Digital Sample Freezing Platform - DSFP

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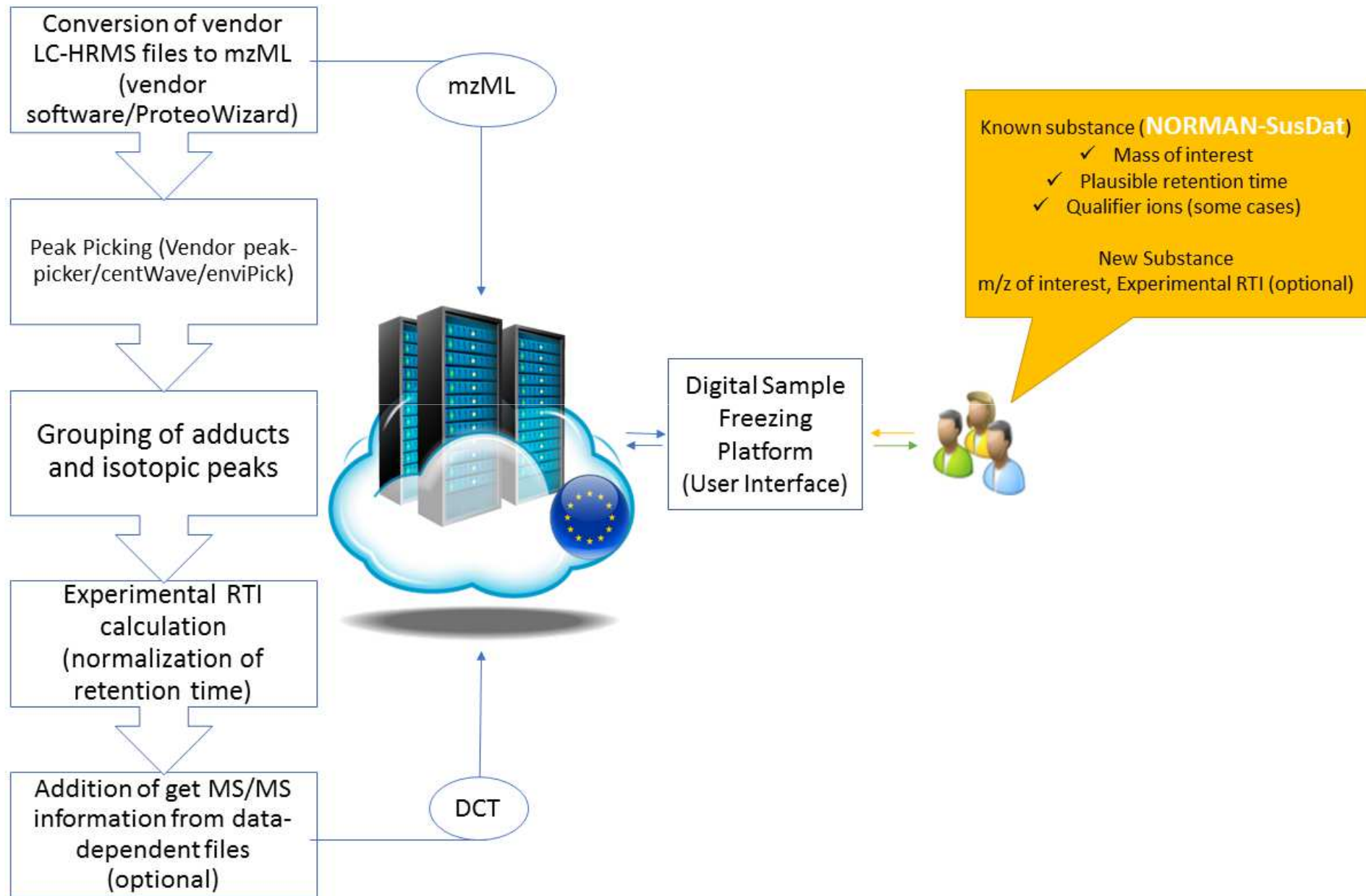

