isoenum-webgui

Release 0.2.0

Aug 14, 2019

Contents:

CHAPTER 1

isoenum-webgui

`isoenum-webgui` provides Flask-based web user interface that uses `isoenum` package to generate accurate InChI (International Chemical Identifier) for NMR metabolite features based on standard NMR experimental descriptions (currently `1D-1H` and `1D-CHSQC`) in order to improve data reusability of metabolomics data.

1.1 Links

- isoenum @ GitHub
- isoenum @ PyPI
- isoenum @ ReadTheDocs

1.2 Installation

The `isoenum-webgui` package runs under Python 3.4+. Use pip to install.

1.2.1 Install on Linux, Mac OS X

```
python3 -m pip install isoenum-webgui
```

1.2.2 Install on Windows

```
py -3 -m pip install isoenum-webgui
```

1.2.3 Dependencies

The `isoenum-webgui` requires a **non-pip-installable** dependency: the Open Babel chemistry library version 2.4.1 or later, which relies on `InChI` library version 1.0.4 or later to perform `InChI` conversions.

Refer to the official documentation to install Open Babel on your system:

- Official Installation Instructions: http://openbabel.org/wiki/Category:Installation

1.3 Development version installation

1.3.1 Install development version on Linux, Mac OS X

```
python3 -m pip install git+git://github.com/MoseleyBioinformaticsLab/isoenum-webgui.
↪git
```

1.3.2 Install development version on Windows

```
py -3 -m pip install git+git://github.com/MoseleyBioinformaticsLab/isoenum-webgui.git
```

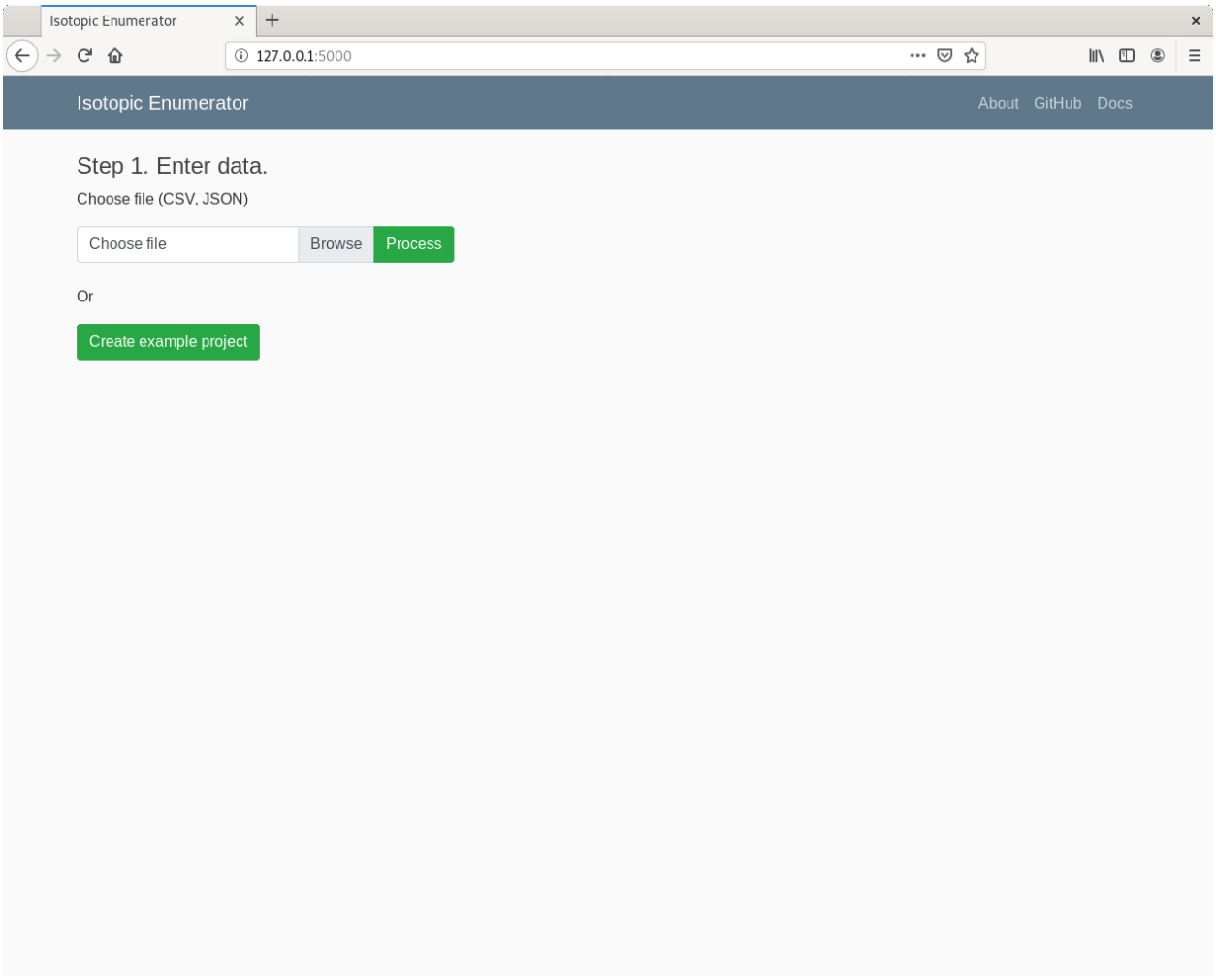
1.4 License

This package is distributed under the BSD license.

1.4.1 The isoenum-webgui GUI Reference

Home View

The home view allows the user to select a CSV or JSON file or create an example project.



Accepted File Formats

CSV

- `CSV` file containing `InChI` strings:

```
Base Identifier
"InChI=1S/C2H4O2/c1-2(3)4/h1H3,(H,3,4)"
"InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H"
"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1"
```

- `CSV` file containing "Base Identifier" header and `InChI` strings:

```
Base Identifier
"InChI=1S/C2H4O2/c1-2(3)4/h1H3,(H,3,4)"
"InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H"
"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1"
```

- `CSV` file saved from the `InChI` Table View:

```
Name,Base Identifier,ISO,CHG,Repr Identifier
acetic acid,"InChI=1S/C2H4O2/c1-2(3)4/h1H3,(H,3,4)",13:C:1<br>13:C:2,O:4:-1,"InChI=1/
↪C2H4O2/c1-2(3)4/h1H3,(H,3,4)/p-1/i1+1,2+1/fC2H3O2/q-1"
benzene,InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H,,,InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H
valine,"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1",,,
↪"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1"
```

