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)

HELMHOLTZ CENTRE FOR ENVIRONMENTAL RESEARCH – UFZ

NORMAN Network and MassBank

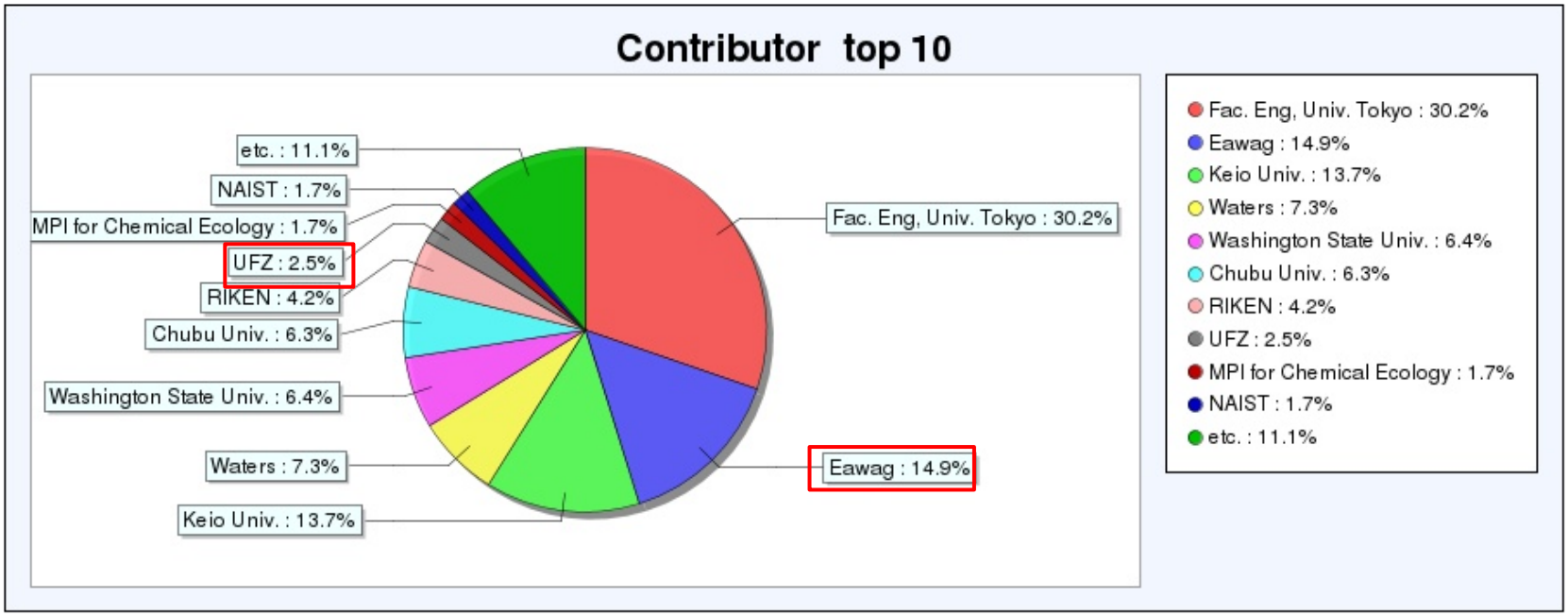
Main goal of NORMAN is to enhance the exchange of knowledge on emerging environmental samples

- 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 environmentaly relevant substances!

MassBank eawag aquatic research norman HELMHOLTZ CENTRE FOR ENVIRONMENTAL RESEARCH – UFZ

