REGIONAL TRAINING COURSE ON METHODS AND TOOLS TO IDENTIFY SOURCES OF AIR POLLUTION

IAEA RER 1013: Supporting Air Quality Management

Quality Control & Preparation of Data Bases for Source Apportionment

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Outline

Case Study

- Project CVdust: Atmospheric aerosol in Cape Verde region: seasonal evaluation of composition, sources and transport

CVDust project

- Motivation / objective
- Sampling and analysis procedures
- Quality control/ database consolidation

Soure apportionment

- Enrichment factors
- PMF
- Contribution of Sahara dust

Databases

- DatabaseCVDust.xlsx
- CVDust-data validation.xlsx

Programs

- PMF3.0
- Excel

Why study atmospheric dust in Cape Verde?

Because of:

- Our previous experience in the study of atmospheric aerosols and dust
- Implementation of scientific relations with research community in Cape Verde
- The global importance of Sahara dust emissions into the atmosphere

CVDust Project - Motivation

Global importance of Sahara dust emissions into the atmosphere

Estimated Global Emission rates of particles into the Atmosphere (Tg yr-1)

	Fine Particles	Coarse Particles
Sea Salt	82.1	2460
Dust	250	1000-4875
Carbon	81	
Sulfate	150	
Nitrate	11.3	
Ammonium	33.6	

- Natural Soil;
- Agriculture (example “Dust Bowl” in USA);
- Transports;
- Industry (cement; mining)

CVDust Project - Motivation

Sources of Soil Dust:

- **North Africa the major source of dust**. Estimates of Sahara emissions: 130-760 Tg yr− 1 (Goudie and Middleton, 2001);
- Recent estimates annual Saharan dust emission of 1600 Tg yr− 1 (Ozer, 2001).
- Sahel cultivation contributes with up to 15% dust North Africa emissions;
- *Other dust sources: Arabian Peninsula, Iran, Turkmenistan, Afghanistan, Pakistan, Northern India, the Namib and Kalahari desert and the Tarim Basin in China.*

CVDust Project - Motivation

Global dust budget – Modeled annually averaged values for emission, atmospheric loading and deposition

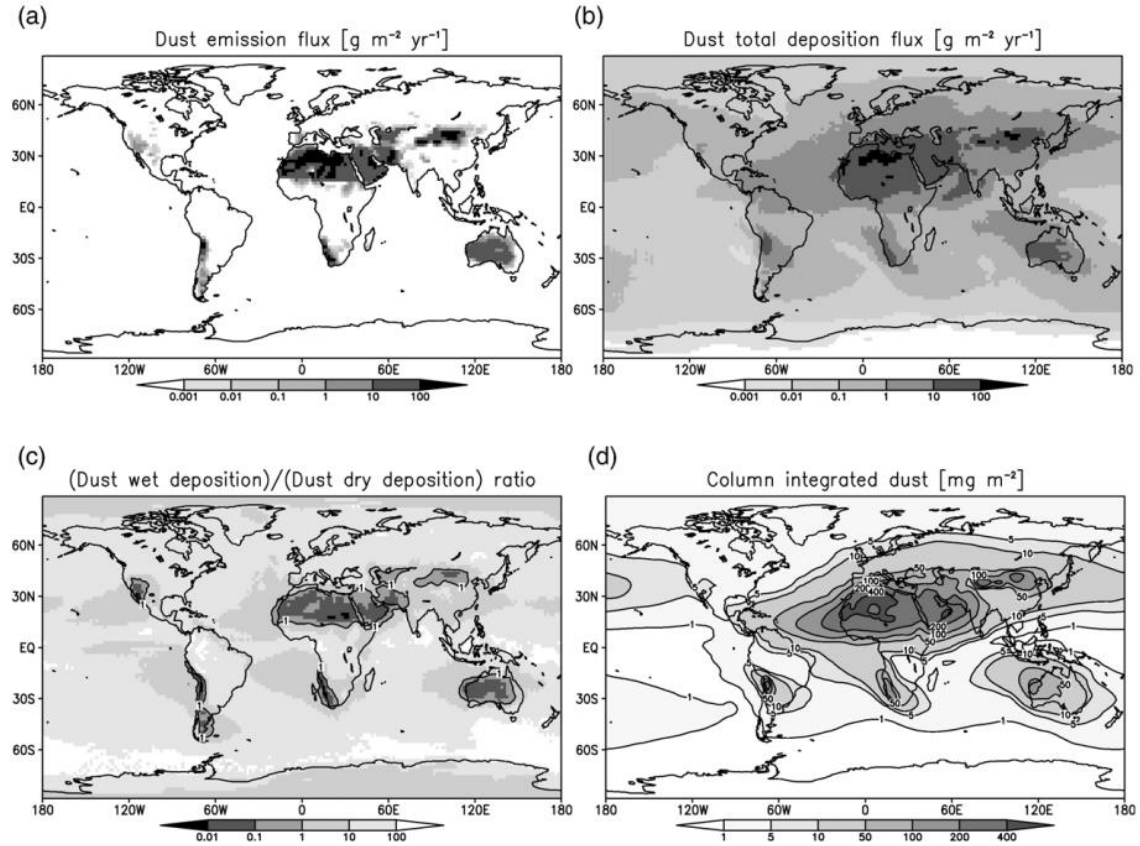


Fig. 4. Simulated annually averaged (a) dust emission flux, (b) total deposition flux, (c) ratio of wet deposition to dry deposition, and (d) atmospheric load.

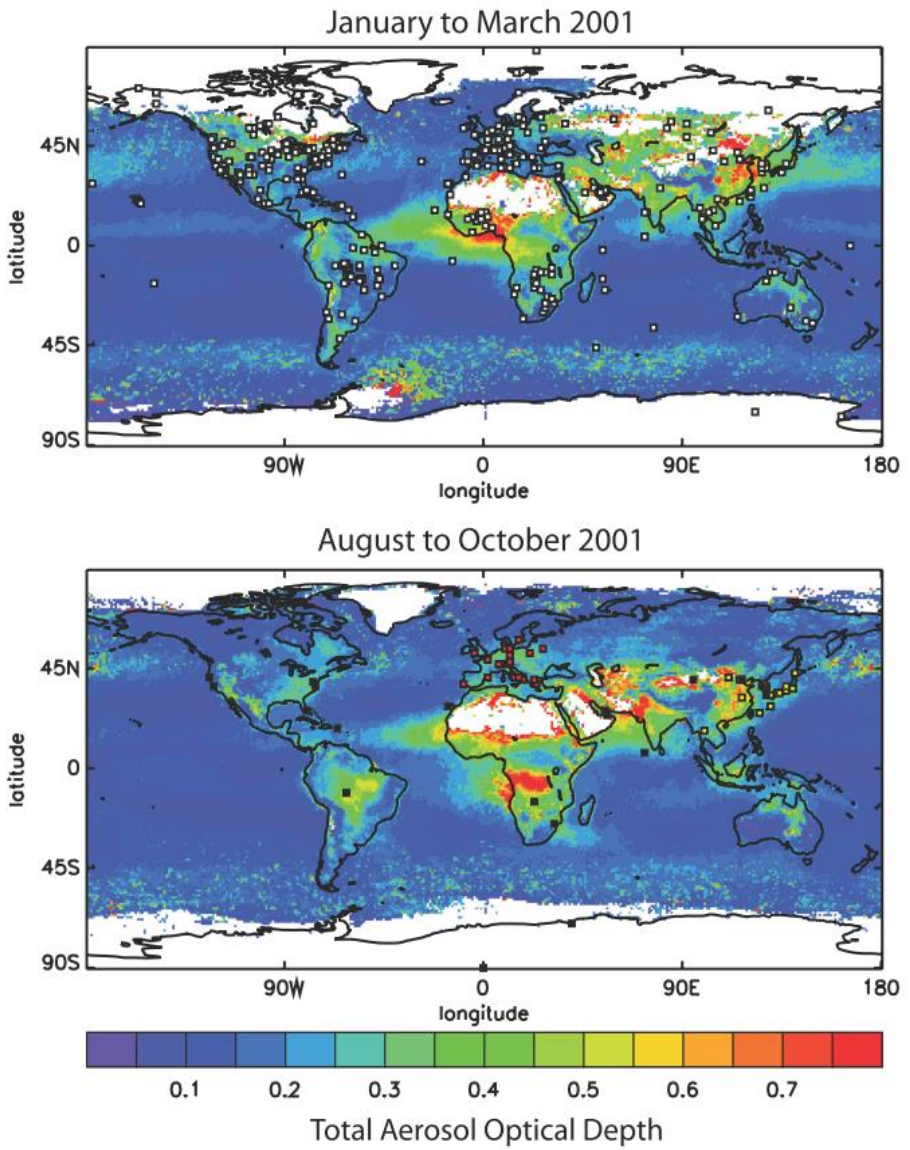
ref: Tanaka and Chiba, (2006)

CVDust Project - Motivation

MODIS Satellites measurements of atmospheric total aerosol optical depth during 2001

Clearly visible the Sahara dust plume over central/north Atlantic

http://modis.gsfc.nasa.gov/index.php



CVDust Project - Motivation

Dust emission Regions in Sahara, from TOMS AbsIndex (1980-92)

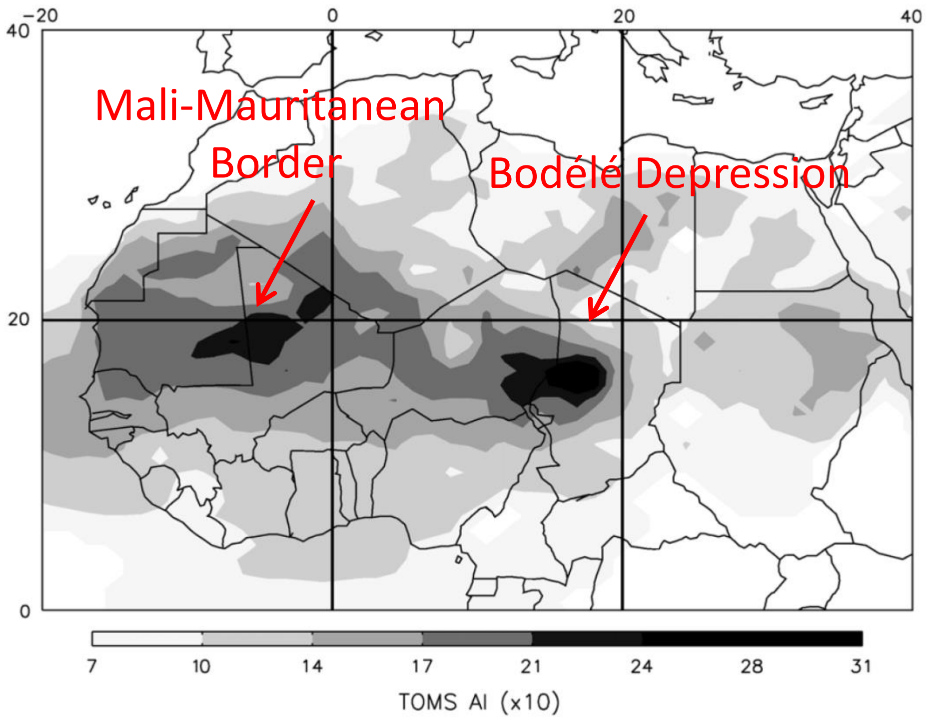


Fig. 3. Long-term mean TOMS AI (×10) (1980–1992).

(ref: Engelstaedter, 2006)

Sinks of out of Sahara emitted dust:

Kaufman et al. (2005) estimate North Africa annual dust transport to west 240±80 Tg:

- 140 Tg are deposited in the Atlantic Ocean,
- 50 Tg fertilize the Amazon Basin
- 50 Tg are transported to the Caribbean.
- 20 Tg are transported towards Europe.