JSON

- `JSON` file saved from the `InChI` Table View:


```
{
    "d3f60ba7-0098-4af7-999a-a506823539c1": {
        "Name": "acetic acid",
        "Base Identifier": "InChI=1S/C2H4O2/c1-2(3)4/h1H3,(H,3,4)",
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↪0\"/>\n<line x1=\"77.6\" y1=\"80.0\" x2=\"77.6\" y2=\"53.0\" stroke=\"rgb(76,76,76)\
↪"  stroke-width=\"2.0\"/>\n<line x1=\"74.6\" y1=\"80.0\" x2=\"51.3\" y2=\"93.5\"␣
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```
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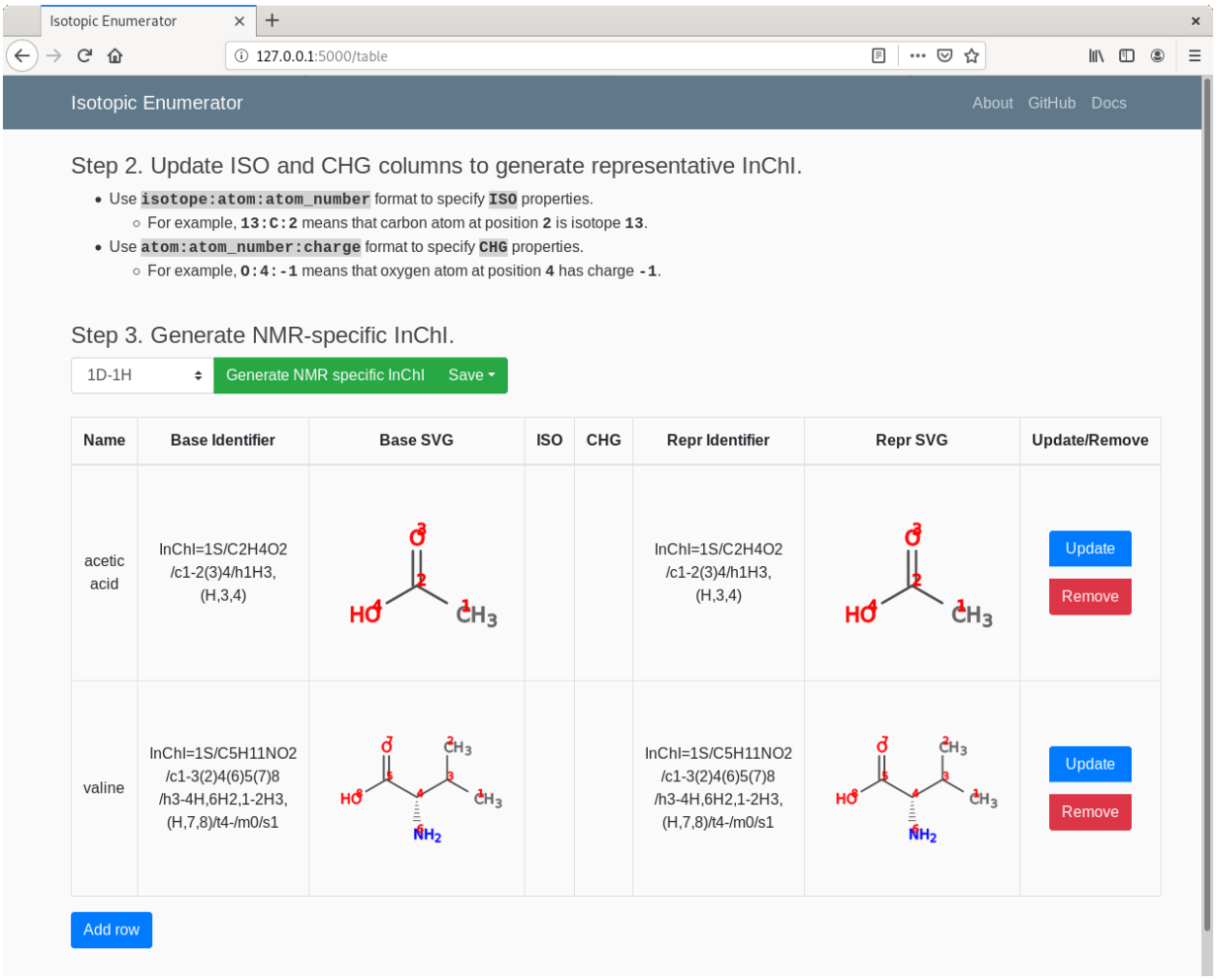
↪fC2H3O2/q-1",
                        "me_group": "ME1",
                        "row_id": "d3f60ba7-0098-4af7-999a-a506823539c1_1"
                    },
                    "d3f60ba7-0098-4af7-999a-a506823539c1_2": {
                        "descr": [
                            "[1H5,1H6,1H7:C1]HResonance",
                            "[1H5,1H6,1H7:13C1]J1CH"
                        ],
                        "inchi": "InChI=1/C2H4O2/c1-2(3)4/h1H3,(H,3,4)/p-1/i1+1H3,2+1/
↪fC2H3O2/q-1",
                        "me_group": "ME2",
                        "row_id": "d3f60ba7-0098-4af7-999a-a506823539c1_2"
                    }
                }
            }
        }
    }
}
```

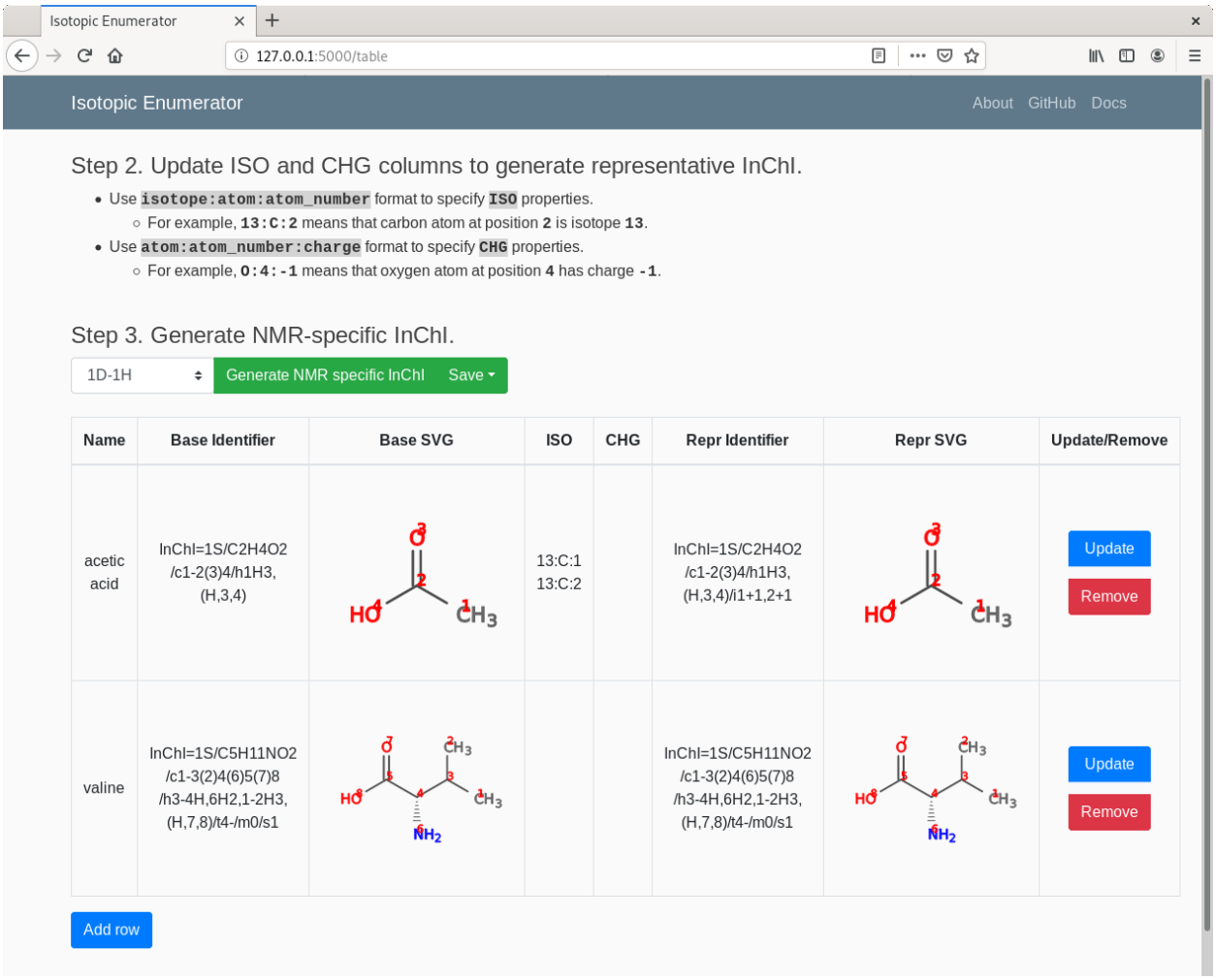

InChI Table View

The `InChI` Table View provides an editable table interface where the user can update/change the metabolite name, base identifier, isotopic properties and atom charges.



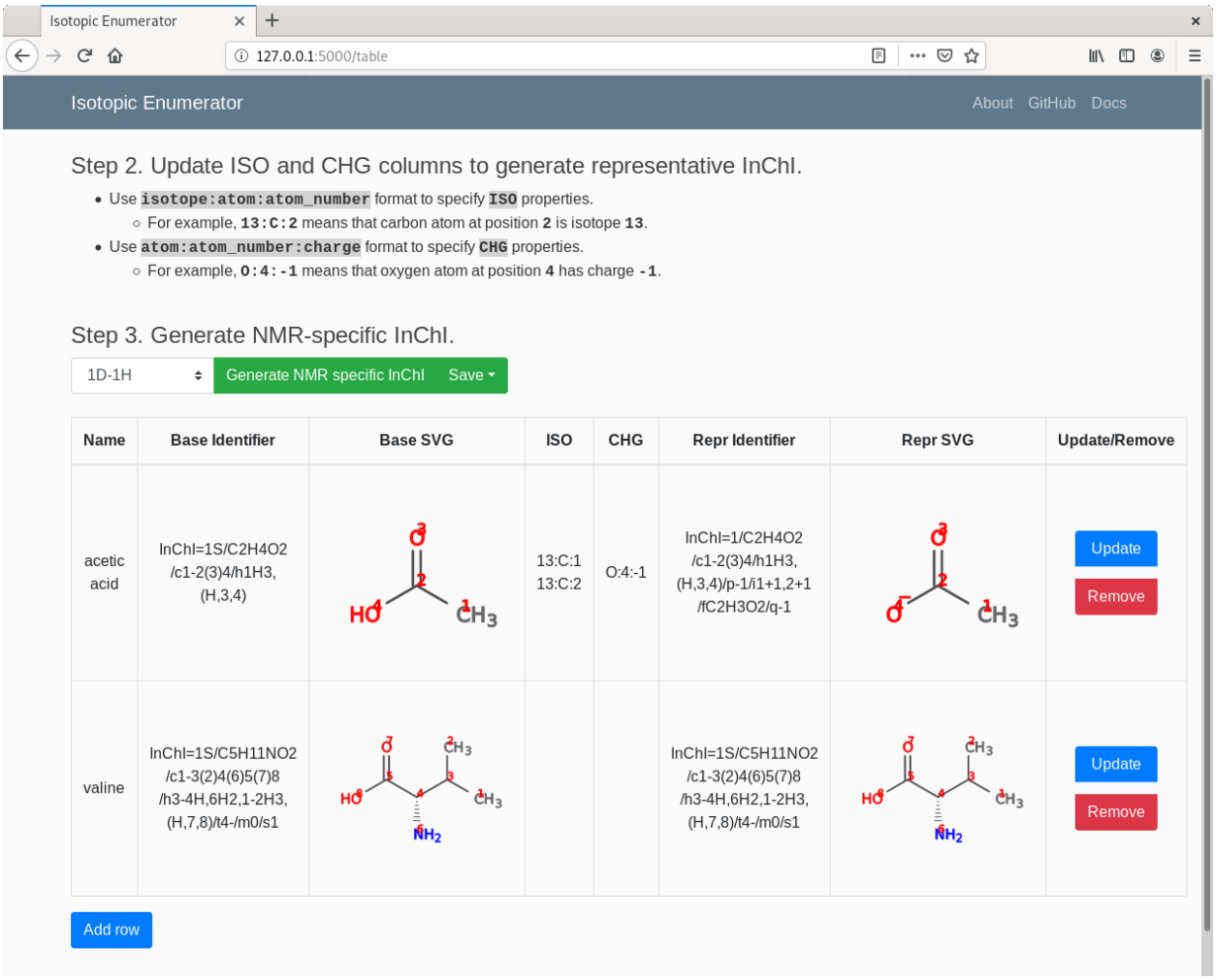
How to update isotopic properties.

