# Database assisted identification of organic substances

# DAIOS

**Wolfgang Schulz and Rudi Winzenbacher**

Landeswasserversorgung Water-supply, Langenau, Germany

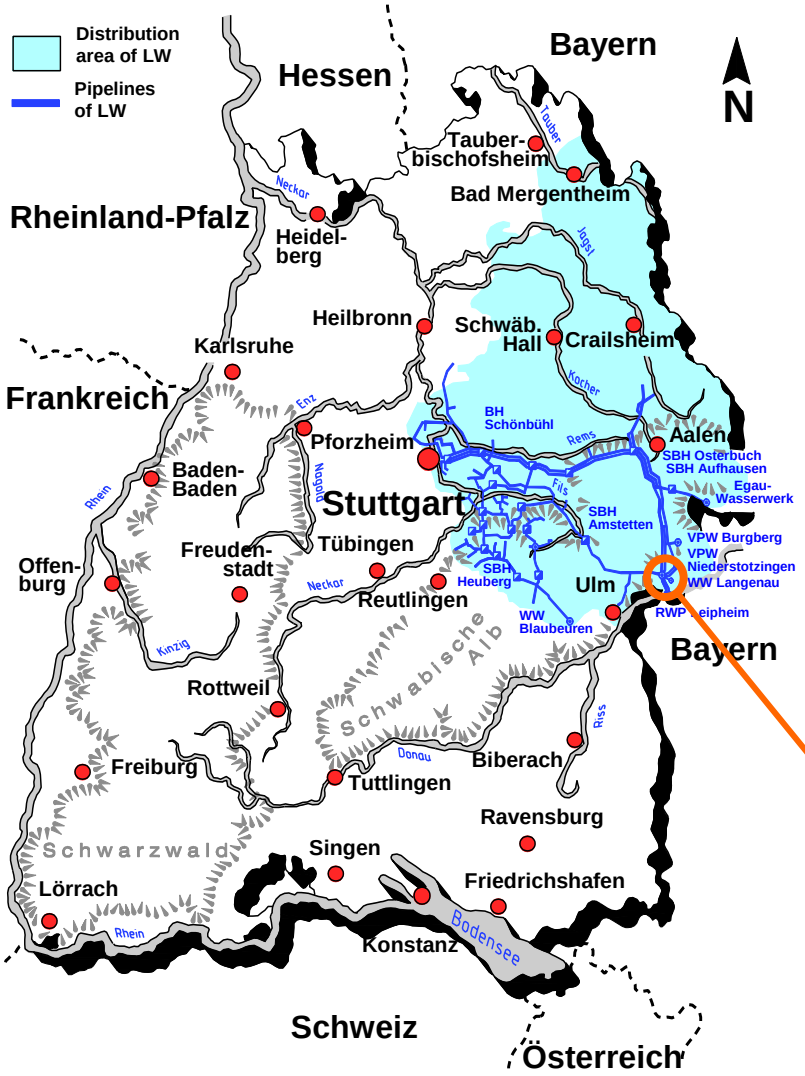
# Outline

- Motivation to built DAIOS
- DAIOS
- Example of application
- Conclusion


http://www.daios-online.de

# Landeswasserversorgung is situated in South Germany

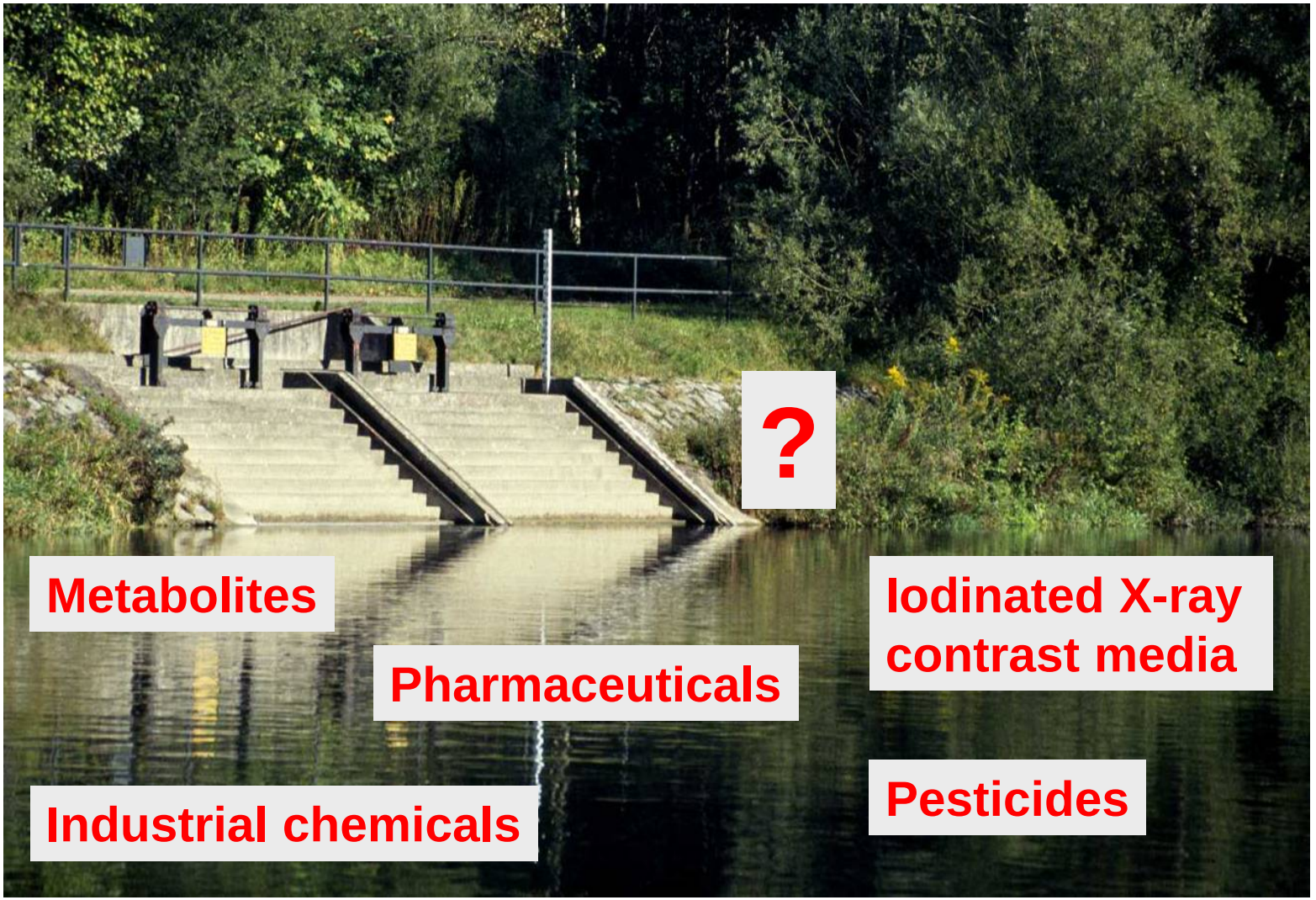
# Distribution area of LW in South West Germany



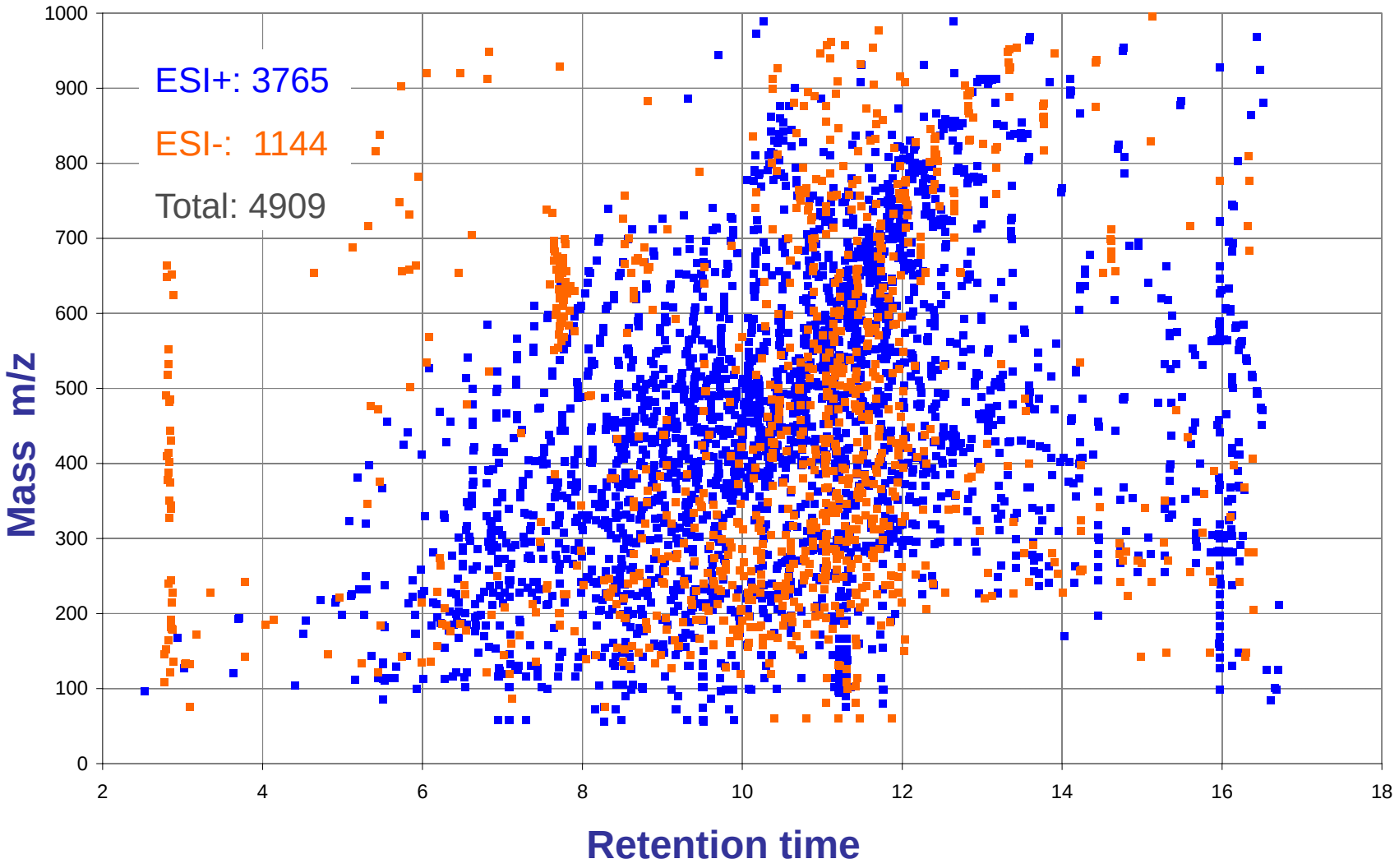

- Distribution area in South West Germany
- 3 Million customers within distribution area about 95 Million m³/Year
- Long-distance water fraction approx. 50%