CVDust Project - Motivation

Impacts of desert dust emissions:

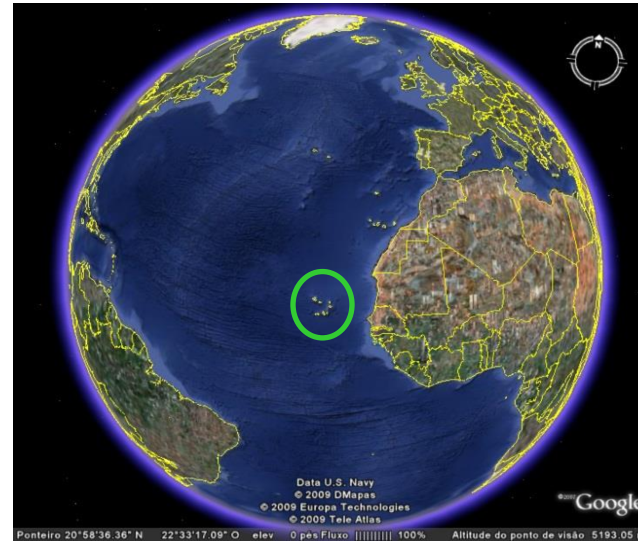
- **Atmospheric Heat Balance and Climate Control**
  - *Weakening of Atlantic Tropical Cyclones*
- **Biogeochemical Cycles**
  - *Biogeochemical Cycles in Atlantic and Amazon Basin*
  - *Toxic Algae Blooms*
- **Human Health**
  - *Spreading of meningitis in Sahel* (Sultan et al., 2005)
  - *Kawasaki disease in Japan and Western USA* (Fraser, 2012)

CVDust Project - Objectives

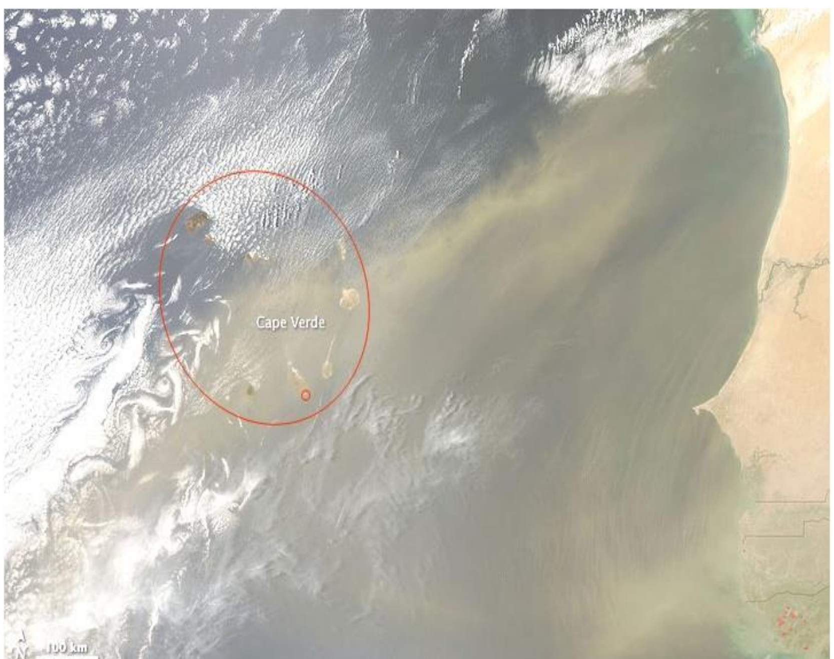
1. **Monitoring and sampling atmospheric dust during one year**
2. **Chemical and structural characterization of collected samples**
    - *Water Soluble ions*
    - *Carbonate and Carbonaceous forms*
    - *Elemental Composition (NAA)*
    - *Mineralogical Composition (XRD; TEM; SEM)*
    - *Organic Species (GC/MS)*
    - *Microbial and fungi characterization*
3. **Source Identification; Transport and Deposition Modeling**
    - *Source Apportionment (PMF; PCA/MLRA)*
    - *Transport Modeling (Trajectory Analysis; DREAM Model)*
4. **Quantify African dust input to Cape Verde Air Quality**
5. **Explain processes governing dust production, transport, and removal from atmosphere over the Atlantic**

CVDust Project - Motivation

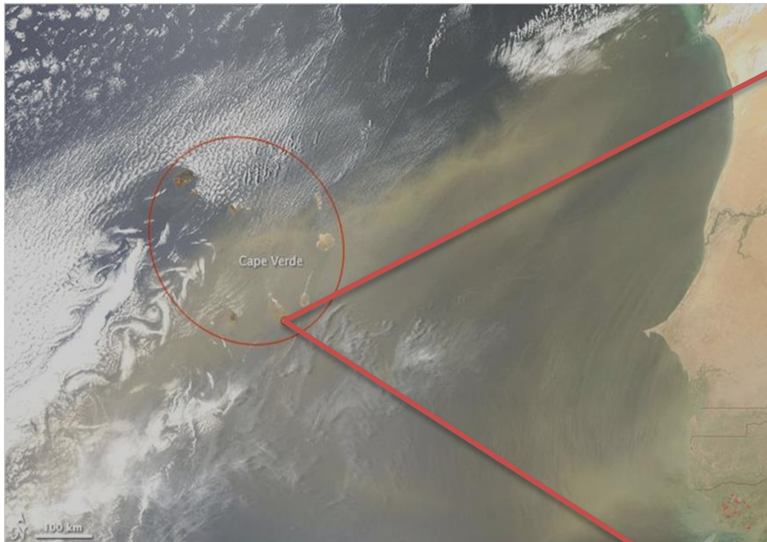
Special Conditions of Cape Verde to perform Sahara Dust Studies:



- Out of West Africa Coast (900 km)
- Dust Season Period (Bruma Seca – Dry Fog)
- Safety and Electricity Supply
- Good relations and Low Cost



CVDust Project – Sampling and analysis



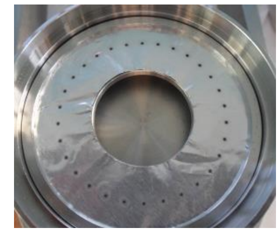
Sampling Location

Santiago Island

Praia

CV Meteorological Institute

CVDust Project – Sampling and analysis



Equipment:

1 GRIMM Aerosol Spectrometer (0.25->32µm) 31 channels
1 Aethalometer (7 wavelength channels)
2 PM10 LowVol filter samplers
1 PM10 HighVol filter Sampler
1 Berner LowVol impactor (0.063-16 µm) 8 stages
1 HighVol impactor (<0.49-10µm) 6 stages
1 Meteo Station

CVDust Project – Sampling and analysis

Sampling equipment	Filters matrix	Species	Technique
Low volume	Teflon filters	Elements	INAA+PIXE
Low volume	Teflon filters	Water soluble ions	Ion chromatography
High volume	Quartz filters	- CO_3^{2-} - OC, EC	- Measuring CO_2 - Thermo-optical transmission technique
Berner low volume	Aluminium foil	Water soluble ions	Ion chromatography

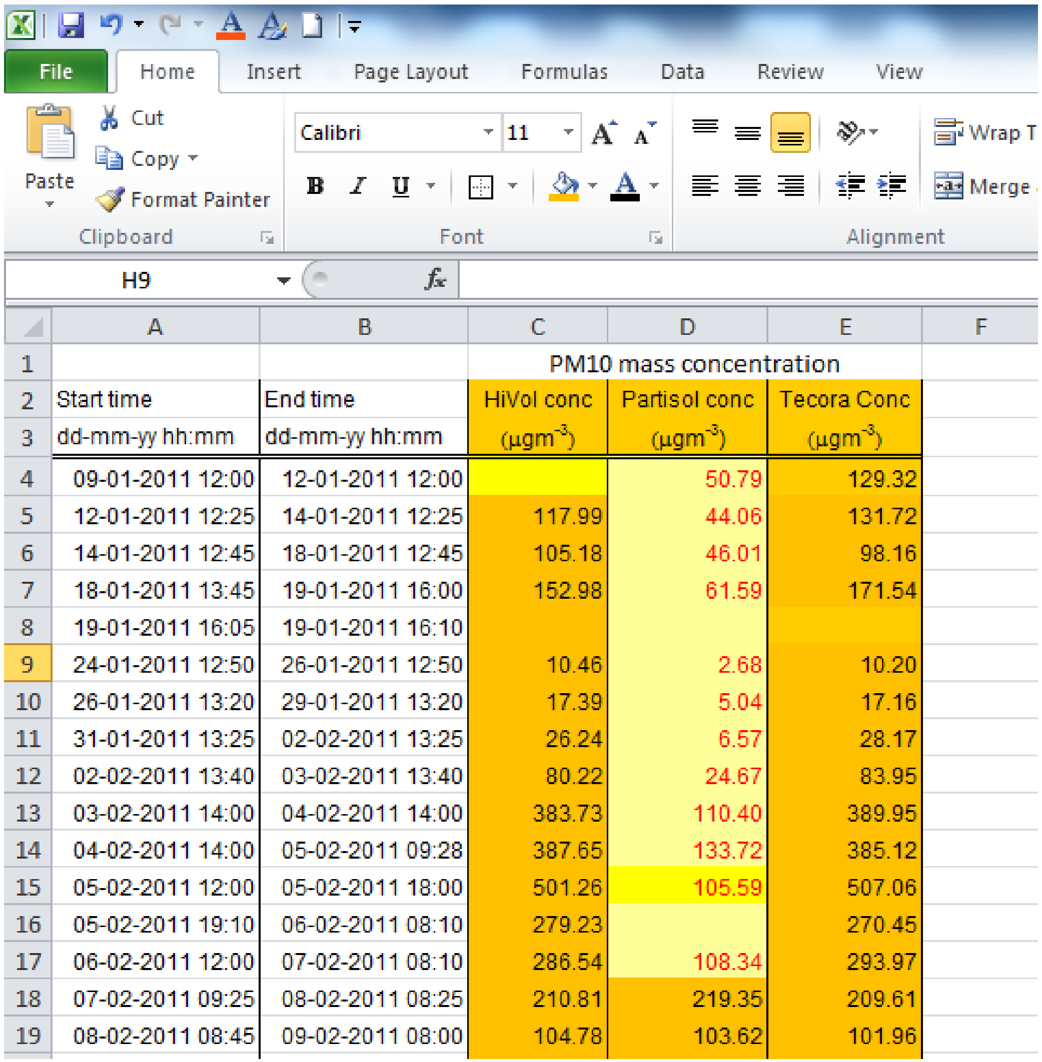
Quality prevention / Quality Control

- Initial station mounting and training at Aveiro
- Prevention for electric supply instabilities and failure
- Joint installing of Station in Praia
- Spare equipment and spare parts
- Tough program of frequent testing, calibration and maintenance
- Close contacts and rapid answer to new situations
- Rapid evaluation of collected samples and data
- Continuous intercomparison of results during analysis