- Use `isotope:atom:atom_number` format to specify `ISO` properties. For example:
  - `13:C:1` means that carbon atom at position `1` is isotope `13`.
  - `13:C:2` means that carbon atom at position `2` is isotope `13`.



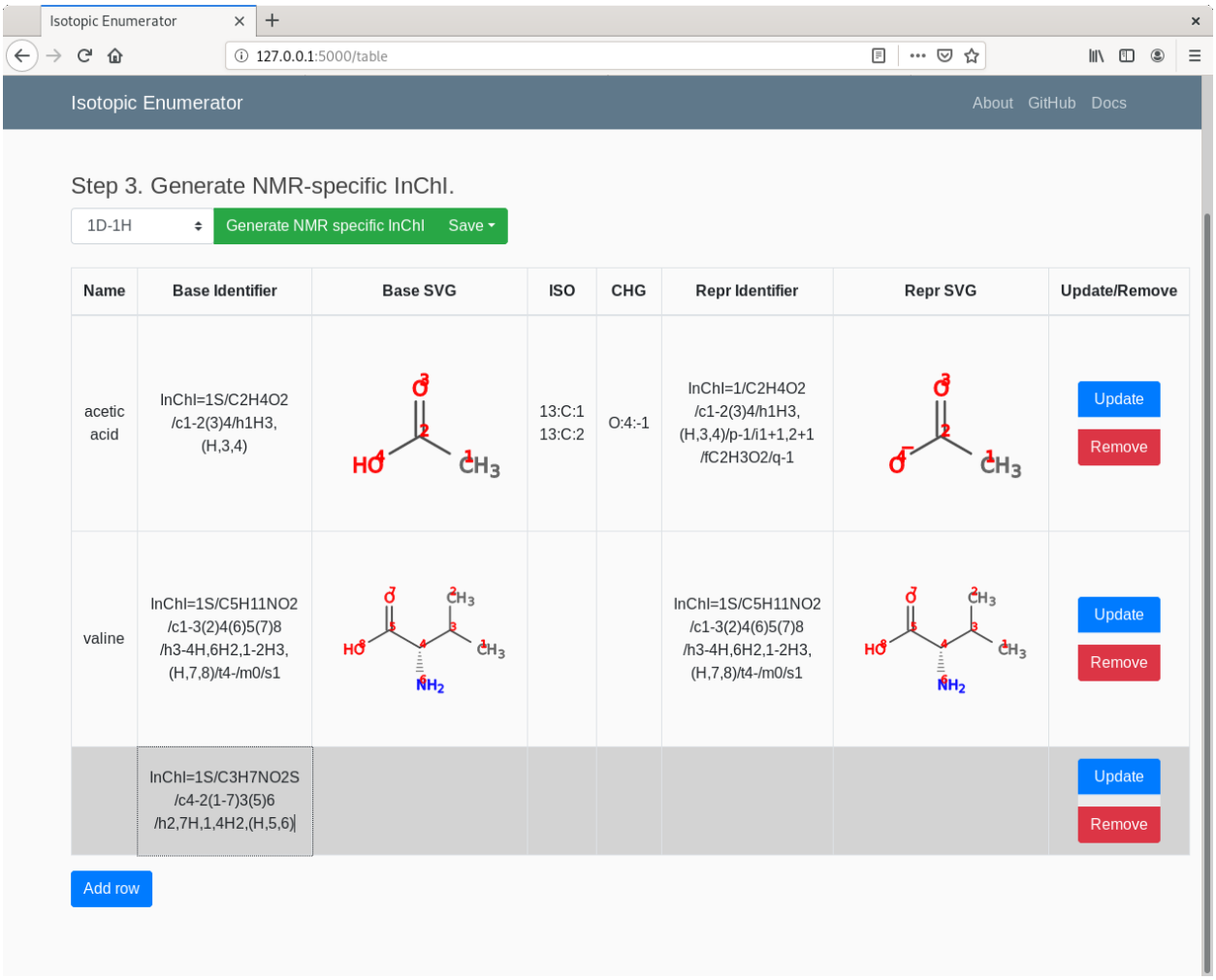
How to update charge properties.

- Use `atom:atom_number:charge` format to specify `CHG` properties. For example:
  - `O:4:-1` means that oxygen atom at position `4` has charge `-1`

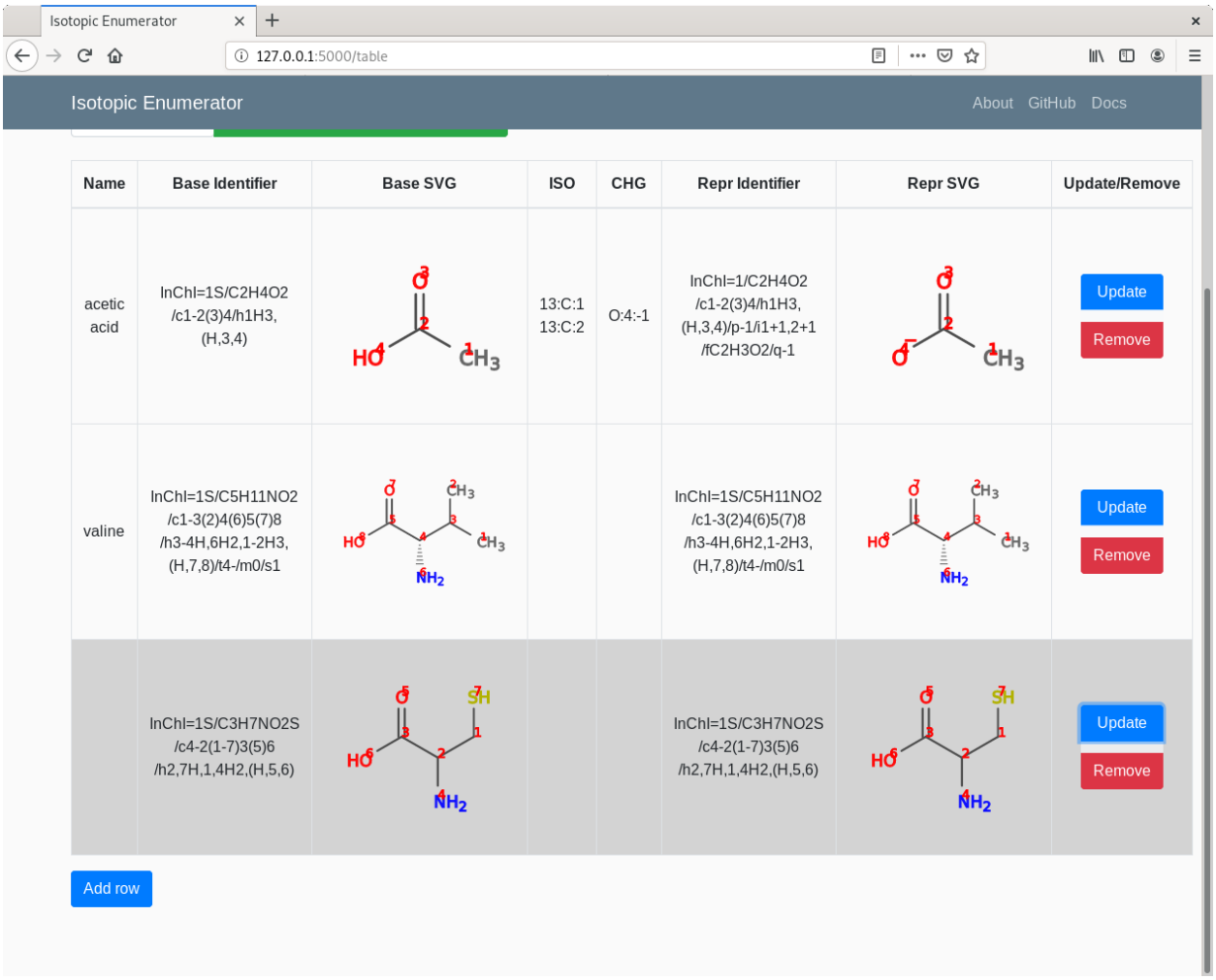


How to add/remove new row to table.

