



Network of reference laboratories and related organisations for monitoring and bio-monitoring of emerging environmental pollutants

NORMAN MassBank

Current state and future activities

Tobias Schulze (UFZ)
Dübendorf (17 Sep 2014)



eawag
aquatic research .o.o



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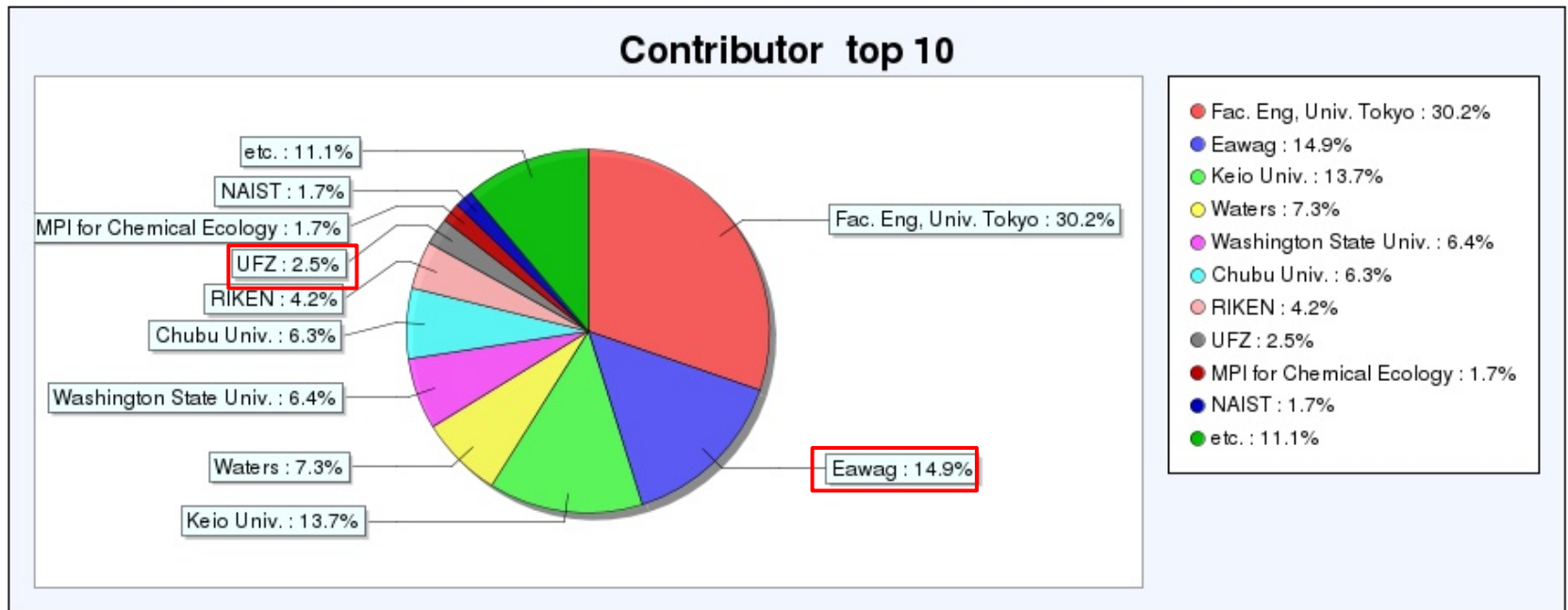
Main goal of NORMAN is to enhance the exchange of knowledge on emerging environmental samples

- Many different laboratories (with different instruments,...)
- Focus on different substances and classes
- Not each member has each reference standard
- „Emerging compounds“ → not yet widely known, not yet in data bases
- Many substances transform in the environment → no standards, no spectra

The main goal of NORMAN MassBank is to improve identification of environmentally relevant substances!



