

**Additional File 1:** One example of use of Query Builder module in MeRy-B.

Objective: Extracting the list of the metabolites identified in the  $^1\text{H}$ -NMR spectra of project T06002: name, chemical shifts, groups and multiplicity.

*This workflow tutorial with step-by-step and with screenshots illustrates how to reach this objective.*

Data consultation module

Tools

Query Builder

The Query Builder shows several tabs: *Attributes*, *Filters*, *Results* *Browse*, which should be filled in sequential order. *Attributes* tab allows the user to select amongst all database controlled fields, the fields shown in *Results* tab. **Add a subset:** (drop-down list)

Choose *Compounds*

Select the attributes in the *compounds* frame in the order wanted by the user, *i.e.* 1 *user synonym*, 2 *nmr shift description*, 3 *nmr multiplicity* and finally 4 *nmr shift*. The selection order will be the field order in the Result table.

The screenshot shows the MeRy-B Query Builder interface. The sidebar on the left contains navigation links: Home, About MeRy-B, News, Data consultation, Projects, Spectra Data, Compounds, and Tools. The main area is titled 'Query Builder' and has tabs for Attributes, Filters, Results, and Browse. Below the tabs are two sections: 'samples' and 'compounds'. The 'samples' section has checkboxes for species, genotype, individual, taxon id, background, sample name, tissue, study type, project id, developmental stage, project name, env condition, and experiment name. The 'compounds' section has checkboxes for compound name, accession id, meryb id, user synonym, compound description, nmr shift, nmr shift description, nmr multiplicity, and experiments set name. At the bottom, there is an 'Add a subset:' dropdown menu and a 'RESET' button.

Select the tab *Filters*

This tab allows the user to select a subset of the whole database using filters.

Add a Filter

Select *Project name* in the drop-down list and type T in the last text box.

Query Builder

Attributes Filters Results Browse Import query Export query COUNT rows

Filter 1

project name -- exact match 11

Add a Filter

- Tomato & long-term cadmium stress - 2010
- Tomato - polyamines Japan
- Tomato HT screening method
- Tomato MeRy-B 2009
- Tomato- Metabolomics - 2006
- Tomato- Plant Physiol. - 2009

Select *Project name* in the drop-down list, *i.e.* Tomato- Metabolomics 2006.

Query Builder

Attributes Filters Results Browse Import query Export query COUNT rows

Filter 1

project name -- exact match Tomato- Metabolomics - 2006

Add a Filter

Select the *Results* tab.

This tab allows the user to process the query. The results may be sorted according to a selected field in the *Attributes* tab.

Select *user synonym* in the drop-down list and click on the *Launch query* button.

Query Builder

Attributes Filters Results Browse Import query Export query COUNT rows

Sort by: user synonym | Launch query

Exports: CSV

Rows: 43 found

| user synonym   | nmr shift                    | description         | nmr multiplicity | nmr shift |
|----------------|------------------------------|---------------------|------------------|-----------|
| Acetylcholine  | N-(C(5)H3)3                  | Singlet             | 3.22             |           |
| Adenosine-like | C1H of ribose                | Doublet             | 6.2              |           |
| Alanine        | C(3)H3                       | Doublet             | 1.48             |           |
| Asparagine     | C(3)H2                       | Multiplet           | 2.92             |           |
| Aspartate      | 1/2(C(3)H2)                  | Multiplet           | 2.81             |           |
| Choline        | N-(C(3)H3)3                  | Singlet             | 3.2              |           |
| Citrate        | C(2)H2+ C(4)H2               | Doublet of doublets | 2.63             |           |
| Formate        | C(1)H                        | Singlet             | 8.47             |           |
| Fructose       | alphaC(3)H+ C(5)H+alphaC(5)H | Multiplet           | 4.12             |           |
| GABA           | C2H2                         | Triplet             | 2.3              |           |
| GABA           | C3H2                         | Multiplet           | 1.92             |           |
| GABA           | C4H2                         | Triplet             | 3.01             |           |
| Glucose        | alpha-C1H                    | Doublet             | 5.25             |           |
| Glucose        | beta-C1H                     | Doublet             | 4.66             |           |
| Glutamate      | C(3)H2                       | Multiplet           | 2.07             |           |
| Glutamine      | C(4)H2                       | Multiplet           | 2.45             |           |
| Isoleucine     | C(6)H3                       | Doublet             | 1.01             |           |
| Leucine        | C(5)H3+ C(6)H3               | Triplet             | 0.96             |           |
| Malate         | C(2)H                        | Doublet of doublets | 4.3              |           |
| Mannose        | C(1)H                        | Doublet             | 5.2              |           |
| Phenylalanine  | C(5)H+ C(6)H+ C(7)H          | Multiplet           | 7.4              |           |
| Sucrose        | Glucopyranosyl-C(1)H         | Doublet             | 5.41             |           |
| Threonine      | C(4)H3                       | Doublet             | 1.33             |           |
| Trigonelline   |                              | Multiplet           | 8.83             |           |
| Trigonelline   |                              | Singlet             | 4.44             |           |
| Trigonelline   |                              | Triplet             | 8.08             |           |

