



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

NORMAN MassBank Status and future plans



Tobias Schulze
Amsterdam, 27 November 2012



Status of NORMAN MassBank

- 2010: First idea to adapt MassBank for NORMAN during WG3 workshop
- 2011:
- NORMAN MassBank server goes online
 - EMPOMASS Database was converted to MassBank format
- 2012:
- First version of RMassBank was available in March
 - NORMAN joined MassBank consortium in August
 - RMassBank package was released via Bioconductor
 - NORMAN MassBank server relaunched in November
 - NORMAN MassBank workshop in Amsterdam



eawag
aquatic research o.o.o



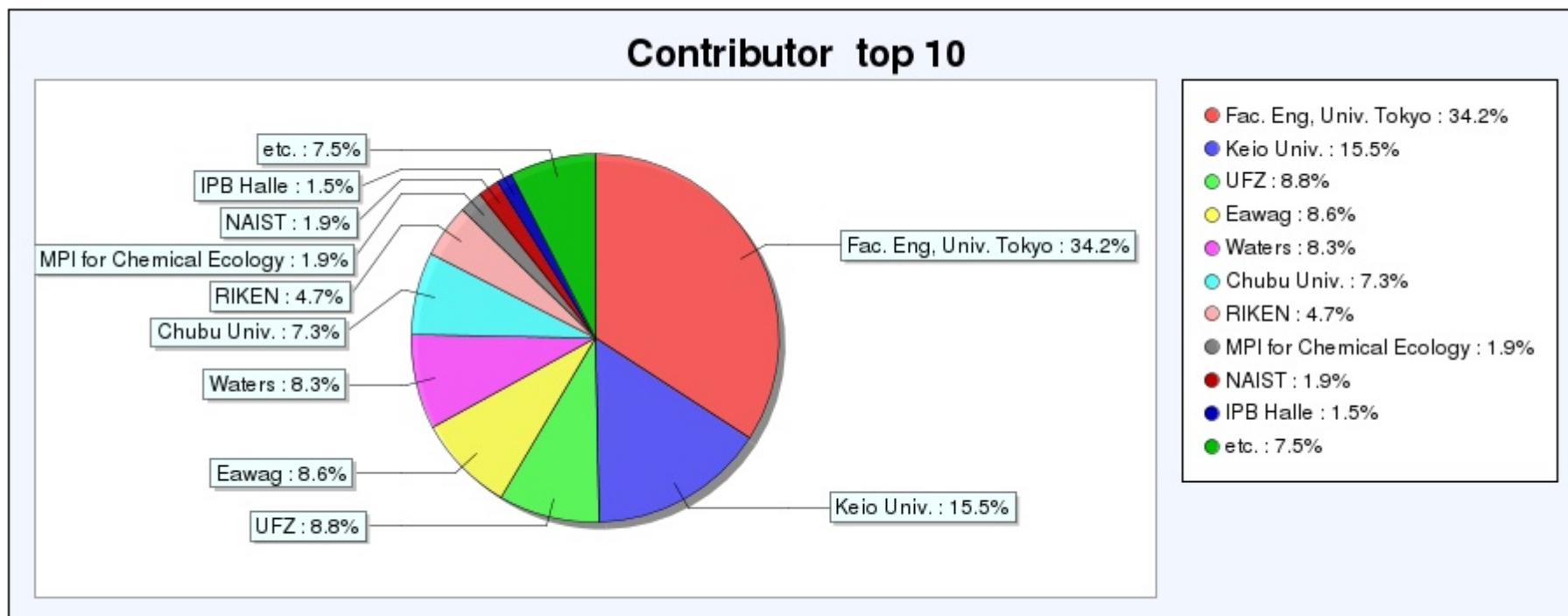
Current content of NORMAN MassBank

Record Index

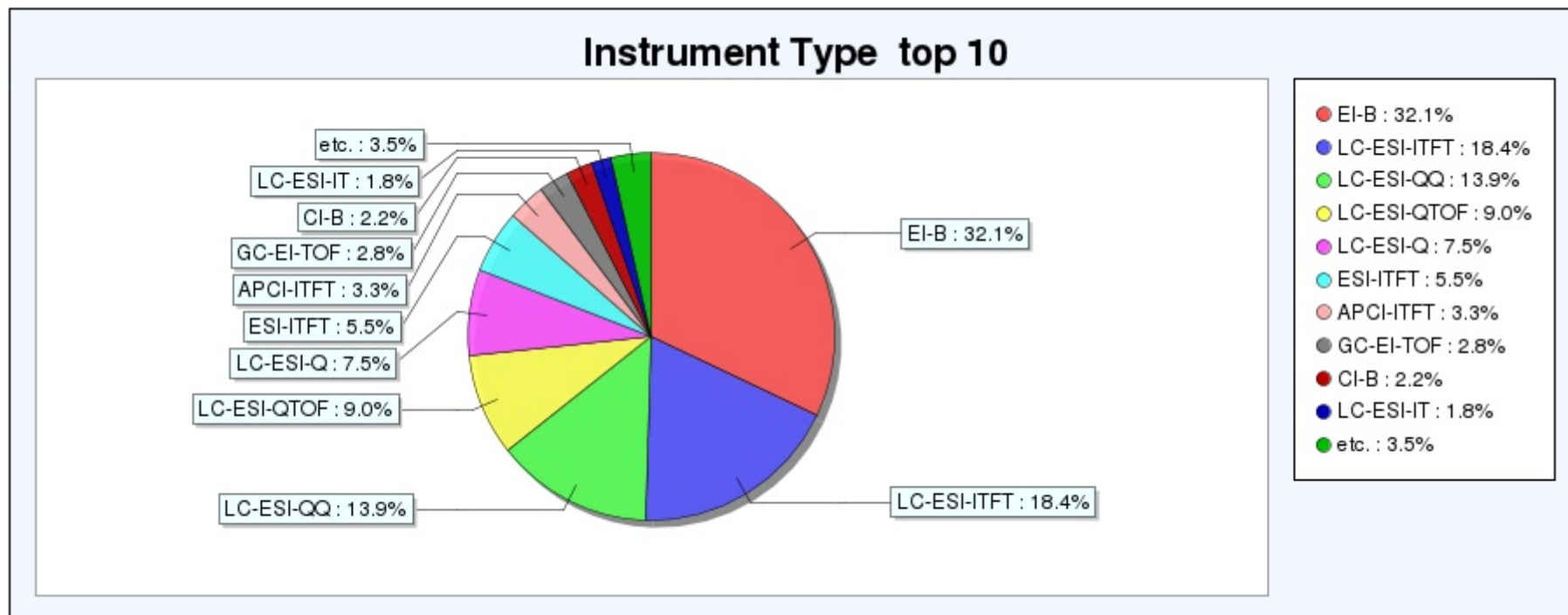
[Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Browser](#) | [Browse](#) | [Index](#) | MassBank ID:

