

Fachtagung

Fortschritte in der Suspected- und Non-target-Analytik

LfU Augsburg 27. - 28. März 2014

Wie kann DAIOS die Identifizierung von Spurenstoffen unterstützen?

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Zweckverband Landeswasserversorgung, Langenau



Zweckverband
Landeswasserversorgung



Handeln | Kommunizieren
RISK IDENT Identifizieren | Bewerten

gefördert vom:
 Bundesministerium
für Bildung
und Forschung

Datenbank DAIOS (www.daios-online.de)



Database Assisted Identification of Organic Substances

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

[» HOME](#) [» REGISTER](#) [» CONTACT](#) [» ABOUT](#)


» LOGIN - LOGGED OUT

WELCOME TO DAIOS-ONLINE



The word DAios is an abbreviation for: DATABASE ASSISTED IDENTIFICATION OF ORGANIC SUBSTANCES.
The database is designed to support Non-Target-Screening research. After your registration you can use this application free of charge. All basic features of the database will then be available for you. In order to participate and generate new data entries you should already be a member of the research group "Non-Target-Screening" of the water chemical community.

So go ahead and get your free guest user now. Just » REGISTER here.
To find out more about the concepts of this database please check out the » ABOUT page.
If you have further questions or suggestions please feel free to » CONTACT us.

Visitors: 805
Users: 49
Substances: 174
Last update: 2009-09-28

Tab „Suchen“

SEARCH

Search Parameter

Exact Mass		Tolerance	ppm	10	0.5			
Precursor Mass		Tolerance	ppm	10	0.5			
Fragment Masses					Tolerance	ppm	10	0.5
Mass range								
Substance Name	Valsartan							

» SHOW/HIDE ADDITIONAL OPTIONS

Tab „Misc“

» HOME » SEARCH » INDEX » NEW SUBSTANCE » ADMIN

» LOGOUT » EDIT USER

PHENAZONE

MAIN SECONDARY DATA **MISC** Ms/Ms CHROMATOGRAPHY TRANSFORMATION TREE

Main Class

Sub Class

Comments

No comments yet

Tab „MS/MS“

VALSARTAN

MAIN SECONDARY DATA MISC **Ms/Ms** CHROMATOGRAPHY TRANSFORMATION TREE

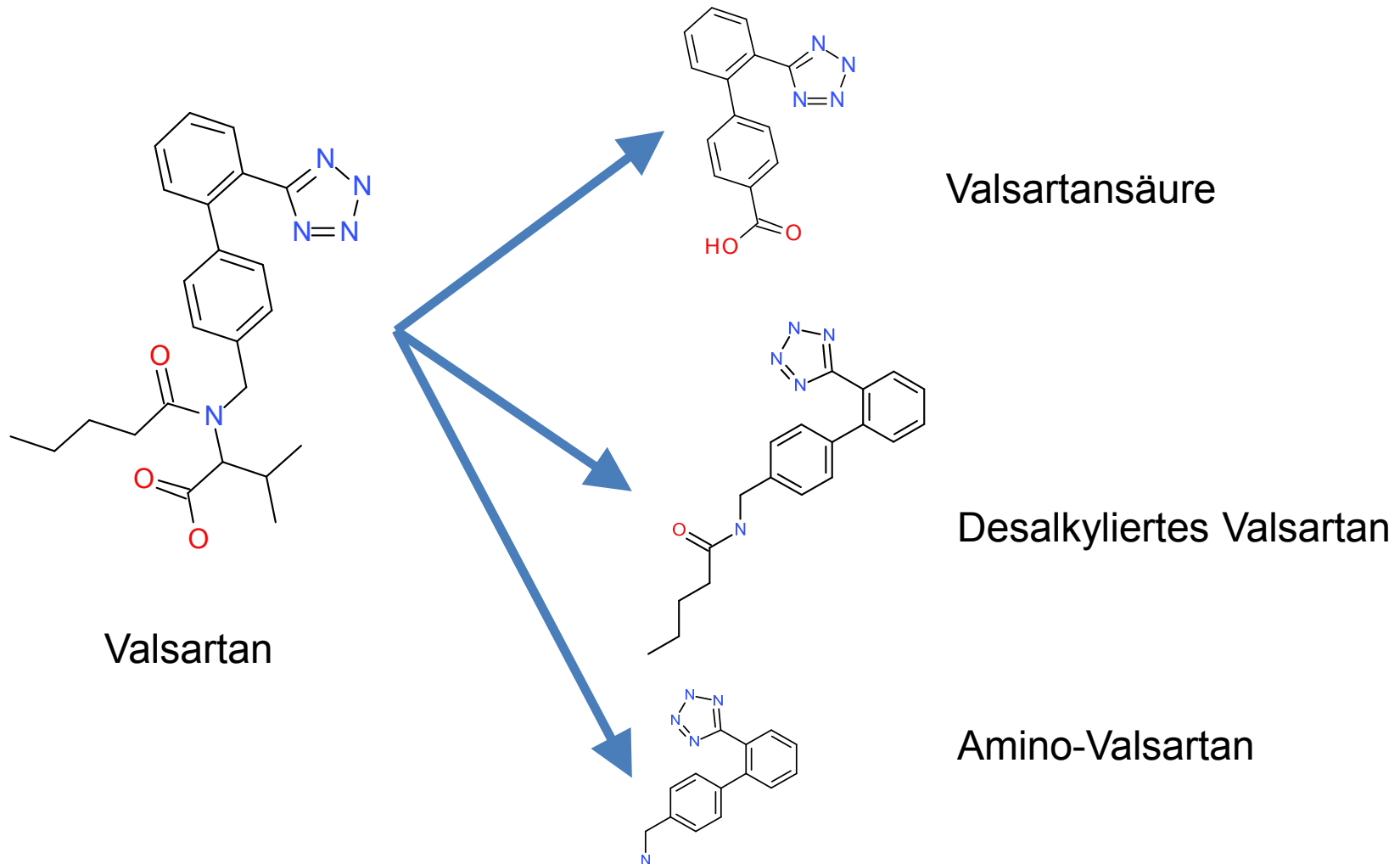
Precursor Mass

☐ H+ ☐ -H+
☐ NH4+ ☐ Cl
☐ Na+ ☐ Br
☐ K+ ☐ HCOO
☐ Other

Fragment Mass

☒	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”

The screenshot shows the DAIOS web application interface. At the top, there is a navigation bar with links: » HOME » SEARCH » INDEX » NEW SUBSTANCE » ADMIN. On the right, there is a logo for DAIOS and links for » LOGOUT » EDIT USER. Below the navigation bar, the page title is VALSARTAN. A tabbed interface shows several tabs: MAIN, SECONDARY DATA, MISC, MS/MS, CHROMATOGRAPHY, and TRANSFORMATION TREE. The TRANSFORMATION TREE tab is active. A warning message states: "Warning: changes take effect immediately, a save is performed automatically". The main content area displays the transformation tree for Valsartan. It includes a list of precursors on the left, a central box for Valsartan (435.227, C24H29NO3), and three boxes for transformation products: Amino-Valsartan (251.117000, C14H13N5), Valsartan acid (266.080300, C14H10N4O2), and Dealkyliertes Valsartan (335.174600, C19H21N5O). Each product box has a "remove" link.

