



FOR-IDENT platform

User Manual

(3. Version, Mai 2017)

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Cite as: Grosse S., Letzel T.: User Manual for FOR-IDENT Database, 2017 (3), 1-35

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1. General information

The database 'STOFF-IDENT' was originally be developed within the research project 'RISK-IDENT', funded by the German Federal Ministry of Education and Research (BMBF) in the time period 11/2011-03/2015. The database is further be developed with new functions as well as with increased amount of compounds and proven data quality in the research project 'FOR-IDENT' funded by the German BMBF in the time period 03/15-02/17.

During the first period of the FOR-IDENT project the original idea of STOFF-IDENT was continued and extended. The basis remained the same, however new requirements and workflow strategies necessitated the following:

- modern and responsive design
- a better support of Excel as import and export format
- easier and innovative development of modules for the integration of other software services
- better focus for the user on his/her workflow and data workout
- Screen with better result presentation
- Drag'n' drop for data files in the search function
- Search-History
- Quality increase of included data and other error eliminations

Primary the compound database 'STOFF-IDENT' is used for identification purposes, more exactly for non-target screening ('Hidden Targets' and/or 'Known Unknown') and suspected-target screening analysis in different parts of water research.¹ This is why just water relevant organic molecules, their transformation products and metabolites that occur in the environment are listed.²

Besides common compound parameters as Name, CAS Number, Formula, InChi key, IUPAC Name, SMILES Code, monoisotopic mass, also physicochemical indications as the logP and the logD value for four different pH values are included.²

The database query is possible by using e.g. the compound name as well as the monoisotopic mass. Also a normalization of the retention time is integrated to use this chromatographic parameter. This tool, called 'Retention Time Index (RTI)' normalizes the retention time based on the logD value. Therefore a standard mixture with 'calibration molecules' has to be measured with the same chromatographic method as for the analytes that will be searched afterwards in the database. You can find an example of such a mixture in the excel data file 'template_RTI.zip' in the sheet 'calibration'. This also can be opened by pressing the 'Help' button in the molecular screening part. Of course also an own composition of calibration molecules can be used. Here it is important just to use neutral charged molecules that include the total logP/logD range of your method. Be aware that the corrections as well as results obtained and published so far are only strictly valid using these calibration molecules as shown on page 23.^{3a,b}

During the second period of the FOR-IDENT Project other open access available databases are connected directly to the platform or Links to the appropriate website is implemented. New formats to import data with MSMS information is now available as well as information about predicted transformation products.

The manual will be updated regularly if new functions are available.

¹ T. Letzel *et al.*, Chemosphere **2015**, 137, 198-206.

² http://risk-ident.hswt.de/media/downloads/STOFF-IDENT%20in%20der%20Anwendung_Dr_%20Marion%20Letzel.pdf (German)

^{3a} [http://risk-ident.hswt.de/media/downloads/Retention%20Time%20Index%20\(RTI\)_Dr_%20Thomas%20Letzel\(1\).pdf](http://risk-ident.hswt.de/media/downloads/Retention%20Time%20Index%20(RTI)_Dr_%20Thomas%20Letzel(1).pdf)

^{3b} http://risk-ident.hswt.de/media/downloads/Statusseminar_TUM.pdf

1.1 Languages, Settings, Home and Logout

Switch between the languages: English and German

Settings: change user setting (e.g. password)

Home: Start page (e.g. FOR-IDENT manual, information of supported formats)

Logout

The image shows two parts of the FOR-IDENT web application. On the left is a sidebar menu with a blue header 'FOR-IDENT'. Below the header are language flags (German and English) and a 'Collapse' button. The menu items are 'Settings' (with a person icon), 'Logout' (with a door icon), and 'Home' (with a house icon). A red rectangle highlights the 'Settings', 'Logout', and 'Home' items. On the right is a modal window titled 'Edit user settings' with a close button (X). It contains several input fields: 'E-Mail (max.60)' with a red error indicator, 'Username (max.60)', 'Password (min.6)', 'Password confirmation', 'First Name (max.40)', 'Last Name (max.40)', and 'Organization (max.80)'. At the bottom right of the modal are 'OK' and 'Close' buttons.

The image shows the main page of the FOR-IDENT web application. It has a dark sidebar on the left with the title 'FOR-IDENT DEV' and a search bar. Below the search bar are links for 'Registrieren', 'Anmelden', 'Start', 'Suche', 'Schnellsuche', 'Indexsuche', 'Processing', and 'Molekülscreening'. The main content area has a blue header 'FOR-IDENT' and a 'Collapse' button. Below the header are links for 'Manual', 'Manual STOFF-IDENT and RTI', 'Method-/data-workout inquiry', and 'STOFF-IDENT contents'. The 'Manual' section is expanded, showing a 'Formats' section with a warning about export files and a list of supported formats: .cef (Agilent), .mzML (Waters), .txt (Sciex), and .xlsx / .csv (Thermo). Below the formats section is a 'Sponsored by' section with logos for the Federal Ministry of Education and Research, Bayerisches Landesamt für Umwelt, Hochschule Weihenstephan-Triesdorf, and TUM. The 'Partner' section shows logos for the Zweckverband Landeswasserversorgung, IWW, and Berliner Wasserbetriebe. The 'Powered by' section shows the logo for the University of Applied Sciences.

2. Abbreviations

| | |
|------------|-------------------------------|
| Da | Dalton |
| M | monoisotopic mass |
| m/z | mass to charge |
| ppm | parts per million |
| RT | retention time |
| RTI | Retention Time Index |
| TP | transformation product |

3. System requirements

All well-established operation software and browsers should be supported.

In general you may use the actual browser version, especially for Internet Explorer use version 9 or higher.

The Excel version should be at least Excel 97.

4. Search tabs

4.1 Quick search

1. Input of Monoisotopic Mass as M or m/z by selection of the Ion species and determination of the mass accuracy (ppm)

The image shows two screenshots of the FOR-IDENT Quick search interface. The left screenshot shows the 'Monoisotopic Mass' field highlighted with a red box. The right screenshot shows the 'Ion species' dropdown menu open, with options ±0, +H, and -H, also highlighted with a red box.

2. Entry of logP value instead of Monoisotopic Mass
(By going with the cursor to the logP field, the possible values appear)

The image shows two screenshots of the FOR-IDENT Quick search interface. The left screenshot shows the 'logP' field highlighted with a red box. The right screenshot shows a list of 'Possible Values' for logP, including 'Exact z.B -1.23', 'Greater then > 1.23', 'Smaller then < 1.23', and 'Range 1.23 - 3.21'.

3. Selection of possible halogens, if known by isotopic pattern

The image shows a screenshot of the FOR-IDENT Quick search interface. The 'Halogens' section is highlighted with a red box. The section contains checkboxes for Cl, Br, F, and I.

4. Selecting the source lists (lists from various owners and institutions)
(select here in which list FOR-IDENT will perform the search; this tool is still under progress and will be extended with every update)

5. Press 'Start search' button (magnifier)
6. By pressing the 'Clear fields' button (rubber) all entries will be set to default values

4.2. Search

1. Entry of Name, CAS Number, Formula, InChi key, IUPAC Name, SMILES Code, STOFF-IDENT ID, Monoisotopic Mass as M or m/z by selection of the ion species and determination of the mass accuracy (ppm)

(By going with the cursor to the Monoisotopic Mass field, the possible values are shown)

and/ or logP value

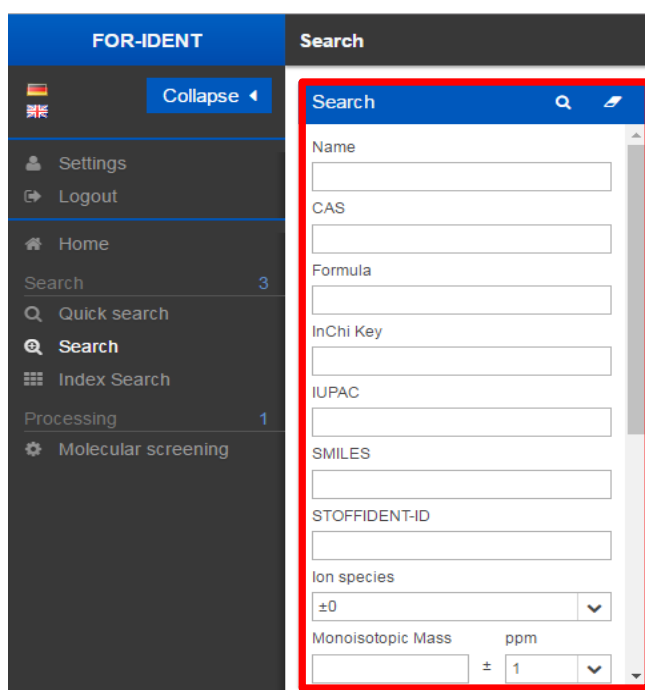
(By going with the cursor to the logP field, the possible values are shown)

and/ or Halogens if known

and/ or selection of a category (this tool is still under progress and will be extended with every update)

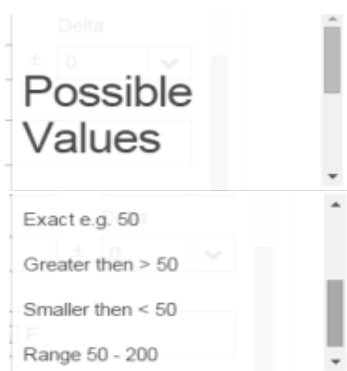
and/ or selecting the source list

(select here in which list FOR-IDENT will perform the search; this tool is still under progress and will be extended with every update))



Mass values

logP values



2. Press 'Start search' button (magnifier)
3. By pressing the 'Clear Fields' button (rubber) all entries will be set to default values

The image displays two side-by-side screenshots of the FOR-IDENT web application's 'Search' interface. Both screenshots show a dark sidebar on the left with navigation options: Settings, Logout, Home, Search (3), Quick search, Search, Index Search, Processing (1), and Molecular screening. The main content area is titled 'Search' and contains input fields for Name, CAS, Formula, InChi Key, IUPAC, SMILES, and STOFFIDENT-ID. It also includes a dropdown for 'Ion species' (set to ±0) and a section for 'Monoisotopic Mass' (ppm) with a value of 1. In the left screenshot, a magnifying glass icon in the top right of the search bar is highlighted with a red box. In the right screenshot, a rubber icon in the top right of the search bar is highlighted with a red box.