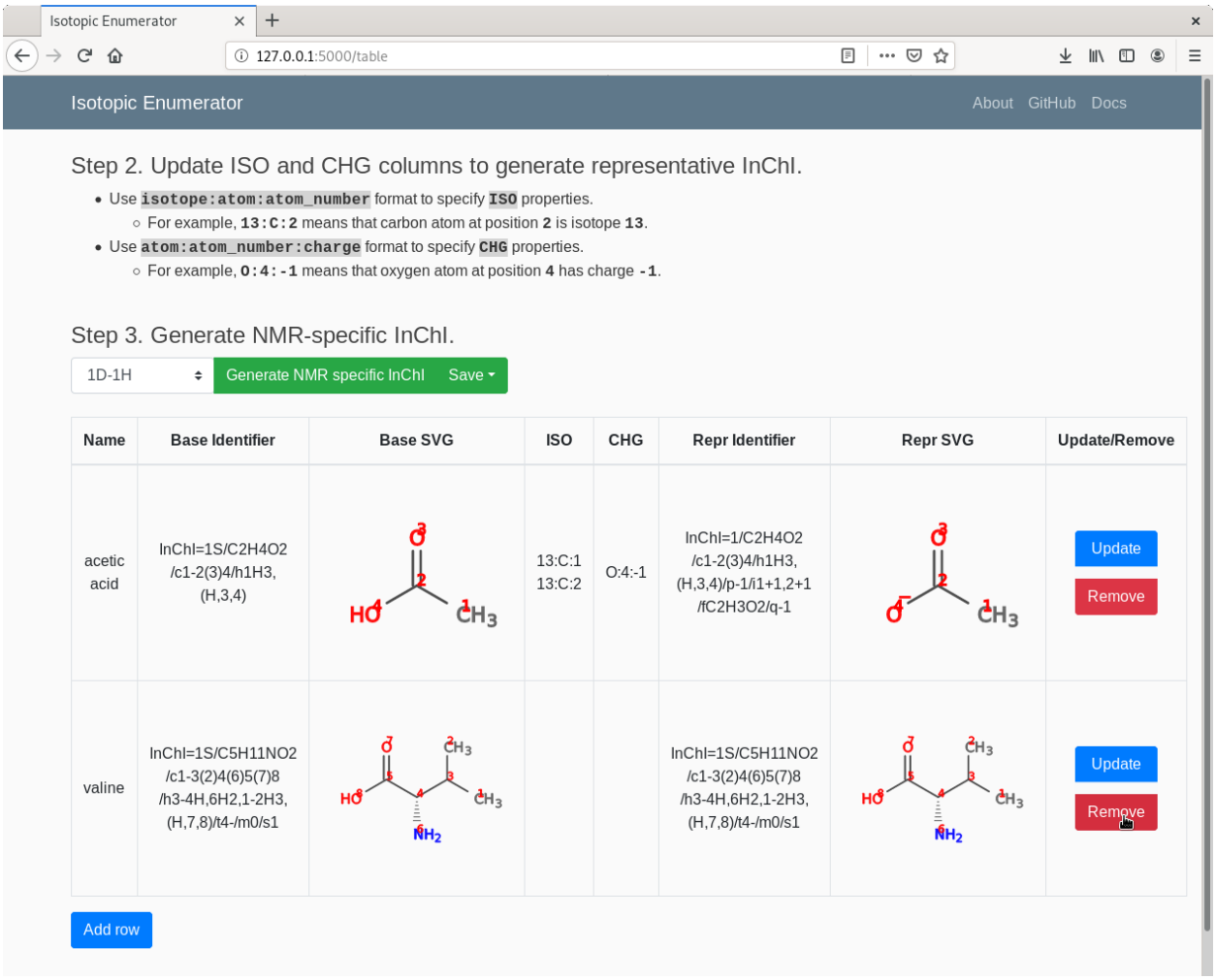
- The user can also add a new editable row by using “Add row” button and insert valid `InChI` string.



- The user can update the row by using the "Update" button to generate base and representative identifiers and their corresponding visualizations.

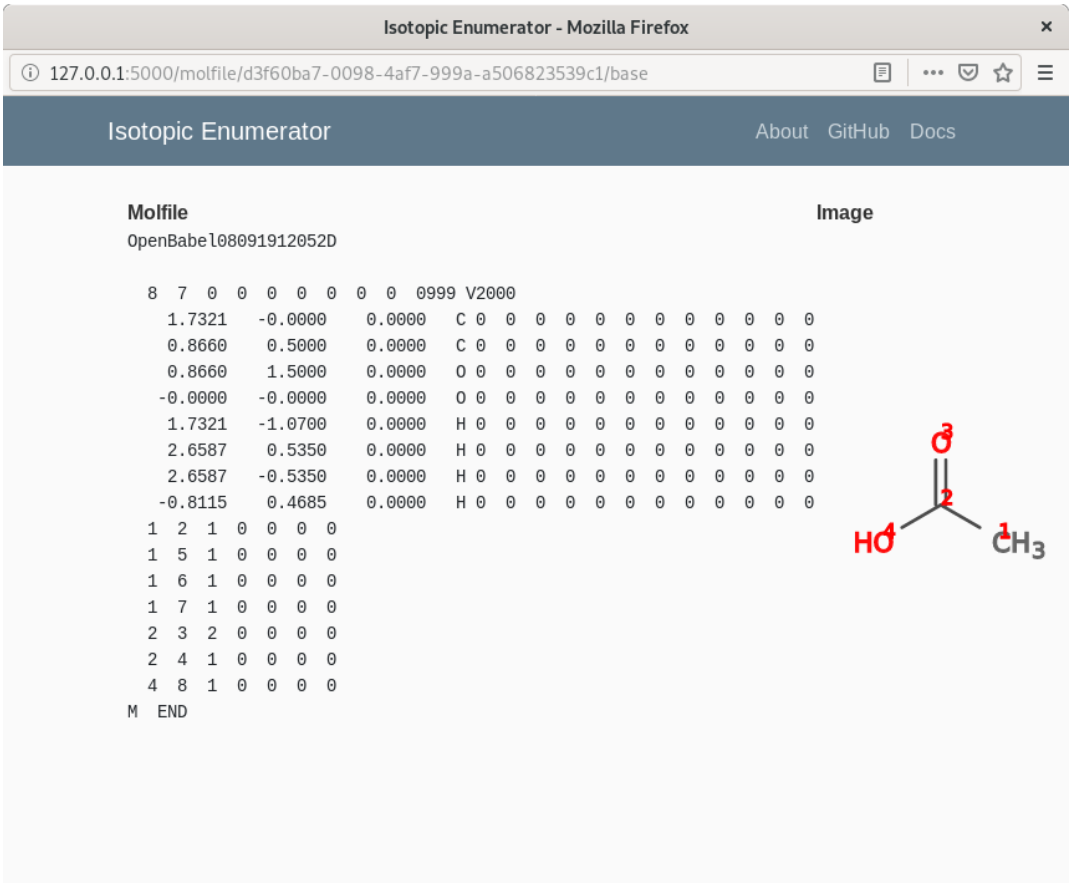


- The user can remove the row by using the “Remove” button in the corresponding table row.

