1.0.0.6933 |
| [2021-03-12T14.34.38] | Peak Report 1.0.0.7139 |
| [2021-03-12T14.34.38] | Mpublish 1.0.0.6695 |
| [2021-03-12T14.34.38] | B2ADF Converter 1.0.0.6496 |
| [2021-03-12T14.34.38] | MS Reaction Optimisation 1.0.0.7110 |
| [2021-03-12T14.34.38] | MS Best Method 1.0.0.6539 |
| [2021-03-12T14.34.57] | Starting MS Scan Engine |
| [2021-03-12T14.34.57] | MS Scan succesfully done in SMPL1 |
| [2021-03-12T14.34.57] | Dataset SMPL1 processed |
| [2021-03-12T14.34.58] | Total elapsed time: 1.31 s |
| | |

Auto Attach traces: Check this option to automatically attach 1D spectra as horizontal and vertical traces in 2D spectra. With this option selected, the HSQC with the 1H spectrum can be correctly added as the horizontal trace in an HSQC spectrum.



- □ Allow events: If checked, Mgears will not block programmed events (Preferences > Scripting > Events).
- □ Autoresume on Critical Error (Not available in Debug Mode): When enabled, Mgears will resume analysis automatically should a critical error occur.
- Retry on Error Opening Dataset: Check this option if you want to force Mgears to retry opening a file after an error occurs (Errors can occur if the file is not in the expected location, or the opening operation fails). Click on the Retry Settings icon to set the number of retries and the time the system must wait between each.



□ **CSV Separator:** Select the CSV separator used in your csv input file in order to be read correctly by Mgears.

| Expert | | |
|-----------------|-------------------|---------------|
| Debug Mod | le (Execu | te All Proces |
| CSV Separator | , – | |
| Notifications - | ; 🔀 Tab | |

3.6.3. Notifications

Mgears can send automatic email notifications to users to inform them about processing status. To set up email notifications, tick the **Notifications** option and fill in the required information.

In the **Setup** tab, configure the email server from which the email will be sent by completing the information about your email server (**Server**, **Port**, **Username**, **Password**, etc).

| ✓ Notifications | | | | | | | | |
|--------------------------|--------------------|-------|---------------|-----------|------|-----------|-------|------|
| Setup Content | Options | | | | | | | |
| Email Server Configura | ation | | | | | | | |
| Server: | localhouse | Port: | 5504 | Username: | Test | Password: | ••••• | |
| Authentication Type: | No authentication | SSL | Test Address: | | | | | Test |
| Receivers | Plain text | | | | | | | |
| Get e-mail from Param | Encrypted password | | | | | | | |
| Fixed List of Receivers: | \sim | | | | | | | |



Once all fields are configured, you can test the notification by adding a Test Address and clicking on Test.

| 5504 | Username: | Test | Password: | ••••• | |
|----------------------------|-----------|------|-----------|-------|------|
| Test Address: user@mestrel | ab.com | | | | Test |
| | | | | | V |

In the **Receivers** section, you can either add a **Fixed List of Receivers** or get the recipients' emails from a **Parameter** in your spectrum.

| | Receivers | | | | | | |
|----|----------------------------|---------------------|--|--|--|--|--|
| | Get e-mail from Parameter: | | | | | | |
| | Fixed List of Receivers: | user2@mestrelab.com | | | | | |
| L. | | | | | | | |

In the **Content** tab, write the notification **Subject** and **Body text**. You can use "\$NAME\$", "\$NMR(Parameter name)\$", "\$MS(Operator)\$", etc., to get analysis-specific information in the subject line and body text. For instance, if you use \$NAME\$, the name of the dataset in hand will be used, whilst if you use \$NMR (parameter name)\$, the actual value of the parameter will be displayed.

The Body text field also admits HTML formatting.





Finally, in the **Options** tab, choose if you want notifications to be sent when a dataset is processed and/or when an error occurs, and choose if you want to attach an Mnova and/or PDF document to the notification.

| ✓ 1 | Votificati | ons | | | | | | | | |
|-----|---------------------------------------|------------|---------|--|--|--|--|--|--|--|
| S | etup | Content | Options | | | | | | | |
| | For Each Processed Group On Error | | | | | | | | | |
| | Attack | n Mnova Do | cument | | | | | | | |
| | Attach PDF Document | | | | | | | | | |
| | | | | | | | | | | |

Top Tip! All of the configuration settings entered in the various Mgears tabs can be saved and recalled in the future. This is particularly useful when you run many different analyses, as it allows a consistent and quick setup when switching between tasks. The Settings files so created (.mgrs) can therefore be thought of as the way to save a complete automation setup.

| Export Settings Save Settings Import Settings Export Settings | Load Settings | Save Settings | 📋 Import Settings | Export Settings |
|---|---------------|---------------|-------------------|-----------------|
|---|---------------|---------------|-------------------|-----------------|

This file can also be used to set up the MyGears workflows, as discussed below.



4. MyGears dialog

MyGears' workflow setup is very similar to Mgears', the main difference being that MyGears will run the automated analysis on a single dataset open in Mnova, and therefore there is no need to configure the **Input** tab.

To create a MyGears workflow from scratch, open the Mgears dialog from the **Automation** section in the Mnova ribbon and proceed as described in sections <u>3.2</u>, <u>3.3</u>, <u>3.4</u>, <u>3.5</u>, and <u>3.6</u> to configure the **Processing**, **Plugins**, **Design**, **Output**, and **Settings** of your analysis. Then, save the settings to a directory of your choice.

To run a MyGears analysis, first open your dataset in Mnova, then open the **MyGears Workflows** from the **Automation** section in Mnova. A dialog with the following buttons opens:

| MestReNova | | \searrow | | |
|----------------------------|----------------------|------------|----------|---|
| Elucidation Chemometri | s Binding | Automation | | |
| Ngears Viewer Mgears | MyGears Workflows | | | |
| MyGears Workflows | [] | × | Button | Description |
| | ‡ | | + | Add Mgears workflow |
| Workflow De | scription | | - | Remove selected workflow |
| | | | | Clear all |
| | | | \$ | Options |
| | | | * | Open MGears with the settings of the selected workflow |
| 4 | | | Ø | Run MyGears |

Click on 🕈 and select the Mgears workflow (.mgrs settings file) you want to run. You can add one or more

workflows, delete a selected workflow, or clear the whole table as needed. The workflows added will be displayed as shown below.

| Gears Work | flows | |
|------------|-------------|--|
| • | | Ø 🏶 🤇 |
| Workflow | Description | Location |
| SMA | | C:/Users/Usuario/Desktop/Datasets/SMA.mgrs |
| Verify+SQA | | C:/Users/Usuario/Desktop/Datasets/Verify+SQA.mgrs |
| veniy+3QA | | c, oseis/ osuano/ besktop/ balasets/ veniy+ Somingis |
| | | |
| | | |
| | | |
| | | |
| | | |

Click on this button 🔨 to launch the analysis. The data in the open document will be processed and the results laid out and saved as specified in the workflow parameters.

If you wish to review the analysis settings before launching the analysis, you can select the workflow you want to review and click on ¹ A dialog asking if you want to load the settings of the selected plugin will appear. Click **Yes**.

| MyGears Work | flows | × | | | | | | | |
|--------------|---|---|----------|--|--|--|--|--|--|
| + | | | | | | | | | |
| Workflow | Description | Location | | | | | | | |
| SMA | | C:/Users/Usuario/Desktop/Datasets/SMA.mgrs | | | | | | | |
| Verify+SQA | | C:/Users/Usuario/Desktop/Datasets/Verify+SQA.mgrs | | | | | | | |
| | | | | | | | | | |
| | | 😢 Question | \times | | | | | | |
| | Do you want to load the settings of the selected Plugins? | | | | | | | | |
| | | Yes No | | | | | | | |



The Mnova Gears dialog will open so you can revise and adjust your analysis configuration as needed, then save the new settings.

| 💩 Mnova Ge | ars | | | | | | ? | > |
|--|--|-------------|------------|--------------|---|-----------------|--------|----|
| 🔁 Input | ve Processing | Plugins | 🔀 Design | 📑 Output | Settings | | | |
| SQA Verify Conce Purity DB Se SMA C Pr SMA C Pr Multi UPAC MS Sc Peak Mput S A DB Se Mput S Sc Sc Sc Sc Sc Sc Sc Sc Sc Sc Sc Sc Sc S | / entration / earch ofiling plet Report C Name can Report olish C C | | | | Add Remove New Custom Plugin Delete Custom Plugin Werify Plugin Settings | i Verify SQA | | |
| Resume | 1 Load Settings | Save Settin | gs 📋 Impor | t Settings 🔹 | Export Settings | * | Cancel | RI |

