Preliminary results of the source apportionment inter-comparison exercise 2015-2016 (part 1)

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and the Fairmode community

Fairmode Technical meeting

Zagreb, 27-29 June 2016

Information that can be obtained from this IE

- Overall model performance on the basis of pre-established criteria,
  - ✓ *for the purposes of air quality management (AQM)*
- Indirect measure of the overall output uncertainty,
- More robust SA results (from a single outcome to an ensemble)
- Cross-validation of obtained results (to overcome the lack in observed data)
- Provide insights to understand the models behavior:
  - ✓ *influence of specific factors (e.g. input data, type of site, type of pollutant, meteorological conditions, etc…)*
  - ✓ *sensitivity to modelling approaches (e.g. RMs vs SMs) and assumptions*

- Additional details about SMs performance
- Integration of RMs outcomes (e.g. Apportionment of secondary pollutants, source-regions apportionment,…)

Main goals

- Contributing to the **harmonization** of Source Apportionment methods and tools

  (development and sharing of Best Practices)

- Contributing to the **integration** of Source and Receptor oriented techniques

  (to provide more robust and complete Source Apportionment information)

- Favoring the **connection** between Source Apportionment and Planning

  (e.g. use of common indicators)

Participant Institutions

AGH-UST, University of Science and Technology
APPA Trento
ARIANET
Aristotle University of Thessaloniki
ARPA Emilia-Romagna
ARPA Lombardia
ARPA Piemonte
ARPA Puglia
ARPA Veneto
CIEMAT
Clarkson University
CNRS - LGGE
Ecole des Mines de Douai
ENEA
Finnish Meteorological Institute
IDAEA-CSIC
IIA - CNR
IMROH
INERIS
INFN
Institute for Nuclear Research, HAS
ISAC -CNR
ISSeP
IST, Universidade de Lisboa
LISA-CNRS
Miguel Hernandez University
NCSR "Demokritos"
Paul Scherrer Institut
Pontificia Universidad Católica de Chile
RIER, University of Cologne
RIVM
RSE
Slovenian Environment Agency
TNO
Università degli Studi di Milano
University College Cork
University of Aveiro
University of Bari
University of Bologna
University of Genoa
University of Helsinki
University of Milano-Bicocca
Warsaw University of Technology

Organization of the IE

- Data distributed in July 2015
- Update in November 2015
- Receptors for CTM in January 2016

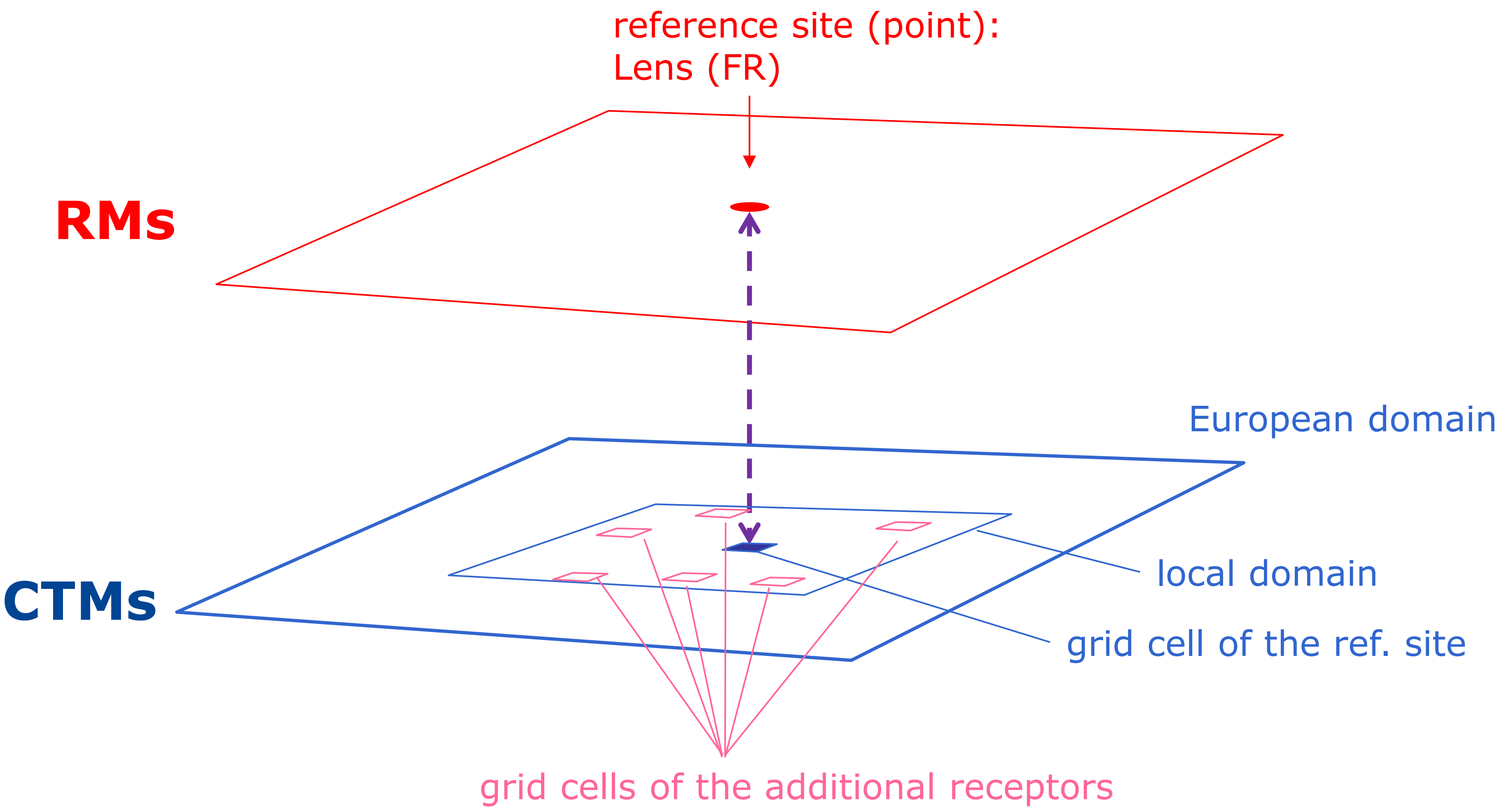
Applications: 79
Withrawed: 39
delivered: 40 teams (33 RM, 7 CTM)

- RM results reported by 33 teams
- CTM results reported by 7 teams
- Many defections and delay in submission of results
- Many requests of clarifications and correction of inconsistencies
- Delay in submission of results and solution of inconsistencies impacted on the timing of the data processing

15 EU countries + USA, Chile

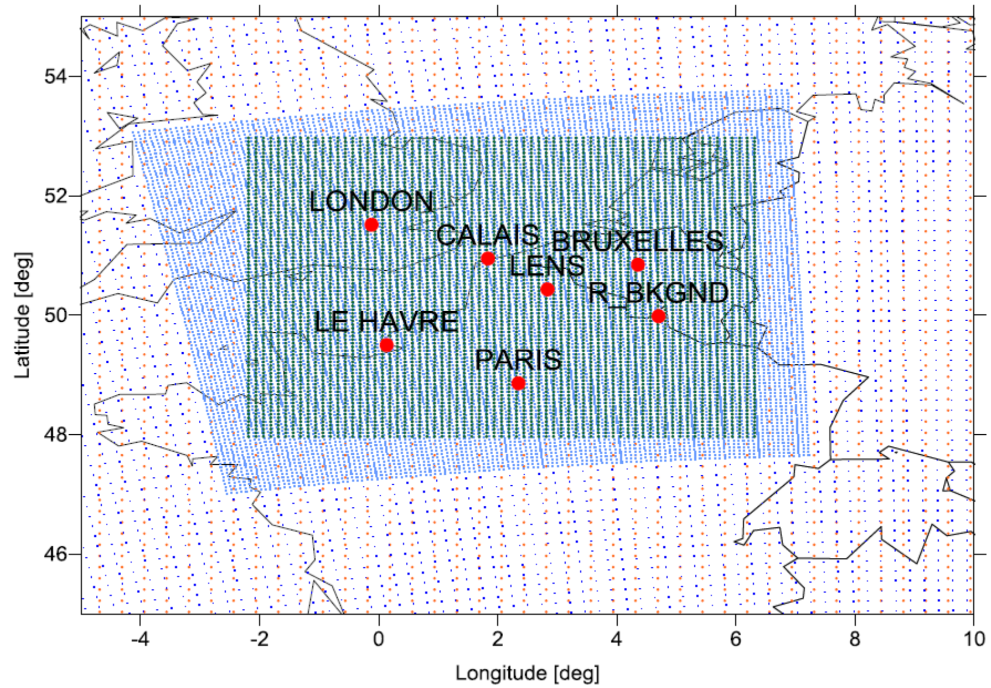
Belgium
Chile
Croatia
Finland
France
Germany
Greece
Hungary
Ireland
Italy
Poland
Portugal
Slovenia
Spain
Switzerland
The Netherlands
USA

How is the intercomparison organized?