4.3. Index Search

1. Selection of search values via single letters or numbers
2. Selecting the source list
(select here in which list FOR-IDENT will perform the search; this tool is still under progress and will be extended with every update)

The image shows the FOR-IDENT 'Index search' interface. The sidebar on the left is identical to the previous screenshots, with 'Index Search' now highlighted. The main content area is titled 'Index search' and contains a search grid. This grid is highlighted with a red border and includes a header 'Search'. The grid consists of letters A through Z (with Z in a single wide box) and numbers 1 through 9, arranged in a 6x5 layout. The letters are in a blue font, and the numbers are in a blue font.

4.4. Search result page

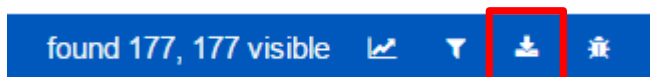
1. After pressing the 'Start search' button (magnifier) the result table appears

| Results found 177, 177 visible | | | | | | |
|---|----------------------|-------------------------|-------------------------------|----------------------|----------------------|----------------------------------|
| Name | CAS Number | SMILES | IUPAC | Formula | Monoisotopic Mass | Tonnage |
| <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> |
| valeric acid | 109-52-4 | CCCCC(O)=O | pentanoic acid | C5H10O2 | 102.068 | 1,000 - 10,000 tonnes per ann... |
| trichloro(hexadecyl)silane | 5894-60-0 | CCCCCCCCCCCCCCCC[Si]... | trichloro(hexadecyl)silane | C16H33Cl3Si | 358.142 | 100 - 1,000 tonnes per annum |
| trans-Zimtsäure | 140-10-3 | OC(=O)C=Cc1ccccc1 | (E)-3-phenylprop-2-enoic acid | C9H8O2 | 148.052 | |

2. A filtering allows to narrow down the results e.g. for Monoisotopic Mass values (left side: min value, right side: max value)

| Results found 177, 177 visible | | | | | | |
|---|----------------------|-------------------------|-------------------------------|----------------------|----------------------|----------------------------------|
| Name | CAS Number | SMILES | IUPAC | Formula | Monoisotopic Mass | Tonnage |
| <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> |
| valeric acid | 109-52-4 | CCCCC(O)=O | pentanoic acid | C5H10O2 | 102.068 | 1,000 - 10,000 tonnes per ann... |
| trichloro(hexadecyl)silane | 5894-60-0 | CCCCCCCCCCCCCCCC[Si]... | trichloro(hexadecyl)silane | C16H33Cl3Si | 358.142 | 100 - 1,000 tonnes per annum |
| trans-Zimtsäure | 140-10-3 | OC(=O)C=Cc1ccccc1 | (E)-3-phenylprop-2-enoic acid | C9H8O2 | 148.052 | |

3. By pressing the 'Download' button, a new window appears
4. Selection of favored parameters for download to excel



Export Results
✕

Filename (max.255)

☐ Include Sources?

Columns

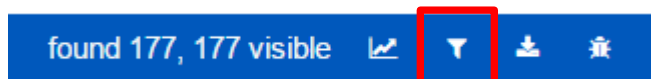
☐ Select/Deselect all

- ☐ STOFFIDENT-ID
- ☐ InChi
- ☐ InChi key
- ☒ CAS
- ☒ Name
- ☐ EC Number
- ☒ SMILES
- ☐ SMILES Structure
- ☒ Elemental formula
- ☒ IUPAC
- ☒ Monoisotopic mass
- ☒ Tonnage
- ☐ logP

Download

Close

5. By pressing the 'Clear filter' Button all filters will be set to default values and the original result table appears



In the 'Search history' area all performed searches were stored and can be reloaded again by 'doubleclick'.

FOR-IDENT

Collapse

Settings

Logout

Home

Search 3

Quick search

Search

Index Search

Processing 1

Molecular screening

Last data update
Jan 30, 2017

Index search

Search

A B C D E

F G H I J

K L M N O

P Q R S T

U V W X Y

Z

1 2 3

4 5 6

7 8 9

Source Lists

☒ Select/Deselect all

☒ NORMANews

☒ NIVA/Waters

☒ STOFF-IDENT

☒ permanent cations

Search history

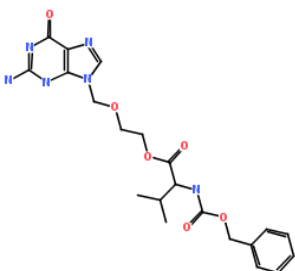
▶ Search1

In the 'Details' tab you can find specific information about the analyte. All information can be downloaded as an excel-file. Besides you have the choice to see the Metadata or not.

Details

Metadata

Structure



General

| | |
|---------------|--|
| Name | 2-[(2-amino-6-oxo-3,6-dihydro-9H-purin-9-yl)methoxy]ethyl N-[(benzyloxy)carbonyl]-L-valinate |
| Source | REACH |
| Last modified | Apr 12, 2016 |
| STOFFIDENT-ID | SI00006435 |
| SMILES | <chem>CC(C)C(NC(=O)OCc1ccccc1)C(=O)OCCOCn1cnc2c1[nH]c(N)nc2=O</chem> |
| Source | chemicalize.org |
| Last modified | Apr 12, 2016 |
| InChi | InChi=1/C21H26N6O6/c1-13(2)15(24-21(30)33-10-14-6-4-3-5-7-14)19(29)32-9-8-31-12-27-11-23-16-17(27)25-20(22)26-18(16)28/h3-7,11,13,15H,8- |

Export Results

Filename (max.255)

☐ Include Sources?

Columns

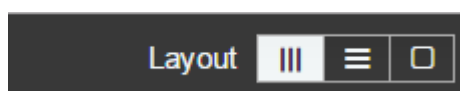
☐ Select/Deselect all

☐ STOFFIDENT-ID
☐ InChi
☐ InChi key
☒ CAS
☒ Name
☐ EC Number
☒ SMILES
☐ SMILES Structure
☒ Elemental formula
☒ IUPAC
☒ Monoisotopic mass
☒ Tonnage
☐ logP

Download

Close

You can change the Layout with three different options



In the Details at the web search part, you can directly search the specific compound via internet or you go to the External Links to get more information of the compound

Web Search

[Google search by Name](#)

[Google search by CAS](#)

[Google search by Inchi](#)

External Links


[Echa's REACH](#)

[EPA Dashboard](#)


www.chemicalize.org

If you find errors in the parameters given, e.g. wrong sum formula, SMILES code, etc. you can use the ‘report record as faulty’ button to send it directly to the software developer team by putting your comments of the fault into the comment field.

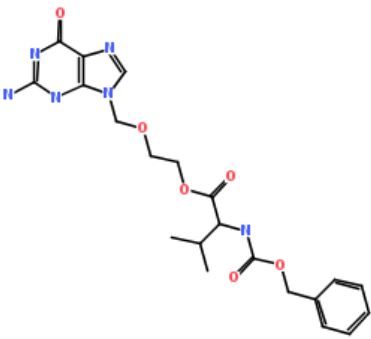
Details



Metadata



Structure



General

Name

2-[(2-amino-6-oxo-3,6-dihydro-9H-purin-9-yl)methoxy]ethyl N-[(benzyloxy)carbonyl]-L-valinate

Source

REACH

Last modified

Apr 12, 2016

Report Window

Preview

Error Report of incorrect entry details
Wed May 04 13:33:21 CEST 2016
Entry:
C₂₄H₂₈N₆O₈

From

Username

Organization

☐ Send error report anonymous

Comment (An explanation of the error helps us enormous to resolve it)

OK

Close

5. Processing

5.1 Molecular Screening

In the Molecular Screening area it is possible to process a list of compounds, e.g. from a non-target screening measurement, by searching the database by mass and/ or formula and if available retention time by using the retention time index function (possible for reversed phase columns) as well as MS/MS information, if available.

The software will perform the database search based on the available information (Mass, RT, RTI calibration, MS/MS) uploaded in the file. Detailed information are given in the following sections.

