

# Digital Sample Freezing Platform - DSFP

Environmental Samples (e.g. WW, SW – Danube, Black Sea)



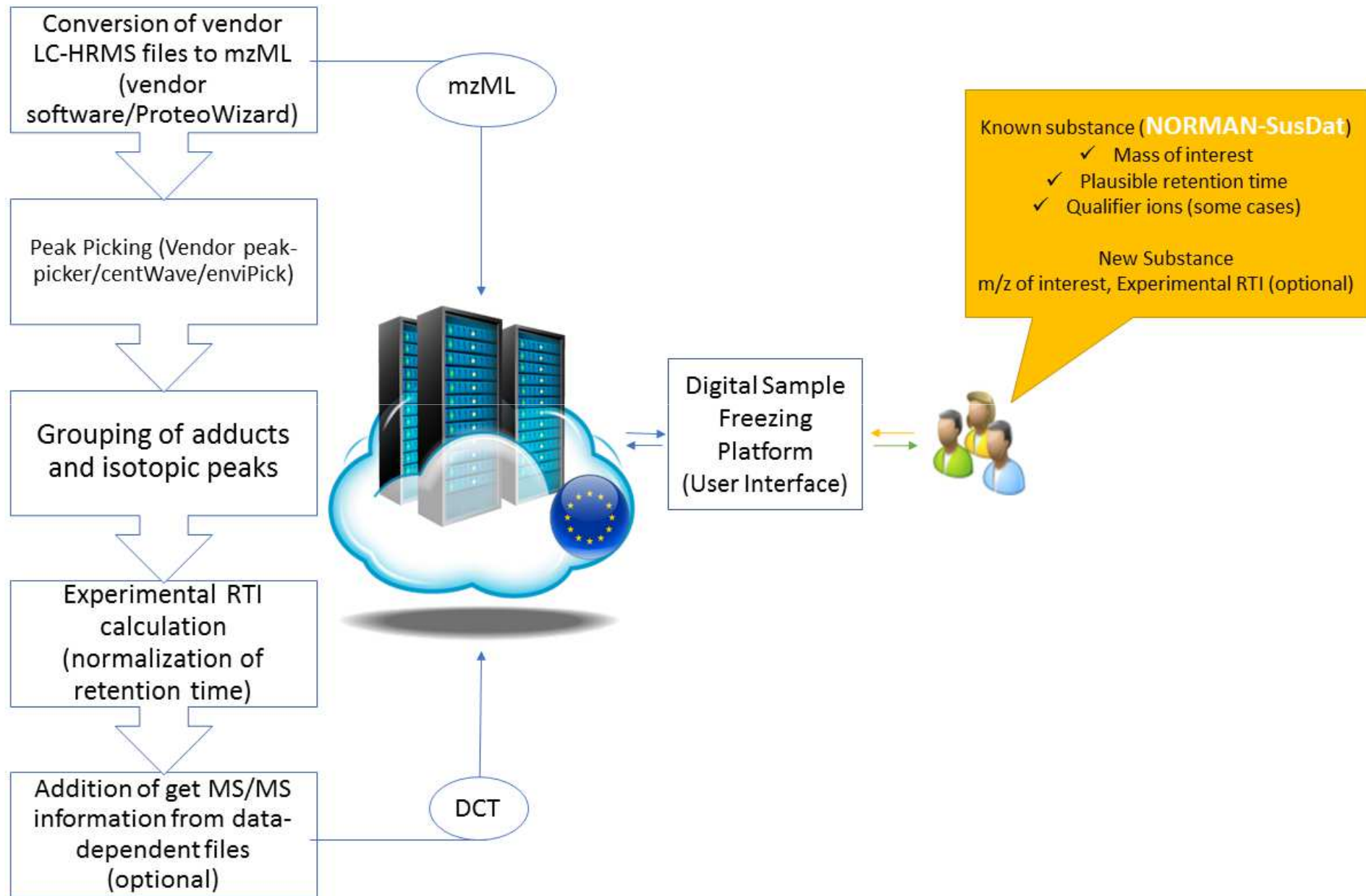
Digital/Virtual Freezing of Samples

Design of platform accessible to everyone (Go-back-in-time capabilities)



Small scale testing of digital freezing

# Digital Sample Freezing Methodology



# Interface for processing recorded LC-HRMS data at [www.norman-data.eu](http://www.norman-data.eu)

Choose Emerging Substance or input mass of interest and experimental RTI

Substance name or CAS or StdInChIKey

Compound

OR

Precursor m/z

254.059389

absolute m/z difference



RTI Tolerance (%)



Submit Job

Contributed Samples Results Chromatograms Interactive Map Help

Show 10 entries

Search:

Select per page

Country

Matrix

Date

Organization

Project

All

All

All

All

All

All

All

1	<input type="checkbox"/>	EI_LC-ESI-QTOF_Danube JDS01 Boefinger Halde_Danube River_Germany_13.08.2013_JDS3_16081301.xlsx	Germany	Water-Surface water-River water	2013-06-13	Environmental Institute	Joint Danube Survey 3
2	<input type="checkbox"/>	EI_LC-ESI-QTOF_Danube JDS02 Kelheim - Gauging station_Danube River_Germany_13.08.2013_JDS3_16082302.xlsx	Germany	Water-Surface water-River water	2013-08-13	Environmental Institute	Joint Danube Survey 3
3	<input type="checkbox"/>	EI_LC-ESI-QTOF_Danube JDS03 Geisling Power Plant_Danube River_Germany_13.08.2013_JDS3_16081303.xlsx	Germany	Water-Surface water-River water	2013-08-13	Environmental Institute	Joint Danube Survey 3
4	<input type="checkbox"/>	EI_LC-ESI-QTOF_Danube JDS04 Deggendorf_Danube River_Germany_15.08.2013_JDS3_21081301.xlsx	Germany	Water-Surface water-River water	2013-08-15	Environmental Institute	Joint Danube Survey 3
5	<input type="checkbox"/>	EI_LC-ESI-QTOF_Danube JDS05 Muehlau_Danube River_Germany_16.08.2013_JDS3_21081302.xlsx	Germany	Water-Surface water-River water	2013-08-16	Environmental Institute	Joint Danube Survey 3
6	<input type="checkbox"/>	EI_LC-ESI-QTOF_Danube JDS06 Jochenstein_Danube River_Germany_17.08.2013_JDS3_21081303.xlsx	Germany	Water-Surface water-River water	2013-08-17	Environmental Institute	Joint Danube Survey 3
7	<input type="checkbox"/>	EI_LC-ESI-QTOF_Danube JDS07 Upstream dam Abwinden-Asten_Danube River_Austria_18.08.2013_JDS3_21081304.xlsx	Austria	Water-Surface water-River water	2013-08-18	Environmental Institute	Joint Danube Survey 3
8	<input type="checkbox"/>	EI_LC-ESI-QTOF_Danube JDS08 Oberloiben_Danube River_Austria_18.08.2013_JDS3_21081305.xlsx	Austria	Water-Surface water-River water	2013-08-18	Environmental Institute	Joint Danube Survey 3
9	<input type="checkbox"/>	EI_LC-ESI-QTOF_Danube JDS09 Klosterneuburg_Danube River_Austria_19.08.2013_JDS3_27081301.xlsx	Austria	Water-Surface water-River water	2013-08-19	Environmental Institute	Joint Danube Survey 3
10	<input type="checkbox"/>	EI_LC-ESI-QTOF_Danube JDS10 Wildungsmauer_Danube River_Austria_20.08.2013_JDS3_27081302.xlsx	Austria	Water-Surface water-River water	2013-08-20	Environmental Institute	Joint Danube Survey 3

Compound selection

Choose Emerging Substance or Input mass of interest and experimental RTI

Substance name or CAS or StdInChIKey

OR

Precursor m/z

absolute m/z difference  
 0.003 0.05

RTI Tolerance (%)  
 0 20 100

Input parameters

Chromatogram selection Panel

show 10 entries

Search:

Select per page

	Country	Matrix	Date	Organization	Project
1	Germany	Water-Surface water- River water	2013-08-13	Environmental Institute	Joint Danube Survey 3
2	Germany	Water-Surface water- River water	2013-08-13	Environmental Institute	Joint Danube Survey 3
3	Germany	Water-Surface water- River water	2013-08-13	Environmental Institute	Joint Danube Survey 3
4	Germany	Water-Surface water- River water	2013-08-15	Environmental Institute	Joint Danube Survey 3
5	Germany	Water-Surface water- River water	2013-08-16	Environmental Institute	Joint Danube Survey 3
6	Germany	Water-Surface water- River water	2013-08-17	Environmental Institute	Joint Danube Survey 3
7	Austria	Water-Surface water- River water	2013-08-18	Environmental Institute	Joint Danube Survey 3
8	Austria	Water-Surface water- River water	2013-08-18	Environmental Institute	Joint Danube Survey 3
9	Austria	Water-Surface water- River water	2013-08-19	Environmental Institute	Joint Danube Survey 3
10	Austria	Water-Surface water- River water	2013-08-20	Environmental Institute	Joint Danube Survey 3

Showing 1 to 10 of 156 entries

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# Compound Selection Module

Substance name or CAS or StdInChIKey

Compound

OR

Precursor m/z

254.059389

Substance name or CAS or StdInChIKey

Sulfamethoxazole [ 723-46-6 ]  
[JLKIGFTWXXRPMT-UHFFFAOYSA-N]

Choose Ionization

Positive

Compound can be ionized positively and negatively!

Adduct

[M+H]<sup>+</sup>

More than 2 possible adducts

Predicted RTI Positive

-58 259 980

-58 48 152 256 300 404 508 672 778 880 980

Reset

Substance name or CAS or StdInChIKey

Trimethoprim [ 738-70-5 ] [IEDVJHCEMCRBQM-UHFFFAOYSA-N]

Choose Ionization

Positive

Adduct

[M+H]<sup>+</sup>

Predicted RTI Positive

-58 283 980

-58 48 152 256 360 464 568 672 778 880 980

Reset

Substance name or CAS or StdInChIKey

Perfluorooctane sulfonic acid (PFOS) [ 1763-23-1 ]  
[YFSUTJLHUFNCNZ-UHFFFAOYSA-N]

Choose Ionization

Negative

Adduct

[M-H]<sup>-</sup>

Predicted RTI Negative

-54 410 1,000

-54 52 156 260 370 478 582 688 794 900 1,000

Reset

Compounds with prior-knowledge on spectral behavior:

- ✓ Ionization pre-selection
- ✓ Adduct pre-selection
- ✓ Qualifier fragments in evaluation of chromatograms module