Current content of NORMAN MassBank



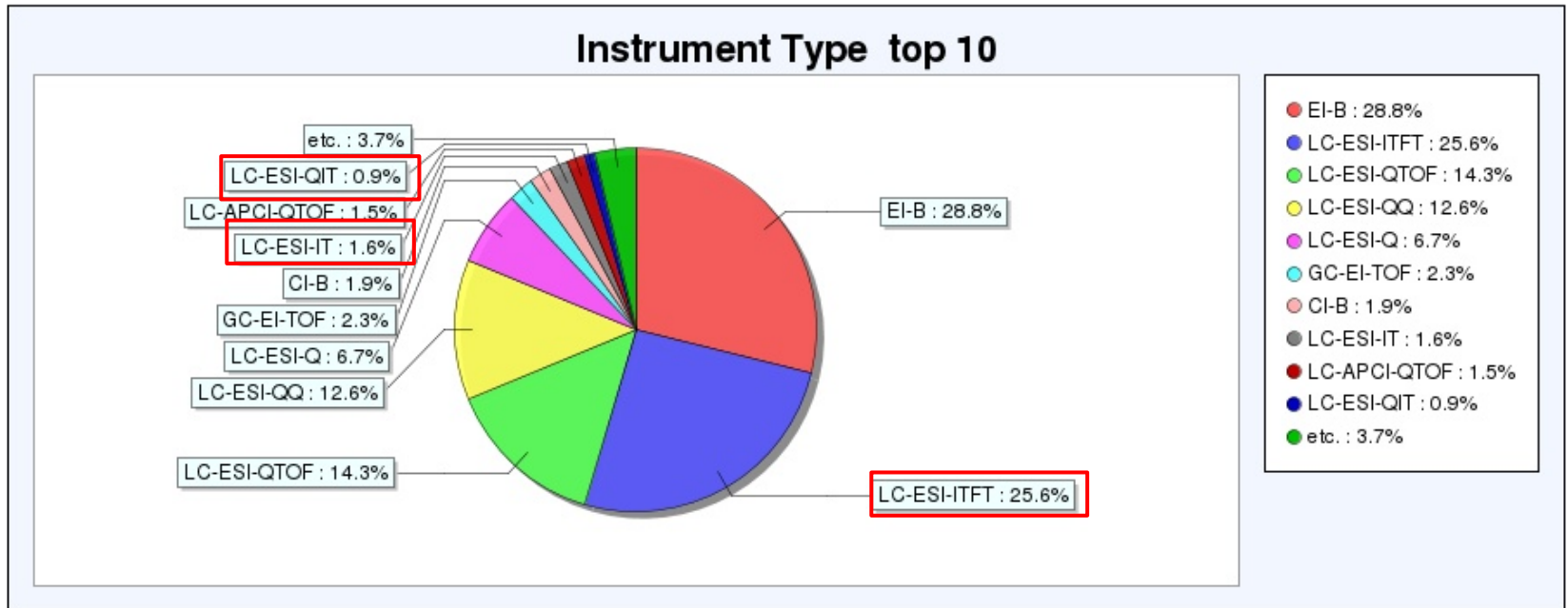
40,953 spectra from different instruments (~15.000)

7,293 mass spectra from NORMAN members (~715)

Contributions from NORMAN member institutes



Current content of NORMAN MassBank



Contributions from NORMAN members have increased the proportion of LC-MS/MS data available in MassBank

 Contributions from NORMAN member institutes



Special features of MassBank.eu

Literature spectra, tentative and additional spectra

- Cannot generate „match values“ if neither spectra are in the library
- Move towards exchanging tentatively identified spectra between institutes
- Provide „Supporting Information“ for publications → repository functions