FOR-IDENT Molecular Screening (Hidden-Target Screening/ Suspected-Target Screening/ Known Unknowns)

Process

Files **Add**

Processes **Edit**

Mass Screening
RTI Screening
MS/MS
Transformation Products
MassBank entry available
Required data available: ☒ or ☐
Processing activated: ☒ or ☐

Parameters **Start**

pH

Source Lists

☒ Select/Deselect all

☒ NORMANews
☒ NINAWaters
☒ STOFF-IDENT
☒ permanent cations

Last processed

Please note:

Each zip file contains two Excel templates, which can be used for the processing. The only difference between both files is an additional sheet, which contains the RTI calibration data. For more information please see the manual below.

- Green indicates neutral molecules with logD values between 0.35 – 4.00. The calculated logD value is directly used.
- Yellow indicates neutral molecules but they are in the lower hydrophobicity of reversed phase columns with logD values < 0.35. The calculated logD value is corrected by subtracting one logD value (-1).
- Purple indicates neutral molecules but they are in the higher hydrophobicity range of reversed phase columns which have logD values > 4.00. The calculated logD value is corrected by adding one logD value (+1).
- Blue indicates negatively charged molecules. The calculated logD value is corrected by subtracting one logD value (-1). The correction is not performed if C18 (polar endcapped) or C18 (polar embedded) was selected as stationary phase.
- Red indicates positively charged molecules. The calculated logD value is corrected by subtracting one logD value (-1).

The mentioned comments are based on results of the project RISK-IDENT from the Technical University of Munich. More details will be published soon

Manual FOR-IDENT

- [Example RTI and search files](#)
- [Example RTI file](#)
- [Example MassHunter export files](#)
- [Example MarkerLynx Marker export files](#)
- [Example MarkerLynx Results export files](#)
- [Example MarkerView export files](#)
- [Example ProFinder export files](#)
- [Example SIEVE export files](#)
- [Example Unifi export files](#)
- [Example MasterView export files](#)
- [Example Compound Discoverer export files](#)

Last data update
Jan 30, 2017

Possible formats

All templates can be found under the 'Help' page.

The 'template_general_search.zip' searches the database only by mass.

By using the 'template_general_RTI.zip' the database is searched by mass or formula and by retention time, including retention time index with calibration data.

Other possible Excel/ Comma separated value formats are:

- Only mass:

template_MH_search.zip; template_ML_marker_search.zip;
template_ML_results_search.zip; template_MV_search.zip; template_MSV_search.zip;
template_PF_search.zip; template_SI_search.zip; template_CD_search.zip;
template_TF_search.zip; template_UN_search.zip

- mass/formula and/or retention time:

template_MH_RTI.zip; template_ML_marker_RTI.zip; template_ML_results_RTI.zip;
template_MV_RTI.zip; template_MSV_RTI.zip; template_PF_RTI.zip;
template_SI_RTI.zip; template_CD_RTI.zip; template_UN_RTI.zip

Explanation to use excel-formats:

Agilent (MH: MassHunter qualitative analysis)

Waters (ML: MassLynx Marker und ML: MassLynx results)

Sciex (MV: MarkerView)

Sciex: (MSV: MasterView)

Agilent (PF: Profinder)

Thermo Scienitific (SI: SIEVE)

Thermo Scientific (CD: Compound Discoverer 2.0)

Thermo Scientific (TF: Tracefinder 4.1)

(For TraceFinder 4.1 and lower versions Excel files may contain duplicates, use Excel function Data-> Remove Duplicates)

Waters (UN: Unifi)

There is also the possibility to use non-excel formats:

.cef (Agilent)

.mzML (Waters)

.txt (Sciex) (please, install the template first. Instructions can be found on the Start page)

.csv (Thermo Scientific)

If you find your export file listed above, you can use it directly without any changes.

To use the retention time index function upload an extra excel-file with the calibration data like template_calibration.

Using the retention time index function requires a single measurement with a set of calibration molecules measured with the same analytical method as the sample (see below). Retention times of the calibration molecules must be filled in column 'rt1' (required), 'rt2' and 'rt3' (optional). Two options are available using the calibration data.

First option is to add a second sheet in the report file of the sample (if the report is an excel-file, otherwise use the second option), which must be named 'calibration' and follows the design showed below on the right. Templates of different vendors can be found under the 'Help' page.

| | A | B | C | D | E | F | | A | B | C | D | E |
|----|------------|---------------|-------------------|------|-----|-----|----|----------------|------|-----|-----|-------|
| 1 | identifier | accurate mass | elemental formula | rt1 | rt2 | rt3 | 1 | substance name | rt1 | rt2 | rt3 | logD |
| 2 | | | | | | | 2 | | | | | |
| 3 | | | | | | | 3 | | | | | |
| 4 | Unknown Y | 164.09495 | | 23.6 | | | 4 | Metformin | 16.9 | | | -1.36 |
| 5 | | | | | | | 5 | Chloridazon | 23.6 | | | 1.11 |
| 6 | | | | | | | 6 | Carbetamide | 25.0 | | | 1.65 |
| 7 | | | | | | | 7 | Monuron | 25.5 | | | 1.93 |
| 8 | | | | | | | 8 | Metobromuron | 27.5 | | | 2.24 |
| 9 | | | | | | | 9 | Chlorbromuron | 29.0 | | | 2.85 |
| 34 | | | | | | | 10 | Metconazole | 29.9 | | | 3.59 |
| 35 | | | | | | | 11 | Diazinon | 31.9 | | | 4.19 |
| 36 | | | | | | | 12 | Quinoxifen | 34.2 | | | 4.98 |
| 37 | | | | | | | 13 | Fenofibrate | 35.1 | | | 5.28 |
| 38 | | | | | | | 14 | | | | | |
| 39 | | | | | | | 40 | | | | | |

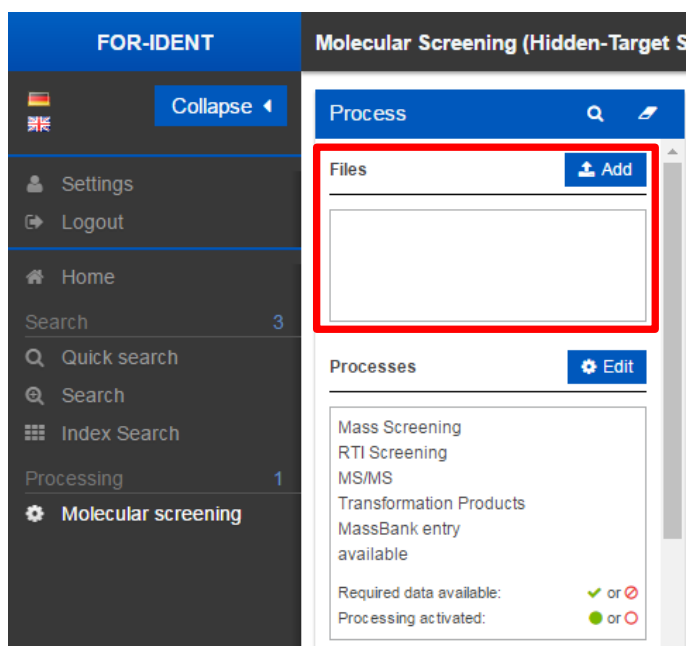
targets calibration targets calibration

Second option is to use an extra excel-file, as can be seen below. A template can be found under the 'Help' page: 'template calibration'.

| | A | B | C | D | E | F |
|----|----------------|------|-----|-----|-------|---|
| 1 | substance name | rt1 | rt2 | rt3 | logD | |
| 2 | | | | | | |
| 3 | | | | | | |
| 4 | Metformin | 16.9 | | | -1.36 | |
| 5 | Chloridazon | 23.6 | | | 1.11 | |
| 6 | Carbetamide | 25.0 | | | 1.65 | |
| 7 | Monuron | 25.5 | | | 1.93 | |
| 8 | Metobromuron | 27.5 | | | 2.24 | |
| 9 | Chlorbromuron | 29.0 | | | 2.85 | |
| 10 | Metconazole | 29.9 | | | 3.59 | |
| 11 | Diazinon | 31.9 | | | 4.19 | |
| 12 | Quinoxifen | 34.2 | | | 4.98 | |
| 13 | Fenofibrate | 35.1 | | | 5.28 | |
| 14 | | | | | | |