# River Danube in South Germany (Leipheim)

# Direct abstraction of river water (near Leipheim)

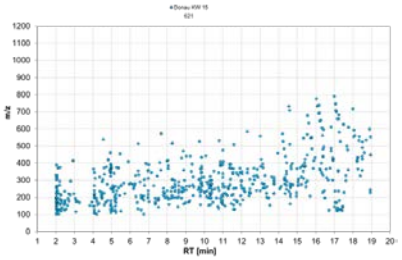


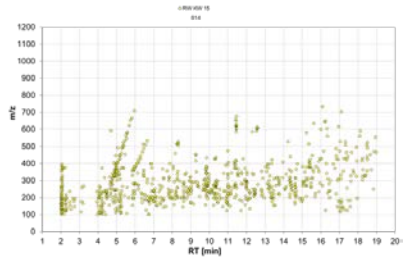
# Mass – RT scatter plot (Groundwater industrially influenced)



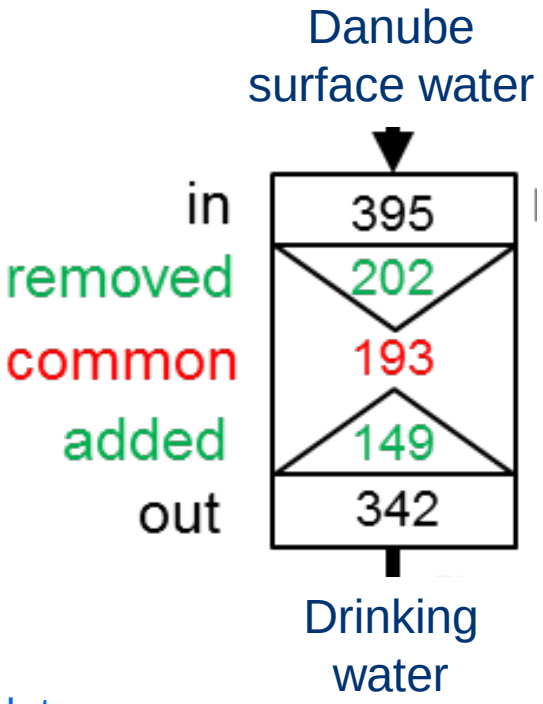
# Removal and formation of organic trace substances during water treatment

| Danube Features | Drinking water Features | Question |
|---|---|---|
| ● | – | removable |
| ● | ● | not or partial removable |
| – | ● | transformation product |





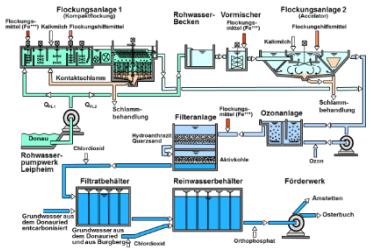
mass - RT scatterplots



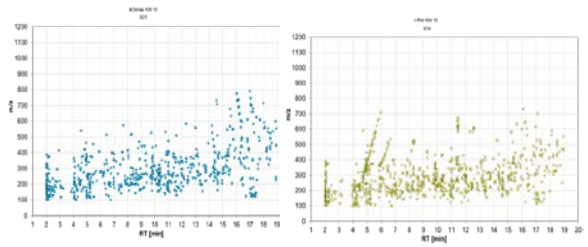
# Non-Target-Screening:
# Comparison of Danube raw water and drinking water

## Danube raw water

## Water treatment




## Drinking water



Scatter plots
for raw and
drinking water

## Non-target screening

| Sample | Number of components (identical) |
|---|---|
| KW 1 | 251 / 170 (85) |
| KW 2 | 374 / 214 (114) |
| KW 3 | 175 / 287 (65) |
| KW 4 | 286 / 301 (98) |

Zweckverband
Landeswasserversorgung

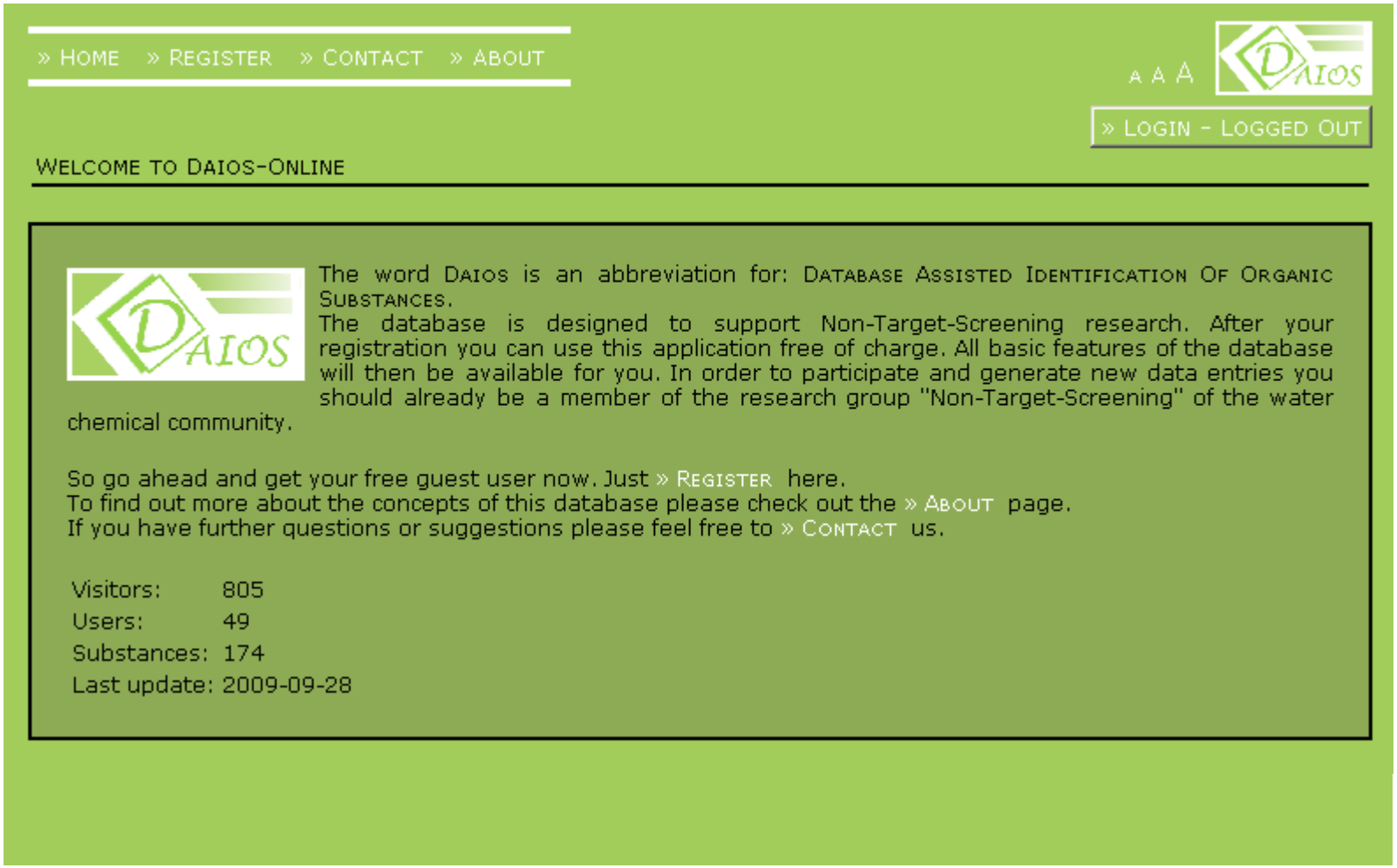
## DAIOS

Aim: Creating a database to support the Identification of compounds in LC-MS and LC-HRMS

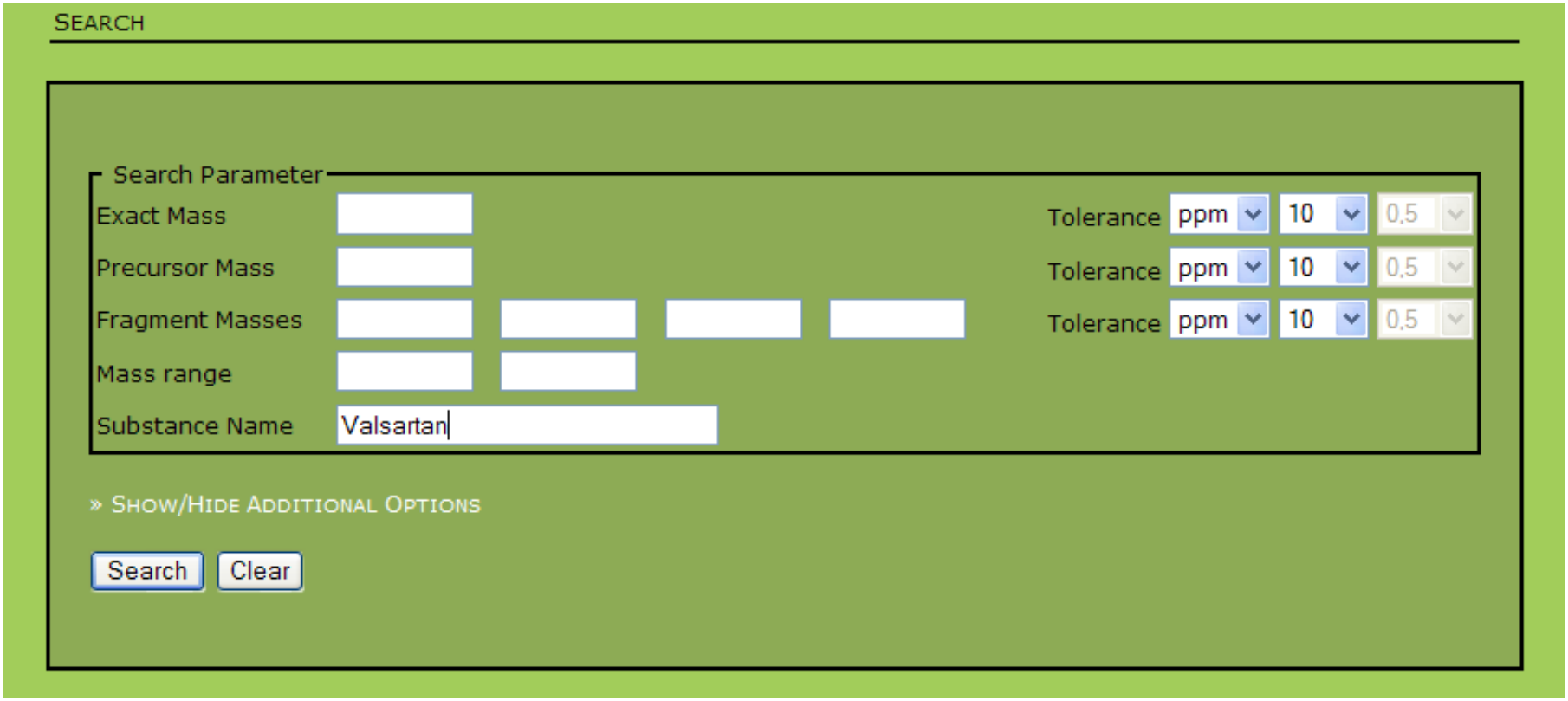
No spectrum library only table of Fragments