» HOME » SEARCH » INDEX » NEW SUBSTANCE » ADMIN

DAIOS

» LOGOUT » EDIT USER

VALSARTAN

MAIN SECONDARY DATA MISC MS/MS CHROMATOGRAPHY TRANSFORMATION TREE

Warning: changes take effect immediately, a save is performed automatically

Precursor
to Valsartan
ADD NEW

(4-(1-Hydroxy-1-meth
1,2,4-Benzenetriol
1,2-Dihydro-4-amino-
1,2-Dihydroxynaphthe
1,3-Benzothiazole-2-s
1,4-Dihydroxynaphthe
1,5-Dimethyl-3,3-diph
1,6-Dihydroxynaphthe

Valsartan
435.227
C24H29NO3

ADD NEW
Decompositions
of Valsartan

Amino-Valsartan
251.117000
C14H13N5
remove

Valsartan acid
266.080300
C14H10N4O2
remove

Dealkyliertes Valsartan
335.174600
C19H21N5O
remove

Ausgangssubstanz

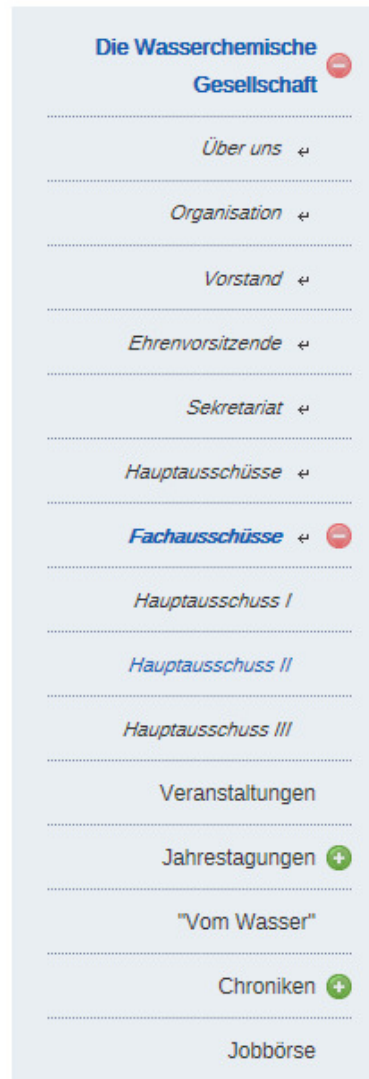
Transformationsprodukte

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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e-Mail: tamara.grummt@uba.de

FA Non Target Screening



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Fax: +49 7345 9638-2290

DAIOS 2.0

Neuprogrammierung durch:

Tobias Placht, Marco Luthardt und
Prof. Frank Leßke

Hochschule Weihenstephan-Triesdorf,
Bioinformatik



DAIOS Login

provided by  developed by 

User:

Password:

Don't have an account? Click [here](#) to register

Login

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 Visible 4

type to filter

Name	CAS	Exact mass	Molare mass
Valsartan	137862-53-4	435.2270	435.52

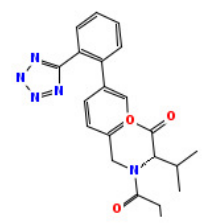
Details Ms/Ms Transformation Tree

Valsartan View Raw Data Download Molfile

General information

Property	Value
Name	Valsartan
IUPAC	N-Pentanoyl-N-{[2'-(2H-tetrazol-5-yl)-4-biphenyl]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

Startseite Wir Stellenangebote Ausschreibungen Kontakt Impressum

Themen Umweltqualität Wirtschaft Kommunen Umweltwissen Publikationen Veranstaltungen Presse

Themen A-Z Abfall Altlasten Analytik/Stoffe Boden Energie Geologie Lärm Luft Natur Strahlung Wasser

Suche Suspected target screening

Über Kontakt Benutzer Ausloggen

Suspected target screening

+ Datei hinzufügen Ausführen

pH 3.00

ppm 5

Ionisierung +H

Stationäre Phase C18

Dateien

Compounds for SI.xls

Filter

Bereichsfilter (z.B. 1.45-2.54) Nur Beste

Target identifier	Best match	Monoisotopic mass	Δ mass	logP	Δ logP	Name	CAS	EC Number	Elemental formula	SMILES
436.2343 / 10.80	X	435.2270	0.0006	5.00	2.51	valsartan	137862-53		C ₂₄ H ₂₉ N ₅ O ₃	CCCCC(=O)N(Cc1ccc(cc1)-
252.1230 / 11.59	X	251.1158	0.0006	2.71	-0.11	Dipropyl pyridine-2,5-dicarboxy	136-45-8	205-245-9	C ₁₃ H ₁₇ N ₄ O ₄	CCCOC(=O)c1ccc(nc1)C(=O
208.1333 / 4.83	X	207.1259	0.0004	2.22	2.09	Ciclopirox	29342-05-1		C ₁₂ H ₁₇ N ₂ O ₂	Cc1cc(C2CCCCC2)n(O)c(=C
209.1174 / 7.05	X	208.1099	0.0003	1.82	0.44	[[p-(2-methoxyethyl)phenoxy]r	56718-70-1	260-353-3	C ₁₂ H ₁₆ O ₃	COCCc1ccc(OCC(CO2)cc1

