
isoenum-webgui

Release 0.2.0

Aug 14, 2019

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`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
```

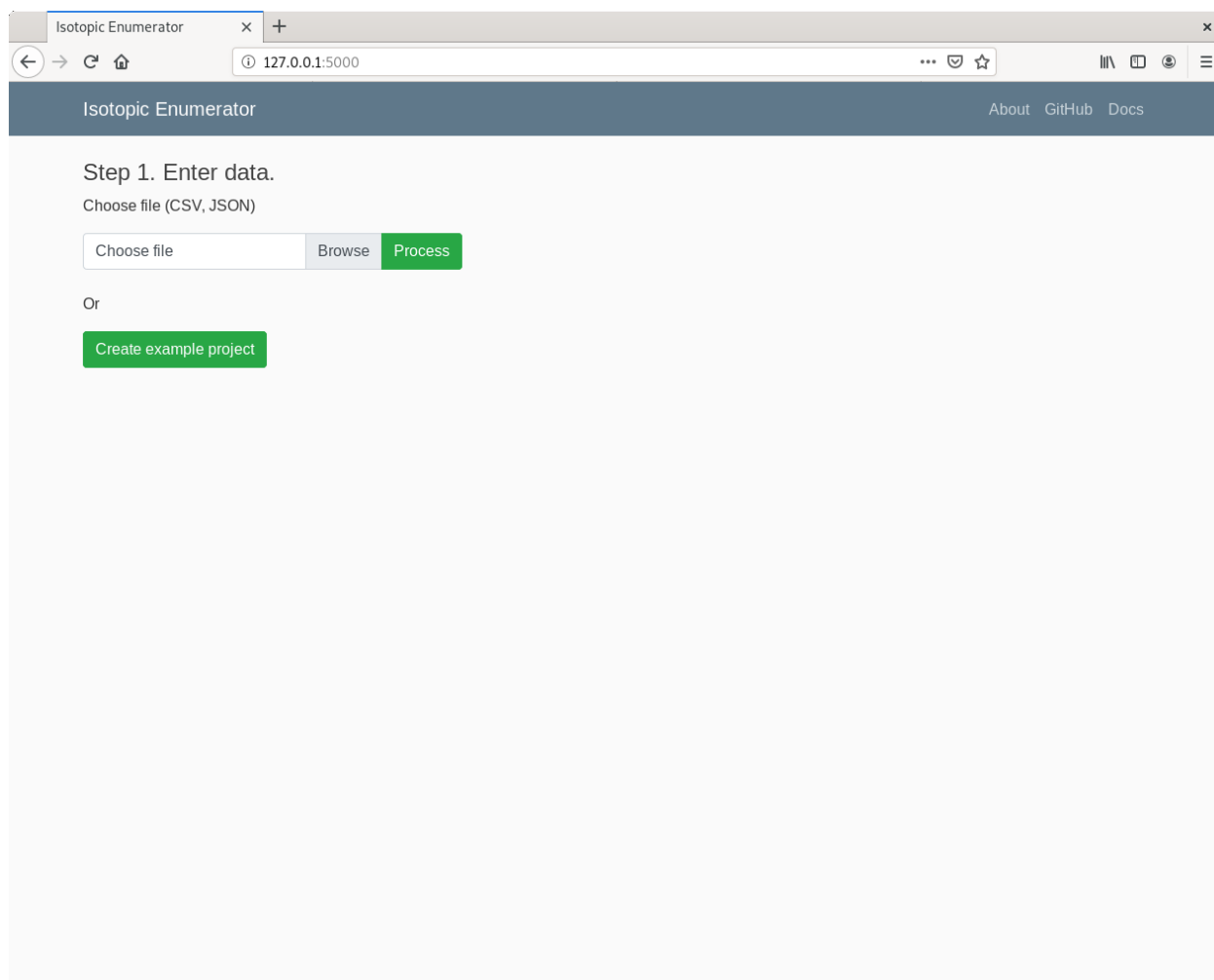
1.4 License

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:

- JSON file saved from the InChI Table View:

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```

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→0000      0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0\n      1.7321   -1.0700   0.0000   H 0
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→0\n      2 3 2 0 0 0 0\n      2 4 1 0 0 0 0\n      4 8 1 0 0 0 0\n      END\n",
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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.

