Fachtagung
Fortschritte in der Suspected- und Non-target-Analytik
LfU Augsburg 27. - 28. März 2014

Wie kann DAIOS die Identifizierung von Spurenstoffen unterstützen?

W. Schulz, N. Jung, T. Lucke und R. Winzenbacher

Zweckverband Landeswasserversorgung, Langenau

ASKURIS
Zweckverband Landeswasserversorgung
RISK IDENT Identifizieren | Bewerten Handeln | Kommunizieren
gefördert vom: Bundesministerium für Bildung und Forschung

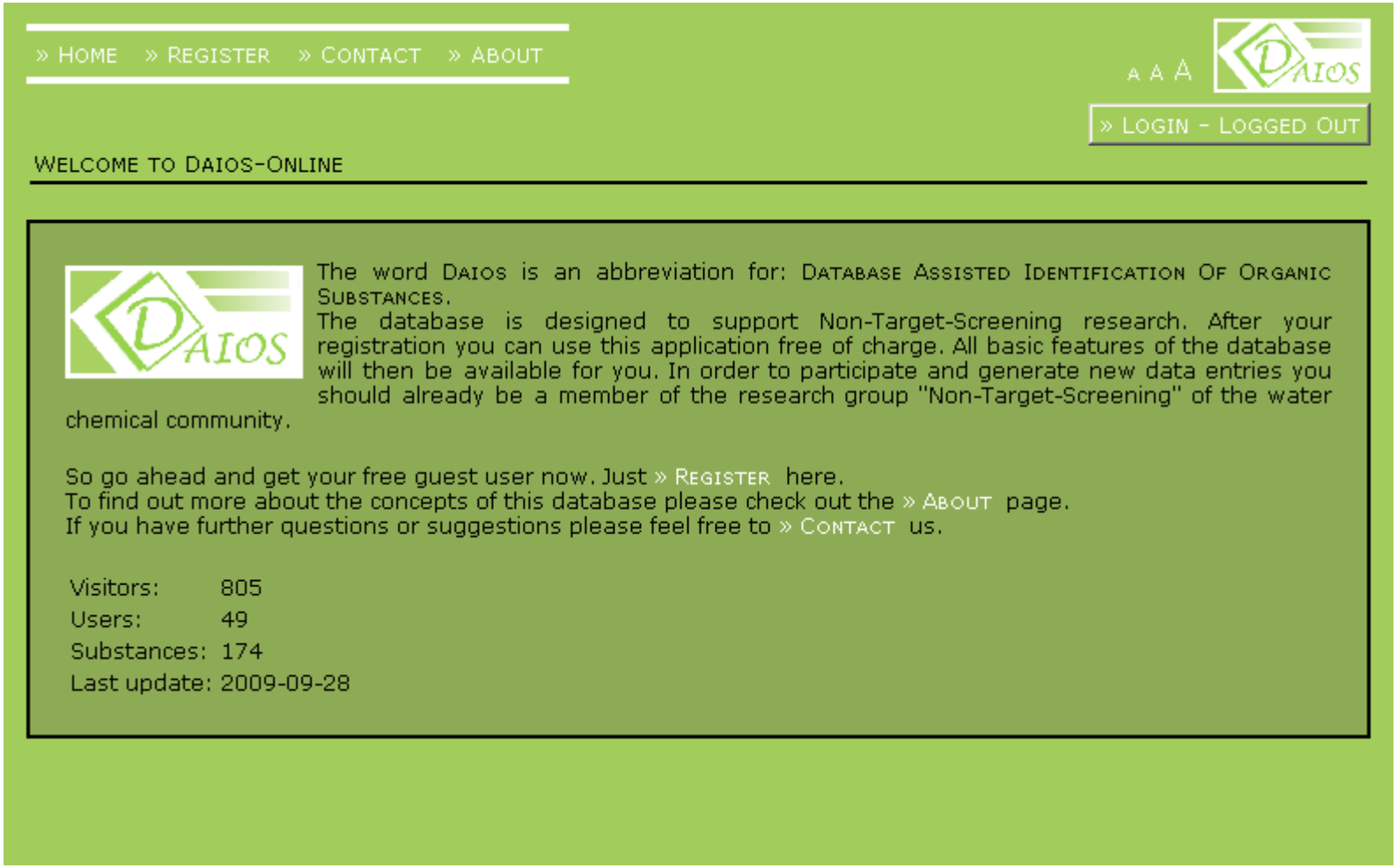
Datenbank DAIOS (www.daios-online.de)

Database **A**ssisted **I**dentification of **O**rganic **S**ubstances

Ziele:

- Unterstützung der Identifizierung bei LC-MS Messung
- keine Spektrenbibliothek (unabhängig von Geräteplattform)
- Einbindung von Meta-Informationen
- frei im Internet verfügbar