Herunterladen

RTI Standard

RTI Berechnung für alle Komponenten

Kalibrationsdaten							Ziele							
Stoffname	RTI	logP	RT Mittel	rt1	rt3	rt2	Identifizier	RTI	logP	Exakte Masse	RT Mittel	rt1	rt3	rt2
Metformin	50.0	-1.36	1.2	1.2			252.1230 / 11.59	112.9	2.82	252.1230	11.6	11.6		
Chloridazon	87.2	1.11	6.4	6.4			267.0878 / 7.27	92.3	1.45	267.0878	7.3	7.3		
Carbetamide	95.3	1.65	7.8	7.8			336.1814 / 9.04	101.4	2.05	336.1814	9.0	9.0		
Monuron	99.5	1.93	8.2	8.2			436.2343 / 10.80	107.9	2.49	436.2343	10.8	10.8		
Metobromuron	104.2	2.24	10.2	10.2			207.1735 / 11.57	113.2	2.83	207.1735	11.6	11.6		
Chlorbromuron	113.4	2.85	11.7	11.7			207.1735 / 4.19	70.6	0.01	207.1735	4.1	4.1		

Suche mit Masse

DAIOS 2.0

Search Edit User administration Edit User Properties Contact Logout

Mass Meta Index

Search Clear

Mass range
to

Exact mass
+/- unit 0.01

Precursor mass
+/- unit 0.01

Mass fragments
+/- unit 0.01

History Clear

Details Ms/Ms Transformation Tree

View Raw Data Download Molfile

Suche mit Namen

DAIOS 2.0

Search Edit User administration 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 Visible 4

type to filter

Name	CAS	Exact mass	Molare mass
Valsartan	137862-53-4	435.2270	435.52

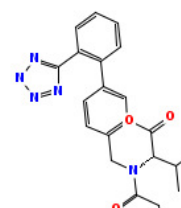
Details Ms/Ms Transformation Tree

Valsartan View Raw Data Download Molfile

General information

Property	Value
Name	Valsartan
IUPAC	N-Pentanoyl-N-{[2'-(2H-tetrazol-5-yl)-4-biphenyl]methyl}-L-valine
Synonym	
CAS Registry Number	137862-53-4
Chemical formula	C ₂₄ H ₂₉ N ₅ O ₃

Secondary Data



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 Visible 4

type to filter

Name	CAS	Exact mass	Molare mass
Valsartan	137862-53-4	435.2270	435.52

Details

Ms/Ms

Transformation Tree

Valsartan

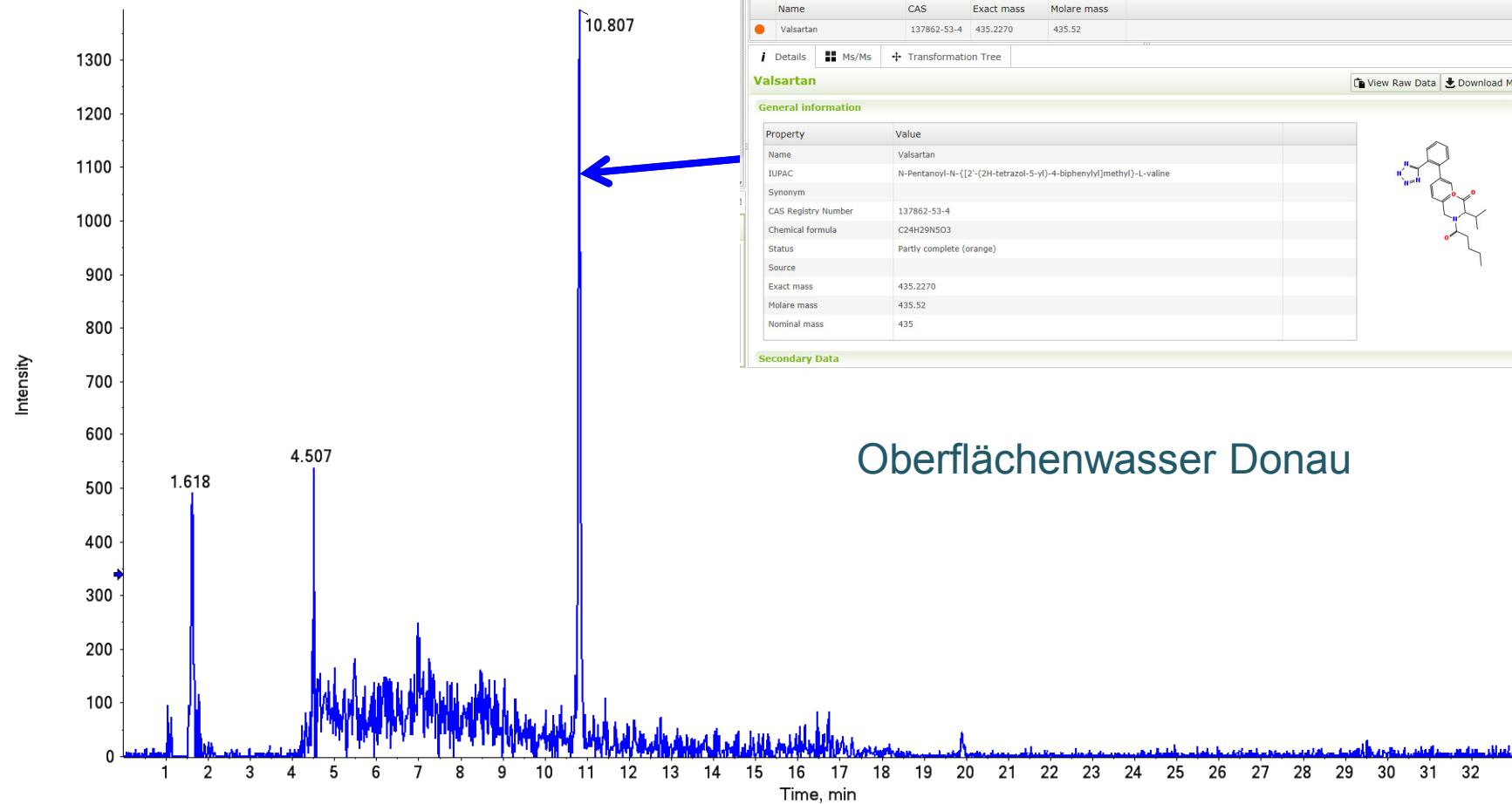
Precursor entries : 2

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

Valsartan XIC from 14-03-04_TOF_BfG_pos_2014-KW10_Donau_04-03-14_05.wiff (sample 1)



