

Workshop on Emerging Environmental Pollutants

Stresa, 19 – 20 June 2006



Sub-project SEARCH

Jaroslav Slobodník

Environmental Institute, Koš, Slovak Republic



Overall objectives

- Emerging substances in EU 25+ water/air/soil/biota matrices
 - Platform for bringing existing knowledge together
 - Framework for systematic elaboration, collection and scientifically sound evaluation of future data

- How?
 - Development and integration of three web-based databases
 - EMPOMAP – WP S1
 - EMPODAT – WP S2
 - EMPOMASS – WP S3

WP S1 – EMPOMAP

Overview

- European map of knowledge in the field of emerging pollutants
 - European leading experts (S1-1)
 - Organisations (S1-2)
 - Projects (S1-3)
- Major goals
 - Definition of the current state and future needs of research on emerging substances in Europe
 - Help to co-ordinate national research programmes in order to avoid duplication of research
- Additional features
 - Targeted identification of experts and stakeholders concerned with a specific emerging pollutant
 - Link to other European databases dealing with related topics (WEKNOW, GEDRI, METROPOLIS, EUGRIS...)

WP S1 - EMPOMAP

Deliverables and milestones

- Definition of the general and specific database parameters;
- Web-based database published on the project web-site (month 13);
- First 100 entries in the database (month 16).

WEKNOW

Web-based European Knowledge Network on Water

[Home](#) > [Search the database](#) > [View Expert](#)

Welcome **anonymous**

[Print current page](#)

Navigation

[Add new entry](#)

[Search the database](#)

[Experts](#)

[Projects](#)

[Organisations](#)

[Edit the database](#)

[Contact](#)

European drinking water EXPERTS

GENERAL COORDINATES - EXPERT

Family name: First name: Mr./Ms.: Title (Prof., Dr., ...):

Ainsworth **Richard** **Mr.** **Dr.**

Organisation (full name in English):

Hydraugen

Current position / job title:

Department / group:

ADDRESSES:

Street name and number:

Lower Common House, The Avenue

Town / City:

Reading, Berks.

Post code:

RG7 6NS

P.O.Box:

Bucklebury

Country:

United Kingdom

Telephone: **+44-118-9712563**

Fax:

E-mail: **r.ainsworth@btinternet.com**

Website:

PERSONAL EXPERTISE:



EUGRIS Portal for Soil and Water management in Europe



Member:
New visitor:

Quick Project & Resource search

Search EUGRIS

[Terms & conditions for use](#) | [About EUGRIS](#) | [What's New on EUGRIS](#) | [Help](#) | [Glossary](#) | [Contact us](#)

[Home](#) | [Country Pages](#) | [Library & links](#) | [Meefings/Training](#) | [News](#) | [Research & funding](#) | [Topics](#) | [Who does what](#)

Search EUGRIS

Which area of EUGRIS do you want to search?

Search using free text

Match: Any word All words Exact Phrase

Within fields: Dated:

And / or search using Keywords (select up to 5 Keywords using ctrl and mouse left click):

- Brownfields
- Contaminated land-->Contaminants-->BTEX
- Contaminated land-->Contaminants-->Chlorinated aliphatics
- Contaminated land-->Contaminants-->Contaminants overview

Search criteria:
 Find Just Free Text Find Just Keywords
 Find Free Text OR Keywords Find Free Text AND Keywords

Sort by:

WP S2 – EMPODAT

Overview

- Collection of monitoring/occurrence data on emerging substances
- Improvement of inter-comparability of the data among all EU MS
 - Harmonisation of formats of data and metadata reporting
 - Unified coding of newly assigned emerging substances, measurement units, etc.

