



# Integration of European Simulation Chambers for Investigating Atmospheric Processes

## N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies

CEAM FOUNDATION

EUROPEAN PHOTOREACTOR –EUPHORE–

**Amalia Muñoz-Cintas**  
**Joaquín Valero-Pinazo**  
**Elena Gómez-Álvarez**  
**Mónica Vázquez-Moreno**

## N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies

Activity N1



Raw Data Analyses,  
Data Inter-comparison  
and Quality Assurance.

Activity N2

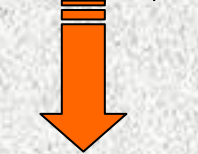


Standardised Data  
Protocol and Central  
Database of  
Environmental Chamber  
Studies.

Activity N3



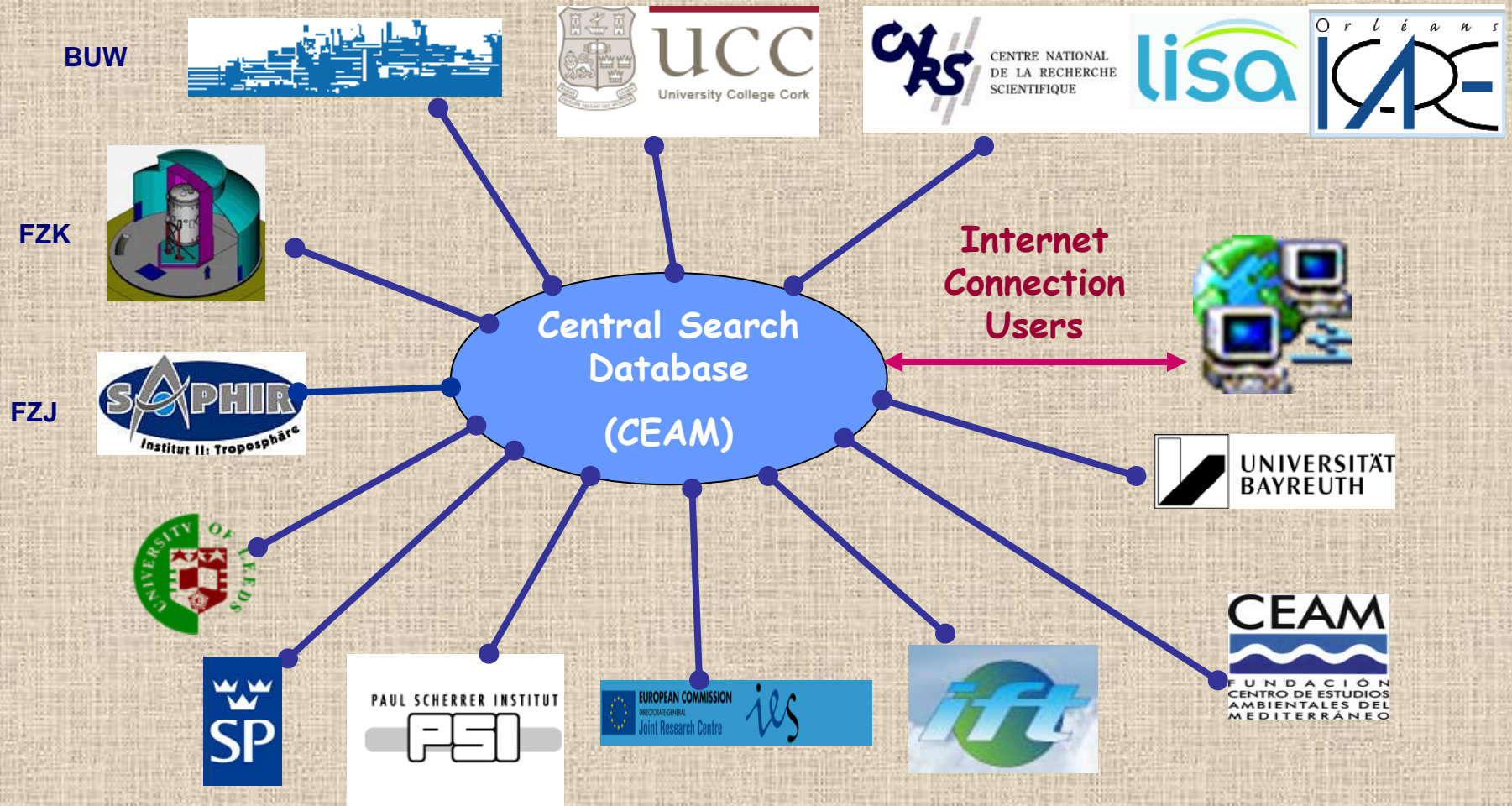
Infrastructure-related  
workshops.



- Tool for atmospheric chemists to obtain kinetic and mechanistic information
- Aims interpretability and comparability between different chambers
- 13 Individual partners
- Database based on a decentralised concept



# N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies





# N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies

## WORKING PLAN

PROJECT MILESTONES AND DELIVERABLES		Year 1				Year 2				Year 3				Year 4				Year 5				
		I	II	III	IV	I	II	III	IV	I	II	III	IV	I	II	III	IV	I	II	III	IV	
N2	STANDARDISED DATA PROTOCOL AND CENTRAL DATABASE OF ENVIRONMENTAL CHAMBER STUDIES																					
	Definition of the standardised data protocol (M)	█	█																			
	Construction of the database (1 <sup>st</sup> version) (M)			█	█																	
	Release of the database on WWW (D)					█																
	Construction of data interfaces by the chamber-operating partners, report (D)			█	█																	
	Linkage between the interfaces and the central database (D)					█	█															
	Improvements of the central database																					

- 2004:** Start database design
- 2005:** First version for testing
- 2006:** Fully functional released version.  
**November:** EUROCHAMP Database workshop (Valencia, Spain)
- 2007-2009:** Database improvements and operation



# N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies

<http://eurochamp-database.es>

## Access as **GUEST**:

- No username or password required.
- All records can be seen, but not all fields.
- There are no privileges to either insert, modify or delete records.

## Access as **USER**:

- Username and password required.
- All records and fields can be seen.
- There are no privileges to either insert, modify or delete records.
- Non-registered users, can apply to register.

## Access as **INSTITUTION**:

- Username and password is required (provided to each partner institution).
- Only the institution own records can be seen.
- Full privileges to insert, modify and delete their own records.

EUROCHAMP Data Server Search Engine

Notice: Web pages are subject to a disclaimer and a copyright notice.

[EUROCHAMP Home Page](#) | [Sixth Framework Programme](#) | [European Commission](#)

## EUROCHAMP Database Server

[Introduction](#)

[Access Database GUEST](#)

[Access Database USERS](#)

[Access Database INSTITUTIONS](#)

[Web Statistics](#)

[Useful Links to Partners](#)

[CEAM EUPHORE Lab.](#)  
[FZJ-ICG-II Homepage](#)  
[FZK AIDA Homepage](#)  
[PC University of Wuppertal](#)  
[UCC-CRAC Homepage](#)  
[JRC-IES Ispra](#)  
[CNRS-LCSR Orleans](#)  
[PSI-LAC Villigen](#)  
[University of Bayreuth](#)  
[Uni. Leeds Chemistry](#)  
[SP Technical Research Institute of Sweden](#)  
[CNRS-LISA Paris](#)  
[IFT Leipzig](#)



### Project Description

EUROCHAMP is a research project funded within the EC 6th Framework Programme, Section "Support for research Infrastructures - Integrated Infrastructure Initiative".

11 European Partners are the backbone of this project, a grid of environmental chambers designed for the scientific investigation of atmospheric transformation processes. A number of associated research groups worldwide contribute to the project providing expert knowledge in specific fields of atmospheric science.

### Database on Environmental Chamber Studies

The search engine will provide access to the data recorded during the experimental runs performed in the environmental simulation chambers of the participating institutes. There is a huge difference in size, scientific scope, technical capabilities and research topics treated among the groups providing the analysed data. The main objective is to give easy access to the data records and associated calibration files, with simple but specific search criteria and an easy to manage download facility.