Note. It is also possible to run a MyGears workflow by pressing the **MyGears** button in the **Automation** tab. In this case, MyGears will run with the configuration stored in the registry.

| Mes | itReNova | | | | | |
|--------------------------|------------------|---------|----------------------|------------|---|--|
| Elucidation Chemometrics | | | Binding | Automation | - | |
| °© | Ð | 0 | | | | |
| Mgears | Mgears Viewer | MyGears | MyGears Workflows | | | |
| | N | 1gears | | | | |



The result folder is saved under the directory previously specified in the **Output** section. This folder contains all the output generated for the current evaluation.

| > M | Scan > MS Scan_Results > | 2021-01-08T08.06.58 | |
|-----|---------------------------|---------------------|--|
| 1 | css | | |
| | data | | |
| | documents | | |
| | images | | |
| | js | | |
| | pdf | | |
| | 2021-01-08T08.06.58 | | |
| | 2021-01-08T08.06.58.resum | ne | |
| | MSScanResults | | |
| X | MSScanResults_03AGA001 | | |
| |] settings.mgrs | | |
| | | | |

Output folders and files may include:

| Туре | Name | Description | | | | | |
|------|---------------------------------------|---|--|--|--|--|--|
| | Css | Part of the html reporting | | | | | |
| | Data | Folder with .result files | | | | | |
| | Documents Folder with Mnova documents | | | | | | |
| | Images Part of the html reporting | | | | | | |
| | Js | Part of the html reporting | | | | | |
| | PDF | Folder with PDF report | | | | | |
| | Plugin specific | With Plugin specific result files (csv, word, mnova, etc) | | | | | |
| D | .log | General log of Mgears (information that you see while Mgears is running) | | | | | |
| D | .resume | File to restart the processing where it was (automatically if there is a crash or manually if the user stops Mgears on purpose) | | | | | |
| D | .html | Html Dynamic report | | | | | |
| D | Settings.mgrs | Mgears settings file | | | | | |
| | | 🗁 Folder 🛛 🗋 File | | | | | |

Plugin-specific results files (.csv, .odt, .mnova files, etc) are generally customizable in the **Plugin Settings** section. For instance, the IUPAC Name plugin can be configured to generate SDF files for each molecule, and MS Scan to lay out results in a CSV document; HTML reports can be set to include specific parameters and exclude others with Purity; and Peak Reports can be formatted as needed, etc.

| Other outputs | Result file content | |
|--|--|----------|
| 🍫 Settings ? 🛛 🗙 | Settings ? | \times |
| Options | Analysis Output | |
| ✓ Draw IUPAC Name | RT Rel Area (%) Rel Height (%) | |
| ✓ Save SDF Files ✓ Create Report | ✓ m/z Area (Abs) Scan | |
| | ✓ Total Rel Area (%) Height (Abs) Start/End Time | |
| Verify Settings ? × Load Settings Save Settings Analysis Layout HTML Report Not Flelds Verify Quality Purity Tests Molecule Image Spectra Image Image Name Documents Verify Ventov PDF | Format and font Image: Chem. Angew. Chem. J. Med. Chem. Manasee Patent Font Polyhedron RSS MS Shell Dlg 2 MS Shell Dlg 2 MS Shell Dlg 2 MS Shell Dlg 2 Bold Italic Bold Italic Bold Italic Bold Italic Strikeout Underline Writing System Ang OK Cance | |





5.1. Mnova Reports

Mnova output files are typically saved under **Documents**. However, it is possible to change the desired destination folder during the setup in the **Output** tab, as explained in the section 3.5.1.1. Other advanced reporting settings are detailed in section 3.5.4.

Mnova reports can be customized to fit a display layout of your choice in the **Design** tab (Section <u>3.4</u>), and to include the specific information (data, metadata, results, etc.) selected in the **Plugin settings**, as shown below.



Here is an example of an Mnova report obtained with the Purity plugin.





5.2. PDF Reports

PDF reports are typically saved under the **PDF** folder. However, it is possible to change the desired destination folder during the setup in the **Output** tab as explained in the section <u>3.5.1.2</u>. Other advanced reporting settings are detailed in section <u>3.5.4</u>.

As with the Mnova reports, PDF reports can be customized to fit a display layout of your choice in the **Design** tab (Section <u>3.4</u>), and to include the specific information (data, metadata, results, etc.) selected in the **Plugin settings**. PDFs are basically a static version of the Mnova reports generated by Mgears.

Below is an example of a PDF report obtained using the Purity plugin.





5.3. CSV Reports

Many Mnova Gears Plugins will generate a CSV file with their results. The content of this CSV file is usually customizable in the **Plugin specific settings,** as with the MS Scan plugin.

| Default | Settings Analysis Output RT Rel m/z Total Rel Area (%) | Custo Area (%) | ? × M. ✓ Rel Height (%) Scan Start/End Time | | | | |
|---------|--|-------------------|---|--------------------|--------------|----------|------------|
| | | Tolerance | Minimum Relative Abudance [%] | Minimum Area Thr | eshold [%] | | |
| | | 0.25 | 5 | 10 | | | |
| | | m/z [Da] | RT [min] | Total Rel Area [%] | Rel Area [%] | Abs Area | Rel Height |
| | | | | 10.28 | 100 | 14523 | 100 |
| | | | 1 | 71.47 | 100 | 100985.5 | 100 |
| | | - | | 0.86 | 73.99 | 1216 | 58.06 |
| | | | | 0.3 | 26.01 | 427.5 | 41.94 |
| | | | | 17.09 | 100 | 24147.5 | 100 |

Sometimes the **Mapping file** used in the **Input** tab can be used to generate final reports including input and output data. In these cases, a configuration of the columns reserved for outputs is possible in the plugin-specific settings dialog, as shown below for the Chrom Reaction Optimization plugin.

| OO CSV | / Inp | n Variables CSV | gurat / File | tion Mnova Par | ameters Table | 2 | | | ? | × | | | | | |
|-------------|-------|-----------------|------------------|-------------------|-----------------|--|----------|--------------|-----------|-----------|------------|---------|----------|----------|--|
| | | Parameter | | Output Colur | nn Outpu | ıt Header | | Print to HTM | 1L | | | | | | |
| | 1 | Name | | 1 | Name | | v | | | | | | | | |
| | 2 | Well | | 0 | Well Pos | ition | | | | | | | | | |
| | 3 | SM (RT) | | 5 | SM (RT) | | v | | | | | | | | |
| F . | 4 | SM (Area) | | 6 | SM (Area | a) | | | | | | | | | |
| | 5 | SM (% Area) | | 7 | SM (% A | rea) | v | | | | | | | | |
| | 6 | P1 (RT) | 90 | CSV Column | Detection | | | | | | | | ? | \times | |
| | 7 | P1 (Area) | Ov | erview of Test | output csv file | t csv file using file undefined as example. Columns that will be printed by the automation | | | | | | | | | |
| | 8 | P1 (% Area) | | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | - | |
| Test Output | | t CSV: 🔍 | 1 2 3 4 | Name | Temperat | Catalyst | Solvent | SM (%) | SM (RT) | SM (Area) | Acquisitio | Column9 | Column10 | | |
| | | | | | CS | SV Input | | Autom | ation var | iables | Mnova p | aramete | rs Ca | ncel | |

HTML reports are commonly generated by Mgears analyses. These global reports include the analysis parameters and allow a dynamic visualization of the analysis results. Direct links to other output files are also embedded in these reports.