DAIOS 1.0 2009



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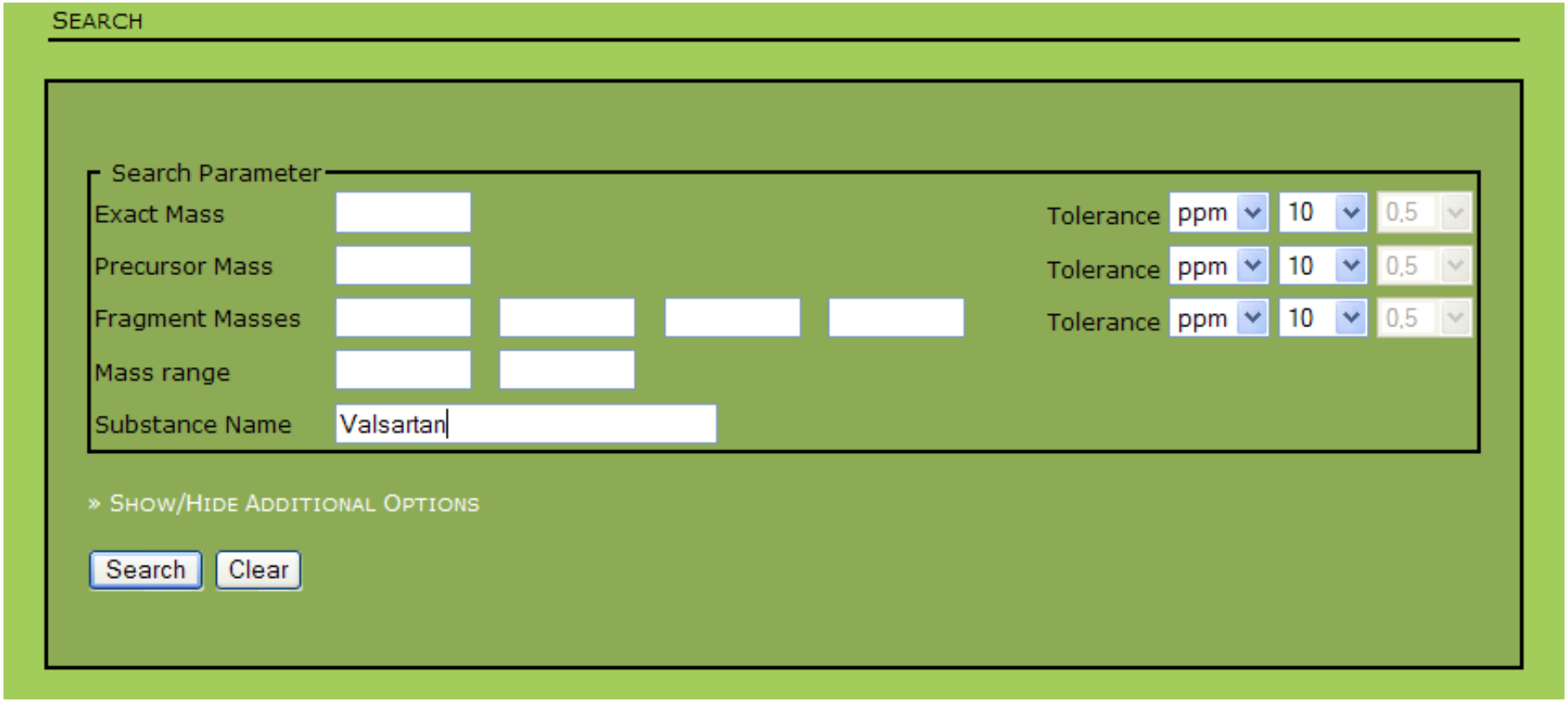
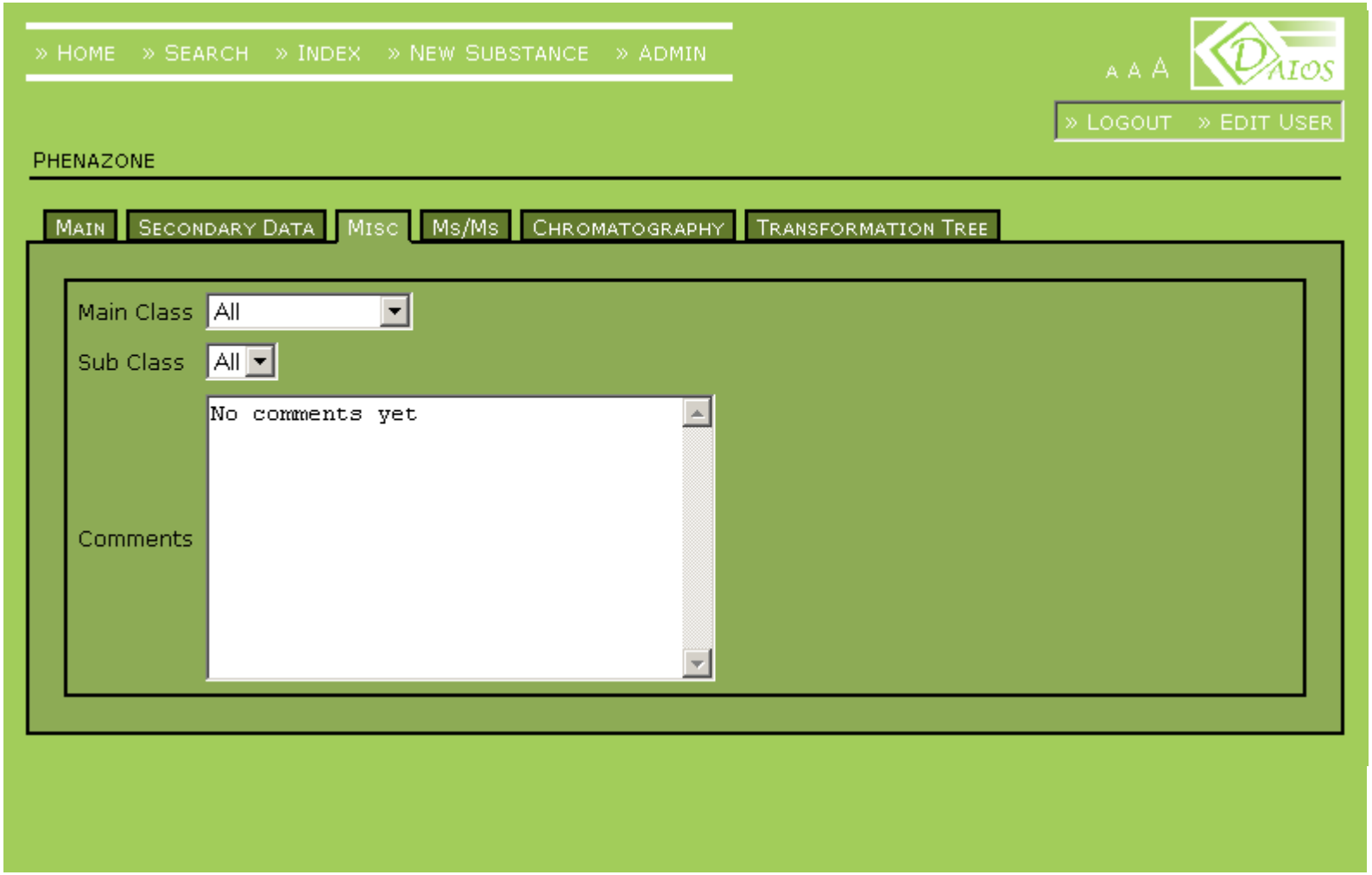
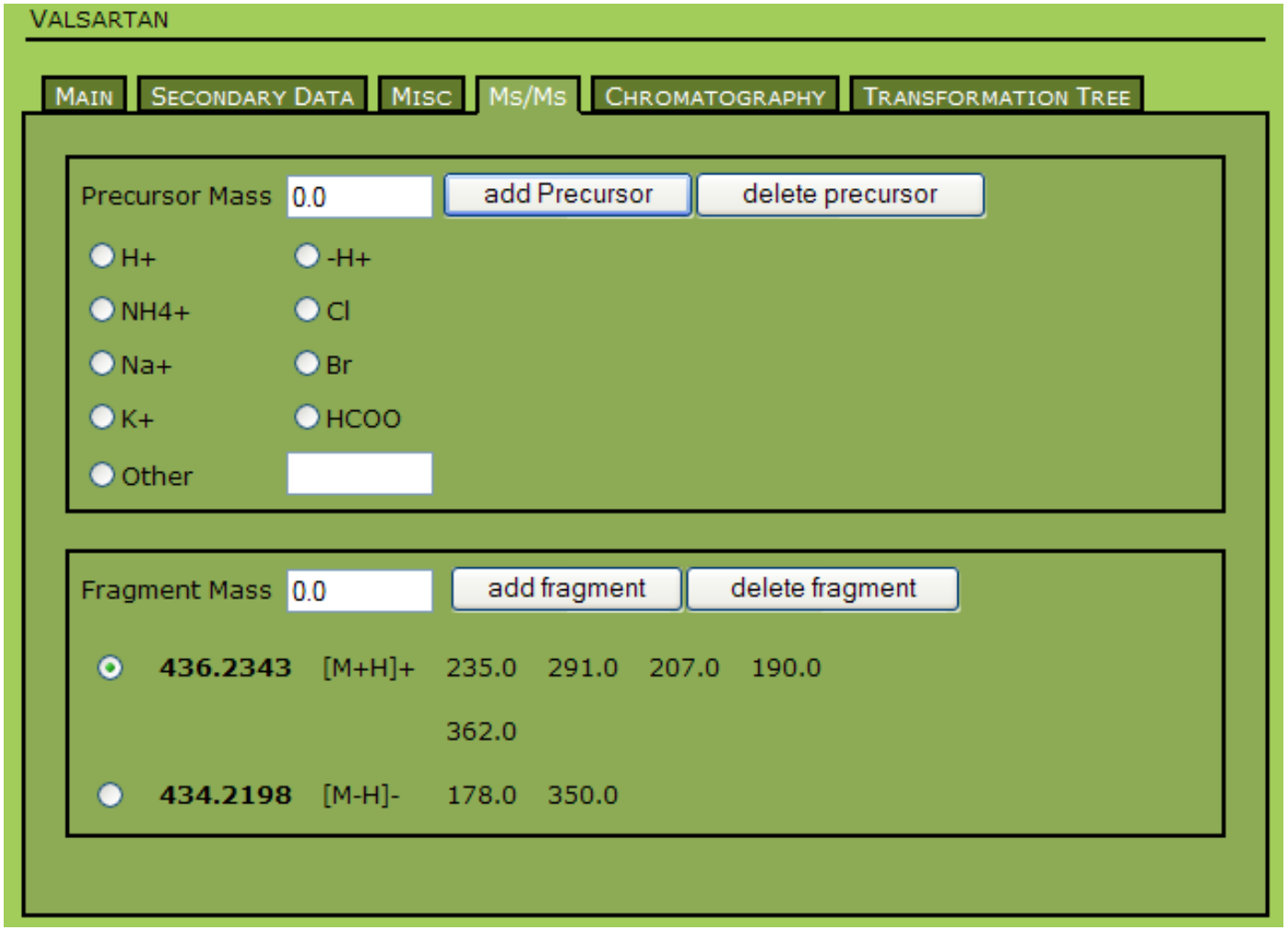