# Sample Selection Module

Contributed Samples   Results   Chromatograms   [Interactive Map](#)   [Help](#)

Show  entries   Search:

Select per page

		Country	Matrix	Date	Organization	Project
	<input type="text" value="All"/>	<input type="text" value="All"/>	<input type="text" value="All"/>	<input type="text" value="All"/>	<input type="text" value="All"/>	<input type="text" value="All"/>
7	<input type="checkbox"/> EI_LC-ESI-QTOF_Danube JDS07 Upstream dam Abwinden-Asten_Danube River_Austria_18.08.2013_JDS3_21081304.xlsx	Austria	Water-Surface water- River water	2013-08-18	Environmental Institute	Joint Danube Survey 3
8	<input type="checkbox"/> EI_LC-ESI-QTOF_Danube JDS08 Oberloiben_Danube River_Austria_18.08.2013_JDS3_21081305.xlsx	Austria	Water-Surface water- River water	2013-08-18	Environmental Institute	Joint Danube Survey 3
9	<input type="checkbox"/> EI_LC-ESI-QTOF_Danube JDS09 Klostemeuburg_Danube River_Austria_19.08.2013_JDS3_27081301.xlsx	Austria	Water-Surface water- River water	2013-08-19	Environmental Institute	Joint Danube Survey 3

The image shows five filter dropdown menus with the following content:

- Country:** Austria, Bulgaria, Canada, Croatia, Georgia, Germany, Greece, Hungary
- Matrix:** Air-Workplace air - Indoor, Biota-Territorial (marine) water, Sediments-Territorial
- Date:** All, 2013-07-09, 2016-08-23
- Organization:** Environmental Institute, Helmholtz Centre for Environmental Research - UFZ, University of Athens
- Project:** EMBLAS\_II, Joint Danube Survey 3, Norman CT2016, TREMEPOL

# Sample Selection Module

## Meta-Data retrieval

241 ☰

☐ UoA\_LC-ESI-QTOF\_Wastewater  
effluent\_Athens\_Greece\_07.03.2015\_TREMEPOL

Greece

Water-Waste water-  
Municipal and Industrial

2015-03-07

University of Athens

TREMEPOL

**Latitude (Decimal):** 37.94051

**Longitude (Decimal):** 23.5883

**Precision of coordinates:** Precise (range 1-10 m)

**Laboratory Name:** Laboratory of Analytical Chemistry

**Organization Country:** Greece

**Laboratory City:** Athens

**Contact Person:** Nikolaos Thomaidis

**Type of data source:** Monitoring data

**Type of monitoring:** Surveillance

**Instrument manufacturer:** Bruker maxis Impact

**Analytical Column:** Thermo Acclaim RSLC C18 2.2um, 2.1x100mm

**Reconstitution solvents:** Methanol/Water 50/50

**Injection volume (ul):** 5

**Column temperature (C):** 25

**Mobile phases** A 90:10 water:methanol with 0.01% formic acid and 5mM ammonium formate; B methanol with 0.01% formic acid and 5mM ammonium formate

**Gradient:** 99% A at 0-1 min; 61% A at 3 min; 0.1% A at 14-16 min; 99% A at 16.1-20 min

**Flow (mL/min):** 200 uL/min at 0-3 min; 400 uL/min at 14 min; 480 uL/min at 16-19 min; 200 uL/min at 19.1-20 min

**MS Scan Range:** 50-1000

**Declared mass accuracy MS1:** 2

**Declared mass accuracy MS2:** 3

**Fragmentation method:** CID

# Results

Contributed Samples Results Chromatograms Interactive Map Help

Column visibility Copy CSV Excel PDF Print Show 100 entries Search:

Select per page

		Retention time [min]	Mass of ion [m/z]	Intensity	Ion Type	MS/MS available	Proposed substance	Molecular Formula	Level of confirmation of identification	RTI
	All								All	
1	<input type="checkbox"/> LC-ESI-QTOF_Seawater JOSS01_Black Sea_Ukraine_04.06.2016_EMBLAS III_17798	4.56	254.0585	1252	-	No	-	-	Mass of interest	248.2
2	<input type="checkbox"/> LC-ESI-QTOF_Seawater JOSS02_Black Sea_Ukraine_26.05.2016_EMBLAS III_17799	4.57	254.0579	1048	-	No	-	-	Mass of interest	249.4
3	<input type="checkbox"/> LC-ESI-QTOF_Seawater JOSS03_Black Sea_Ukraine_03.06.2016_EMBLAS III_17800	4.56	254.0592	816	-	No	-	-	Mass of interest	248.1
4	<input type="checkbox"/> LC-ESI-QTOF_Seawater JOSS04_Black Sea_Ukraine_27.05.2016_EMBLAS III_17801	4.57	254.0588	948	-	No	-	-	Mass of interest	249.1
5	<input type="checkbox"/> LC-ESI-QTOF_Seawater JOSS05_Black Sea_Ukraine_26.05.2016_EMBLAS	4.55	254.0581	1024	-	No	-	-	Mass of interest	247.9