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

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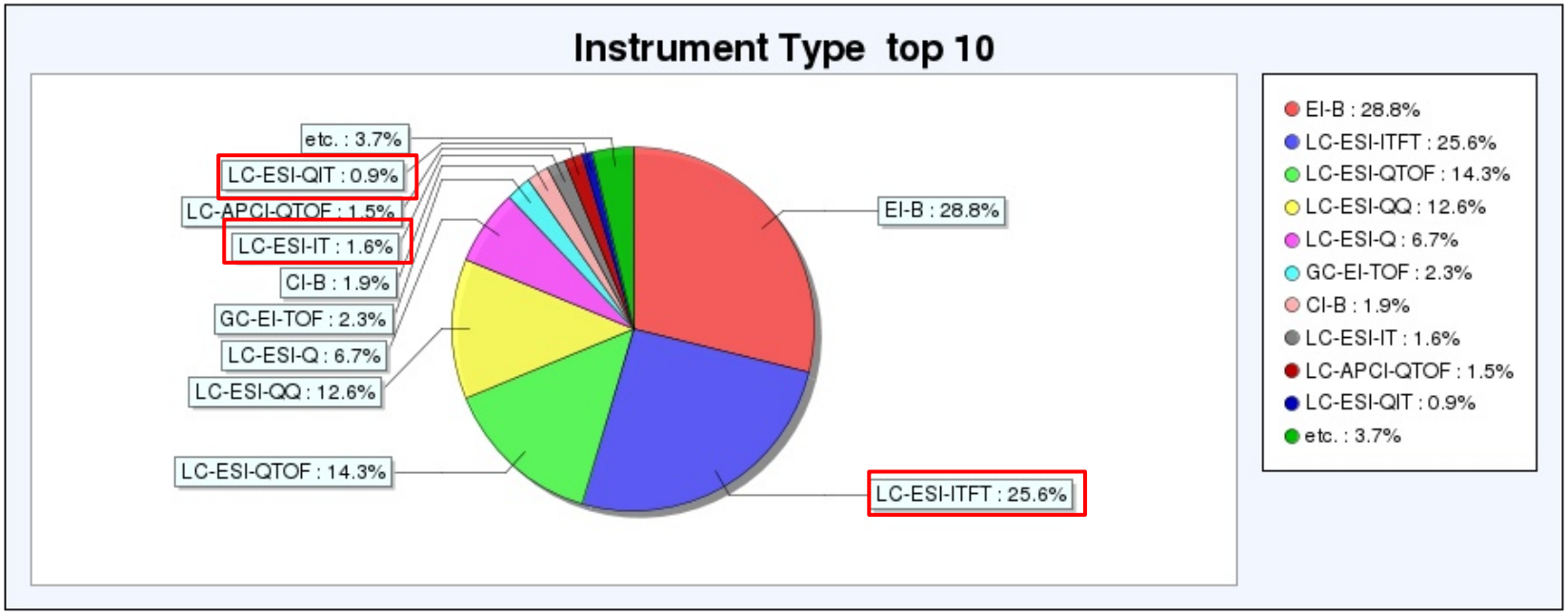
Current content of NORMAN MassBank



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, tentatative and additional specta

- 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)	

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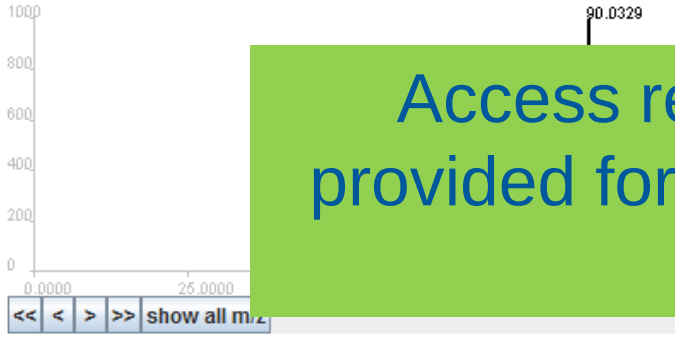
Example of an additional spectra

MassBank Record: ETS00107

Home | Spectrum | Quick | Peak | Substructure | Browser | Batch | Browse | Index | MassBank ID: Go