Hosted at [Fundación Centro de Estudios Ambientales del Mediterráneo - CEAM](#)

[Parque Tecnológico](#) - C/ Charles R. Darwin, 14 46980 - PATERNA - VALENCIA - ESPAÑA

Created by: EUROCHAMP - EU 6th FP Infrastructure Initiative Web-site contact e-mail address: [eurochamp\\_master@ceam.es](mailto:eurochamp_master@ceam.es)



• **Open source software packages**



# N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies

## INPUT FILES

**EUROCHAMP Network Activity 2 Database Insert/Update Records**

Insert a new record

Required fields are in red.

Date of experiment  Please use the format yyyy-mm-dd or yyyy-mm-dd if you add a series.

Type of experiment  Please select from the drop down menu.

Keywords  Enter different key words separated by a comma. A keyword list can be obtained from the

Reactants  Please enter the chemical names separated by comma.

Smiles  Please enter the SMILES separated by comma. [HELP](#)

CAS number  Enter the CAS number using the following format 1234-45-6.

Parameters  Please fill the field with the parameters separated by comma.

Pressure [Pa]  Give the mean pressure in Pa.

Temperature [K]  Give the mean temperature in K.

Light source used  Please select from the drop-down menu.

Reactive species  Please select from the drop down menu.

Resource link  Please enter the URL of the original data record linked to this entry.

Project name  Enter the project name and acronym.

Institute  Please enter your institute name from the drop down menu.

Experimental Reference Number  Please enter a unique number to identify the experiment.

Description  Please introduce the url of the pdf file.

Formula\_Index  Enter the Formula index of your reagents.

Option  Option field for additional information.

Insert a new record

(Total records:0) [Home](#) | [Insert](#) | [Search](#) | [Show all](#) | [Logout](#) | [Top](#)  
[data\\_records](#)

[Data introduction in the EUROCHAMP database: documents required](#)  
[Format established for introduction of files](#)

[Database Home](#) // [Access GUEST](#) // [Access USER](#) // [Access INSTITUTION](#)

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Parque Tecnológico "Dr Charles R. Darwin, 14 46100 - PATERNA - VALENCIA - ESPAÑA  
Created by: EUROCHAMP - EV 5th FP Infrastructure Initiative, Web-site contact e-mail address: [suexchamp\\_master@ceam.es](mailto:suexchamp_master@ceam.es)

- Date of experiment
- Type of experiments
- Keywords
- Reactants
- Smiles notation
- CAS number
- Parameters
- Pressure
- Temperature
- Light source used
- Reactive species
- Resource link
- Project name
- Institute
- Experimental Conditions
- Description
- Formula\_index
- Option

➤ Data introduction in the EUROCHAMP database: documents required

➤ Format established for introduction of files



# N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies

## Eurochamp Database Format: EDF (Text/Ascii)

<http://saphir.fz-juelich.de/eurochamp/>

Activity N1

### Tools

- edf template generator
- edf file checker
- edf file creator
- edf file merger
- edf file correlator
- edf file converter
- edf idl routines
- How to create edf files

Navigation: [SAPHIR @ ICG-2](#) / [wikis @ ICG-2](#) / [ICG-2 home page](#) / [FZJ home page](#)



# EUROCHAMP

Integration of European Simulation Chambers for Investigating Atmospheric Processes

A Research Project within the:  
  
EC 6th Framework Programme

### EUROCHAMP in general

**EUROCHAMP** is a research project funded within the [EC 6th Framework Programme](#), Section "Support for research Infrastructures - Integrated Infrastructure Initiative". [Twelve European partners](#) are the backbone of this project, which provides a grid of environmental chambers designed for the scientific investigation of atmospheric chemical processes. For further details see the new [EUROCHAMP web page](#) and references therein. An [overview on the technical data and publications](#) of the different chambers within EUROCHAMP is provided on this server.

### EUROCHAMP data format

New file format in use, now version 2, with support of 2-d data. Please read the pdf file [EUROCHAMP data format \(edf\)](#) and email comments [here](#). A history of previous versions can be seen at [the fileformats page](#). The following list of programs is intended to help you with the correct creation of the files. These programs are part of EUROCHAMP's *Networking Activity N1: Raw Data Analysis, Data Inter-comparison and Quality Assurance*. These programs provide a well defined interface for all chamber data which are accessible through the EUROCHAMP data base. The edf file format primarily supports time series as recorded in most chambers, e.g. concentration profiles. Now (2008-7-3) it supports 2-d data, i.e. time series of spectra. Pictures and movies and 3-d or 4-d data not supported.

1. [edf template generator](#) interactively creates a edf header template which can be downloaded and used as header for your data. This program is **already running** and [comments are welcome](#).
2. [edf file checker](#) reads your edf file which you upload to our server. You will receive a log file of the tests done on your file. If all tests are passed the data in your file will be plotted and you can download the figures. Under construction! Please [email comments](#).
3. [edf file creator](#) makes an edf file from data you submit to our server. This is still under construction! Email suggestions [here](#).
4. [edf file merger](#) combines a number of edf files into one edf file with a common time axis. A [detailed description](#) is provided. There are number of open questions and software issues. Therefore this routine is also under construction and will not be



# N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies

## Search for records

All the conditions required

Date of experiment is equal to

Last update 01 01 1968

Type of experiment is equal to

Keywords contains

Reactants contains

Smiles contains

CAS number is equal to

Parameters is equal to

Pressure [Pa] is equal to

Temperature [K] is equal to

Light source used is equal to

Reactive species is equal to

Project name contains

Institute is equal to

Experimental Reference Number is equal to

Formula\_Index is equal to

Search for record

(Total records:296)











[All Records](#) | [Search](#) | [Show all](#) | [Logout](#) | [Top](#)

# N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies

## EUROCHAMP Network Activity 2 Database

289 records found

Page 10 of 29 [1](#) [2](#) [3](#) [4](#) [5](#) [6](#) [7](#) [8](#) [9](#) [10](#) [>](#) [>>](#)

	Date of experiment	Type of experiment	Reactants	Parameters	Reactive species	Institute
	2002-05-30	Ozonolysis product study radical scavenger ambient temperature	propene, ozone, 500ppmV carbonmonoxide	p, T, O3, C3H6, H2O, HCHO, Gas Flow	O3 ozone	Forschungszentrum Juelich GmbH ICG-II
	2002-06-04	Ozonolysis product study radical scavenger ambient temperature	ethene, ozone, 500ppmV carbonmonoxide	p, T, O3, C2H4, H2O, HCHO, Gas Flow	O3 ozone	Forschungszentrum Juelich GmbH ICG-II
	2002-06-07	Ozonolysis product study radical scavenger ambient temperature	Z-2-butene, E-2-butene, ozone	p, T, O3, C4H8, H2O, HCHO, Gas Flow	O3 ozone	Forschungszentrum Juelich GmbH ICG-II
	2002-06-08	Ozonolysis product study radical scavenger ambient temperature	E-2-butene, ozone, 500ppmV carbonmonoxide	p, T, O3, C4H8, H2O, HCHO, Gas Flow	O3 ozone	Forschungszentrum Juelich GmbH ICG-II
	2002-07-03	OH product study ambient temperature NOx	p-xylene	p-xylene, P, T, NO, NO2, NOx, O3, J(NO2), Formaldehyde, Nitric Acid, Formic Acid, Glyoxal	OH hydroxyl radical	EUPHORE Laboratories, Fundación CEAM
	2002-07-06	Ozonolysis product study radical scavenger ambient temperature	1-butene, ozone, 500ppmV carbonmonoxide	p, T, O3, C4H8, H2O, HCHO, Gas Flow	O3 ozone	Forschungszentrum Juelich GmbH ICG-II
	2002-07-12	Photolysis ambient temperature	propyl nitrite, CO	Time, CH3CH2CH2ONO, CH3CH2CH2ONO2, CO, CH3CH2CHO, CH3C(O)CH3, HCHO, NO2, O3		LISA-ERMAS University of Paris
	2002-07-12	Ozonolysis product study radical scavenger ambient temperature	i-butene, ozone	p, T, O3, C4H8, H2O, HCHO, Gas Flow	O3 ozone	Forschungszentrum Juelich GmbH ICG-II
	2002-07-18	Photolysis ambient temperature	propyl nitrite, CO	Time, CH3CH2CH2ONO, CH3CH2CH2ONO2, CO, CH3CH2CHO, CH3C(O)CH3, HCHO, NO2, O3		LISA-ERMAS University of Paris
	2002-07-18	OH product study ambient temperature NOx	p-xylene	p-xylene, P, T, NO, NO2, NOx, O3, Nitric Acid, HONO, J(NO2), Formaldehyde	OH hydroxyl radical	EUPHORE Laboratories, Fundación CEAM