WP S2 – EMPODAT

Overview

■ Chemical data (S2-1)

- Substances known to be present in environment, not yet included in routine monitoring programmes
- Basic information on:
 - Concentration, sample matrix, geographical co-ordinates of the sampling site, sampling date, detailed information on the analytical methodology, QA/QC measures
 - Link to the IUCLID database, recommendations by IUPAC

■ Field data from bio-monitoring (S2-2)

- Biological effects measured by bio-assays and biomarkers

WP S2 – EMPODAT

Deliverables and milestones

- **Guidance document** on the agreed data and metadata reporting formats and methodologies used for the (targeted) risk assessment;
- **Protocol** for the evaluation of data availability and quality;
- **Protocol** for unified coding of newly assigned emerging substances;
- **Protocol** with minimum information requirements for emerging substances and establishment of new databases;

- **Web-based database published on the project web-site (month 18).**
- **First 10.000 entries in the database starting with data on the selected emerging pollutants from the CASE studies (month 24).**



- Objectives
 - Organisation
 - Work/Tasks
 - News/Events**
 - Info Exchange
 - Downloads
- [\[News/Events\]](#) [\[Newsletter\]](#) [\[Update\]](#) [\[Join\]](#)

→ NEWS

- Metropolis database on-line** (News from: 12-05-2004)
The Metropolis database on bio-monitoring assays and...

Metropolis database on-line (News from: 12-05-2004)

The Metropolis database on bio-monitoring assays and chemical analytical methods is on-line on this web-site at the address <http://metropolis.speciation.net/>. The size of the database is intended to increase further thanks to the contributions from the participants in the Metropolis network and the external users. You can enter new methods in the database either by on-line submission of the data or by using an Excel template, as explained in the user instructions. The database also allows for practitioners from routine laboratories, research institutes, etc. to submit their comments, as experts using these methods. Click on >> more ... for direct access to the Metropolis database

[>> more...](#)

Metropolis, an innovative approach to research networking for improving environmental monitoring across Europe.

METROLOGY IN SUPPORT OF PRECAUTIONARY SCIENCES AND SUSTAINABLE DEVELOPMENT POLICIES



Assay Database

[Home](#) [Search](#) [Supply a new assay](#) [Need for research](#) [Ongoing research](#) [Help](#) [Log in](#)

Search the database for a specific method/ assay

Matrix

Substance

Bio-effect

Standardised

Show

Empty fields will search all possible parameters.

Keyword Search

Search for

Show all methods/ assays in the database

Order by

Show all substances

Order by



EUROWATERNET/WISE

Objectives

- Harmonisation and streamlining the reporting and information collection needs in line with the EU directives and national obligations;
- Use of the same national data sets for reporting to the EEA and other institutions.

WISE - Water Information System for Europe

- Shared pool of common and timely data and information on the state of, and pressures on, Europe's water that meets the needs of all those organisations requiring to report and make assessments at the European level.

Need for agreement on the:

- Determinants
- Level of data aggregation
- Spatial and temporal resolution
- Metadata

Tools to populate WISE – REPORTNET, EUROWATERNET (EIONET-water)

- Water Indicator Report 2003
 - Nutrients
 - Oxygen consuming substances
 - Hazardous substances (metals)
 - Hazardous substances (organics)
 - Hazardous substances (pesticides)



European Environment Information and Observation Network (EIONET)

Networking improving Europe's environment

Search Eionet

EIONET Topic areas Water Eionet-Water Data ...

Services

Helpdesk
CIRCA
EIONET Planner
Topics

Reportnet services

ROD Obligations
CDR Repository
Content Registry
Data Dictionary
Directory
IMS Indicators

Not logged in

Login

Find a member

Shortcuts for members

Directory
NFP/EIONET IG

News Item: Eionet-Water Data Request 2005

Released: 2005/08/12

To: [EIONET PCPs and NRCs for Rivers and Lakes](#)
 To: [EIONET PCPs and NRCs for Groundwater](#)
 To: [EIONET PCPs and NRCs for Marine and Coastal Environment](#)
 To: [EIONET PCPs and NRCs Water Quantity and Use](#)
 Cc: [EIONET National Focal Points](#)

From: Niels Thyssen, EEA

Date: 12 August 2005

Dear Colleague

I am writing to inform you of the detailed plans for the Eionet-Water annual data flow that is, as you know, one of the agreed EIONET Priority Data Flows.