SEARCH
Search Parameter
Exact Mass
Precursor Mass
Fragment Masses
Mass range
Substance Name
Valsartan
Tolerance
ppm
10
0,5
Tolerance
ppm
10
0,5
Tolerance
ppm
10
0,5
» SHOW/HIDE ADDITIONAL OPTIONS
Search
Clear

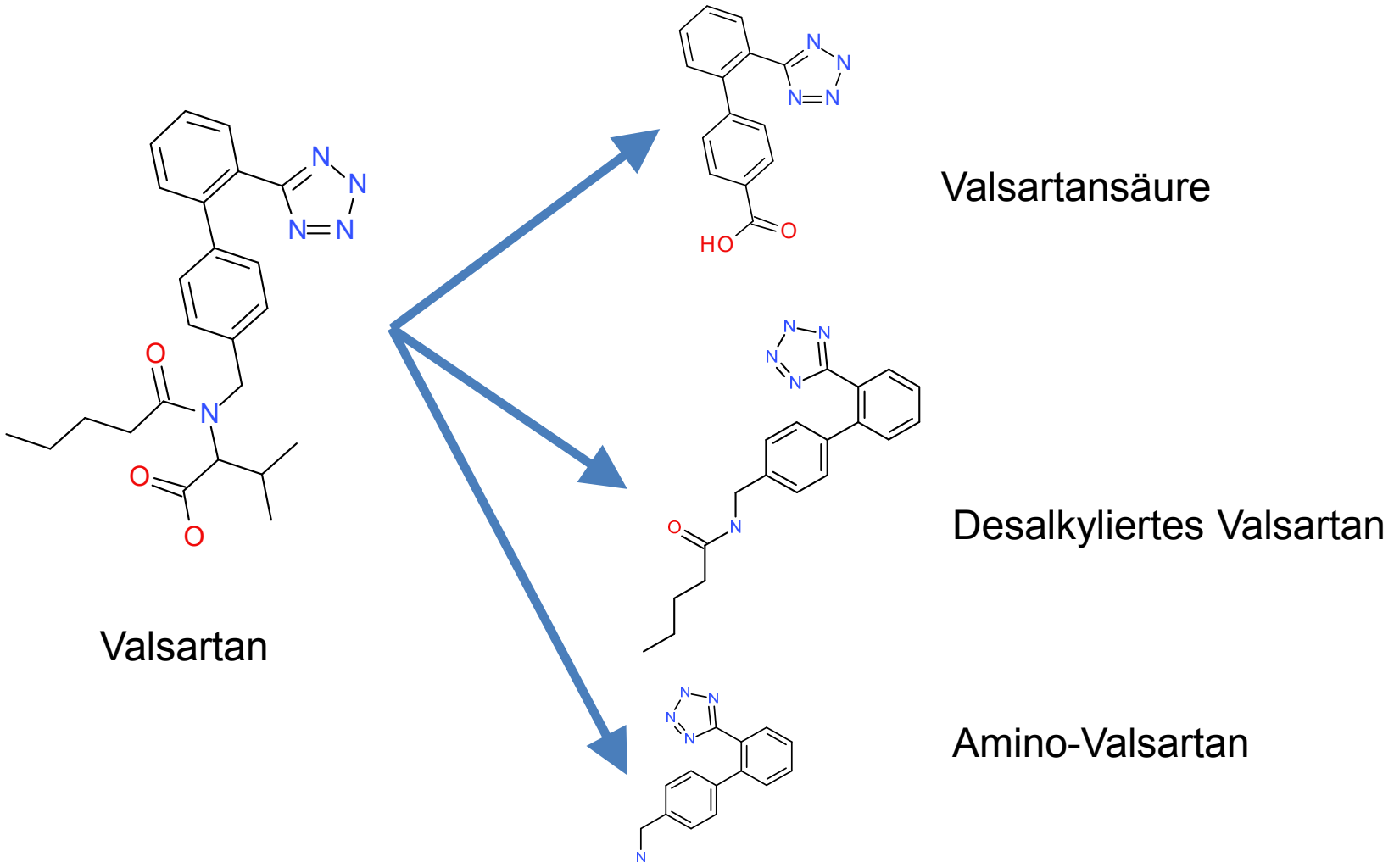
Tab „Misc“


» HOME
» SEARCH
» INDEX
» NEW SUBSTANCE
» ADMIN
A A A
» LOGOUT
» EDIT USER
PHENAZONE
MAIN
SECONDARY DATA
MISC
MS/MS
CHROMATOGRAPHY
TRANSFORMATION TREE
Main Class
All
Sub Class
All
No comments yet
Comments

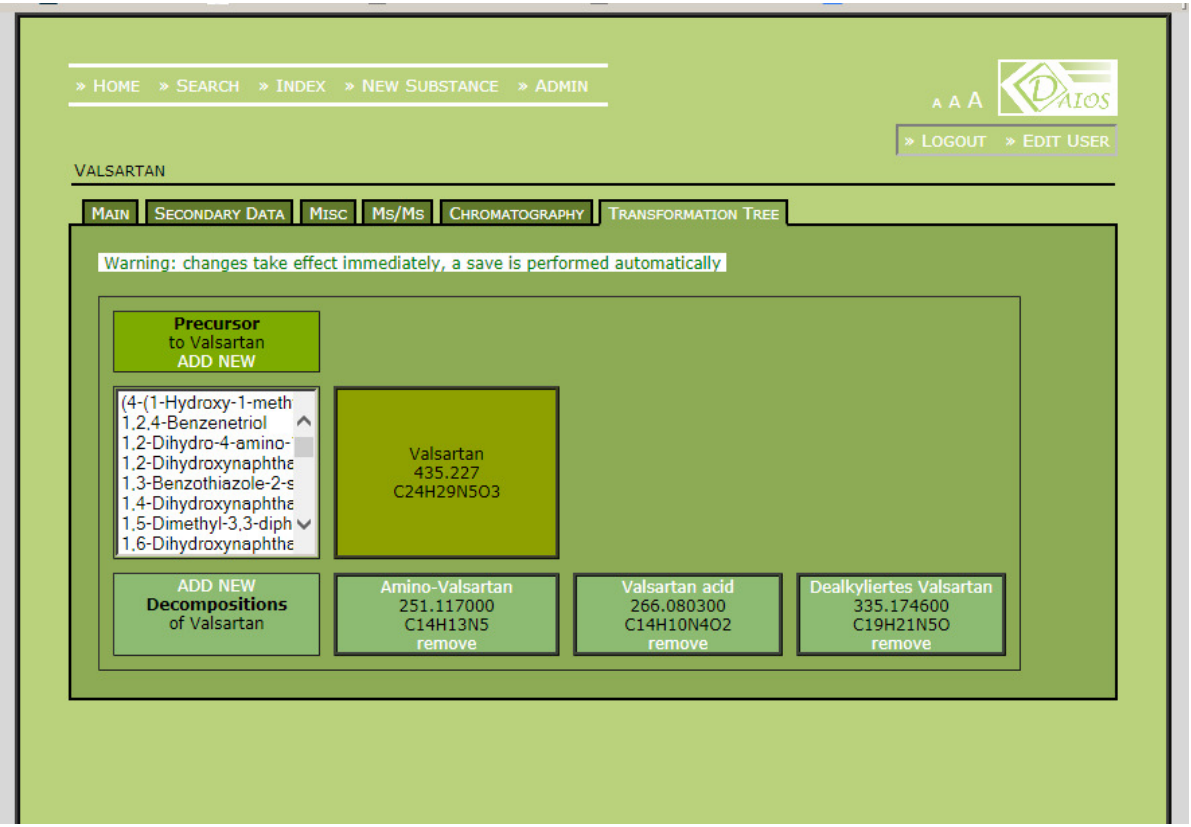
Tab „MS/MS“


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

Transformation Tree Valsartan



Tab “Transformation Tree”