2008 DAIOS 1.0

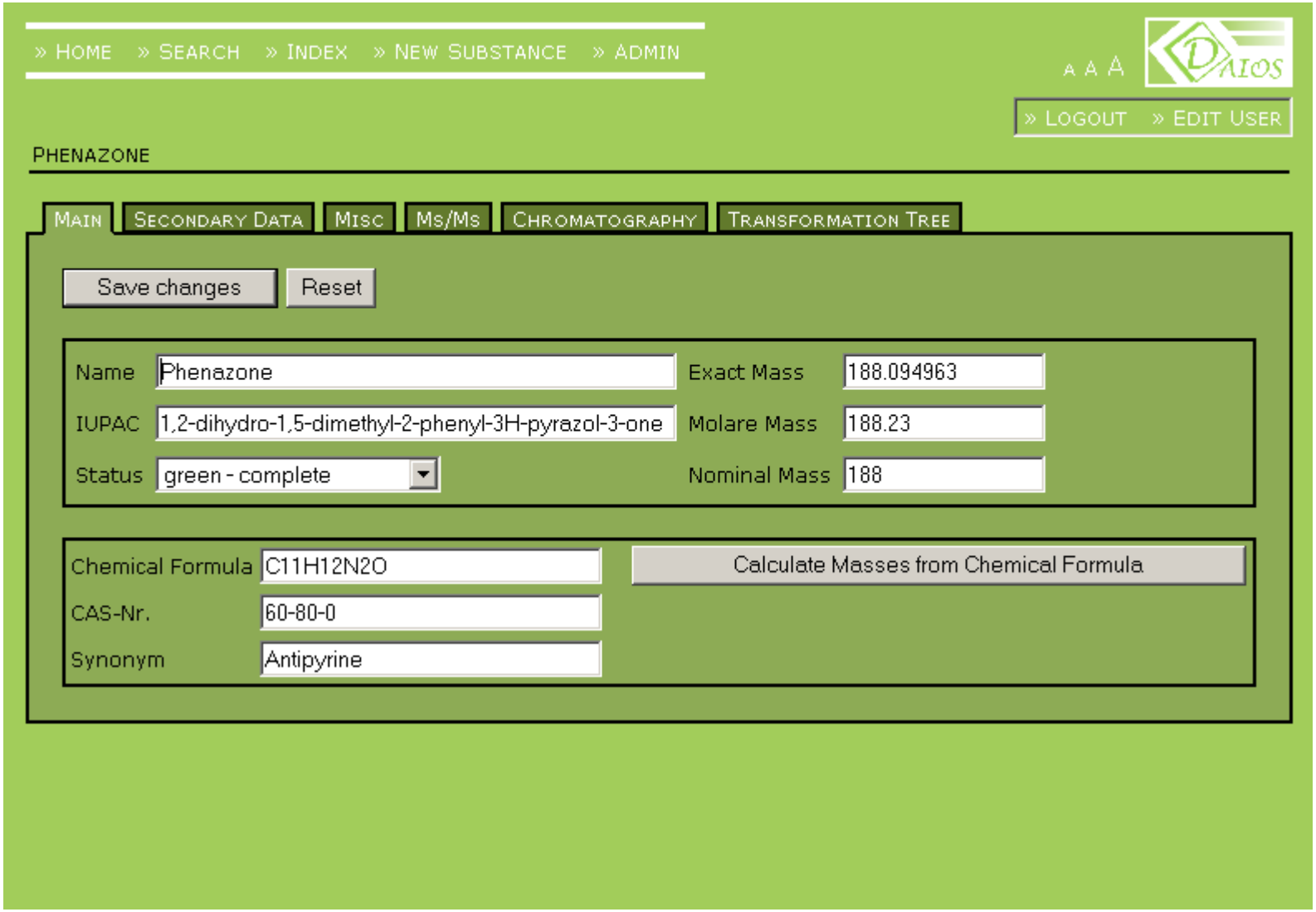
# DAIOS 1.0 2009



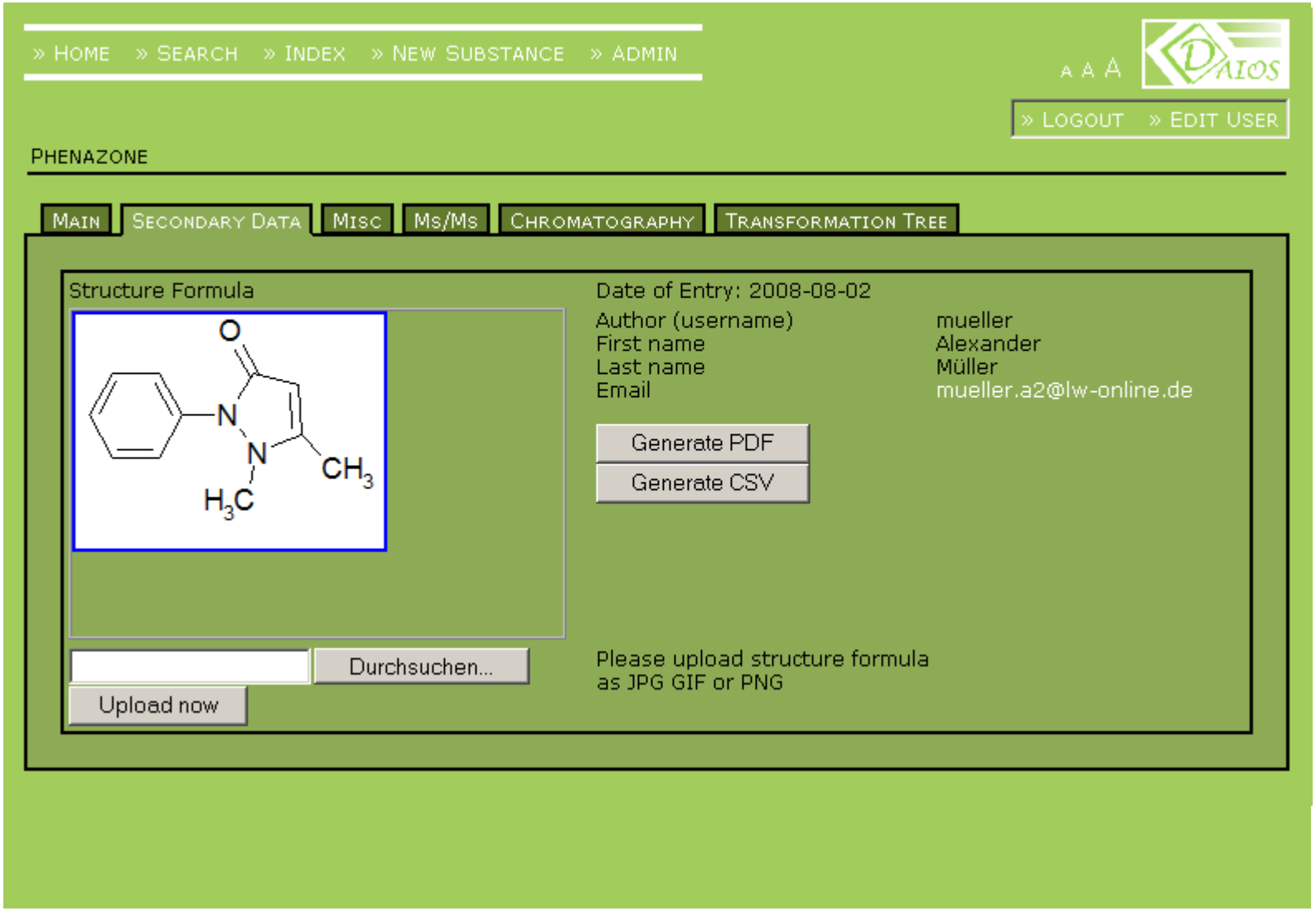
# Tab „Search“


SEARCH
Search Parameter
Exact Mass
Precursor Mass
Fragment Masses
Mass range
Substance Name
Valsartan
Tolerance
ppm
10
0,5
Tolerance
ppm
10
0,5
Tolerance
ppm
10
0,5
» SHOW/HIDE ADDITIONAL OPTIONS
Search
Clear