Contributor	: CASMI (26)	Chubu Univ. (2,628)	Eawag (3,102)
	Fac. Eng. Univ. Tokyo (12,379)	Fukuyama Univ. (340)	IPB Halle (528)
	JEOL Ltd. (45)	KWR UV (3)	Kazusa (273)
	Keio Univ. (5,619)	Kyoto Univ. (185)	MPI for Chemical Ecology (691)
	Metabolon (149)	NAIST (680)	NORMAN MassBank (0)
	Nihon Univ. (75)	Osaka MCHRI (20)	Osaka Univ. (502)
	PFOS research group (277)	RIKEN (1,719)	Tottori Univ. (16)
	UFZ (3,193)	UOEH (35)	Univ. Connecticut (510)
	Univ. Toyama (253)	Waters (2,992)	
Instrument Type	: APCI-ITFT (1,206)	CE-ESI-TOF (20)	CI-B (796)
	EI-B (11,636)	EI-EBEB (12)	ESI-ITFT (1,994)
	FAB-B (26)	FAB-EB (5)	FAB-EBEB (173)
	FD-B (41)	FI-B (1)	GC-EI-TOF (1,016)
	LC-APCI-ITFT (10)	LC-APPI-QQ (277)	LC-ESI-IT (664)
	LC-ESI-ITFT (6,662)	LC-ESI-ITTOF (253)	LC-ESI-Q (2,719)
	LC-ESI-QIT (378)	LC-ESI-QQ (5,028)	LC-ESI-QTOF (3,258)
	MALDI-TOF (17)	MALDI-TOFTOF (45)	UV (3)