Intercomparison outline – Source oriented Models

- **Common input dataset**
  - ECMWF meteorology
  - TNO emissions
  - MACC chemical fields
- **Centralized MPE**
  - LENS dataset
  - AIRBASE sites
  - Local networks
- **Set of receptors (10)**
  - Lens
  - Urban sites
  - Coastal sites
  - Background sites



8 - 14 source categories
3 + 3 summer/winter months
Hourly concentrations
Primary and secondary PM
PM precursors

Evaluation Methodology (RM)

European Commission

Complementary tests: provide ancillary information about the solutions' performance

- Mass apportionment
- Number of factor/sources

Preliminary tests: test if source/factors belong to a given source category

- Chemical profiles → Pearson distance, SID, WD
- Time-trends → Pearson distance
- Contribution-to-species (%) → Pearson distance

= % of species total matrix (EPA PMF v3) = explained variation (PMF 2) = contribution by species (CMB 8.2)

Performance tests Evaluate if source/factor SCEs fall within an established quality objective

- Z-scores → test solution bias coherence with the quality objective (σ_p)
- Z'-scores → test SCE reported uncertainty coherence with the one of the reference
- RMSD* → test the bias, amplitude and phase of the SCE time trends

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A new methodology to assess the performance and uncertainty of source apportionment models in intercomparison exercises

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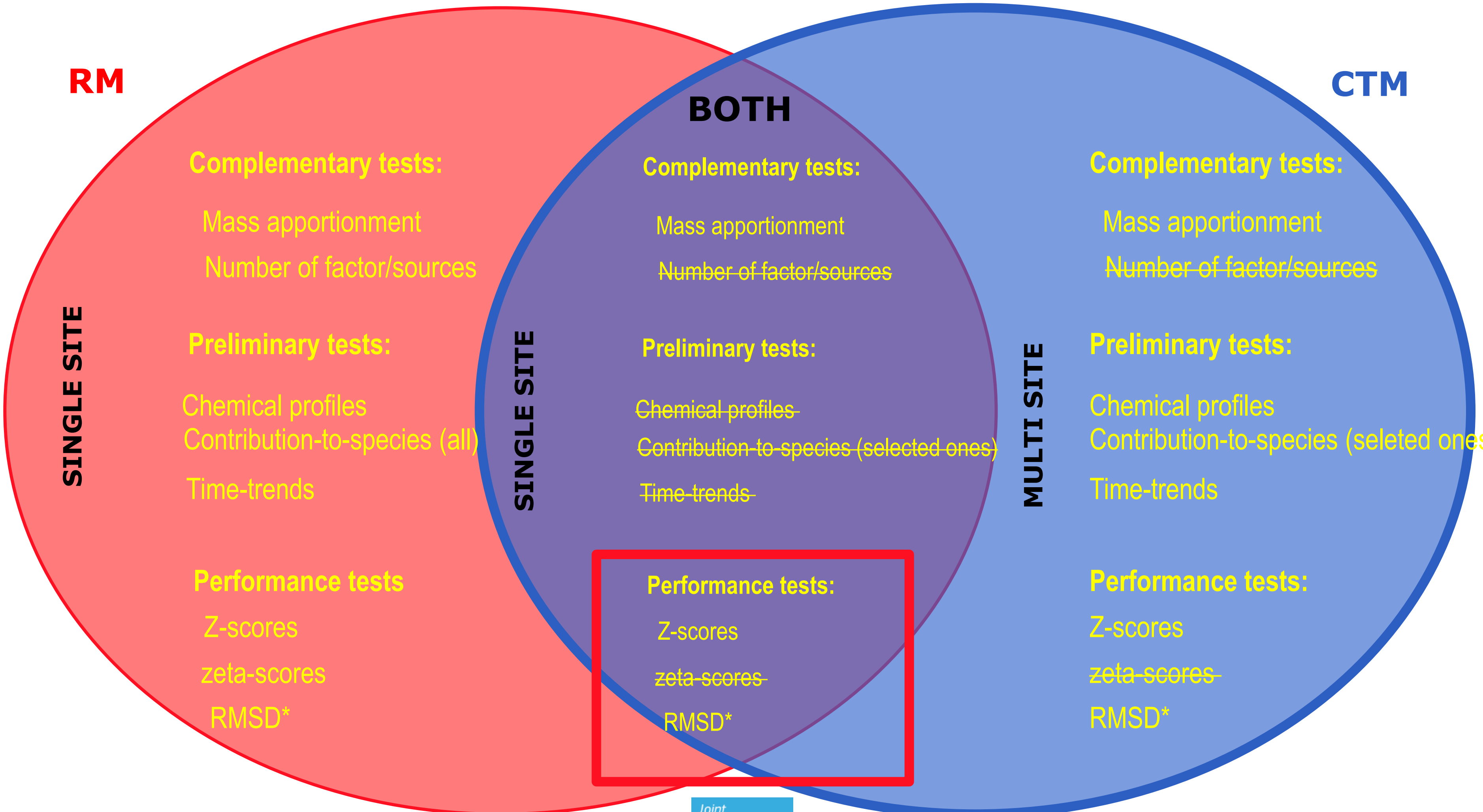
ELSEVIER

A new methodology to assess the performance and uncertainty of source apportionment models II: The results of two European intercomparison exercises

C.A. Belis [a,*], F. Karagulian [a], F. Amato [b], M. Almeida [c], P. Artaxo [d], D.C.S. Beddows [e], V. Bernardoni [f], M.C. Bove [g], S. Carbone [h], D. Cesari [i], D. Contini [i], E. Cuccia [g], E. Diapouli [j], K. Eleftheriadis [j], O. Favez [k], I. El Haddad [l], R.M. Harrison [e,m], S. Hellebust [n], J. Hovorka [o], E. Jang [e], H. Jorquera [p], T. Kammermeier [q], M. Karl [r], F. Lucarelli [s], D. Mooibroek [t], S. Nava [s], J.K. Nøjgaard [u], P. Paatero [v], M. Pandolfi [b], M.G. Perrone [w], J.E. Petit [l,z], A. Pietrodangelo [x], P. Pokorná [o], P. Prati [h], A.S.H. Prevot [m], U. Quass [q], X. Querol [b], D. Saraga [y], J. Sciare [z], A. Sfetsos [y], G. Valli [g], R. Vecchi [g], M. Vestenius [i], E. Yubero [aa], P.K. Hopke [ab]

Evaluation in this IE



Introduction to RM tests

European Commission

Intercomparison outline – Receptor oriented models

DATA SET WITH SPECIATED PM (including organic markers)

COUNTRY	France
PERIOD	03.2011 to 03.2012
TIME RES.	every 3 days
DURATION OF SAMPLING	24 hours
TYPE OF SITE	Urban background
	PM10
N SAMPLES	116
IONS	ok (8 species)
EC/OC	ok
TRACE ELEMENTS	ok (25 species)
PAHs	ok (15 species)
LEVO/MANN	ok + galacto
HOPANES	ok (10 species)
N-ALKANES	ok (29 species)
CHOLESTEROL	
SOA MARKERS	ok
OTHER	Pristane, Phytane, Glucose

LGGE
Laboratoire de Glaciologie et Géophysique de l'Environnement

LCME
Laboratoire Chimie Moléculaire et Environnement

INERIS
maîtriser le risque pour un développement durable

MINES Douai

Atmo Nord - Pas de Calais
Surveillance de la qualité de l'air

RM PARTICIPANTS

AGH-UST	ISAC LE	RIVM
APPATN	FMI	SAGE
ARPA ER	IDAEA_T	UCC
ARPA LO	IDAEA_A	UMH
ARPA PU	IMROH	UNIBO
ARSO	ISSeP	UNIHE
AUTH	IST	UNIMI
CARES	LGGE+	UNMIB
CNR IIA	NCSR	UNIFI
ENEA	PSI	UNIGE
ISAC BO	PUC	WUT