Digital/Virtual Freezing of Samples

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

norma n**E**ws

Small scale testing of digital freezing

Digital Sample Freezing Methodology

Interface for processing recorded LC-HRMS data at www.norman-data.eu

NORMAN Digital Sample Freezing Platform | Main Page | Batch mode | Contribute

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

0.003   0.05

0.0 0.005   0.005   0.01   0.015   0.02   0.025   0.03   0.035   0.04   0.045   0.05

RTI Tolerance (%)

0   20   100

0   10   20   30   40   50   60   70   80   90   100

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
1 ⊕	EI_LC-ESI-QTOF_Danube JDS01 Boefinger Halde_Danube River_Germany_13.08.2013_JDS3_16081301.xlsx	Germany	Water-Surface water-River water	2013-08-13	Environmental Institute	Joint Danube Survey 3
2 ⊕	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 ⊕	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 ⊕	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 ⊕	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 ⊕	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 ⊕	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 ⊕	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 ⊕	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
10 ⊕	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

Showing 1 to 10 of 156 entries   Previous 1 2 3 4 5 ... 16 Next

Compound selection

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

0.003   0.05

0.0,005 0.005 0.01 0.015 0.02 0.025 0.03 0.035 0.04 0.045 0.05

RTI Tolerance (%)

0   20   100

0 10 20 30 40 50 60 70 80 90 100

Submit Job

Input parameters

Chromatogram selection Panel

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
1	ⓘ	☐ EI_LC-ESI-QTOF_Danube JDS01 Boefinger Halde_Danube River_Germany_13.08.2013_JDS3_16081301.xlsx	Germany	Water-Surface water-River water	2013 08 13	Environmental Institute	Joint Danube Survey 3
2	⊕	☐ 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	⊕	☐ 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	⊕	☐ 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	⊕	☐ 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	⊕	☐ 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	⊕	☐ 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	⊕	☐ 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	⊕	☐ 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
10	⊕	☐ 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

Showing 1 to 10 of 156 entries   Previous   1   2   3   4   5   ...   16   Next

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]+ ▾

More than 2 possible adducts
Predicted RTI Positive

-56   259   980

-56 48 152 256 360 464 568 672 776 880 980

Reset

Substance name or CAS or StdInChIKey

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

Choose Ionization

Positive ▾

Adduct

[M+H]+ ▾

Predicted RTI Positive

-56   283   980

-56 48 152 256 360 464 568 672 776 880 980

Reset

Substance name or CAS or StdInChIKey

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

Choose Ionization

Negative ▾

Adduct

[M-H]- ▾

Predicted RTI Negative

-54   410   1,000

-54 52 158 264 370 476 582 688 794 900 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

Show [10 ▼] entries

Search: [_____]

		Select per page	Country ▲	Matrix ⬍	Date ⬍	Organization ⬍	Project ⬍
		All	All	All	All	All	All
7	⊕	☐ 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	⊕	☐ 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	⊕	☐ 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

[|]
Austria
Bulgaria
Canada
Croatia
Georgia
Germany
Greece
Hungary

[|]
Air-Workplace air - Indoor
Biota-Teritorial (marine) water
Sediments-Territorial

[All]

[All]
2013-07-09   2016-08-23

[|]
Environmental Institute
Helmholtz Centre for Environmental Research - UFZ
University of Athens

[|]
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

Column visibility | Copy | CSV | Excel | PDF | Print   Show 100 ▾ entries   Search: [ ]