87% measuring efficiency

140 PM10 filtering periods
11 HV Impactor sampling periods
5 Berner Impactor sampling periods

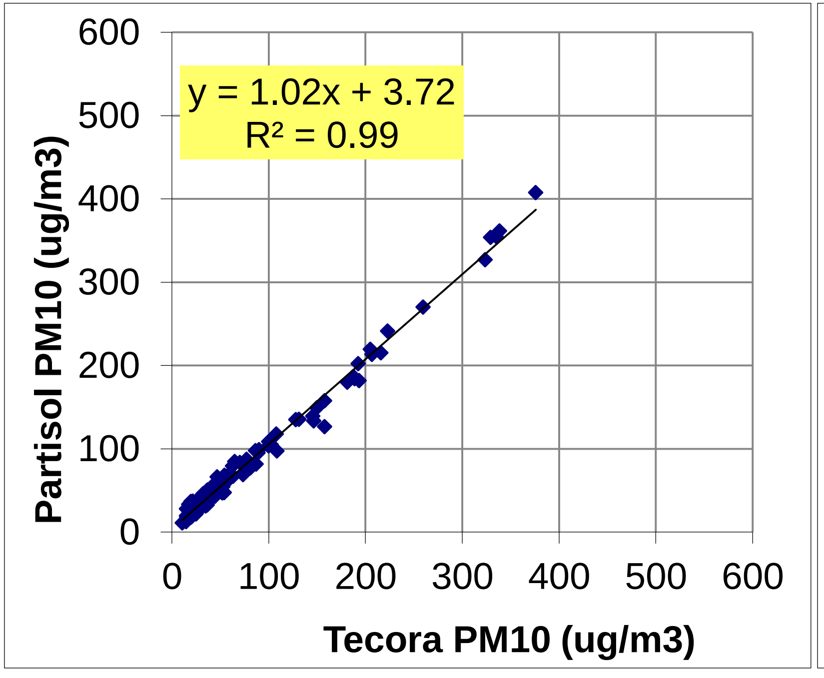
Detection of sampling errors

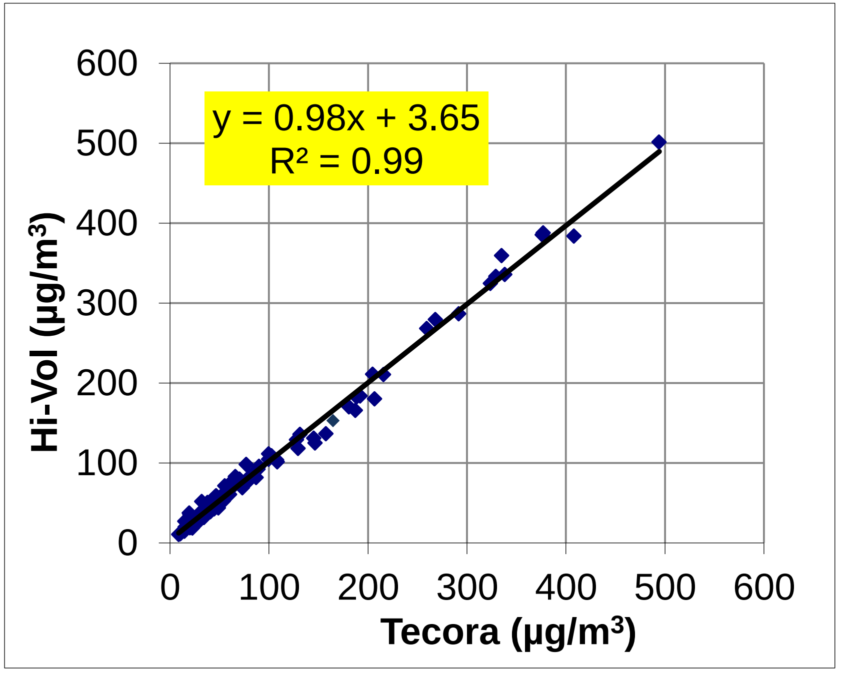


	A	B	C	D	E
1			PM10 mass concentration		
2	Start time	End time	HiVol conc	Partisol conc	Tecora Conc
3	dd-mm-yy hh:mm	dd-mm-yy hh:mm	(μgm^{-3})	(μgm^{-3})	(μgm^{-3})
4	09-01-2011 12:00	12-01-2011 12:00		50.79	129.32
5	12-01-2011 12:25	14-01-2011 12:25	117.99	44.06	131.72
6	14-01-2011 12:45	18-01-2011 12:45	105.18	46.01	98.16
7	18-01-2011 13:45	19-01-2011 16:00	152.98	61.59	171.54
8	19-01-2011 16:05	19-01-2011 16:10			
9	24-01-2011 12:50	26-01-2011 12:50	10.46	2.68	10.20
10	26-01-2011 13:20	29-01-2011 13:20	17.39	5.04	17.16
11	31-01-2011 13:25	02-02-2011 13:25	26.24	6.57	28.17
12	02-02-2011 13:40	03-02-2011 13:40	80.22	24.67	83.95
13	03-02-2011 14:00	04-02-2011 14:00	383.73	110.40	389.95
14	04-02-2011 14:00	05-02-2011 09:28	387.65	133.72	385.12
15	05-02-2011 12:00	05-02-2011 18:00	501.26	105.59	507.06
16	05-02-2011 19:10	06-02-2011 08:10	279.23		270.45
17	06-02-2011 12:00	07-02-2011 08:10	286.54	108.34	293.97
18	07-02-2011 09:25	08-02-2011 08:25	210.81	219.35	209.61
19	08-02-2011 08:45	09-02-2011 08:00	104.78	103.62	101.96

Work on file
CVDust-data validation.xlsx
to detect sampling errors.

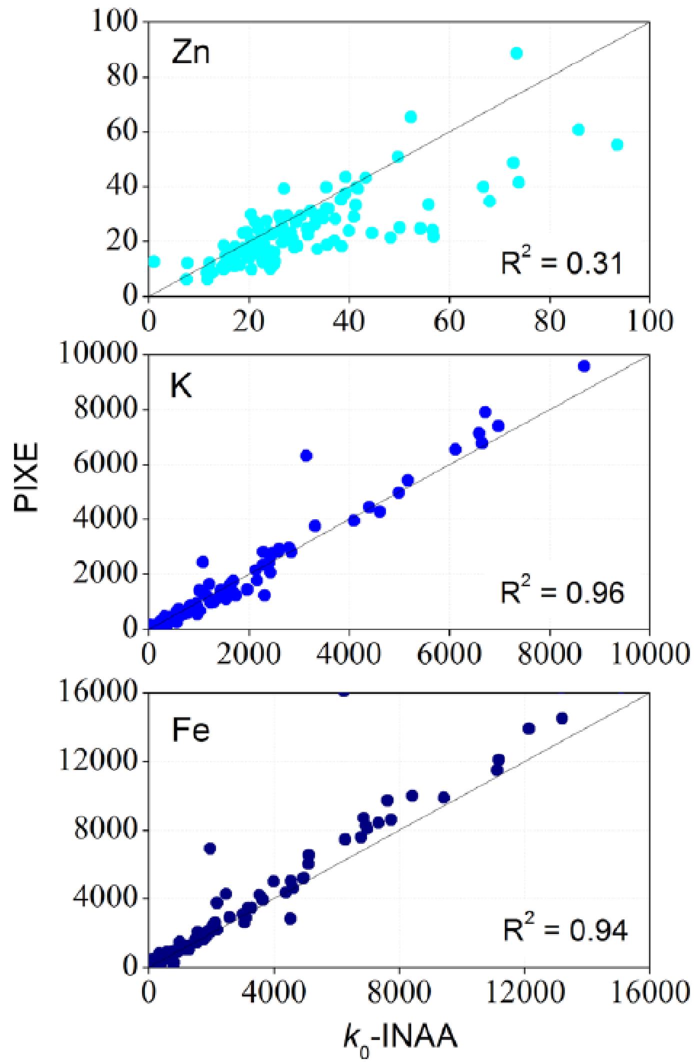
Detection of sampling errors





Measurement of PM10 mass for 3 parallel sampling devices and 2 weighting labs

Control of INAA and PIXE analysis



M. Almeida-Silva, S.M. Almeida, J. Cardoso, T. Nunes, M.A. Reis, P.C. Chaves, C.A. Pio (2014) Characterization of the Aeolian aerosol from Cape Verde by k0-INAA and PIXE, Journal of Radioanalytical and Nuclear Chemistry 300, 629-635. http://dx.doi.org/10.1007/s10967-014-2957-9.

Analysis of Internal Quality Data - INAA

- Participation in Inter-comparision exercises;
- Irradiating reference materials with all batch of samples;
- Evaluating the internal quality data.

$$\zeta = \frac{x_{\text{lab}} - x_{\text{ref}}}{\sqrt{u_{\text{lab}}^2 + u_{\text{ref}}^2}}$$

$|\zeta| \leq 2$	Questionable
$2 < |\zeta| < 3$	Satisfatory
$|\zeta| \geq 3$	Unsatisfatory

S.M. Almeida, M. Almeida-Silva, C. Galinha, C.A. Ramos, J. Lage, N. Canha, A.V. Silva, P. Bode (2014) Assessment of the Portuguese k0-INAA laboratory performance by evaluating internal quality control data, Journal of Radioanalytical and Nuclear Chemistry 300, 581-587. http://dx.doi.org/10.1007/s10967-014-2987-3.

CVDust Project – Data validation

- 10 types of RM were analyzed

Reference Material		No. of analysed RM	Associated samples	Irradiated mass (mg)	Irradiation conditions: Thermal Flux ($cm^{-2}s^{-1}$)	f	α	Irr.T (h)	Wait T (d)	Meas T (h)	Measuring conditions: Wait T (d)	Meas T (h)
NIST-1633a	Coal Fly Ash	119	Aerosols	11-474	7.0×10^{12}	50	0.005	5	3-4	7	28	7
IAEA-336	Lichens	36	Lichens	134-474	3.87×10^{12}	69	0.045	5	3-4	2	28	2
IAEA-Soil7	Soil	12	Soils	139-207	3.87×10^{12}	69	0.045	1	3-4	1.5	28	2.5
GBW07406	Soil	11	Soils	65-151	3.87×10^{12}	69	0.045	1	3-4	1.5	28	2.5
GBW07404	Soil	5	Soils	65-111	3.87×10^{12}	69	0.045	1	3-4	1.5	28	2.5
NIST-1568a	Rice Flour	14	Cereals	49-246	3.87×10^{12}	69	0.045	5	3-4	4	28	4
NIST-1567a	Wheat Flour	3	Cereals	77-126	3.87×10^{12}	69	0.045	5	3-4	4	28	4
NIST-1572	Citrus Leaves	10	Plants	135-143	3.87×10^{12}	69	0.045	5	3-4	3	28	3
INCT-OBTL5	Oriental Tobacco Leaves	4	Plants	149-152	3.87×10^{12}	69	0.045	5	3-4	3	28	3
NIST-1575	Pine Needles	4	Plants	149-153	3.87×10^{12}	69	0.045	5	3-4	3	28	3