Selection of results for deeper inspection from experts



# Module for Evaluation of Chromatograms

Contributed Samples Results Chromatograms Interactive Map Help

## Select Chromatogram

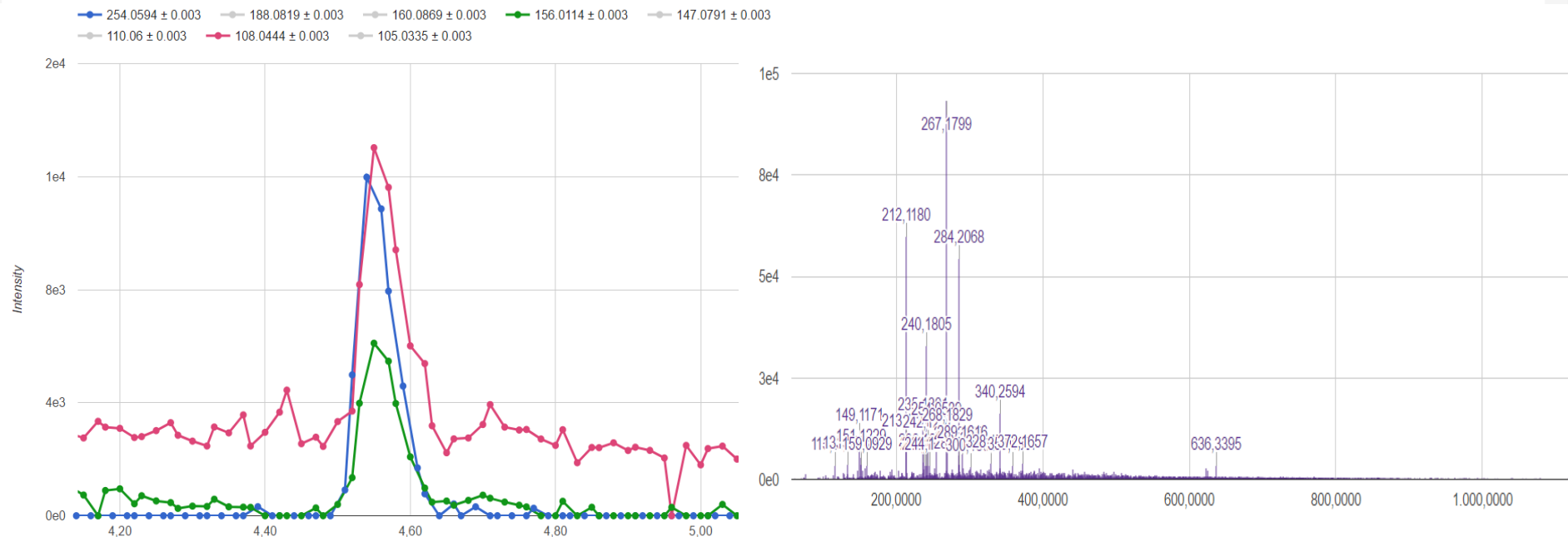
UoA\_LC-ESI-QTOF\_Seawater UA07\_Black Sea\_Ukraine\_19.05.2016\_EMBLAS II\_17856.xlsx