The 2005 Eionet-Water annual data flow is the fifth formal Eionet-Water (formerly known as Eurowaternet) data collection and will run **from now until Friday, 28 October 2005**. All relevant information for data providers (guidelines, table and data element definitions, templates, code lists, etc.) can be viewed at and downloaded from the [Reportnet Data Dictionary](#).

Rivers, Lakes, Groundwater and Transitional, Coastal and Marine Waters

The data to be collected will cover the state of, and pressures on, Europe's rivers, lakes, groundwater and transitional, coastal and marine waters. Quality determinands include those relating to nutrients, organic pollution indicators and hazardous substances.



Elements

Short name	Datatype	Element type
CountryCode^C	string	Fixed values
NationalStationID^C	string	Quantitative
Year^C	integer	Quantitative
Month^C	integer	Quantitative
Day^C	integer	Quantitative
Determinand_HazSubs^C	string	Quantitative
Unit_HazSubs^C	string	Quantitative
CASNumber^C	string	Quantitative
SampleAnalysis^C	string	Fixed values
LimitFlag^C	string	Quantitative
LimitOfDetection^C	float	Quantitative
LimitOfDetermination^C	float	Quantitative
Concentration^C	float	Quantitative
Remarks^C	string	Quantitative

(the ^C sign marks a common element)

Complex attributes

RegistrationAuthority	EEA European Environment Agency www.eea.eu.int
SubmitOrganisation	European Topic Centre on Water ETC-W Dr Tim Lack lack@wrcplc.co.uk water.eionet.eu.int

WP S3 – EMPOMASS

Overview

- Geo-referenced data of “unknown” and “provisionally identified” substances
 - **Numeric information extracted from the screening results**
 - E.g, major ions in the mass spectrum of the compound, retention characteristics, match factor, proposed structure, CAS number, molecular mass, etc.
 - **Raw mass spectra organised and searchable in the emerging substances library**
- **Goals:**
 - Occurrence and pollution trends for substances currently not included in major monitoring schemes because of the lack of knowledge on their identity
 - Definition of new emerging threats
 - Interpretation of historical data
 - Definition of needs for targeted research to identify the detected unknown substances

WP S3 – EMPOMASS

Deliverables and milestones

- Definition of the general and specific database parameters;
- Web-based database published on the project web-site (month 13);
- First 2.000 entries in the database (month 18);
- A set of criteria to judge whether additional targeted research is needed on identification of the detected unknown substances (month 24).