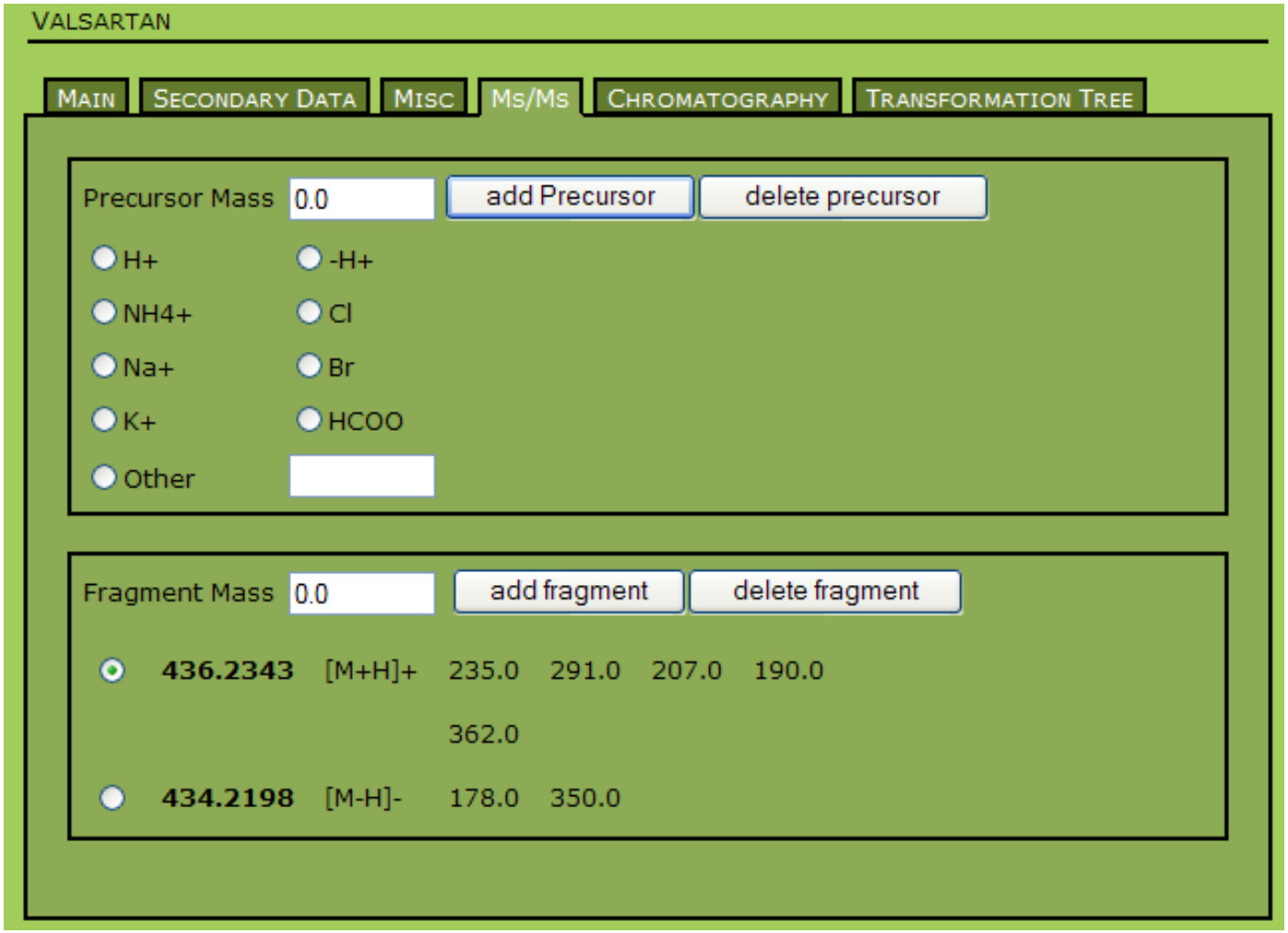
# Tab „Main“


» HOME
» SEARCH
» INDEX
» NEW SUBSTANCE
» ADMIN
A A A
DAIOS
» LOGOUT
» EDIT USER
PHENAZONE
MAIN
SECONDARY DATA
MISC
MS/MS
CHROMATOGRAPHY
TRANSFORMATION TREE
Save changes
Reset
Name
Phenazone
Exact Mass
188.094963
IUPAC
1,2-dihydro-1,5-dimethyl-2-phenyl-3H-pyrazol-3-one
Molare Mass
188.23
Status
green - complete
Nominal Mass
188
Chemical Formula
C11H12N2O
Calculate Masses from Chemical Formula
CAS-Nr.
60-80-0
Synonym
Antipyrine

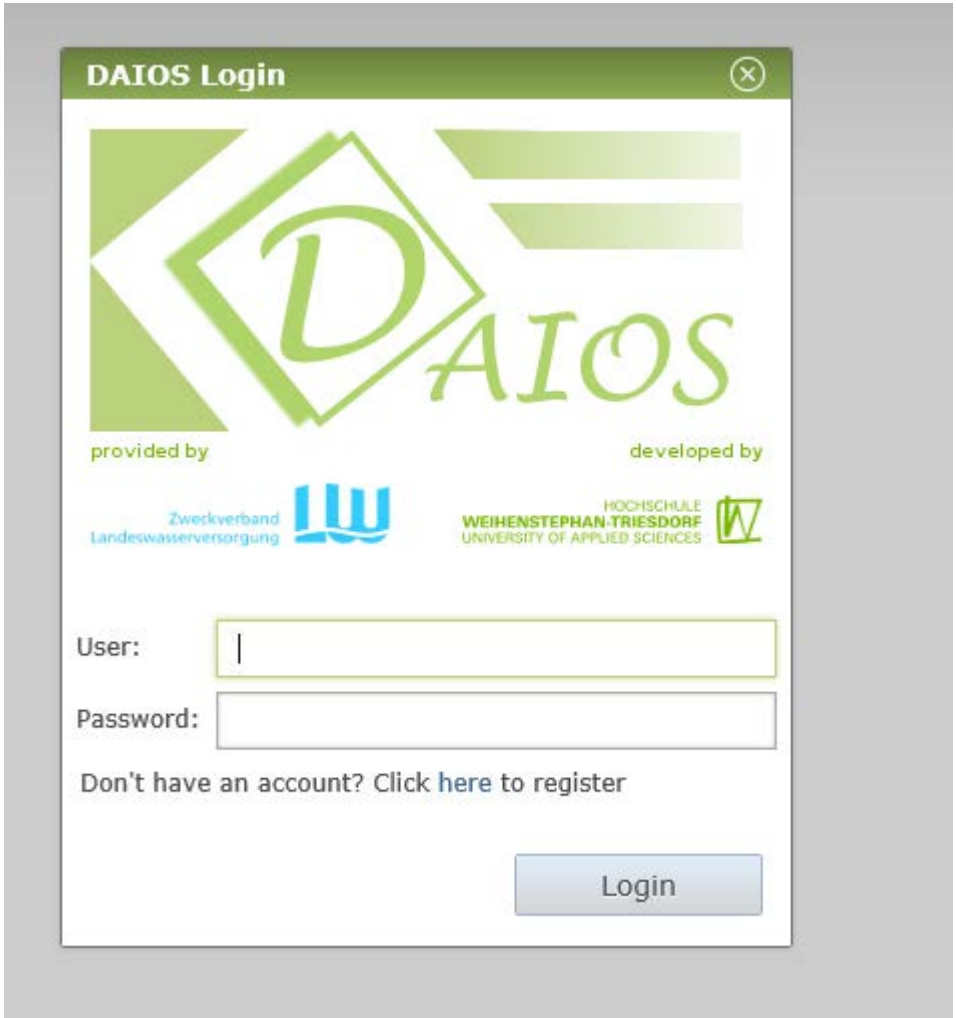
# Tab „Secondary data“



# Tab „MS/MS“


VALSARTAN
Main
Secondary Data
Misc
Ms/Ms
Chromatography
Transformation Tree
Precursor Mass
0.0
add Precursor
delete precursor
H+
-H+
NH4+
Cl
Na+
Br
K+
HCOO
Other
Fragment Mass
0.0
add fragment
delete fragment
436.2343 [M+H]+ 235.0 291.0 207.0 190.0 362.0
434.2198 [M-H]- 178.0 350.0