RM MODELS

PMF5

ME-2

PMF4

PNF3

PMF2

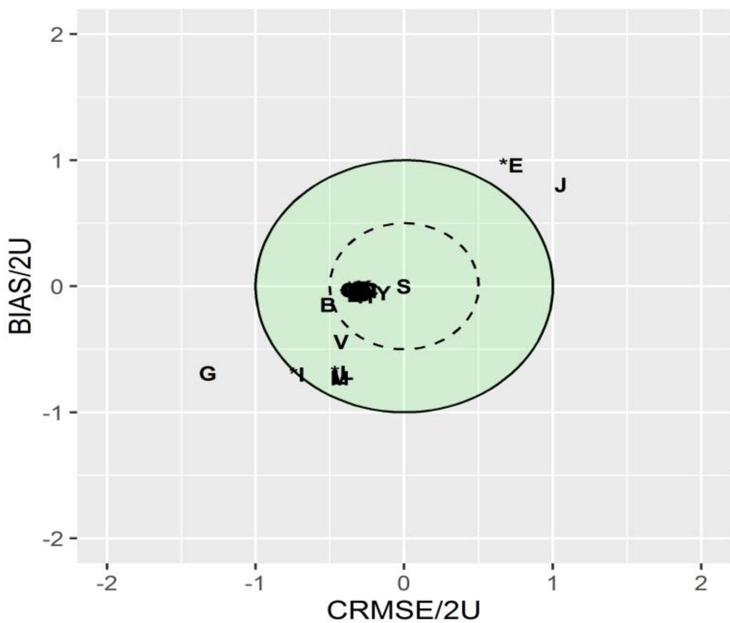
RCMB

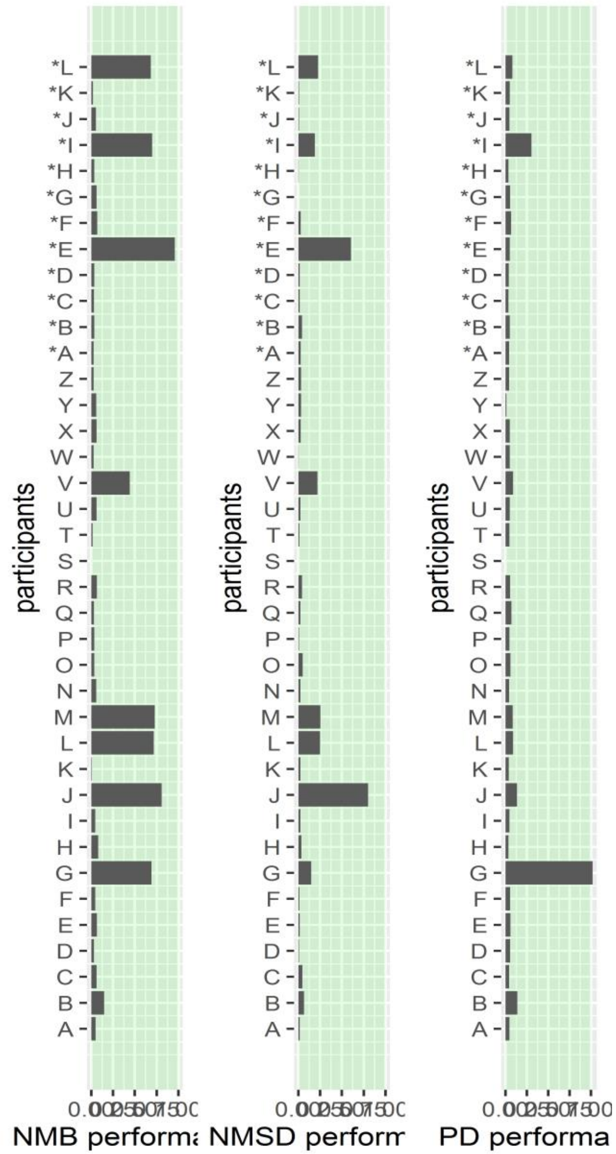
RM SOURCE CATEGORIES (SPECIEUROPE)

1	traffic
2	exhaust
10	soil
12	marine fresh
20	industry
30	fuel oil
31	coal
37	ship
40	biomass burning
41	wood burning
5	road dust
60	SIA
61	ammonium nitrate
62	ammonium sulphate
66	deicing salt
70	POA
71	aged sea salt
74	combustion

RM preliminary tests

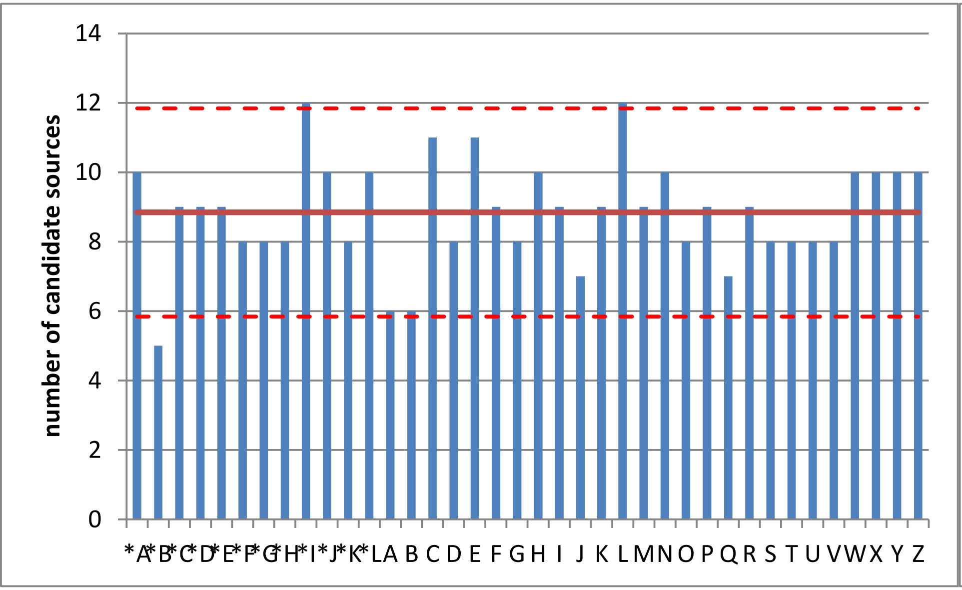
MASS CLOSURE

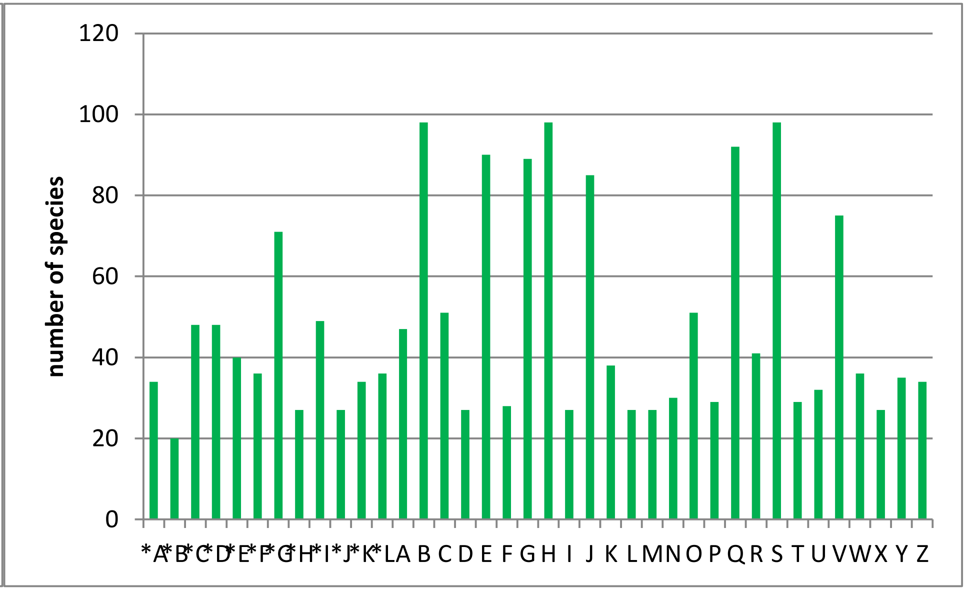




The majority of the results reproduce the gravimetric mass accurately. Some results do not explain all the gravimetric mass but fall in the area of acceptance. A few results over- or underestimate the total PM mass.

candidate sources and species



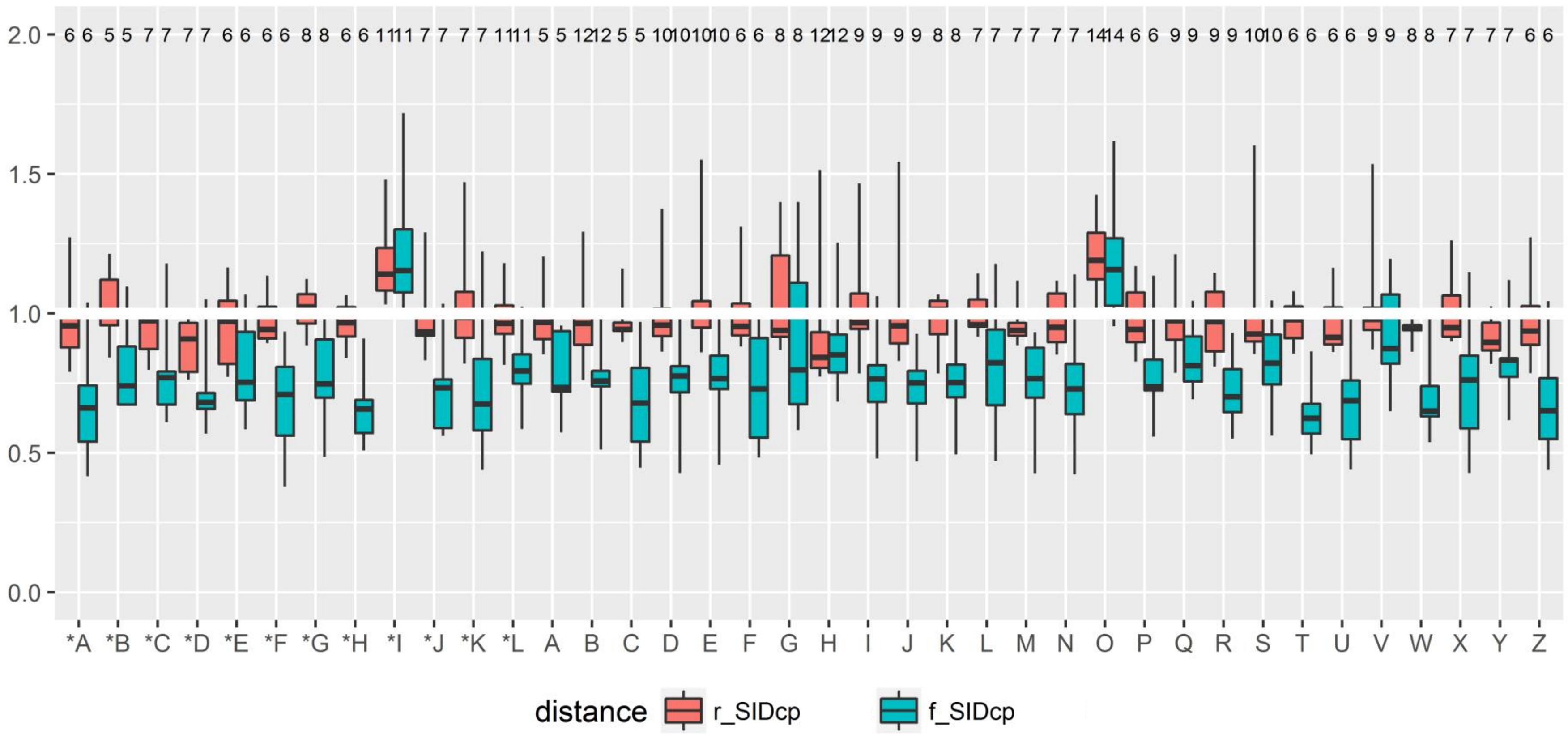


- red solid line bar average (9)
- red broken lines represent avg. +-3
- 84% of the results within the range average+-2 sources