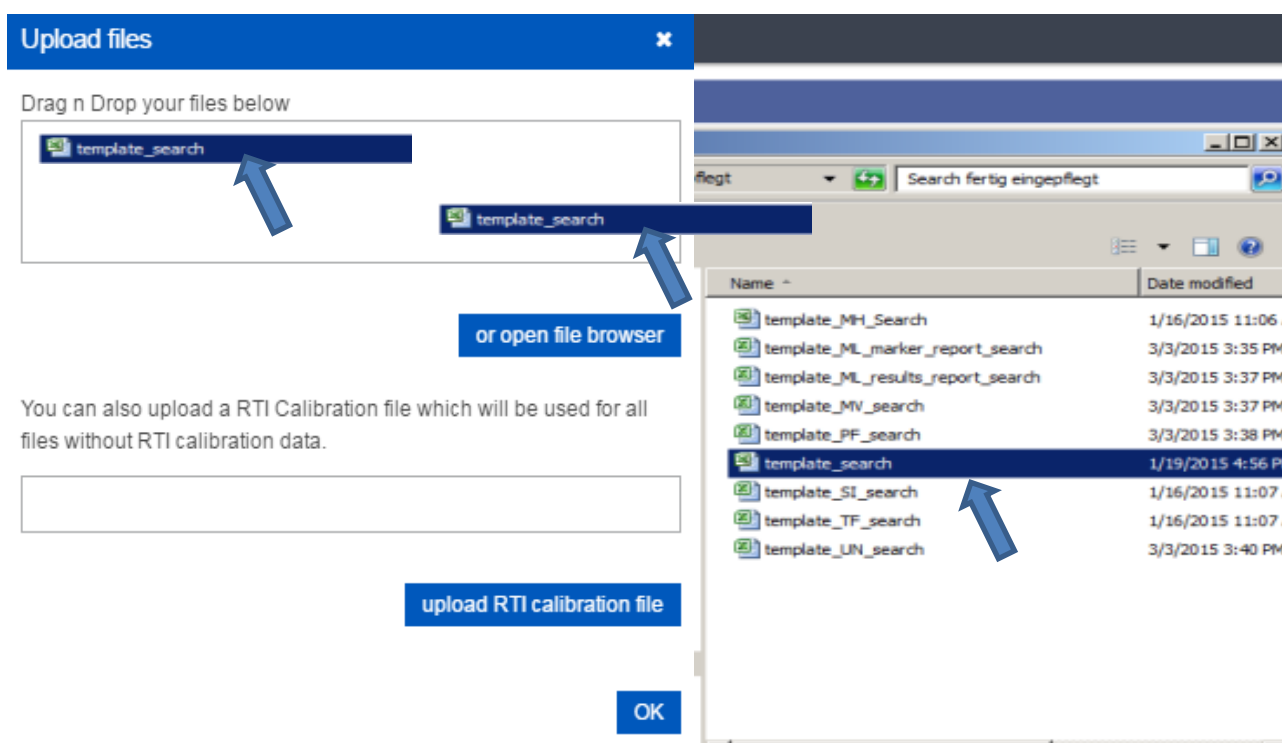
calibration

1. Press 'Add File' to upload data files



There are 2 options to import excel-files or other formats
You have the possibility to import one or more files at the same time
(refer to part 'possible formats' for more details on supported formats)

a) Drag`n Drop the file(s)



b) ...or open file browser and select one or more files

Upload files

Drag n Drop your files below

or open file browser

You can also upload a RTI Calibration file which will be used for all files without RTI calibration data.

upload RTI calibration file

OK

| Name | Date modified | Type | Size |
|--------------------------------|-------------------|------------------------|-------|
| template_MH_RTI | 3/3/2015 3:41 PM | Microsoft Excel 97... | 30 KB |
| template_MH_RTI | 7/8/2015 2:20 PM | Compressed (zippe... | 7 KB |
| template_ML_marker_report_RTI | 3/3/2015 3:42 PM | Microsoft Excel Wor... | 12 KB |
| template_ML_marker_report_RTI | 7/8/2015 2:20 PM | Compressed (zippe... | 9 KB |
| template_ML_results_report_RTI | 3/3/2015 3:44 PM | Microsoft Excel Wor... | 11 KB |
| template_ML_results_report_RTI | 7/8/2015 2:20 PM | Compressed (zippe... | 9 KB |
| template_MV_RTI | 3/3/2015 3:45 PM | Microsoft Excel Wor... | 11 KB |
| template_MV_RTI | 7/8/2015 2:20 PM | Compressed (zippe... | 9 KB |
| template_PF_RTI | 3/3/2015 3:46 PM | Microsoft Excel Wor... | 11 KB |
| template_PF_RTI | 7/8/2015 2:20 PM | Compressed (zippe... | 9 KB |
| template_RTI | 5/10/2016 6:05 PM | Microsoft Excel 97... | 27 KB |
| template_RTI | 7/8/2015 2:20 PM | Compressed (zippe... | 8 KB |
| template_SI_RTI | 1/21/2015 4:38 PM | Microsoft Excel Wor... | 14 KB |
| template_SI_RTI | 7/8/2015 2:20 PM | Compressed (zippe... | 11 KB |
| template_TF_RTI | 1/21/2015 4:38 PM | Microsoft Excel Wor... | 11 KB |
| template_TF_RTI | 7/8/2015 2:20 PM | Compressed (zippe... | 0 KB |

File name: template_RTI

Open

Cancel

If needed it is possible to upload an extra excel-file with the RTI calibration data. This file will be used for all files uploaded in the upper part.

Upload files

Drag n Drop your files below

or open file browser

You can also upload a RTI Calibration file which will be used for all files without RTI calibration data.

upload RTI calibration file

OK

Name

template_calibration

By using a series of different files in one batch, especially with and without RTI calibration data, the extra excel-file will be used, only if the uploaded file doesn't contain the second sheet 'calibration'.

2. Selecting the Process Settings

By clicking on ,Edit' a new window appears. This gives you the possibility to choose the weights of the different functions by your own experience.

Note that the sum has to be 100 %.

The screenshot shows the FOR-IDENT Molecular Screening (Hidden-Target Search) interface. The left sidebar contains navigation options: Settings, Logout, Home, Search (3), Quick search, Search, Index Search, Processing (1), and Molecular screening. The main area displays the 'Process' settings. A red box highlights the 'Processes' section, which lists the following processes and their weights:

| Process | Weight | Status |
|--------------------------|--------|--------|
| Mass Screening | 25% | Active |
| RTI Screening | 25% | Active |
| MS/MS | 25% | Active |
| Transformation Products | 0% | Active |
| MassBank entry available | 25% | Active |

Below the list, the 'Required data available' status is shown as 'or' (green circle) and 'or' (red circle). The 'Processing activated' status is shown as 'or' (green circle) and 'or' (red circle). The 'Process Settings' window is open, showing a table of process weights and a 'Sum: 100%' indicator.

| Process | Data Available | Activated | Weight |
|--------------------------|----------------|-----------|--------|
| Mass Screening | ✓ | ✓ | 10% |
| RTI / Screening | ✓ | ✓ | 40% |
| MS/MS | ✓ | ✓ | 35% |
| Transformation Products | ✓ | ✓ | 0% |
| MassBank entry available | ✓ | ✓ | 15% |

The 'Sum: 100%' indicator is highlighted in a red box. The 'Required data available' status is shown as 'or' (green circle) and 'or' (red circle). The 'Processing activated' status is shown as 'or' (green circle) and 'or' (red circle). The 'Process Settings' window is open, showing a table of process weights and a 'Sum: 100%' indicator.

3. Selection of chromatographic and mass spectrometric parameters, like pH value of used solvents, mass accuracy of precursor ion and fragment ions [ppm], intensity threshold of an uploaded MSMS spectra, Ion species and Stationary phase

The screenshot shows the FOR-IDENT Molecular Screening (Hidden-Target Search) interface. The left sidebar contains navigation options: Settings, Logout, Home, Search (3), Quick search, Search, Index Search, Processing (1), and Molecular screening. The main area displays the 'Parameters' section, which is highlighted with a red box. The parameters are as follows:

| Parameter | Value |
|---------------------|-------|
| pH | 3 |
| ppm precursor ion | 5 |
| ppm fragment ions | 5 |
| Intensity threshold | 0 |
| Ion species | ±0 |
| Stationary phase | C18 |

convincing results are tested for the following stationary phases so far: C18, C18 (polar endcapped), C18 (polar embedded), Phenyl and PFP (in-house column study) Other material gives probably uncertainties.

Once a selection is chosen for an uploaded file, it is kept even if you upload the next one

Besides or instead of the monoisotopic mass or m/z also the elemental formula can be used. The exact mass is then calculated by the database automatically and the accuracy is set to 0.01 ppm.

If just the monoisotopic mass or m/z is entered the accuracy is considered from 'ppm' field.

4. Selecting the source list

(select here in which list FOR-IDENT will perform the search; this tool is still under progress and will be extended with every update)

FOR-IDENT

Molecular Screening (Hidden-Target S)