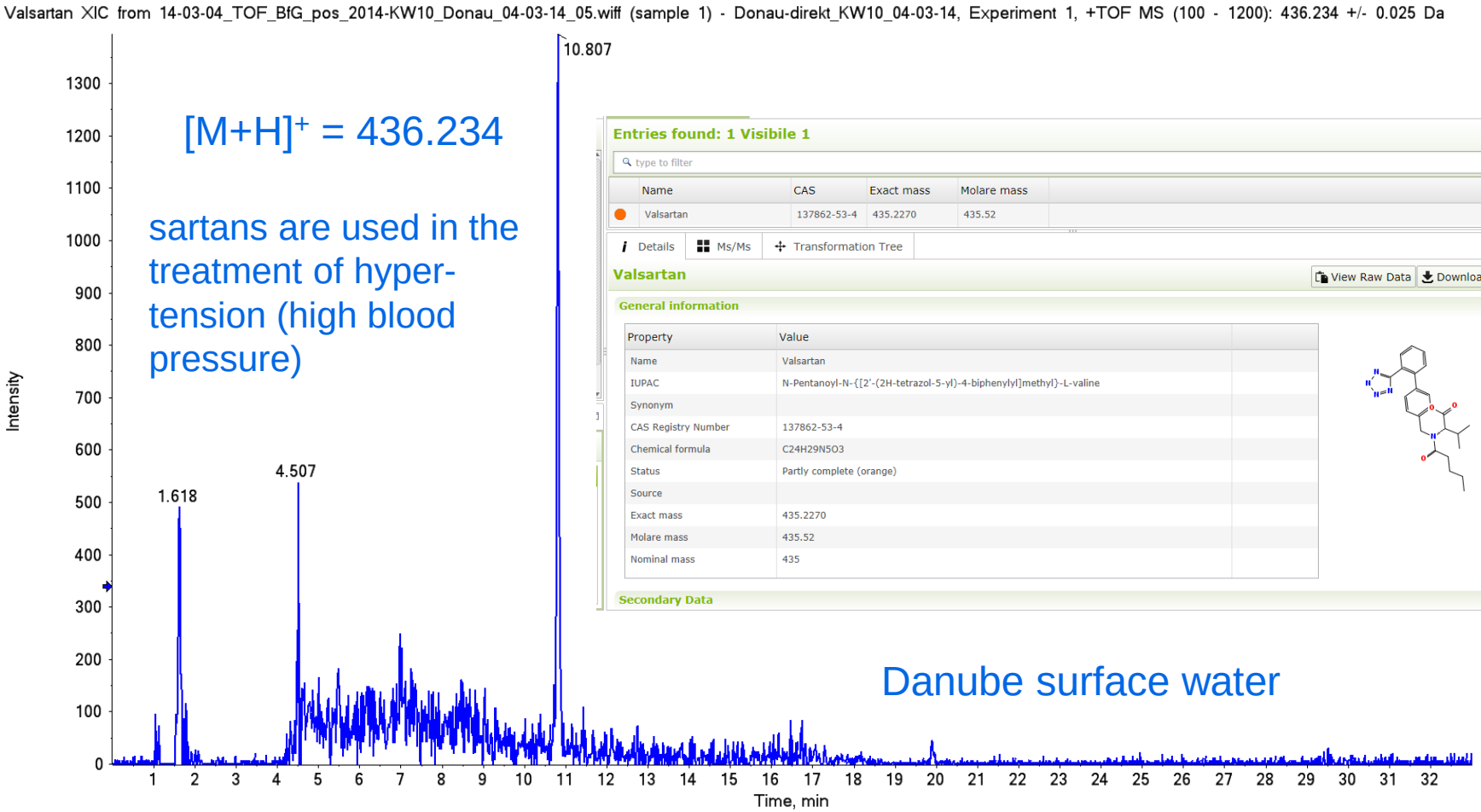
# Database for identification



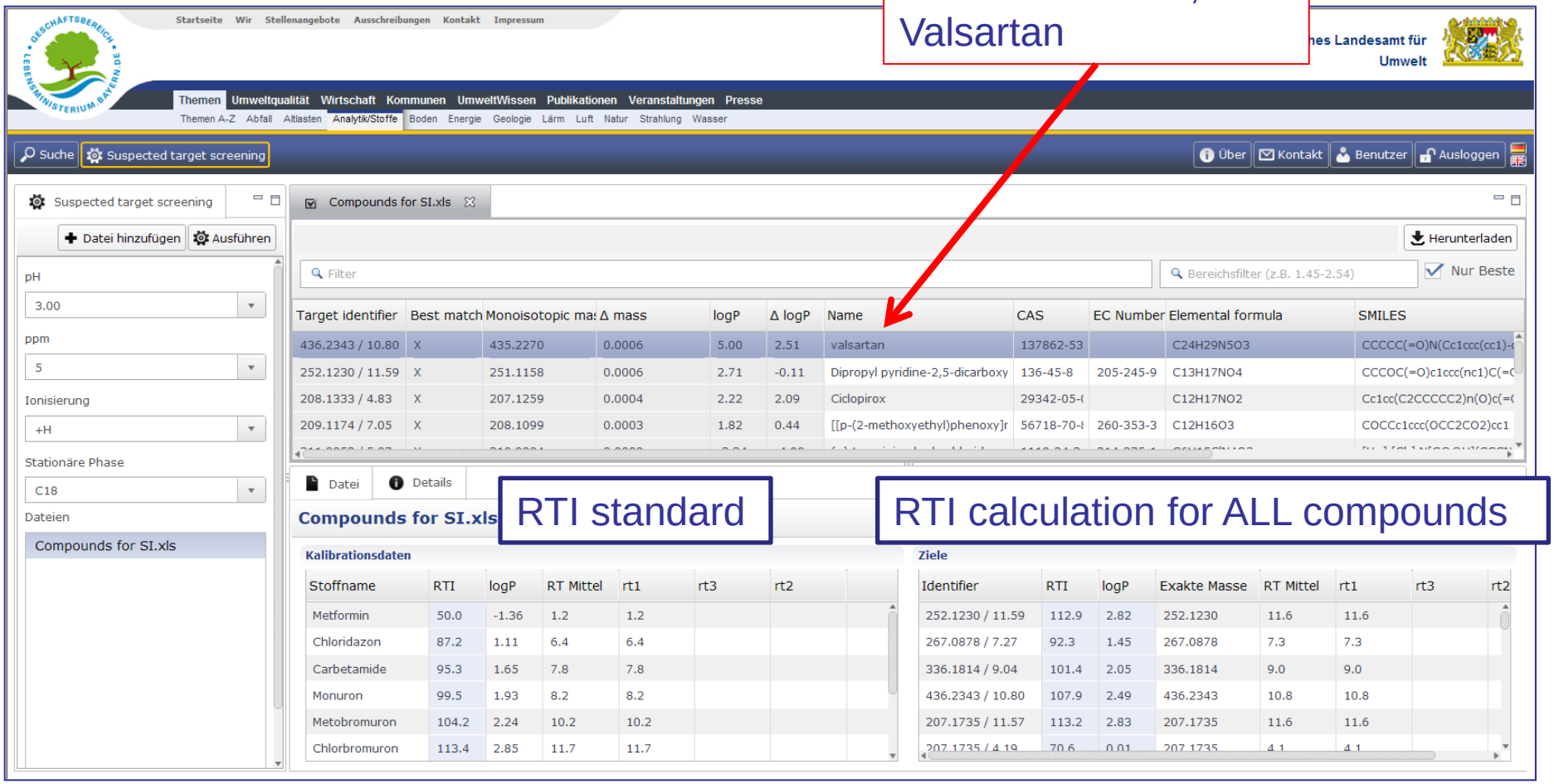

http://www.daios-online.de

DAIOS 2.0 built 2013
by T. Placht and M Luthardt
University of applied sciences
Weihenstephan - Triesdorf