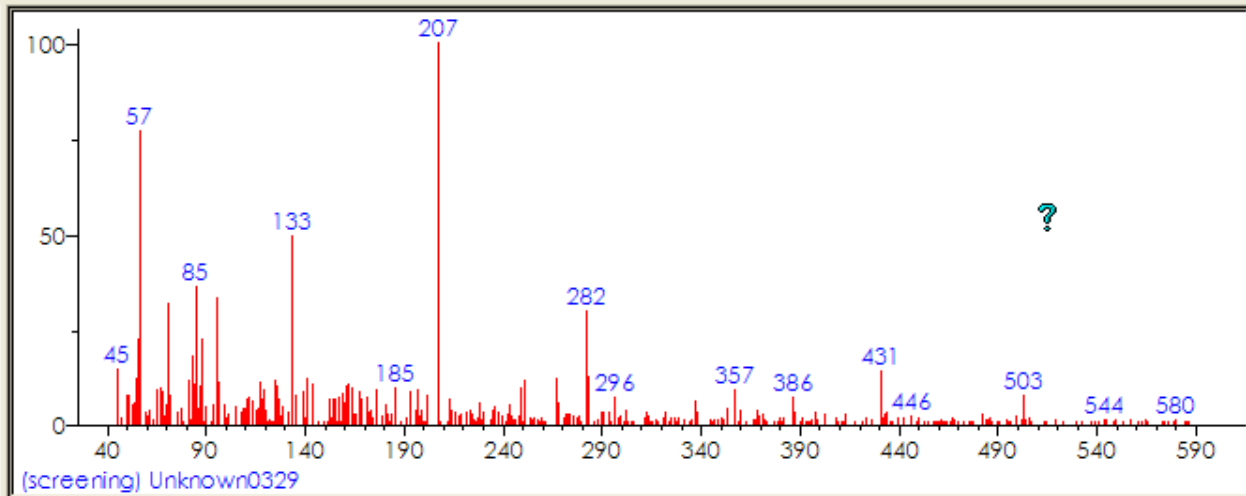
UNKNOWN0329

Clear

a-z

screening

- Unknown0322
- Unknown0323
- Unknown0324
- Unknown0325
- Unknown0326
- Unknown0327
- Unknown0328
- Unknown0329
- Unknown0330
- Unknown0331
- Unknown0332
- Unknown0333
- Unknown0334
- Unknown0335
- Unknown0336
- Unknown0337
- Unknown0338
- Unknown0339
- Unknown0340
- Unknown0341
- Unknown0342
- Unknown0343
- Unknown0344
- Unknown0345
- Unknown0346
- Unknown0347
- Unknown0348
- Unknown0349
- Unknown0350
- Unknown0351
- Unknown0352
- Unknown0353
- Unknown0354
- Vanillin
- Z-7-Hexadecenoic acid



Name: Unknown0329
 Formula:
 MW: N/A CAS#: N/A NIST#: N/A ID#: 786 DB: screening
 Other DBs: None
 Comment: SHMU5/HN07OV
 10 largest peaks:
 207 999 | 57 767 | 133 491 | 85 358 | 95 333 |
 71 315 | 282 295 | 56 225 | 88 222 | 83 179 |
 Synonyms:
 1 r = 1.645

Names Structures

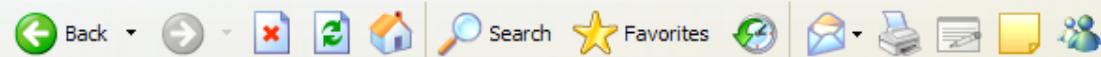
PlotText Plot

Lib. Search Other Search Names Compare Librarian



Feedback

- Who is going to be the user(s) of the database?
- What do you want to get out of the database?
- How can the data producers be motivated to contribute their data to the databases?
- What should be the minimum QA/QC metadata information (next to the name of the compound and its concentration) in order you would trust the data?



Database NORMAN – EMPOMAP

Navigation

- [Home page](#)
- [Search the database](#)
- [Contact](#)

- [Add new entry or Edit the database](#)

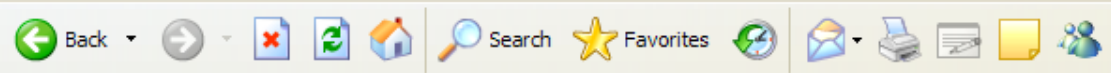
NORMAN - EMPOMAP

Database of European Experts, Organizations and Projects dealing with emerging substances.

This database is part of NORMAN SEARCH sub-project, with modules containing links to the leading European Experts (S1-1), Organizations (S1-2) and Projects (S1-3). It is developed as a web application, using MySQL software.

The database can be searched through keywords and entry categories. Therefore it is essential to use as many Keywords as possible, to identify all of the major research areas and topics (e.g. in the summaries, additional information, using the most indicative titles of the publications, etc.)

To create entries into the database of Experts/Organizations/Projects, please, navigate to 'Add new entry or Edit the database'. A notification e-mail will be sent to you after successful entries of the data.