Current content of NORMAN MassBank

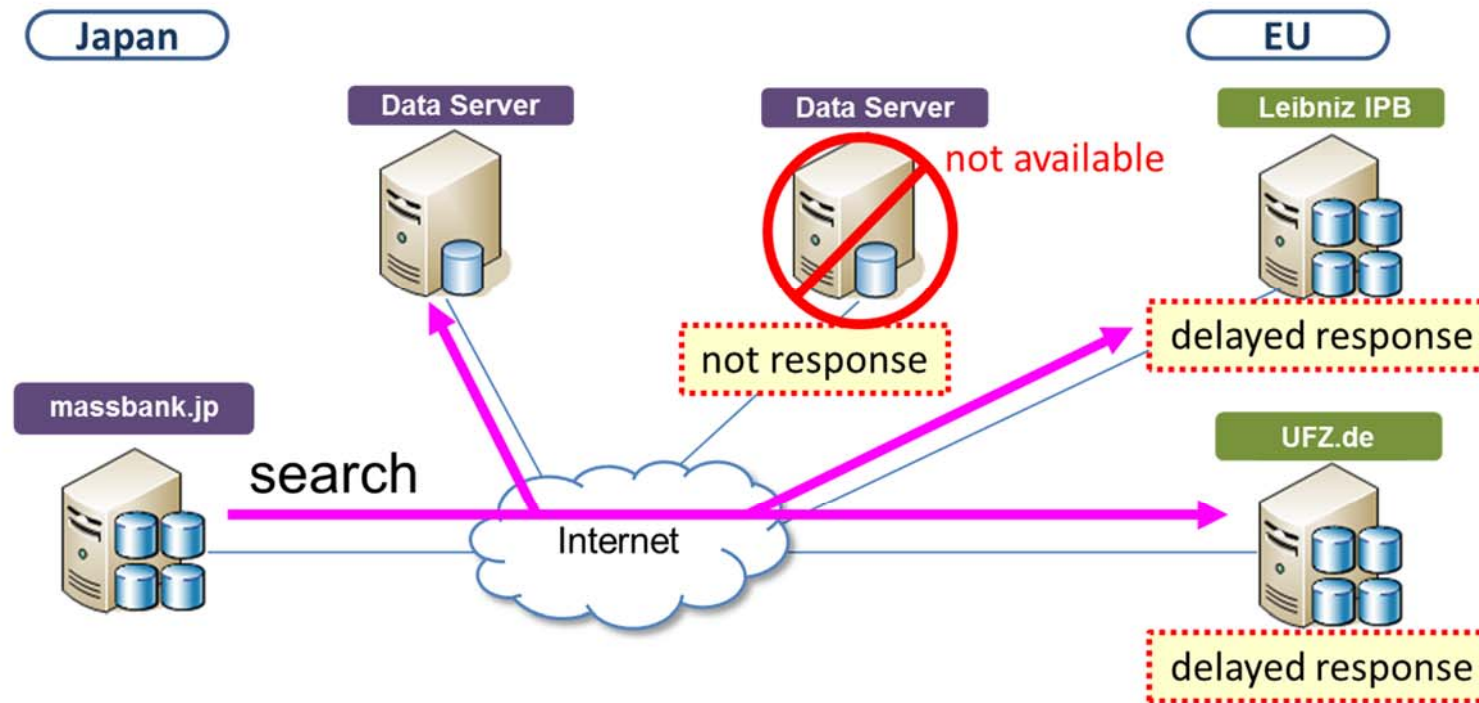


Current content of NORMAN MassBank



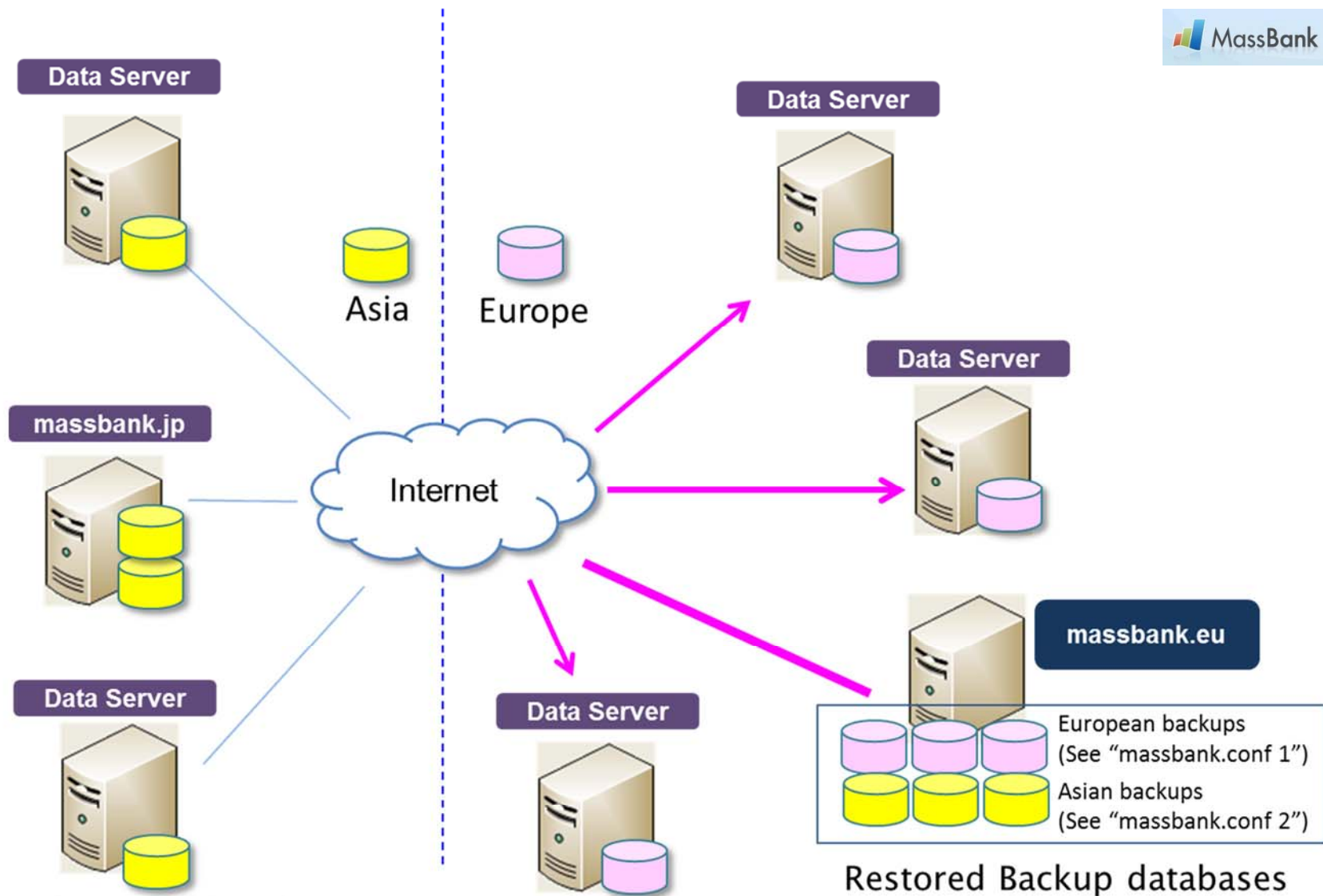
The problem of distributed databases

1. It affects the search results significantly which one of the data servers is unavailable .
2. Transcontinental accesses to MassBank.jp from European users are worse in the responses.