# XIC (extracted ion chromatogram) of Valsartan

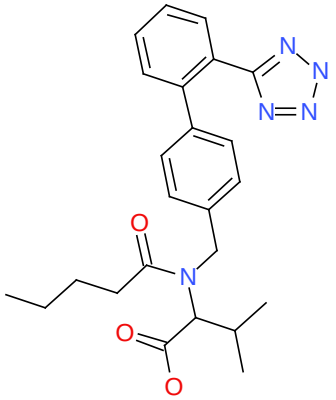


# Stoff-Ident Database Search with RTI-Calculation (Bavarian environmental Agency)

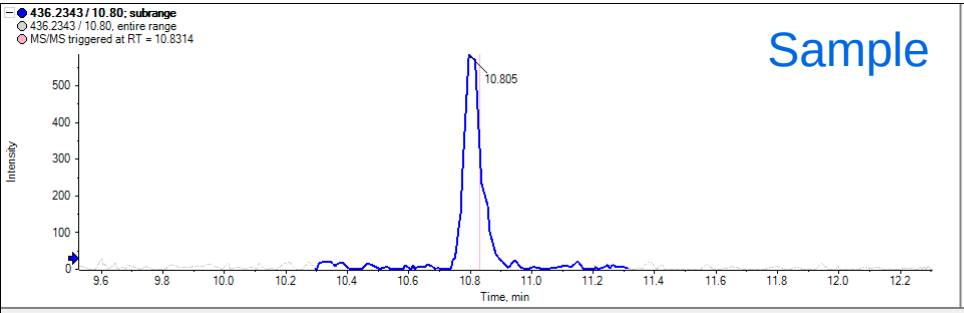


# Identification using DAIOS
# IDA-MS/MS

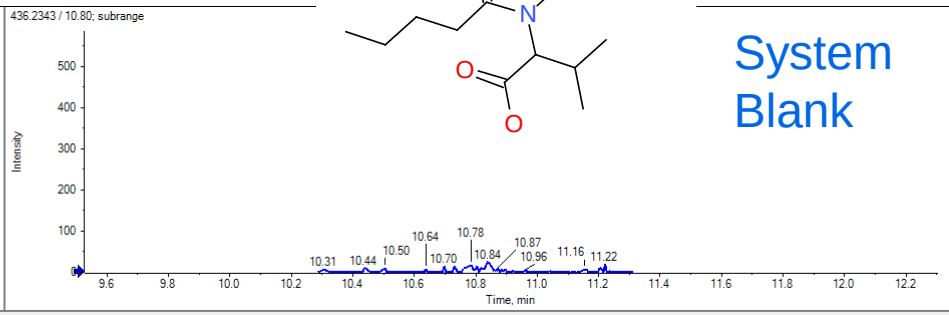
## Valsartan

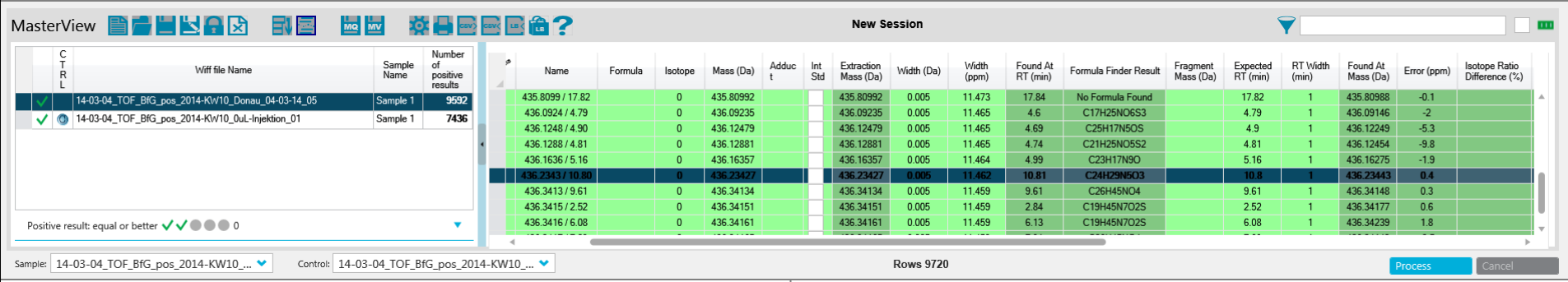


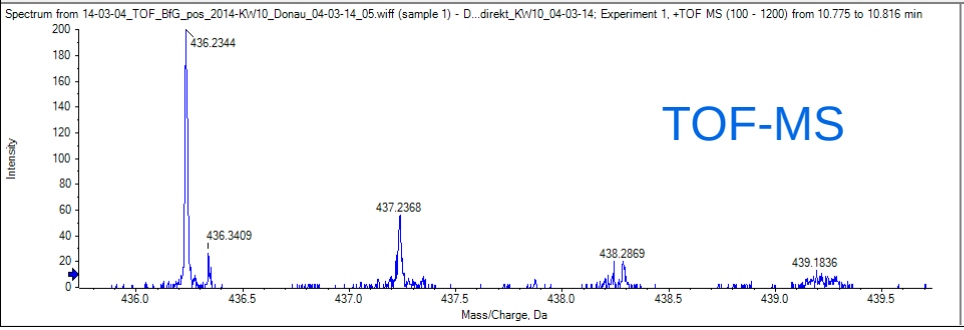
Sample



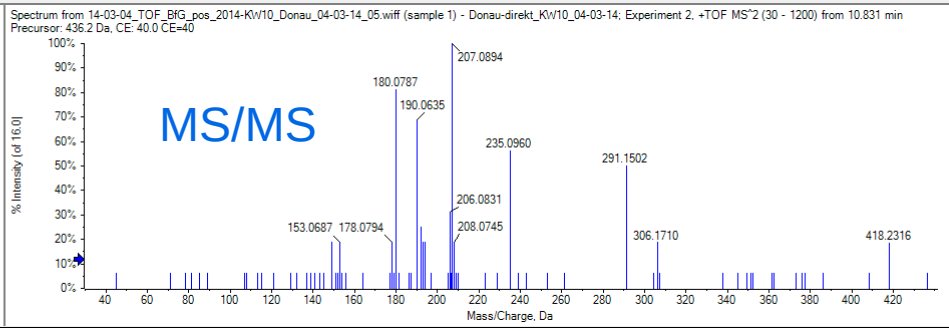

System Blank



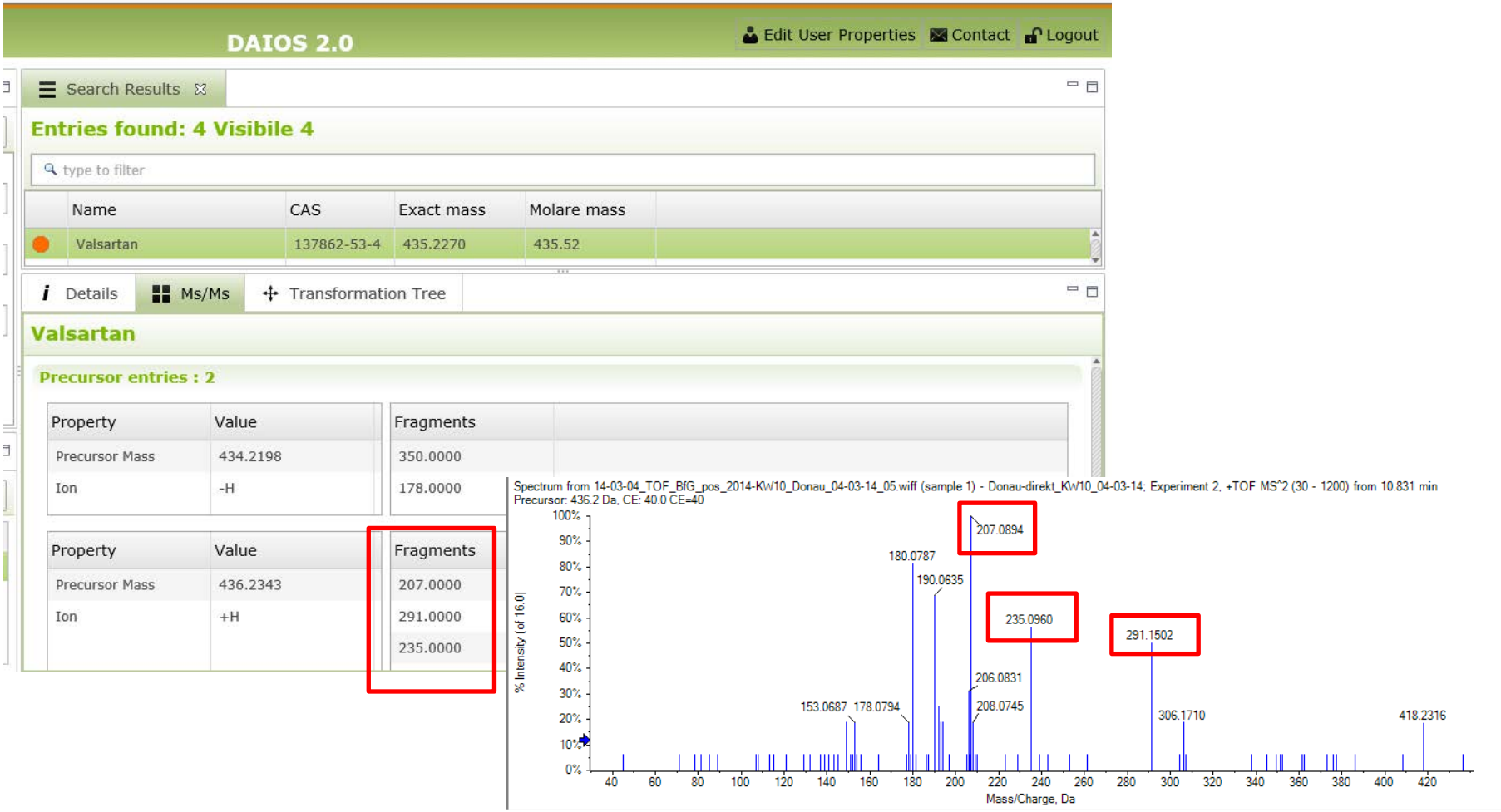



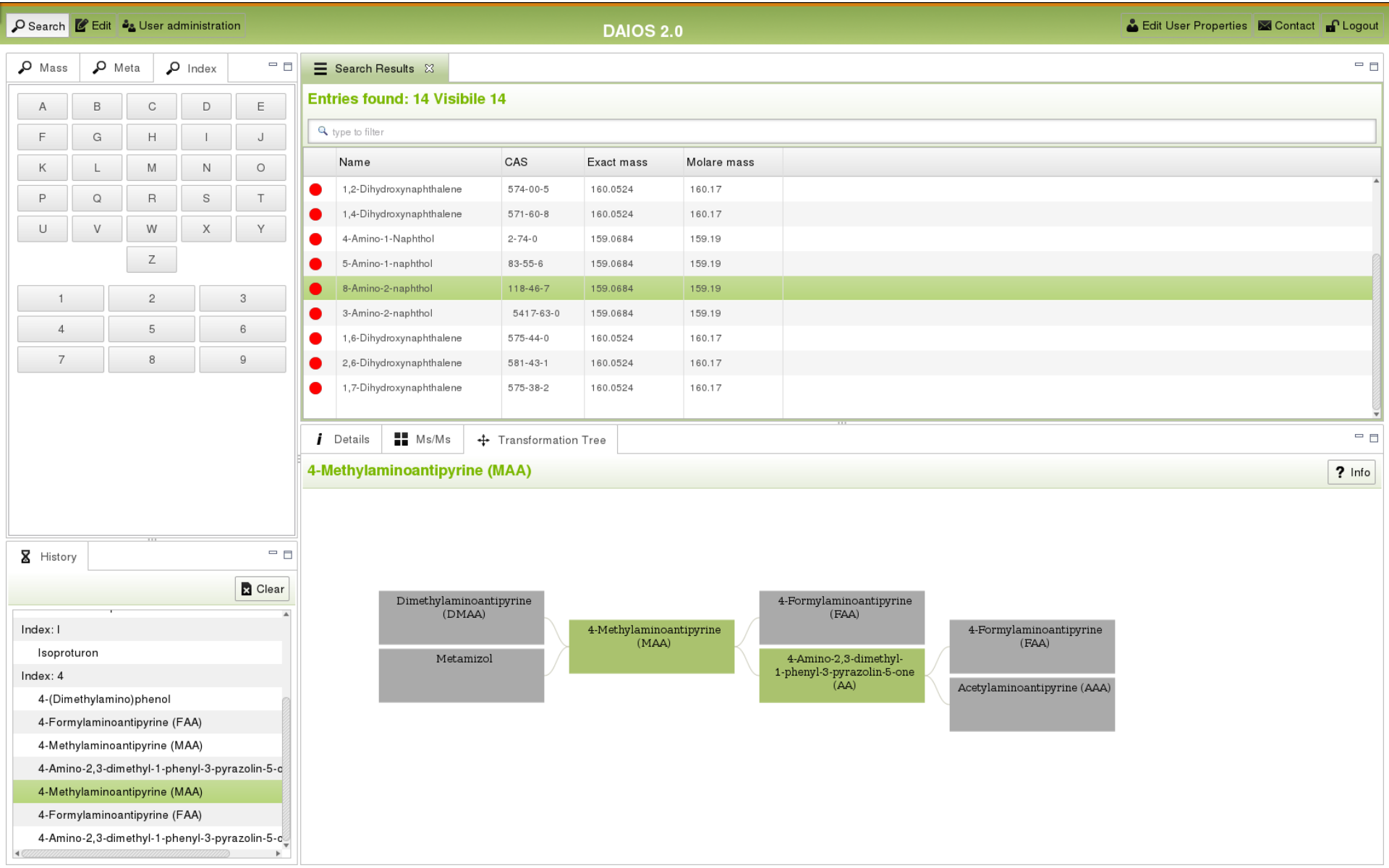

TOF-MS



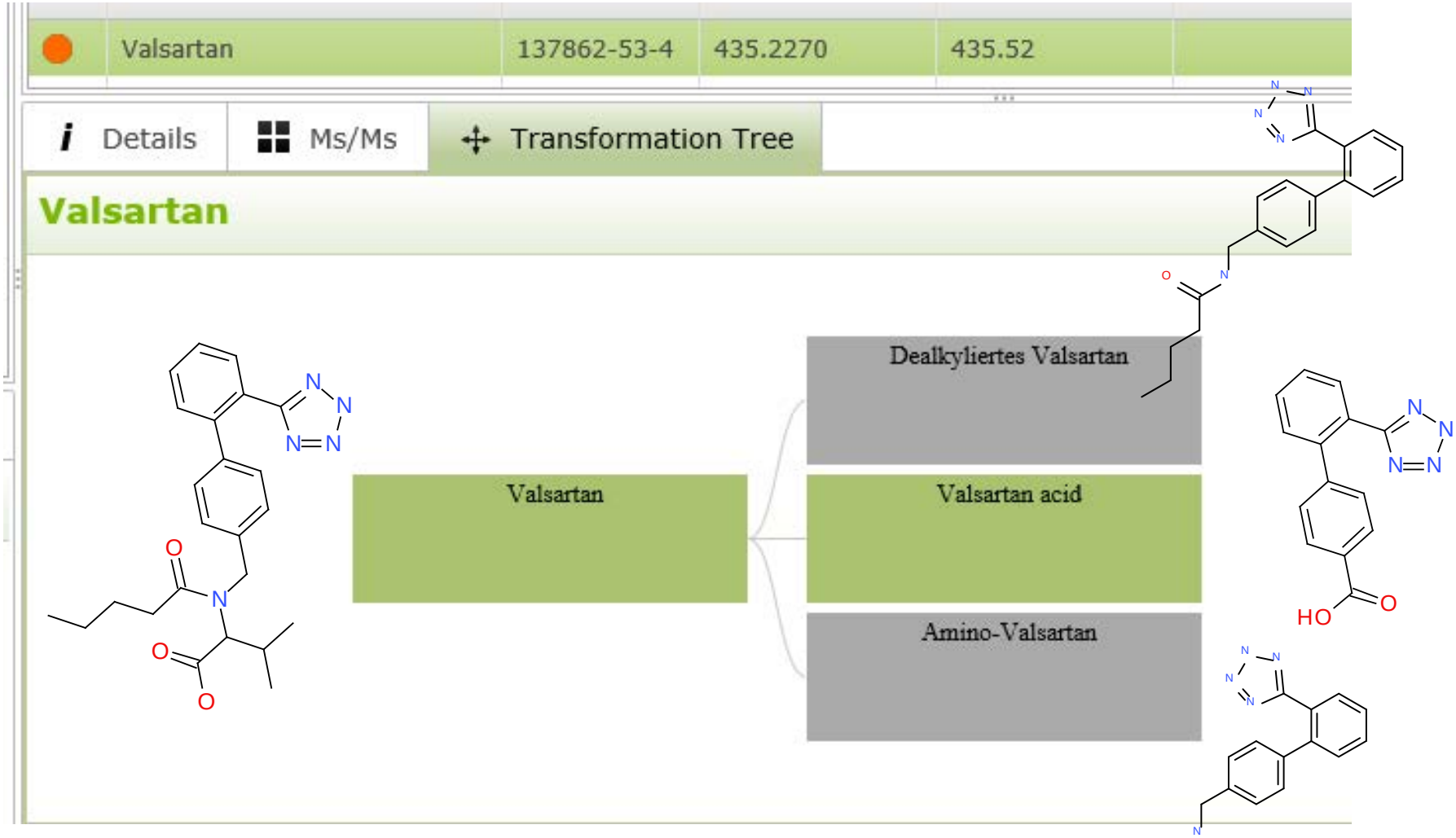

MS/MS

# Database assisted identification of organic substances

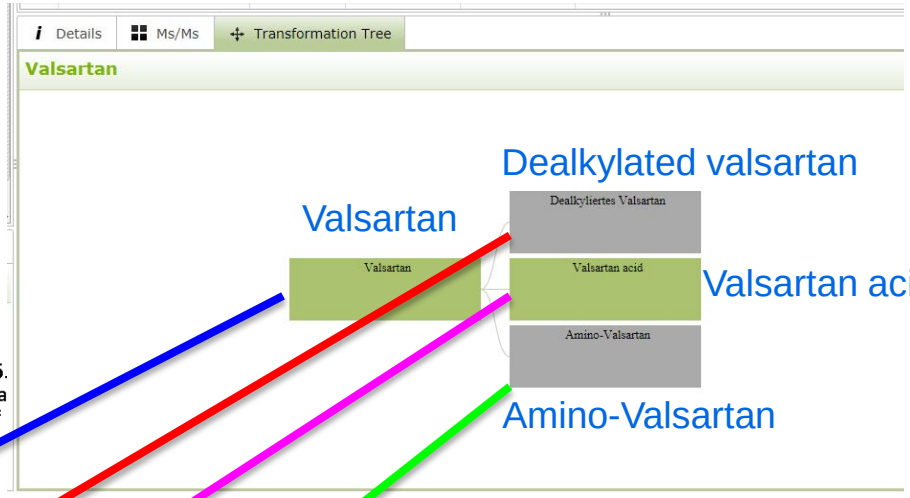


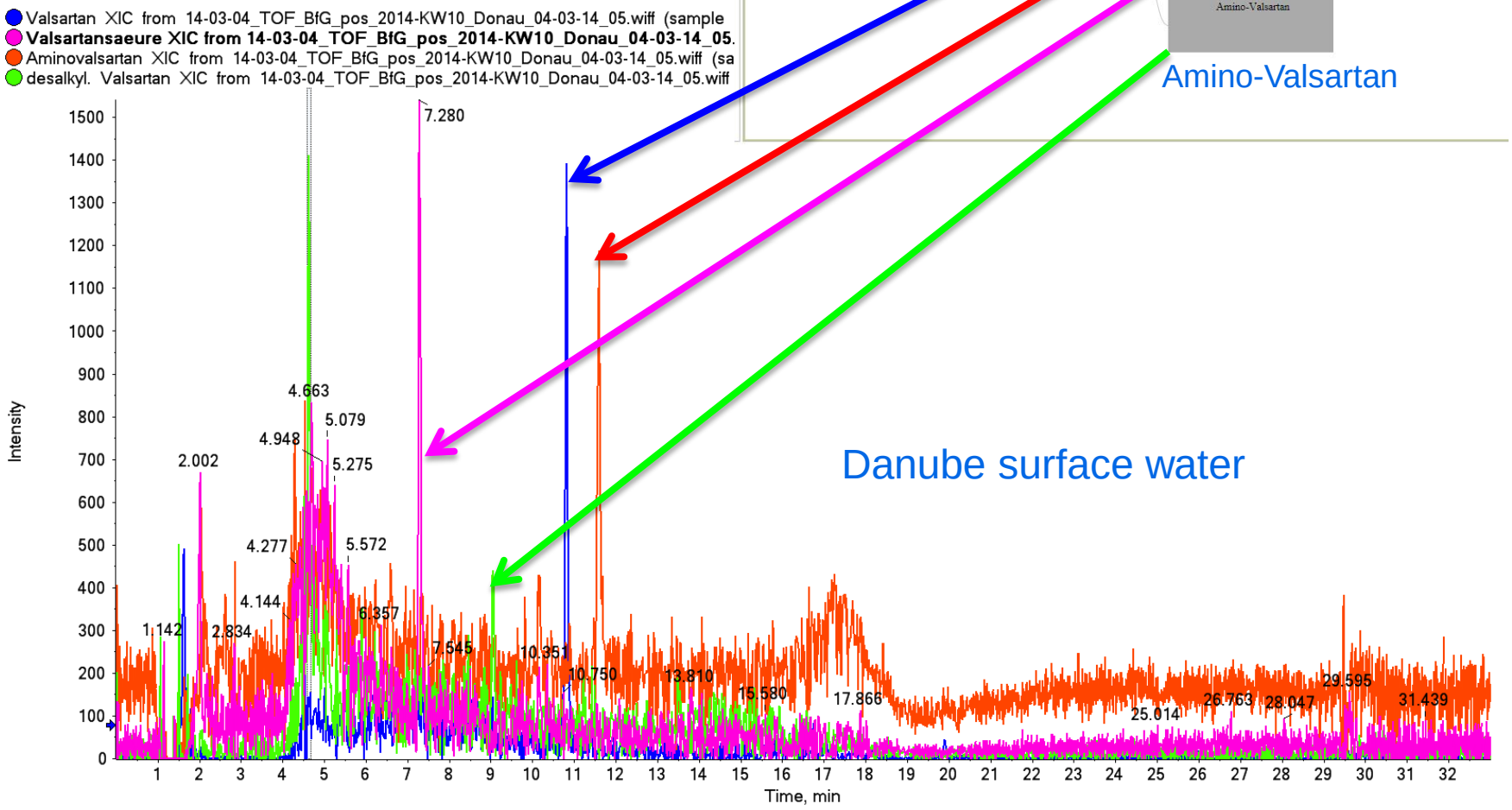

Search
Edit
User administration
DAIOS 2.0
Edit User Properties
Contact
Logout
Mass
Meta
Index
A B C D E
F G H I J
K L M N O
P Q R S T
U V W X Y
Z
1 2 3
4 5 6
7 8 9
History
Clear
Index: I
Isoproturon
Index: 4
4-(Dimethylamino)phenol
4-Formylaminoantipyrine (FAA)
4-Methylaminoantipyrine (MAA)
4-Amino-2,3-dimethyl-1-phenyl-3-pyrazolin-5-c
4-Methylaminoantipyrine (MAA)
4-Formylaminoantipyrine (FAA)
4-Amino-2,3-dimethyl-1-phenyl-3-pyrazolin-5-c
Search Results
Entries found: 14 Visibile 14
type to filter
Name
CAS
Exact mass
Molare mass
1,2-Dihydroxynaphthalene 574-00-5 160.0524 160.17