(Total records:289)

[All Records](#) | [Search](#) | [Show all](#) | [Logout](#) | [Top](#)



# N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies



## EUROCHAMP Network Activity 2 Database

### Details of the record

**Date of experiment** 2002-07-03

**Upload date** 15 Jan 2007

**Last update**

**Type of experiment** OH product study ambient temperature NO<sub>x</sub>

**Keywords** p-xylene, photooxidation, VOCs, NO<sub>x</sub>

**Reactants** p-xylene

**Smiles** c1c(ccc(c1)C)C

**CAS number** 106-42-3

**Parameters** p-xylene, P, T, NO, NO<sub>2</sub>, NO<sub>x</sub>, O<sub>3</sub>, J(NO<sub>2</sub>), Formaldehyde, Nitric Acid, Formic Acid, Glyoxal

**Pressure [Pa]** 0

**Temperature [K]** 0

**Light source used** Natural sunlight none

**Reactive species** OH hydroxyl radical

**Resource link** [http://80.24.165.149/files/eurochamp/Chamber\\_A/2002\\_07\\_03/2002\\_07\\_03\\_chA\\_lkas.htm](http://80.24.165.149/files/eurochamp/Chamber_A/2002_07_03/2002_07_03_chA_lkas.htm)

**Project name** Effects of the oxidation of the aromatic compounds in the troposphere (EXACT)

**Institute** EUPHORE Laboratories, Fundación CEAM

**Experimental Reference Number** 2002\_07\_03\_chA

**Description** [http://80.24.165.149/files/eurochamp/Chamber\\_A/2002\\_07\\_03/documents/2002\\_07\\_03\\_chA\\_mvfg.pdf](http://80.24.165.149/files/eurochamp/Chamber_A/2002_07_03/documents/2002_07_03_chA_mvfg.pdf)

**Formula\_Index** C<sub>8</sub>H<sub>10</sub>

**Option**


(Total records:289)

[All Records](#) | [Search](#) | [Show all](#) | [Logout](#) | [Top](#)

# N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies

## Ozonolysis of methyl vinyl ketone (MVK)

Date: 2004\_03\_12 / Uploaded: 2006\_04\_28

Institute	Fundación CEAM	
Experiment Reference Number	2004_03_12_chB	
Experiment Type	Ozonolysis - room temperature	

### Available Data Files

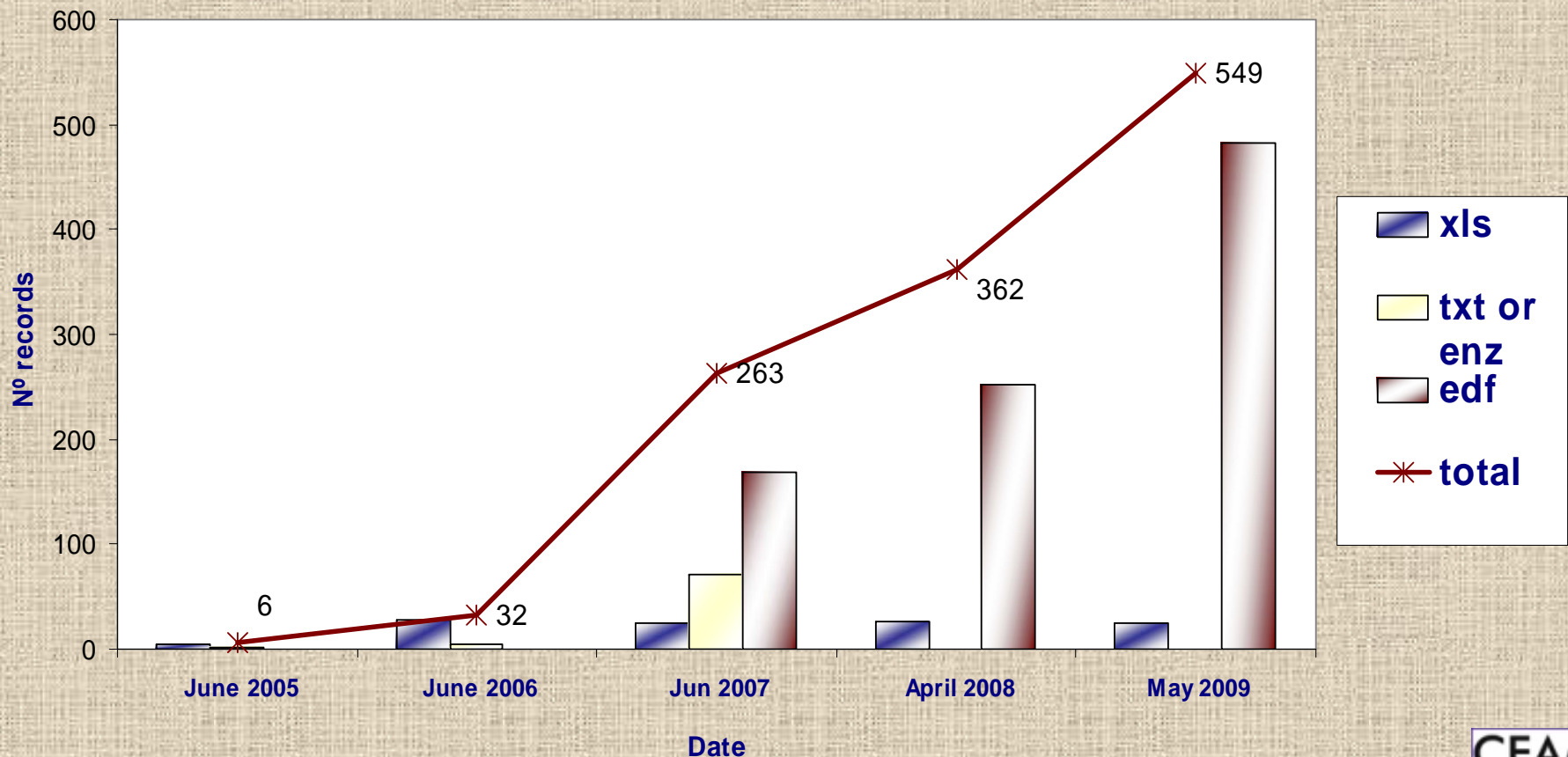
Data Category	Parameters	Description	Download File
Monitor Data	T, P, mbar H <sub>2</sub> O, JNO <sub>2</sub> , NO, NO <sub>2</sub>	Generic Instruments	<a href="#">Monitor data file</a>
Particles Data	Mass concentration	TEOM	<a href="#">Particles data file</a>
Gas Chromatographic Data	VOCs	GC-FID/PID	<a href="#">Gas products data file</a>
Gas Chromatographic Data	VOCs	GC-MS	<a href="#">Gas products data file</a>
Gas Chromatographic Data	VOCs	GC-PAN	<a href="#">Gas products data file</a>
Gas Chromatographic Data	VOCs	GC-TGA	<a href="#">Gas products data file</a>
Packed file		All data files can be downloaded as *.zip file	<a href="#">All data files.zip</a>