- 55% of the results were obtained with less than 40 species
- 18 % of the results were obtained with more than 80 species
- many results with merged species

RM similarity tests

SID all particpants



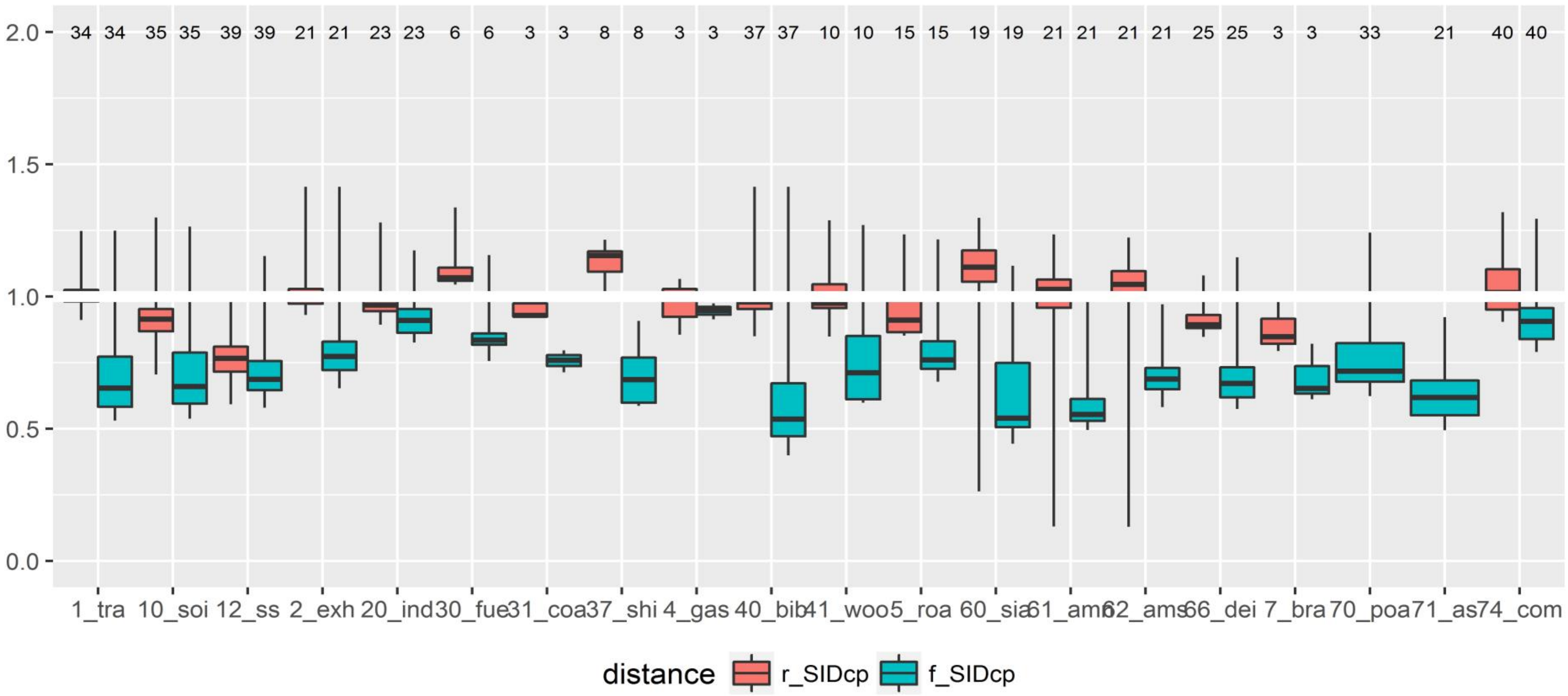
r = distances to the reference chemical profiles (cp) in SPECIATE and SPECIEUROPE

f = distances among the candidate sources

top = number of candidate sources

Results *I and O show the majority of cp not comparable with the reference and with the other results. Half of results with more than 25% of candidate sources not comparable to the reference sources.

SID by sources



r = distances to the reference chemical profiles (cp) in SPECIATE and SPECIEUROPE

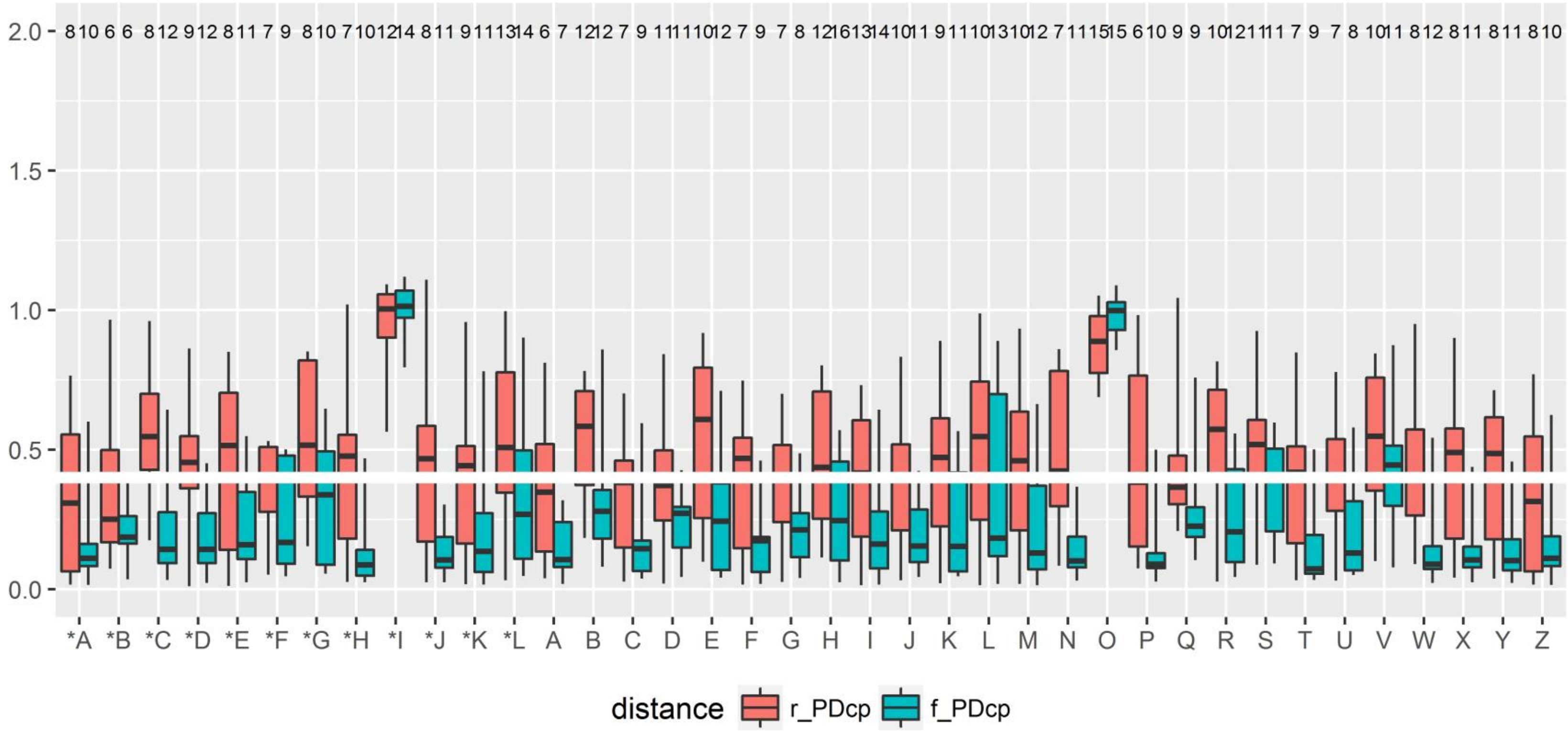
f = distances among the candidate sources

top = number of candidate sources

Fuel oil, ship, SIA and, to a lesser extent, undefined combustion are the most critical source categories