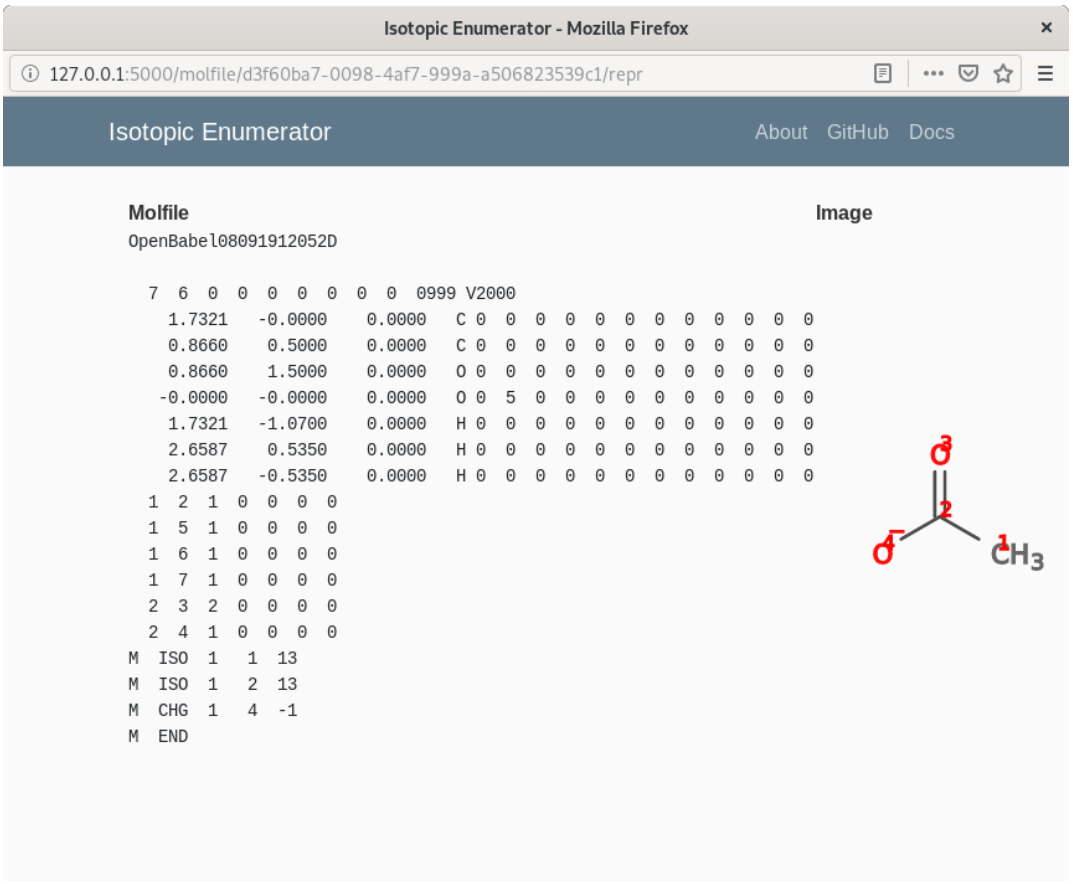


How to view corresponding Molfile.

- The user can view the corresponding `Molfile` for both base and representative `InChI` by clicking on the metabolite image (i.e. Base SVG or Repr SVG columns).
  - Base `Molfile`:

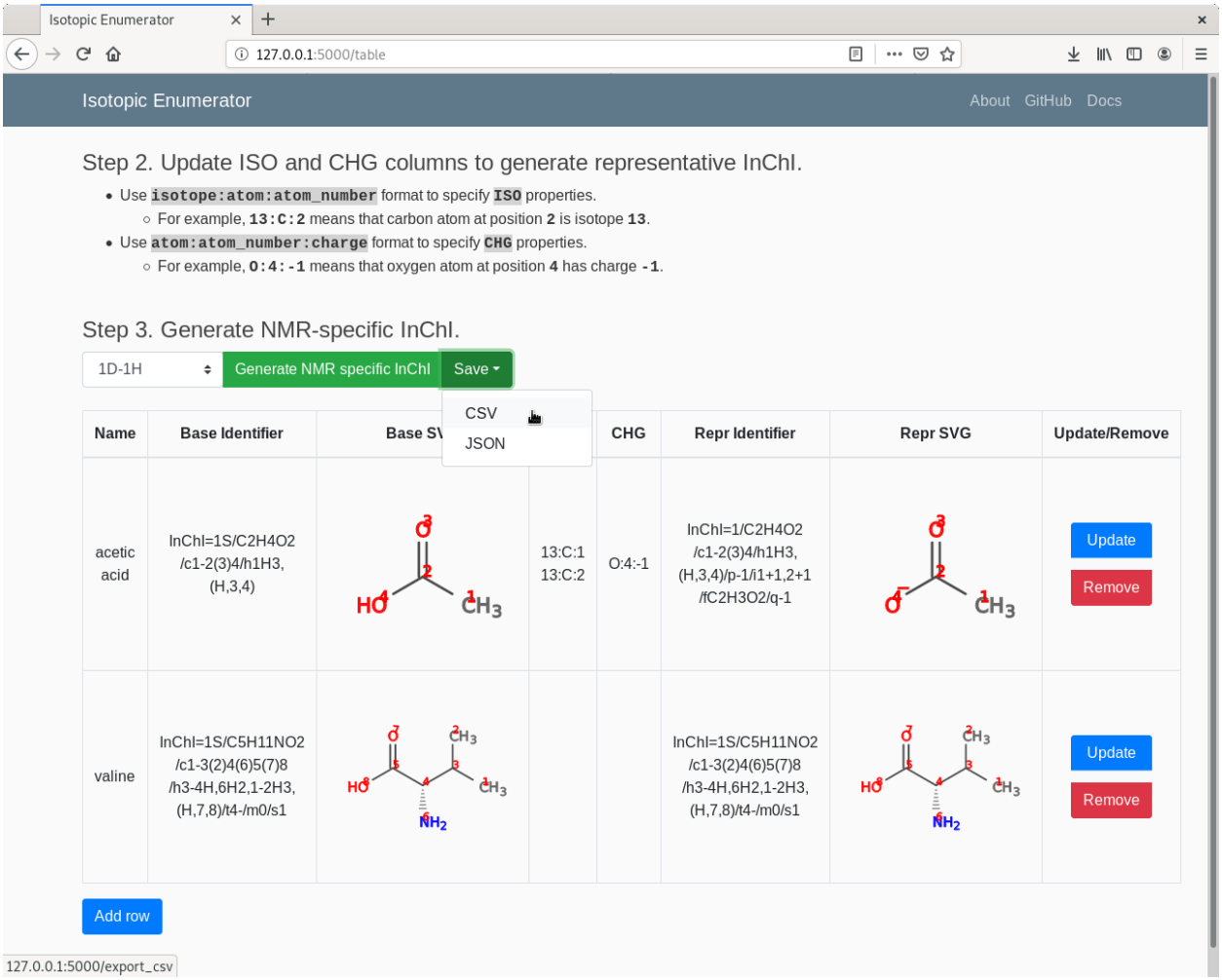


– Repr `Molfile`:



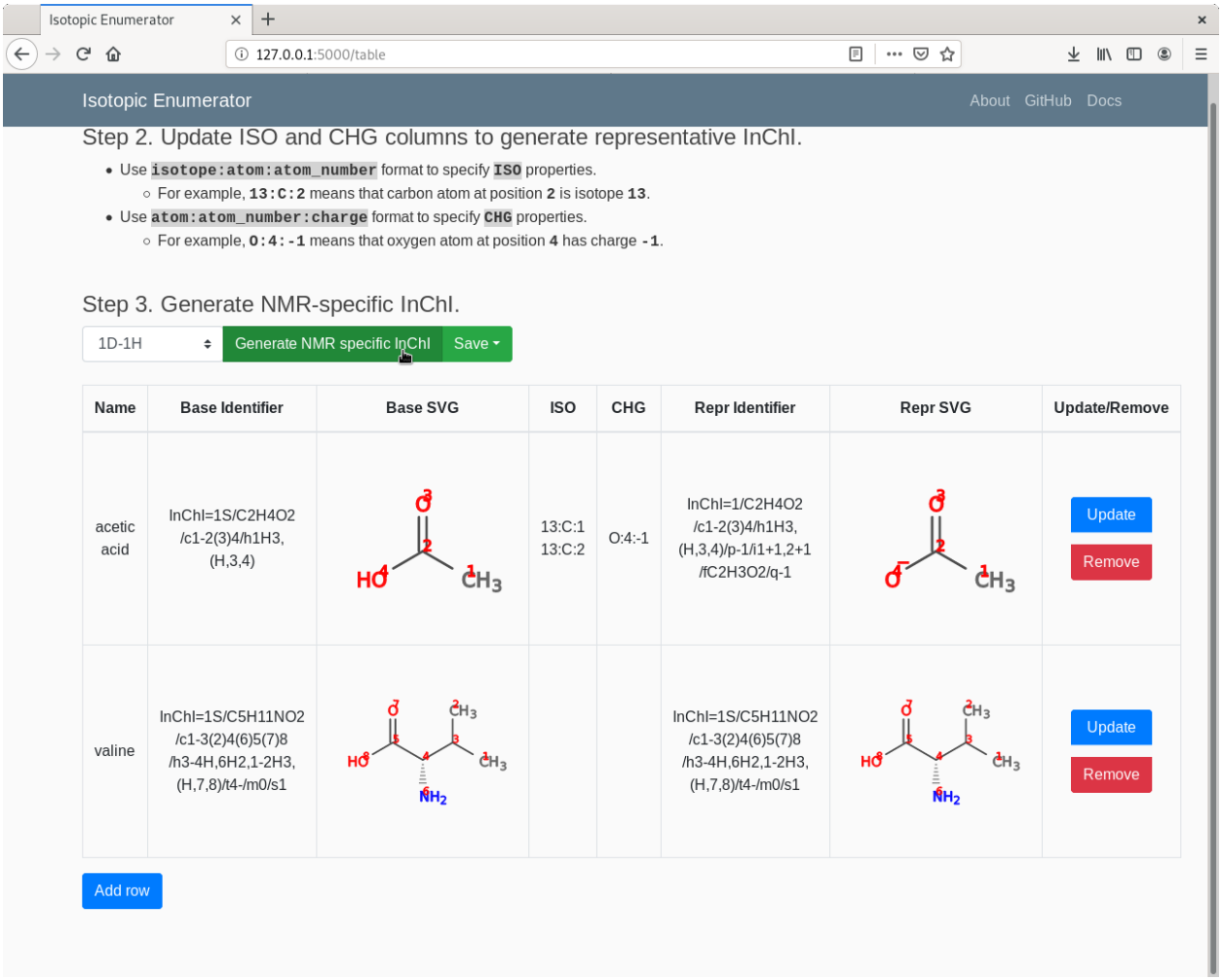
How to save table view.