Isotopic Enumerator

Step 2. Update ISO and CHG columns to generate representative InChI.

- Use **isotope:atom:atom_number** format to specify **ISO** properties.
 - For example, **13:C:2** means that carbon atom at position **2** is isotope **13**.
- Use **atom:atom_number:charge** format to specify **CHG** properties.
 - For example, **0:4:-1** means that oxygen atom at position **4** has charge **-1**.

Step 3. Generate NMR-specific InChI.

1D-1H Generate NMR specific InChI Save

Name	Base Identifier	Base SVG	ISO	CHG	Repr Identifier	Repr SVG	Update/Remove
acetic acid	InChI=1S/C2H4O2 /c1-2(3)/h1H3, (H,3,4)				InChI=1S/C2H4O2 /c1-2(3)/h1H3, (H,3,4)		Update Remove
valine	InChI=1S/C5H11NO2 /c1-3(2)4(6)5(7)8 /h3-4H,6H2,1-2H3, (H,7,8)/t4-m/s1				InChI=1S/C5H11NO2 /c1-3(2)4(6)5(7)8 /h3-4H,6H2,1-2H3, (H,7,8)/t4-m/s1		Update Remove

Add row

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**.

Isotopic Enumerator

127.0.0.1:5000/table

About GitHub Docs

Step 2. Update ISO and CHG columns to generate representative InChI.

- Use `isotope:atom:atom_number` format to specify **ISO** properties.
 - For example, `13:C:2` means that carbon atom at position **2** is isotope **13**.
- Use `atom:atom_number:charge` format to specify **CHG** properties.
 - For example, `0:4:-1` means that oxygen atom at position **4** has charge **-1**.

Step 3. Generate NMR-specific InChI.

1D-1H

Generate NMR specific InChI

Save

Name	Base Identifier	Base SVG	ISO	CHG	Repr Identifier	Repr SVG	Update/Remove
acetic acid	InChI=1S/C2H4O2 /c1-2(3)4/h1H3, (H,3,4)		13:C:1 13:C:2		InChI=1S/C2H4O2 /c1-2(3)4/h1H3, (H,3,4)/1+1,2+1		Update Remove
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		Update Remove

Add row

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**

Isotopic Enumerator

127.0.0.1:5000/table

About GitHub Docs

Step 2. Update ISO and CHG columns to generate representative InChI.

- Use **isotope:atom:atom_number** format to specify **ISO** properties.
 - For example, **13:C:2** means that carbon atom at position **2** is isotope **13**.
- Use **atom:atom_number:charge** format to specify **CHG** properties.
 - For example, **0:4:-1** means that oxygen atom at position **4** has charge **-1**.

Step 3. Generate NMR-specific InChI.

1D-1H

Generate NMR specific InChI

Save

Name	Base Identifier	Base SVG	ISO	CHG	Repr Identifier	Repr SVG	Update/Remove
acetic acid	InChI=1S/C2H4O2 /c1-2(3)4/h1H3, (H,3,4)		13:C:1 13:C:2	O:4:-1	InChI=1/C2H4O2 /c1-2(3)4/h1H3, (H,3,4)/p-1/f1+1,2+1 /C2H3O2/q-1		Update Remove
valine	InChI=1S/C5H11NO2 /c1-3(2)4(6)5(7)8 /h3-4H,6H2,1-2H3, (H,7,8)/t4-m/s1				InChI=1S/C5H11NO2 /c1-3(2)4(6)5(7)8 /h3-4H,6H2,1-2H3, (H,7,8)/t4-m/s1		Update Remove

Add row

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.

Isotopic Enumerator
 127.0.0.1:5000/table

About GitHub Docs

Step 3. Generate NMR-specific InChI.