Pearson distance (PD) all particpants

European Commission



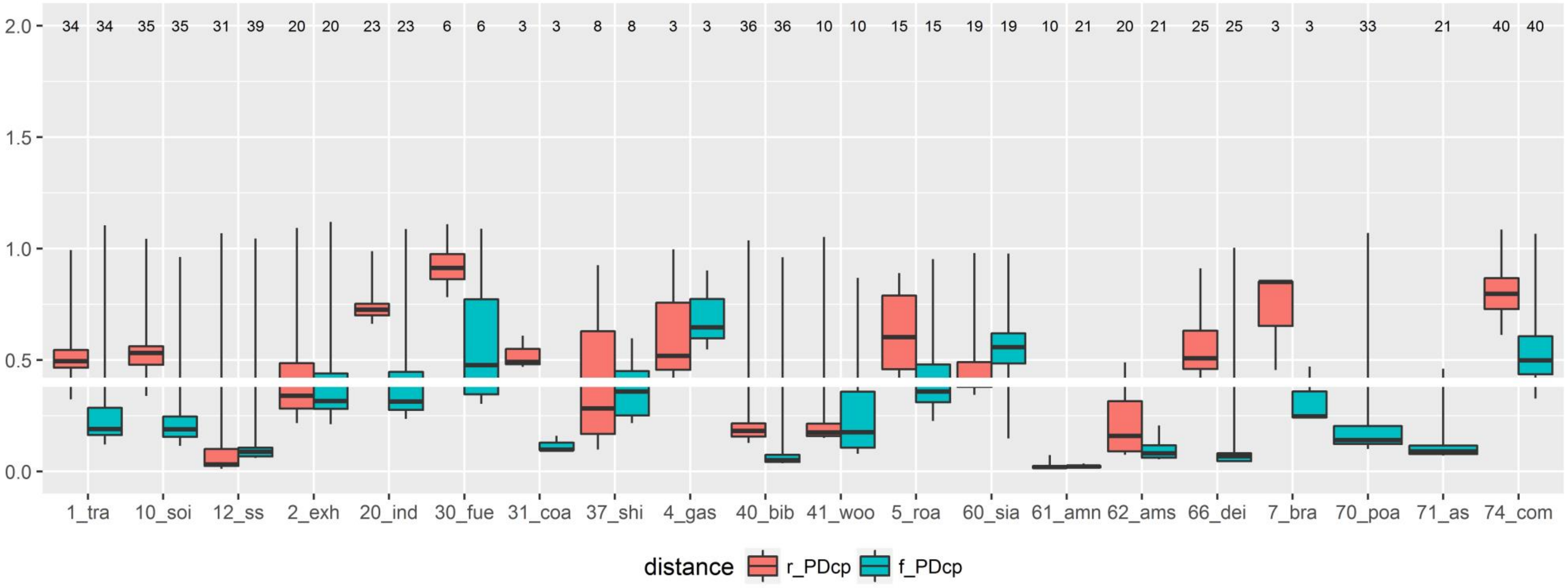
r = distances to the reference chemical profiles (cp) in SPECIATE and SPECIEUROPE

f = distances among the candidate sources

top = number of candidate sources

Results *I and O majority of cp not comparable with the reference and with the other results. Majority of results with more than 50% of candidate sources not comparable to the reference sources.

Pearson distance (PD) all particpants



r = distances to the reference chemical profiles (cp) in SPECIATE and SPECIEUROPE

f = distances among the candidate sources

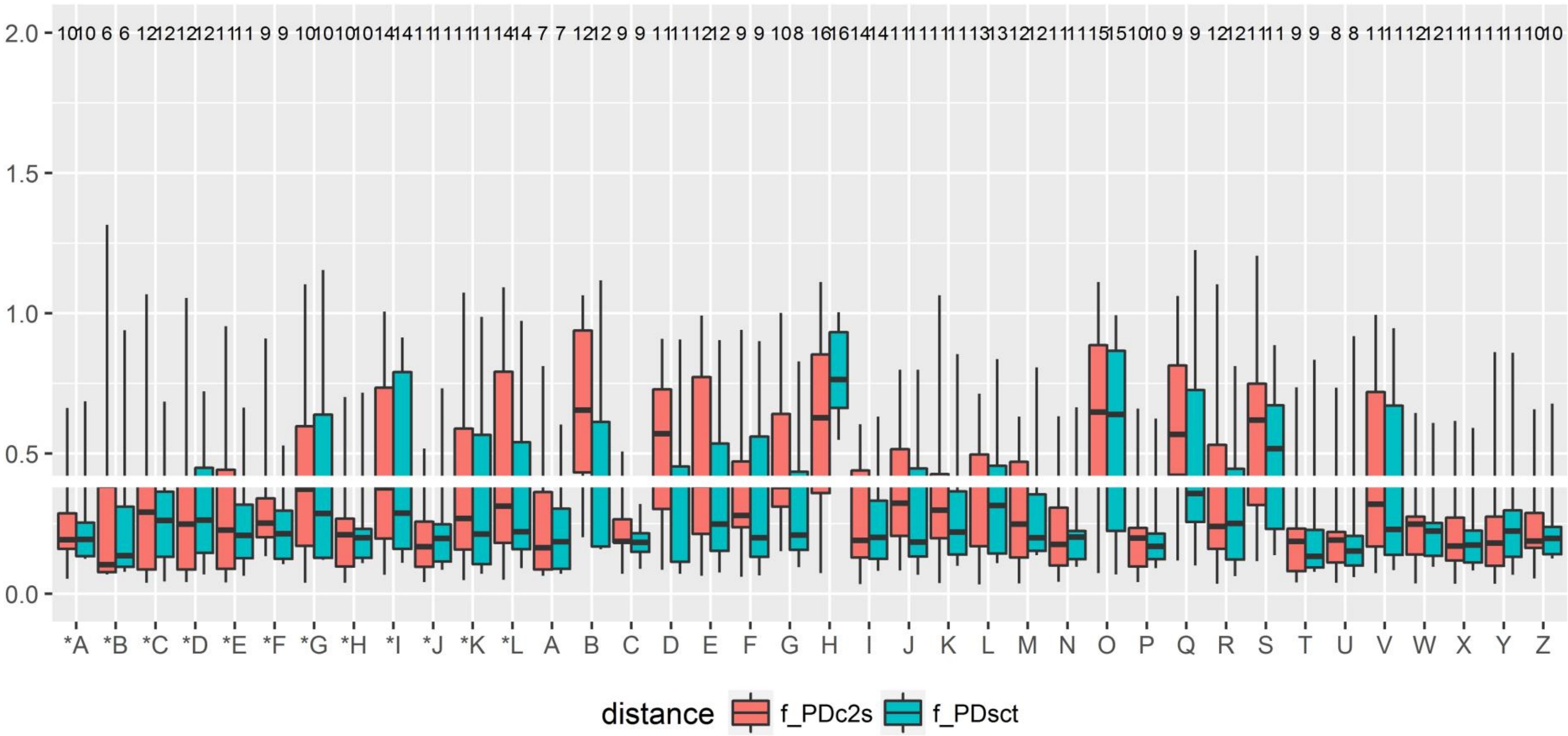
top = number of candidate sources

industry, fuel oil, undefined combustion, traffic, exhaust, road dust soil are the most critical source categories.

For gasoline, fuel oil, SIA and undefined combustion there is little agreement among participant results.

Pearson distance (PD) time series and contribution-to-species

European Commission



f = distances among the candidate sources

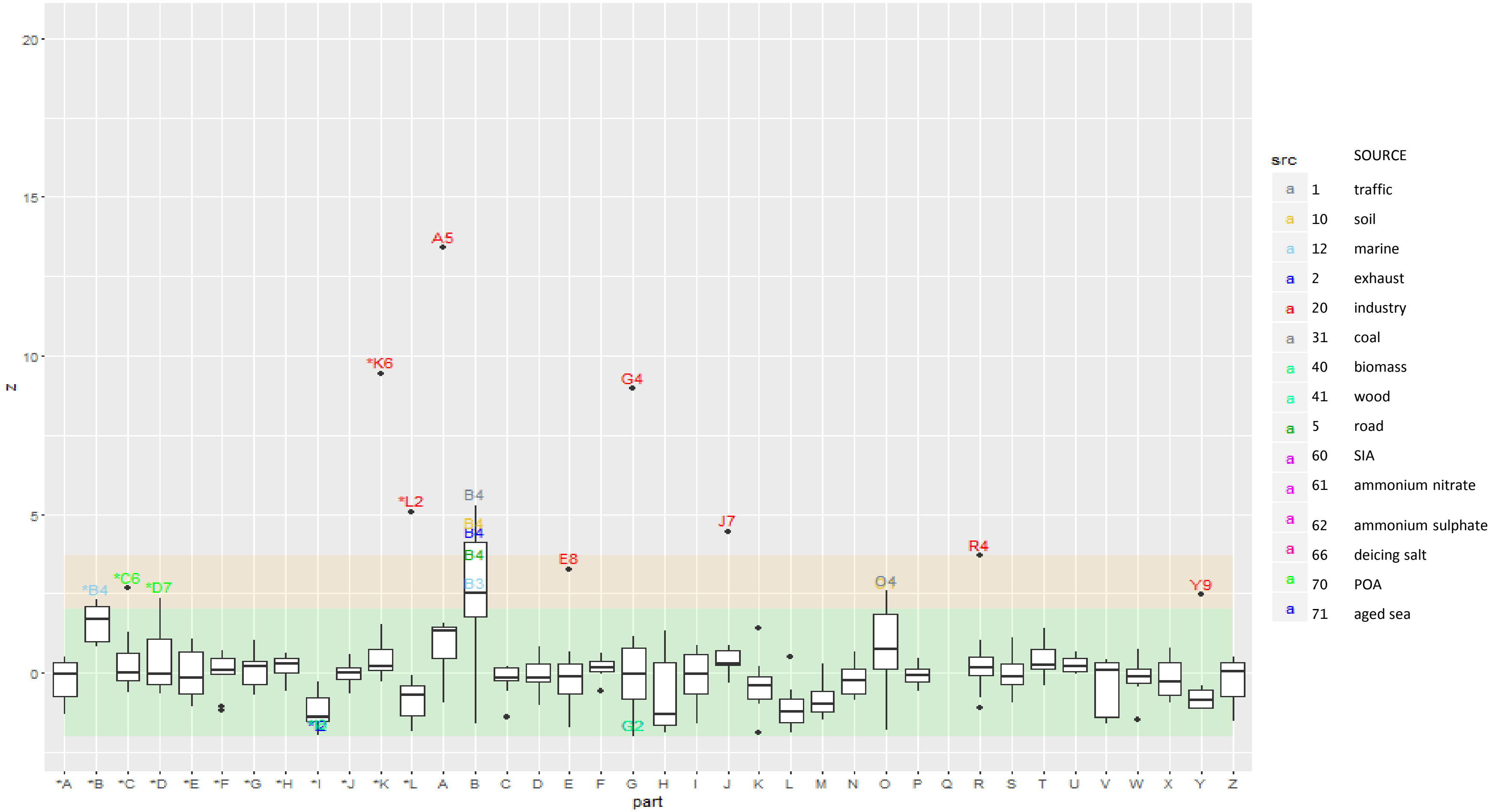
top = number of candidate sources

c2s = contribution to species; sct= source contribution estimate time series

General good agreement between participants. Results H, O and S present atypical time trends. Results B, D, H, O, Q and S show contribution-to-species not comparable with the rest.