- The user can save the table into CSV or JSON files to save their progress.



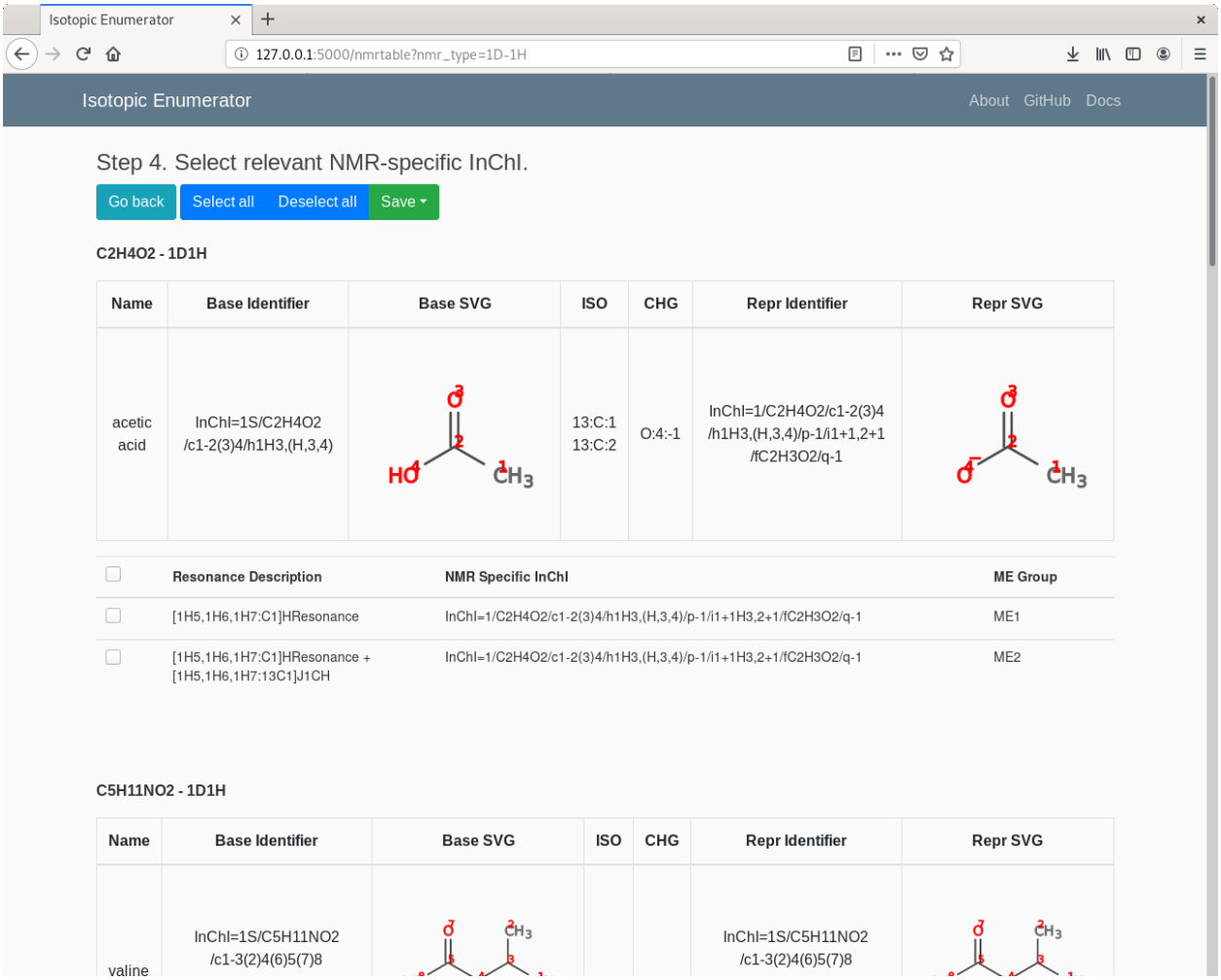
How to generate NMR specific InChI.

- To generate NMR specific InChI for metabolites, the user needs to select the appropriate NMR experiment type and click the “Use NMR specific InChI”.



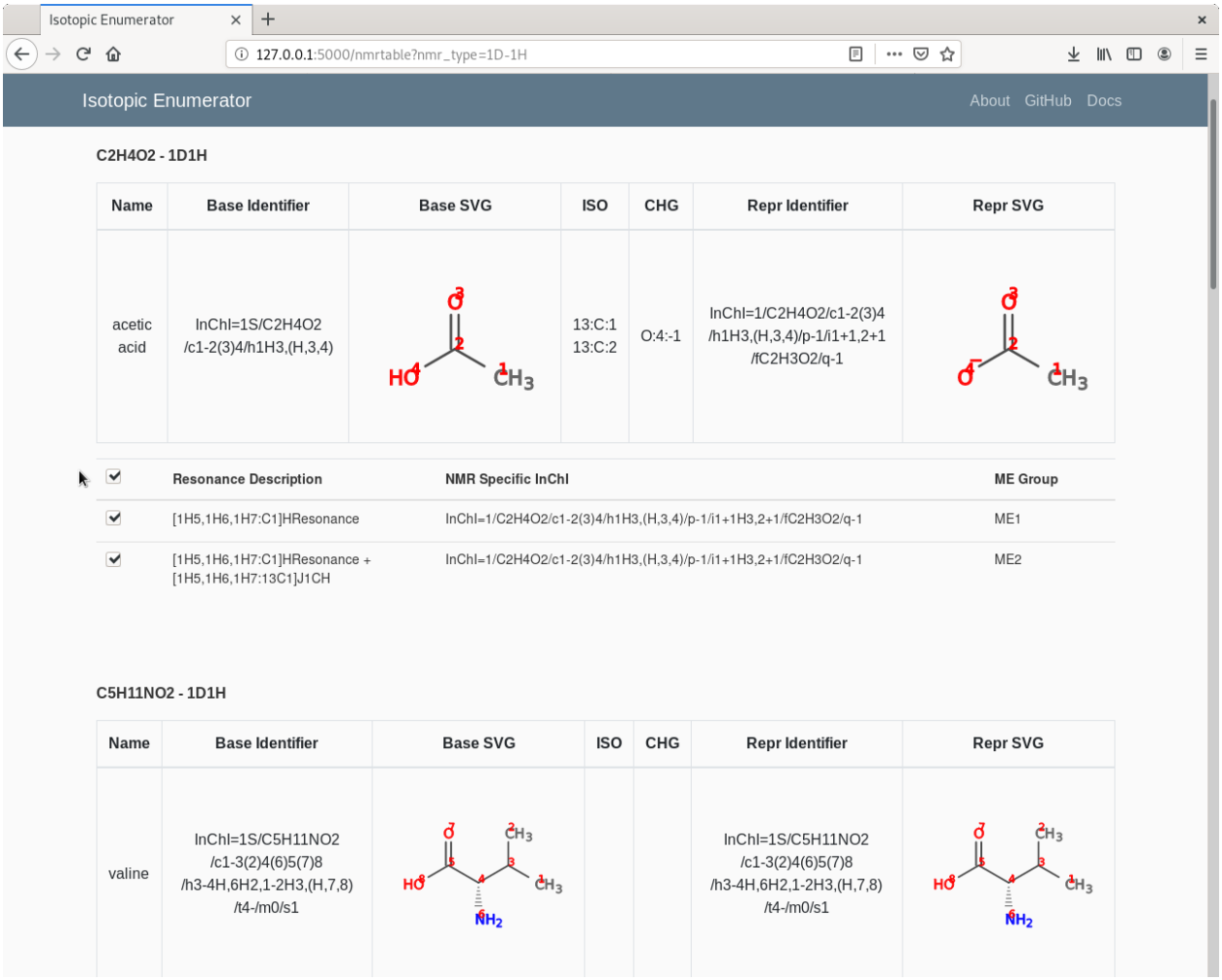
NMR specific InChI Table View

- NMR specific `InChI` table view provides the interface where the user can see NMR specific `InChI` tables based upon selected NMR experiment type description.