Contributor	: Athens Univ. (0)	Boise State Univ. (4)	Chubu Univ. (2,563)
	Eawag (6,106)	Eawag Additional Specs (50)	FIOCRUZ (597)
	Fac. Eng. Univ. Tokyo (12,379)	Fukuyama Univ. (340)	GL Sciences Inc. (174)
	IPB Halle (528)	JEOL Ltd. (45)	Kazusa (273)
	Keio Univ. (5,619)	Kyoto Univ. (185)	Literature Specs (39)
	MPI for Chemical Ecology (691)	Metabolon (149)	NAIST (676)
	NORMAN MassBank (0)	Nihon Univ. (365)	Osaka MCHRI (20)
	Osaka Univ. (449)	PFOS research group (413)	RIKEN (1,719)
	Tottori Univ. (16)	UFZ (1,030)	UFZ Additional Specs (107)
	UOEH (35)	Univ. Connecticut (510)	Univ. Toyama (253)
	Washington State Univ. (2,626)	Waters (2,992)	



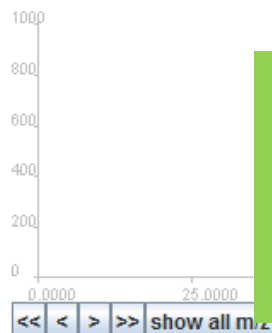
Example of an additional spectra

MassBank Record: ETS00107

[Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Browser](#) | [Batch](#) | [Browse](#) | [Index](#) | MassBank ID:

1H-Benzotriazole-4-carboxylic acid (Tentative); LC-ESI-ITFT; MS2; 80-110; R=7500; [M+H]⁺

Mass Spectrum



Chemical Structure

Access restricted folders could be provided for review purposes to browse record files

ACCESSION: ETS00107

RECORD_TITLE: 1H-Benzotriazole-4-carboxylic acid (Tentative); LC-ESI-ITFT; MS2; 80-110; R=7500; [M+H]⁺

DATE: 2014.06.27

AUTHORS: Huntscha S, Schymanski E, Hofstetter TB, Spahr S, Hollender J, Department of Environmental Chemistry, Eawag

LICENSE: CC BY-SA

COPYRIGHT: Copyright (C) 2014 Eawag, Duebendorf, Switzerland

PUBLICATION: Huntscha S, Hofstetter TB, Schymanski E, Spahr S, Hollender J (2014) Environ. Sci. Technol, 48:4435-4443, DOI: 10.1021/acs.est.5b01001

COMMENT: CONFIDENCE TENTATIVELY IDENTIFIED ONLY! Most likely isomer

COMMENT: Source; 164m0445a_MSMS.txt

COMMENT: Structure/data is 1H-Benzotriazole-4-carboxylic acid; other isomers possible (but less likely)



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Linking to Gazetter service

ACCESSION: ETS00106
RECORD_TITLE: 1H-Benzotriazole TP10 (Tentative); LC-ESI-ITFT; MS2; 80-110; R=7500; [M+H]⁺
DATE: 2014.06.27
AUTHORS: Huntscha S, Schymanski E, Hofstetter TB, Spahr S, Hollender J, Department of Environmental Chemistry, Eawag
LICENSE: CC BY-SA
COPYRIGHT: Copyright (C) 2014 Eawag, Duebendorf, Switzerland
PUBLICATION: Huntscha S, Hofstetter TB, Schymanski E, Spahr S, Hollender J (2014) Environ. Sci. Technol, 48:4435-4443, DOI:10.1021/es4
COMMENT: CONFIDENCE MOLECULAR FORMULA IDENTIFIED ONLY!
COMMENT: Source: 156m0396b_MSMS.txt

CH\$NAME: 1H-Benzotriazole TP10 (Tentative)
CH\$NAME: 1H-Benzotriazole Transformation Product 10 (TP10)
CH\$COMPOUND_CLASS: N/A; Biotransformation Product
CH\$FORMULA: C5HSN3O3
CH\$EXACT_MASS: 155.0330
CH\$SMILES: N/A
CH\$IUPAC: N/A

SP\$SAMPLE: LOCATION [GAZ:00064414](#) [GAZ:00113795](#)