RM performance tests

Performance RMs
z-score (overall sce)



z score thresholds from kernel curve (Belis et al., 2015)

Result Q (out of scale) and B present the majority of the source candidates out of the acceptability zone. Most of the sce attributed to industry are overestimated.

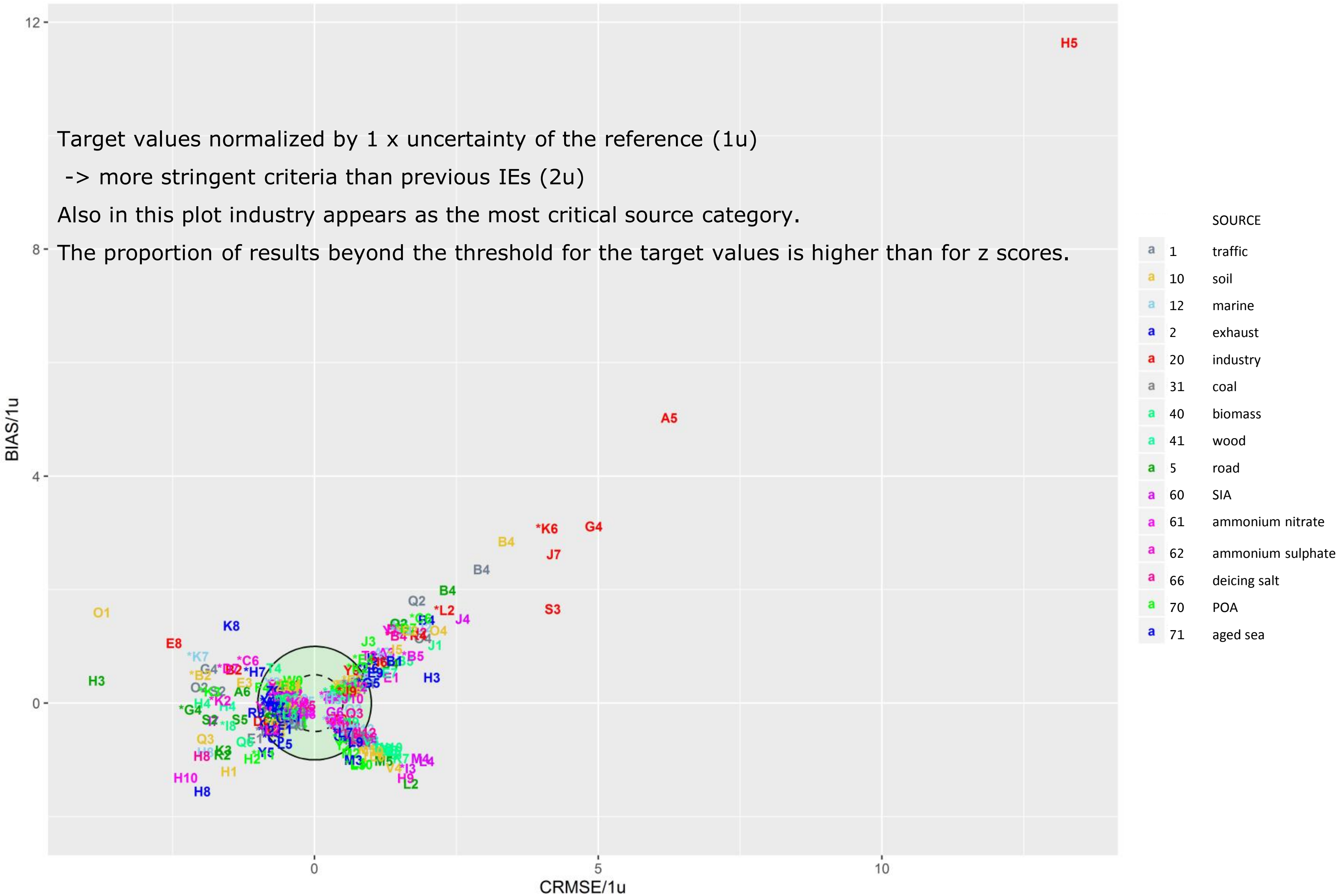
Performance RMs
Target plot (sce time series)

Target values normalized by 1 x uncertainty of the reference (1u)

-> more stringent criteria than previous IEs (2u)

Also in this plot industry appears as the most critical source category.

The proportion of results beyond the threshold for the target values is higher than for z scores.

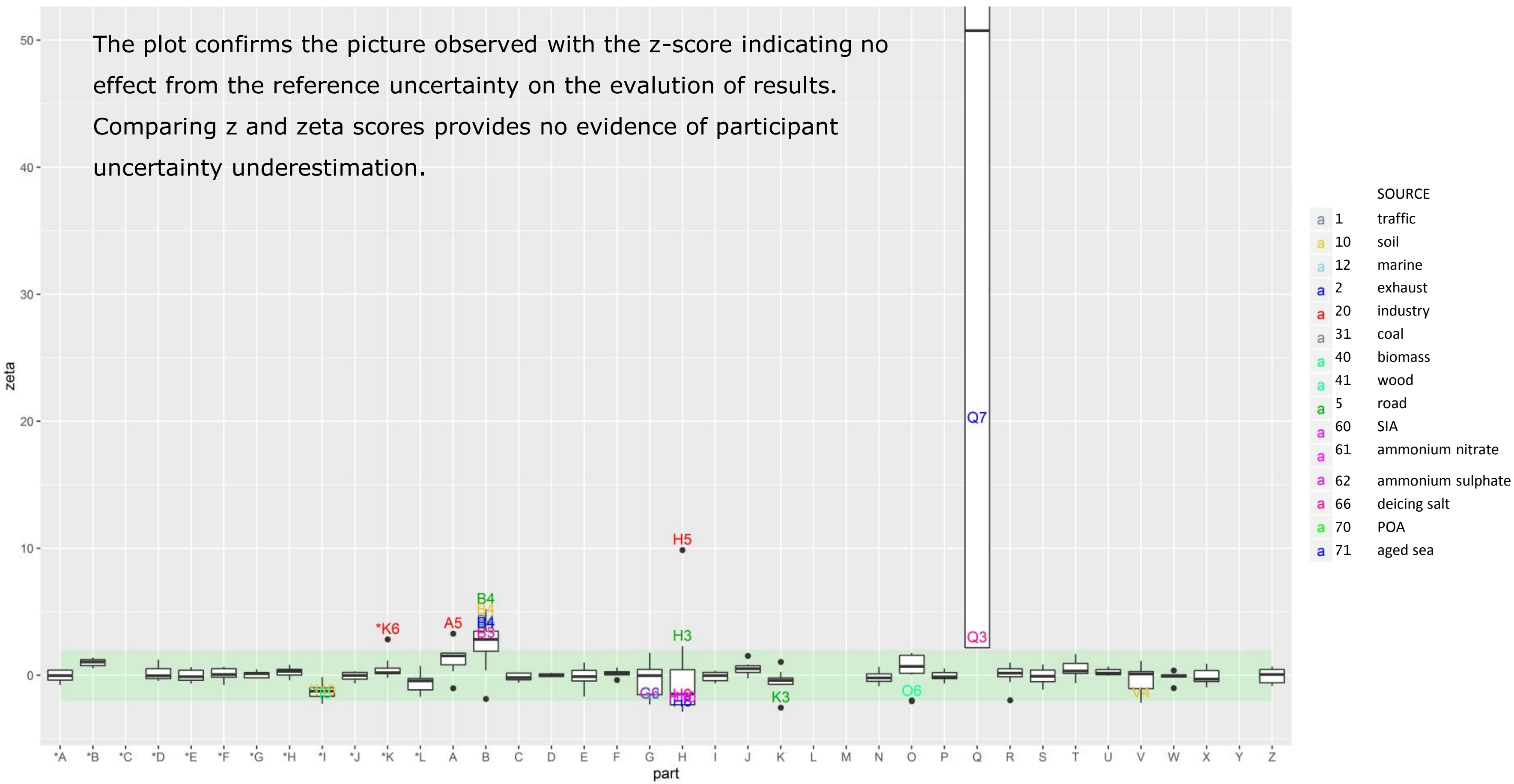


Performance RMs
zeta-score (overall sce)