# N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies

## Database Status 7.05.2009

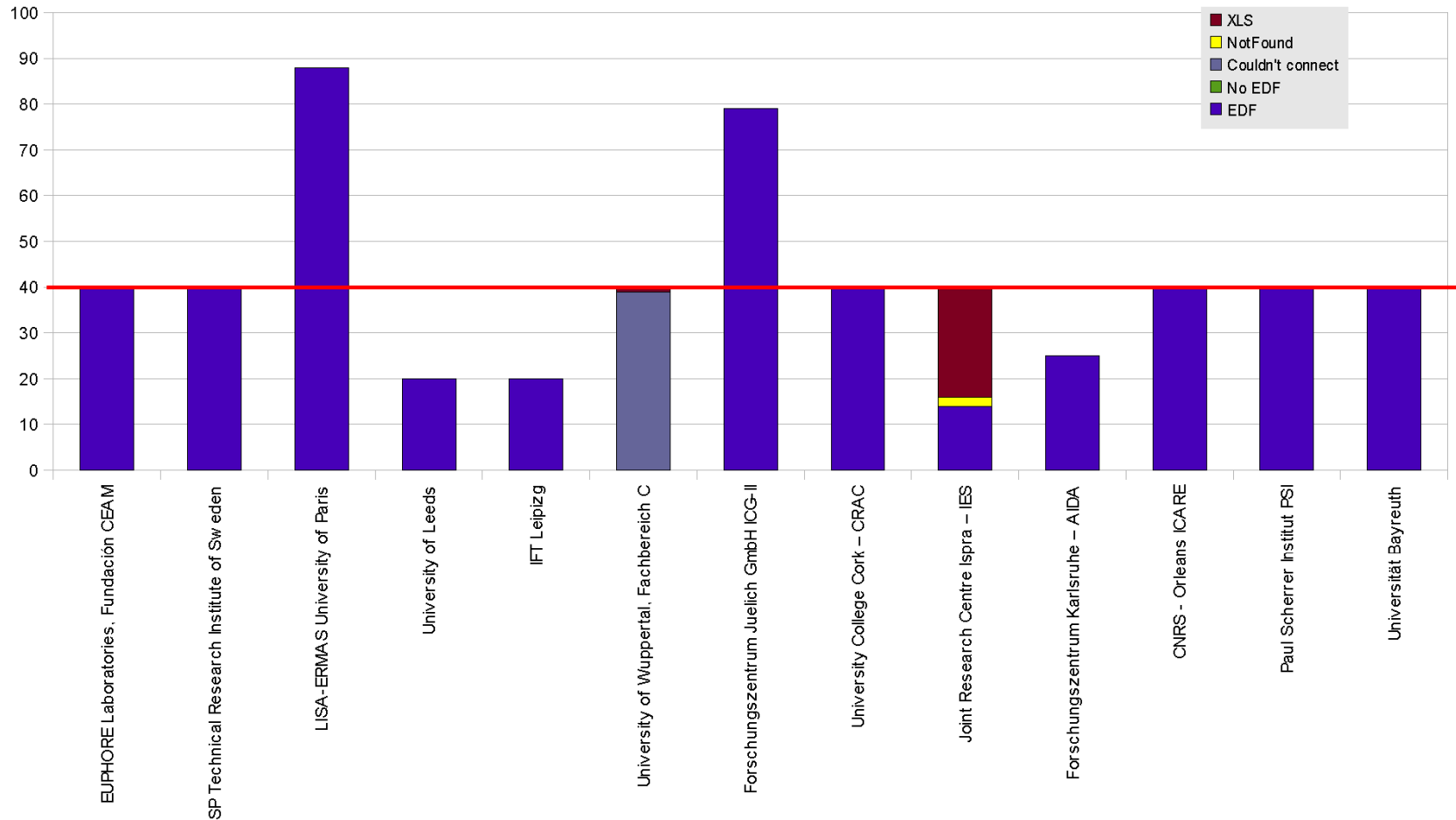
Evolution of the number and format of the records





# N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies

## Database Status 11.05.2009 (File type)





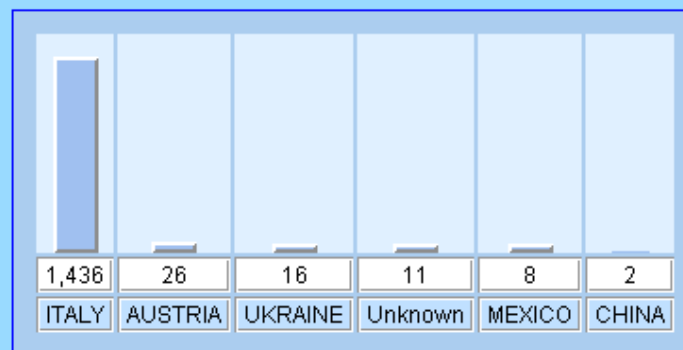
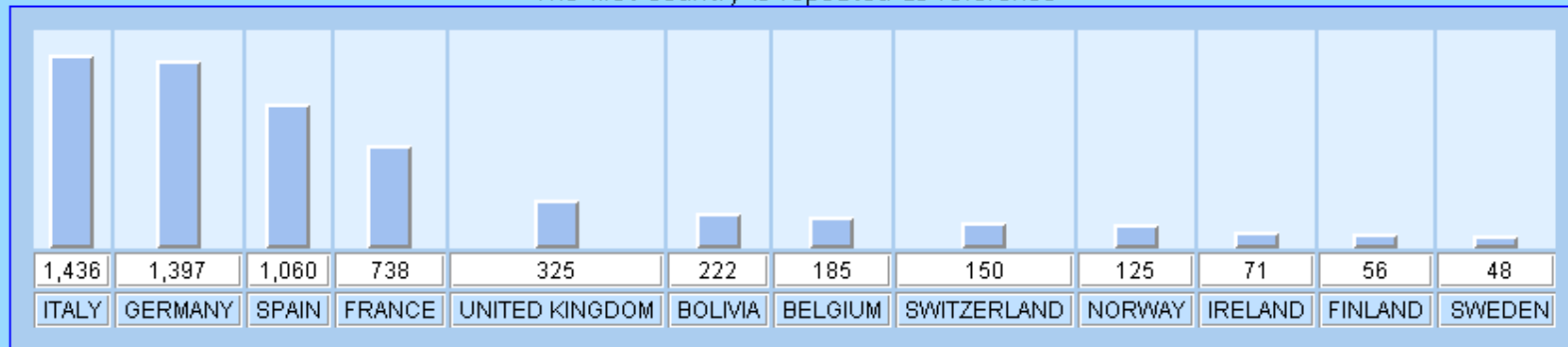
# N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies

## STATISTICS (Update: 7.05.2009)

Visits as users.

### Geographic distribution

The first country is repeated as reference





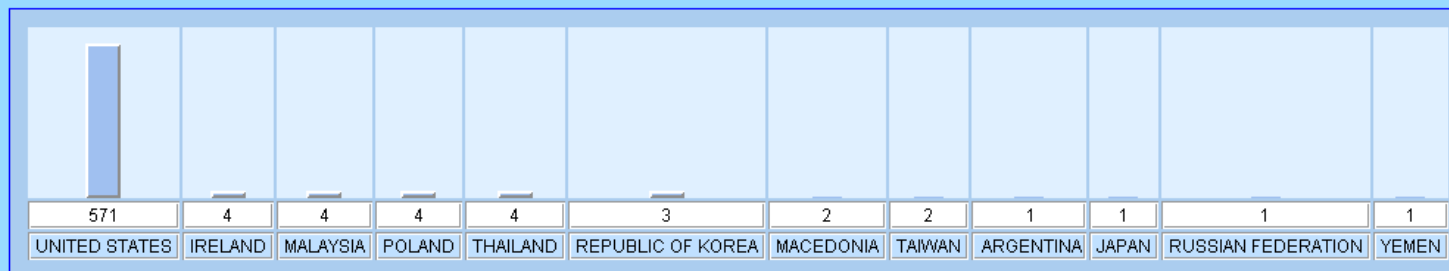
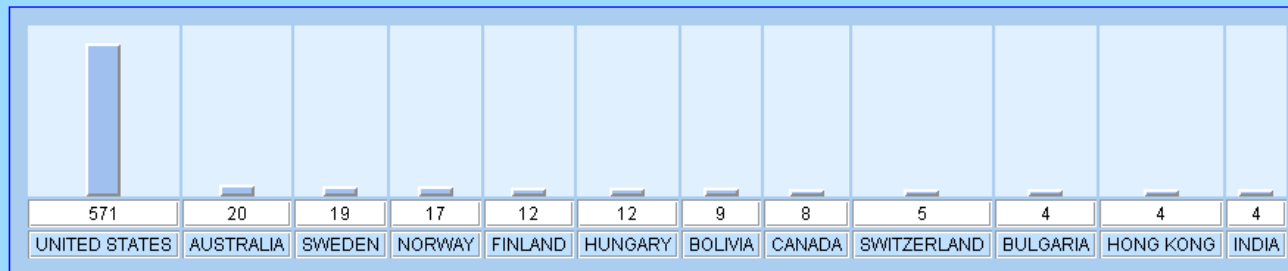
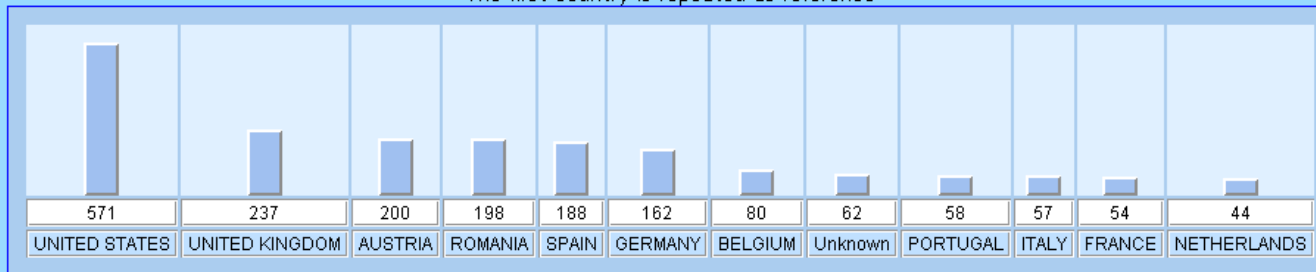
# N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies

## STATISTICS (Update: 7.05.2009)

Visits as *guest*.