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, DO
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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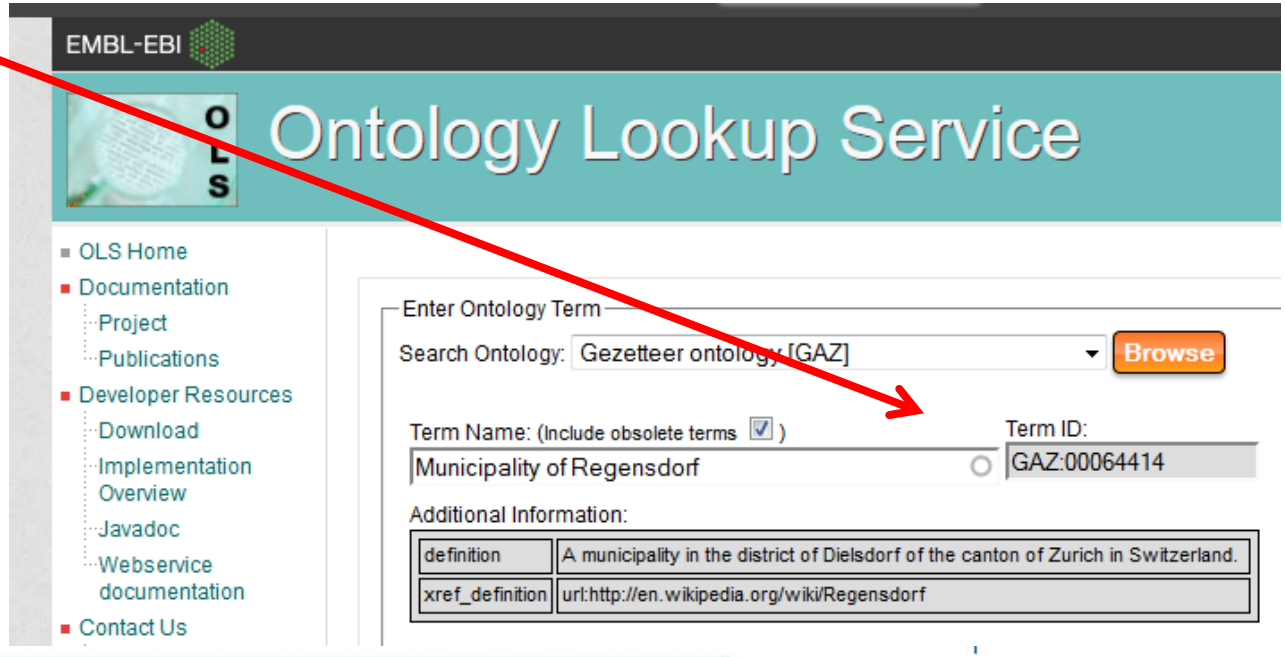
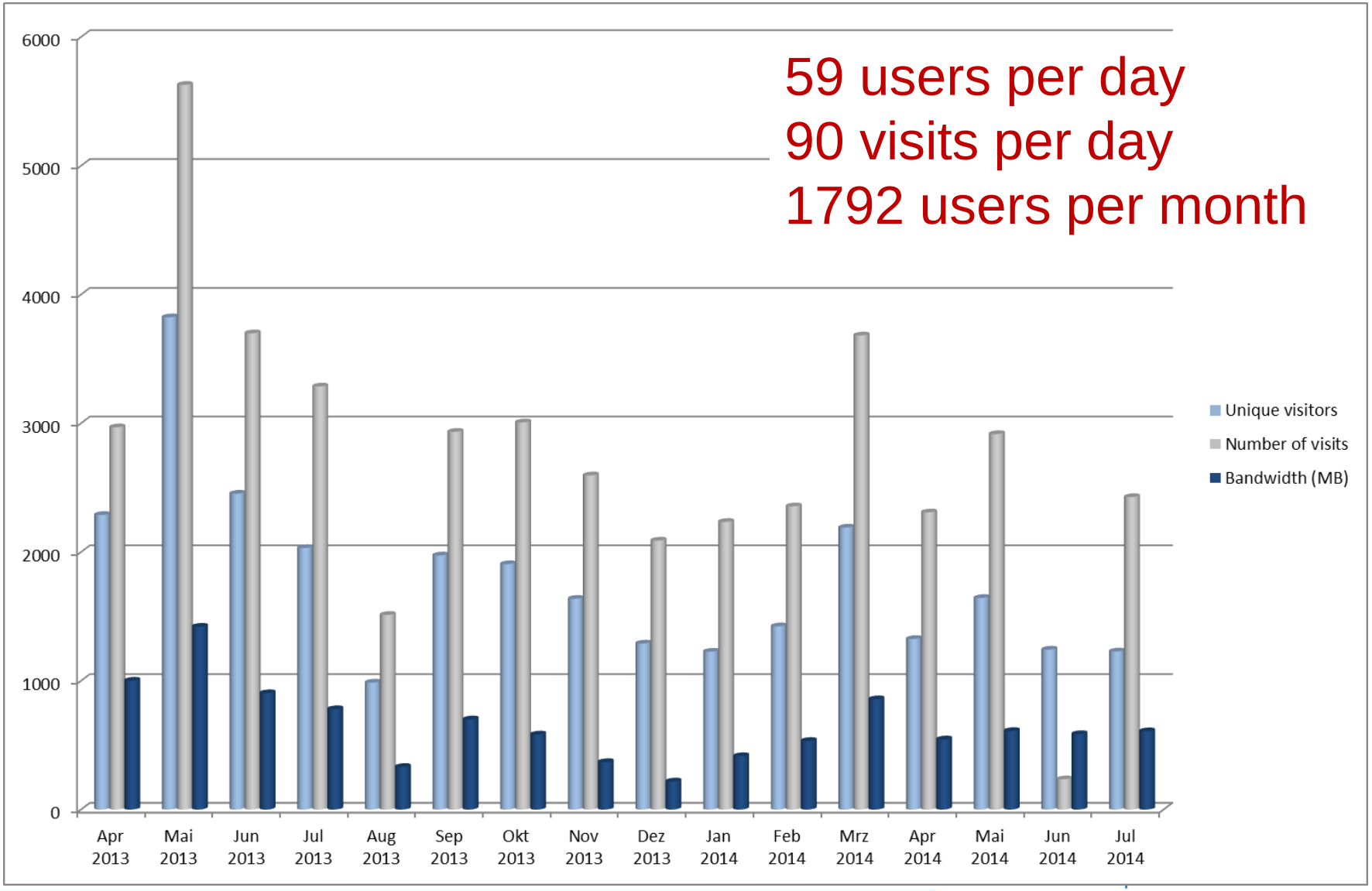
Linking to Gazetter service