| Parameters | 1 | | | | | | | | | | |
|---|---|---------------------|---------------------|--|--|--|---|--|--|--|--|
| Parameter | J | Value | | | | | | | | | |
| Results Directory | | C:/Users/Us | suario/Deskto | p/Results/MS Scan/20 | 021-03-12T09.59.15 | | | | | | |
| Started On | | 2021-03-12T09:59:15 | | | | | | | | | |
| Completed On | | 2021-03-12 | 2021-03-12108:58:15 | | | | | | | | |
| Minimum Relative Abundance | | 5% | | | | | | | | | |
| Tolerance | | 0.25 Da | | | | | | | | | |
| Minimum Area Threshold | | 10.00 % | | | | | | | | | |
| Show 100 ventries Output csv | Output mnova | Copy | CSV C | Columns PDF F | Print a [%] Rel Area [%] | Search: Abs Area | Rel Height [%] | | | | |
| Show 100 ventries Output csv | Output mnova | Copy | CSV C | Columns PDF F Total Rel Area 10.09 | Print a [%] | Search: Abs Area 14523.000 | Rel Height [%] | | | | |
| Show 100 ventries Output csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv | Output mnova SMPL1.mnova SMPL1.mnova | Copy m/z [Da] | CSV C | Columns PDF F I I IIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII | Print a [%] Rel Area [%] 100.00 100.00 | Search: Abs Area Abs Area 14523.000 100985.500 | Rel Height [%] | | | | |
| Show 100 entries Output csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv | Output mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova | Copy | CSV C | Columns PDF F 1 0.09 Total Rel Area 10.09 70.13 0.84 | Print a [%] Rel Area [%] 100.00 100.00 73.99 | Search: Abs Area (*) 14523.000 100985.500 1216.000 | Rel Height [%] 100.00 100.00 58.06 | | | | |
| Show 100 entries Output csv A MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv | Output mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova | Copy | CSV C | PDF F Image: Columns PDF F Image: Columns Total Rel Area Image: Columns Total Rel Area< | Print (%) (%) (%) (%) (%) (%) (%) (%) (%) (%) | Search: Abs Area () Abs Area () 14523.000 100985.500 1216.000 427.500 | Rel Height [%] 100.00 100.00 58.06 41.94 | | | | |
| Show 100 entries Output csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv | Output mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova | Copy m/z [Da] | CSV C | PDF F Image: Delement of the second se | Print Rel Area [%] 100.00 100.00 100.00 20.01 26.01 100.00 | Search: Abs Area 14523.000 100985.500 1216.000 427.500 24147.500 | Rel Height [%] 100.00 100.00 58.06 41.94 100.00 | | | | |
| Show 100 entries Output csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv | Output mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova | Copy m/z [Da] | CSV C | PDF P 10.09 70.13 0.84 0.30 16.77 0.14 | Print Rel Area [%] 100.00 100.00 100.00 26.01 100.00 48.38 | Search: Abs Area 14523.000 100985.500 1216.000 427.500 24147.500 198.112 | Rel Height [%] 100.00 100.00 58.06 41.94 100.00 49.36 | | | | |
| Show 100 entries Output csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv | Output mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova | Copy m/z [Da] | CSV C | PDF F Image: Columns PDF F 10.09 Total Rel Area 0.0.4 0.30 16.77 0.14 0.15 0.15 | Print Rel Area [%] 100.00 100.00 73.99 26.01 100.00 48.38 51.62 51.62 | Search: Abs Area 14523.000 100985.500 1216.000 427.500 24147.500 198.112 211.400 | Rel Height [%] 100.00 58.06 41.94 100.00 49.36 50.64 | | | | |
| Show 100 entries Output csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv | Output mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova | Copy m/z [Da] | CSV C | PDF F 10.09 10.09 70.13 0.84 0.30 16.77 0.14 0.15 0.11 10.11 | Print Rel Area [%] 100.00 100.00 100.00 26.01 100.00 48.38 51.62 28.65 | Search: Abs Area 14523.000 100985.500 1216.000 427.500 24147.500 198.112 211.400 162.000 | Rel Height [%] 100.00 100.00 58.06 41.94 100.00 49.38 50.64 17.40 | | | | |
| Show 100 ventries Output csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv | Output mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova | Copy miz [Da] | CSV C | PDF F 10.09 10.09 70.13 0.84 0.30 16.77 0.14 0.15 0.11 0.08 | Print Rel Area [%] 100.00 100.00 100.00 26.01 100.00 48.38 51.62 28.65 20.34 20.34 | Search: Abs Area Abs Are | Rel Height [%] 100.00 100.00 58.06 41.94 100.00 49.38 50.64 17.40 18.62 | | | | |
| Show 100 ventries Output csv A MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv MSScanResults_SMPL1.csv | Output mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova SMPL1.mnova | Copy m/z [Da] | CSV C | PDF F 10.09 70.13 70.13 0.84 0.30 16.77 0.14 0.15 0.11 0.08 0.13 0.13 | Print Rel Area [%] 100.00 100.00 100.00 26.01 100.00 48.38 51.62 28.65 20.34 32.63 | Search: Abs Area 14523.000 100985.500 1216.000 427.500 24147.500 198.112 211.400 162.000 115.000 184.500 | Rel Height [%] 100.00 100.00 58.06 41.94 100.00 49.36 50.64 17.40 18.62 24.41 | | | | |

In some cases, HTML reports can include graphics to better represent the results.

| how | 5 v entries | | | | | Copy C | SV Columns | PDF Print | | | | Sear | ch: | | | | |
|--------|----------------------------------|--------|------------|-------------|---------|--------------|--------------------|---------------|-----------|---------------|--------------|----------------|---------------|-----------------|----------------------------|-------------|-------|
| * | Name | Cpd X | Cpd | Y | 0 | EDTA 🕴 | d-glucose | glycerin |) hipp | uric_acid 0 | quinic_acid | 0 taurin | Trig_HCI | t xylitol | þ | | |
| | Sample 1 | 0.0000 | | 0.0000 | | 1.0000 | 0.0000 | 0.0000 | | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | | | |
| : : | Sample 2 | 0.0000 | | 0.0000 | | 0.0000 | 0.6150 | 0.0000 | | 0.0000 | 0.2492 | 0.1358 | 0.0000 | 0.0000 | | | |
| } | Sample 3 | 0.0000 | | 0.2665 | | 0.0000 | 0.4327 | 0.0000 | | 0.0000 | 0.0000 | 0.0898 | | 0.0000 | | | |
| 4 | Sample 4 | 0.1108 | <i>,</i> , |) loture | Product |) (%) Bis | is-add (%) Pie Cha | ert Bar Chart | 0 Name | Well Position | Product (RT) | Product (Area) | Biss-add (RT) | Biss-add (Area) | MS | Mnova File | Pdf |
| iowing | 5 ample 5 1 to 5 of 5 entries | 0.0000 | 1 | D-1 | 60 | ٥ | G | | L20-1 | A1 | | 1147649 | | | | L20-1.mnova | L20-1 |
| | | | 2 | 6-1 | 0 | ٥ | - | | L26-1 | A2 | | | | | | L25-1.mnova | L26- |
| | | | 3 | 7-1 | 2 | ٠ | • | | L27-1 | A3 | | 26796 | | 81570 | | L27-1.mnova | L27-1 |
| | | | 4 | 61 | 2 | 5 | - | | L28-1 | м | | 33299 | - | 107348 | Land and the second second | L28-1.mnova | L28-1 |
| | | | 5 | 12 | 1 | 5 | _ | | L28-2 | AS | | 28634 | | 124689 | Constraint Sector | L28-2.mnova | L28-1 |

M



| | Сору | CSV | Columns | PDF | Print |
|---|---------|-------|-----------------------|-----------------|-------|
| m | /z [Da] | RT (r | Output cs | v | [%] 🔶 |
| 5 | 000 | 1.36 | Output m m/z [Da] | nova | |
| 5 | - 000 | 1.86 | RT [min] | | |
| 5 | 0000 | 1,40 | Total Rel Rel Area | Area [%] [%] | |
| 5 | 0000 | 2.00 | Abs Area | [,.] | |
| 6 | 0000 | 1.76 | Rel Heigh | nt [%] | |

6. Mnova Gears Results Viewer

One of the most interesting features of Mnova Gears is its results viewer, which allows live interaction, reviewing, and rapid update of analysis results once an Mgears analysis has been completed.