### Geographic distribution

The first country is repeated as reference

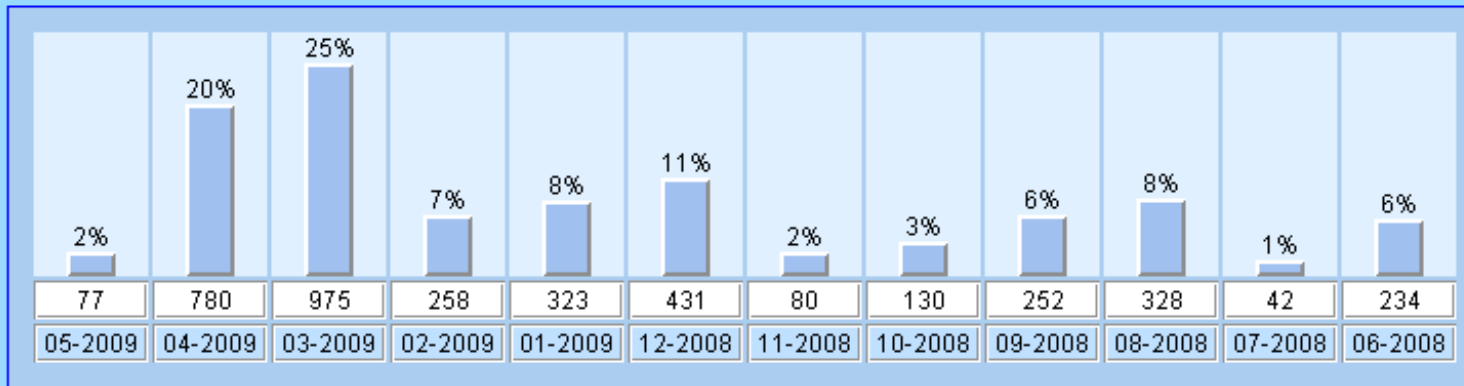




# N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies

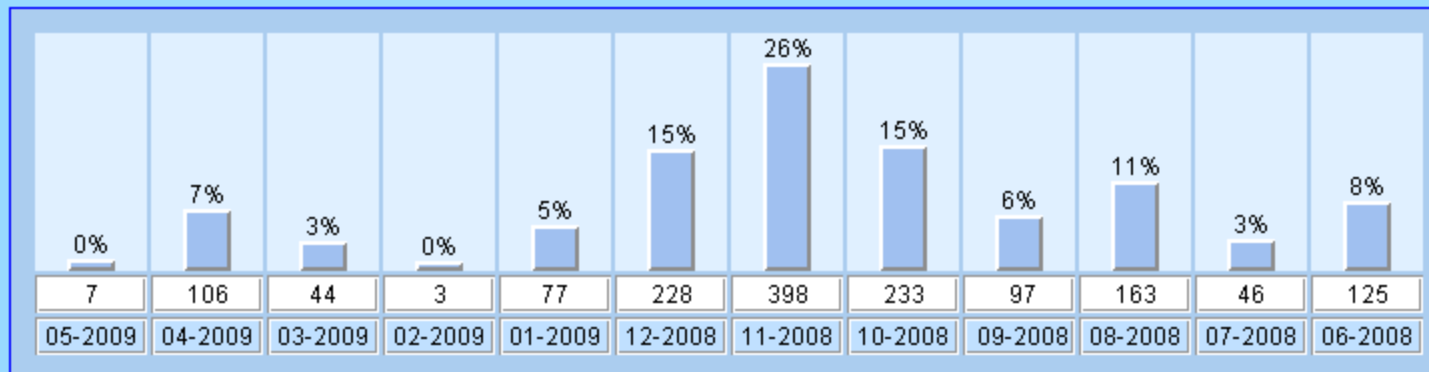
## STATISTICS (Update: 7.05.2009)

Visits last months



**USERS**

Visits last months



**GUESTS**



## **N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies**

### **POTENTIAL BENEFITS AND APPLICATIONS OF THE EUROCHAMP DATABASE**

- 1. Platform to develop and intercompare models**
  - 1. University of Leeds**
  - 2. SOA (JRA-2 WP-3)**
- 2. Validation of instrumentation**
  - 1. OVOC (Jülich, January 2005)**
  - 2. HO<sub>x</sub> (Jülich, July 2005)**
  - 3. NO<sub>3</sub>/N<sub>2</sub>O<sub>5</sub> (Jülich, June 2007)**
  - 4. HONO (EUPHORE, May 2010)**
- 3. Intercomparison of chambers**



# N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies

## Univ. Leeds modelisation of experiments performed at EUPHORE

### JRA2-WP4

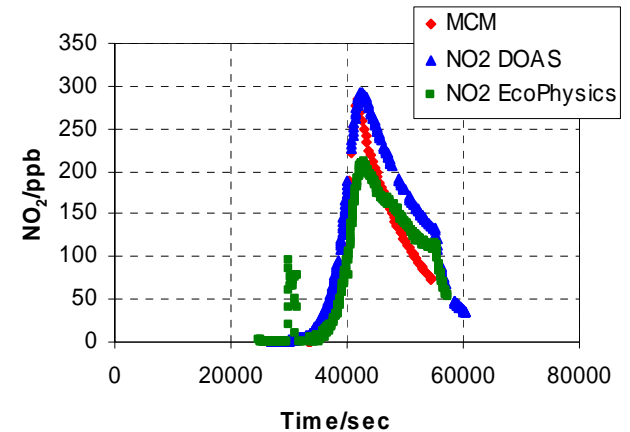
Smog Chamber Study on DVE-1 under VOC-limiting conditions (ethylene glycol di-vinyl ether,  $\text{CH}_2=\text{CHOCH}_2\text{CH}_2\text{CHO}=\text{CH}_2$ )

12/04/2005

14/04/2005

Interface creation for the modeling of the experiments carried out in the EUPHORE chambers

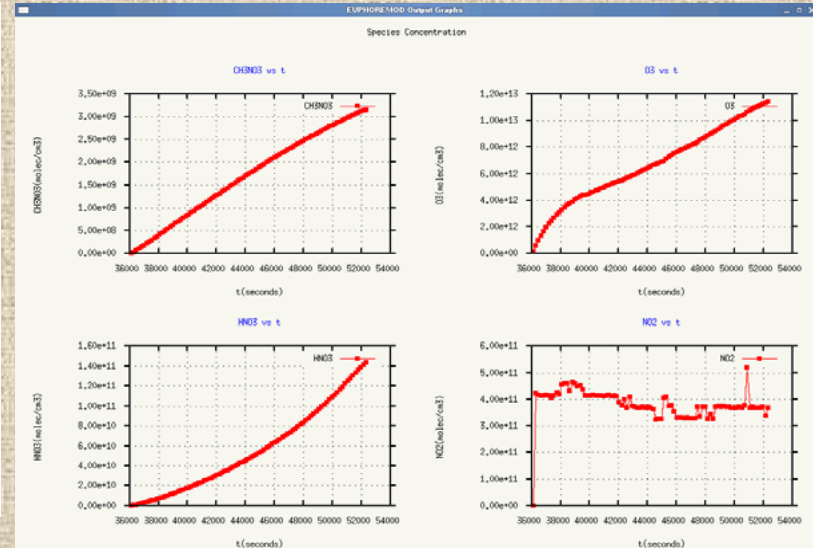
NO<sub>2</sub> comparison MCM-DOAS-NOx Monitor