Oberflächenwasser Donau

Transformation Tree

DAIOS 2.0

Search Edit User administration Edit User Properties Contact Logout

Mass Meta Index Search Results

Search Clear

Name
valsartan

CAS

Chemical Formula

History Clear

Meta: Name = valsartan
Valsartan

Entries found: 4 Visible 4

type to filter

Name	CAS	Exact mass	Molare mass
Valsartan	137862-53-4	435.2270	435.52

Details Ms/Ms Transformation Tree

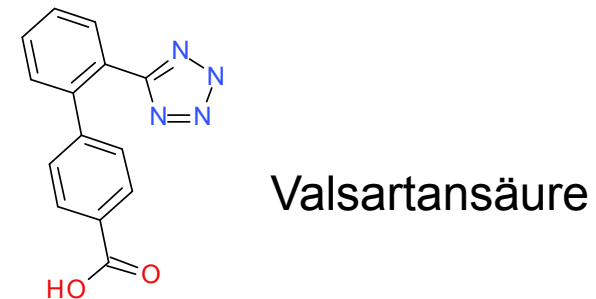
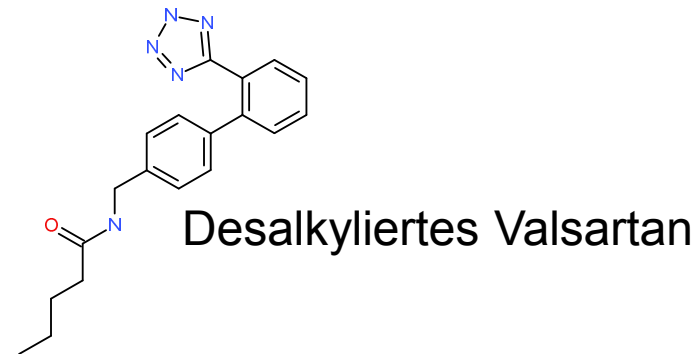
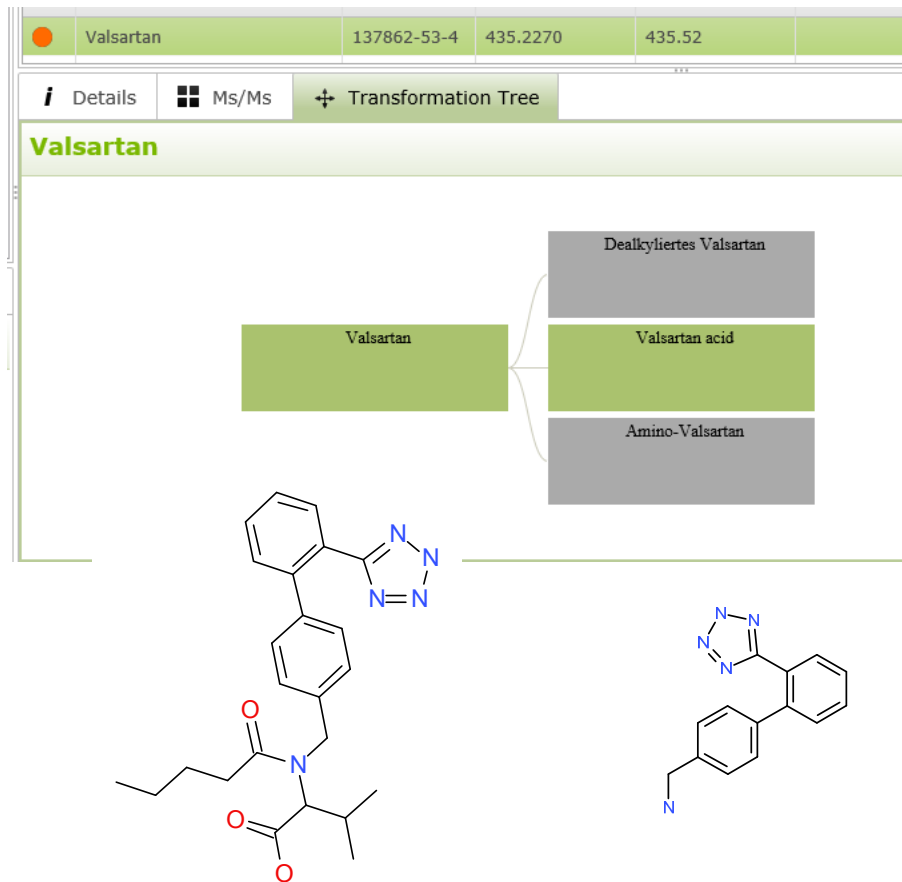
Valsartan ? Info

```

graph LR
    Valsartan[Valsartan] --- Dealkyliertes_Valsartan[Dealkyliertes Valsartan]
    Valsartan --- Valsartan_acid[Valsartan acid]
    Valsartan --- Amino_Valsartan[Amino-Valsartan]
  
```

Transformationsprodukte

Valsartan



Valsartansäure

DAIOS 2.0

Search Edit User administration Edit User Properties Contact Logout

Mass Meta Index Search Clear

Name: valsartan

CAS:

Chemical Formula:

History Clear

Meta: Name = valsartan

Valsartan

Valsartan acid

Search Results

Entries found: 4 Visible 4

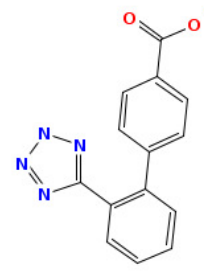
type to filter

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	C ₁₄ H ₁₀ N ₄ O ₂
Status	Incomplete (red)
Source	
Exact mass	266.0803
Molare mass	266.26



The chemical structure of Valsartan acid is shown, featuring a 1,2,4-triazole ring system connected to a biphenyl moiety, which is further substituted with a carboxylate group (COO⁻).