The **Mgears Viewer** is accessible from the Mnova **Automation** section. When open, the dialog presents several action buttons described in the table below.

| Me | stReNova | Mg | jears | Viewei | | | | | | | ć | F × |
|------------------|--|----|---------|--------|-----|-----------|------|---|-----|----------|----------------------|-----|
| Elucidatio | on Chemometrics Binding Automation | | | 8 | 5 | | \$ | | | | O Analyz Agair | e – |
| Mgears | Mgears Viewer Mgears Workflows | | # | Ti | tle | Docum | nent | | l | Location | | |
| Button | Description | | | ta | | | | | | | | |
| | Load data | | eli Pia | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 0 | 1 |
| F | Get latest results from MyGears | | 1 | 2 | 5 | т | 5 | 0 | · · | 0 | 9 | 1 |
| 5 | Connect the Viewer to a results folder to get the results on-the-fly | | | | | | | | | | | |
| H | Save data | | | | | | | | | | | |
| | Save and database the current result | | | | | | | | | | | |
| | Clear results | | | | | | | | | | | |
| ¢ | Settings | | | | | | | | | | | |
| ŵ | Open the Mgears dialog with the current settings | Re | esults | | | | | | | | | 1 |
| | Show/Hide the samples table | | | | | | | | | | | |
| | Show/Hide the wellplate | | | | | | | | | | | |
| | Show/Hide the details of the results | | | | | | | | | | | |
| Analyze Again | Run analysis again for the active document | | | | | | | | | | | |



6.1. Loading results

To load analysis results, click on the load button and select the data folder in the predefined output location. Alternatively, click the small arrow next to the **Load** button to see a list of the 10 most recent results for easy access.

| Mgea | ars Viewer Chemometrics |
|------|---|
| | |
| Ø | kysers/Usuario/Desktop/Results/Chrom Reaction Optimization/2022-04-25T12.29.22_LastAnalysis |
| 0 | C:/Users/Usuario/Desktop/Results/Chrom Reaction Optimization/2023-10-04T11.48.06_NegTIC |
| 0 | C:/Users/Usuario/Desktop/Results/Chrom Reaction Optimization/2023-07-17T17.28.53 |
| 0 | C:/Users/Usuario/Desktop/Results/QC Profiling/2021-06-18T13.33.44 |
| 0 | C:/Users/Usuario/Desktop/Results/QC Profiling/2023-10-04T17.25.24_NewVersion |
| 0 | C:/Users/Usuario/Desktop/Results/Affinity Screen/2023-07-20T18.13.02_UserManual |
| ۲ | C:/Users/Usuario/Desktop/Results/Affinity Screen/2023-07-27T17.39.51_UserManual |
| 0 | C:/Users/Usuario/Desktop/Results/Affinity Screen |
| 0 | C:/Users/Usuario/Desktop/Results/Chrom Reaction Optimization/2023-09-28T15.36.03_LastAnalysis |
| 0 | C:/Users/Usuario/Desktop/Results/Chrom Reaction Optimization/2023-07-17T16.34.55 |

All samples processed in the selected analysis are loaded into the Mgears viewer's main list and well plate overview. Detailed results are visible at the bottom section.

When the viewer is connected to a folder 🖾, the results saved to that folder are automatically loaded (onthe-fly) once the analysis is completed.

Note that the Mgears viewer shows the results of one automation run at a time. When using MyGears, it will show the latest results.

| ~ | | 5 | HE | | ¢. | ê 🗄 | | Ê | | | Д | Naly Agai |
|-------|-------------------------------------|--|---|---|--|---------------------------------|--------------------------------|----------|---------------------------|-------|--------------------------------------|--------------|
| ŧ | | Title | | Doc | ument | | | | | | | |
| | RE/ | ACTION | I-02 RE | ACTION | 1-02.m | nova C:/ | Users/ | /Usuario | o/Deskt | op/Re | sults/(| Chro |
| | RE/ | ACTION | I-03 RE | ACTION | 1-03.mr | nova C:/ | Users/ | /Usuario | o/Deskt | op/Re | sults/0 | Chro |
| | | | | | | | | | | | | |
| l Pla | te – | 2 | 2 | 1 | 5 | 6 | 7 | 0 | 0 | 10 | | |
| 1 | | 2 07.44 | 5 | 4 | 5 | 0 | , , | 0 | 9 | 10 | | |
| Chro | m R | eaction | Optimiz | ation | | | | | | | | _ |
| Chro | m R esul | eaction t in Well sults | Optimiz Plate: Unkno | SM (% A | Area) Metadat | ta Co | • ntrols | RT | س لم Statistics | Ē | ŵ | |
| R | m R esult Res Na | eaction of the time of time of the time of the time of tim | Optimiza Plate: Unkno ACTIO | SM (% A wns N-01 | Area) Metadat | ta Co | • ntrols | RT : | ₩ Statistics | | ŵ | |
| R | m R esult Res Na | eaction t in Well sults ell: A1 Name | Optimiz Plate: Unkno ACTIO | ation SM (% A wns N-01 ype | Area) Metadat RT | a Co Are | ntrols 2a | RT S | Statistics % Area | | ÷ | |
| R | m R esult Res Na We | eaction of t in Well sults me: RE ell: At Name SM | Optimizi Plate: Unkno ACTIOI | SM (% A wns N-01 ype Material | Area) Metadat RT 0.959 | ta Co Are 246812 | ntrols | RT 9 | Statistics % Area | | ÷ | |
| R | m R esult Res Na W 1 | eaction of t in Well sults anne: RE ell: A1 Name SM P1 | Optimiza Plate: Unkno ACTIOI Start I Produ | ation SM (% A wns N-01 ype Material uct | Area) Metadat RT 0.959 0.576 | a Co Are 246812 271113 | ntrols ea 28377 35381 | RT 9 | Statistics % Area | | •••••••••••••••••••••••••••••••••••• | |



6.1.1. Main list section

In the upper part of the Mgears Viewer, analysis samples are listed and numbered with certain details such as **Title**, **Document**, and **Location**. It is possible to change the configuration of this table. To do so, click on the **Settings** button is and customize the **Main List** visualization by checking/unchecking the available items.

| | # | Title | Document | Location |
|-------------|-------------|--------------|--------------|--------------|
| /isible | / | \checkmark | \checkmark | \checkmark |
| | | | | |
| | | | | |
| ell Plate – | | | | |
| | | | | 42 |
| | (olumpine: | | | 12 |

The Main list can be completely hidden from the Mgears Viewer by clicking on this button \blacksquare .