Model Parameters

Number of Steps	256
Step Size	180.0e+00 seconds
Species Interpolation Method	4 cubic spline=1, cubic spline linear=2, piecewise constant=3, piecewise linear=4
Conditions Interpolation Method	4 cubic spline=1, cubic spline linear=2, piecewise constant=3, piecewise linear=4
Dec Interpolation Method	4 cubic spline=1, cubic spline linear=2, piecewise constant=3, piecewise linear=4
Maximum number of data points in constraint files	10000
Maximum number of constrained species	150
Rates output step size	3600 seconds
Model start time	36120 seconds
Jacobian output step size	3600 seconds
Latitude	39.5e00 degree
Longitude	-0.5e+00 degree
Day	6
Month	4
Year	2004

Edit Default Values Clear All Save Parameters





## **N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies**

### **Intercomparison of aerosol models using the EUROCHAMP database as a platform**

#### **JRA2-WP3**

#### **AIM**

To test some of the **existing models** for simulation of **SOA formation against experimental data** from a set of selected chamber experiments in order to get a basis for analysing the differences between the different modelling approaches and possibly improve the models.

#### **CURRENT STATUS**

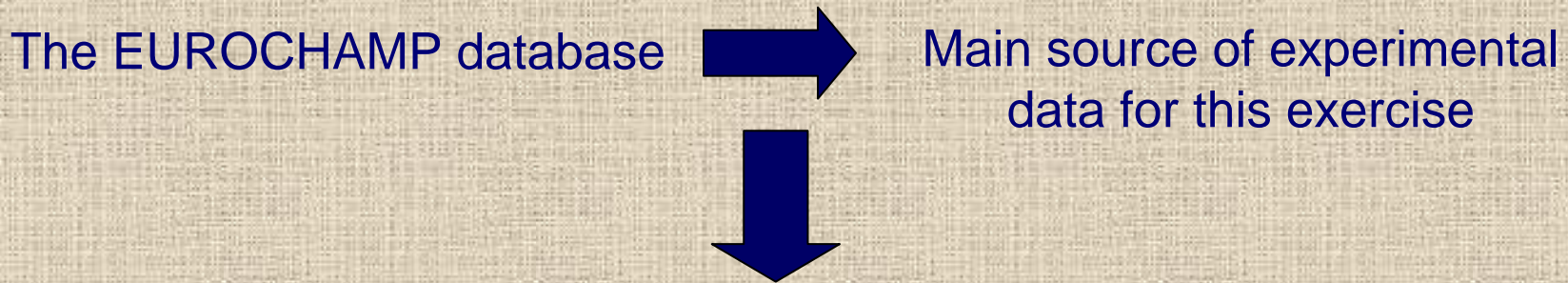
- Selection of experimental runs
- Workshop in Arona (Italy), April 2009: preliminary modelling results and further actions



## N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies

### Intercomparison of aerosol models using the EUROCHAMP database as a platform

#### JRA2-WP3



SOA formation from ozonolysis and photo-oxidation of  $\alpha$ -pinene  
(Comparable data from different chambers,  
Previous studies information of SOA products available)

As much information as possible about relevant chamber artefacts (wall source of OH, dilution rate,...) and wall loss rates should be collected



# N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies

## Intercomparison of instrumentation

### OVOC CAMPAIGN

## Intercomparison of Oxygenated Volatile Organic (OVOC) measurements at the SAPHIR atmosphere simulation chamber in Jan 2005

Data introduced on the EUROCHAMP Database

#### Paper:

E.C. Apel; T. Brauers; R. Koppmann; R. Tillmann; C. Holzke; R. Wegener; J. Boßmeyer; A. Brunner; Ruuskanen, T. ; M. Jocher; C. Spirig; R. Steinbrecher; R. Meier; D. Steigner; E. Gómez Alvarez; K. Müller; S.J. Solomon; G. Schade; D. Young; P. Simmonds; J.R. Hopkins; A.C. Lewis; G. Legreid; A. Wisthaler; A. Hansel; R. Blake; K. Wyche; A. Ellis; P.S. Monks. ***Intercomparison of oxygenated volatile organic compound (OVOC) measurements at the SAPHIR atmosphere simulation chamber.*** Journal of Geophysical Research, JGR, 113 (2008), D20307, doi:10.1029/2008JD009865.



## N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies

### Dissemination

- A. Muñoz. E. Gomez-Alvarez. **Overview of the EUROCHAMP Database of European Atmosphere Simulation Chambers.** Book: Simulation and Assessment of Chemical Processes in a Multiphase Environment. Nato Science for Peace and Security Series –C: Environmental Security. 61-70. 2008. Springer. Edited by I. Barnes an M. M. Kharytonov. **Ukraine**
- E. Gómez-Alvarez; M. Vázquez; A. Muñoz; J. Hjorth; M.Pilling; H. Saathoff; T. Brauers. **The EUROCHAMP chamber experiment database: Goals and Uses. Present and future potential benefits.** Book: Simulation and Assessment of Chemical Processes in a Multiphase Environment. Nato Science for Peace and Security Series –C: Environmental Security. 61-70. 2008. Springer. Edited by I. Barnes an M. M. Kharytonov. **Ukraine**
- A. Muñoz, B Correa, E. Gómez-Alvarez, E. Borrás, T. Vera, M. Vázquez, M. Ródenas, A Carrascosa, and K. Wirtz. **Ceam contribution to the Eurochamp activity N2. Central database of environmental chamber studies.** 19th International Symposium on Gas Kinetics 2006. 22-27 July. **Orleans (France).**
- A. Muñoz; E. Schlosser; E. Gómez; E. Borrás; M.Ródenas; T. Vera; M.Vázquez; A. Carrascosa; T. Brauers. **Eurochamp activity N2: central database of environmental chamber studies.** Poster. Second ACCENT Symposium 2007 Atmospheric Composition Change. Causes and Consequences- Local to Global. **Urbino (Italy).** July 2007



## N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies

### Dissemination

- A. Muñoz, E. Gómez-Alvarez, J. Valero. **The EUROCHAMP Database of European Atmosphere Simulation Chambers**. Poster. EGU General Assembly 2008. Geophysical Research Abstracts. Vol. 10, EGU2008-A-03357, April 2008. **Vienna (Austria)**
- A. Muñoz, E. Gómez-Alvarez, J. Valero, Esther Borrás. **The Eurochamp Database Of European Atmospheric Simulation Chambers**. Poster. Atmospheric Chemical Mechanisms. **UC Davis California (USA)** 10-12 December 2008.
- A. Muñoz, E. Gómez-Alvarez, J. Valero. **The Eurochamp Database Of Atmosphere Simulation Chambers**. Poster. 1st Sino-French Joint Workshop on Atmospheric Environment. Urban and Regional Air Quality: Emissions, Processes, Monitoring and Regulations. Publicación: Book of abstracts. **Beijing, (China)**. 29-31 October 2008
- A. Muñoz, E. Gómez-Alvarez, J. Valero, M. Vázquez, M. Ródenas. **The Eurochamp Database Of European Atmospheric Simulation Chambers**. Poster. INTROP Final Conference Tropospheric Chemistry. 14-17 April 2009, **Portoroz (Slovenia)**



# N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies

## DATABASE TECHNICAL IMPROVEMENTS

Joaquín Valero-Pinazo



# N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies

- See all records in one page



## EUROCHAMP Network Activity 2 Database

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Date of experiment	Type of experiment	Reactants	Parameters	Reactive species	Institute
1991-05-29	OH kinetic study relative method ambient temperature	Benzene, Toluene, p-Xylene	Reaction time, GC-FID area of the reactants.	OH hydroxyl radical	Universität Bayreuth
1991-06-06	OH kinetic study relative method ambient temperature	Benzene, Toluene, p-Xylene			
1991-06-13	OH kinetic study relative method ambient temperature	Benzene, Toluene, p-Xylene			
1991-07-17	OH kinetic study relative method ambient temperature	p-Xylene, Benzene, Toluene			
1991-07-25	OH kinetic study relative method ambient temperature	Benzene, Toluene, p-Xylene			