Ausgangssubstanz

Transformationsprodukte

gefördert vom: Bundesministerium für Bildung und Forschung

Wasserchemische Gesellschaft
Fachgruppe in der GDCh

http://www.wasserchemische-gesellschaft.de/de/

Fachausschuss (FA) Non-Target-Screening

Fachausschüsse - Hauptausschuss II

- Stoffe und Gewässergüte -

FA Biologische Verfahren zur Beurteilung der Gewässergüte

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Fax: +49 37437 76 219
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Tel.: +49 7345 9638-2291
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DAIOS 2.0

Neuprogrammierung durch:

Tobias Placht, Marco Luthardt und Prof. Frank Leßke

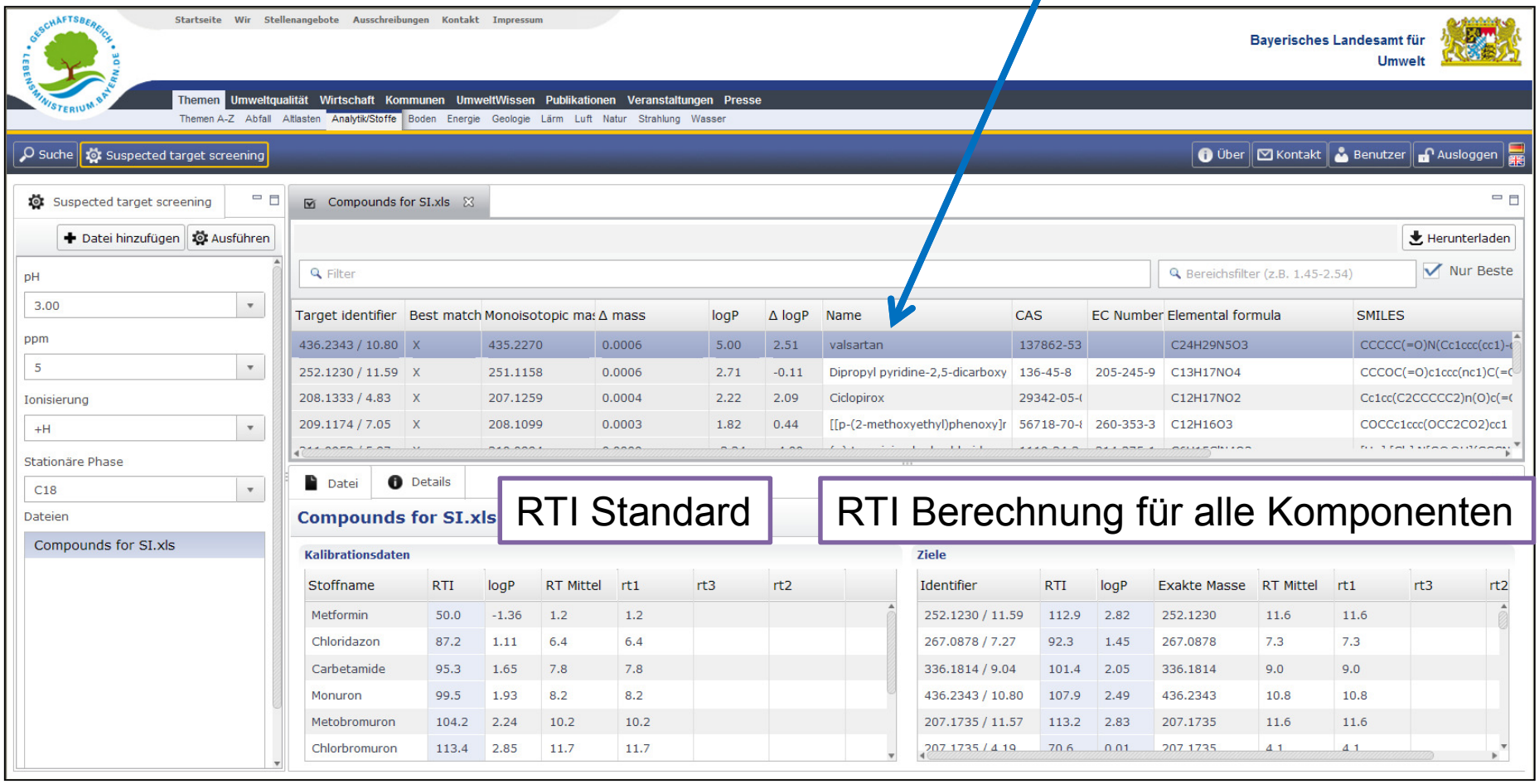
Hochschule Weihenstephan-Triesdorf, Bioinformatik

DAIOS 2.0


Search
Edit
User administration
DAIOS 2.0
Edit User Properties
Contact
Logout
Mass
Meta
Index
Search
Clear
Name
valsartan
CAS
Chemical Formula
History
Clear
Meta: Name = valsartan
Valsartan
Search Results
Entries found: 4 Visibile 4
type to filter
Name
CAS
Exact mass
Molare mass
Valsartan
137862-53-4
435.2270
435.52
Details
Ms/Ms
Transformation Tree
Valsartan
View Raw Data
Download Molfile
General information
Property
Value
Name
Valsartan
IUPAC
N-Pentanoyl-N-{[2'-(2H-tetrazol-5-yl)-4-biphenylyl]methyl}-L-valine
Synonym
CAS Registry Number
137862-53-4
Chemical formula
C24H29N5O3
Secondary Data