Address <http://www.ei.sk/norman/search.php>

Go Links >>



Database NORMAN – EMPOMAP

Navigation

- [Home page](#)
- [Search the database](#)
- [Contact](#)
- [Add new entry or Edit the database](#)

Search the database

Select database:

- Expert
- Organisation
- Project



You are logged in as Admin Admin (Username: admin)

Database NORMAN – EMPOMAP

EUROPEAN EMERGING SUBSTANCES EXPERTS INVENTORY SUBMISSION

Please, complete the following form to submit your profile for the **NORMAN** inventory (i.e., Network of reference laboratories and related organisations for monitoring and bio-monitoring of environmental pollutants).

NOTE: Those FIELDS IN RED ARE MANDATORY and unless these fields are filled in, the entry will not be accepted by the database.

GENERAL COORDINATES - EXPERT

- Navigation**
- [Home page](#)
 - [Search the database](#)
 - [Contact](#)
 - [Add new entry or Edit the database](#)
 - [Your Profile](#)
 - [Logout](#)

Family name:

First name:

Mr./Ms.:

Title (Prof., Dr., etc. ...):

Current position/job title:

Department/group:

Organisation (full name):

Address

Street name and number:

P.O. Box (if applicable):

Town/City:

Post code:

Country:

Telephone (+XX-XXX-XXXXXXX):

Fax:

E-mail:

Web-site:

Type of organisation (please select ONE as appropriate):

- Governmental organisation/regulatory body
- International organisation
- National reference laboratory or equivalent
- Non-governmental organisation (NGO)
- Private consulting company
- Private research institute
- Public research institute
- River water authority
- University/other academic institution
- Other (please specify):
- Number of employees:

Scope of activities (please select ALL that apply):

- Bio-assays
- Bioindicators
- Biomarkers
- Bio-monitoring
- Database development
- Development/validation of analytical methods
- Emerging substances in air
- Emerging substances in biota
- Emerging substances in soils, suspended matters, sediments
- Emerging substances in water
- Environmental risk assessment
- Health aspects related to emerging substances
- Identification of emerging substances by mass spectrometry techniques
- Legislation/networking
- Monitoring of emerging substances
- Quality assurance/quality control
- Quality standards/guideline values for emerging substances

**Project primary focus (please select ALL that apply):**

- Monitoring of emerging substances
- Analytical method development/validation
- Exposure assessment
- Hazard assessment
- Risk assessment
- Legislation/quality standards/networking
- Treatment technologies

Others (please specify): **Project specific focus (tick all that apply):**Monitoring of emerging substances

- Chemical quality analysis – metals and metal species
- Chemical quality analysis – organic micropollutants
- Chemical quality analysis – radioactivity
- Development of databases
- Development of monitoring strategies
- Identification of unknown pollutants

Others (please specify): Analytical method development/validation

- Criteria for method acceptance
- Development of new methodologies
- Quality assurance/quality control

Others (please specify): Exposure assessment

- Biomarkers of exposure
- Modelling
- Pharmaco-kinetic

You are logged in as **Admin Admin** (Username: admin)

Navigation

- [Home page](#)
- [Search the database](#)
- [Contact](#)
- [Add new entry or Edit the database](#)
- [Your Profile](#)
- [Logout](#)

Search EXPERT

PLEASE SELECT FIELDS IN WHICH YOU WANT TO SEARCH

Search options:

At least one of the selected criteria must comply ▼

Search criteria:

Primary field of work: PLEASE SELECT ONE ▼

Additional field of work: PLEASE SELECT ONE ▼

Other additional field of work: PLEASE SELECT ONE ▼

Country: PLEASE SELECT ONE ▼

Please, select **ADDITIONAL** search criteria: ▼ ⓘ ▼ ⓘ ▼ ⓘ

Search

Reset



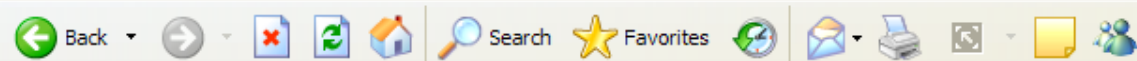
Database NORMAN – EMPOMASS

Navigation

- [Home page](#)
- [Search the database](#)
- [Contact](#)
- [Add new entry or Edit the database](#)