(Total records: 548)



## EUROCHAMP Network Activity 2 Database

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Date of experiment	Type of experiment	Reactants	Parameters	Reactive species	Institute
1996-08-23	OH kinetic study relative method ambient temperature	MVT, isobutene, OH	Time, MVT, isobutene	OH hydroxyl radical	Joint Research Centre Ispra - IES
1996-08-26	Ozonolysis room temperature	MVT, isobutene, cyclohexane, OH	Time, MVT, isobutene	O3 ozone	Joint Research Centre Ispra - IES
1996-08-30	NO3 radical reaction kinetic study	Nopinone, propene	Time, nopinone, propene	NO3 nitrate radical	Joint Research Centre Ispra - IES
1996-08-30	NO3 radical reaction kinetic study	IPOH, isobutene, NO3	Time, IPOH, NO3	NO3 nitrate radical	Joint Research Centre Ispra - IES
1996-11-20	NO3 radical reaction kinetic study	MVT, 1-butene, NO3	Time, MVT, 1-butene	NO3 nitrate radical	Joint Research Centre Ispra - IES
1997-04-09	Cl atom initiated oxidation kinetic study	Isoprene, ethene, Cl2	Time, isoprene, ethene	Cl chlorine atom	Joint Research Centre Ispra - IES
1997-04-11	Cl atom initiated oxidation kinetic study	MBO, ethene, Cl2	Time, methylbutenol, ethene	Cl chlorine atom	Joint Research Centre Ispra - IES
1997-09-17	Cl atom initiated oxidation kinetic study	Toluene, ethene, CH3ONO	Time, toluene, ethene	Cl chlorine atom	Joint Research Centre Ispra - IES
1997-10-02	Cl atom initiated oxidation kinetic study	Benzene, methane, Cl2	Time, benzene, methane	Cl chlorine atom	Joint Research Centre Ispra - IES
1997-11-27	OH product study ambient temperature NOx	Perfluoroethene, OH	Time, perfluoroethene, CF2O	OH hydroxyl radical	Joint Research Centre Ispra - IES
1997-11-28	OH kinetic study relative method ambient temperature	Perfluoroethene, cyclohexane, CH3ONO	Time, perfluoroethene, cyclohexane	OH hydroxyl radical	Joint Research Centre Ispra - IES
1997-12-11	Ozonolysis product study radical scavenger ambient temperature	Perfluoroethene, O3	Time, perfluoroethene, CF2O	O3 ozone	Joint Research Centre Ispra - IES
1997-12-17	Ozonolysis room temperature	Perfluoroethene, O3, cyclohexane	Time, perfluoroethene, Ozone	O3 ozone	Joint Research Centre Ispra - IES
1997-12-19	NO3 radical reaction product study	Perfluoroethene, NO3	Time, perfluoroethene, CF2O	NO3 nitrate radical	Joint Research Centre Ispra - IES
1998-01-15	NO3 radical reaction kinetic study	Perfluoroethene, propene, NO3	Time, perfluoroethene, propene	NO3 nitrate radical	Joint Research Centre Ispra - IES





## N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies

- **Allow updating a set of records**
  - To update a bunch of records with the same information
  - It allows to change more than a field at a time
  - Useful to change the web address of all the experiments of an institution



# N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies



## EUROCHAMP Network Activity 2 Database Insert/Update Records

### Details of the record

**ID** 437  
**Date of experiment** 2007-04-23  
**Upload date** 16 Dec 2008  
**Last update** 16 Dec 2008  
**Type of experiment** Photolysis ambient temperature  
**Keywords** hymexazol, Pesticides, HCHO, Acetaldehyde, Acetone, Glyoxal, Methylglyoxal  
**Reactants** hymexazol, HCHO, Acetaldehyde, Acetone, Glyoxal, Methylglyoxal  
**Smiles** O=C1/C=C(\ON1)C  
**CAS number** 10004-44-1  
**Parameters** Pressure, Temperature, Dewpoint, Relative humidity, Ozone, NO, NO2, NOx, NOy, CO, JNO2  
**Pressure [Pa]** 100885  
**Temperature [K]** 289.85  
**Light source used** Natural sunlight none  
**Reactive species**  
**Resource link** [http://80.24.165.149/files/EUROCHAMP/Chamber\\_B/2007\\_04\\_23/2007\\_04\\_23\\_ChB\\_wp2r.html](http://80.24.165.149/files/EUROCHAMP/Chamber_B/2007_04_23/2007_04_23_ChB_wp2r.html)  
**Project name** ECOPEST  
**Institute** EUPHORE Laboratories, Fundación CEAM  
**Experimental Reference Number** 2255  
**Description** [http://80.24.165.149/files/EUROCHAMP/Chamber\\_B/2007\\_04\\_23/23\\_04\\_2007\\_expe\\_descr.pdf](http://80.24.165.149/files/EUROCHAMP/Chamber_B/2007_04_23/23_04_2007_expe_descr.pdf)  
**Formula\_Index**  
**Option**

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# N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies

## Insert/Update Records

The aim of multiupdate is to update a bunch of records with the same information

### Step 1. Select the option or fill in the text that you want to be replaced

Date of experiment  Please use the format yyyy-mm-dd or yyyy-mm-dd to yyyy-mm-dd if you add a series.

Type of experiment  Please select from the drop down menu.

Keywords  Enter different key words separated by a comma. A keyword list can be obtained from the

Reactants  Please enter the chemical names separated by comma.

Smiles  Please enter the SMILES separated by comma.

CAS number  Enter the CAS number using the following format 1234-45-6.

Parameters  Please fill the field with the parameters separated by comma.

Pressure [Pa]  Give the mean pressure in Pa.

Temperature [K]  Give the mean temperature in K.

Light source used  Please select from the drop-down menu.

Reactive species  Please select from the drop down menu.

Resource link  Please enter the URL of the original data record linked to this entry.  
*Duplication is not allowed.*

Project name  Enter the project name and acronym.

Institute  Please enter your institute name from the drop down menu.

Experimental Reference Number  Please enter a unique number to identify the experiment.

Description  Please enter the URL of the pdf file.

Formula\_Index  Enter the Formula index of your reagents.

Option

# N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies

## Insert/Update Records

### Step 2. Select or fill in the new data

Date of experiment  Please use the format yyyy-mm-dd or yyyy-mm-dd to yyyy-mm-dd if you add a series.

Type of experiment  Please select from the drop down menu.

Keywords  Enter different key words separated by a comma. A keyword list can be obtained from the

Reactants  Please enter the chemical names separated by comma.

Smiles  Please enter the SMILES separated by comma.

CAS number  Enter the CAS number using the following format 1234-45-6.

Parameters  Please fill the field with the parameters separated by comma.

Pressure [Pa]  Give the mean pressure in Pa.

Temperature [K]  Give the mean temperature in K.

Light source used  Please select from the drop-down menu.

Reactive species  Please select from the drop down menu.

Resource link  Please enter the URL of the original data record linked to this entry.  
*Duplication is not allowed.*

Project name  Enter the project name and acronym.

Institute  Please enter your institute name from the drop down menu.

Experimental Reference Number  Please enter a unique number to identify the experiment.

Description  Please enter the URL of the pdf file.

Formula\_Index  Enter the Formula index of your reagents.

Option  Option field for additional information.