Data-Independent

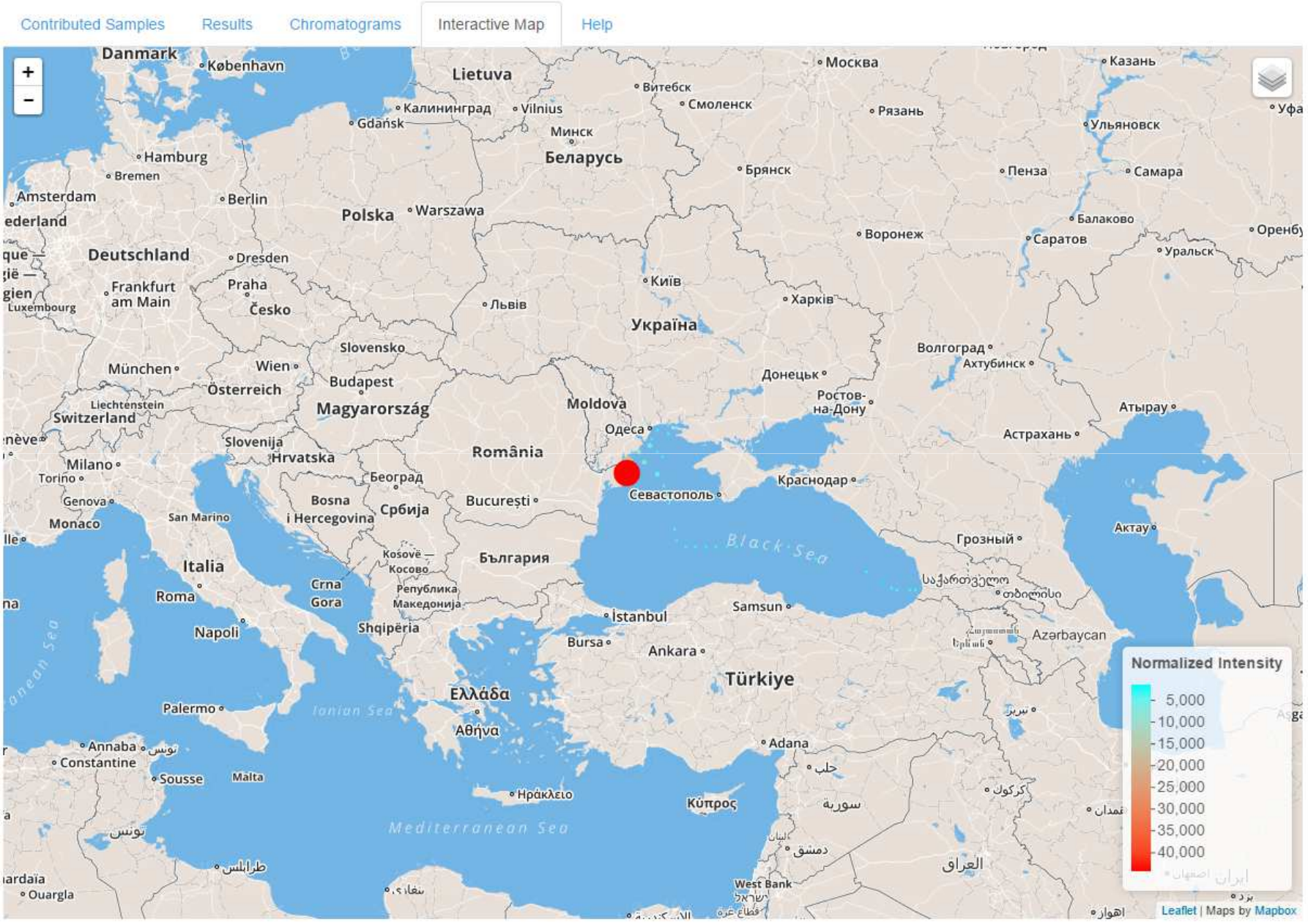
Data-Dependent

	show	mz	accuracy_mDa	chromatogram
1	<input checked="" type="checkbox"/>	254.0594	0.0030	UoA_POS_4eV_LC-ESI-QTOF_Seawater UA07_Black Sea_Ukraine_19.05.2016_EMBLAS II_17856.mzML
2	<input type="checkbox"/>	188.0819	0.0030	UoA_POS_25eV_LC-ESI-QTOF_Seawater UA07_Black Sea_Ukraine_19.05.2016_EMBLAS II_17856.mzML
3	<input type="checkbox"/>	160.0869	0.0030	UoA_POS_25eV_LC-ESI-QTOF_Seawater UA07_Black Sea_Ukraine_19.05.2016_EMBLAS II_17856.mzML
4	<input type="checkbox"/>	156.0114	0.0030	UoA_POS_25eV_LC-ESI-QTOF_Seawater UA07_Black Sea_Ukraine_19.05.2016_EMBLAS II_17856.mzML
5	<input type="checkbox"/>	147.0791	0.0030	UoA_POS_25eV_LC-ESI-QTOF_Seawater UA07_Black Sea_Ukraine_19.05.2016_EMBLAS II_17856.mzML
6	<input type="checkbox"/>	110.0600	0.0030	UoA_POS_25eV_LC-ESI-QTOF_Seawater UA07_Black Sea_Ukraine_19.05.2016_EMBLAS II_17856.mzML
7	<input type="checkbox"/>	108.0444	0.0030	UoA_POS_25eV_LC-ESI-QTOF_Seawater UA07_Black Sea_Ukraine_19.05.2016_EMBLAS II_17856.mzML
8	<input type="checkbox"/>	105.0335	0.0030	UoA_POS_25eV_LC-ESI-QTOF_Seawater UA07_Black Sea_Ukraine_19.05.2016_EMBLAS II_17856.mzML

Submit (Press the button everytime changes are done to the table above)



# 1-Click Interactive Spatial Distribution Map



# Batch Mode Module

Create Results Visualization

Step 1: Select compounds that you want to screen

You selected 0 compound. This is beta-version. Therefore, only the first 500 compounds will be processed

Select/Deselect

Show 10 entries

Search:

	Name	Formula	CAS number	InChIKey	Source	ChemspiderID
	<input type="text" value="All"/>	<input type="text" value="All"/>	<input type="text" value="All"/>	<input type="text" value="All"/>	<input type="text" value="All"/>	<input type="text" value="All"/>
1	Sulfaclozine	C10H9CIN4O2S	102-65-8	QKLPUVXBJHRFQZ-UHFFFAOYSA-N	Alygizakis	60252
2	Sulfachlorpyridazine	C10H9CIN4O2S	80-32-0	XOXHILFPRYWFOU-UHFFFAOYSA-N	Alygizakis	6382
3	Sulfaguanidine	C7H10N4O2S	57-67-0	BRBKOPJOKNSWSG-UHFFFAOYSA-N	Alygizakis	5133
4	Sulfamerazine	C11H12N4O2S	127-79-7	QPPBRPIAZZHUNT-UHFFFAOYSA-N	Alygizakis	5134
5	Sulfamethizole	C9H10N4O2S2	144-82-1	VACCAVUAMIDAGB-UHFFFAOYSA-N	Alygizakis	5137
6	Sulfamoxole	C11H13N3O3S	729-99-7	CYFLXLSBHQBMFT-UHFFFAOYSA-N	Alygizakis	12361
7	Sulfanilamide	C6H8N2O2S	1337-39-9	FDDDEECHVMSUSB-UHFFFAOYSA-N	Alygizakis	5142
8	Cefoperazone	C25H27N9O8S2	62893-19-0	GCFBRXLXSHGKWDW-WJONJSRFSAN	Alygizakis	5408849
9	Tiamulin	C28H47NO4S	55297-95-5	UURAUHCOJAIIRQ-QGLSALSOSAN	Alygizakis	571196
10	Albendazole Sulfoxide	C12H15N3O3S	54029-12-8	VXTGHWHFYNYFFV-UHFFFAOYSA-N	UOA	75767