1D-1H
 Generate NMR specific InChI
Save

Name	Base Identifier	Base SVG	ISO	CHG	Repr Identifier	Repr SVG	Update/Remove
acetic acid	InChI=1S/C2H4O2 /c1-2(3)4/h1H3, (H,3,4)		13:C:1 13:C:2	O:4:-1	InChI=1/C2H4O2 /c1-2(3)4/h1H3, (H,3,4)/p-1/r1+1,2+1 /C2H3O2/q-1		Update Remove
valine	InChI=1S/C5H11NO2 /c1-3(2)4(6)5(7)8 /h3-4H,6H2,1-2H3, (H,7,8)/t4-m/s1				InChI=1S/C5H11NO2 /c1-3(2)4(6)5(7)8 /h3-4H,6H2,1-2H3, (H,7,8)/t4-m/s1		Update Remove
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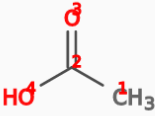
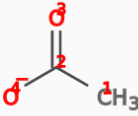
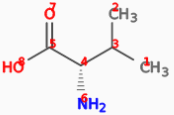
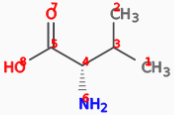
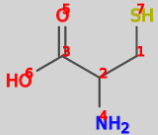
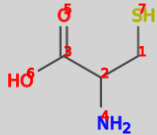
Add row

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

Isotopic Enumerator

127.0.0.1:5000/table

About GitHub Docs

Name	Base Identifier	Base SVG	ISO	CHG	Repr Identifier	Repr SVG	Update/Remove
acetic acid	InChI=1S/C2H4O2 /c1-2(3)/h1H3, (H,3,4)		13:C:1 13:C:2	O:4:-1	InChI=1/C2H4O2 /c1-2(3)/h1H3, (H,3,4)/p-1/1+1,2+1 /tC2H3O2/q-1		Update Remove
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		Update Remove
	InChI=1S/C3H7NO2S /c4-2(1-7)3(5)6 /h2,7H,1,4H2,(H,5,6)				InChI=1S/C3H7NO2S /c4-2(1-7)3(5)6 /h2,7H,1,4H2,(H,5,6)		Update Remove

Add row

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

Isotopic Enumerator

Step 2. Update ISO and CHG columns to generate representative InChI.

- Use **isotope:atom:atom_number** format to specify **ISO** properties.
 - For example, **13:C:2** means that carbon atom at position **2** is isotope **13**.
- Use **atom:atom_number:charge** format to specify **CHG** properties.
 - For example, **0:4:-1** means that oxygen atom at position **4** has charge **-1**.

Step 3. Generate NMR-specific InChI.

1D-1H Generate NMR specific InChI Save

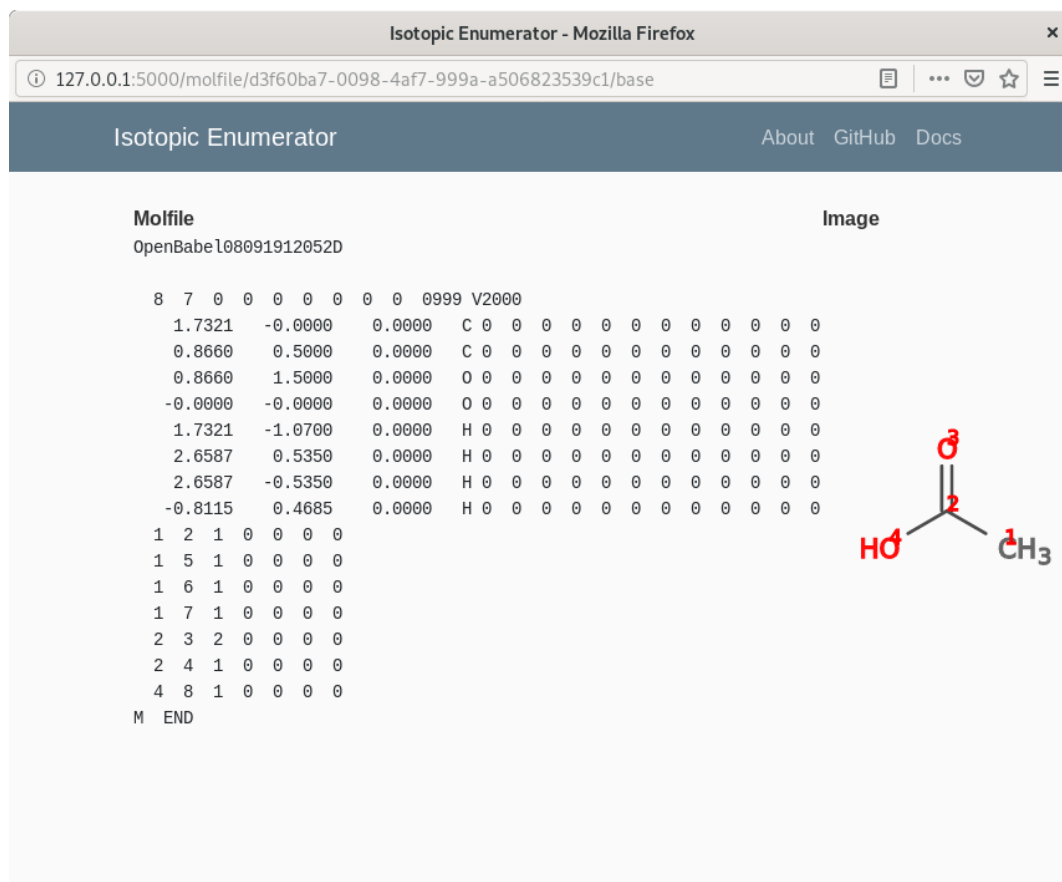
Name	Base Identifier	Base SVG	ISO	CHG	Repr Identifier	Repr SVG	Update/Remove
acetic acid	InChI=1S/C2H4O2 /c1-2(3)/h1H3, (H,3,4)		13:C:1 13:C:2	O:4:-1	InChI=1/C2H4O2 /c1-2(3)/h1H3, (H,3,4)/p-1/f1+1,2+1 /tC2H3O2/q-1		Update Remove