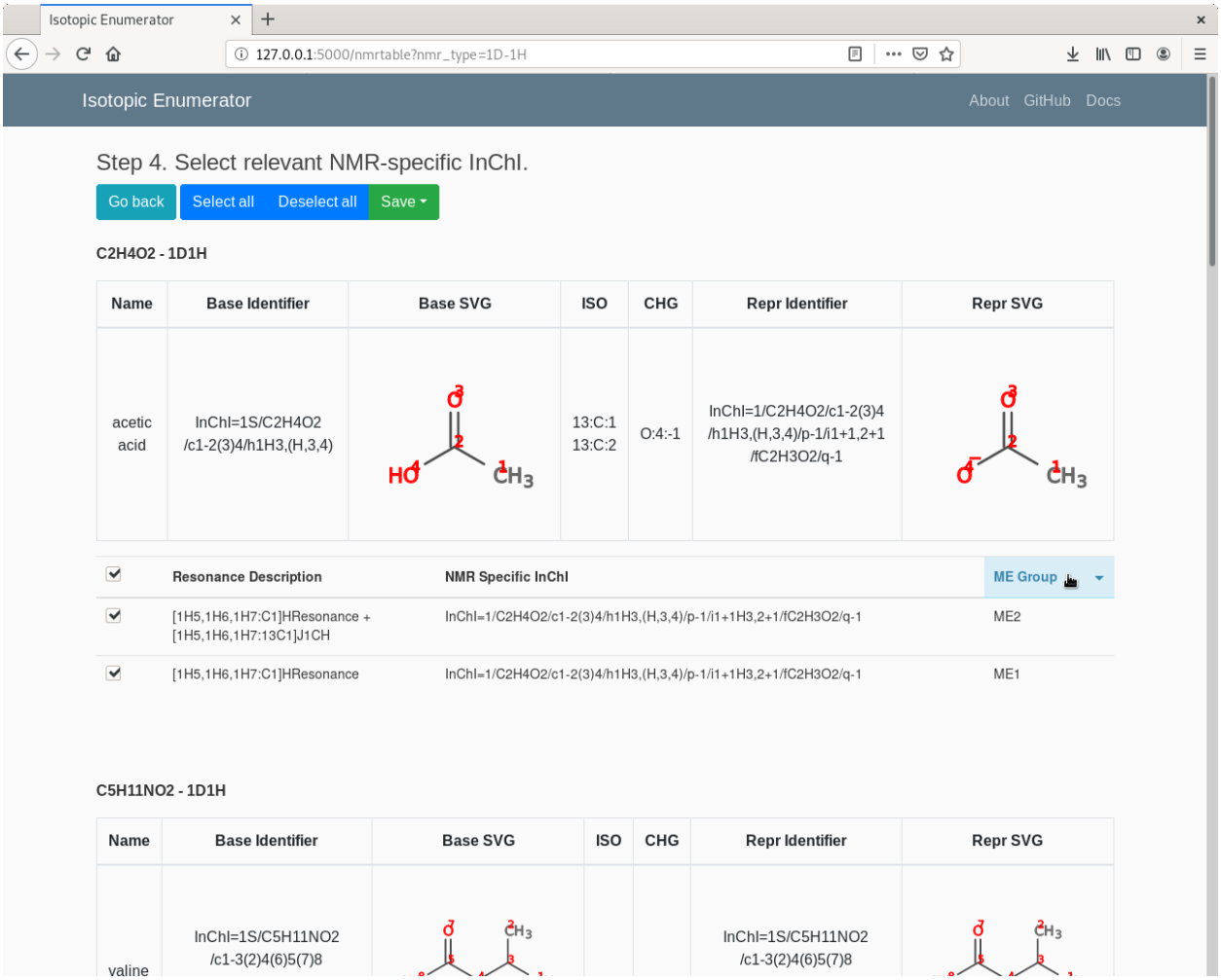


How to select NMR specific InChI.

- The user can examine tables that contain “Resonance Description” and corresponding “NMR specific InChI” to save the appropriate identifiers that correspond to peaks in their NMR spectra.

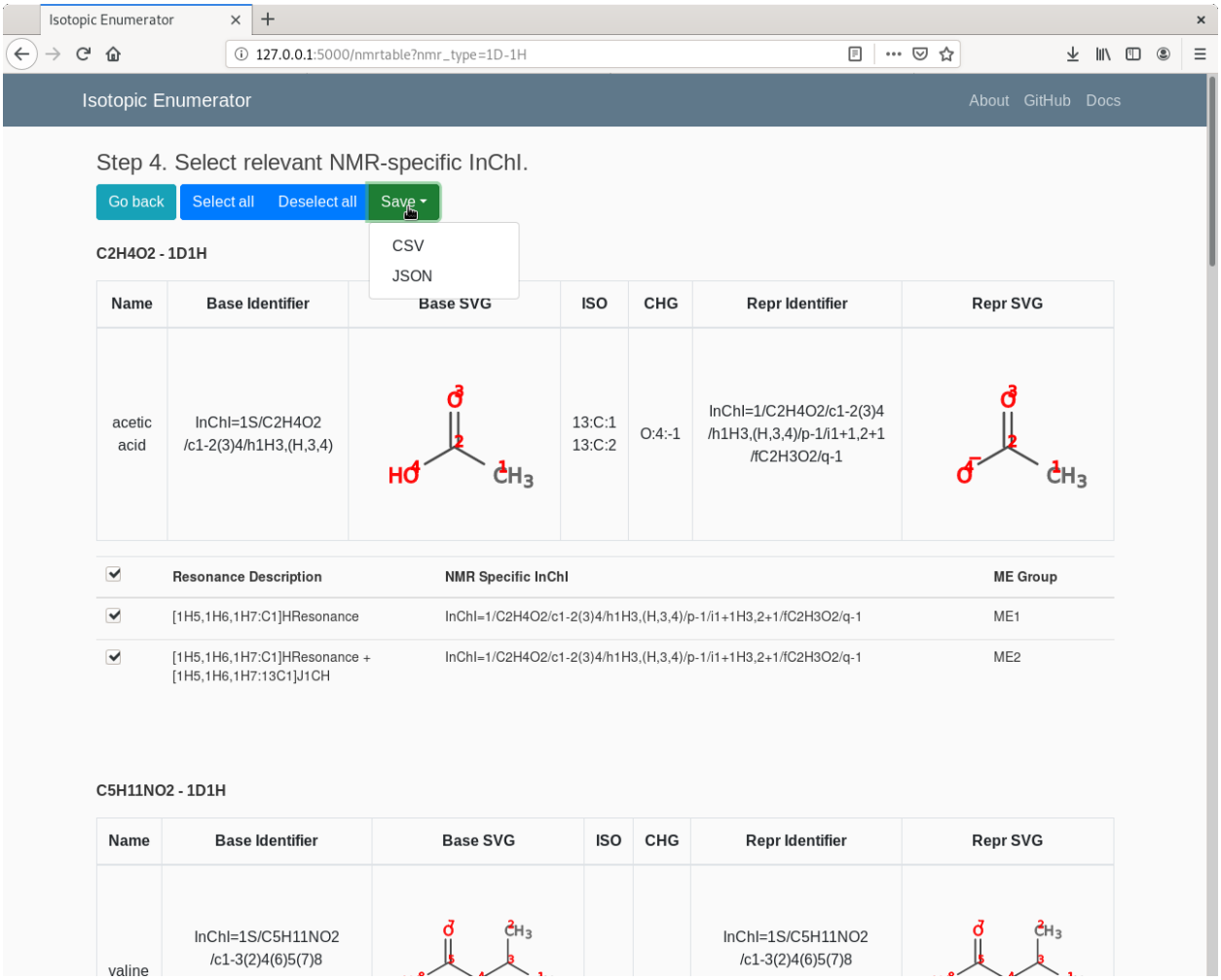


- The user can sort NMR specific tables by “Resonance Description”, “NMR specific InChI”, and “ME Group”. “ME” stands for “Magnetically Equivalent” `InChI` - ones that have similar “Resonance Description” and identical `InChI` strings.



How to save NMR table view.

- The user can save the NMR table into CSV or JSON files to save their progress.