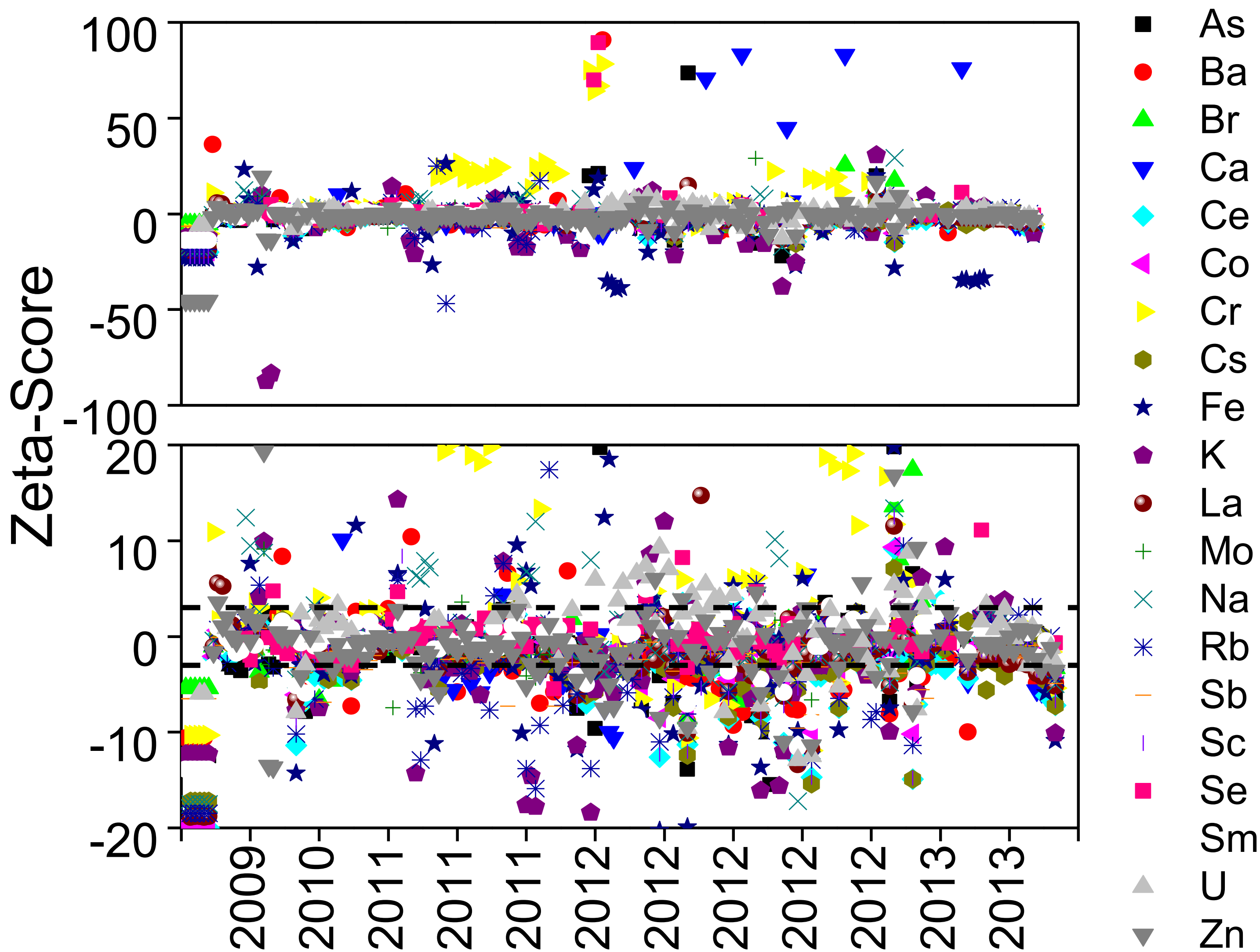
- 20 elements were evaluated

As, Ba, Br, Ca, Ce, Co, Cr, Cs, Fe, K, La, Mo, Na, Rb, Sb, Sc, Se, Sm, U, and Zn

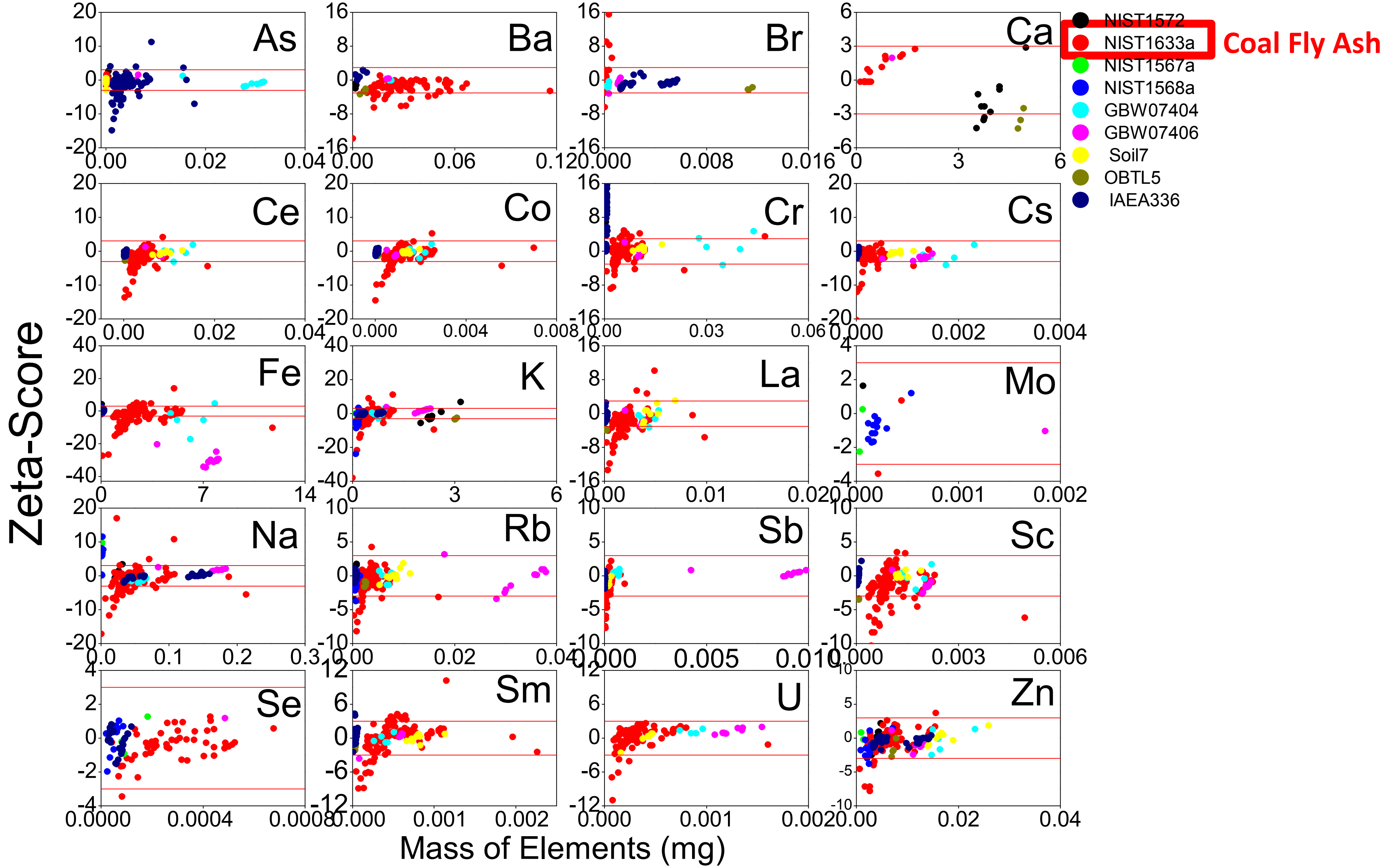
- Results from 6 operators were assessed

- Corresponded to the analysis of approximately 1500 samples and generation of 30 000 element concentrations.

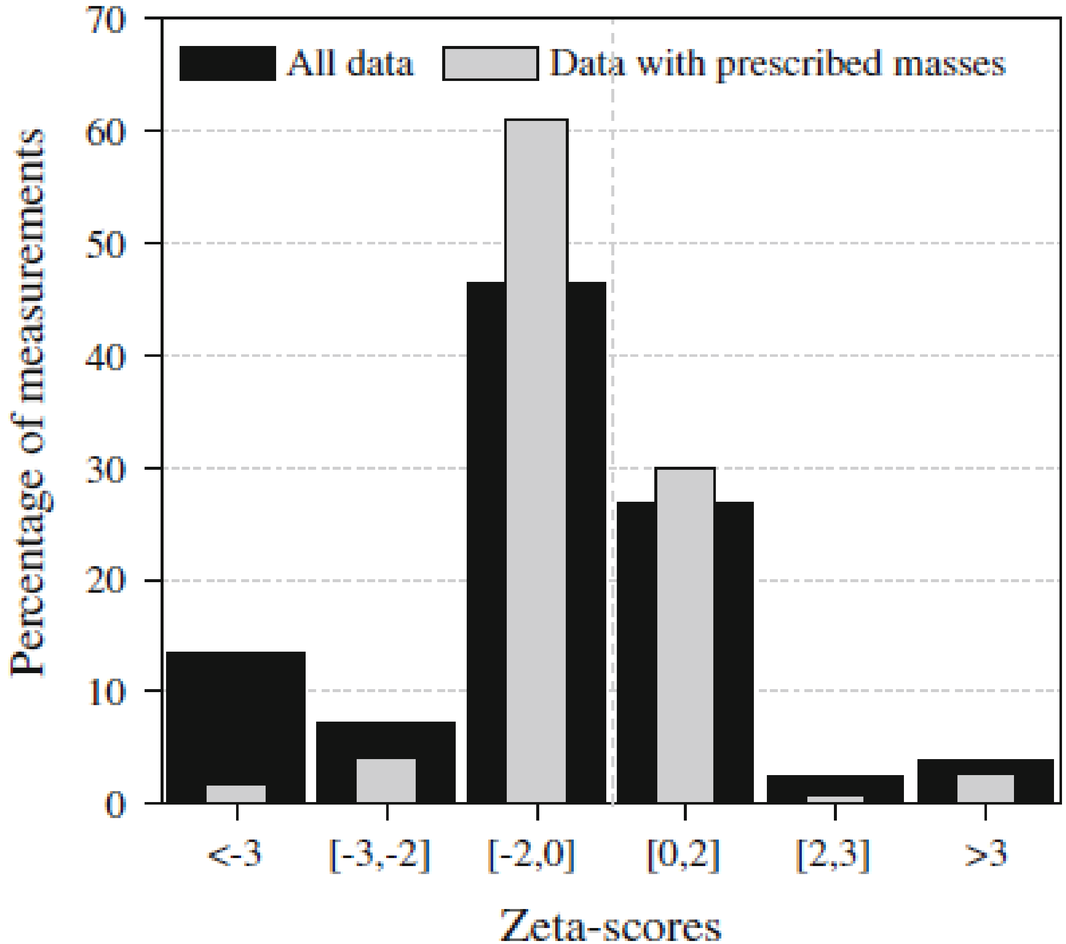
Quality Control – Zeta-score for all RM and elements