MS/MS Fragmente Valsartansäure

DAIOS 2.0

Search Edit User administration Edit User Properties Contact Logout

Mass Meta Index Search Clear

Name
valsartan

CAS

Chemical Formula

History Clear

Meta: Name = valsartan
Valsartan
Valsartan acid

Search Results

Entries found: 4 Visible 4

type to filter

Details Ms/Ms Transformation Tree

Valsartan acid

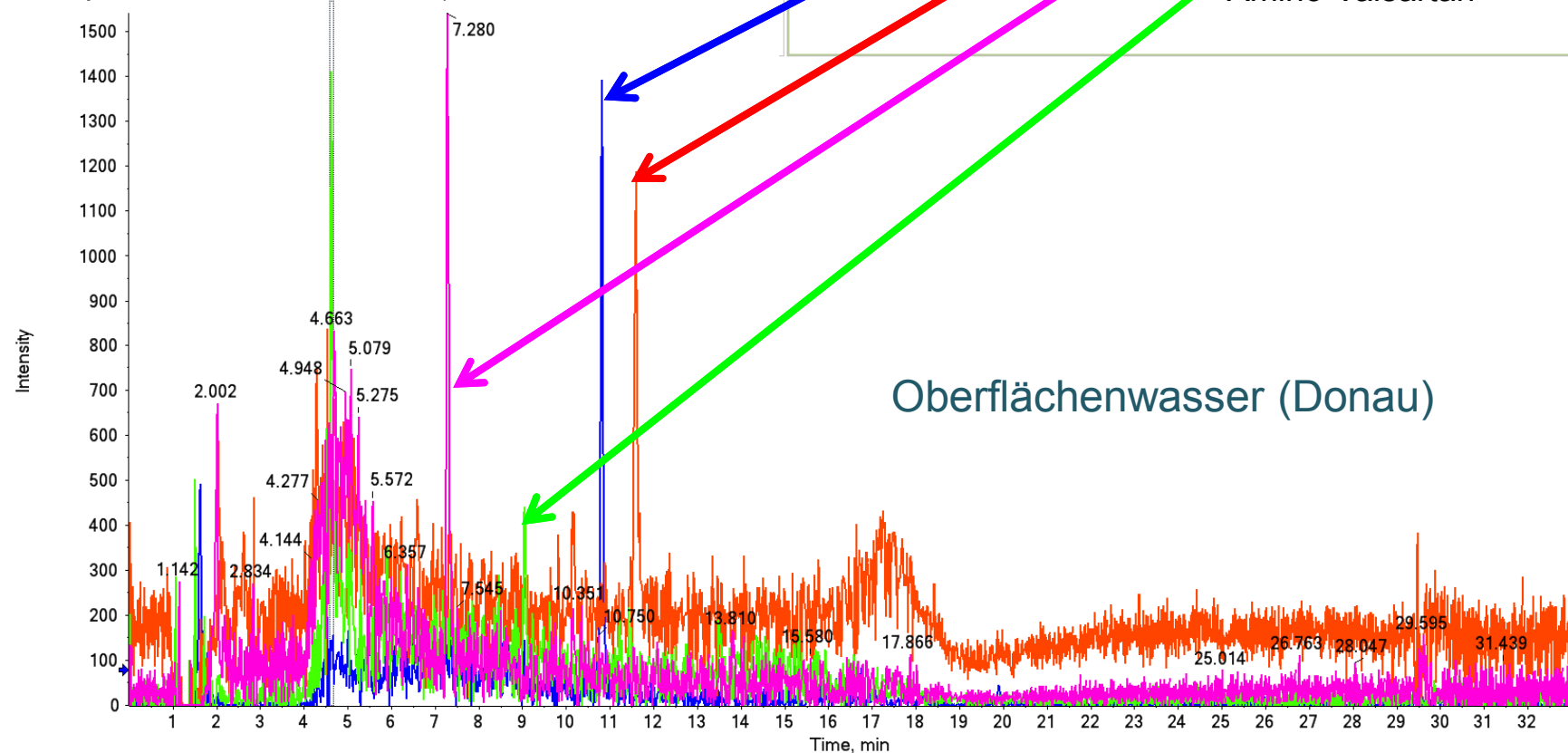
Precursor entries : 2

Property	Value	Fragments
Precursor Mass	265.0731	165.0000
Ion	-H	193.0000

Property	Value	Fragments
Precursor Mass	267.0876	206.0000
Ion	+H	178.0000
		151.0000

XICs von Valsartan und seinen Transformationsprodukten

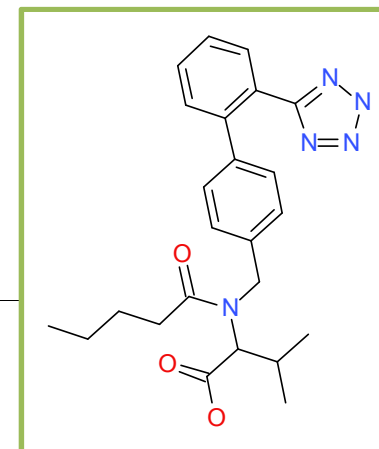
- Valsartan XIC from 14-03-04_TOF_BfG_pos_2014-KW10_Donau_04-03-14_05.wiff (sample)
- Valsartansäure XIC from 14-03-04_TOF_BfG_pos_2014-KW10_Donau_04-03-14_05.wiff (sa)
- Aminovalsartan XIC from 14-03-04_TOF_BfG_pos_2014-KW10_Donau_04-03-14_05.wiff (sa)
- desalkyl. Valsartan XIC from 14-03-04_TOF_BfG_pos_2014-KW10_Donau_04-03-14_05.wiff



Oberflächenwasser (Donau)

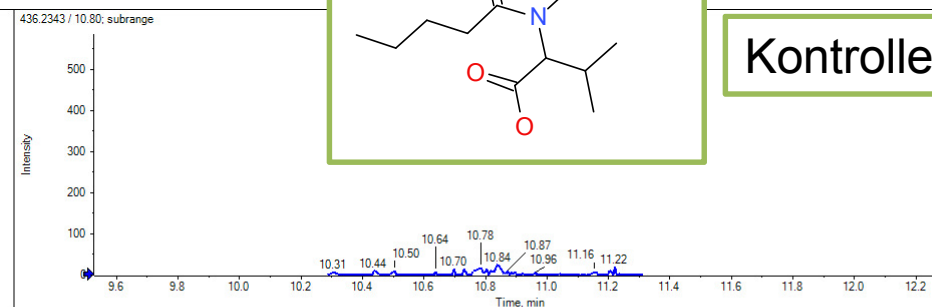
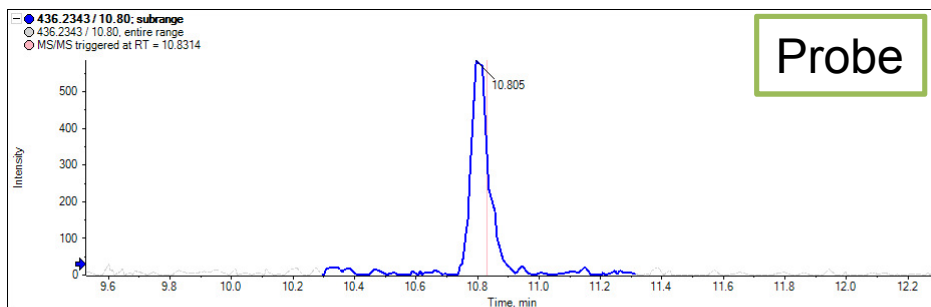
Identifizierung mit DAIOS IDA-MS/MS