1,4-Dihydroxynaphthalene 571-60-8 160.0524 160.17
4-Amino-1-Naphthol 2-74-0 159.0684 159.19
5-Amino-1-naphthol 83-55-6 159.0684 159.19
8-Amino-2-naphthol 118-46-7 159.0684 159.19
3-Amino-2-naphthol 5417-63-0 159.0684 159.19
1,6-Dihydroxynaphthalene 575-44-0 160.0524 160.17
2,6-Dihydroxynaphthalene 581-43-1 160.0524 160.17
1,7-Dihydroxynaphthalene 575-38-2 160.0524 160.17
Details
Ms/Ms
Transformation Tree
4-Methylaminoantipyrine (MAA)
Info
Dimethylaminoantipyrine (DMAA)
Metamizol
4-Methylaminoantipyrine (MAA)
4-Formylaminoantipyrine (FAA)
4-Amino-2,3-dimethyl-1-phenyl-3-pyrazolin-5-one (AA)
4-Formylaminoantipyrine (FAA)
Acetylaminoantipyrine (AAA)

# DAIOS Transformation Tree



# XICs of Valsartan and its transformation products




Danube surface water

# Database assisted identification of organic substances

DAIOS 2.0

Edit User Properties | Contact | Logout

Search Results

Entries found: 4 Visibile 4

type to filter

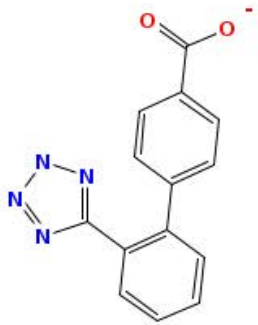
Details | Ms/Ms | Transformation Tree

## Valsartan acid

View Raw Data | Download Molfile

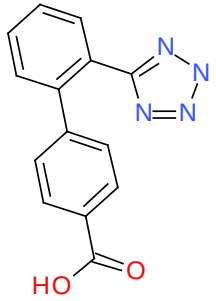
### General information

| Property | Value |
|---|---|
| Name | Valsartan acid |
| IUPAC | |
| Synonym | |
| CAS Registry Number | |
| Chemical formula | C14H10N4O2 |
| Status | Incomplete (red) |
| Source | |
| Exact mass | 266.0803 |
| Molare mass | 266.26 |