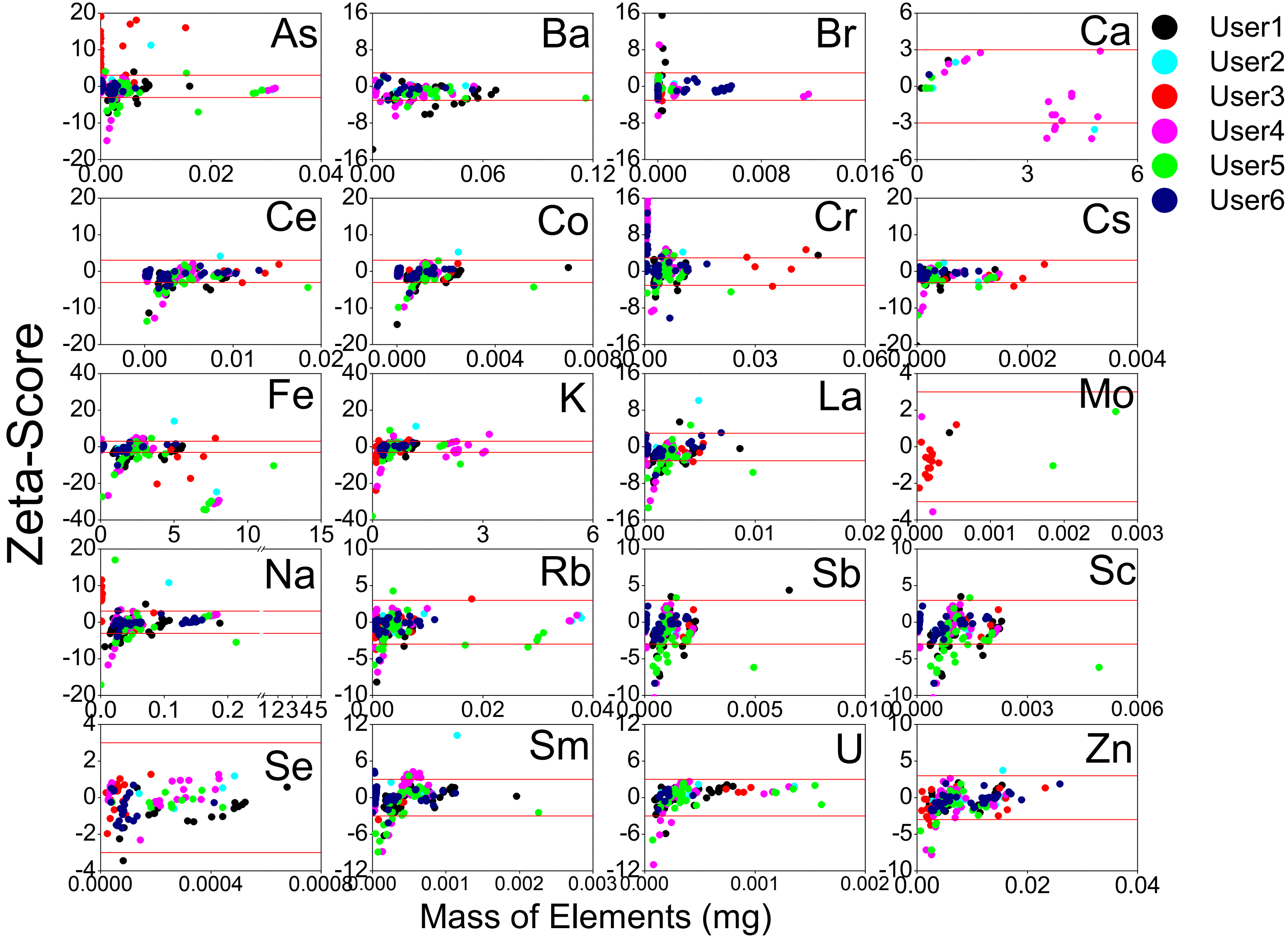
Zeta-score per element mass and RM



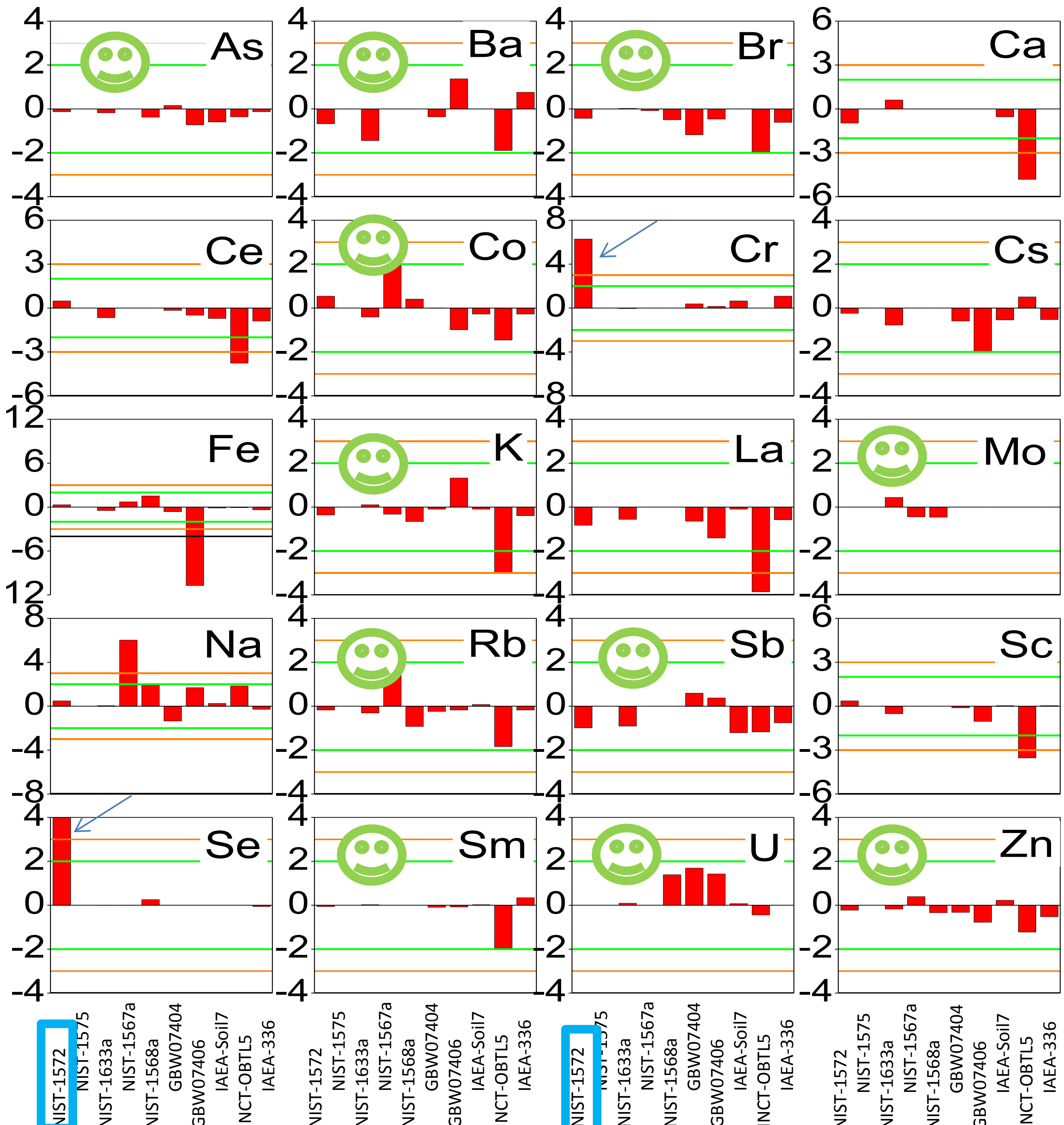
Zeta-Scores (2009-2013)



Zeta-score per element mass and user



Zeta-score per element and RM



NIST 1572 - Citrus Leaves

Control of Water Soluble Ion Analysis

*Charge

/Molecular weight

Principle:

1)In an electrolytic solution the concentrations of all the ionic species are such that the solution as a whole is neutral.

2) Considering that we measured the major ions

3) ∑ cations = ∑ anions (in equivalent)

	A	B	C	D	E	F	G	H	I	J	K	L
1		Neq/µmol	1000	1000	1000	2000	1000	1000	1000	2000	2000	2000
2		Mol Weig	35.45	79.9	62	96	23	18	39.1	24.3	40.1	60
3	Start Time		Cl^-	Br	NO_3^-	SO_4^{2-}	Na^+	NH_4^+	K^+	Mg^{2+}	Ca^{2+}	CO_3^{2-}
4			(µg/m³)	(µg/m³)	(µg/m³)	(µg/m³)	(µg/m³)	(µg/m³)	(µg/m³)	(µg/m³)	(µg/m³)	(µg/m³)
5	09-01-2011 12:00		6.275	0.011	1.046	1.721	4.629	0.051	0.266	0.422	1.049	0.94
6	12-01-2011 12:25		3.605	0.009	1.076	1.625	2.368	0.082	0.249	0.325	1.190	1.89
7	14-01-2011 12:45		1.346	0.005	0.442	0.616	0.846	0.020	0.097	0.142	0.487	1.81
8	18-01-2011 13:45		4.332	0.009	1.606	1.442	2.886	0.121	0.280	0.289	0.896	0.71
9	24-01-2011 12:50		1.017	0.003	0.237	0.386	0.816	0.091	0.058	0.073	0.073	0.32
10	26-01-2011 13:20		2.230	0.002	0.536	1.155	2.037	0.158	0.093	0.205	0.121	0.06
11	31-01-2011 13:25		3.168	0.007	0.429	0.769	2.264	0.050	0.105	0.205	0.471	0.77
12	02-02-2011 13:40		7.543	0.019	1.091	1.991	5.384	0.064	0.299	0.512	2.014	3.16
13	03-02-2011 14:00		10.312	0.028	1.301	4.298	8.254	0.176	0.629	0.929	6.681	13.40
14	04-02-2011 14:00		8.929	0.029	1.462	3.736	6.295	0.116	0.520	0.600	4.133	9.94
15	05-02-2011 12:00		25.853	0.021	8.085	13.824	22.008	0.479	1.931	2.186	13.759	16.34
16	05-02-2011 19:10		7.589	0.017	1.630	2.712	5.984	0.269	0.606	0.634	3.420	4.45
17	06-02-2011 12:00		7.606	0.022	1.674	3.698	5.363	0.087	0.544	0.644	4.901	9.17
18	07-02-2011 09:25		5.940	0.015	1.884	3.072	4.447	0.064	0.385	0.456	2.937	4.82
19	08-02-2011 08:45		9.738	0.006	4.390	6.996	2.996	3.470	0.254	0.425	1.848	1.96
20	09-02-2011 08:30		4.005	0.010	1.071	1.330	2.705	0.081	0.127	0.270	0.722	0.65
21	11-02-2011 08:20		6.509	0.010	0.797	1.409	4.765	0.161	0.202	0.434	0.500	0.11
22	13-02-2011 12:45		6.605	0.020	0.877	1.294	5.564	0.154	0.205	0.485	0.464	0.30
23	15-02-2011 13:00		7.324	0.008	1.089	1.710	5.478	0.212	0.188	0.486	0.290	0.05
24	17-02-2011 13:20		5.981	0.010	1.007	1.379	4.502	0.149	0.160	0.408	0.283	0.09
25	19-02-2011 13:35		5.237	0.012	0.757	1.038	3.717	0.102	0.120	0.339	0.311	0.29
26	21-02-2011 13:50		7.328	0.012	1.261	2.067	5.367	0.156	0.233	0.503	1.427	1.40
27	23-02-2011 14:10		9.079	0.014	2.147	2.797	6.803	0.308	0.323	0.663	1.845	1.41
28	24-02-2011 14:30		8.267	0.015	1.751	3.019	6.275	0.198	0.345	0.607	2.506	3.81
29	27-02-2011 18:15		8.306	0.023	1.370	4.059	6.351	0.052	0.489	0.563	5.455	10.58
30	28-02-2011 08:35		7.805	0.014	1.757	3.146	6.277	0.137	0.474	0.614	5.250	8.01
31	28-02-2011 18:50		5.672	0.012	1.329	2.129	4.274	0.083	0.233	0.424	2.621	3.69
32	01-03-2011 14:30		8.080	0.013	1.662	2.130	6.223	0.145	0.237	0.593	0.963	0.61
33	03-03-2011 14:50		6.094	0.007	1.503	1.707	4.625	0.298	0.219	0.436	0.655	0.26
34	08-03-2011 08:10		3.768	0.004	0.637	0.950	2.898	0.177	0.115	0.264	0.191	0.09
35	13-03-2011 11:45		4.646	0.006	0.453	0.974	3.525	0.077	0.133	0.328	0.202	0.06
36	16-03-2011 13:00		9.378	0.014	1.250	1.888	6.461	0.171	0.230	0.606	0.697	0.37
37	18-03-2011 13:10		8.679	0.008	0.891	1.782	5.622	0.150	0.267	0.528	0.514	0.11
38	21-03-2011 14:00		5.968	0.009	0.822	1.537	4.308	0.285	0.185	0.386	0.350	0.07
39	23-03-2011 14:30		8.666	0.012	1.689	3.690	7.219	0.281	0.349	0.654	1.837	1.67
40	28-03-2011 09:00		10.033	0.010	1.697	2.846	7.200	0.422	0.330	0.682	1.910	1.72
41	30-03-2011 13:30		10.600	0.010	1.227	2.784	7.335	0.365	0.295	0.646	0.793	0.17
42	02-04-2011 17:20		7.971	0.012	0.898	2.165	5.815	0.245	0.253	0.549	0.958	0.99
43	05-04-2011 14:15		7.571	0.010	1.435	2.041	5.601	0.228	0.229	0.472	1.164	0.90