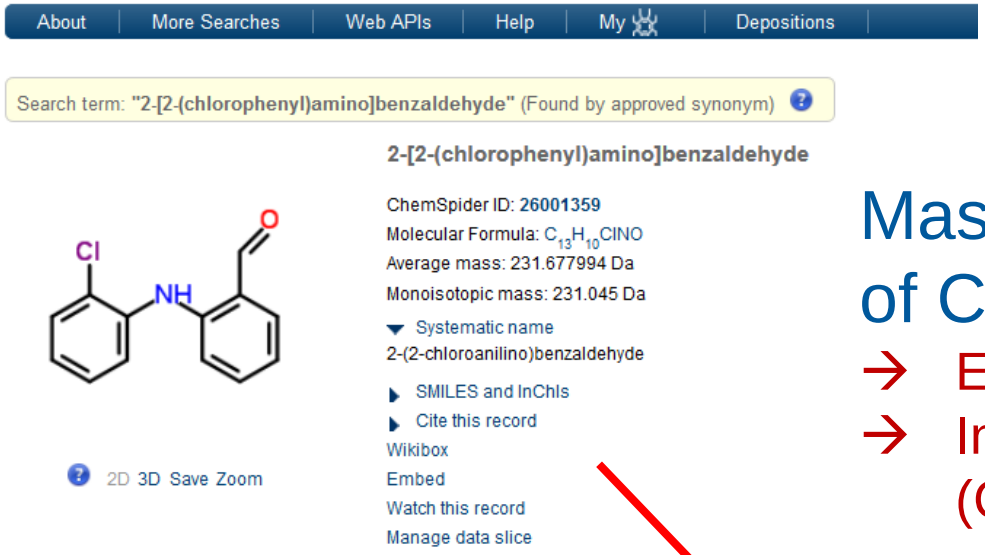
```
ACCESSION: ETS00106
RECORD_TITLE: 1H-Benzotriazole TP10 (Tentative); LC-ESI-ITFT; MS2; 80-110; R=7500; [M+H]+
DATE: 2014.06.27
AUTHORS: Huntscha S, Schymanski E, Hofstetter TB, Spahr S, Hollender J, Department of Environmental Chemistry, Eawag
LICENSE: CC BY-SA
COPYRIGHT: Copyright (C) 2014 Eawag, 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: C5H5N3O3
CH$EXACT_MASS: 155.0330
CH$SMILES: N/A
CH$IUPAC: N/A

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



Frequency of server usage



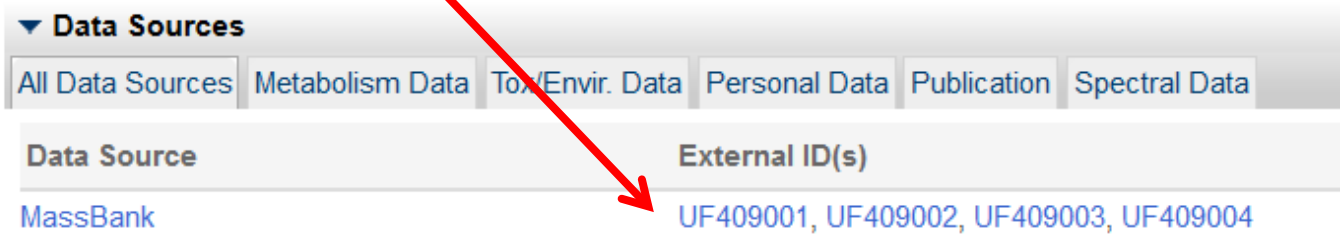
MassBank as ChemSpider data source



MassBank is a data source of ChemSpider