~~SP\$SAMPLE: COMMENT: 4-Me-BT samples collected from Duebendorf (GAZ:00113795), 4Me- and 5-Me-BT samples from Regensdorf (GAZ:00064414)~~

EMBL-EBI 

Ontology Lookup Service

- OLS Home
- Documentation
 - Project
 - Publications
- Developer Resources
 - Download
 - Implementation Overview
 - Javadoc
 - Webservice documentation
- Contact Us

Enter Ontology Term

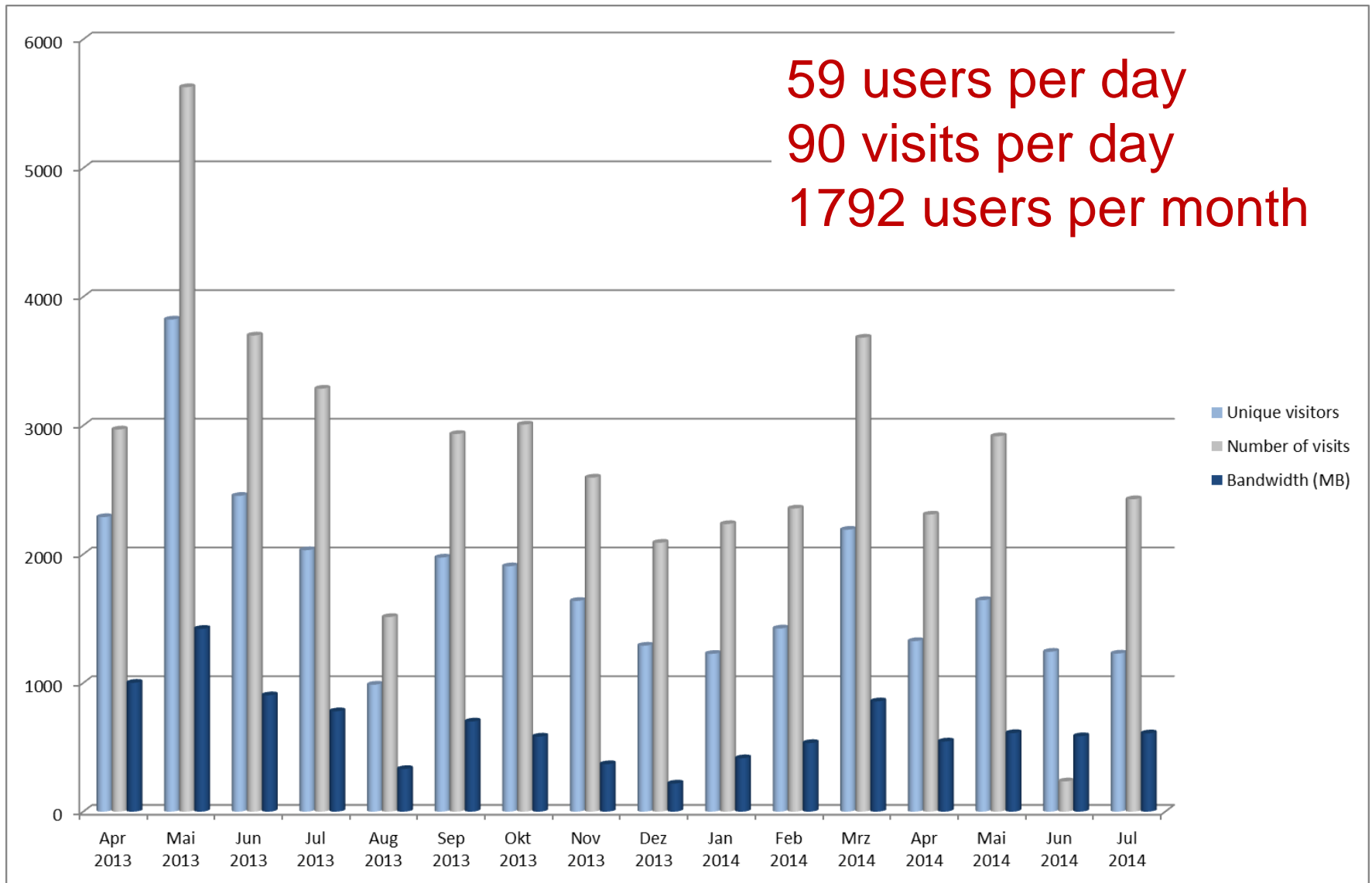
Search Ontology:

Term Name: (Include obsolete terms) Term ID:


Additional Information:


definition	A municipality in the district of Dielsdorf of the canton of Zurich in Switzerland.
xref_definition	url:http://en.wikipedia.org/wiki/Regensdorf

Frequency of server usage

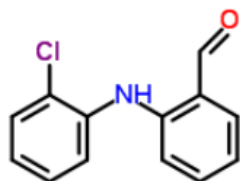



MassBank as ChemSpider data source

About More Searches Web APIs Help My  Depositions

Search term: "2-[2-(chlorophenyl)amino]benzaldehyde" (Found by approved synonym) 

2-[2-(chlorophenyl)amino]benzaldehyde



 2D 3D Save Zoom

ChemSpider ID: 26001359
Molecular Formula: C₁₃H₁₀ClNO
Average mass: 231.677994 Da
Monoisotopic mass: 231.045 Da
▼ Systematic name
2-(2-chloroanilino)benzaldehyde
▶ SMILES and InChIs
▶ Cite this record
Wikibox
Embed
Watch this record
Manage data slice

MassBank is a data source of ChemSpider

- Enhances visibility
- Includes all opendata records (CC-BY-SA)

▼ Data Sources

All Data Sources Metabolism Data Tox/Envir. Data Personal Data Publication Spectral Data

Data Source

External ID(s)

MassBank

UF409001, UF409002, UF409003, UF409004



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Linkage of MassBank and Stoff-Ident

The main goal of Stoff-Ident is to provide a database for aquatic-relevant pollutants

REACH registered compounds

Other registered compounds (e.g pesticide, biocides, pharmaceuticals)

WFD and river basin specific compounds

Transformation products

The main goal of linking MassBank and Stoff-Ident is to improve the identification of those compounds

Stoff-Ident links to mass spectra provided in MassBank

Stoff-Ident should feed back on missing compounds

Ranking on most important compounds (e.g. toxicity predictions) to prioritise spectra generation

<http://risk-ident.hswt.de/pages/en/tasks/wp-1-database.php?lang=EN>

MassBank in Data Citation Index

Save to EndNote online Add to Marked List Back to List 1 of 1

MassBank.

By: Nishioka, Takaaki; Oda, Yoshiya; Arita, Masanori; Neumann, Steffen; Schulze, Tobias; Schymanski, Emma L

MassBank
Source URL: <http://www.massbank.jp/?lang=en>
Viewed Date: 04 Apr 2013
Published: 2006

Abstract

MassBank is the first public repository of mass spectral data designed for sharing amongst the scientific community. MassBank data are useful for the chemical identification and structure elucidation of chemical compounds detected by mass spectrometry. Project

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Funding

Close funding text
MassBank was supported by the Grant for Life Science Databases from Institute for Bioinformatics Research and Development, Japan Science and Technology Agency (JST) 10.

Categories and Classification

Research Areas: Chemistry
Web of Science Category: Chemistry, Analytical

Document Information

Document Type: Repository
Language: English
Accession Number: DRCI:DATA2013097003561029

Citation Network

0 Times Cited
0 Cited References
[Create Citation Alert](#)
(data from Web of Science™ Core Collection)

All Times Cited Counts

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0 in SciELO Citation Index

This record is from:
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If you would like to improve the quality of the data in this record, please suggest a correction.