The EMPOMASS database (WP S3) focuses on the collection of geo-referenced data of "unknown" and "provisionally identified" substances in various environmental compartments. Mass spectra obtained from GC-MS screening in electron impact mode are widely accepted as unique fingerprints of individual organic compounds and therefore will form its basis. However, with a view to the latest scientific achievements in the field of mass spectrometry, the database format will be designed to also accommodate information on LCMS(MS) and exact mass measurement data. The database consists of two modules: one containing numeric information extracted from the screening results such as major ions in the mass spectrum of the compound, retention characteristics, match factor, proposed structure, CAS number, molecular mass, etc. (S3-1), and the other containing raw mass spectra organised and searchable in the specific emerging substances library (S3-2). A specific protocol will be developed and validated for estimation of the concentrations of "unknown" substances, for which the standard chemical is not available. The database will allow the user to trace occurrence and pollution trends for substances, which are currently not included in major monitoring schemes because of the lack of knowledge on their identity. A set of criteria will be developed to judge whether additional targeted research is needed to identify the detected unknown substances, e.g., based on the frequency of occurrence, concentrations or evidence of biological impact in the vicinity of the sampling site(s). Extensive European research resources have already been invested in identification of substances not having mass spectra in the commercially available libraries. It is expected that the EMPOMASS database will bring all this knowledge together and also aid the interpretation of historical data by simple reprocessing of "old" mass spectra of as yet unidentified compounds. Similar to the EMPODAT database, existing data of

NORMAN network members will be inserted into the database and links to the existing national (e.g., GC-MS database of RIZA, the Netherlands) or international (e.g., JDS Database of the ICPDR) databases will be created.

**Database NORMAN – EMPOMASS****Navigation**

- [Home page](#)
- [Search the database](#)
- [Contact](#)

- [Add new entry or Edit the database](#)

Search the database**Select database of substances:**

- Provisionally identified
- Unknown

Select analytical method:

- GC-MS
- LC-MS(MS)
- Exact mass measurement data

**Database NORMAN – EMPOMASS****Navigation**

- [Home page](#)
- [Search the database](#)
- [Contact](#)
- [Add new entry or Edit the database](#)

Search Provisionally identified, Unknown substances: GC-MS**PLEASE SELECT FIELDS IN WHICH YOU WANT TO SEARCH****Search options:**At least one of the selected criteria must comply **Search criteria:**Country: River: River length [km]: Sampling site: Matrix: Base ion: Provisionally identifiedAdditional ions: Unknown UnknownDeterminant: CAS number: Determinant code: Match factor [%]: Molecular weight: Chem. formula:

**Database NORMAN – EMPOMASS****Navigation**

- [Home page](#)
- [Search the database](#)
- [Contact](#)

- [Add new entry or Edit the database](#)

Search Provisionally identified, Unknown substances: GC-MS**PLEASE SELECT FIELDS IN WHICH YOU WANT TO SEARCH****Search options:**

At least one of the selected criteria must comply ▼

Search criteria:

Country:

River:

River length [km]:

Sampling site:

Matrix:

Base ion:

Provisionally identified

Additional ions:

Determinant:

CAS number:

Determinant code:

Match factor [%]:

Molecular weight:

Chem. formula:



Database NORMAN – EMPOMASS

Navigation

- [Home page](#)
- [Search the database](#)
- [Contact](#)
- [Add new entry or Edit the database](#)