Process

MassBank entry available 25%

Required data available: ✓ or ✗

Processing activated: ● or ○

Parameters **Start**

pH
3

ppm precursor ion
5

ppm fragment ions
5

Intensity threshold
0

Ion species
±0

Stationary phase
C18

Source Lists

☒ Select/Deselect all

☒ NORMANews

☒ NIVA/Waters

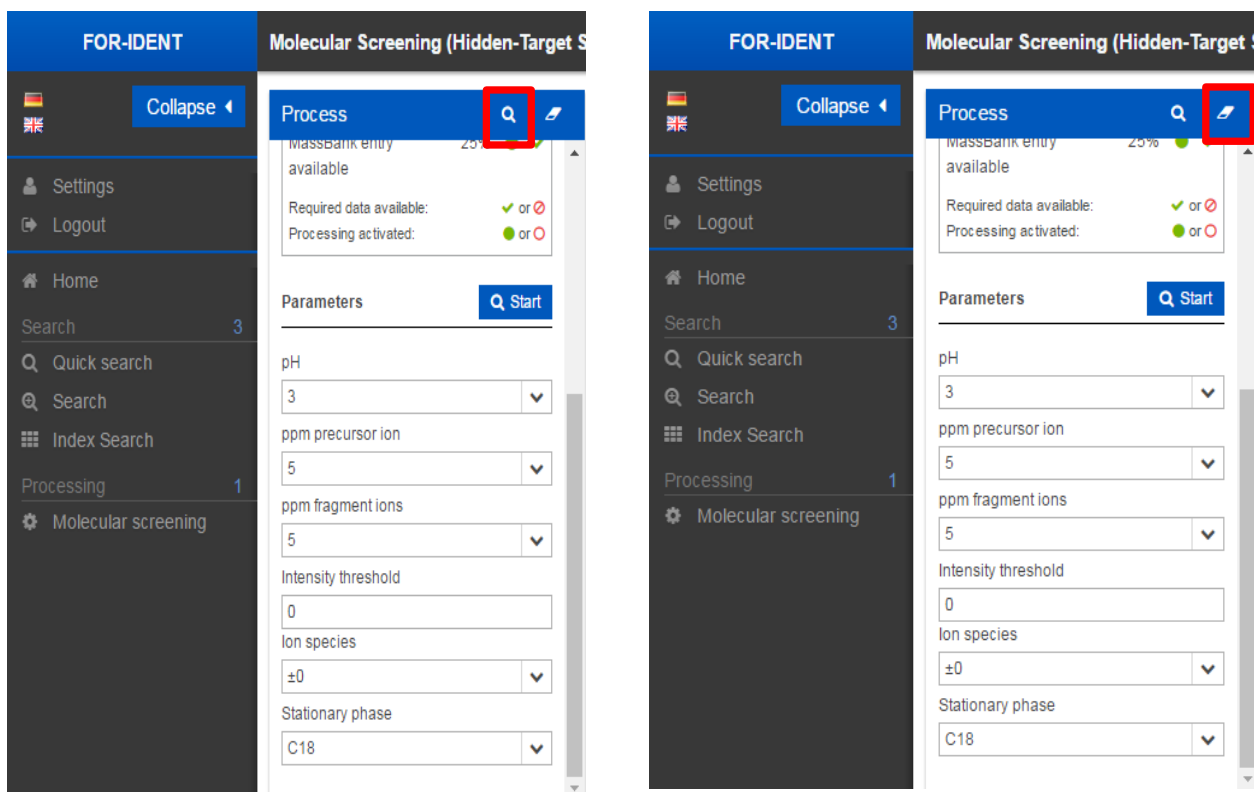
☒ STOFF-IDENT

☒ permanent cations

Last processed

Last data update
Jan 30, 2017

- Press 'Start search' button (magnifier)
- By pressing the 'Clear fields' button (rubber) all entries will be set to default values



5.2 result page

5.2.1 Explanation of the result table

Under the first tab 'Results' the hits for the uploaded file is shown (explained in detail starting with 5.2.1.1)

| FOR-IDENT | | | | | | | | | |
|---|------------|-----|----------------|---------|-------|----------|----------|-------|---------|
| Molecular Screening (Hidden-Target S) | | | | | | | | | |
| <div> <div> <div>FOR-IDENT</div> <div>Collapse</div> </div> <div> <div>Settings</div> <div>Logout</div> </div> <div> <div>Home</div> <div>Search 3</div> <div>Quick search</div> <div>Search</div> <div>Index Search</div> </div> <div> <div>Processing 1</div> <div>Molecular screening</div> </div> </div> <div> <div>Process</div> <div> <div>MassBank entry available</div> <div>Required data available: ✓ or ✗</div> <div>Processing activated: ✓ or ✗</div> </div> <div>Parameters</div> <div> <div>Start</div> <div>pH: 3</div> <div>ppm precursor ion: 5</div> <div>ppm fragment ions: 5</div> <div>Intensity threshold: 0</div> <div>Ion species: ±0</div> <div>Stationary phase: C18</div> </div> </div> | | | | | | | | | |
| Results | | | | | | | | | |
| Details | Target | RT | Result name | Look At | Score | Mass ... | RTI S... | MS/MS | MassB.. |
| | | | | | | | | | |
| Show | Amantadin | 5.1 | amantadine | ● | | | | | |
| Show | Amantadin | 5.1 | 3,7-dimethy... | | | | | | |
| Show | Metoprolol | 5.6 | Metoprolol | ● | | | | | |
| Show | Metoprolol | 5.6 | butoxamine | | | | | | |

Under the second tab 'Search content' the data of the uploaded file is shown (in the upper part the calibration data, in the lower part the targets), with the calculation of RTI and determined logD values

| Results Search content Help | | | | | | |
|-----------------------------|------------|---------------|-----------------|-------|------------------|------|
| Substance | Valid RT | RTI | logD | RT | Calibration data | |
| Metformin | ✓ | 50,0 | -1,36 | 16,91 | | |
| Chloridazon | ✓ | 87,2 | 1,11 | 23,56 | | |
| Carbetamide | ✓ | 95,3 | 1,65 | 25,01 | | |
| Monuron | ✓ | 99,5 | 1,93 | 25,49 | | |
| Metobromu... | ✓ | 104,2 | 2,24 | 27,53 | | |
| Chlorbromu... | ✓ | 113,4 | 2,85 | 29,03 | | |
| Metconazole | ✓ | 124,5 | 3,59 | 29,92 | | |
| Diazinon | ✓ | 133,6 | 4,19 | 31,87 | | |
| Quinoxifen | ✓ | 145,5 | 4,98 | 34,22 | | |
| Fenofibrate | ✓ | 150,0 | 5,28 | 35,14 | | |
| Target | Exact mass | Elemental ... | Calculated mass | RT | RTI | logD |
| Amantadin | 152,1433 | C10H17N | ✓ | 5,08 | 74,0 | 0,57 |
| Metoprolol | 268,1915 | C15H25NO3 | ✓ | 5,57 | 77,1 | 0,76 |
| Targets | | | | | | |

Under the third tab 'Help' the explanation of pH dependency is given and all templates are listed as well as the user manual can be found

| Results Search content Help | | | | | | |
|---|--|--|--|--|--|--|
| <p>Please note:</p> <p>Each zip file contains two Excel templates, which can be used for the processing. The only difference between both files is an additional sheet, which contains the RTI calibration data. For more information please see the manual below.</p> <ul style="list-style-type: none"> Green indicates neutral molecules with logD values between 0.35 – 4.00. The calculated logD value is directly used. Yellow indicates neutral molecules but they are in the lower hydrophobicity of reversed phase columns with logD values < 0.35. The calculated logD value is corrected by subtracting one logD value (-1). Purple indicates neutral molecules but they are in the higher hydrophobicity range of reversed phase columns which have logD values > 4.00. The calculated logD value is corrected by adding one logD value (+1). Blue indicates negatively charged molecules. The calculated logD value is corrected by subtracting one logD value (-1). The correction is not performed if C18 (polar endcapped) or C18 (polar embedded) was selected as stationary phase. Red indicates positively charged molecules. The calculated logD value is corrected by subtracting one logD value (-1). <p>The mentioned comments are based on results of the project RISK-IDENT from the Technical University of Munich. More details will be published soon</p> <p>Manual FOR-IDENT</p> <p>Example RTI and search files</p> <p>Example RTI file</p> <p>Example MassHunter export files</p> <p>Example MarkerLynx Marker export files</p> <p>Example MarkerLynx Results export files</p> <p>Example MarkerView export files</p> <p>Example ProFinder export files</p> <p>Example SIEVE export files</p> <p>Example Unifi export files</p> <p>Example MasterView export files</p> <p>Example Compound Discoverer export files</p> | | | | | | |

5.2.1.1 columns Target and RT

In the column 'Target' the name is shown which was used in the uploaded report file as identifier and in the column 'RT' the retention time, if uploaded.

| Results | | | | | | Scoring | | | |
|---------|----------------------|----------------------|----------------------|----------------------|-------|----------|----------|-------|---------|
| Details | Target | RT | Result name | Look At | Score | Mass ... | RTI S... | MS/MS | MassB.. |
| | <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> | | | | | |
| Show | Amantadin | 5.1 | amantadine | | | | | | |
| Show | Amantadin | 5.1 | 3,7-dimethy... | | | | | | |
| Show | Metoprolol | 5.6 | Metoprolol | | | | | | |
| Show | Metoprolol | 5.6 | butoxamine | | | | | | |

5.2.1.2 columns Result name and pH dependency

The column pH dependency shows the charge of the molecule at a definite pH value and in which range the logD value is, as the software calculates an automatic correction of the logD value depending on the color code.

Details of the color code are as follows:

Green indicates molecules, which are charged neutral for each pH value. The calculated logD value is directly used.

Yellow indicated molecules are charged neutral for each pH value, but are in the lower hydrophobicity range of reversed phase columns with log D values < 0.35. The calculated log D value is corrected by subtracting one logD value (-1).

Purple indicated molecules are charged neutral for each pH value, but are in the upper hydrophobicity range of reversed phase columns with logD values > 4.00. The calculated logD value is corrected by adding one logD value (+1).

Blue indicated molecules are charged negative. The calculated logD value is corrected by subtracting one logD value (-1). The correction is not performed, if C18 (polar endcapped) or C18 (polar embedded) columns are selected as stationary phase.

Red indicated molecules are charged positive. The calculated logD value is corrected by subtracting one logD value (-1).

The correction, if necessary, is automatically done by the database.