Valsartan



Probe

Kontrolle



MasterView

New Session

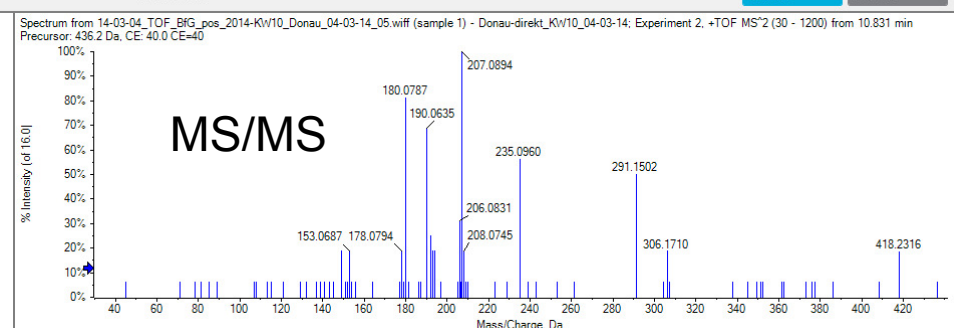
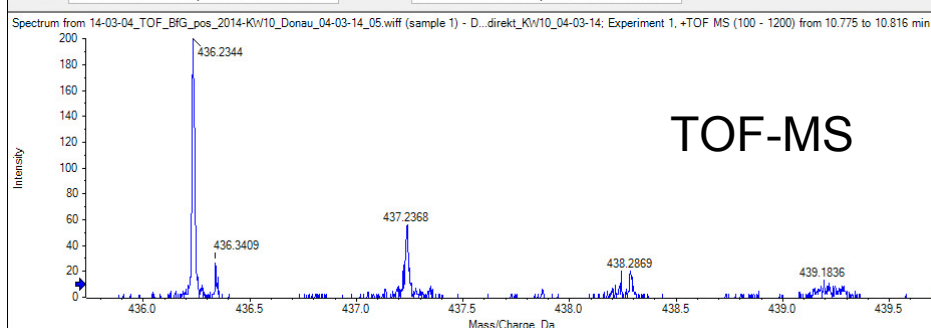
CT	Wiff file Name	Sample Name	Number of positive results	Name	Formula	Isotope	Mass (Da)	Adduct	Int. Std.	Extraction Mass (Da)	Width (Da)	Width (ppm)	Found At RT (min)	Formula Finder Result	Fragment Mass (Da)	Expected RT (min)	RT Width (min)	Found At Mass (Da)	Error (ppm)	Isotope Ratio Difference (%)
✓	14-03-04_TOF_BfG_pos_2014-KW10_Donau_04-03-14_05	Sample 1	9532	435.8099 / 17.82		0	435.80992			435.80992	0.005	11.473	17.84	No Formula Found		17.82	1	435.80988	-0.1	
✓	14-03-04_TOF_BfG_pos_2014-KW10_OuL-Injektion_01	Sample 1	7436	436.0924 / 4.79		0	436.09235			436.09235	0.005	11.465	4.6	C17H25NO6S3		4.79	1	436.09146	-2	
				436.1248 / 4.90		0	436.12479			436.12479	0.005	11.465	4.69	C25H17N5OS		4.9	1	436.12249	-5.3	
				436.1288 / 4.81		0	436.12881			436.12881	0.005	11.465	4.74	C21H25NO5S2		4.81	1	436.12454	-9.8	
				436.1636 / 5.16		0	436.16357			436.16357	0.005	11.464	4.99	C23H17N9O		5.16	1	436.16275	-1.9	
				436.2343 / 10.80		0	436.23427			436.23427	0.005	11.462	10.81	C24H29N5O3		10.8	1	436.23443	0.4	
				436.3413 / 9.61		0	436.34134			436.34134	0.005	11.459	9.61	C26H45NO4		9.61	1	436.34148	0.3	
				436.3415 / 2.52		0	436.34151			436.34151	0.005	11.459	2.84	C19H45N7O2S		2.52	1	436.34177	0.6	
				436.3416 / 6.08		0	436.34161			436.34161	0.005	11.459	6.13	C19H45N7O2S		6.08	1	436.34239	1.8	

Positive result: equal or better ✓✓✓●●●0

Sample: 14-03-04_TOF_BfG_pos_2014-KW10_... Control: 14-03-04_TOF_BfG_pos_2014-KW10_...

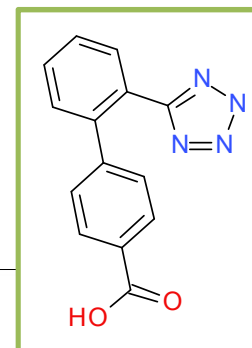
Rows 9720

Process Cancel



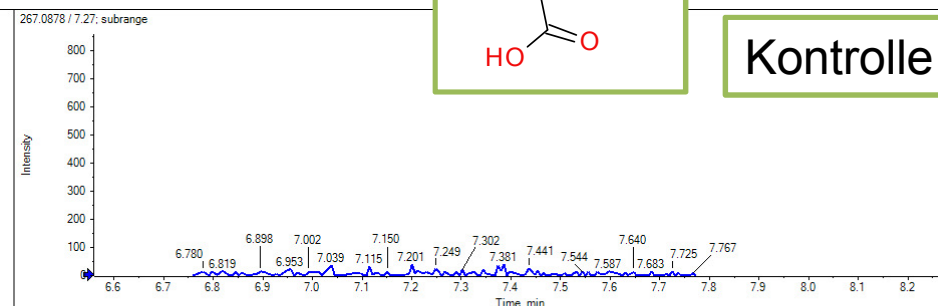
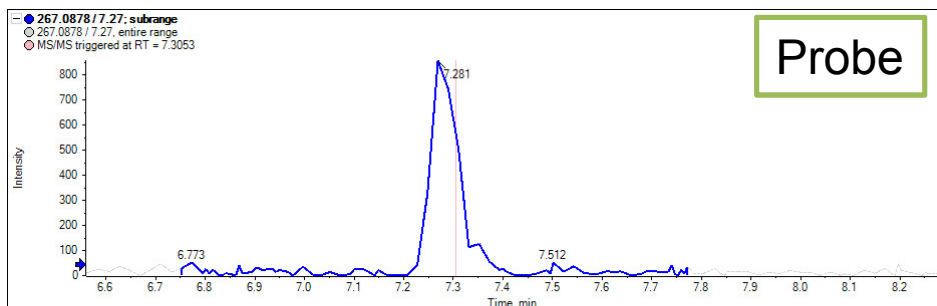
Identifizierung mit DAIOS IDA-MS/MS