European Commission

Influence of the uncertainty of the reference

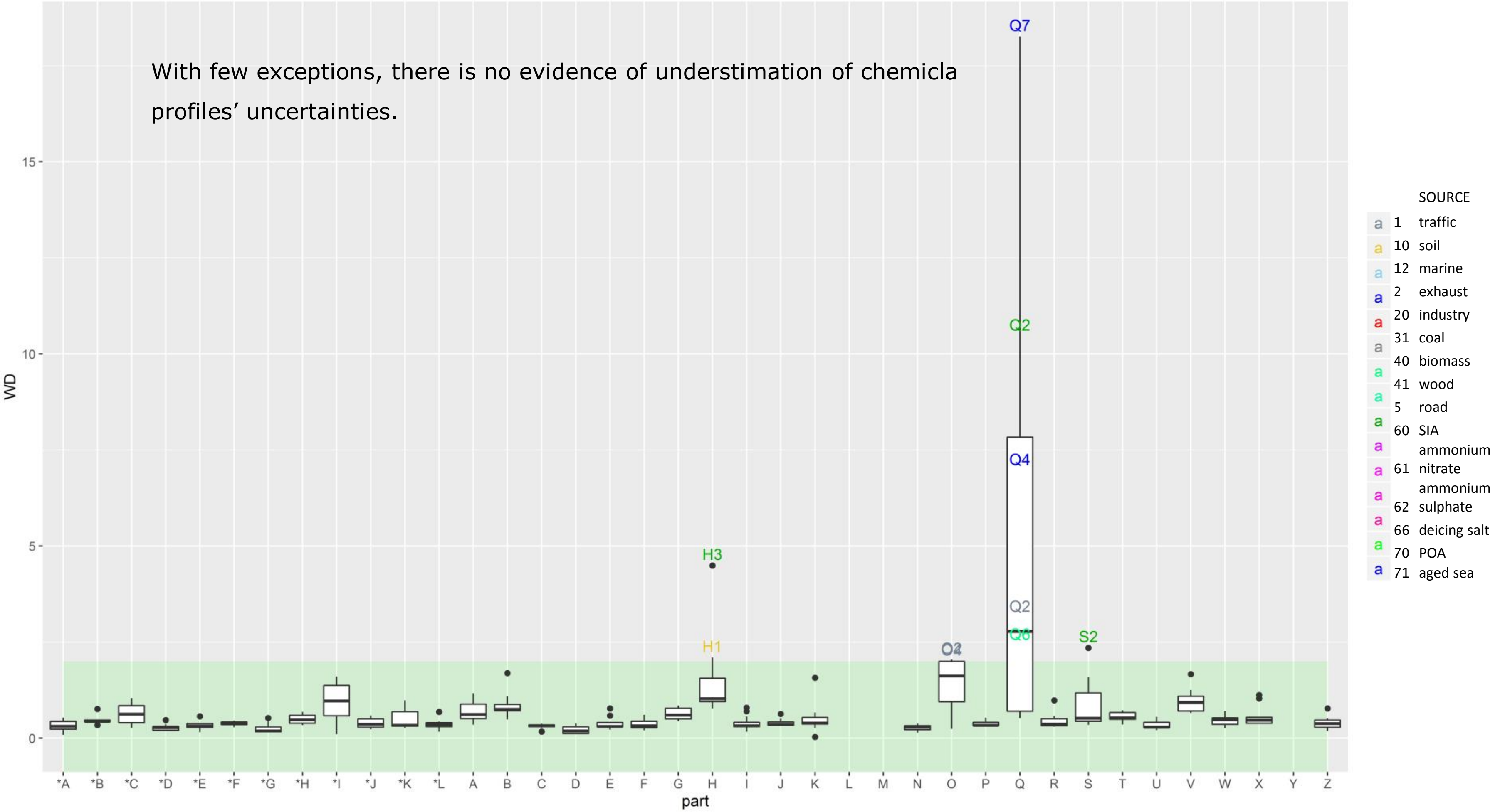
The plot confirms the picture observed with the z-score indicating no effect from the reference uncertainty on the evalution of results. Comparing z and zeta scores provides no evidence of participant uncertainty underestimation.



RMs
Weighted Distance (WD)

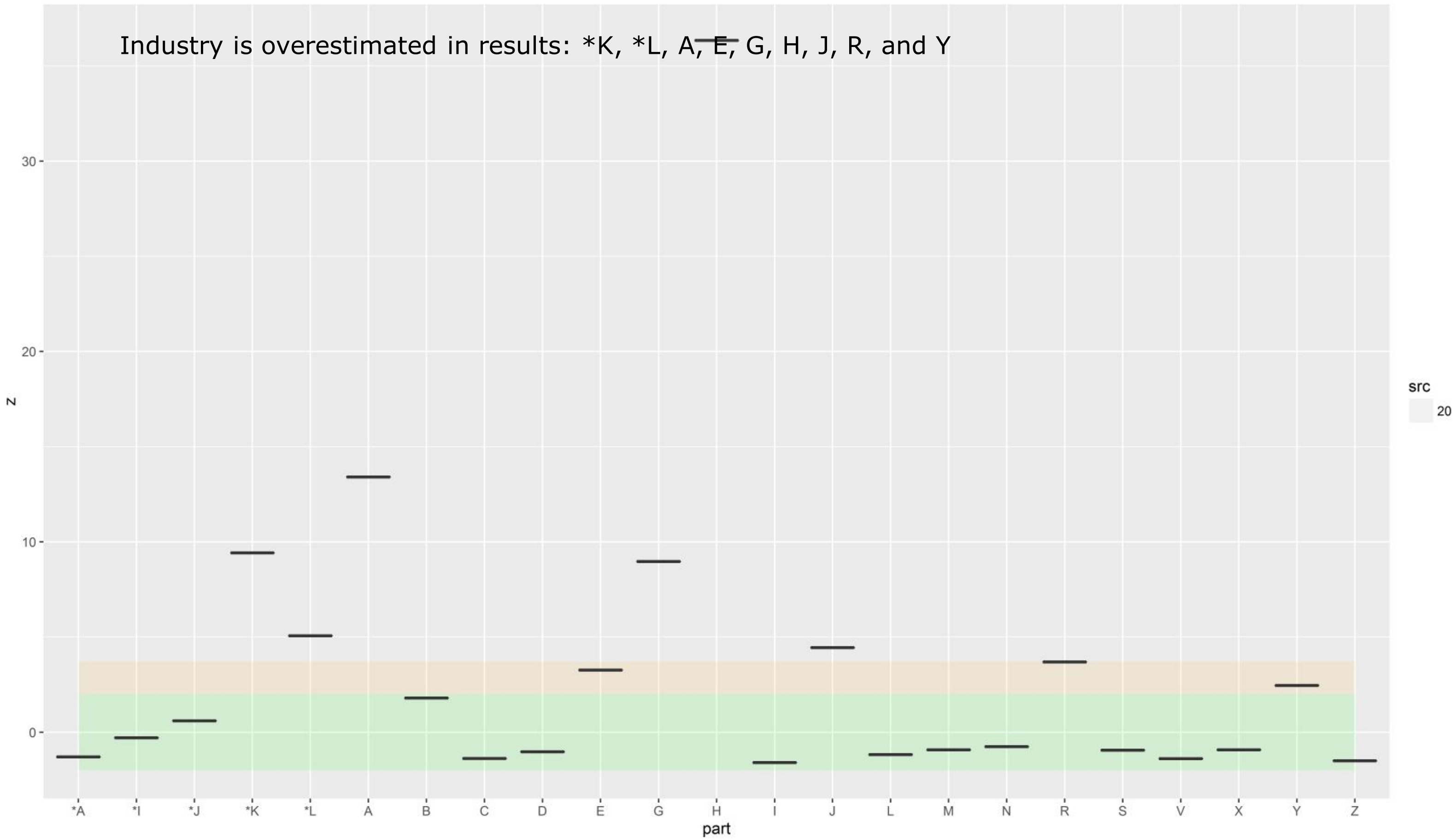
uncertainty of the chemical profiles

With few exceptions, there is no evidence of understimation of chemicla profiles' uncertainties.



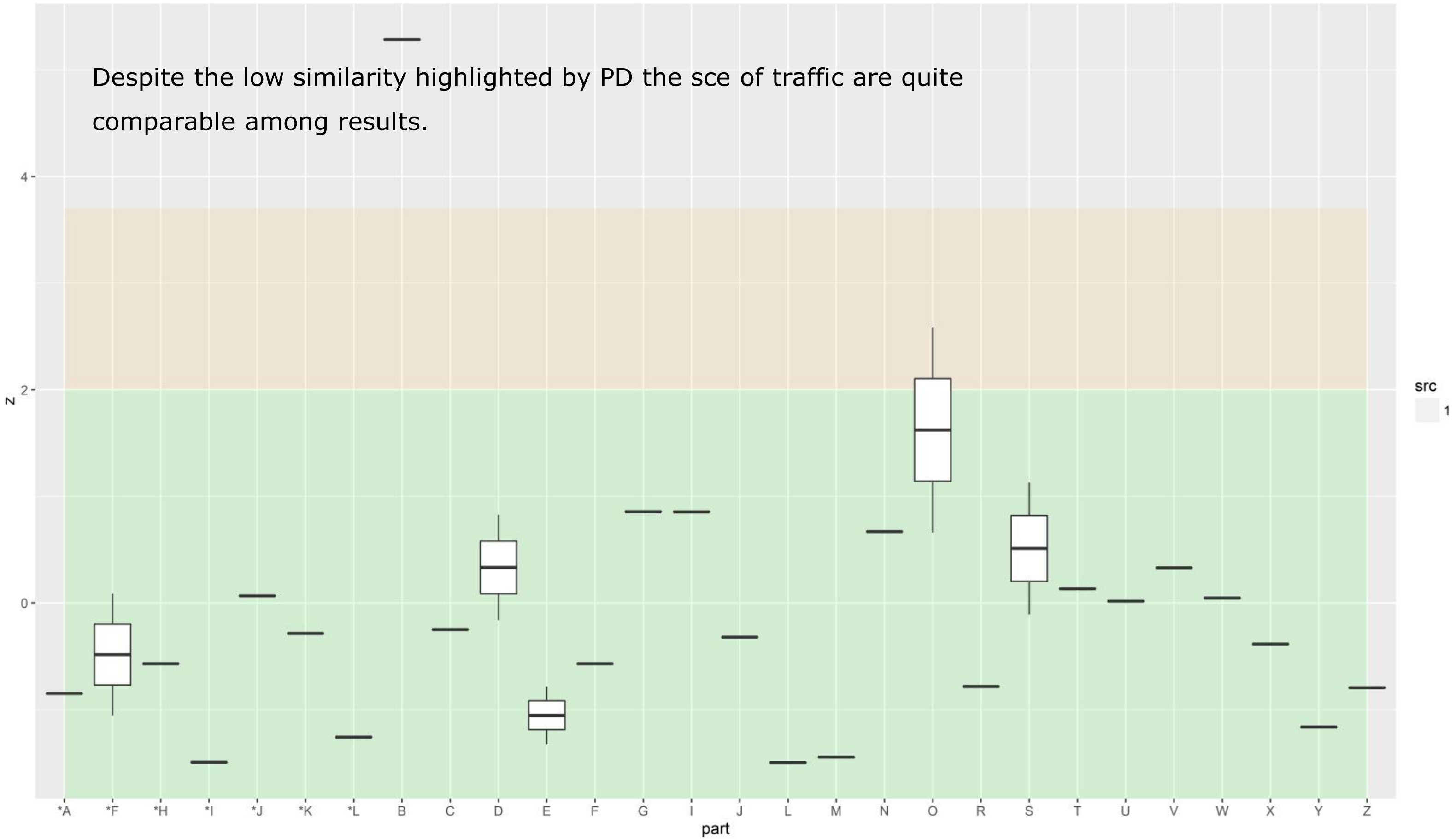
Performance RMs
z score plot (sce time series)