In the column 'Result name' the name of the database hit of the target analyte is shown with its pH dependency color code in column 'pH dep'.

| Results Search content Help | | | | | | |
|-----------------------------|----------------------|---|----------------------|------------------------|------------------------|------------|
| | Results | | | | | RTI Screen |
| Details | Target | RT | Result name | Look At | Score | pH dep |
| | <input type="text"/> | <input type="text"/> <input type="text"/> | <input type="text"/> | <input type="text"/> ▼ | | |
| Show | Amantadin | 5.1 | amantadine | ● | <div><div></div></div> | ● |
| Show | Amantadin | 5.1 | 3,7-dimethy... | | <div><div></div></div> | ● |
| Show | Metoprolol | 5.6 | Metoprolol | ● | <div><div></div></div> | ● |
| Show | Metoprolol | 5.6 | butoxamine | | <div><div></div></div> | ● |

5.2.1.3 columns Scoring: Mass Screening, RTI Screening, MS/MS and MassBank

| Results Search content Help | | | | | | | | | |
|-----------------------------|----------------------|---|----------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|
| | Results | | | | | Scoring | | | |
| Details | Target | RT | Result name | Look At | Score | Mass Screening | RTI Screening | MS/MS | MassBank |
| | <input type="text"/> | <input type="text"/> <input type="text"/> | <input type="text"/> | <input type="text"/> ▼ | | | | | |
| Show | Amantadin | 5.1 | amantadine | ● | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> |
| Show | Amantadin | 5.1 | 3,7-dimethy... | | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> |
| Show | Metoprolol | 5.6 | Metoprolol | ● | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> |
| Show | Metoprolol | 5.6 | butoxamine | | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> |

To evaluate the hits suggested for one target analyte by STOFF-IDENT the scoring bars indicates the likelihood of each function, especially if several hits are suggested for one target analyte.

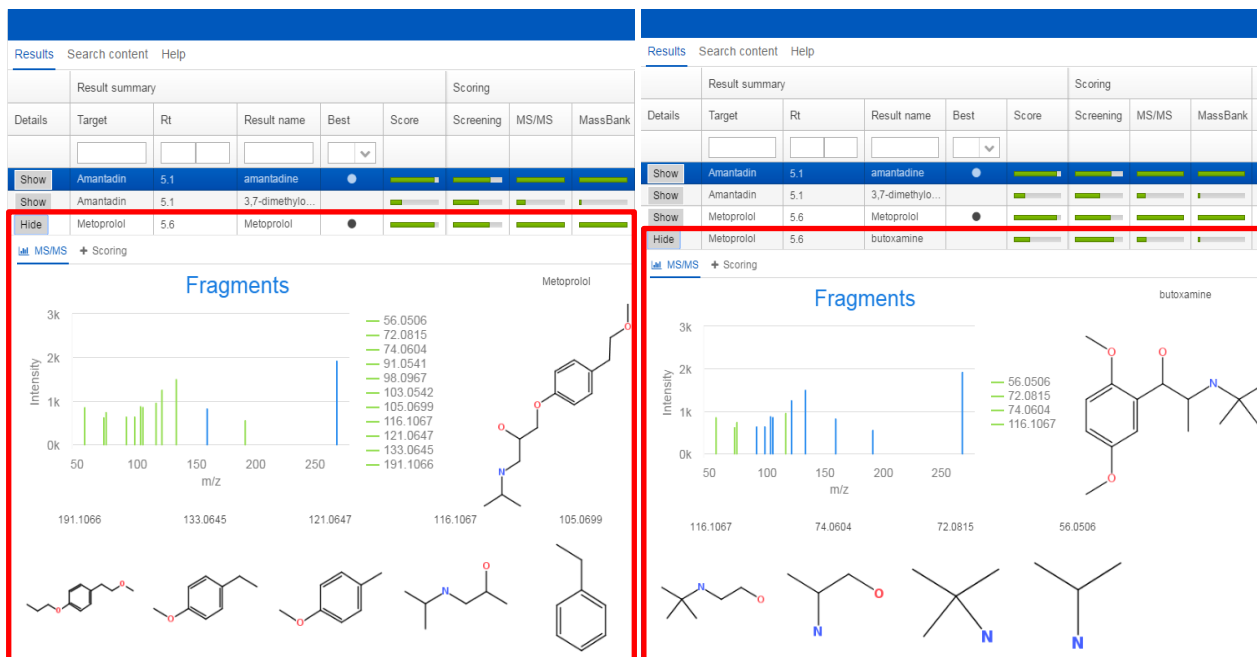
The Mass Screening Score represents the difference between the measured mass and the one listed in the database (column 'Δ mass').

The RTI Screening Score represents the difference between the determined logD value via RTI normalization and the one listed in the database (column 'Δ logD (Adj.-DB)').

A full green bar indicates very low difference while as smaller the bar indicates as higher the difference.

The MS/MS Score describes the differences between the uploaded MS/MS fragments and the ones, which MetFrag predicts in silico. The real MetFrag score is used, which includes some other rules and parameters. A scoring is just possible, if two or more hits are given for one target analyte. Refer to section “additional information” in this part for more details.

By pressing the ‘Show’ Button the comparison of uploaded fragments and in silico fragments of MetFrag is shown. Green indicates a fragment mass match and blue a mismatch of fragment. Below also the matched fragment structures are shown.



The MassBank Score represents, if the database hit has an experimental determined spectra in the MassBank database (Links are shown in the ‘Details’ area).

A full bar means at least one spectra available, an empty bar means no spectra available in MassBank database. No comparison of fragmentation spectra are performed.

Details Metadata

Source PubChem

Name Adamantanamine

Source PubChem

Name Adamantylamine

Source PubChem

MassBank

[MassBank EU ID: KO002184](#)

[MassBank EU ID: UF414704](#)

[MassBank EU ID: UF414701](#)

[MassBank EU ID: KO002187](#)

Triangles in the Score columns

- a) **missing RTI Screening Score: A logD value cannot be determined via RTI, if the RT of the target analyte is outside the calibration area of the RTI calibration molecules**
- b) **missing MSMS Score: A scoring can only be given, if at least two candidates are found for one target. Or if problems by parsing SMILES code occurred**
- c) **missing Score: The overall Score is missing, if one of the single Score gives no value**

| found 3 | | | | | | | | | |
|---------|----------------------|----------------------|----------------------|----------------------|---------|----------------|---------------|-------------|-------------|
| Results | Search content | Help | | | | | | | |
| | Results | | | | Scoring | | | | |
| Details | Target | RT | Result name | Look At | Score | Mass Screening | RTI Screening | MS/MS | MassBank |
| | <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> | | | | | |
| Show | Amantadin | 16.0 | amantadine | ● | ▲ | <div></div> | ▲ | <div></div> | <div></div> |
| Show | Amantadin | 16.0 | 3,7-dimethy... | | ▲ | <div></div> | ▲ | <div></div> | <div></div> |
| Show | Atrazine | 9.7 | Wonuk | ● | ▲ | <div></div> | | ▲ | <div></div> |
| Show | Atrazine-2-... | 5.0 | Atrazine-2-... | ● | | <div></div> | | | <div></div> |

No overall score available, due to missing scores

The screening score is not available, because the RT is not given or out of bounds of the calibration range.

The MS/MS provided by MetFrag is only supported for a list of candidates, not for single candidates. Also problems with parsing the SMILES can result in no MS/MS score.

5.2.1.4 columns Look At and Score

If several hits are suggested for one target analyte by STOFF-IDENT, in the column 'Look At' and 'Score' a summary of the single Scores is shown. The one with the highest overall Score, depending on the weight chosen by the operator, is marked with '●'.

| Results | Search content | Help | | | | | | | |
|---------|----------------------|----------------------|----------------------|----------------------|-------------|----------------|---------------|-------------|-------------|
| | Results | | | | Scoring | | | | |
| Details | Target | RT | Result name | Look At | Score | Mass Screening | RTI Screening | MS/MS | MassBank |
| | <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> | | | | | |
| Show | Amantadin | 5.1 | amantadine | ● | <div></div> | <div></div> | <div></div> | <div></div> | <div></div> |
| Show | Amantadin | 5.1 | 3,7-dimethy... | | <div></div> | <div></div> | <div></div> | <div></div> | <div></div> |
| Show | Metoprolol | 5.6 | Metoprolol | ● | <div></div> | <div></div> | <div></div> | <div></div> | <div></div> |
| Show | Metoprolol | 5.6 | butoxamine | | <div></div> | <div></div> | <div></div> | <div></div> | <div></div> |

A filtering of the results on all the 'Look At' molecules is easily available by selecting '●' in the 'Look At' column.

The result can be exported separately.