Graphik: Takaaki Nishioka

The solution – automated replication of DBs



Graphik: Takaaki Nishioka

Future perspectives

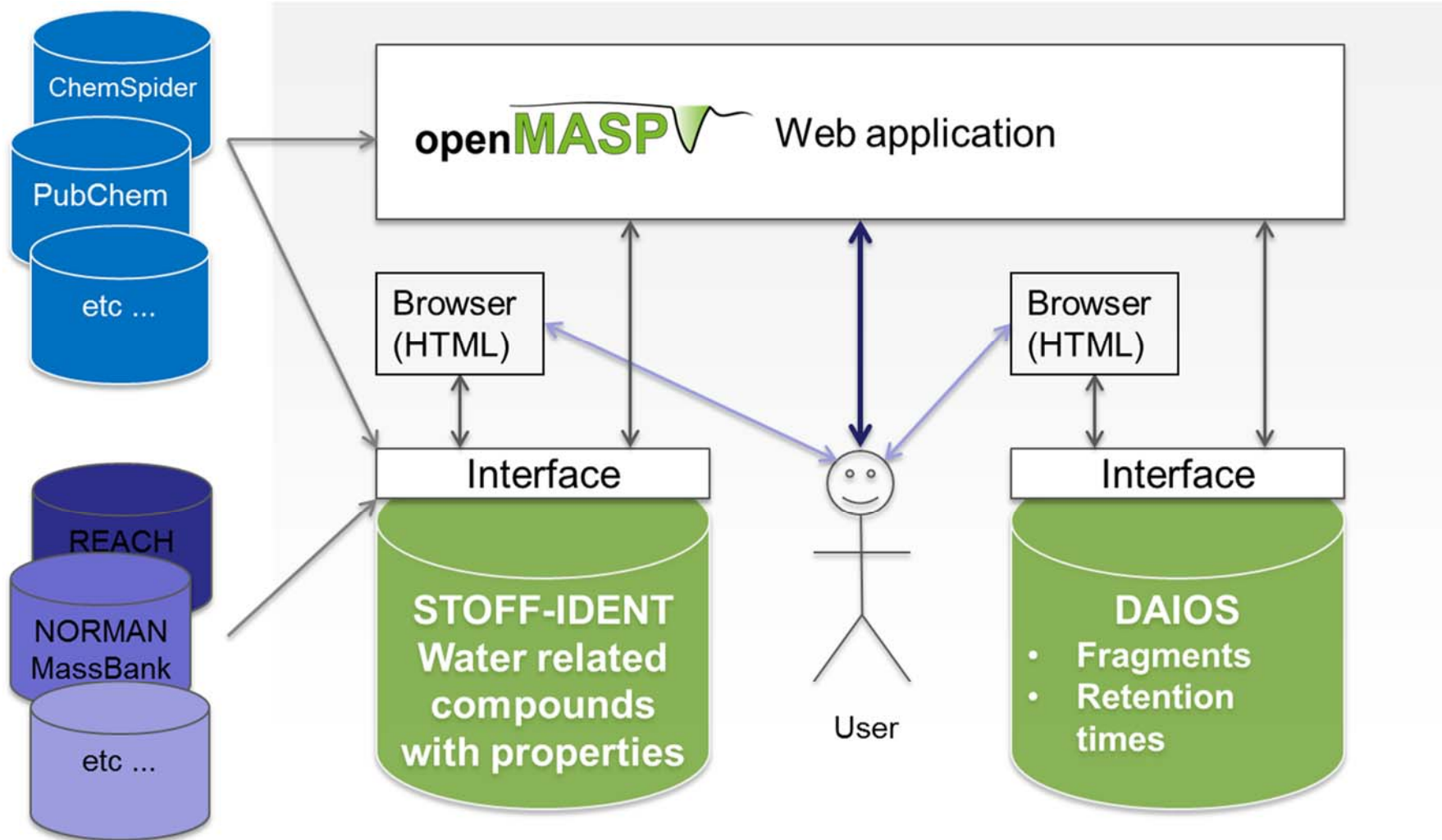
- Development of a workflow for easy upload of GC-MS data
 - Development of an automated quality assurance tool to check MassBank records before upload
 - Further development of RMassBank to be available for other instruments than Orbitrap
 - Many new spectra and compounds!
 - Integration of NORMAN MassBank in the OpenMasp platforms as linked mass spectra database



eawag
aquatic research o.o.o



Integration of MassBank in the openMASP platform



Graphik: Risk-Ident consortium (modified)

<http://openmasp.hswt.de/>
<http://risk-ident.hswt.de/>

The End

Thank you for your attention!

Questions or comments?

Contact: tobias.schulze@ufz.de