| 📑 🐻 | | \$ | õ 🖽 | •••• | Ê | | | ļ | 🚍 · 🛱 🔽 🖨 🗖 👘 🔛 💼 🗎 | 1 |
|---|--|---|---|--|---|--------------------------------------|-------|----------|--|----------------|
| Title | Dor | ument | | | | | | | Well Plate | |
| PEACTION | | NL-02 m | | orc/l | Isuario | /Dockte | op/Po | culte/ | 1 2 3 4 5 6 7 8 9 | 10 |
| NLACTION | | N-02.111 | 10va C./U | 5015/0 | , sudito | Desku | op/ne | suits/ | A 28.99 27.44 45.29 48.75 0.00 45.18 38.58 24.56 0.00 | 57.60 |
| REACTION | N-03 REACTIO | N-03.m | nova C:/U | sers/L | Jsuario | /Deskto | op/Re | sults/ | | |
| ate | | _ | _ | _ | _ | _ | _ | _ | | |
| 2 | 3 4 | 5 | 6 | 7 | 8 | 9 | 10 | | Results | |
| 99 27.44 | 45.29 48.75 | 0.00 | 45.18 38 | .58 | 24.56 | 0.00 | 57.60 | 0 | Chrom Reaction Optimization | |
| om Reaction | Optimization | | | | (b) | <i>î</i> = | r#1 | | Result in Well Plate: SM (% Area) - JA JA Results Unknowns Metadata Controls RT Statistics Name: REACTION-01 Well: A1 | i 👘 |
| om Reaction tesult in Wel | Optimization | Area) | | • | y j j | <u>v∫t</u> ≜ | Ē | 1 | Result in Well Plate: SM (% Area) - JA JA Results Unknowns Metadata Controls RT Statistics Name: REACTION-01 Well: A1 Name Type RT Area % Area | 5 20 |
| om Reaction Result in Wel Results | Optimization | Area) Metadal | a Cont | * rols | ¥∫≜ RT S | √ ↓ tatistics | Ē | 1 | Result in Well Plate: SM (% Area) J Results Unknowns Metadata Controls Name: REACTION-01 Well: A1 Name Type RT Area % Area 1 Start Material 0.959 2468128377 | 20 |
| om Reaction Result in Wel Results Name: R Well: A | Optimization II Plate: SM (% Unknowns EACTION-01 1 | Area) Metadal | a Cont | ▼ rols | ¥∫≧ RT S | √ I _A tatistics | Ē | | Result in Well Plate: SM (% Area) Results Unknowns Metadata Controls RT Statistics Name: REACTION-01 Well: A1 Name Type RT Area % Area 1 SM Start Material 0.959 2468128377 28.99 2 P1 Product 0.576 2711135381 31.85 | 2a |
| m Reaction Result in Wel Results Name: R Well: A Name | Optimization II Plate: SM (% Unknowns EACTION-01 1 e Type | Area) Metadal RT | a Cont | • rols | T RT S 9 | tatistics | Ē | ÷ | Result in Well Plate: SM (% Area) Results Unknowns Metadata Controls RT Statistics Name: REACTION-01 Well: A1 Name Type RT Area % Area 1 Start Material 0.959 2468128377 28.99 2 P1 Product 0.576 2711135381 31.85 3 82 By Product 0.485 3258906350 38.28 | s |
| m Reaction tesult in Wel Results Name: R Well: A Name 1 SM | Optimization II Plate: SM (% Unknowns EACTION-01 1 e Type Start Materia | Area) Metadal RT I 0.959 | a Cont Area 2468128 | • rols 377 2 | ₹ RT S % 28.99 | یل <u>ت</u> tatistics 5 Area | | | Name Type RT Area % Area 1 SM Start Material 0.959 2468128377 28.99 2 P1 Product 0.576 2711135381 31.85 3 \$22 By Product 0.485 3258906350 38.28 4 P3 Ignored - - - | 2a |
| m Reaction Result in Wel Name: R Well: A Name 1 SM 2 P1 | Optimization II Plate: SM (% Unknowns EACTION-01 1 e Type Start Materia Product | Area) Metadat RT I 0.959 0.576 | a Cont Area 2468128 2711135 | • rols 377 2 381 3 | ₹ RT S 94 28.99 31.85 | ±∫ tatistics 5 Area | Ē | ÷ | Result in Well Plate: SM (% Area) J J J Results Unknowns Metadata Controls RT Statistics Name: REACTION-01 Well: A1 1 SM Start Material 0.959 2468128377 28.99 2 P1 Product 0.576 2711135381 31.85 3 B2 By Product 0.485 3258906350 38.28 4 P3 Ignored - - - | 2a |
| m Reaction Result in Wel Name: R Well: A Name 1 SM 2 P1 3 P2 | Optimization II Plate: SM (% Unknowns EACTION-01 1 e Type Start Materia Product By Product | Area) Metadal I 0.959 0.576 0.485 | a Cont Area 2468128 2711135 3258906 | * rols 3377 2 3381 3 350 3 | RT S RT S 28.99 31.85 38.28 | tatistics | | ▲ | Result in Well Plate: SM (% Area) J_A J_A Results Unknowns Metadata Controls RT Statistics Name: REACTION-01 Well: A1 Area % Area 1 SM Start Material 0.959 2468128377 28.99 2 P1 Product 0.576 2711135381 31.85 3 P2 By Product 0.485 3258906350 38.28 4 P3 Ignored - - | 20 20 20 |



6.1.2. Well plate section

A **Well Plate** overview is available and can be particularly useful when analysis samples are loaded in a well plate. The dimensions of the well plate can be defined in the **Mgears Viewer Settings** dialog.

| | # | Title | Document | Location |
|------------|----------|----------|---|---|
| Visible | v | v | Image: A start of the start of | Image: A start of the start of |
| | | | | |
| | | | | |
| Well Plate | 9 | | | |
| | | | | 12 |

Watch out! If a Mapping file is used in an analysis, and the option for reading position in the well plate is selected in the advanced filtering options, then the dimensions of the well plate will be automatically set and will not be editable in the **Mgears Viewer Settings** dialog.

| -Well Plate Number Of Columns: | Disabled \rightarrow | 12 🗘 |
|---|------------------------|------|
| Options Apply Design After Running Analyze Again | | |

An option to **Draw Well Plate with Enhanced Graphics** is available in the **Mgears Viewer Settings** too. This feature allows you to choose between displaying **Bubble** plots or a **Heat Map** within the well plate, instead of presenting numerical results. The **Text font** and **size** can be customized. See the example below.

| Draw Well Plate with Enhanced Gra | phics | | | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 0 | 1 |
|---|---|----------------------------|------|-------|-------|---------------------|-------|-------|-------|-------|-------|-------|------|
| Bubbles | Heat Map Text font | Show Numbers in Heat Map | -> A | 29.20 | 27.71 | 45.43 | 41.10 | 67.31 | 45.31 | 39.02 | 24.80 | 30.74 | 58. |
| | Segoe UI | ▼ 9pt \$ | | | | | | | | | | | |
| Draw Well Plate with Enhanced Gra | phics | | | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 0 | 1 |
| Bubbles | Heat Map | ✓ Show Numbers in Heat Map | | 1 | 2 | 5 | - | | 0 | | 0 | 9 | 1 |
| | Text font | | -> A | • | • | • | • | | • | • | • | • | |
| | | | | | | | | | | | | | _ |
| ✓ Draw Well Plate with Enhanced Gra | phics | | | | 2 | 2 | 4 | F | 6 | 7 | 0 | 0 | 4 |
| O Bubbles | Heat Map | Show Numbers in Heat Map | _ | 1 | 2 | 3 | 4 | 5 | 0 | / | 8 | 9 | 10 |
| | Text font | | → A | | | | | | | | | | |
| | Segoe UI | - 9pt - | | | | | | | | | | | |
| Draw Well Plate with Enhanced Gra | phics | | | | 2 | 2 | | - | 6 | - | 0 | 0 | |
| O Bubbles | Heat Map | ✓ Show Numbers in Heat Map | | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| | Text font Segoe UI | ✓ 9pt ¹ | → A | 29.20 | 27.71 | <mark>45.4</mark> 3 | 41.10 | 67.31 | 45.31 | 39.02 | 24.80 | 30.74 | 58.2 |



| | / | Add Suffi | x to Valu | es in the | Well Plate | e % | | | | | | |
|---|----|------------|-----------|-----------|------------|--------|--------|--------|--------|--------|---|---|
| | We | ll Plate — | | | | | | | | | | |
| | | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 4 | • |
| | Α | 29.20% | 27.71% | 45.43% | 41.10% | 67.31% | 45.31% | 39.02% | 24.80% | 30.74% | 5 | , |
| Į | • | | | | | | | | | Þ | , | |

The **Well plate** overview can be completely hidden from the Mgears Viewer by clicking on this button **III**.

| | Mgears Viewer - 2022-04-25T12.29.22_LastAnalysis |
|--|--|
| | |
| # Title Document | # Title Document |
| REACTION-02 REACTION-02.mnova C:/Users/Usuario/Desktop/Results/Chrom | 2 REACTION-02 REACTION-02.mnova C:/Users/Usuario/Desktop/Results/Chrom |
| REACTION-03 REACTION-03.mnova C:/Users/Usuario/Desktop/Results/Chrom 💌 | 3 REACTION-03 REACTION-03.mnova C:/Users/Usuario/Desktop/Results/Chrom |
| Mall Diste | 4 |
| 1 2 3 4 5 6 7 8 9 10 | |
| A 28.99 27.44 45.29 48.75 0.00 45.18 38.58 24.56 0.00 57.60 | Chrom Reaction Optimization |
| | No. of ACTION AL |
| Result in Well Plate: SM (% Area) 🔹 🌿 🏂 📸 | Wall: A1 |
| Result in Well Plate: SM (% Area) Results Unknowns Metadata Controls RT Statistics | Well: A1 Name Type RT Area |
| Result in Well Plate: SM (% Area) Results Unknowns Metadata Controls RT Statistics Name: REACTION-01 Well: A1 | Name Type RT Area % Area 1 Start Material 0.959 2468128377 28.99 |
| Result in Well Plate: SM (% Area) Results Unknowns Metadata Controls RT Statistics Name: REACTION-01 Well: A1 Name Type RT Area % Area | Name Type RT Area % Area 1 SM Start Material 0.959 2468128377 28.99 2 P1 Product 0.576 2711135381 31.85 |
| Result in Well Plate: SM (% Area) Image: Plate: Image: Plate: SM (% Area) Image: Plate: Image: Plate: SM (% Area) Image: Plate: Image: Plate: SM (% Area) Image: Plate: <td>Name Type RT Area % Area 1 SM Start Material 0.959 2468128377 28.99 2 P1 Product 0.576 2711135381 31.85 3 P2 By Product 0.485 3258906350 38.28</td> | Name Type RT Area % Area 1 SM Start Material 0.959 2468128377 28.99 2 P1 Product 0.576 2711135381 31.85 3 P2 By Product 0.485 3258906350 38.28 |
| Result in Well Plate: SM (% Area) Results Unknowns Metadata Controls RT Statistics Name: REACTION-01 Well: A1 Name Type RT Area % Area 1 SM Start Material 0.959 2468128377 28.99 2 P1 Product 0.576 2711135381 31.85 | Name Type RT Area % Area 1 SM Start Material 0.959 2468128377 28.99 2 P1 Product 0.576 2711135381 31.85 3 PZ By Product 0.485 3258906350 38.28 4 P3 Ignored - - - |
| N (% Area) Image: Image | Name Type RT Area % Area 1 SM Start Material 0.959 2468128377 28.99 2 P1 Product 0.576 2711135381 31.85 3 P2 By Product 0.485 3258906350 38.28 4 P3 Ignored - - - |
| Result in Well Plate: SM (% Area) Image: Area Image: REACTION-01 Well: A1 Name: REACTION-01 Well: A1 Name: Type R Area % Area 1 SM Start Material 0.959 2 P1 Product 0.576 3 P2 By Product 0.485 3 P2 | Well: A1 Name Type RT Area % Area 1 SM Start Material 0.959 2468128377 28.99 2 P1 Product 0.576 2711135381 31.85 3 P2 By Product 0.485 3258906350 38.28 4 P3 Ignored - - |