Search Provisionally identified, Unknown substances: GC-MS

64 match(es) found to your query

		Sampling site	Sampling date	Matrix	Determinant	SCAN number
3	<input type="checkbox"/>	Volkswagen Slovakia a.s.	01.10.2003	Waste water	Hexa(methoxymethyl)melamine	2727
4	<input type="checkbox"/>	Volkswagen Slovakia a.s.	01.10.2003	Waste water		2444
6	<input type="checkbox"/>	Istrochem a.s.	01.10.2003	Waste water	Cyclohexanamine	268
7	<input type="checkbox"/>	Istrochem a.s.	01.10.2003	Waste water	Aniline	492
8	<input type="checkbox"/>	Istrochem a.s.	01.10.2003	Waste water	Cyclohexane, isocyanato-	547
9	<input type="checkbox"/>	Istrochem a.s.	01.10.2003	Waste water	Aniline, N-methyl-	674
11	<input type="checkbox"/>	Istrochem a.s.	01.10.2003	Waste water	Benzenamine, N,N-dimethyl-	755
14	<input type="checkbox"/>	Istrochem a.s.	01.10.2003	Waste water	Tributylamine	982
15	<input type="checkbox"/>	Istrochem a.s.	01.10.2003	Waste water	Benzothiazole	1024
16	<input type="checkbox"/>	Istrochem a.s.	01.10.2003	Waste water	Phenol, 4-chloro-2-methyl-	1072
17	<input type="checkbox"/>	Istrochem a.s.	01.10.2003	Waste water	Benzothiazole, 2-methyl-	1147
18	<input type="checkbox"/>	Istrochem a.s.	01.10.2003	Waste water	1,2-Benzisothiazole, 3-methyl-	1176
19	<input type="checkbox"/>	Istrochem a.s.	01.10.2003	Waste water		1312
20	<input type="checkbox"/>	Istrochem a.s.	01.10.2003	Waste water		1351
21	<input type="checkbox"/>	Istrochem a.s.	01.10.2003	Waste water	N-Cyclohexylidene-N-cyclohexylamine	1432
22	<input type="checkbox"/>	Istrochem a.s.	01.10.2003	Waste water	1H-Pyrazole, 4-chloro-1-phenyl-	1467

http://www.ei.sk - Provisionally identified substances: GC-MS - ...

Country:	Slovak Republic
River:	Morava
River length [km]:	0.55
Sampling site:	Volkswagen Slovakia a.s.
Sampling date:	01.10.2003
Matrix:	Waste water
Base ion:	343
Additional ions:	267, 207, 163, 177, 375
Determinant:	Hexa(methoxymethyl)melamine
CAS number:	680002-20-0
Determinant code:	
Identified by:	NIST lib.
Match factor [%]:	90.5
Molecular weight:	390
Chem. formula:	C15H30N6O6
Reduced time:	1.33
SCAN number:	2727
Raw chromatogram:	3.MS
Internal standard:	Propazine
Mass spectrum snapshot:	3.gif
Standard operation procedure:	STN EN ISO 6468
Sample preparation technique:	SPE cartridge
Sample volume [ml]:	100 ml
Instrument:	HP 6890
Injector:	LVI, PTV-LVI
Injector conditions:	70°C(0.5 min)-720°C/min-280°C
Carrier gas:	H2
Column:	HP-MS1; 30m x 0.1mm x 0.1um
Temperature program:	60°C(2 min)-5°C/min-180°C-10°C/min-280°C (10 min)
Flow rate [ml/min]:	1.2
Derivatization:	No
Detector type:	Quadrupole
Scan range [amu]:	45-500
Scan frequency [scan/s]:	1.2

norman

stances: GC-MS

Matrix	Determinant	SCAN number
Waste water	Hexa(methoxymethyl)melamine	2727
Waste water		2444
Waste water	Cyclohexanamine	268
Waste water	Aniline	492
Waste water	Cyclohexane, isocyanato-	547
Waste water	Aniline, N-methyl-	674
Waste water	Benzenamine, N,N-dimethyl-	755
Waste water	Tributylamine	982
Waste water	Benzothiazole	1024
Waste water	Phenol, 4-chloro-2-methyl-	1072
Waste water	Benzothiazole, 2-methyl-	1147
Waste water	1,2-Benzisothiazole, 3-methyl-	1176
Waste water		1312
Waste water		1351
Waste water	N-Cyclohexylidene-N-cyclohexylamine	1432
Waste water	1H-Pyrazole, 4-chloro-1-phenyl-	1467