Suche in der Datenbank Stoff-Ident mit RTI-Berechnung RISK-IDENT

Treffer Valsartan für Masse 435.2270



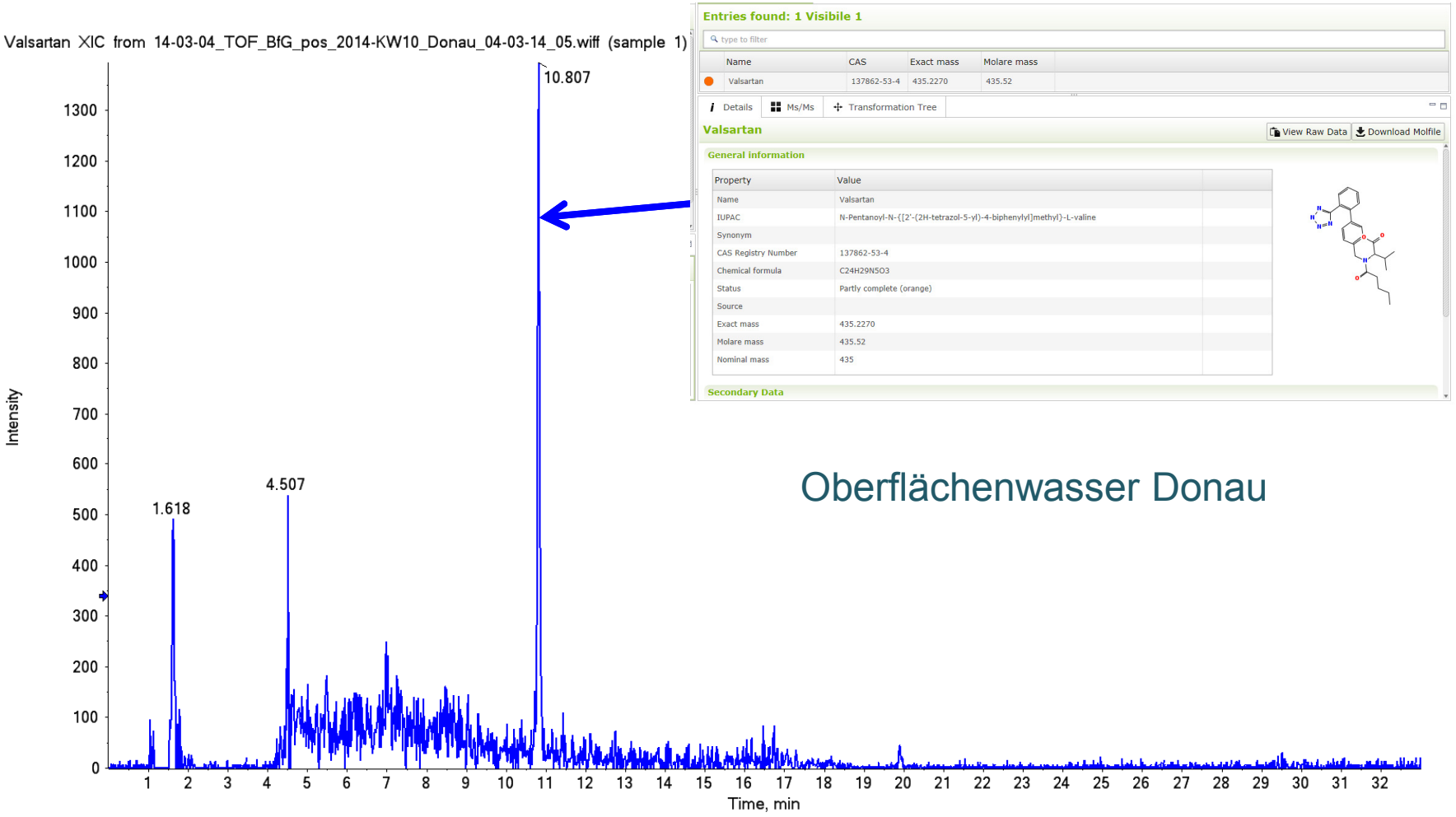
Suche mit Masse

Suche mit Namen

MS/MS Daten


Search
Edit
User administration
DAIOS 2.0
Edit User Properties
Contact
Logout
Mass
Meta
Index
Search
Clear
Name
valsartan
CAS
Chemical Formula
History
Clear
Meta: Name = valsartan
Valsartan
Search Results
Entries found: 4 Visibile 4
type to filter
Name
CAS
Exact mass
Molare mass
Valsartan
137862-53-4
435.2270
435.52
Details
Ms/Ms
Transformation Tree
Valsartan
Precursor entries : 2
Property
Value
Fragments
Precursor Mass
434.2198
350.0000
Ion
-H
178.0000
Property
Value
Fragments
Precursor Mass
436.2343
207.0000
Ion
+H
291.0000
235.0000

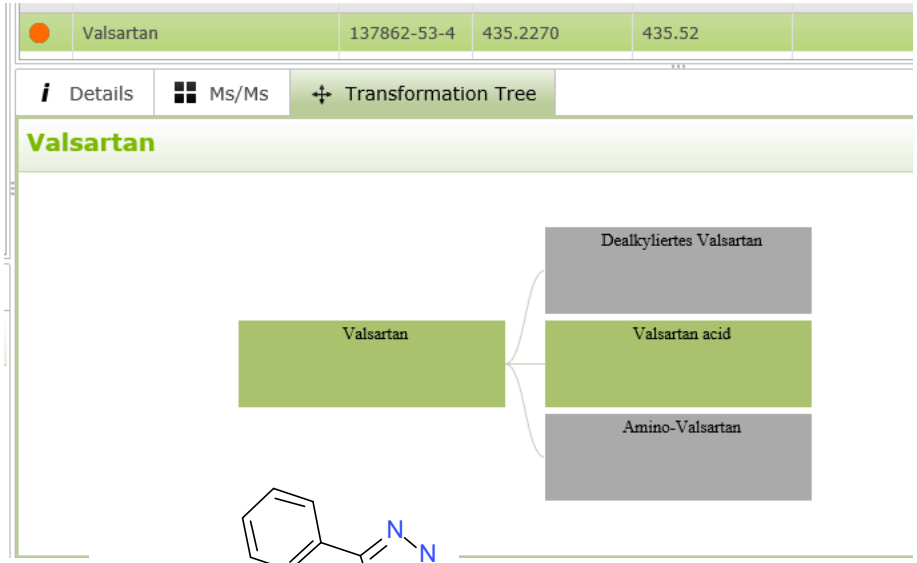
XIC (extracted ion chromatogram) von Valsartan