MassBank is recognised

Screenshot by Megan Force (Thomson-Reuters)

MassBank in Data Citation Index

The screenshot shows a record page on the Web of Science platform. The main title is "L-Glutamine; GC-EI-QQ; MS; 3 TBDMS; RT:916.38 sec". The record is from the MassBank repository, authored by Dempo, Y; Bamba, T; Fukusaki, E. The source URL is <http://www.massbank.jp/jsp/FwdRecord.jsp?id=OUF01015>, viewed on 24 Jul 2013, and published in 2013. The abstract states: "This file contains mass spectral peak data for a compound analyzed by one of several contributing research groups. Copyright: Funkusaki Lab. in Osaka Univ." The author information lists an address at Osaka University, Engineering Department, Japan. The record is classified under Spectroscopy. Document information includes a data set type in English with accession number DRCI:DATA2014022003747151. Other information includes instrument GC-EI-QQ and formula C5H10N2O3, with 0 cited references in the Data Citation Index.

WEB OF SCIENCE™ THOMSON REUTERS™

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L-Glutamine; GC-EI-QQ; MS; 3 TBDMS; RT:916.38 sec

From Repository: [MassBank](#)
By: Dempo, Y; Bamba, T; Fukusaki, E

MassBank
Source URL: <http://www.massbank.jp/jsp/FwdRecord.jsp?id=OUF01015>
Viewed Date: 24 Jul 2013
Published: 2013

Abstract

This file contains mass spectral peak data for a compound analyzed by one of several contributing research groups. Copyright: Funkusaki Lab. in Osaka Univ.

Author Information

Addresses:
1. Osaka University, Engineering Department, Japan

Categories / Classification

Research Areas: Spectroscopy
Web of Science Category: Spectroscopy

Document Information

Document Type: Data set
Language: English
Accession Number: DRCI:DATA2014022003747151

Other Information

Miscellaneous: instrument: GC-EI-QQ; formula: C5H10N2O3
Cited References in Data Citation Index: 0

Citation Network

0 Times Cited
0 Cited References
[Create Citation Alert](#)
(data from Web of Science™ Core Collection)

All Times Cited Counts

0 in All Databases
0 in Web of Science Core Collection
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0 in Data Citation Index
0 in SciELO Citation Index

This record is from:
Data Citation Index™

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Suggest a correction
If you would like to improve the quality of the data in this record, please [suggest a correction](#).

Additional information is needed to connect WLAN-GLOBAL.

Screenshot by Megan Force (Thomson-Reuters)

- Commitment with UFZ IT management for a long-term perspective of MassBank hosting (agreement for 3 years)
- Migration of server operating system from openSUSE 12 to Ubuntu Server 14.04 LTS (long-term updates, SVN release of opendata records)
- Relaunch of NORMAN MassBank web-site
- Interlinkage of MassBank and Stoff-Ident / ChemSpider



- Updating more spectra from current contributors (esp. Eawag, UFZ)
- Updating spectra from new contributors
 - Contributions from MassBank workshop
 - University of Gdansk announced interest to contribute MS of some TPs of pharmaceuticals
- NORMAN MassBank web-site will be more narrative regarding activities (similar to MassBank.jp)
- SVN release of records and mol-files of openData records (CC-BY-SA)

Funding (EU side):

- NORMAN network and in-kind contributions
- Eawag Discretionary Funds
- UFZ for funding Erik Müller

MassBank.jp

- Prof. Takaaki Nishioka, NAIST, Japan
- Prof. Masanori Arita, NIG, Japan

MassBank.eu

- Emma Schymanski, Michael Stravs, Eawag
- Steffen Neumann, IPB Halle
- Erik Müller, Guido Schramm, Tobias Schulze, UFZ

All contributors to MassBank



Thank you for your attention!

Questions or comments?

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<http://massbank.eu/MassBank>



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