Next step



# N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies



## EUROCHAMP Network Activity 2 Database Insert/Update Records

### Step 3. Experiments involved

These experiments will be updated

Exp date	Project name	Reactants
1 2001-09-27	Effects of the oxidation of the aromatic compounds in the troposphere (EXACT)	Toluene
2 2002-01-11		O3, NO, NO2, NOX, CO, alpha-pinene
3 2002-01-14		O3, NO, NO2, NOX, CO, alpha-pinene
4 2002-01-16		O3, NO, NO2, NOX, CO
5 2002-01-17		O3, NO, NO2, NOX, CO
6 2002-04-15	OSOA Origin and Formation of Secondary Organic Aerosol	a-pinene, a-pinene, O3
7 2002-04-16	OSOA Origin and Formation of Secondary Organic Aerosol	a-pinene, NOx, SF6
8 2002-04-17	OSOA Origin and Formation of Secondary Organic Aerosol	a-pinene, NOx, SF6, H2O
9 2002-04-18	OSOA Origin and Formation of Secondary Organic Aerosol	a-pinene, HONO, SF6, H2O
10 2002-04-19	OSOA Origin and Formation of Secondary Organic Aerosol	a-pinene, NOx, SF6
11 2002-07-03	Effects of the oxidation of the aromatic compounds in the troposphere (EXACT)	p-xylene
12 2002-07-18	Effects of the oxidation of the aromatic compounds in the troposphere (EXACT)	p-xylene
13 2004-03-09	MOST	ethylene glycol vinyl ether
14 2004-03-10	MOST	acrylic acid
15 2004-03-11	MOST	Allyl alcohol
16 2004-03-12	MOST	Methyl vinyl ketone
17 2004-03-23	EUPHORE	Isoprene
18 2004-03-24	MOST	3-methylfuran, methacrolein, methyl vinyl ketone
19 2004-03-30	IALSI	1-octene
20 2004-03-31	IALSI	CO
21 2004-04-01	IALSI	H2
22 2004-04-02	IALSI, EUROCHAMP	HCHO
23 2004-04-03	IALSI	Glycolaldehyde
24 2004-04-06	EUPHORE	Isoprene
25 2004-05-06	MOST	Ethylene Glycol Vinyl Ether
26 2004-05-07	MOST	Ethylene glycol vinyl ether
27 2004-06-16	IMSEUR	Ethylbenzene
28 2004-06-17	IMSEUR	ethylbenzene
29 2004-06-22	IMSEUR	Ethylbenzene
30 2004-06-23	IMSEUR	Ethylbenzene
31 2004-07-06	IMSEUR	Ethyl vinyl ketone
32 2005-04-12	MOST	NO, SF6, Ethylene Glycol Diethyl Ether
33 2005-04-14	MOST	NO, SF6, Ethylene Glycol Diethyl Ether
34 2005-04-15	MOST	Ethene, NO, SF6
35 2007-04-23	ECOPEST	hymexazol, HCHO, Acetaldehyde, Acetone, Glyoxal, Methylglyoxal
36 2007-04-25	ECOPEST	Hymexazol, O3, SF6, Formic acid, Toluene, HONO, HNO3
37 2007-06-12	ECOPEST	Chloropicrin, Phosgene, HNO3, HCHO, Acetaldehyde, Acetone
38 2007-07-17	NITROPHEN	2-nitrophenol, CO, NO, NO2, O3
39 2007-07-19	NITROPHEN	2-nitrophenol, CO, NO, NO2, O3
40 2007-11-14	ECOPEST	Chloropicrin, 1,3,5-TMB, 2,3-dimethyl-2-butene, Cyclohexane, O3, NO

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Array ( [substituir] => Array ( [EXP\_date] => [Type\_of\_exp] => [keywords] => [Reactants] => [Smiles] => [CAS\_number] => [Parameters] => [Pressure] => [Temperature] => [Light\_source] => [Reactive\_species] => [Resource\_link] => EUROCHAMP [Project\_name] => [Institute] => [Exp\_ref\_num] => [Description] => [Formula\_Index] => [Option] => ) [substituto] => Array ( [Resource\_link] => EUROCHAMP1 ) )



# N2 Activity: Standardised Data Protocol and Central Database of Environmental Chamber Studies



## EUROCHAMP Network Activity 2 Database Insert/Update Records

### Details of the record

**ID** 386  
**Date of experiment** 2002-04-16  
**Upload date** 26 Dec 2007  
**Last update** 8 May 2009  
**Type of experiment** OH product study ambient temperature NOx  
**Keywords**  
**Reactants** a-pinene, NOx, SF6  
**Smiles** CC1(C)[C@H]2C(C)=CC[C@@H]1[C@]2(C)C  
**CAS number** 80-56-8  
**Parameters** a-pinene, NOx, SF6, T, P, Humidity  
**Pressure [Pa]** 100385  
**Temperature [K]** 285.22  
**Light source used** Natural sunlight none  
**Reactive species** OH hydroxyl radical  
**Resource link** [http://80.24.165.149/files/EUROCHAMP1/chamber\\_B/2002\\_04\\_16/2002\\_04\\_16\\_ChB\\_OSOA.htm](http://80.24.165.149/files/EUROCHAMP1/chamber_B/2002_04_16/2002_04_16_ChB_OSOA.htm)  
**Project name** OSOA Origin and Formation of Secondary Organic Aerosol  
**Institute** EUPHORE Laboratories, Fundación CEAM  
**Experimental Reference Number** 1613  
**Description** [http://80.24.165.149/files/eurochamp/chamber\\_B/2002\\_04\\_16/documents/2002\\_04\\_16\\_Experimental\\_Description.pdf](http://80.24.165.149/files/eurochamp/chamber_B/2002_04_16/documents/2002_04_16_Experimental_Description.pdf)  
**Formula\_Index**  
**Option** Controlled constant [NOx]

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- **Improve Check EDF**
  - analyze the ZIP content





## EUROCHAMP Network Activity 2 Database Tools

- [Add user](#), lists and manages users. From table of applications to admitted.
- [Summary of experiments](#), counts the number of experiments per institution.
- [Broken links](#), looks for broken links in field  (optionaly in experiments wiht Id greater than  )
- [Check EDF](#), looks for EDF files in field  (optionaly in experiments wiht Id greater than  )

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## EUROCHAMP Network Activity 2 Database Tools

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### Looking for EDF files

ID	Exp_date	Institute	result	protocol	extension	Resource_link
4	1999-10-06	6 Forschungszentrum Karlsruhe - AIDA	EDF	http	html	<a href="http://imk-aida.fzk.de/data/AIDA/1999/10/06/diesel_soot_99.html">http://imk-aida.fzk.de/data/AIDA/1999/10/06/diesel_soot_99.html</a>
6	2000-03-01	5 Joint Research Centre Ispra - IES	EDF	http	dynamic_page	<a href="http://ccu.jrc.it/EUROCHAMP/2000_03_01a.cfm">http://ccu.jrc.it/EUROCHAMP/2000_03_01a.cfm</a>
7	2003-04-30	8 Paul Scherrer Institut PSI	EDF	http	directory	<a href="http://psi-smog:smochada1@eurochamp.web.psi.ch/ec_downloads/psi_20030430/">http://psi-smog:smochada1@eurochamp.web.psi.ch/ec_downloads/psi_20030430/</a>
12	1999-10-29	11 LISA-ERMAS University of Paris	EDF in ZIP	http	html	<a href="http://www.lisa.univ-paris12.fr/ERMAS/Eurochamp/ethylac2910.htm">http://www.lisa.univ-paris12.fr/ERMAS/Eurochamp/ethylac2910.htm</a>
14	2004-03-10	1 EUPHORE Laboratories, Fundación CEAM	EDF	http	html	<a href="http://80.24.165.149/files/eurochamp/Chamber_B/2004_03_10/2004_03_10_chB_tqv1.htm">http://80.24.165.149/files/eurochamp/Chamber_B/2004_03_10/2004_03_10_chB_tqv1.htm</a>
15	2004-03-09	1 EUPHORE Laboratories, Fundación CEAM	EDF	http	html	<a href="http://80.24.165.149/files/eurochamp/Chamber_B/2004_03_09/2004_03_09_chB_wbka.htm">http://80.24.165.149/files/eurochamp/Chamber_B/2004_03_09/2004_03_09_chB_wbka.htm</a>
16	2004-03-11	1 EUPHORE Laboratories, Fundación CEAM	EDF	http	html	<a href="http://80.24.165.149/files/eurochamp/Chamber_B/2004_03_11/2004_03_11_chB_slvo.htm">http://80.24.165.149/files/eurochamp/Chamber_B/2004_03_11/2004_03_11_chB_slvo.htm</a>
17	2004-03-12	1 EUPHORE Laboratories, Fundación CEAM	EDF	http	html	<a href="http://80.24.165.149/files/eurochamp/Chamber_B/2004_03_12/2004_03_12_chB_wkd2.htm">http://80.24.165.149/files/eurochamp/Chamber_B/2004_03_12/2004_03_12_chB_wkd2.htm</a>

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