valine	InChI=1S/C5H11NO2 /c1-3(2)4(6)5(7)8 /h3-4H,6H2,1-2H3, (H,7,8)/t4-m/s1				InChI=1S/C5H11NO2 /c1-3(2)4(6)5(7)8 /h3-4H,6H2,1-2H3, (H,7,8)/t4-m/s1		Update Remove

Add 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:

Isotopic Enumerator - Mozilla Firefox

127.0.0.1:5000/molfile/d3f60ba7-0098-4af7-999a-a506823539c1/repr

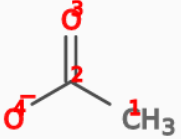
Isotopic Enumerator [About](#) [GitHub](#) [Docs](#)

Molfile

OpenBabel08091912052D

```
7 6 0 0 0 0 0 0 0 0999 V2000
  1.7321 -0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
  0.8660 0.5000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
  0.8660 1.5000 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0
 -0.0000 -0.0000 0.0000 O 0 5 0 0 0 0 0 0 0 0 0 0
  1.7321 -1.0700 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0
  2.6587 0.5350 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0
  2.6587 -0.5350 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0
1 2 1 0 0 0 0
1 5 1 0 0 0 0
1 6 1 0 0 0 0
1 7 1 0 0 0 0
2 3 2 0 0 0 0
2 4 1 0 0 0 0
M ISO 1 1 13
M ISO 1 2 13
M CHG 1 4 -1
M END
```

Image



How to save table view.

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

Isotopic Enumerator

127.0.0.1:5000/table

About GitHub Docs

Step 2. Update ISO and CHG columns to generate representative InChI.

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

Step 3. Generate NMR-specific InChI.

1D-1H Generate NMR specific InChI Save

Name	Base Identifier	Base SV	CHG	Repr Identifier	Repr SVG	Update/Remove
acetic acid	InChI=1S/C2H4O2 /c1-2(3)4/h1H3, (H,3,4)		13:C:1 13:C:2	O:4:-1 InChI=1/C2H4O2 /c1-2(3)4/h1H3, (H,3,4)/p-1/f1+1,2+1 /tC2H3O2/q-1		Update Remove
valine	InChI=1S/C5H11NO2 /c1-3(2)4(6)5(7)8 /h3-4H,6H2,1-2H3, (H,7,8)/t4-m/s1			InChI=1S/C5H11NO2 /c1-3(2)4(6)5(7)8 /h3-4H,6H2,1-2H3, (H,7,8)/t4-m/s1		Update Remove

Add row

127.0.0.1:5000/export_csv

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”.

Isotopic Enumerator

Step 2. Update ISO and CHG columns to generate representative InChI.

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

Step 3. Generate NMR-specific InChI.