		Retention time [min]	Mass of ion [m/z]	Intensity	Ion Type	MS/MS available	Proposed substance	Molecular Formula	Level of confirmation of identification	RTI
☐ Select per page										
	All						A		All	
1	☐ LC-ESI-QTOF_Seawater JOSS01_Black Sea_Ukraine_04.06.2016_EMBLAS II_17798	4.56	254.0585	1252	-	No	-	-	Mass of interest	248.2
2	☐ LC-ESI-QTOF_Seawater JOSS02_Black Sea_Ukraine_26.05.2016_EMBLAS II_17799	4.57	254.0579	1048	-	No	-	-	Mass of interest	249.4
3	☐ LC-ESI-QTOF_Seawater JOSS03_Black Sea_Ukraine_03.06.2016_EMBLAS II_17800	4.56	254.0592	816	-	No	-	-	Mass of interest	248.1
4	☐ LC-ESI-QTOF_Seawater JOSS04_Black Sea_Ukraine_27.05.2016_EMBLAS II_17801	4.57	254.0588	948	-	No	-	-	Mass of interest	249.1
5	☐ 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

1-Click Interactive Spatial Distribution Map

Batch Mode Module

Easy 4-step batch-mode screening

Heatmap Module
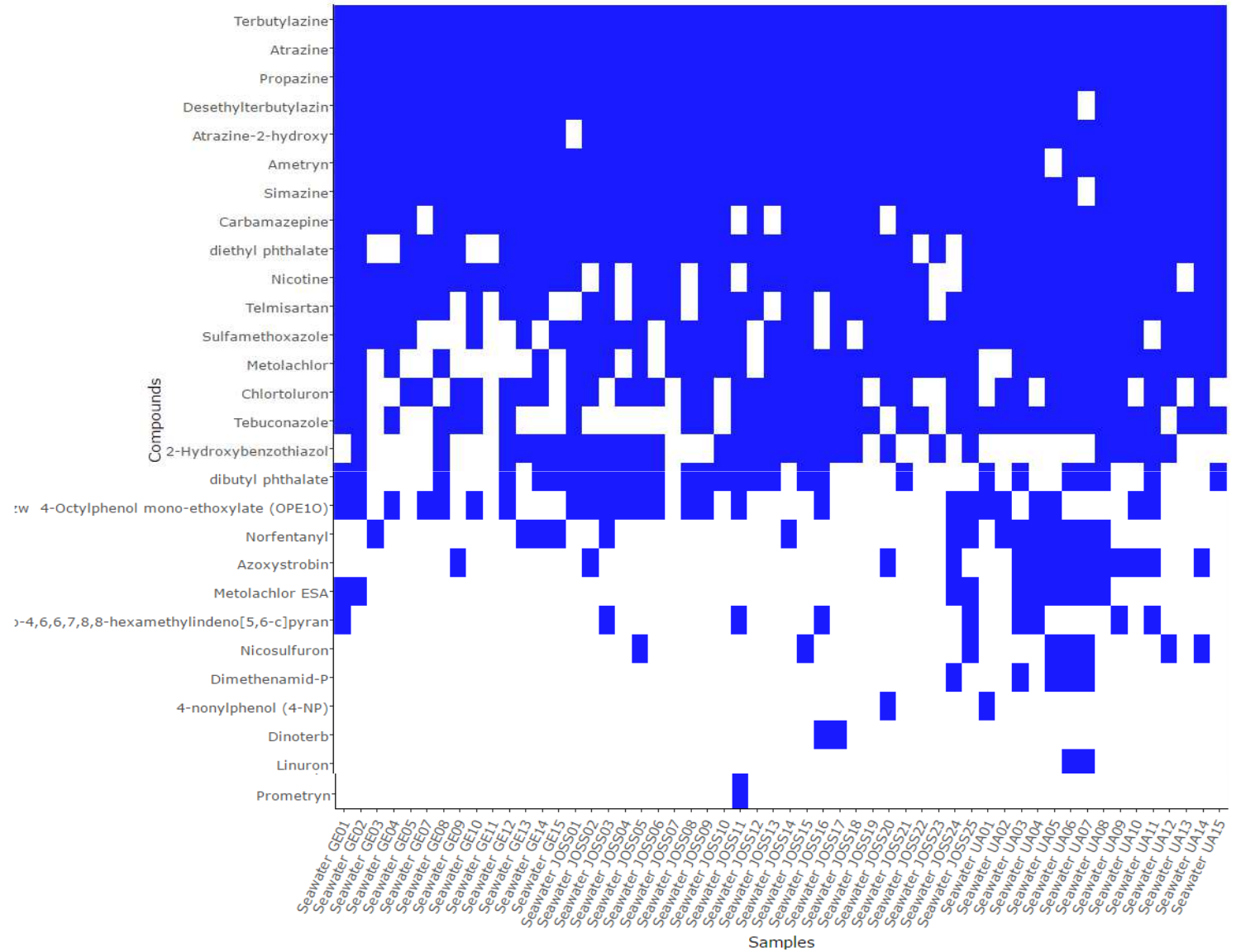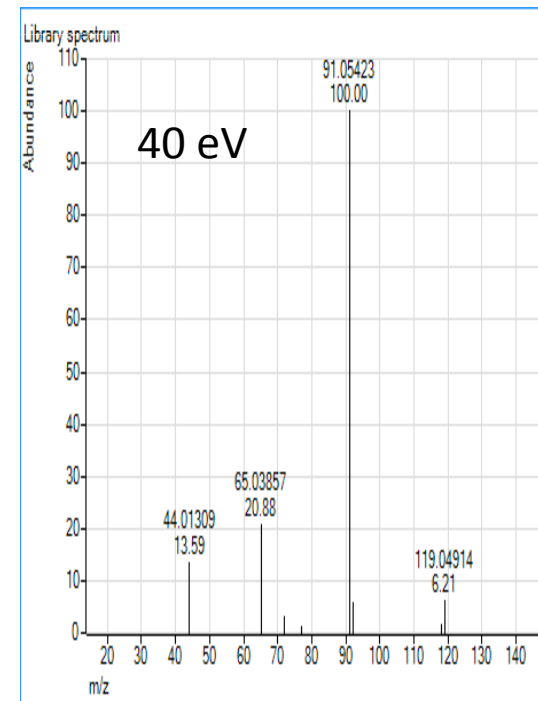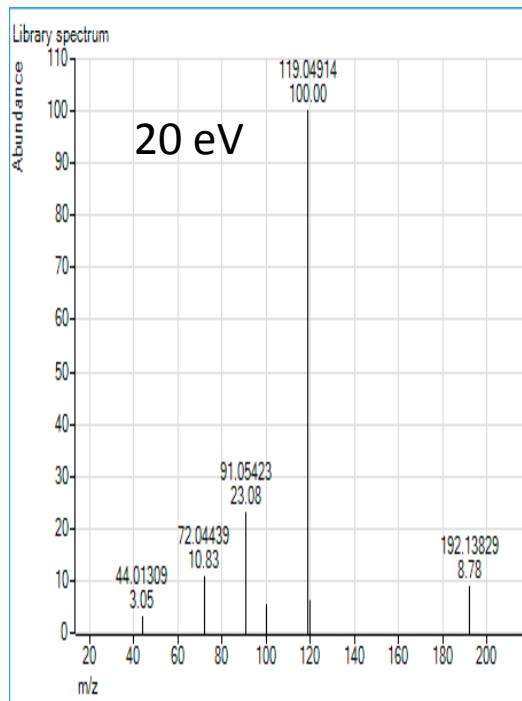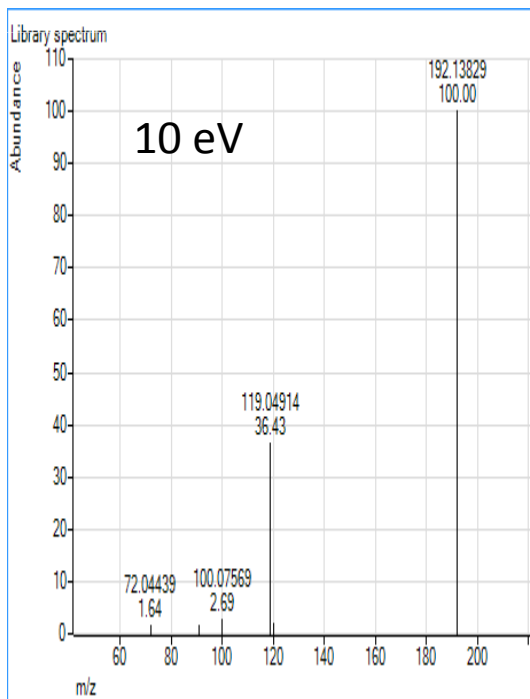