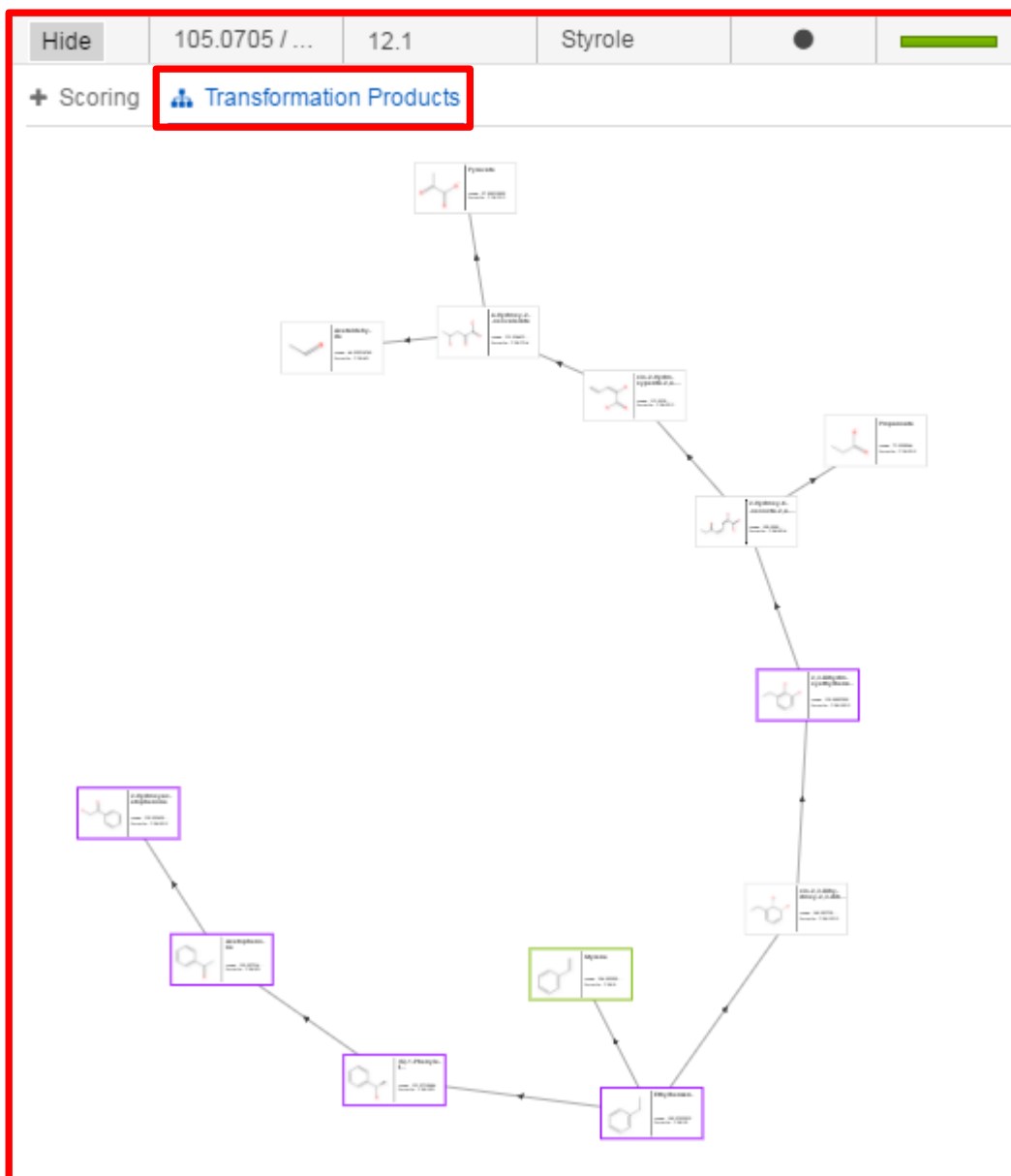
| fo | | | | | | | | | |
|-----------------------------|----------------------|----------------------|----------------------|------------------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|
| Results Search content Help | | | | | | | | | |
| | Results | | | | Scoring | | | | |
| Details | Target | RT | Result name | Look At | Score | Mass Screening | RTI Screening | MS/MS | MassBank |
| | <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="button" value="●"/> ▼ | | | | | |
| Show | Amantadin | 5.1 | amantadine | ● | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> |
| Show | Metoprolol | 5.6 | Metoprolol | ● | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> |

5.2.1.5 column Pathways available

Transformation products are predicted by the EnviPath database using the software tool of EAWAG-BBD. If a pathway exist for one suggested hit in the database, it is marked with '●' in the column 'pathways available'.

| found 31, 31 visible | | | | | | | | | |
|-----------------------------|----------------------|----------------------|----------------------|------------------------------------|------------------------|------------------------|------------------------|-------------------|--|
| Results Search content Help | | | | | | | | | |
| | Results | | | | Scoring | | | | |
| Details | Target | RT | Result name | Look At | Score | Mass Screening | MassBank | Pathway available | |
| | <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="button" value="●"/> ▼ | | | | | |
| Show | 103.0752 / ... | 2.0 | (Cycloprop... | | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | | |
| Show | 103.0752 / ... | 2.0 | 1,3-dioxepa... | | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | | |
| Show | 105.0705 / ... | 12.1 | Styrole | ● | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | ● | |

By pressing the 'Show' Button and using the Tab 'Transformation products' the predicted pathway is shown. This tool is still under progress and will be extended soon.



Description of pathway colors:

Green Box: selected database hit

Blue Box: parent compound

Purple Box: transformation product found in the uploaded datafile

Grey Box: transformation product not found in the uploaded datafile

5.2.1.6 columns Target mass and Δ mass

In the column 'Target mass' the monoisotopic mass of the uploaded target is shown.

In the column ' Δ mass' the difference between the mass of the database hit and the Target mass is calculated and shown automatically.

| Results Search content Help | | | | | | | |
|-----------------------------|----------------------|----------------------|----------------------|-----------------------|------------------------|----------------------|----------------------|
| Results | | | | | | Mass Screening | |
| Details | Target | RT | Result name | Look At | Score | Target mass | Δ mass |
| | <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> |
| Show | Amantadin | 5.1 | amantadine | <input type="radio"/> | <div><div></div></div> | 151.1361 | 0.0000 |
| Show | Amantadin | 5.1 | 3,7-dimethy... | <input type="radio"/> | <div><div></div></div> | 151.1361 | 0.0000 |
| Show | Metoprolol | 5.6 | Metoprolol | <input type="radio"/> | <div><div></div></div> | 267.1834 | 0.0000 |
| Show | Metoprolol | 5.6 | butoxamine | <input type="radio"/> | <div><div></div></div> | 267.1834 | 0.0000 |

5.2.1.7 columns RTI, logD DB, logD RTI, Δ logD (RTI-DB), Adj. logD RTI und Δ logD (Adj.-DB)

The column RTI contains the RTI values normalized via the calibration standards of the target analyte.

The column logD DB contains the logD value of the entered pH value of the substance, listed in the database, which was found as a hit via STOFF-IDENT.

The column logD RTI contains the logD value of the target analyte, calculated via RTI.

In the column Δ logD (RTI-DB) the difference between the logD value calculated via RTI and the one that is listed in the database is calculated and shown automatically.

In the column Adj. logD RTI an automatic correction like written in 5.2.1.2 is done, if necessary.

In column Δ logD (Adj.-DB) the difference between the adjusted logD value and the one listed in the database is calculated and shown.

| Results Search content Help | | | | | | | | | | | |
|-----------------------------|----------------------|----------------------|----------------------|-----------------------|------------------------|----------------------|----------------------|----------------------|------------------------|----------------------|-------------------------|
| Results | | | | | | log | | | | | |
| Details | Target | RT | Result name | Look At | Score | RTI | logD DB | logD RTI | Δ logD (RTI-DB) | adj. logD RTI | Δ logD (adj.-DB) |
| | <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> | <input type="text"/> |
| Show | Amantadin | 5.1 | amantadine | <input type="radio"/> | <div><div></div></div> | 74.0 | -1.57 | 0.57 | 2.14 | -0.43 | 1.14 |
| Show | Amantadin | 5.1 | 3,7-dimethy... | <input type="radio"/> | <div><div></div></div> | 74.0 | 2.93 | 0.57 | -2.36 | 0.57 | -2.36 |
| Show | Metoprolol | 5.6 | Metoprolol | <input type="radio"/> | <div><div></div></div> | 77.1 | -1.48 | 0.76 | 2.24 | -0.24 | 1.24 |
| Show | Metoprolol | 5.6 | butoxamine | <input type="radio"/> | <div><div></div></div> | 77.1 | -1.19 | 0.76 | 1.95 | -0.24 | 0.95 |

5.2.1.8 CAS number, SMILES, IUPAC, Formula and Tonnage

In the following columns CAS number, SMILES, IUPAC, Formula and Tonnage all in the database listed information for the found hits are shown

| Results Search content Help | | | | | | | | | | |
|-----------------------------|------------|-----|----------------|---------|-------|------------|------------------------------|-----------------------------------|-----------|-------------------------|
| Results | | | | | | Substance | | | | |
| Details | Target | RT | Result name | Look At | Score | CAS Number | SMILES | IUPAC | Formula | Tonnage |
| | | | | | | | | | | |
| Show | Amantadin | 5.1 | amantadine | | | 768-94-5 | NC12CC3CC(C(C3)C1)C2 | adamantan-1-amine | C10H17N | Intermediate Use Only |
| Show | Amantadin | 5.1 | 3,7-dimethy... | | | 51566-62-2 | CC(CCC=C(C)C)CC#N | 3,7-dimethyloct-6-enenitrile | C10H17N | 100 - 1,000 tonnes p... |
| Show | Metoprolol | 5.6 | Metoprolol | | | 37350-58-6 | COCc1ccc(OCC(O)CNC(C)... | 1-{4-(2-Methoxyethyl)phenoxy... | C15H25NO3 | |
| Show | Metoprolol | 5.6 | butoxamine | | | 2922-20-5 | COC1ccc(OC)c(c1)C(O)C(C)N... | 2-(tert-butylamino)-1-(2,5-dim... | C15H25NO3 | |