6.1.3. Results section

In the **Results** section, detailed analysis results are displayed.

| Result: 0.83 | | | | |
|-----------------------------|---------|-------|--------------|--|
| Tosts | | | | |
| Name | Quality | Score | Significance | |
| 1H Global Counts | 0.59 | 1.00 | 1.43 | |
| 1H Prediction Bounds Metric | 0.67 | 1.00 | 1.99 | |
| 1H Assignments | 0.67 | 0.84 | 4.12 | |
| HSQC Global Counts | 0.60 | 1.00 | 1.48 | |
| HSQC Assignments | 0.80 | 1.00 | 4.04 | |
| Predictions Congruence | 0.21 | 0.31 | 1.97 | |

If the analysis performed generates multiple results per sample, the Mgears viewer provides flexibility to display those results.

| Results | Results |
|---|--|
| Results Chrom Reaction Optimization Result in Well Plate: SM (% Area) SM (% Area) P1 (% Area) P2 (% Area) Name: REACTIO Vell: A1 Bar Chart Areas Pie Chart With Unknowns % Area | Results MS Scan Settings Mass Spectrum Extraction Minimum Relative Abundance : 5 % Tolerance : 0.25 Da Minimum Area Threshold : 10 % Results RT ranges: m/z: EIC 2: 5 0 Da |
| 1 SM Start Controls Chart 2 P1 Product 0.576 2711135381 31.85 | m/z [Da] RT [min] Total Rel EIC 3: 5 0 Da ea 1 5 0 1. 70.13 100.00 100985.500 |



| Mgears | Viewer - | 2021-0 | 6-18T13 | .33.44_Re | port | | | 8 × |
|----------|--|---|--|--|---|--|---------------|-----------|
| - | 3 | HE | | ‡ 🏟 | | | Analy Agai | ze 👻 n |
| # 3 | РКОТО | Title N_ETHY | LBENZEN | NE PROTO | Docum N_ETHYLB | nent ENZENE | .mnova | |
| 4 | QUININ | IE | | QUININ | IE.mnova | | | Ţ |
| 4 | | | | | | | Þ | |
| Well Pla | ate | | | | | | | |
| | 2 | | 3 | | 4 | 5 | 6 | 7 |
| A FEL | ODIPINE | PROTO | N_ETHY | LBENZENE | QUININE | | | |
| 4 | | | | | _ | | | |
| Well Dia | to Chowin | | | Dook B | loport Docu | 1+ | | ų |
| well Pla | te showin | iy. | | Peak N | teport Resu | it. | | |
| Results | | | | | | | | |
| Peak | Report R | Result | Multiple | t Report Re | sult | | | H |
| Rep | ort: 1.5, 1.5, 1.6, 1.7, 1.8, 2.3, 2.7, 3.1, 3.4, 4.9, 5.5, 7.3 | MR(CD 1.5, 1.5 1.5, 1.6 1.6, 1.6 1.7, 1.7 1.8, 1.9 2.3, 2.3 2.7, 2.7 3.1, 3.2 3.4, 3.4 4.9, 4.9 5.7, 5.7 7.4 7.4 7.4 7.4 7.4 7.4 7.4 7 | Cl3, 400 l 5, 1.5, 1.5 5, 1.6, 1.6 5, 1.7, 1.7 7, 1.8, 1.8 9, 2.3, 2.3 9, 2.3, 2.3 1, 2.7, 2.7 2, 3.2, 3.2 1, 3.4, 3.4 9, 5.0, 5.0 1, 5.8, 5.8 1, 7, 5, 7, 5 1, 7, 7 1, 7, 7 | $\begin{array}{l} MHz): \ \delta = 0\\ i, \ 1.5, \ 1.5, \\ i, \ 1.6, \ 1.6, \\ i, \ 1.7, \ 1.7, \\ i, \ 1.8, \ 1.8, \\ i, \ 2.3, \ 2.3, \\ i, \ 2.6, \ 2.6, \\ i, \ 2.7, \ 2.7, \\ i, \ 3.2, \ 3.2, \\ i, \ 3.4, \ 3.4, \\ i, \ 5.0, \ 5.0, \\ i, \ 5.8, \ 5.8, \\ i, \ 5.0, \ 5.0, \ 5.0, \\ i, \ 5.0, \ 5.0, \ 5.0, \ 5.0, \\ i, \ 5.0, \ $ |).8, 0.8, 0.8, 0.8, 1.5, 1.5, 1.5, 1.5, 1.5, 1.1, 1.6, 1.6, 1.4, 1.4, 1.4, 1.4, 1.4, 2.3, 2.3, 2.3, 2.3, 2.3, 2.3, 2.3, 2.4, 3.4, 3.4, 3.4, 3.4, 3.4, 3.4, 3.4, 3 | 8, 1.4, 5, 1.5, 6, 1.6, 7, 1.7, 8, 1.8, 3, 2.3, 7, 2.7, 1, 3.1, 4, 3.4, 9, 4.9, 0, 5.5, 3, 7.3, | | |

The **Results** section can also be completely hidden from the Mgears Viewer by clicking on this button

| Agears Viewer | - 2022-04-25T12. | 29.22_L | astAnalysis | | | | × | M | gears | Viewer - 2 | 2022- | 04-25T12 | 29.22_ | LastAna | alysis | | | | |
|-------------------|--------------------|------------|----------------|--------------|----------|-----------------|------|---|---------|------------|-------|----------|--------|---------|---------|---------|--------|---------|------------------------------|
| • | 5 8 8 8 | ¢ (| ð 🔳 🖽 | Ê | | Analyz Agair | ze 👻 | 7 | - | i | H | 8 🗖 | Φ | ÷ [| | ľ9 | | | Co Analyz Again |
| # T | tle Doc | ument | | | | | | | # | Title | | Doc | ument | | | | | | |
| REACT | ION-02 REACTION | 1-02.m | nova C:/Users, | /Usuario/Des | ktop/Re | sults/Chro | m | 2 | | REACTIO | N-02 | REACTIO | N-02.m | nova (| :/Users | /Usuari | o/Desk | top/Res | ults/Chror |
| REACT | ION-03 REACTION | N-03.mi | nova C:/Users, | /Usuario/Des | ktop/Res | sults/Chro | m 👻 | 3 | | REACTIO | N-03 | REACTIO | N-03.m | nova (| :/Users | /Usuari | o/Desk | top/Res | ults/Chror |
| | | | | | | 1 | | 4 | | REACTIO | N-04 | REACTIO | N-04.m | nova (| :/Users | /Usuari | o/Desk | top/Res | ults/Chror |
| 1 2 | 3 4 | 5 | 6 7 | 8 9 | 10 | | | 5 | | REACTIO | N-05 | REACTIO | N-05.m | nova (| :/Users | /Usuari | o/Desk | top/Res | ults/Chror |
| A 28.99 27. | 45.29 48.75 | 0.00 | 45.18 38.58 | 24.56 0.00 | 57.60 | | | 6 | | REACTIO | N-06 | REACTIO | N-06.m | nova (| :/Users | /Usuari | o/Desk | top/Res | ults/Chror |
| | | | | | | | | 7 | | REACTIO | N-07 | REACTIO | N-07.m | nova (| :/Users | /Usuari | o/Desk | top/Res | ults/Chror |
| esults | | | | | | | | 8 | | REACTIO | N-08 | REACTIO | N-08.m | nova (| :/Users | /Usuari | o/Desk | top/Res | ults/Chror |
| Chrom Read | ion Optimization | | | | | | | 9 | | REACTIO | N-09 | REACTIO | N-09.m | nova (| :/Users | /Usuari | o/Desk | top/Res | ults/Chror |
| Result in | Woll Diato: SM (%) | Area) | | ./@ ./t | Ê | | | 4 | | | | | | | | | | | Þ |
| Results | Unknowns | Motadal | a Controls | | er EQ | | | W | ell Pla | te 2 | 3 | 4 | 5 | 6 | 7 | 8 | 0 | 10 | 1 |
| Name | : REACTION-01 | rietada | a condois | KI Staust | 103 | | | A | 28.9 | 99 27.44 | 45.2 | 9 48.75 | 0.00 | 45.18 | 38.58 | 24.56 | 0.00 | 57.60 | |
| Well: | A1 | | | | | _ | | | | | | | | | | | | | |
| Na | ime Type | RT | Area | % Are | ea . | ^ | | | | | | | | | | | | | |
| 1 SN | Start Material | 0.959 | 2468128377 | 28.99 | | | | | | | | | | | | | | | |
| 2 <mark>P1</mark> | Product | 0.576 | 2711135381 | 31.85 | | | | | | | | | | | | | | | |
| 3 P2 | By Product | 0.485 | 3258906350 | 38.28 | | - | | | | | | | | | | | | | |
| | | | | | | | | | | | | | | | | | | | |
| | | | | | | | | | | | | | | | | | | | |