Blue color indicates that compound was detected in the corresponding sample
White color indicates that compound was not detected

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
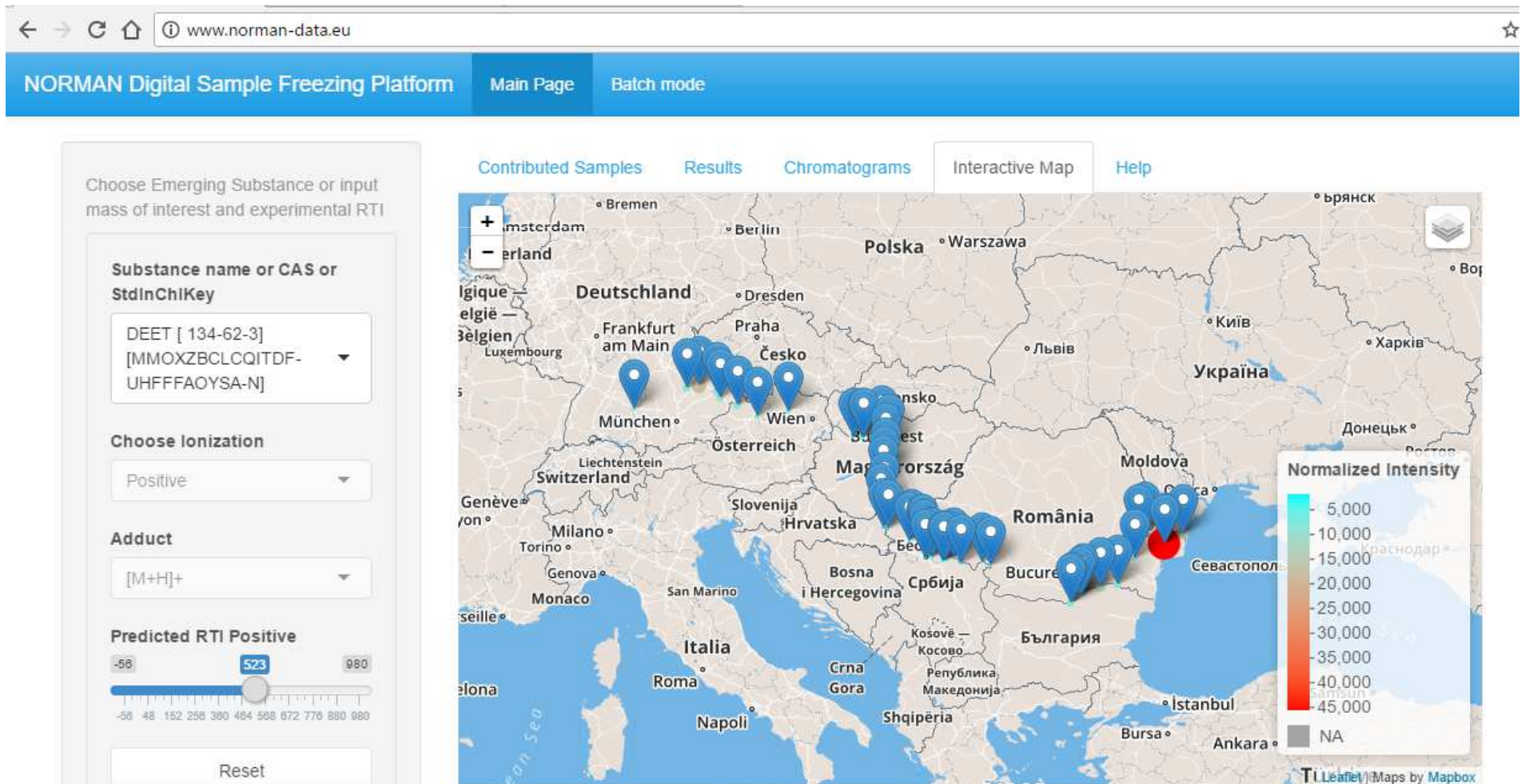- Tools: - predicted RTI (±), mass accuracy (±), specific fragments
- JDS-58-Arges – unambiguously positive for DEET
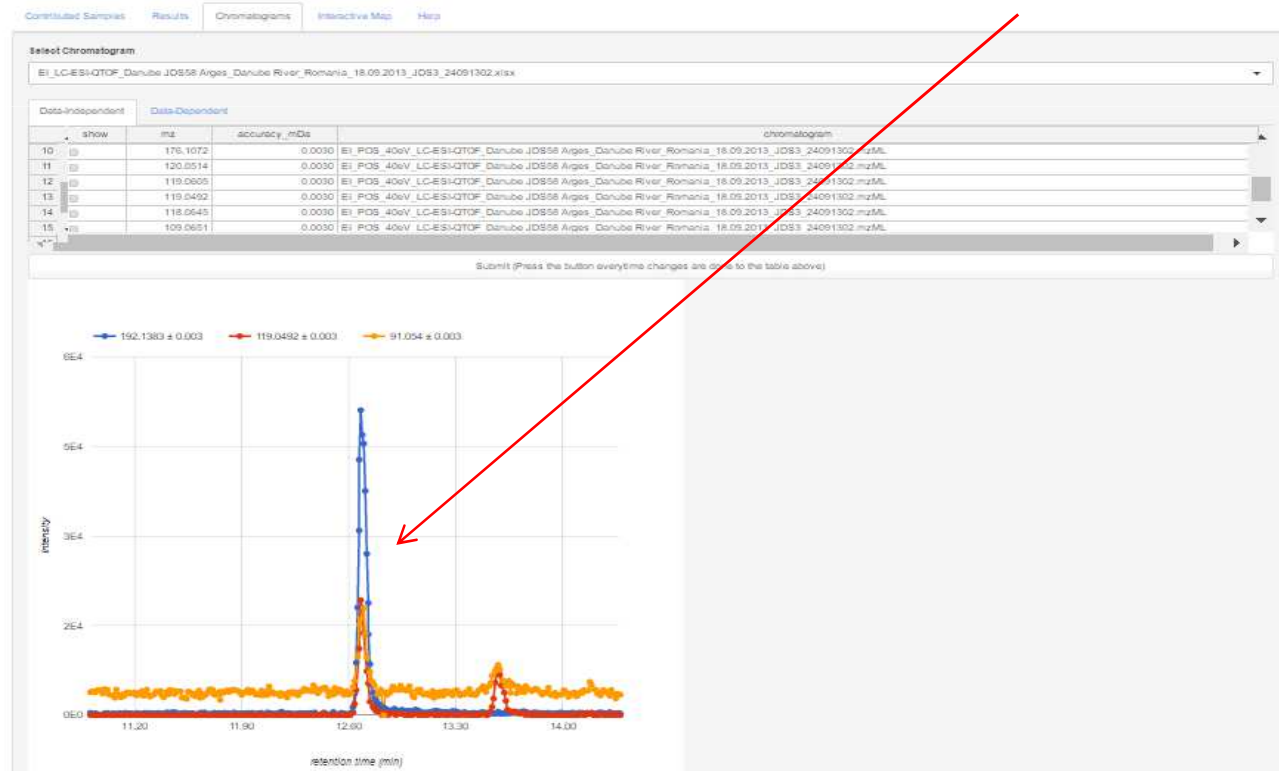
DSFP - retrospective search

- 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