Showing 1 to 10 of 14,633 entries

Previous  2 3 4 5 ... 1464 Next

Step 2: Select parameters

Step 3: Select samples that you want to screen

Step 4: Submit your request

[Download](#) [Visualize the data](#)

## Easy 4-step batch-mode screening

# Heatmap Module

Create Results

Visualization

Height

330

Width

300

Size Letters Y

10

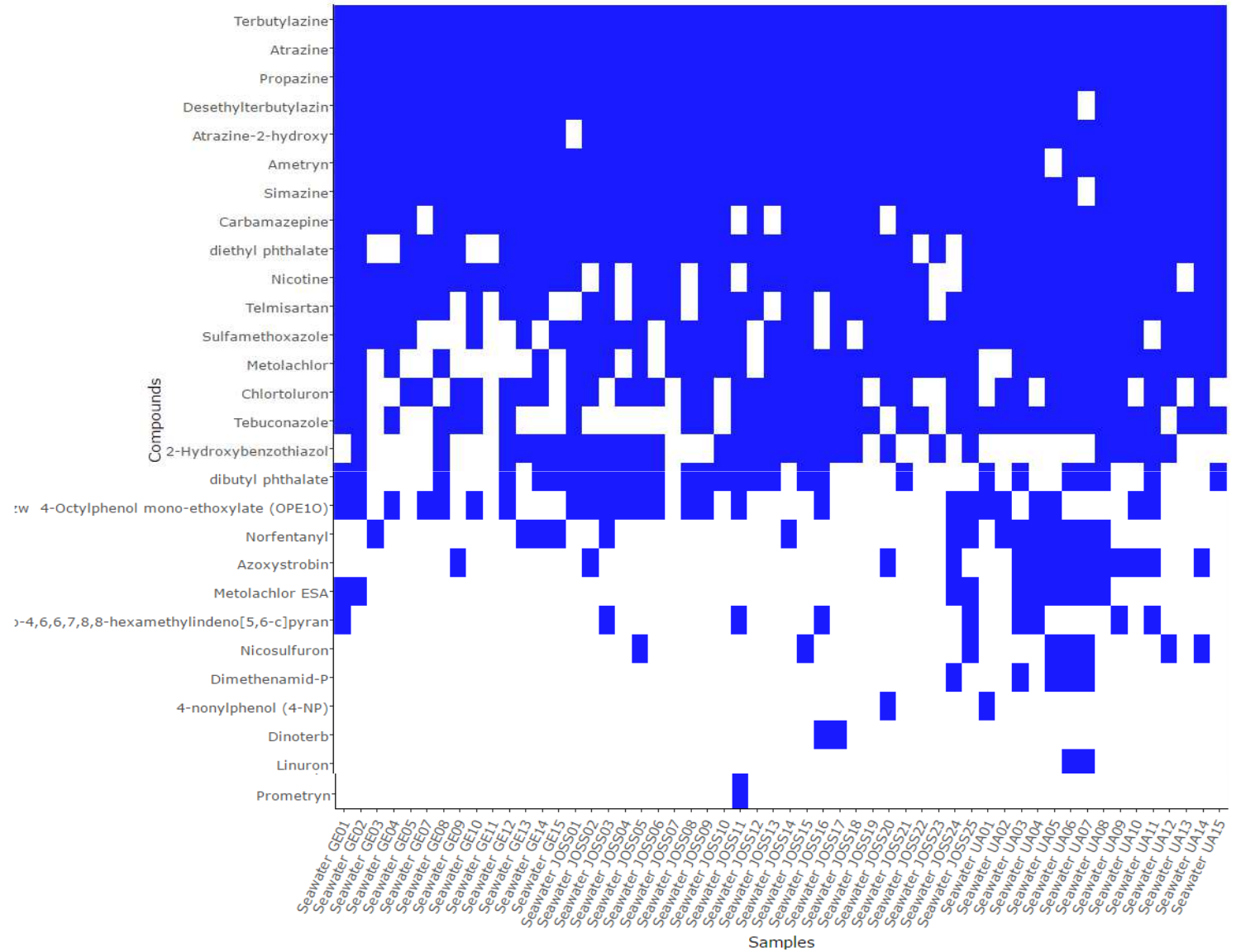
Size Letters X

10

Rotation of labels on x-axis

65

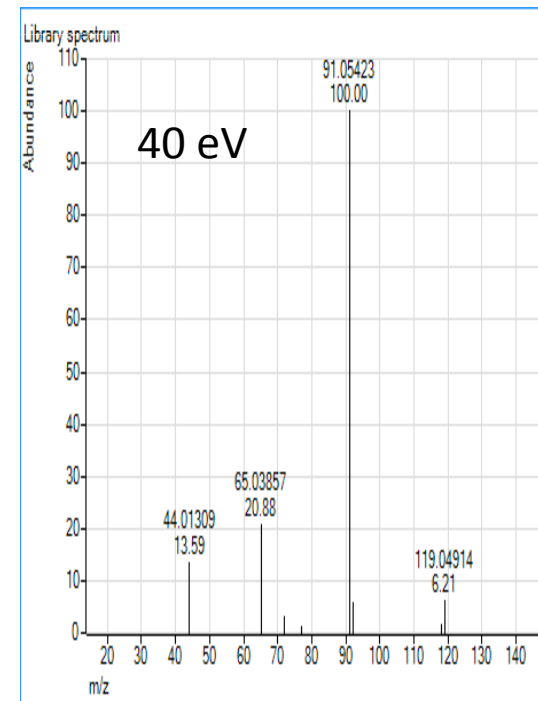
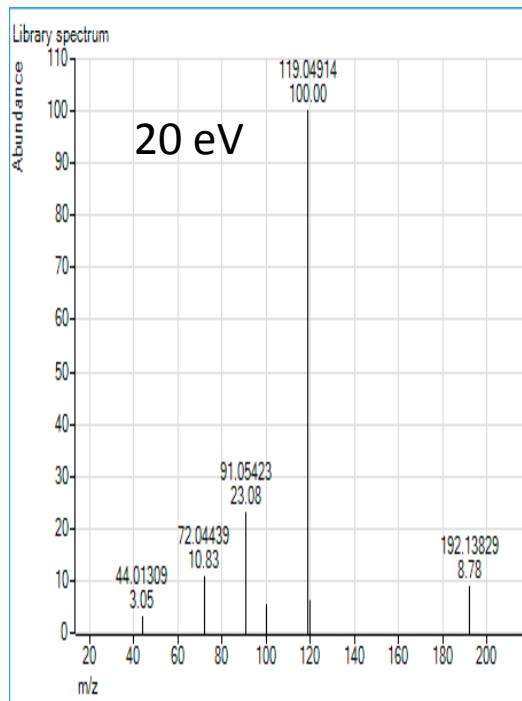
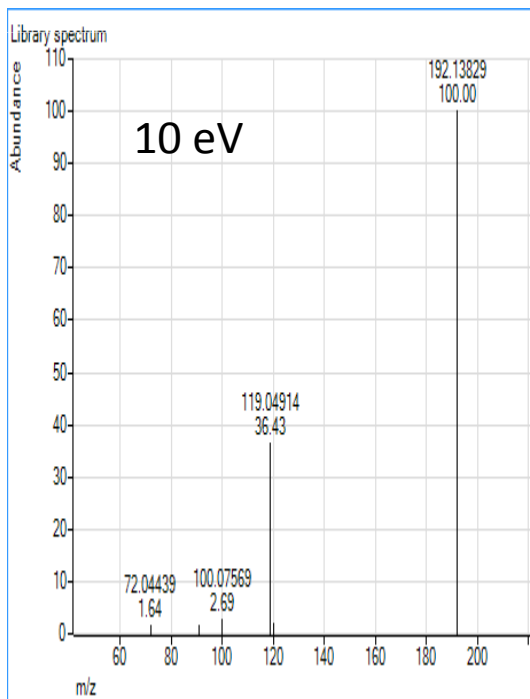
## Occurrence Results



Blue color indicates that compound was detected in the corresponding sample  
White color indicates that compound was not detected

# DSFP - retrospective search

- DEET - the most common active ingredient in insect repellents,
- MS/MS spectra at three different collision energies



# DSFP - retrospective search

- Task: - the presence of DEET during JDS3 survey
- Tools: - predicted RTI ( $\pm$ ), mass accuracy ( $\pm$ ), specific fragments
- JDS-58-Arges – unambiguously positive for DEET

Choose Emerging Substance or input mass of interest and experimental RTI

Substance name or CAS or SMILESKey  
DEET [ 134-62-3 ] (MMOXZBCLQIQDFJHFFRQYSAAN)