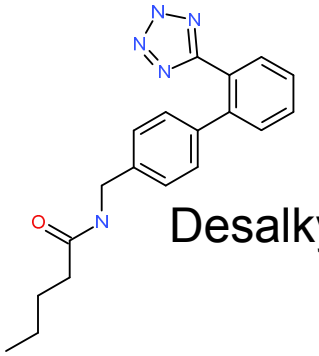


Oberflächenwasser Donau

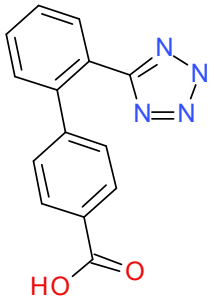
Transformation Tree

Transformationsprodukte
Valsartan

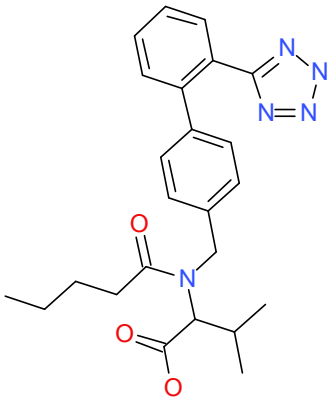


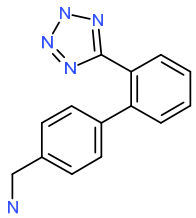


Desalkyliertes Valsartan



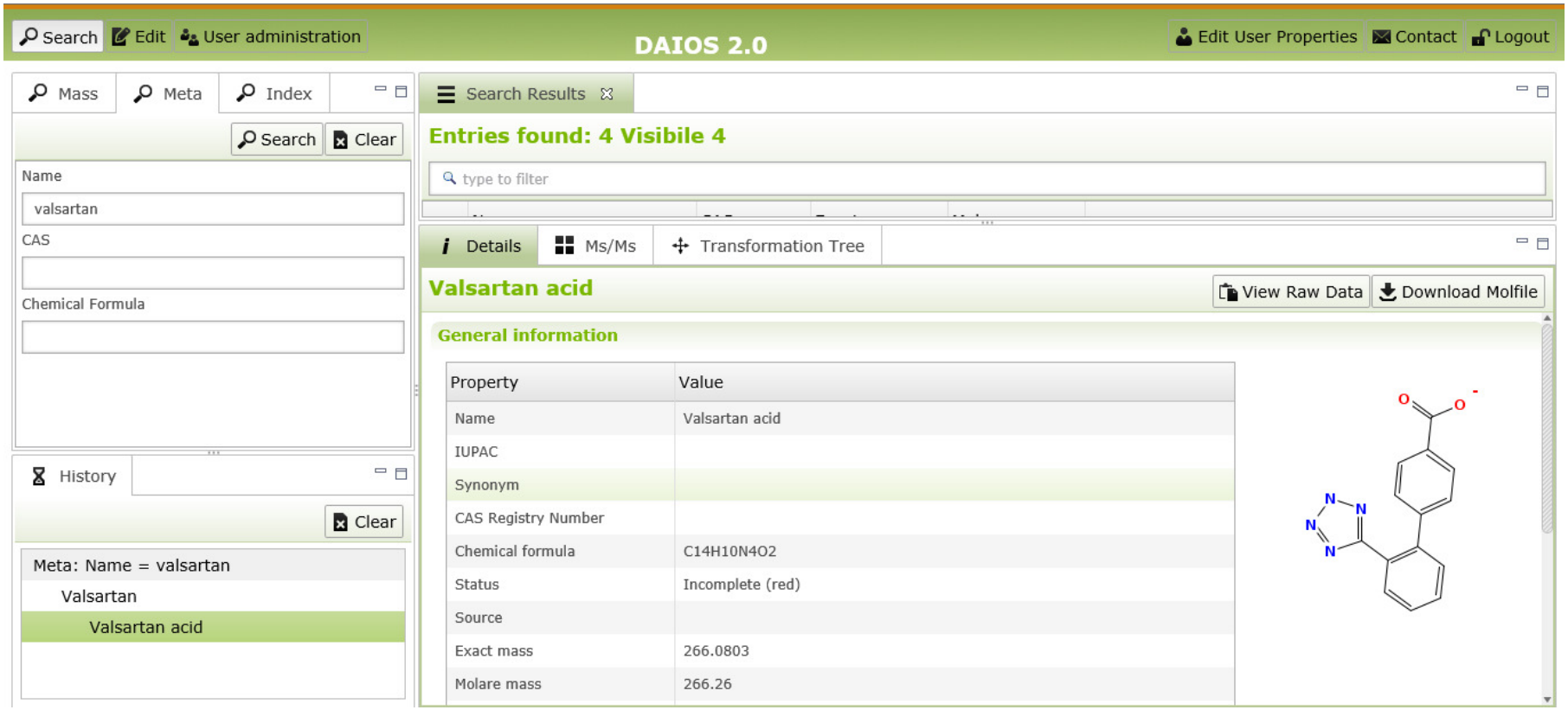
Valsartansäure





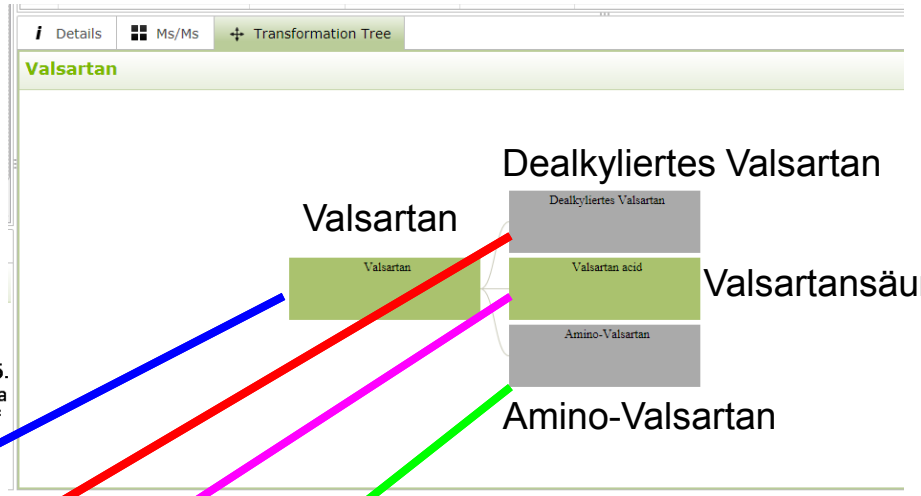
Amino-Valsartan

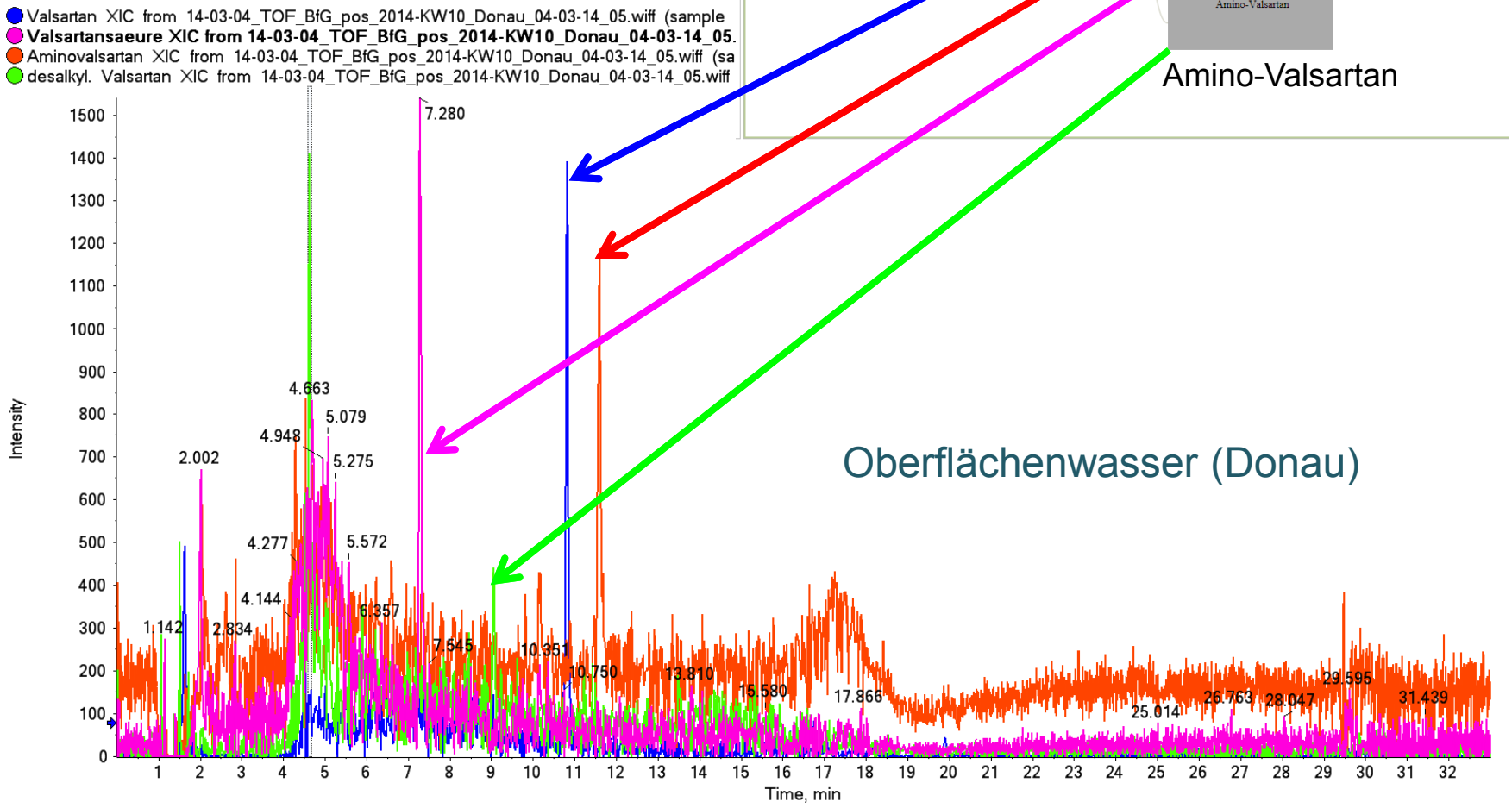
Valsartansäure



MS/MS Fragmente Valsartansäure

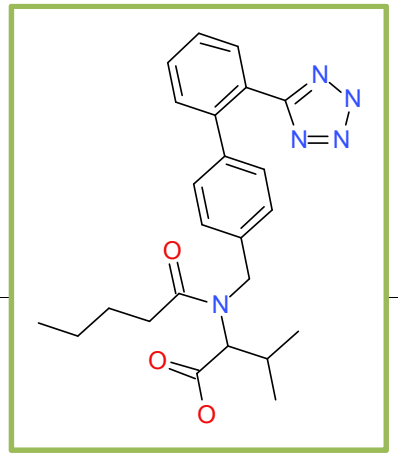
XICs von Valsartan und seinen Transformationsprodukten