→ Enhances visibility

→ Includes all opendata records (CC-BY-SA)



Linkage of MassBank and Stoff-Ident

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

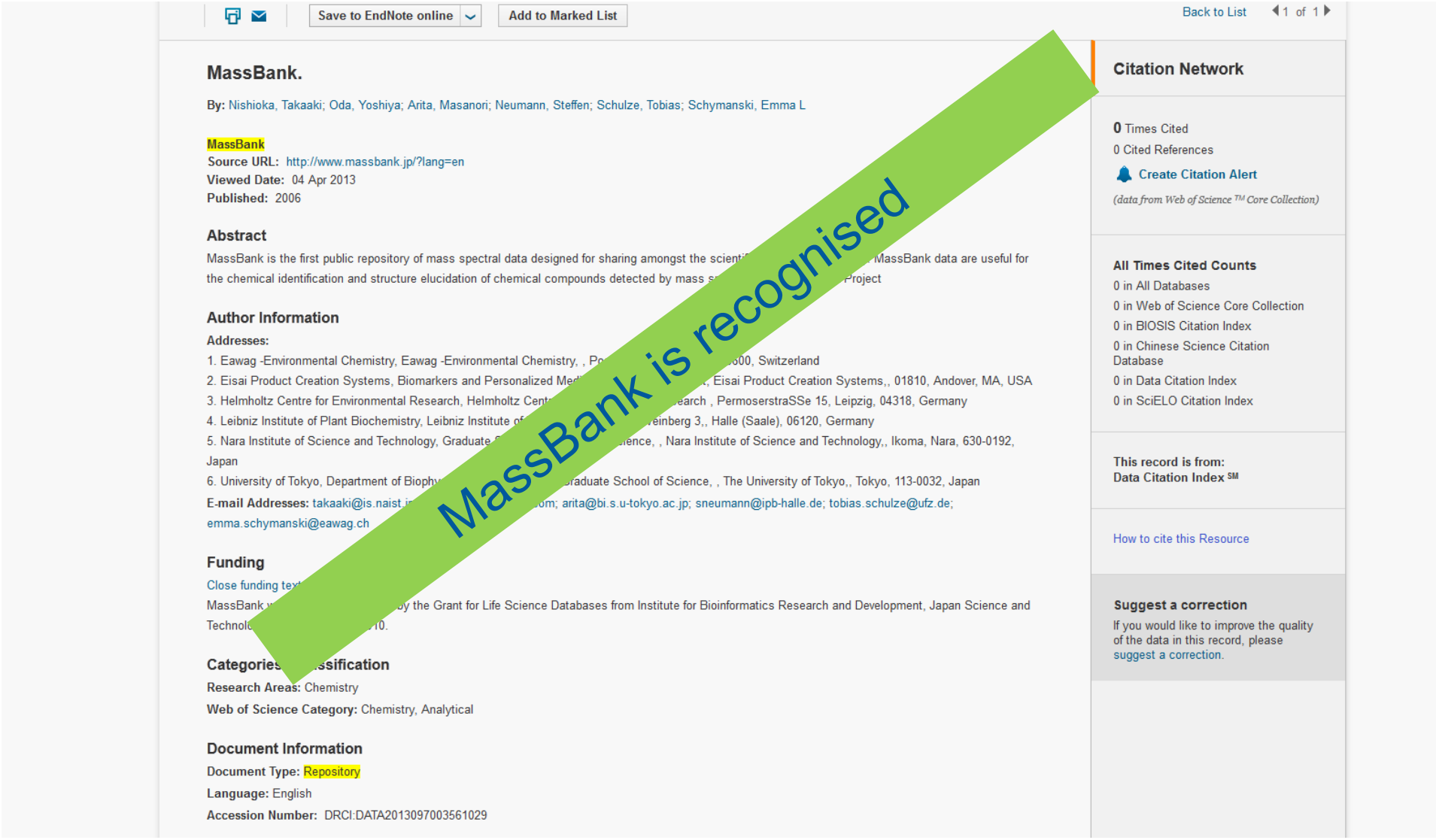
- REACH registered compounds
- Other registered compounds (e.g pesticide, biocides, pharmaceuticals)
- WFD and river basin specific compounds
- Transformation products

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

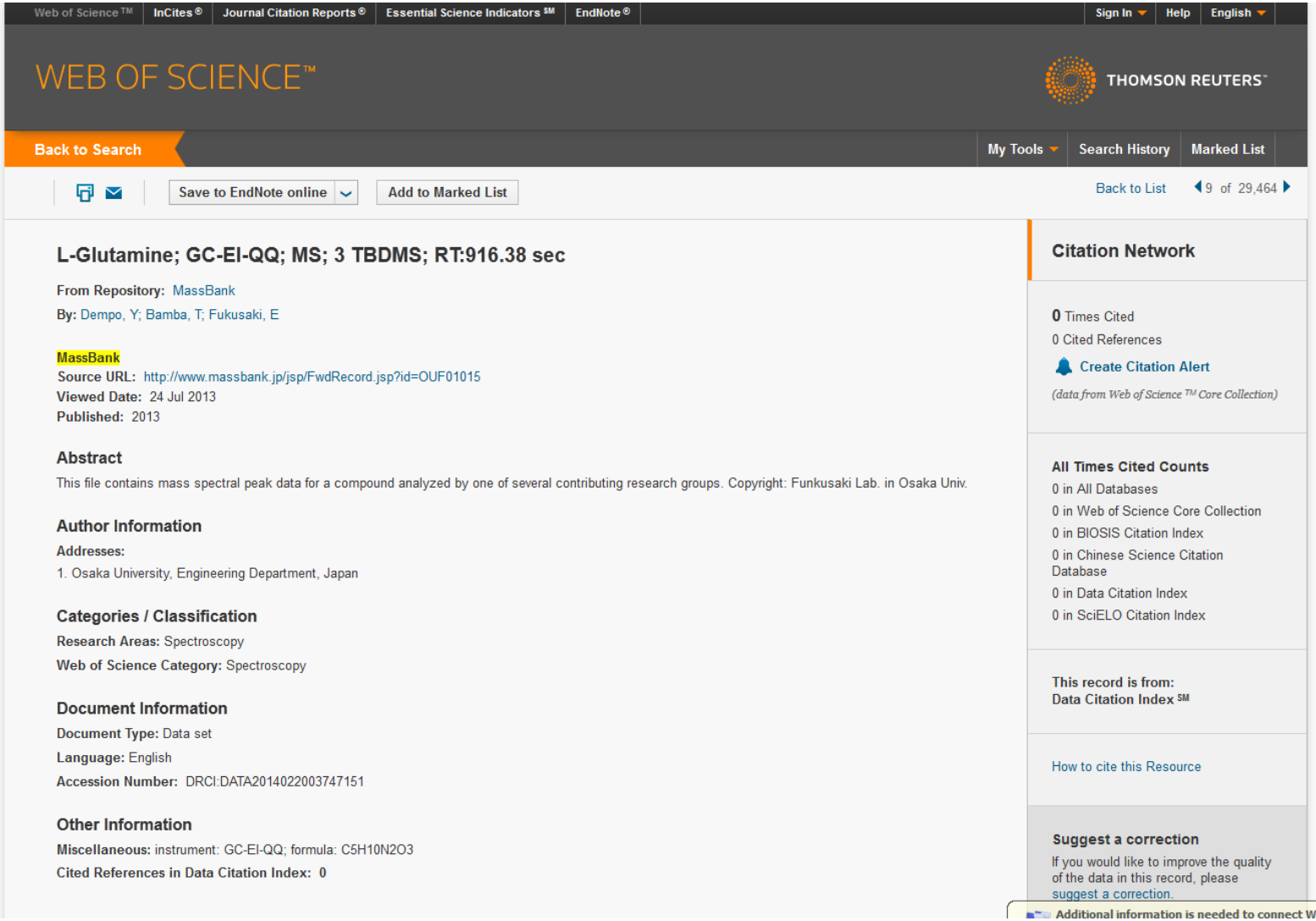
http://risk-ident.hswt.de/pages/en/tasks/wp-1-database.php?lang=EN

MassBank in Data Citation Index



Screenshot by Megan Force (Thomson-Reuters)

MassBank in Data Citation Index



Screenshot by Megan Force (Thomson-Reuters)

Current activities

- 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

Future activities

- 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)

Acknowledgements

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- NORMAN network and in-kind contributions
- Eawag Discretionary Funds
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MassBank.jp

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- 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

The End

Thank you for your attention!

Questions or comments?

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http://massbank.eu/MassBank