1D-1H Generate NMR specific InChI Save

Name	Base Identifier	Base SVG	ISO	CHG	Repr Identifier	Repr SVG	Update/Remove
acetic acid	InChI=1S/C2H4O2 /c1-2(3)4/h1H3, (H,3,4)		13:C:1 13:C:2	O:4:-1	InChI=1/C2H4O2 /c1-2(3)4/h1H3, (H,3,4)/p-1/i+1,2+1 /tC2H3O2/q-1		Update Remove
valine	InChI=1S/C5H11NO2 /c1-3(2)4(6)5(7)8 /h3-4H,6H2,1-2H3, (H,7,8)/t4-m/s1				InChI=1S/C5H11NO2 /c1-3(2)4(6)5(7)8 /h3-4H,6H2,1-2H3, (H,7,8)/t4-m/s1		Update Remove

Add row

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.

Isotopic Enumerator

127.0.0.1:5000/nmrtable?nmr_type=1D-1H

About GitHub Docs

Step 4. Select relevant NMR-specific InChI.

Go back Select all Deselect all Save

C2H4O2 - 1D1H

Name	Base Identifier	Base SVG	ISO	CHG	Repr Identifier	Repr SVG
acetic acid	InChI=1S/C2H4O2/c1-2(3)4/h1H3,(H,3,4)		13:C:1 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	

☐	Resonance Description	NMR Specific InChI	ME Group
☐	[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	ME1
☐	[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	ME2

C5H11NO2 - 1D1H

Name	Base Identifier	Base SVG	ISO	CHG	Repr Identifier	Repr SVG
valine	InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8				InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8	

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.

Isotopic Enumerator

127.0.0.1:5000/nmrtable?nmr_type=1D-1H

Isotopic Enumerator

About GitHub Docs

C2H4O2 - 1D1H

Name	Base Identifier	Base SVG	ISO	CHG	Repr Identifier	Repr SVG
acetic acid	InChI=1S/C2H4O2/c1-2(3)4/h1H3,(H,3,4)		13:C:1 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	

☒ Resonance Description
 ☒ NMR Specific InChI
 ☐ ME Group

☒	[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	ME1
☒	[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	ME2

C5H11NO2 - 1D1H

Name	Base Identifier	Base SVG	ISO	CHG	Repr Identifier	Repr SVG
valine	InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-m/s1				InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8/h3-4H,6H2,1-2H3,(H,7,8)/t4-m/s1	

- 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.

Isotopic Enumerator

Step 4. Select relevant NMR-specific InChI.

Go back Select all Deselect all Save

C2H4O2 - 1D1H

Name	Base Identifier	Base SVG	ISO	CHG	Repr Identifier	Repr SVG
acetic acid	InChI=1S/C2H4O2/c1-2(3)4/h1H3,(H,3,4)		13:C:1 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	

☒	Resonance Description	NMR Specific InChI	ME Group
☒	[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	ME2
☒	[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	ME1

C5H11NO2 - 1D1H

Name	Base Identifier	Base SVG	ISO	CHG	Repr Identifier	Repr SVG
valine	InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8				InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8	

How to save NMR table view.

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

Isotopic Enumerator

127.0.0.1:5000/nmrtable?nmr_type=1D-1H

About GitHub Docs

Step 4. Select relevant NMR-specific InChI.

Go back Select all Deselect all Save

C2H4O2 - 1D1H

CSV
JSON

Name	Base Identifier	Base SVG	ISO	CHG	Repr Identifier	Repr SVG
acetic acid	InChI=1S/C2H4O2/c1-2(3)4/h1H3,(H,3,4)		13:C:1 13:C:2	O:4:-1	InChI=1/C2H4O2/c1-2(3)4/h1H3,(H,3,4)/p-1/i1+1H3,2+1/fC2H3O2/q-1	

☒	Resonance Description	NMR Specific InChI	ME Group
☒	[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	ME1
☒	[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	ME2

C5H11NO2 - 1D1H

Name	Base Identifier	Base SVG	ISO	CHG	Repr Identifier	Repr SVG
valine	InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8				InChI=1S/C5H11NO2/c1-3(2)4(6)5(7)8	

- 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** (*str*) – 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

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