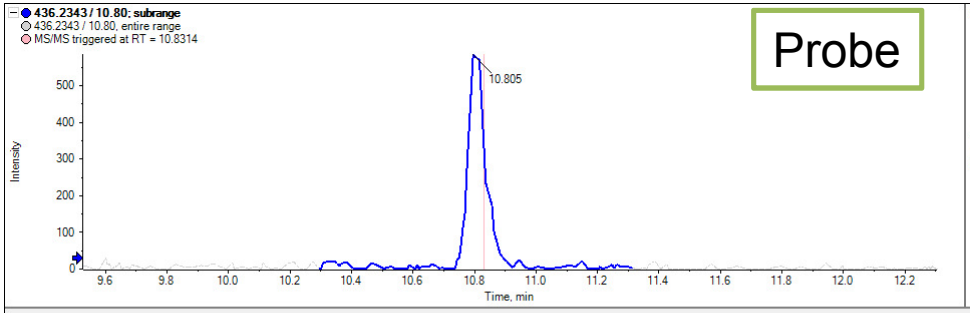


Identifizierung mit DAIOS
IDA-MS/MS

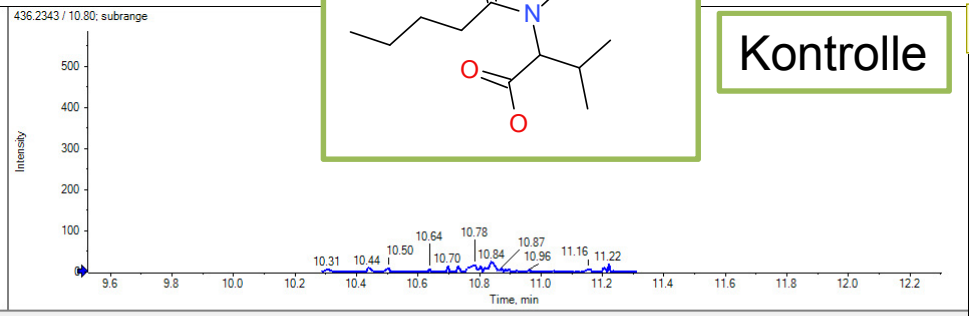
Valsartan

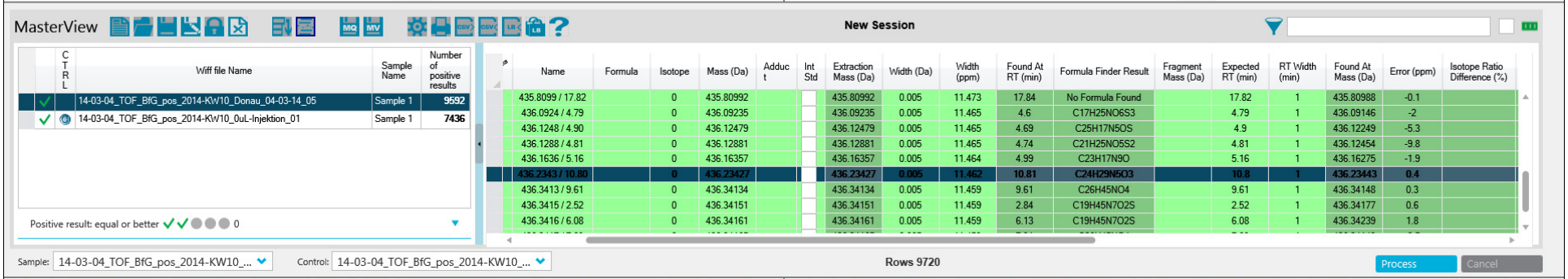


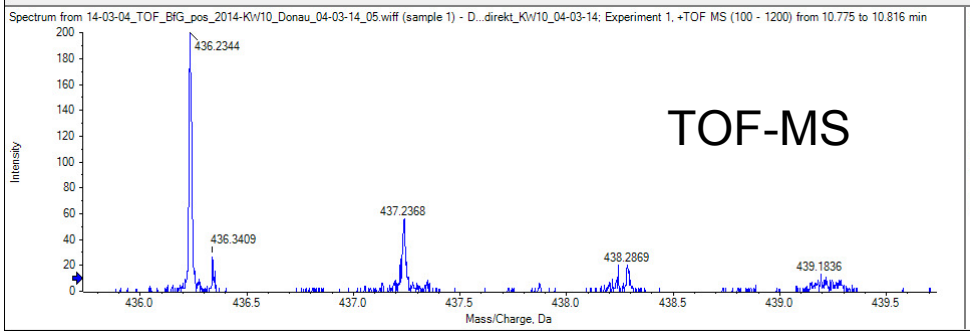
Probe



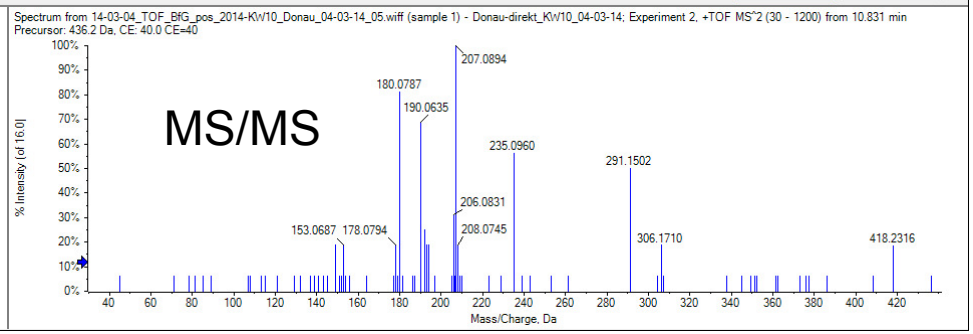
Kontrolle







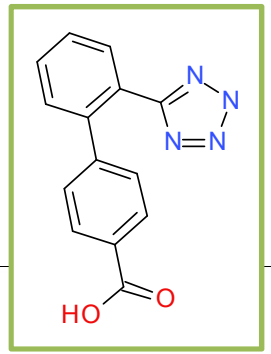
TOF-MS



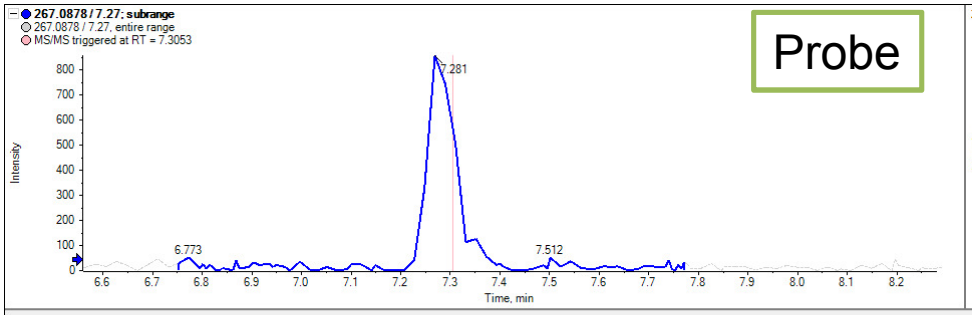
MS/MS

Identifizierung mit DAIOS
IDA-MS/MS

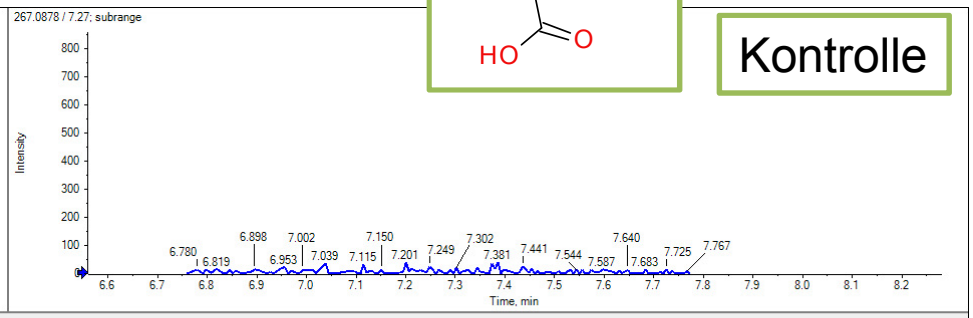
Valsartan Acid

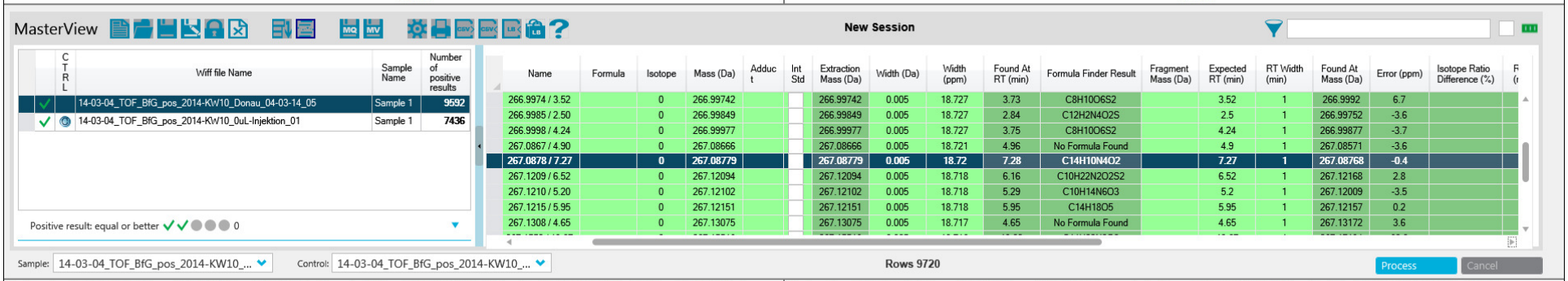


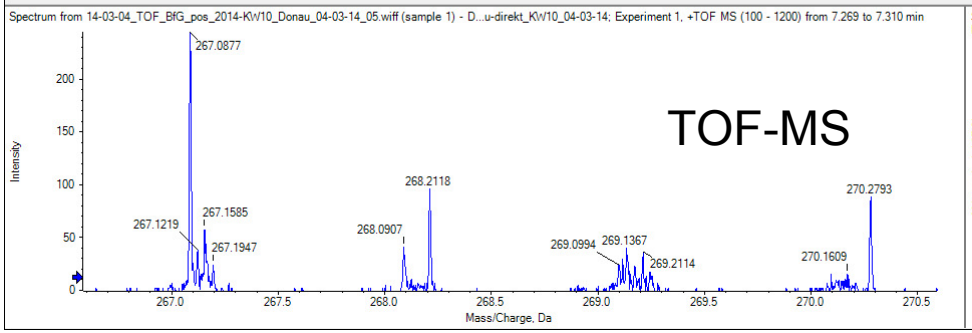
Probe

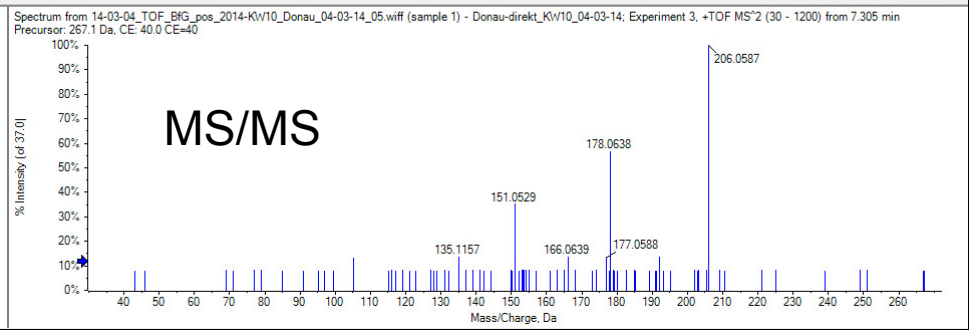


Kontrolle









Vergleich von MS/MS Daten aus DAIOS mit IDA-Spektrum

Database Hit Valsartan mit MS/MS-Data