6.2. Reviewing results

Reviewing analysis results is available for most plugins and can be done on a sample-by-sample basis. Click on a sample (table row or well from the plate overview) to load the corresponding Mnova result document and detailed results.



You can review and edit your results using the standard tools from Mnova.

6.2.1. Changing analysis settings

Mgears allows you to modify your current settings and re-run calculations on your data. Depending on what you wish to modify you can either:

a. Click the brick icon in the top bar of the Mgears Viewer. This opens the Mgears dialog with the current settings. The **Input**, **Processing**, **Output**, and **Setting** tabs are not editable, but you can make changes in the **Design** and **Plugins** tab. After making desired adjustments, click **Update**, and then **Analyze Again** to relaunch the analysis with the updated settings.

| Note. To access | these Mgears settings from the M | gears Viewer, make sure to en | able the option Show |
|------------------|--|-------------------------------|-----------------------------|
| Button to Open | Setting in Mgears in the Mgears | Viewer Settings 🌣 . Without | this option enabled, |
| the brick icon w | on't appear in the top bar of the N | 1gears viewer. | |
| | Add Suffix to Values in the Well Plate | | |
| | ✓ Show Button to Open Settings in Mgears | | |
| | Reset My Gears List | | |
| | | OK Can | zel |

| ts 💡 | Mnova Gears |
|--|---|
| nrom Reaction Optimization | 🖓 Input 😵 Processing 🚱 Plugins 🧏 Design 📑 Output 🏟 Settings |
| Result in Well Plate: SM (Results Unknowns | Using Automatic Detection Experiments Selection C/Users/Usuario/Desktop/Datasets/By Plugin/Affinity Screen/Input |
| Name: REACTION-04 Well: A4 | Pointin Drectory - NUM 1H 13C 1H 13C COSY NOESY HMBC ROESY COSY NOESY HMBC ROESY COSY NOESY HMBC ROESY TOCSY NOESY HMBC ROESY TOCSY NOESY GC/LC/MS Chromatography UV/IR/Raman/Fluorescence Mnova Documents Orders Custom Format |
| 1 SM Start Mate 2 P1 Product 3 P2 By Product | Advanced Options |
| 4 P3 Ignored | Main SDF File: |

b. For some bricks, you can access specific settings directly by clicking the brick 👼 icon in the Results section of the Mgears Viewer. This provides access to brick-specific settings, bypassing the Mgears tabs.

| | Anal Ag | yze 👻 | | | | | | | | | | Λ | |
|---------------------------|------------|-------|-------|-------|------------------|--------|-------------|----------|----------------|--------|------------|-------|---------|
| 7 8 9 10 | 11 12 | Chi | rom | React | ion Optimizatio | n Sei | tings | | | | | : | × |
| | 11 12 | | Н | | | | | | | | | | 0 |
| , 🍊 🗭 🕰 | | Inpu | ıt | Analy | sis Quality C | Contro | ls Out | put | | | | | |
| | | Read | tion | Compo | onents | | | | | | | | |
| | / | | | Name | Туре | | Mol. File | Smiles | Mol. Formula | MZ | RT | Color | Externa |
| | / | | 1 | SM | Start Material | * | | | | | 0.9500 | | |
| | | | 2 | P1 | Product | * | | | | | 0.5600 | | |
| Metadata Controls RT Stat | istics | | 3 | P2 | By Product | * | | | | | 0.4800 | | |
| | | | 4 | P3 | Ignored | * | | | | | 0.4700 | | |
| Area % Area | | | | | | | | | | | | | |
| 3937169 29.20 | | | • | | | | | | | | | | • |
| 1935555 31.49 | | CSV | _ | | | | | | | | | | |
| 4576553 37.93 | | CSV | File: | C:/Us | ers/Usuario/Desk | top/D | Datasets/By | Plugin/C | Chrom RO/Datas | et/Map | ping file. | CSV | |
| | - | | | | | | | | | | ОК | | Cancel |



6.2.2. Result reviewing tools

In the **Results** section, you will discover a range of tools to enhance and update your analysis results. These tools may include manual peak assignment, adding comments, overriding results, and more. The specific options available depend on the Mgears brick in use. See some examples in the image below.

| | QC Profiling Viewer |
|--|--|
| Reaction Optimization | Data ID: Sample A03-2 |
| ult in Well Plate: Pie Chart Areas - 🧏 🌿 🗟 👘 | Content m/z Group |
| sults Unknowns Formulas Metadata Controls RT Statistics | 1 FP1 6584.4 Final Product |
| ame: REACTION-01 Madify pool accimpont | 2 FP2 6598.4 Final Product |
| Name Type | S 3 FP3 6681.5 Final Product |
| SM Start Material | Adding/removing/editing |
| P1 Product 0.576 2851035555 31.49 | 6 SM3 6502 Startin m/z included in the analysi |
| | |
| P2 By Product 0.485 3434576553 37.93 | |
| | OC Broßling |
| | |
| | Result in Well Plate: Final Product (%) 🔽 🚔 🎼 |
| Affinity Screen Viewer | |
| Lizzad N010 | General Groups Peaks Deconvolution Controls |
| | |
| Matched as (5 420 1100 | Total (%) Comment |
| Matched M/z 429.1180 | Total (%) Comment |
| Matched m/z 429.1180 Matched RT 2.587 Qualifier Overriding results | Total (%) Comment Comm |
| Matched m/z 429.1180 Matched RT 2.587 Qualifier Overriding results Score 0.781 | Total (%) Comment 1 18 which column 2 74 1000000000000000000000000000000000000 |
| Matched m/z 429.1180 Matched RT 2.587 Qualifier Score 0.781 Status Matched | Total (%) Comment 1 18 which column 2 74 3 3 1%), (1.600, 2%) (2.020, 1%) 9 ✓ Mgears QC Profiling ? × |
| Image: Notify and Constraints Matched m/z 429.1180 Matched RT 2.587 Qualifier Overriding results Score 0.781 Status Matched Not matched | I Total (%) Comment 1 18 which column 2 74 1 3 1%), (1.600, 2%) (2.020, 1%) 9 ✓ Mgears QC Profiling ? × |
| Light Nors Matched m/z 429.1180 Matched RT 2.587 Qualifier Overriding results Score 0.781 Status Matched Not matched Matched | Total (%) Comment 1 18 which column 2 74 3 3 1%), (1.600, 200, 100, 0 9 74 With column 74 74 74 3 1%), (1.600, 200, 100, 0 9 74 74 New Comment for Group Starting Material ? × |
| Light Nors Matched m/z 429.1180 Matched RT 2.587 Qualifier Overriding results Score 0.781 Status Matched Not matched Matched Hit Matched | I Total (%) Comment 1 18 which column 2 74 Image: Comment of the second |

6.2.3. Advanced result reviewing with Mnova plugins

An advanced review of the sample results can sometimes be achieved with the Mnova Standard plugins, as is the case with Purity and SMA, for example.