The table can be exported as CSV file by clicking the button CSV and opened in a spreadsheet software (e.g. MS Excel), see below. The *Browse* tab shows the user all available fields and field values.

| G6 <span>▼</span> <span><i>f<sub>x</sub></i></span> |                |                                         |                     |           |   |
|-----------------------------------------------------|----------------|-----------------------------------------|---------------------|-----------|---|
|                                                     | A              | B                                       | C                   | D         | E |
| 1                                                   | #43 rows       |                                         |                     |           |   |
| 2                                                   | user_synonym   | nmr_shift_description                   | nmr_multiplicity    | nmr_shift |   |
| 3                                                   | Acetylcholine  | N-(C(5)H <sub>3</sub> ) <sub>3</sub>    | Singlet             | 3.22      |   |
| 4                                                   | Adenosine-like | C1H of ribose                           | Doublet             | 6.2       |   |
| 5                                                   | Alanine        | C(3)H <sub>3</sub>                      | Doublet             | 1.48      |   |
| 6                                                   | Asparagine     | C(3)H <sub>2</sub>                      | Multiplet           | 2.92      |   |
| 7                                                   | Aspartate      | 1/2(C(3)H <sub>2</sub> )                | Multiplet           | 2.81      |   |
| 8                                                   | Choline        | N-(C(3)H <sub>3</sub> ) <sub>3</sub>    | Singlet             | 3.2       |   |
| 9                                                   | Citrate        | C(2)H <sub>2</sub> + C(4)H <sub>2</sub> | Doublet of doublets | 2.63      |   |
| 10                                                  | Formate        | C(1)H                                   | Singlet             | 8.47      |   |
| 11                                                  | Fructose       | alphaC(3)H+ C(5)H+alphaC(5)H            | Multiplet           | 4.12      |   |
| 12                                                  | GABA           | C <sub>2</sub> H <sub>2</sub>           | Triplet             | 2.3       |   |
| 13                                                  | GABA           | C <sub>3</sub> H <sub>2</sub>           | Multiplet           | 1.92      |   |
| 14                                                  | GABA           | C <sub>4</sub> H <sub>2</sub>           | Triplet             | 3.01      |   |
| 15                                                  | Glucose        | alpha-C <sub>1</sub> H                  | Doublet             | 5.25      |   |
| 16                                                  | Glucose        | β-C <sub>1</sub> H                      | Doublet             | 4.66      |   |
| 17                                                  | Glutamate      | C(3)H <sub>2</sub>                      | Multiplet           | 2.07      |   |
| 18                                                  | Glutamine      | C(4)H <sub>2</sub>                      | Multiplet           | 2.45      |   |
| 19                                                  | Isoleucine     | C(6)H <sub>3</sub>                      | Doublet             | 1.01      |   |
| 20                                                  | Leucine        | C(5)H <sub>3</sub> + C(6)H <sub>3</sub> | Triplet             | 0.96      |   |
| 21                                                  | Malate         | C(2)H                                   | Doublet of doublets | 4.3       |   |
| 22                                                  | Mannose        | C(1)H                                   | Doublet             | 5.2       |   |
| 23                                                  | Phenylalanine  | C(5)H+ C(6)H+ C(7)H                     | Multiplet           | 7.4       |   |
| 24                                                  | Sucrose        | Glucopyranosyl-C(1)H                    | Doublet             | 5.41      |   |
| 25                                                  | Threonine      | C(4)H <sub>3</sub>                      | Doublet             | 1.33      |   |
| 26                                                  | Trigonelline   |                                         | Multiplet           | 8.83      |   |
| 27                                                  | Trigonelline   |                                         | Singlet             | 4.44      |   |
| 28                                                  | Trigonelline   |                                         | Triplet             | 8.08      |   |
| 29                                                  | Trigonelline   | C(3)H                                   | Singlet             | 9.13      |   |

Such table is often compulsory in metabolomics publications or reports and the Query Builder tool provides an easy and rapid way to generate it.