Details | Ms/Ms | Transformation Tree

Valsartan

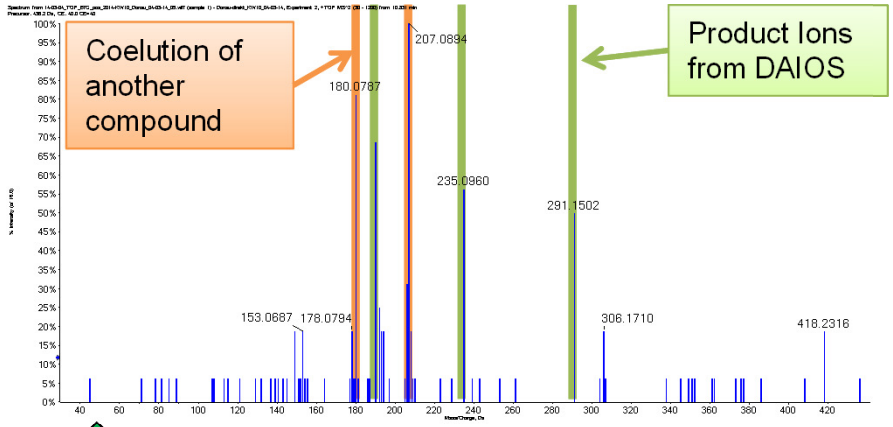
Precursor entries : 2

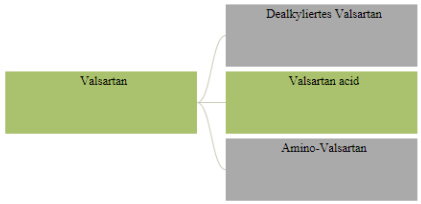
Property	Value
Precursor Mass	434.2198
Ion	-H

Fragments
350.0000
178.0000

Property	Value
Precursor Mass	436.2343
Ion	+H

Fragments
207.0000
291.0000
235.0000
190.0000
362.0000





TP von DAIOS: Valsartan Acid mit MS/MS-Data

Database assissted identification of unknown compounds

Details | Ms/Ms | Transformation Tree

Valsartan acid

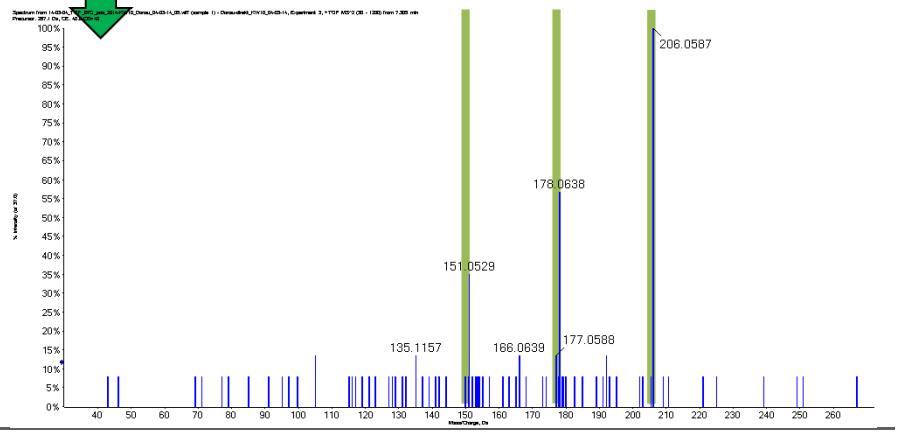
Precursor entries : 2

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



Quantitative Bestimmung von Valsartan und Valsartansäure

Nicole Jung (jung.n@lw-online.de)

Vielen Dank für Ihre Aufmerksamkeit