You have the possibility to check or uncheck columns of interest by using the drop down menu

| Results Search content Help | | | | | | | | | | |
|-----------------------------|----------------|------|----------------|---------|-------|-------|---------|----------|-----------------|---------------|
| found 31, 31 visible | | | | | | | | | | |
| Results | | | | | | ng | | | | |
| Details | Target | RT | Result name | Look At | Score | RTI | logD DB | logD RTI | Δ logD (RTI-DB) | adj. logD RTI |
| | | | | | | | | | | |
| Show | Amantadin | 16.0 | amantadine | | | | -1.57 | | | |
| Show | Amantadin | 16.0 | 3,7-dimethy... | | | | 2.93 | | | |
| Show | Atrazine | 9.7 | Wonuk | | | 102.2 | 1.79 | 2.31 | 0.52 | 1.31 |
| Show | Atrazine-2-... | 5.0 | Atrazine-2-... | | | 73.4 | -0.00 | 0.53 | 0.53 | -0.47 |
| Show | Atrazine-2-... | 5.0 | Simeton | | | 73.4 | -0.30 | 0.53 | 0.83 | -0.47 |
| Show | Chloridazon | 6.5 | Chloridazon | | | 82.8 | 1.11 | 1.11 | 0.01 | 1.11 |

- ✓ RTI
- ✓ logD DB
- ✓ logD RTI
- ✓ Delta Log D Rti Db
- ✓ adj. logD RTI
- ✓ Delta Log D Adjusted Db
- ✓ CAS Number
- ✓ SMILES
- ✓ IUPAC
- ✓ Formula
- ✓ Tonnage

Via the 'Download' button and choosing 'Results' the results table can be exported in excel with all favored parameters.

Screening/ Suspected-Target Screening/ Known Unknowns)

Results Search content Help

Results Non Results Complete

| | Results | Scoring | | | | Mass Screening | | | | |
|---------|----------------|---------|----------------|------|-------|----------------|---------------|-------|----------|-------------|
| Details | Target | RT | Result name | Best | Score | Mass Screening | RTI Screening | MS/MS | MassBank | Target mass |
| Show | Amantadin | 5.1 | amantadine | ● | | | | | | 151.1361 |
| Show | Amantadin | 5.1 | 3,7-dimeth... | | | | | | | 151.1361 |
| Show | Atrazine | 9.7 | Wonuk | ● | | | | | | 215.0938 |
| Show | Atrazine-2-... | 5.0 | Atrazine-2-... | ● | | | | | | 197.1277 |

Export Results ✕

Filename (max.255)

results.xls

☐ Include Sources?

Columns

☐ Select/Deselect all

- ☒ Overall score
- ☒ Massbank simple score
- ☒ Overall best match
- ☐ Measured RT
- ☒ pH dependency
- ☐ RTI best match
- ☒ RTI score
- ☒ Target
- ☒ Target Rt
- ☒ Target mass
- ☒ Target logD
- ☐ Target pH
- ☐ RTI

Download **Close**

Besides exporting the FOR-IDENT results there is also the option to download the 'non results' or the complete set. By pressing the 'Download' button and choosing 'non results' the list of targets with no hit in STOFF-IDENT can be exported in an extra excel file with all favored parameters, e.g. RTI.

Export Results

Filename (max.255)

vendor_File_inkl.Formula_results.xls

☐ Include Sources?

Columns

☒ Select/Deselect all

☒ id

☒ precursor mass

☒ Formula

☒ RTI

☒ RT

☒ formula derived mass

☒ neutral mass

☒ Mass calculated

Download

Close

By pressing the ‘Show summary’ button a summary window appears and shows the values of uploaded features, database hits and non database hits



| <div> <div>Results</div> <div>Search content</div> <div>Help</div> </div> | | | | | | | | | | | |
|---|----------------------|---|----------------------|----------------------|------------------------|------------------------|------------------------|------------------------|------------------------|---|---|
| Result summary | | | | | | Scoring | | | Molecular screening | | |
| Details | Target | RT | Result name | Best | Score | Screening | MS/MS | MassBank | pH dep | Target mass | Δ mass |
| | <input type="text"/> | <input type="text"/> <input type="text"/> | <input type="text"/> | <input type="text"/> | | | | | | <input type="text"/> <input type="text"/> | <input type="text"/> <input type="text"/> |
| Show | Amantadin | 5.1 | amantadine | | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | 151.1361 | 0.0000 |
| Show | Amantadin | 5.1 | 3,7-dimethylo... | | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | 151.1361 | 0.0000 |
| Show | Metoprolol | 5.6 | Metoprolol | | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | 267.1834 | 0.0000 |
| Show | Metoprolol | 5.6 | butoxamine | | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | <div><div></div></div> | 267.1834 | 0.0000 |

| RTI search | |
|--------------------|----|
| Features | 14 |
| Located features | 14 |
| Candidates found | 29 |
| Unlocated features | 0 |

OK

In the 'Last processed' area all performed searches were stored and can be reloaded again by 'doubleclick'.

FOR-IDENT



Collapse

Settings

Logout

Home

Search 3

Quick search

Search

Index Search

Processing 1

Molecular screening

Last data update

Jan 30, 2017

Molecular Screening (Hidden-Target S

Process

Files

Data_pos2_1.xlsx (14)

vendor_File_inkl.Formula... (107)

Pathway-Example.xls (6426)

Processes

Mass Screening 25% ✓

RTI Screening 25% ✓

MS/MS 25% ✓

Transformation Products 0% ✓

MassBank entry 25% ✓

available

Required data available: ✓ or ✗

Processing activated: ● or ○

Parameters

pH

3

Source Lists

Select/Deselect all

NORMANews

NIVA/Waters

STOFF-IDENT

permanent cations

Last processed

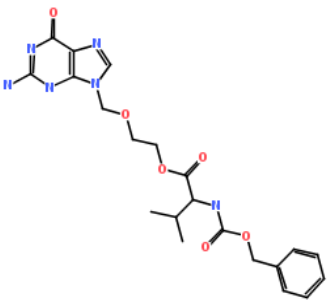
▶ Data_pos2_1.xlsx

In the 'Details' tab you can find specific information about the analyte. All information can be downloaded as an excel-file. Besides you have the choice to see the Metadata or not.

Details

Metadata

Structure



General

| | |
|---------------|--|
| Name | 2-[(2-amino-6-oxo-3,6-dihydro-9H-purin-9-yl)methoxy]ethyl N-[(benzyloxy)carbonyl]-L-valinate |
| Source | REACH |
| Last modified | Apr 12, 2016 |
| STOFFIDENT-ID | SI00006435 |
| SMILES | <chem>CC(C)C(NC(=O)OCc1ccccc1)C(=O)OCCOCn1cnc2c1[nH]c(N)nc2=O</chem> |
| Source | chemicalize.org |
| Last modified | Apr 12, 2016 |
| Inchi | InChI=1/C21H26N6O6/c1-13(2)15(24-21(30)33-10-14-6-4-3-5-7-14)19(29)32-9-8-31-12-27-11-23-16-17(27)25-20(22)26-18(16)28/h3-7,11,13,15H,8- |

Export Results

Filename (max.255)

results.xls

☐ Include Sources?

Columns

☐ Select/Deselect all

☐ STOFFIDENT-ID
☐ InChi
☐ InChi key
☒ CAS
☒ Name
☐ EC Number
☒ SMILES
☐ SMILES Structure
☒ Elemental formula
☒ IUPAC
☒ Monoisotopic mass
☒ Tonnage
☐ logP

Download

Close

You can change the Layout with three different options

Layout

In the Details at the web search part, you can directly search the specific compound via internet or you go to the External Links to get more information of the compound

Web Search

[Google search by Name](#)

[Google search by CAS](#)

[Google search by Inchi](#)


External Links

[Echa's REACH](#)

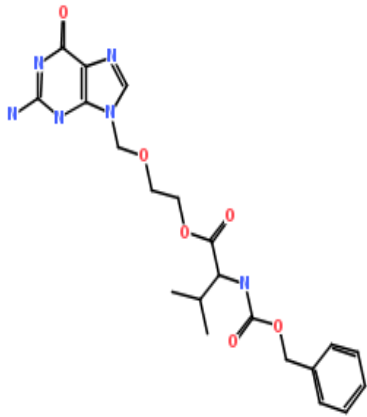
[EPA Dashboard](#)

www.chemicalize.org

If you find errors in the parameters given, e.g. wrong sum formula, SMILES code, etc. you can use the 'report record as faulty' button to send it directly to the software developer team by putting your comments of the fault into the comment field.

Details

Metadata

Structure



General

Name2-[(2-amino-6-oxo-3,6-dihydro-9H-purin-9-yl)methoxy]ethyl N-[(benzyloxy)carbonyl]-L-valinate

SourceREACH

Last modifiedApr 12, 2016

Report Window

Preview

Error Report of incorrect entry details

Wed May 04 13:33:21 CEST 2016

Entry:

From

Username

Organization

☐ Send error report anonymous

Comment (An explanation of the error helps us enormous to resolve it)

OK

Close