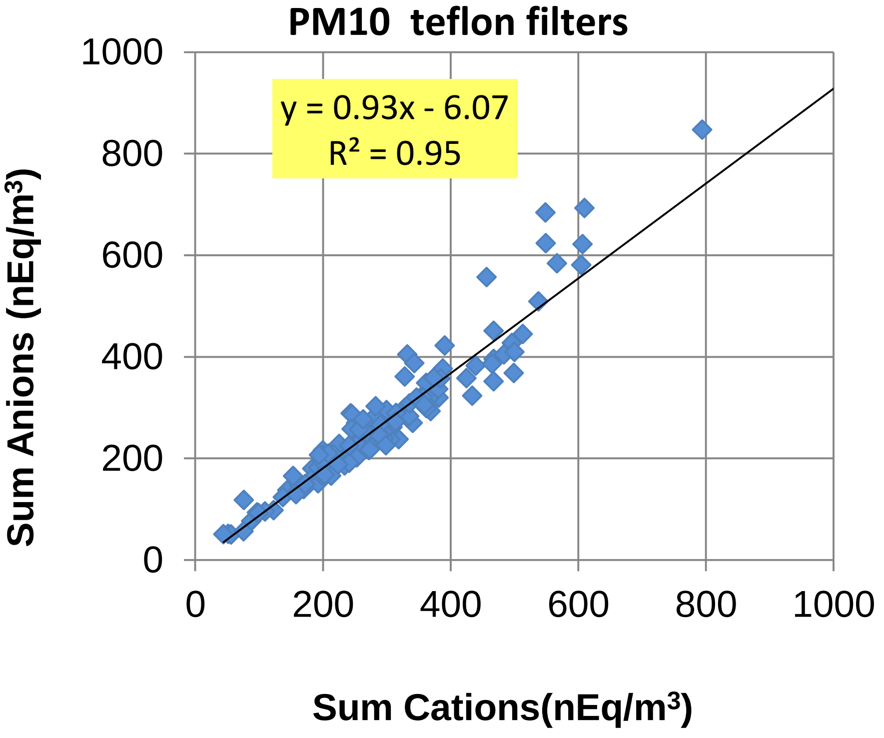
	M	N	O	P	Q	R	S	T	U	V	W	X	Y
2											Bal Ion		
3	Cl^-	Br	NO_3^-	SO_4^{2-}	Na^+	NH_4^+	K^+	Mg^{2+}	Ca^{2+}	CO_3^{2-}	ΣAn	Σcat	ΣCat/ΣAn
4	(nEq/m3)	(nEq/m3)	(nEq/m3)	(nEq/m3)	(nEq/m3)	(nEq/m3)	(nEq/m3)	(nEq/m3)	(nEq/m3)	(nEq/m3)	(nEq/m3)	(nEq/m3)	
5	177.01	0.14	16.87	35.86	201.27	2.85	6.80	34.77	52.34	31.34			
6	101.70	0.12	17.35	33.85	102.98	4.57	6.37	26.79	59.36	62.94			
7	37.97	0.07	7.13	12.83	36.80	1.09	2.47	11.68	24.30	60.26			
8	122.20	0.11	25.90	30.04	125.49	6.74	7.16	23.82	44.67	23.77			
9	28.68	0.04	3.83	8.04	35.47	5.05	1.48	6.02	3.65	10.68			
10	62.90	0.03	8.65	24.06	88.59	8.78	2.37	16.88	6.04	2.10			
11	89.36	0.09	6.92	16.02	98.45	2.77	2.68	16.87	23.49	25.58			
12	212.77	0.24	17.60	41.47	234.10	3.56	7.65	42.17	100.47	105.44			
13	290.88	0.35	20.98	89.55	358.89	9.77	16.08	76.48	333.21	446.51			
14	251.89	0.36	23.58	77.83	273.69	6.45	13.31	49.37	206.12	331.28			
15	729.28	0.26	130.40	288.00	956.86	26.60	49.38	179.93	686.25	544.83			
16	214.08	0.21	26.29	56.51	260.17	14.92	15.49	52.21	170.56	148.48			
17	214.55	0.28	26.99	77.03	233.18	4.83	13.92	53.02	244.45	305.66			
18	167.55	0.19	30.39	63.99	193.37	3.57	9.84	37.54	146.50	160.58			
19	274.70	0.08	70.81	145.75	130.26	192.78	6.51	34.94	92.16	65.42			
20	112.97	0.13	17.28	27.70	117.61	4.49	3.26	22.22	36.03	21.74			
21	183.60	0.13	12.85	29.35	207.18	8.97	5.18	35.76	24.95	3.81			
22	186.31	0.25	14.15	26.95	241.89	8.57	5.23	39.93	23.16	10.16			
23	206.61	0.11	17.57	35.63	238.15	11.79	4.81	40.01	14.46	1.51			
24	168.72	0.12	16.25	28.74	195.72	8.26	4.09	33.60	14.11	3.15			
25	147.74	0.15	12.21	21.62	161.62	5.64	3.08	27.87	15.50	9.71			
26	206.72	0.15	20.33	43.07	233.35	8.66	5.96	41.36	71.18	46.76			
27	256.11	0.18	34.64	58.27	295.76	17.11	8.25	54.60	92.01	46.99			
28	233.20	0.18	28.25	62.90	272.81	11.02	8.83	49.98	125.00	127.09			
29	234.30	0.29	22.10	84.57	276.12	2.87	12.51	46.37	272.07	352.65			
30	220.18	0.17	28.35	65.55	272.90	7.61	12.13	50.55	261.83	267.02			
31	160.01	0.15	21.44	44.35	185.84	4.61	5.95	34.92	130.70	123.13			
32	227.92	0.17	26.80	44.37	270.57	8.08	6.06	48.83	48.02	20.20			
33	171.89	0.09	24.24	35.56	201.10	16.58	5.61	35.90	32.69	8.55			
34	106.30	0.06	10.27	19.80	125.99	9.83	2.95	21.71	9.52	2.90			
35	131.06	0.07	7.31	20.30	153.28	4.30	3.40	26.99	10.07	1.88			
36	264.54	0.17	20.16	39.32	280.92	9.53	5.88	49.84	34.77	12.34			
37	244.81	0.09	14.36	37.12	244.43	8.32	6.82	43.42	25.61	3.63			
38	168.36	0.11	13.26	32.03	187.32	15.85	4.72	31.80	17.45	2.49			
39	244.45	0.15	27.25	76.87	313.86	15.60	8.92	53.86	91.62	55.78			
40	283.02	0.13	27.36	59.29	313.04	23.44	8.45	56.14	95.24	57.44			
41	299.02	0.12	19.79	58.00	318.91	20.29	7.55	53.20	39.56	5.67			
42	224.85	0.15	14.48	45.11	252.81	13.64	6.46	45.20	47.77	33.10			
43	213.56	0.13	23.15	42.51	243.54	12.65	5.87	38.83	58.06	30.16			