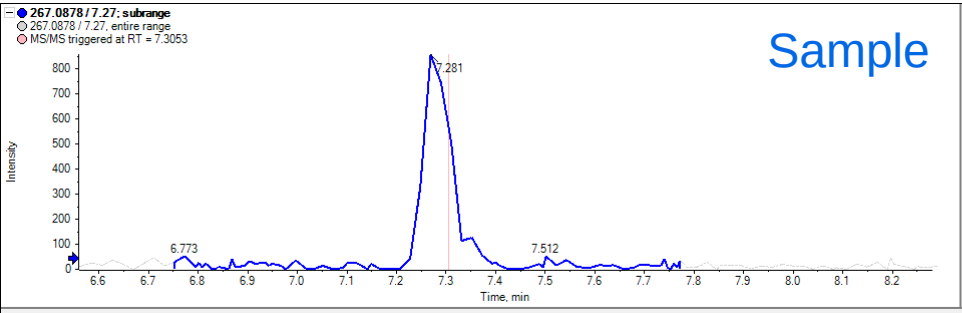


# Identification using DAIOS
# IDA-MS/MS

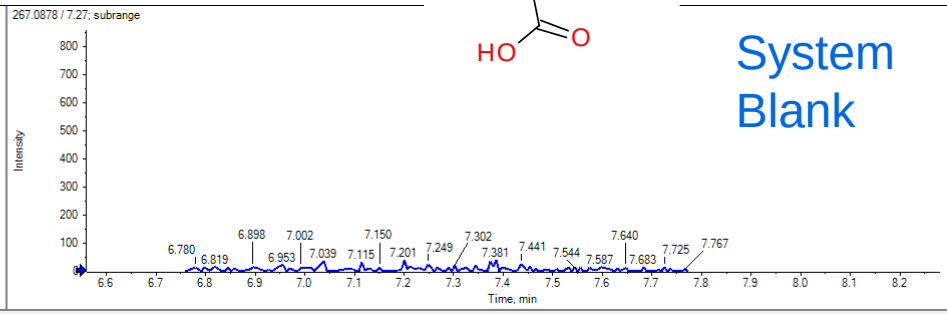
## Valsartan Acid

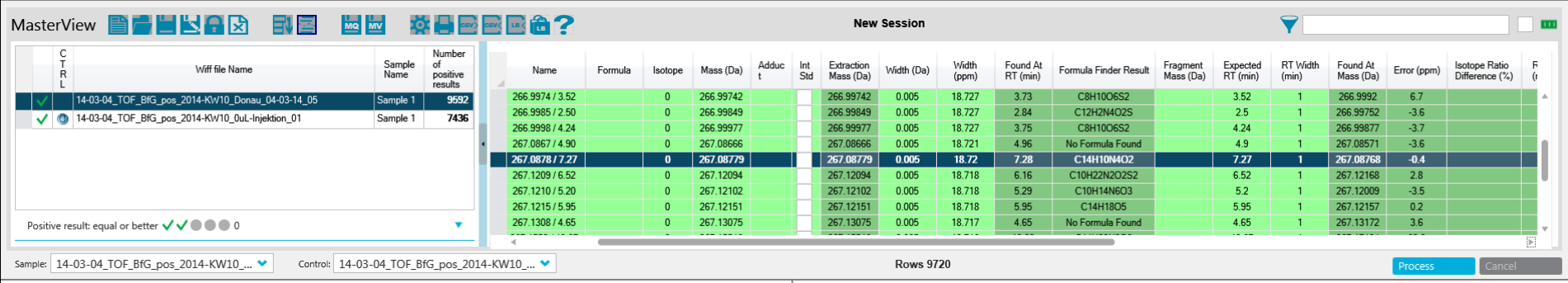


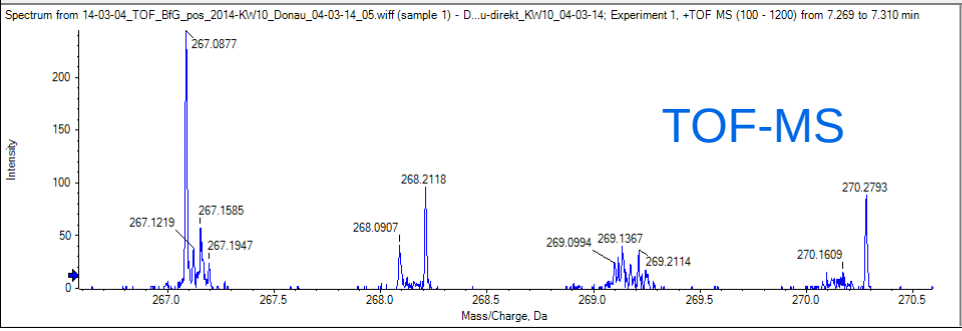

Sample

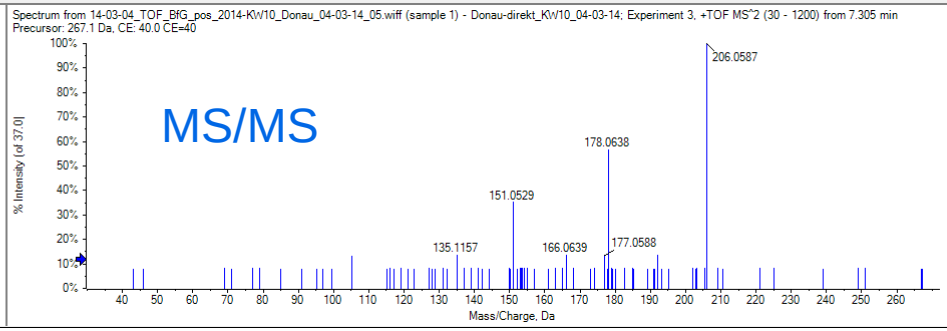



System Blank



# Identification of valsartan acid with DAIOS

DAIOS 2.0

Edit User Properties | Contact | Logout

Search Results

Entries found: 4 Visibile 4

type to filter

Details | Ms/Ms | Transformation Tree

## Valsartan acid

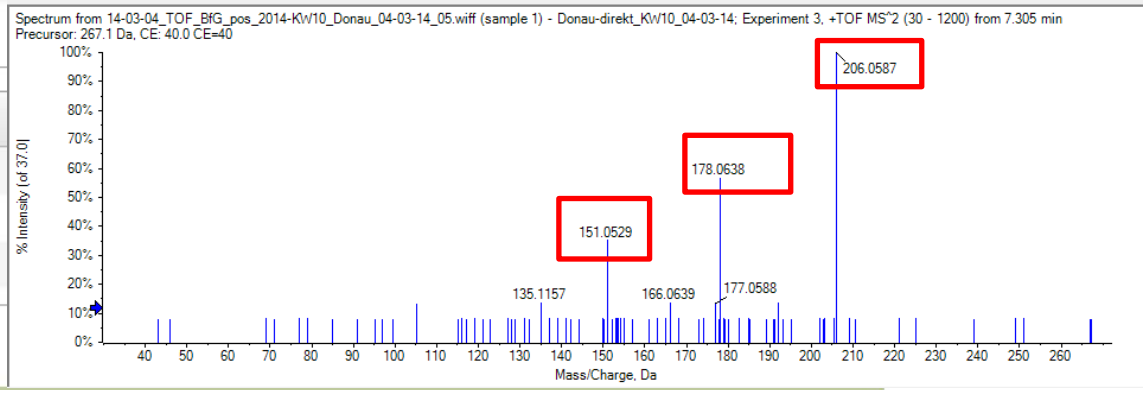
Precursor entries : 2

| Property | Value |
|---|---|
| Precursor Mass | 265.0731 |
| Ion | -H |

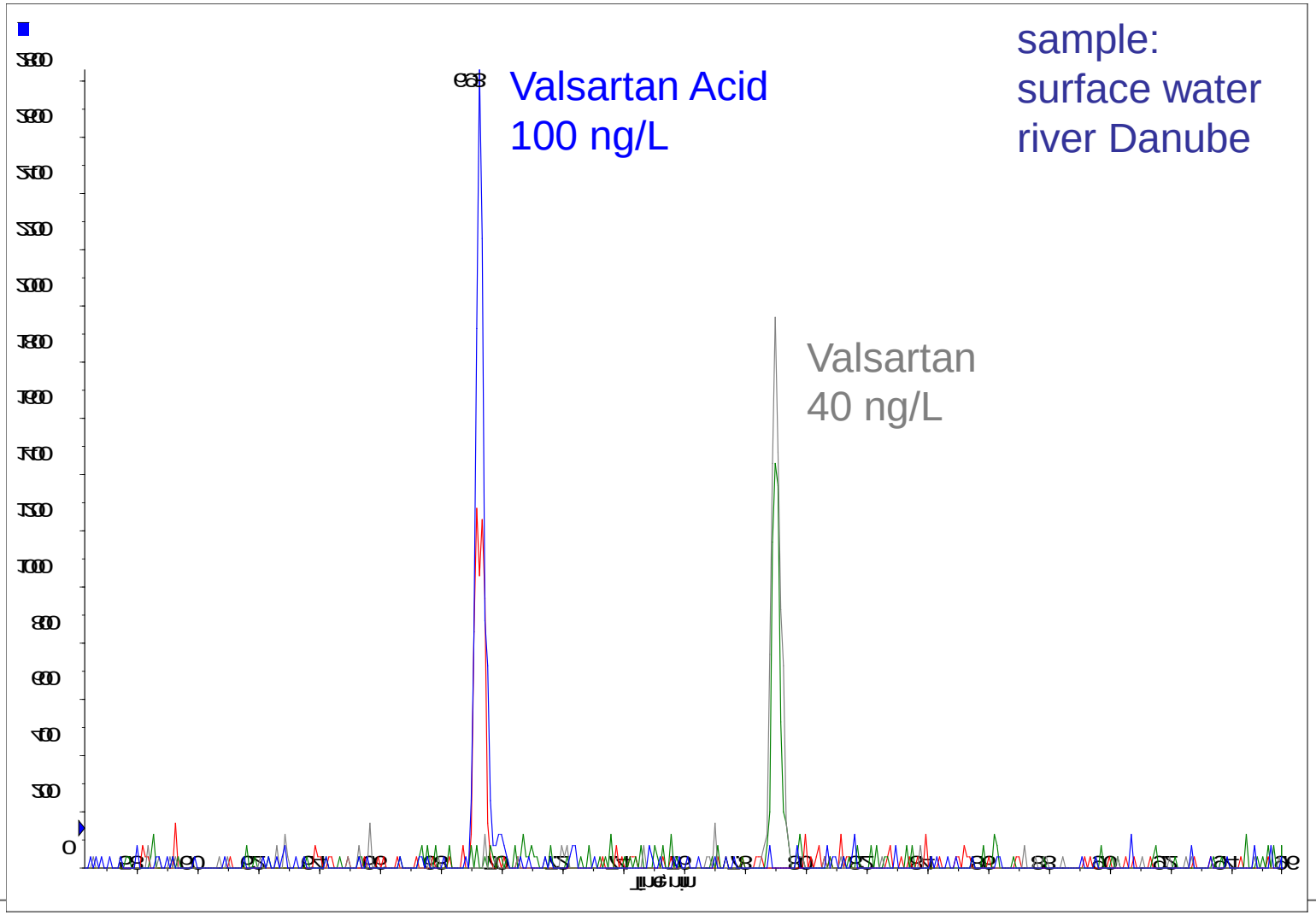
| Fragments |
|---|
| 165.0000 |
| 193.0000 |

| Property | Value |
|---|---|
| Precursor Mass | 267.0876 |
| Ion | +H |

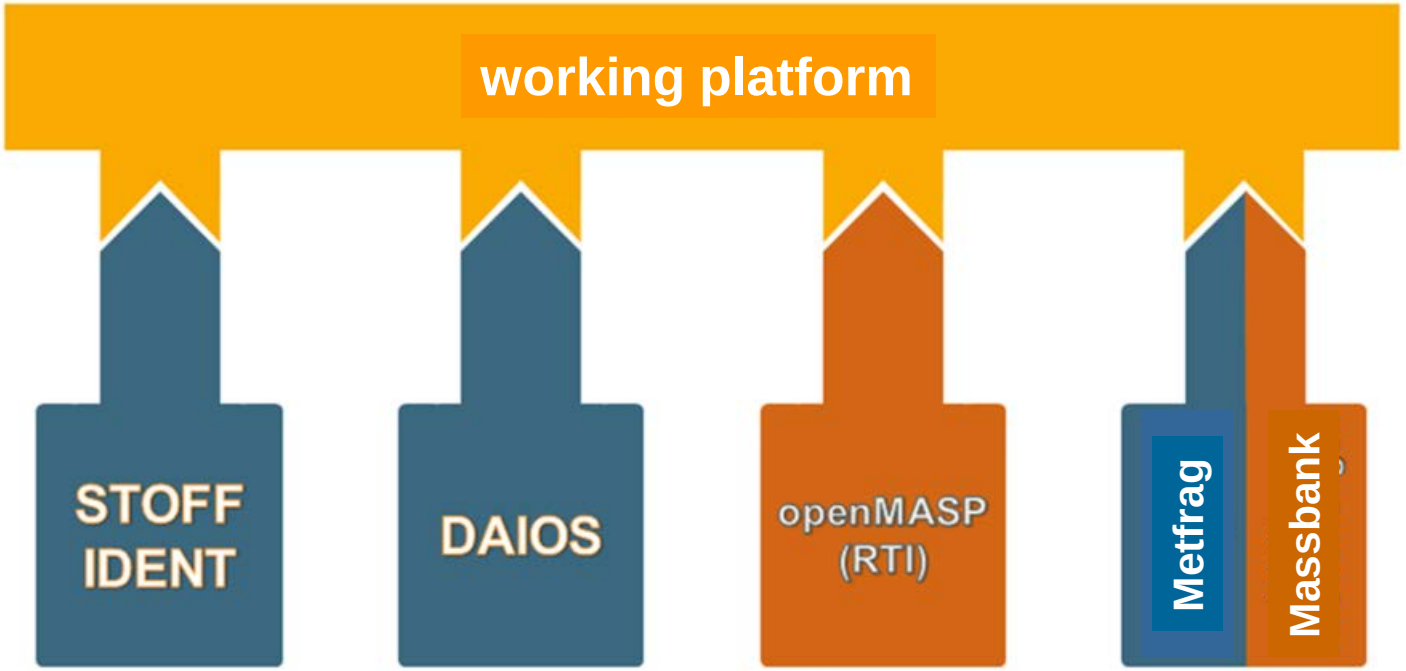
| Fragments |
|---|
| 206.0000 |
| 178.0000 |
| 151.0000 |



# Quantification of Valsartan an Valsartan Acid



# Concept for the identification



# Thank you