Valsartan Acid



Probe

Kontrolle



MasterView

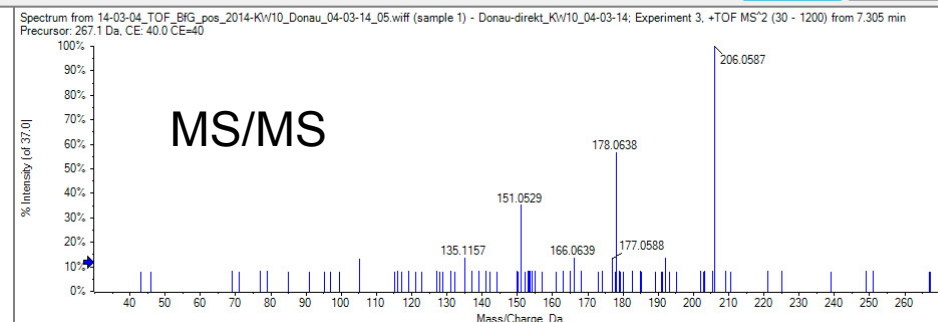
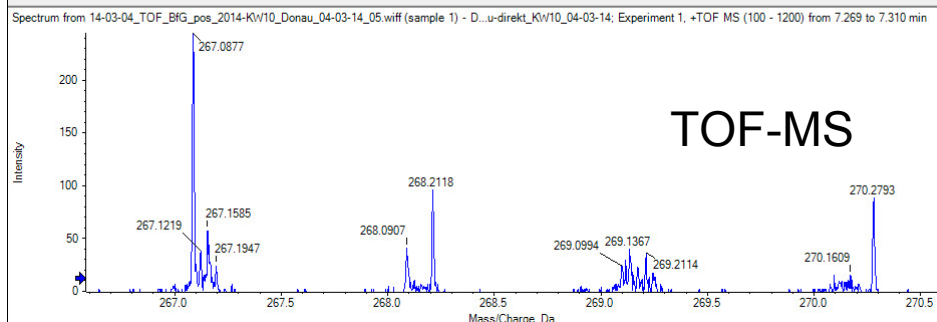
New Session

CT	Wiff file Name	Sample Name	Number of positive results	Name	Formula	Isotope	Mass (Da)	Adduct	Int. Std.	Extraction Mass (Da)	Width (Da)	Width (ppm)	Found At RT (min)	Formula Finder Result	Fragment Mass (Da)	Expected RT (min)	RT Width (min)	Found At Mass (Da)	Error (ppm)	Isotope Ratio Difference (%)	F (t)
✓	14-03-04_TOF_BfG_pos_2014-KW10_Donau_04-03-14_05	Sample 1	9532	266.9974 / 3.52		0	266.99742		266.99742	0.005	18.727	3.73	3.73	C8H10O6S2		3.52	1	266.9992	6.7		
✓	14-03-04_TOF_BfG_pos_2014-KW10_0uL-Injektion_01	Sample 1	7436	266.9985 / 2.50		0	266.99849		266.99849	0.005	18.727	2.84	2.84	C12H2N4O2S		2.5	1	266.99752	-3.6		
✓				266.9998 / 4.24		0	266.99977		266.99977	0.005	18.727	3.75	3.75	C8H10O6S2		4.24	1	266.99877	-3.7		
✓				267.0867 / 4.90		0	267.08666		267.08666	0.005	18.721	4.96	4.96	No Formula Found		4.9	1	267.08571	-3.6		
✓				267.0878 / 7.27		0	267.08779		267.08779	0.005	18.72	7.28	7.28	C14H10N4O2		7.27	1	267.08768	-0.4		
✓				267.1209 / 6.52		0	267.12094		267.12094	0.005	18.718	6.16	6.16	C10H22N2O2S2		6.52	1	267.12168	2.8		
✓				267.1210 / 5.20		0	267.12102		267.12102	0.005	18.718	5.29	5.29	C10H14N6O3		5.2	1	267.12009	-3.5		
✓				267.1215 / 5.95		0	267.12151		267.12151	0.005	18.718	5.95	5.95	C14H18O5		5.95	1	267.12157	0.2		
✓				267.1308 / 4.65		0	267.13075		267.13075	0.005	18.717	4.65	4.65	No Formula Found		4.65	1	267.13172	3.6		

Positive result: equal or better ✓✓✓●●●0

Sample: 14-03-04_TOF_BfG_pos_2014-KW10_... Control: 14-03-04_TOF_BfG_pos_2014-KW10_... Rows 9720

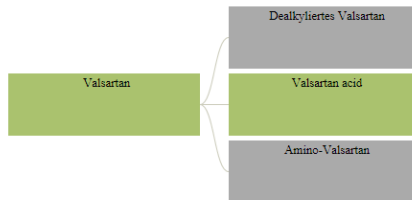
Process Cancel



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

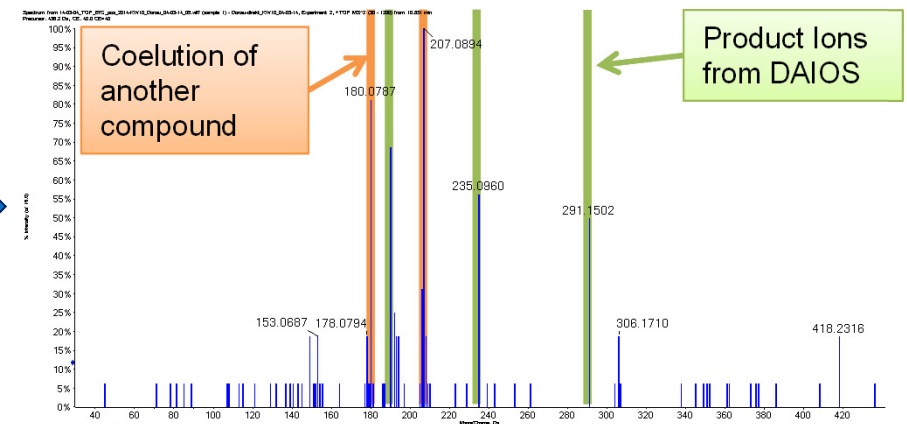
Database Hit
Valsartan mit
MS/MS-Data

i Details			Ms/Ms		Transformation Tree	
Valsartan						
Precursor entries : 2						
Property	Value		Fragments			
Precursor Mass	434.2198		350.0000			
Ion	-H		178.0000			
Precursor Mass	436.2343		207.0000			
Ion	+H		291.0000			
			235.0000			
			190.0000			
			362.0000			