sampling errors | Water soluble ions analysis | Sheet3

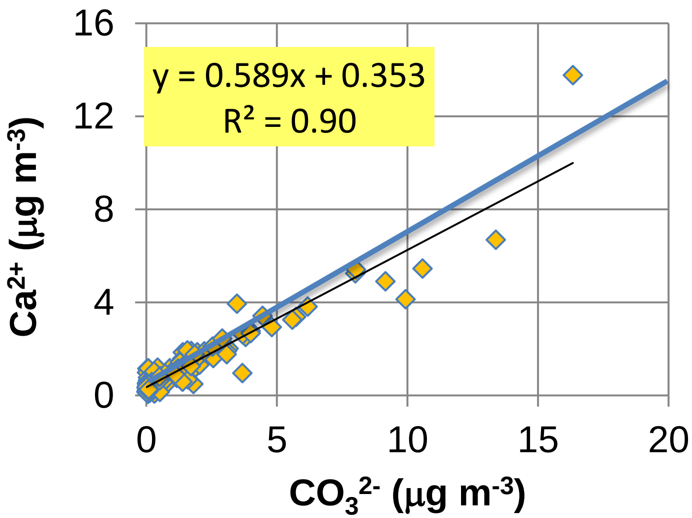
Ready 90%

CVDust Project – Data validation

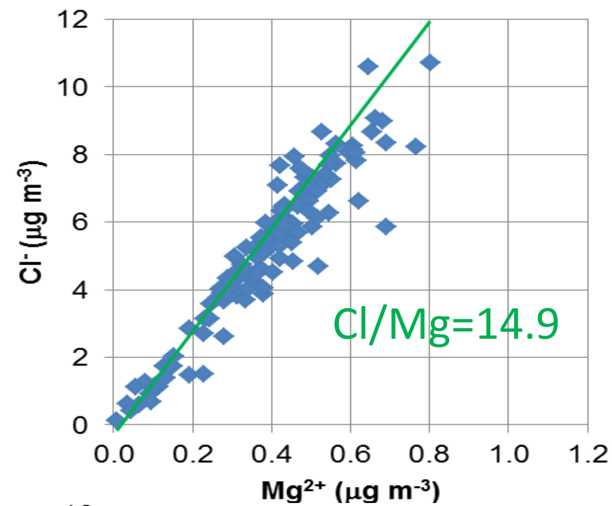
Control of Water Soluble Ion Analysis

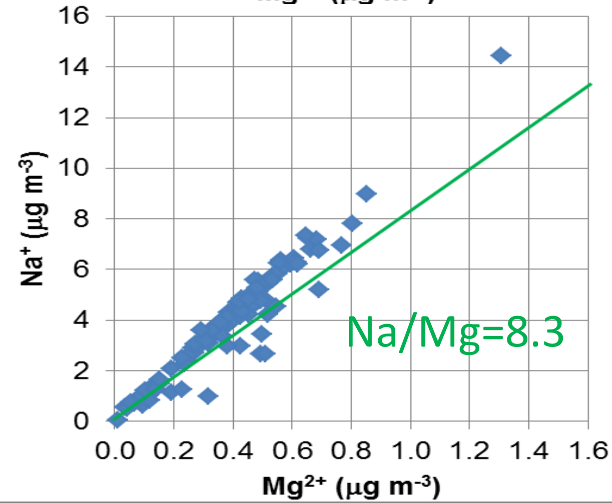


Control of Water Soluble Ion Analysis



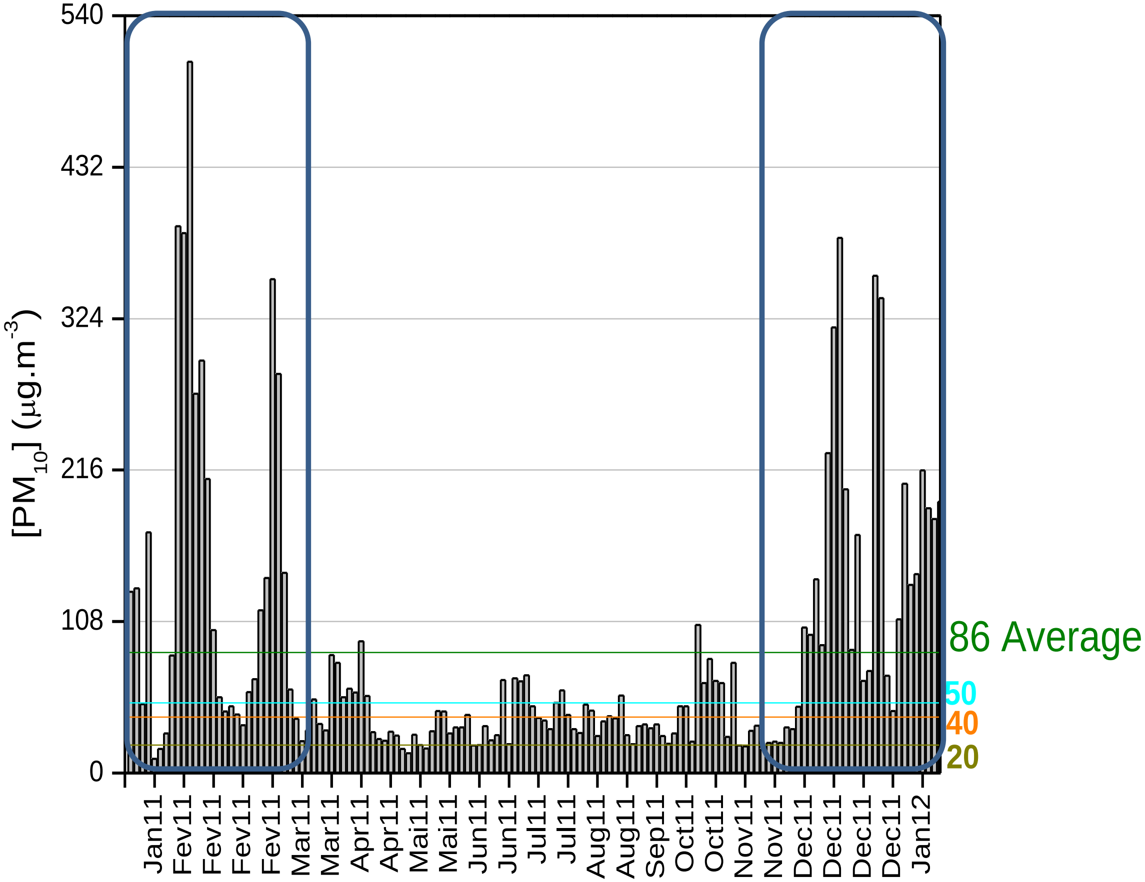
Blue line- Calcium carbonate





Green- Sea salt composition

Control of Concentration time series



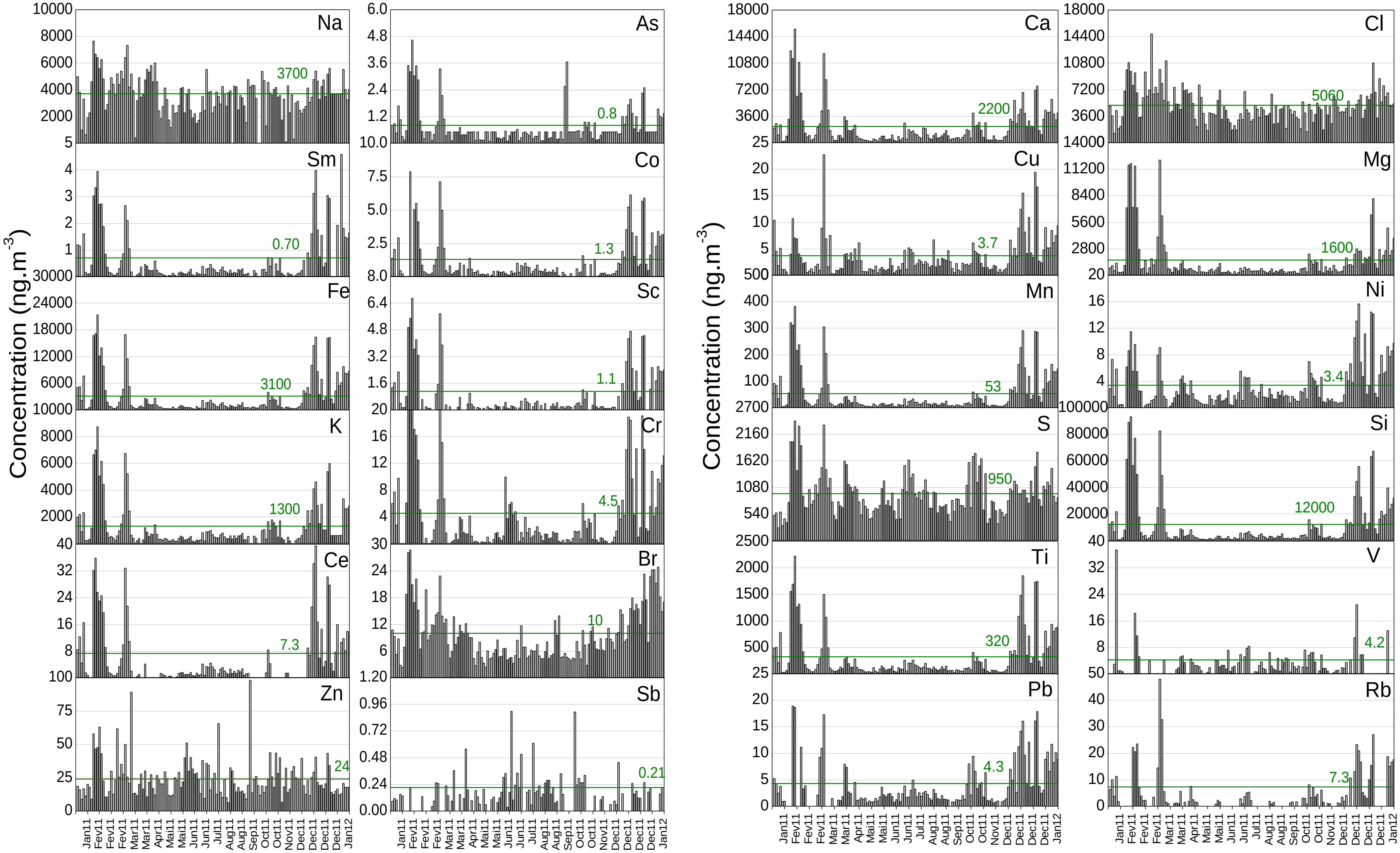
Objective:

- to find outliers
- to observe trends

The season between **December to March** are defined as **DRY SEASON**, as well as, **HARMATTAN** (Simonson, 1995).

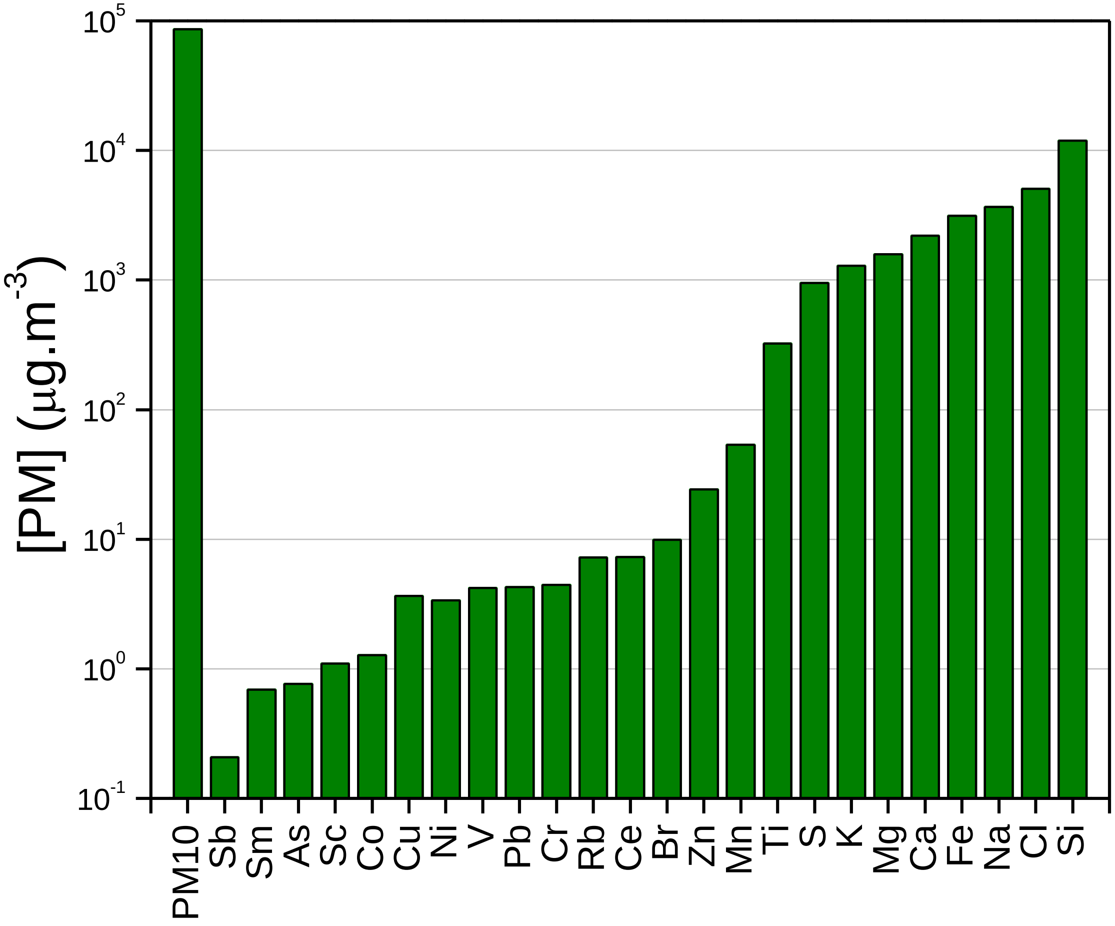
M. Almeida-Silva, S.M. Almeida, M.C. Freitas, C.A. Pio, T. Nunes, J. Cardoso (2013) Impact of Sahara Dust transport on Cape Verde atmospheric element particles, Journal of Toxicology & Environmental Health – Part A 76 (4-5), 240-251. http://dx.doi.org/10.1080/15287394.2013.757200.

Control of Concentration time series



— Average from Cape Verde

Average Concentrations



Should be compared with other places

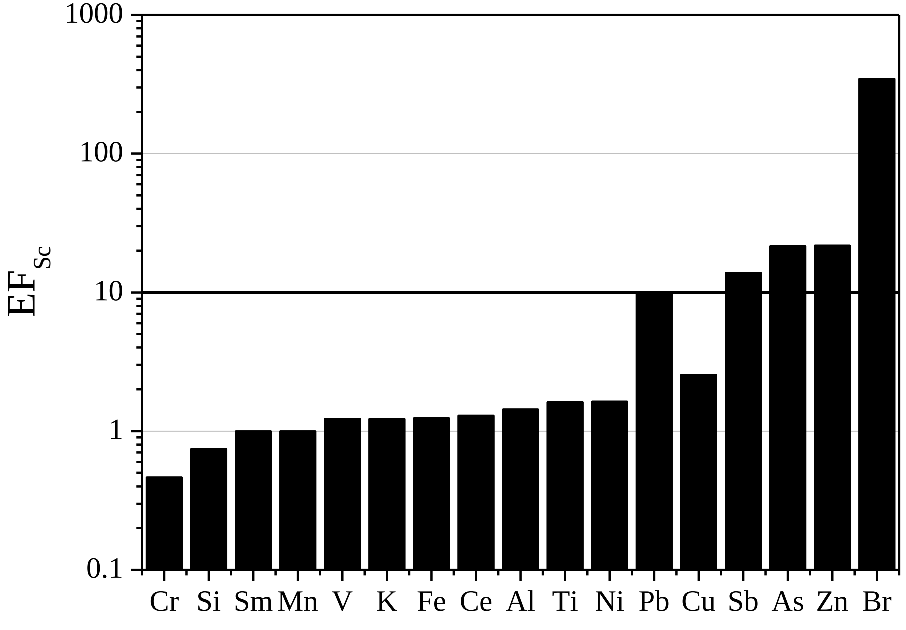
Enrichment factors

$$EF_{Sc} = \frac{\left(\frac{[X]}{[Sc]}\right)_{PM}}{\left(\frac{[X]}{[Sc]}\right)_{crust}}$$

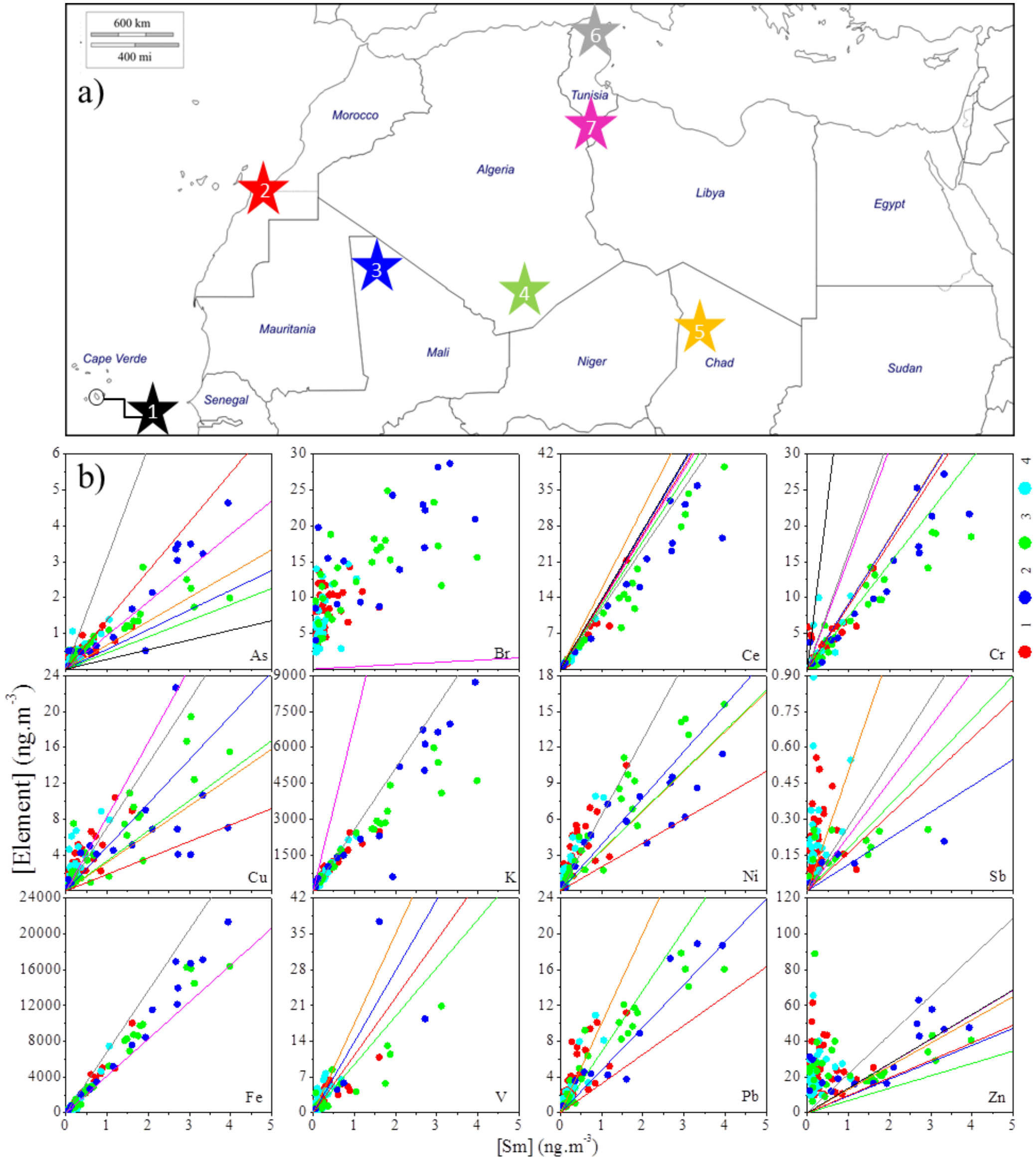
$[X]_{PM}$ - concentration of the element X in PM
$[Sc]_{PM}$ - concentration of Sc in PM
$[X]_{crust}$ - concentration of the X element in soil
$[Sc]_{crust}$ - Sc concentration in soil