In the example below, an open Mgears results document is loaded into the Mnova Purity dialog:

- 1- Click on sample to view results in Mgears viewer.
- 2- Open Purity plugin in the Mnova **Quantitation** ribbon.
- 3- Then, click on 👻 to load the Purity results from the open Mnova document.
- 4- Sample and reference details, as well as all spectral multiplets, are loaded in the **Purity** dialog.
- 5- Revise and edit sample results.
- 6- Edited results will be automatically updated in the Mgears Viewer and Mnova document.
Open a sample result in the Mgears Viewer



Open Mnova Purity plugin

| Purity | 2 | | | | | | | <i>6</i> × |
|----------|-----------|-------|-------|------|----------------|--------|--------|------------|
| D | simonta | 0 | | | Ф | | | |
| Sample | Dotails - | | | Rofo | rence Det | aile — | | _ |
| Mol Wei | nht. | | * | Nam | o. [| 4115 | - | 2 |
| Weight (| (ma). | | - | Weig | e. ht (ma): | | | |
| Desulte | (ing). | | | weig | int (ing). | | | 4 |
| Results | | | | | | | | |
| Purity A | verage: | | | RSD | %: | | | U |
| Name | Score | Shift | Range | Hs | Purity | SNR | Abs In | e |
| | | | | Lo | ad r | esu | lts | |
| | | | | | | | | 1 |
| | | | | | | | | - 24 |
| | | | | | | | | Ch |
| | | | | | | | | |

| Mol We Re Pur | Weight: ight (mg): sults ity Average: | 384. 11.6 99.42 | 2538 ~ 310 | Name: T Weight (mg): 8 RSD%: 0.1 | FCNB 8.182 244 | | • | |
|------------------------|--|-----------------------|--------------------------|--|----------------------|------------------|---|----------|
| | Name | oselec | Shift | Range | Hs | Purity | ^ | - |
| 1 | 🗹 12(dd) | 1 | 7.37 | 7.39227.3465 | 1 | 99.269 | | <u>_</u> |
| 2 | 🗹 11(t) | 1 | 7.23 | 7.25797.2018 | 1 | 99.069 | | |
| 3 | 🗹 19(t) | 1 | 1.06 | 1.08941.0260 | 3 | 99.592 | | đ |
| 4 | 6(s) | 0 | 8.90 | 8.91408.8840 | 1 | 95.239 | | |
| 5 | 🗆 San | nple | e re | sults lo | ad | ed ₅₇ | | |
| 6 | 3(s) | 0 | 5.31 | 5.32305.2930 | 1 | 101.586 | | |
| 7 | 🗌 18(m) | 0 | 3.94 | 3.99983.8891 | 2 | 101.335 | | |
| 8 | 25(s) | 0 | 3.48 | 3.49873.4687 | 3 | 94.799 | | |
| • | 20 21(d) | 0 | 2 23 | 2 2535 2 2103 | 6 | 97 409 | | |

| Mo We | ight (mg): | 384.2538 × 11.6310 | Name: Weight | TCNB (mg): 8.182 | | | • | (|
|----------|------------------------|-----------------------|-----------------|---------------------|-----|---------|---|---|
| Re Pu | sults rity Average: | 99.169 | | RSD%: 0.101 | | | • | |
| | Name | Autoselected | Shift | Range | Hs | Purity | • | 4 |
| 1 | 🗹 12(dd) | 1 | 7.37 | 7.3927.346 | 1 | 99.269 | | 9 |
| 2 | 🗹 11(t) | 1 | 7.23 | 7.2587.202 | 1 | 99.069 | | 6 |
| 3 | [19(t) | 1 | 1.06 | 1.0891.026 | 3 | 99.592 | | |
| 4 | | 0 | 8.90 | 8.9148.884 | 1 | 95.239 | | |
| 5 | 10(dd) | Desele | ect | a mul | tip | let | | |
| 6 | 3(s) | 0 | 5.31 | 5.3235.293 | 1 | 101.586 | | |
| 7 | 18(m) | 0 | 3.94 | 4.0003.889 | 2 | 101.335 | | |
| 8 | 25(s) | 0 | 3.48 | 3.4993.469 | 3 | 94.799 | | |
| • | 20.21(d) | 0 | 2.23 | 2,254,2,210 | 6 | 97 409 | | |

Results automatically updated in the Mgears Viewer







6.3. Saving results

When revising your results, you may want to reanalyze your dataset with the changes you made. To do so, click on the **Analyze Again** button at the top-right side of the **Mgears Viewer**. The analysis results will be automatically updated in the open document, as seen in the example below for the Multiplet report plugin.



If you wish to reanalyze the whole batch, click on the little arrow next the the **Analyze Again** button and choose **Analyse Again All Results**. Mgears will recalculate and update the results for the whole well plate.



If you are happy with these new results, you can click on Η to save them to the output folder.



Top Tip! Enable the option **Save Automatically upon Clicking Analyze Again** in the **Mgears Viewer Settings**. The results will then be automatically saved to the output folder without the need to hit **Save** every time you reanalyze a sample.

| -Visualization | | | | |
|-----------------------------------|---|---|----------------|--------------|
| -Main List - | | Tul | | |
| | # | litle | Document | |
| Visible | \checkmark | \checkmark | \checkmark | \checkmark |
| Options ✓ Apply D ✓ Save Au | esign After Running tomatically upon Cli | Analyze Again cking Analyze Agair need Granhics | | |
| Bubbl | es | O He | eat Map 🗹 Show | / Numb |
| | | Text f | ont | |
| | | Sea | e I II | |

7. Scripting and customization

Mgears provides options for customization using scripts at various points in the process, as seen throughout this User Manual. For example:

- On the input tab, a custom script can be provided to read a structured input file (a csv or xml) from another system and use it to drive Mgears input, or to retrieve an identifier from within a parameter file and use that for grouping. It is even possible to change the whole algorithm of detection in batch mode.
- A processing script can be invoked on the processing tab, where there is even the possibility of being able to run a 'pre'-script before individual file processing starts.
- A custom design script can be used to meet complex layout requirements that would not otherwise be easily achieved in a template.
- A custom script can also be used to create a new plugin for running your own analyses.
- Finally, a custom output script and/or a summary scipt can be used to allow a highly complex and specific output to be generated, as is sometimes required by some downstream system in the workflow.

The possibilities are only limited by programming ingenuity.

You can create and save your own scripts in the **Script Editor** accessible form the **Tools** section in Mnova.

Chemical Shift

Perturbation

Binding

Edit

Script



An Mnova scripting document is available to help you with Mnova's extensions. Click on 😢 to access this documentation.

| | Mnova Exter | sions to QtScript | |
|---|---|-------------------|-------------|
| Application AreaSeries Arrow ASVSettings ASVSettings ASVWarning Atom AtomNNRAssignmentData AtomNNRAPredictionData Attachment AuditTrailCommand AuditTrailCommand AuditTrailLem AuditTrailCommand AuditTrailLem AuditTrailCommand AuditTrailLem AuditTrailCommand AuditTrailLem AuditTraiL | Application Application object Table of contents 1. Properties 2. Functions Properties | | |
| BarCategoryAxis BarSeries | Name | Туре | Comments |
| BarSet BaseSpectrum | applicationName | String | |
| BinaryStream | clipboard | Clipboard | |
| Bond | identityManager | IdentityManager | [read-only] |
| ByteArray CanvasItemView | mainWindow | MainWindow | [read-only] |
| CategoryAxis Chart | name | String | [read-only] |
| ChartView CheckBox | organizationName | String | |
| ChemometricsData Chromatogram | version | Object | [read-only] |
| ChromatogramItem | version.build | Number | [read-only] |
| ChromatogramProcParams ChromNormalizationParams | version.full | String | [read-only] |
| ChromPlotAxesProps ChromPlotProperties | version.major | Number | [read-only] |
| ChromPlugin ChromTimeShiftParams | version.minor | Number | [read-only] |

8. Conclusion

Mnova Gears provides a robust platform for automation of workflows, and limitless possibilities for customization. Please contact us with your inquiries at <u>info@mestrelab.com</u> and let us help to set up your powerful automation system.