Choose Ionization  
Positive

Adduct  
[M+H]<sup>+</sup>

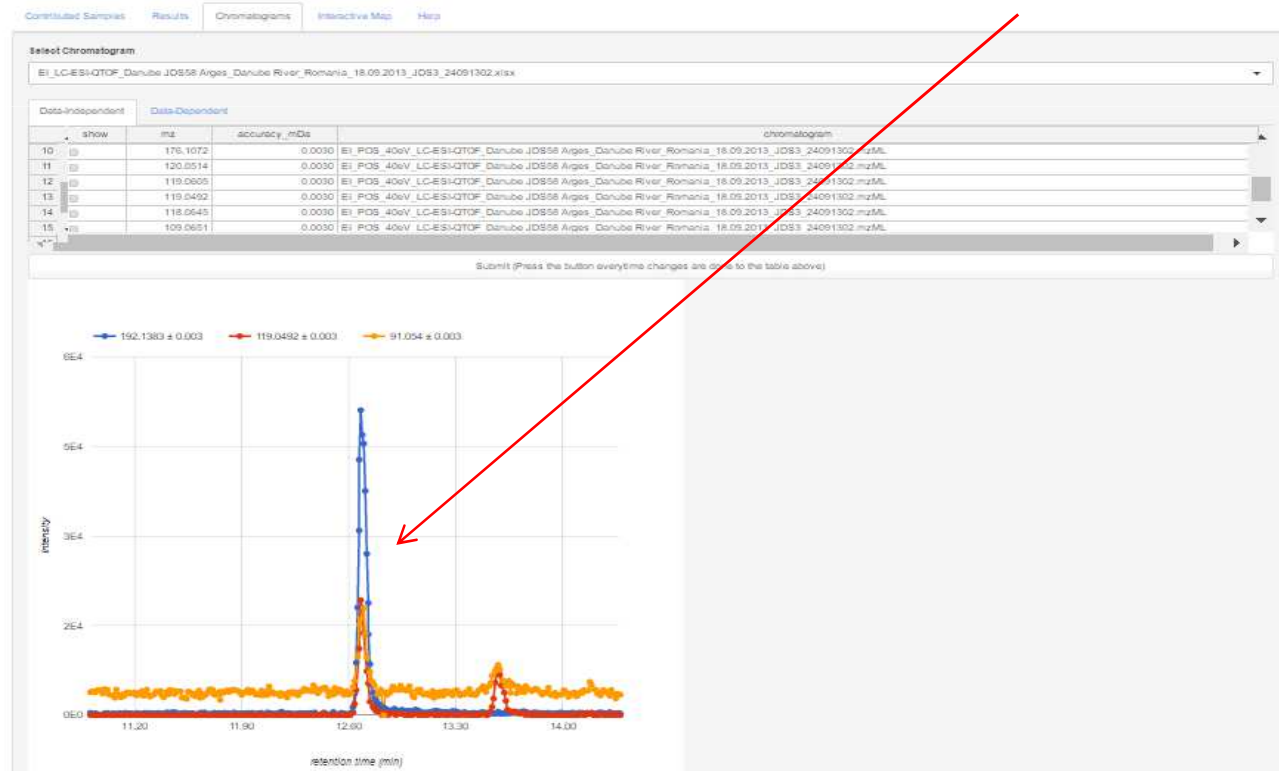
Predicted RTI Positive  
300

Submit Job

absolute m/z difference  
0.003

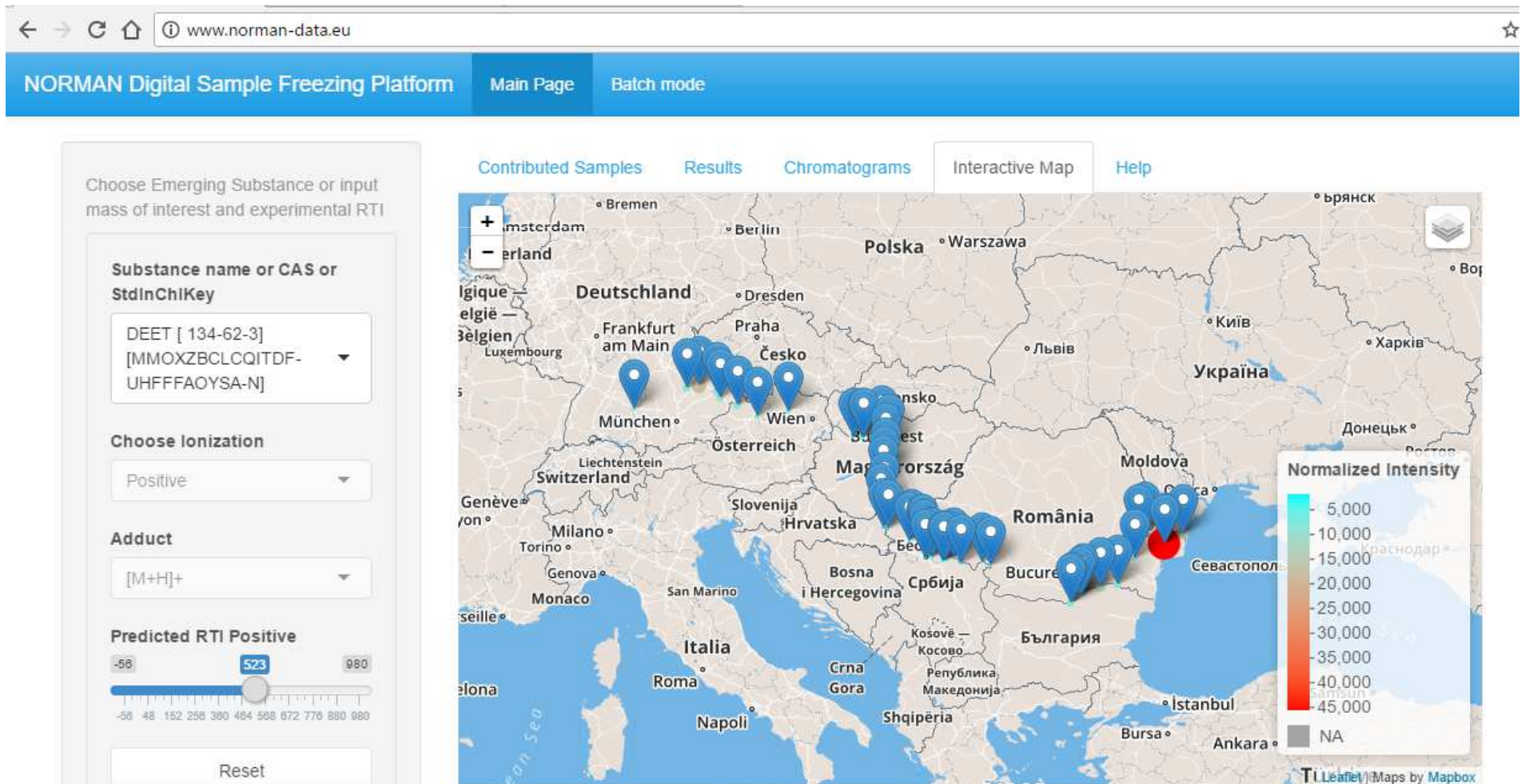
RTI Tolerance (%)  
300

Submit Job



# DSFP - retrospective search

- JDS\_3 - results: - 53 out of 68 sampling points were positive for DEET



# DSFP - retrospective search

- EMBLAS - results: - 32 out of 55 sampling points were positive for DEET