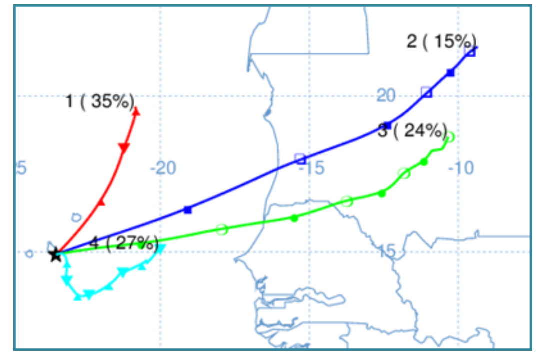
$$EF_{Na} = \frac{\left(\frac{[X]}{[Na]}\right)_{PM}}{\left(\frac{[X]}{[Na]}\right)_{sea}}$$

$[X]_{PM}$ - concentration of the element X in PM
$[Na]_{PM}$ - concentration of Na in PM
$[X]_{sea}$ - concentration of the X element in sea
$[Na]_{sea}$ – Na concentration in sea



Sahara contribution





TÉCNICO LISBOA

Preparation of database

Input files

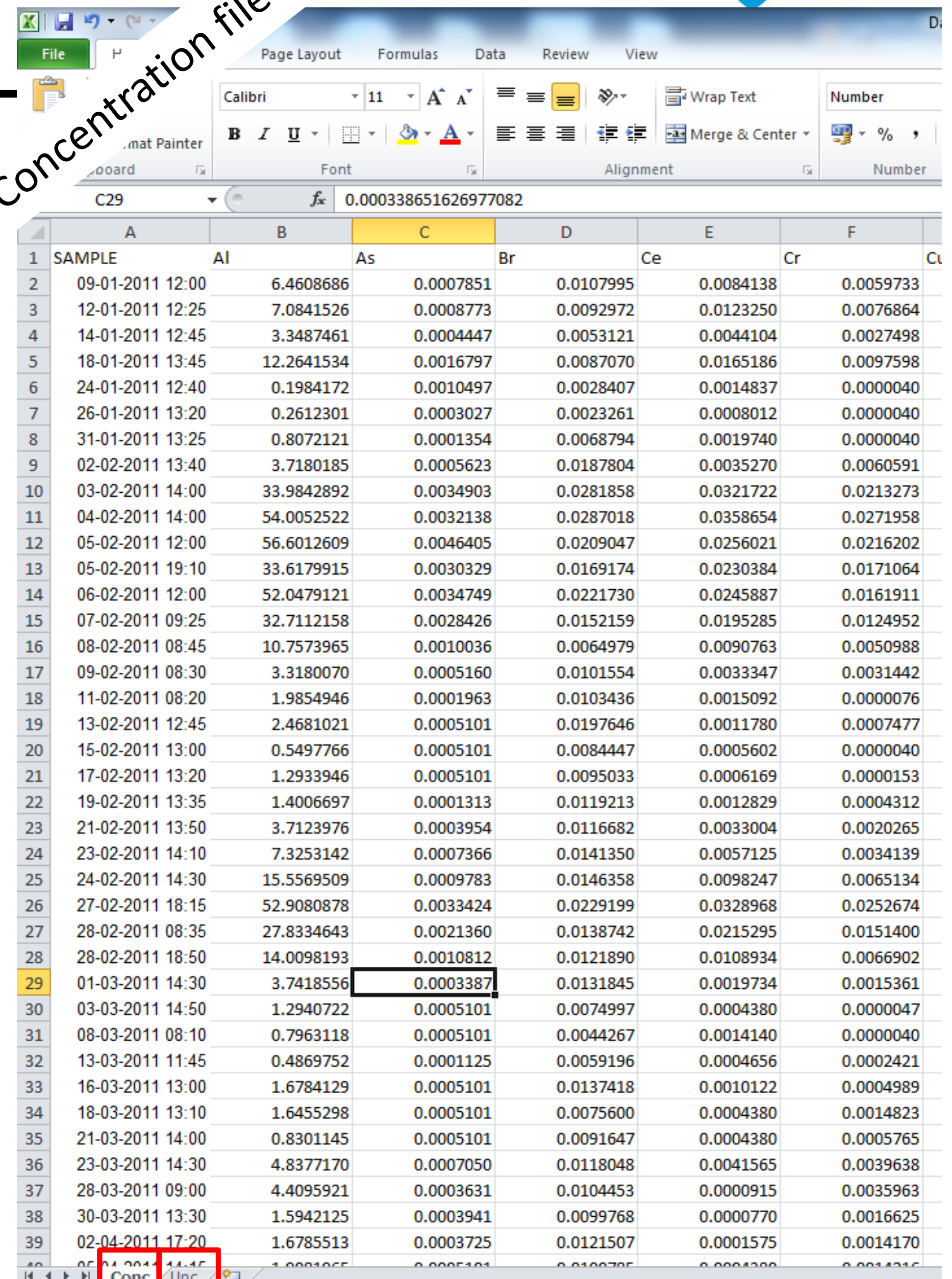
1. Concentration of chemical species
2. Uncertainties

Accepted formats

1. Tab-delimited (.txt)
2. Comma-separated value (.csv)
3. MS Excel (.xls)

Blank cells are not accepted

Factor analysis technique provides a robust solution when the number of samples minus the number of variable is at least 30 (Henry, 1991)



	A	B	C	D	E	F
1	SAMPLE	Al	As	Br	Ce	Cr
2	09-01-2011 12:00	6.4608686	0.0007851	0.0107995	0.0084138	0.0059733
3	12-01-2011 12:25	7.0841526	0.0008773	0.0092972	0.0123250	0.0076864
4	14-01-2011 12:45	3.3487461	0.0004447	0.0053121	0.0044104	0.0027498
5	18-01-2011 13:45	12.2641534	0.0016797	0.0087070	0.0165186	0.0097598
6	24-01-2011 12:40	0.1984172	0.0010497	0.0028407	0.0014837	0.0000040
7	26-01-2011 13:20	0.2612301	0.0003027	0.0023261	0.0008012	0.0000040
8	31-01-2011 13:25	0.8072121	0.0001354	0.0068794	0.0019740	0.0000040
9	02-02-2011 13:40	3.7180185	0.0005623	0.0187804	0.0035270	0.0060591
10	03-02-2011 14:00	33.9842892	0.0034903	0.0281858	0.0321722	0.0213273
11	04-02-2011 14:00	54.0052522	0.0032138	0.0287018	0.0358654	0.0271958
12	05-02-2011 12:00	56.6012609	0.0046405	0.0209047	0.0256021	0.0216202
13	05-02-2011 19:10	33.6179915	0.0030329	0.0169174	0.0230384	0.0171064
14	06-02-2011 12:00	52.0479121	0.0034749	0.0221730	0.0245887	0.0161911
15	07-02-2011 09:25	32.7112158	0.0028426	0.0152159	0.0195285	0.0124952
16	08-02-2011 08:45	10.7573965	0.0010036	0.0064979	0.0090763	0.0050988
17	09-02-2011 08:30	3.3180070	0.0005160	0.0101554	0.0033347	0.0031442
18	11-02-2011 08:20	1.9854946	0.0001963	0.0103436	0.0015092	0.0000076
19	13-02-2011 12:45	2.4681021	0.0005101	0.0197646	0.0011780	0.0007477
20	15-02-2011 13:00	0.5497766	0.0005101	0.0084447	0.0005602	0.0000040
21	17-02-2011 13:20	1.2933946	0.0005101	0.0095033	0.0006169	0.0000153
22	19-02-2011 13:35	1.4006697	0.0001313	0.0119213	0.0012829	0.0004312
23	21-02-2011 13:50	3.7123976	0.0003954	0.0116682	0.0033004	0.0020265
24	23-02-2011 14:10	7.3253142	0.0007366	0.0141350	0.0057125	0.0034139
25	24-02-2011 14:30	15.5569509	0.0009783	0.0146358	0.0098247	0.0065134
26	27-02-2011 18:15	52.9080878	0.0033424	0.0229199	0.0328968	0.0252674
27	28-02-2011 08:35	27.8334643	0.0021360	0.0138742	0.0215295	0.0151400
28	28-02-2011 18:50	14.0098193	0.0010812	0.0121890	0.0108934	0.0066902
29	01-03-2011 14:30	3.7418556	0.0003387	0.0131845	0.0019734	0.0015361
30	03-03-2011 14:50	1.2940722	0.0005101	0.0074997	0.0004380	0.0000047
31	08-03-2011 08:10	0.7963118	0.0005101	0.0044267	0.0014140	0.0000040
32	13-03-2011 11:45	0.4869752	0.0001125	0.0059196	0.0004656	0.0002421
33	16-03-2011 13:00	1.6784129	0.0005101	0.0137418	0.0010122	0.0004989
34	18-03-2011 13:10	1.6455298	0.0005101	0.0075600	0.0004380	0.0014823
35	21-03-2011 14:00	0.8301145	0.0005101	0.0091647	0.0004380	0.0005765
36	23-03-2011 14:30	4.8377170	0.0007050	0.0118048	0.0041565	0.0039638
37	28-03-2011 09:00	4.4095921	0.0003631	0.0104453	0.0000915	0.0035963
38	30-03-2011 13:30	1.5942125	0.0003941	0.0099768	0.0000770	0.0016625
39	02-04-2011 17:20	1.6785513	0.0003725	0.0121507	0.0001575	0.0014170

Preparation of database

Types of Uncertainties files

1. Sample specific – Uncertainty file provides na estimate of the uncertainty for each sample of each species;

2. Equation-based – file provides species-specific parameters that PMF uses to calculate uncertainties for each sample.

1. Sample specific Uncertainty file

	A	B	C	D	E
1		Al	As	Br	Ce
2	1-2011 12:00	0.323043	0.000384	0.000841	0.0006
3	12-01-2011 12:25	0.354208	0.000135	0.000894	0.0005
4	14-01-2011 12:45	0.167437	7.82E-05	0.000426	0.0001
5	18-01-2011 13:45	0.613208	0.000504	0.001086	0.0022
6	24-01-2011 12:40	0.009921	7.17E-05	0.000431	0.0002
7	26-01-2011 13:20	0.013062	0.00013	0.000223	7.85E-
8	31-01-2011 13:25	0.040361	5.12E-05	0.000494	0.003
9	02-02-2011 13:40	0.185901	0.000125	0.001243	0.0058
10	03-02-2011 14:00	1.699214	0.000395	0.004335	0.0063
11	04-02-2011 14:00	2.700263	0.000274	0.002741	0.0121

2. Equation based Uncertainty file

	A	B	C	D
1	Al	As	Br	Ce
2	0.006021	0.002	0.004	0.0005
3	4	9	6	9
4				
5				

Row 2: Method Detection Limit (MDL)

Row 3: Error fraction (in percentage)

If concentration ≤ Detection limit => $Unc = \frac{5}{6} \times MDL$

If concentration > Detection limit => $Unc = \sqrt{((Error\ Fraction \times concentration)^2 + (MDL)^2}$

Preparation of database

Missing values in the data base

	Concentration	Uncertainty
Concentration < MDL	½ MDL	5/6 MDL
Missing values	Geometric Mean	4 × Geometric Mean

Thank you for your attention