- Save to `JSON` is intended to save the project state, while save to `CSV` will create a `CSV` file that will contain NMR specific `InChI` that can be directly used for data deposition.

```
Name,Base Identifier,Repr Identifier,Resonance Description,NMR Specific InChI
acetic acid,"InChI=1S/C2H4O2/c1-2(3)4/h1H3,(H,3,4)","InChI=1/C2H4O2/c1-2(3)4/h1H3,(H,
↪3,4)/p-1/i1+1,2+1/fC2H3O2/q-1","[1H5,1H6,1H7:C1]HResonance","InChI=1/C2H4O2/c1-
↪2(3)4/h1H3,(H,3,4)/p-1/i1+1H3,2+1/fC2H3O2/q-1"
acetic acid,"InChI=1S/C2H4O2/c1-2(3)4/h1H3,(H,3,4)","InChI=1/C2H4O2/c1-2(3)4/h1H3,(H,
↪3,4)/p-1/i1+1,2+1/fC2H3O2/q-1","[1H5,1H6,1H7:C1]HResonance + [1H5,1H6,1H7:13C1]J1CH
↪","InChI=1/C2H4O2/c1-2(3)4/h1H3,(H,3,4)/p-1/i1+1H3,2+1/fC2H3O2/q-1"
valine,"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1",
↪"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1","[1H9,1H10,
↪1H11:C1]HResonance","InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/
↪m0/s1/i1H3/t3?,4-"
valine,"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1",
↪"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1","[1H9,1H10,
↪1H11:C1]HResonance + [1H9,1H10,1H11:13C1]J1CH","InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/
↪h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1/i1+1H3/t3?,4-"
valine,"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1",
↪"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1","[1H9,1H10,
↪1H11:C1]HResonance + [1H9,1H10,1H11:1H15]J3HH","InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/
↪h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1/i1H3,3H/t3?,4-"
valine,"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1",
↪"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1","[1H9,1H10,
↪1H11:C1]HResonance + [1H9,1H10,1H11:13C1]J1CH + [1H9,1H10,1H11:1H15]J3HH","InChI=1S/
↪C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1/i1+1H3,3H/t3?,4-"
```

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```
valine,"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1",
↪"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1","[1H12,1H13,
↪1H14:C2]HResonance","InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/
↪m0/s1/i1H3/t3?,4-"
valine,"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1",
↪"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1","[1H12,1H13,
↪1H14:C2]HResonance + [1H12,1H13,1H14:13C2]J1CH","InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/
↪h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1/i1+1H3/t3?,4-"
valine,"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1",
↪"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1","[1H12,1H13,
↪1H14:C2]HResonance + [1H12,1H13,1H14:1H15]J3HH","InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/
↪h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1/i1H3,3H/t3?,4-"
valine,"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1",
↪"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1","[1H12,1H13,
↪1H14:C2]HResonance + [1H12,1H13,1H14:13C2]J1CH + [1H12,1H13,1H14:1H15]J3HH",
↪"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1/i1+1H3,3H/t3?,
↪4-"
valine,"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1",
↪"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1",
↪[1H15:C3]HResonance,"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/
↪m0/s1/i3H"
valine,"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1",
↪"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1",
↪[1H15:C3]HResonance + [1H15:13C3]J1CH,"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,
↪1-2H3,(H,7,8)/t4-/m0/s1/i3+1H"
valine,"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1",
↪"InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1",
↪"[1H15:C3]HResonance + [1H15:1H9,1H10,1H11]J3HH","InChI=1S/C5H11NO2/c1-
↪3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-/m0/s1/i1H3,3H/t3?,4-"
```

1.4.2 The isoenum-webgui CLI Reference

The isoenum-webgui command-line interface

Usage: isoenum_webgui -h | –help

isoenum_webgui –version

isoenum_webgui [–port=<port>] [–browser] [–debug]

Options:

-h, --help	Show this screen.
--version	Show version.
-b, --browser	Open isoenum-webgui in a default browser.
-p, --port=<port>	Port [default: 5000].
--debug	Debug mode flag.

`isoenum_webgui.cli.`**`cli`**(*cmdargs*)

Command-line interface entry point.

Parameters **`cmdargs`** (*dict*) – Command-line arguments from docopt.

Returns None.

Return type None

1.4.3 The isoenum-webgui API Reference

Isotopic enumerator web interface.

isoenum_webgui.proc

This module contains *isoenum-webgui* data processing/transformation logic, i.e. it calls the appropriate *isoenum* API methods in order to generate correct *InChI*, *Molfile's and SVG images based upon input from the 'isoenum-webgui*.

isoenum_webgui.proc.**generate_repr_molfile**(*inchi_str*, *iso_str*, *chg_str*)
Generate representative *Molfile* using isotope and charge specification strings.

Parameters

- **inchi_str** (*str*) – *InChI* string.
- **iso_str** (*str*) – Isotope specification.
- **chg_str** (*str*) – Charge specification.

Returns Representative *Molfile*.

Return type Molfile

isoenum_webgui.proc.**generate_table**(*records*)
Generate *InChI* table.

Parameters **records** (*dict*) – Global RECORDS store.

isoenum_webgui.proc.**create_initial_record**(*header*, *row*)
Initialize record.

Parameters

- **header** (*list*) – Record keys.
- **row** (*list*) – Record values.

Returns Record dictionary.

Return type dict

isoenum_webgui.proc.**update_record**(*record*)
Update record.

Parameters **record** (*dict*) – Record.

Returns Updated record.

Return type dict

isoenum_webgui.proc.**create_repr_inchi**(*base_inchi_str*, *iso_str*, *chg_str*)
Create representative *InChI* string.

Parameters

- **base_inchi_str** (*str*) – Base *InChI* string
- **iso_str** (*srr*) – Isotope specification.
- **chg_str** (*str*) – Charge specification.

Returns Representative *InChI* string.

Return type str

isoenum_webgui.proc.**create_svg**(*inchi_str*)
Create SVG from *InChI* string.

Parameters **inchi_str** (*str*) – *InChI* string.

Returns SVG string.

Return type str

isoenum_webgui.proc.**create_svg_link**(*svg_str*, *record_id*, *record_type*)
Create SVG link.

Parameters

- **svg_str** (*str*) – SVG string.
- **record_id** (*str*) – Record id.
- **record_type** (*str*) – Record type: base or repr.

Returns SVG link.

Return type str

isoenum_webgui.proc.**generate_nmr**(*nmr_experiment_type*, *records*)
Generate NMR specific *InChI* tables.

Parameters

- **nmr_experiment_type** (*str*) – NMR experiment type.
- **records** (*dict*) – Global RECORDS dictionary.

Returns None.

Return type None

isoenum_webgui.proc.**create_record_id**()
Create record id.

Returns Record id string.

Return type str

isoenum_webgui.proc.**create_empty_record**()
Create empty record.

Returns Empty record dictionary.

Return type dict

isoenum_webgui.routes

Isotopic enumerator web interface routes.

isoenum_webgui.routes.**home**()
Home.

isoenum_webgui.routes.**example_project**()
Example project.

isoenum_webgui.routes.**table**()
Display base and representative InChI.

isoenum_webgui.routes.**nmrtable**()
Display NMR-specific InChI.

isoenum_webgui.routes.**update**()
Update record.

isoenum_webgui.routes.**add**()
Add empty record.

isoenum_webgui.routes.**remove**()
Remove record.

isoenum_webgui.routes.**display_molfile**(*record_id*, *record_type*)
Display Molfile.

isoenum_webgui.routes.**export_json**()
Export as JSON.

isoenum_webgui.routes.**export_csv**()
Export as CSV.

isoenum_webgui.routes.**export_nmr_csv**()
Export NMR-specific InChI as CSV.

isoenum_webgui.routes.**about**()
About page.

isoenum_webgui.routes.**after_request**(*response*)
Do not cache responses.

isoenum_webgui.forms

Isotopic enumerator web interface forms.

class isoenum_webgui.forms.**FileForm**(*formdata=<object object>*, ***kwargs*)
File input form with validation.

isoenum_webgui.config

This module contains *isoenum-webgui* application configurations.

class isoenum_webgui.config.**Config**
Set *isoenum-webgui* Flask app configuration.

isoenum_webgui.errors

Isotopic enumerator web interface custom exception handling.

isoenum_webgui.errors.**handle_error**(*error*)
Custom error handler.

1.4.4 Release History

0.2.0 (2019-08-14)

Improvements

- Added popup window for base and representative molfiles.
- Strip out html on paste event for editable table.

- Updated templates.
- Added error handling for “Base Identifier” column.
- Added CLI, GUI, API documentation.
- Added “isoenum_webgui” entry point.

0.1.0 (2019-07-30)

- Initial public release.

1.4.5 License

CHAPTER 2

Indices and tables

- genindex
- modindex
- search

Python Module Index

i

Index