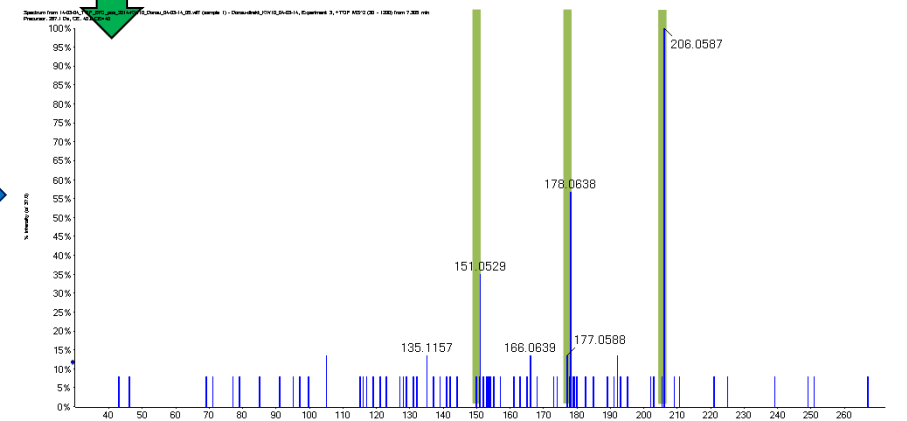


TP von DAIOS:
Valsartan Acid
mit MS/MS-Data

i Details			Ms/Ms		Transformation Tree	
Valsartan acid						
Precursor entries : 2						
Property	Value		Fragments			
Precursor Mass	265.0731		165.0000			
Ion	-H		193.0000			
Precursor Mass	267.0876		206.0000			
Ion	+H		178.0000			
			151.0000			



Database assisted identification
of unknown compounds



Quantitative Bestimmung von Valsartan und Valsartansäure

XIC of +MRM(18 pairs): 267.000/206.000 Da ID: Valsartan Acid-1 from Sample 53 (Donau) of 14-03-03_Sartane_MV_LWVAesser_Lu.wiff (Tur...

Max. 2840.0 cps.

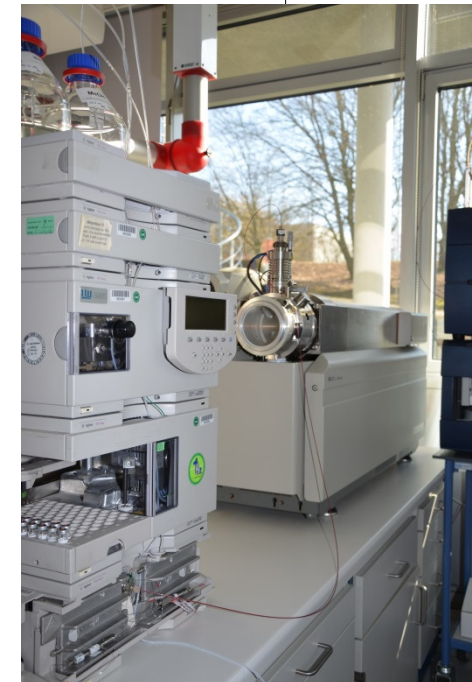
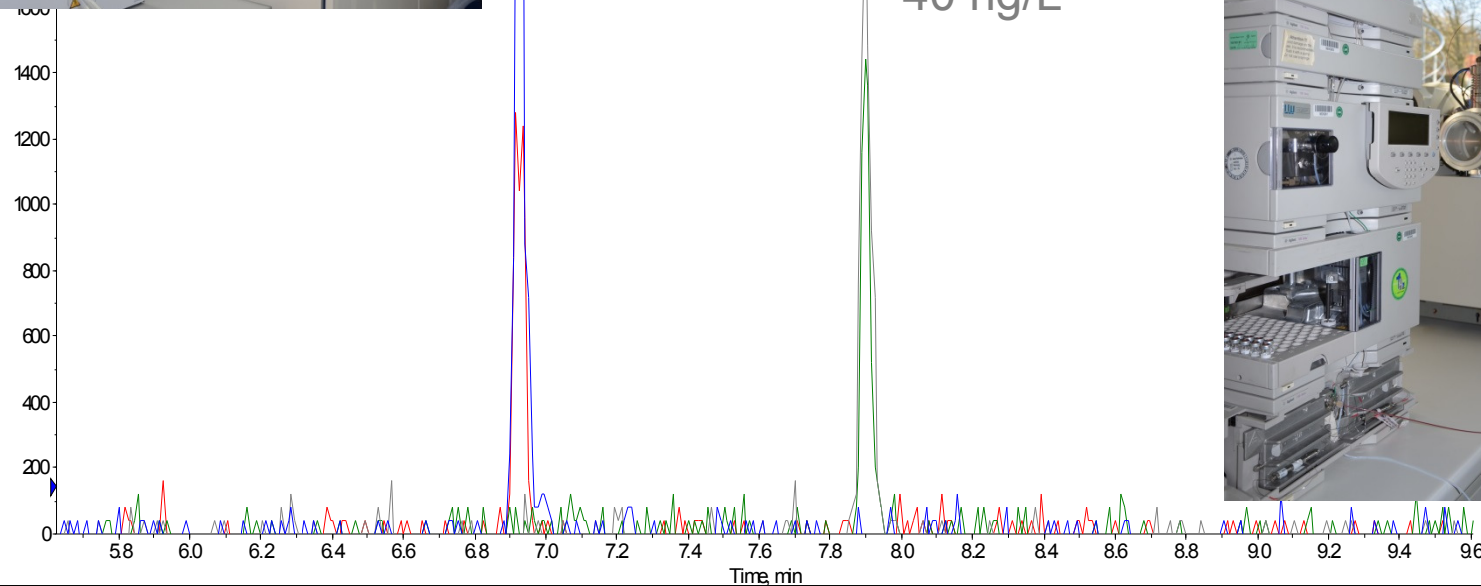


6.93

Valsartansäure
100 ng/L

Donau

Valsartan
40 ng/L



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

DAIOS Login

DAIOS

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Vielen Dank für Ihre Aufmerksamkeit