Industry



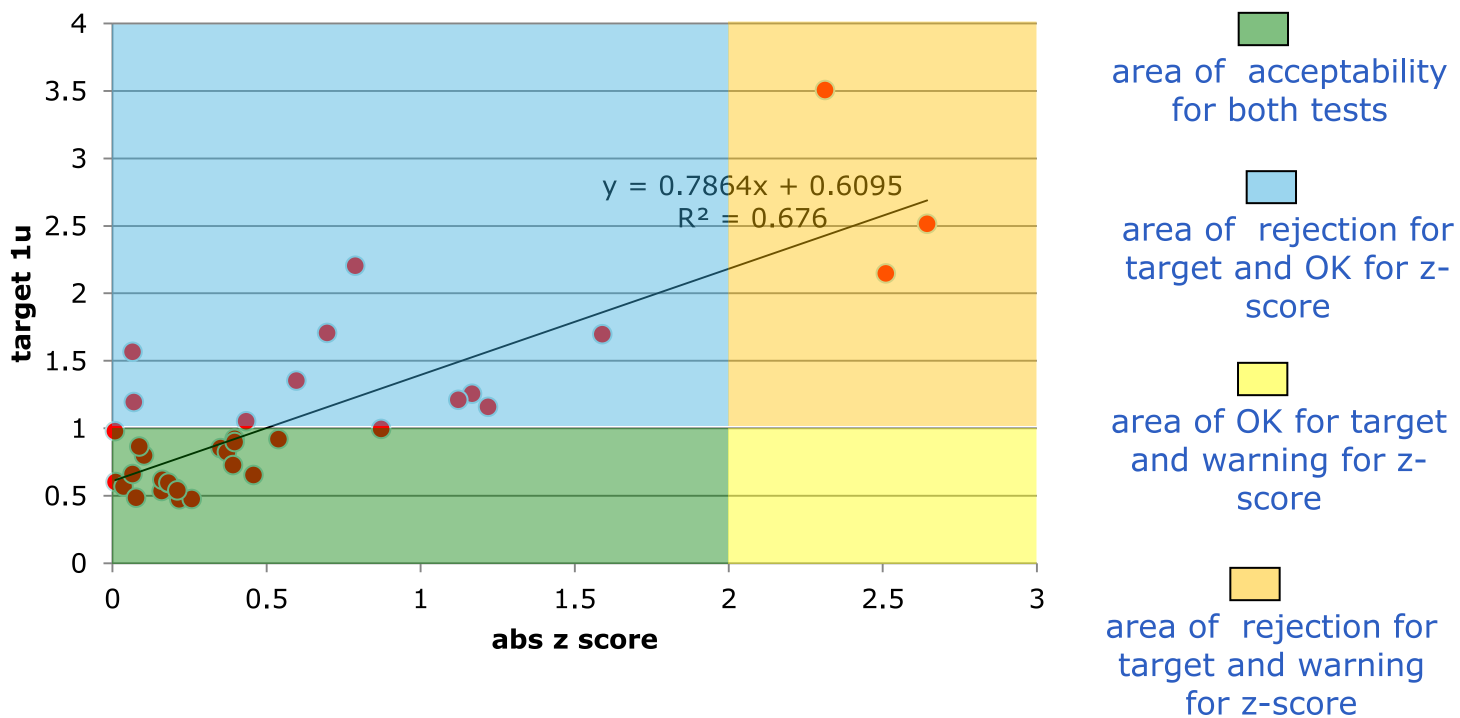
Performance RMs
Z-score (sce time series)

traffic



Additional analysis of RM results

RM analysis
Target vs z-score



Average of the scores of all candidate sources in every RM result (red dots)

Target and z-score are correlated. Target test is more severe because assess every single time step.

RM analysis

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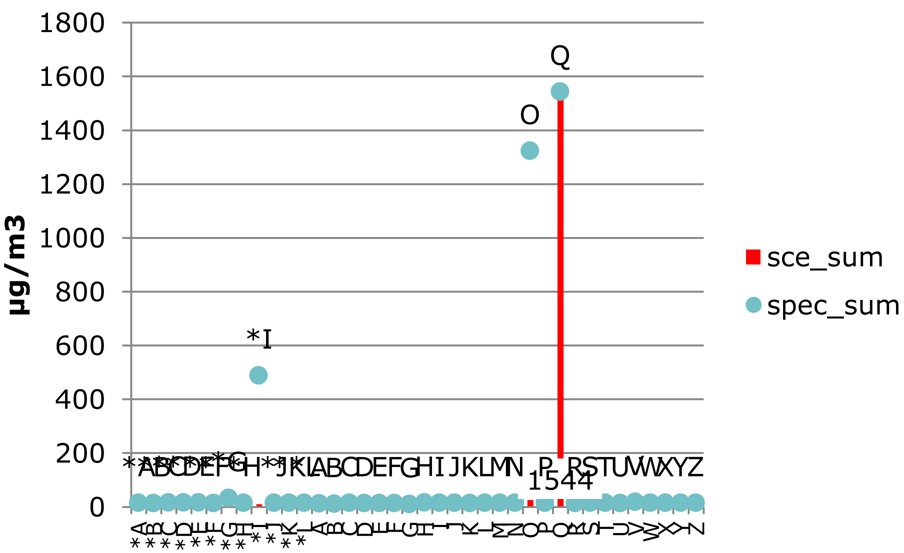
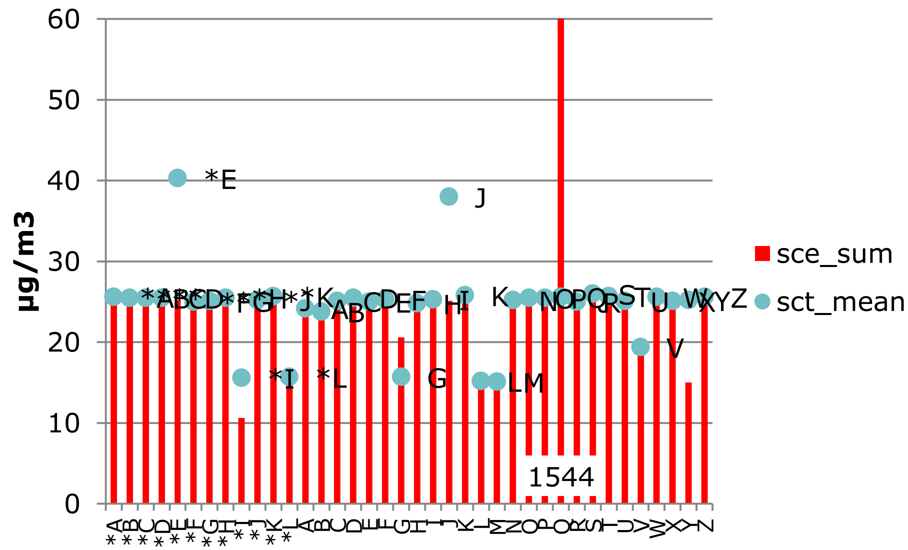




Coherence between the sum of the mass of the sources (sce provided by participants, red bar) and the sum of the mass of the species (blue dots)

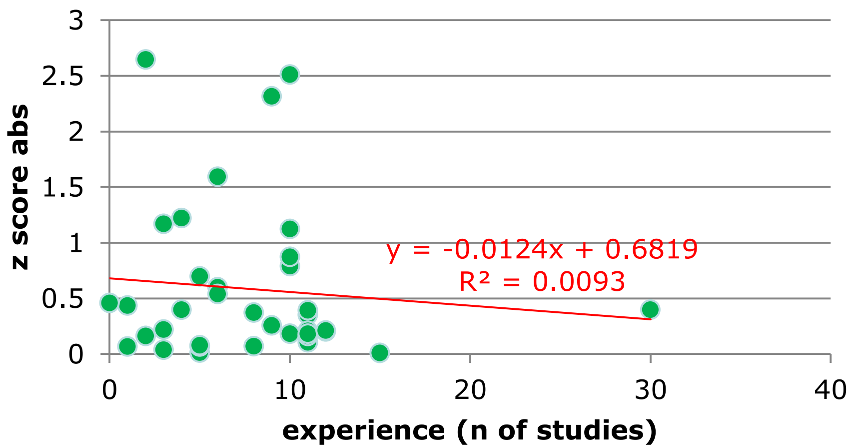
Problems for *I, O and Q

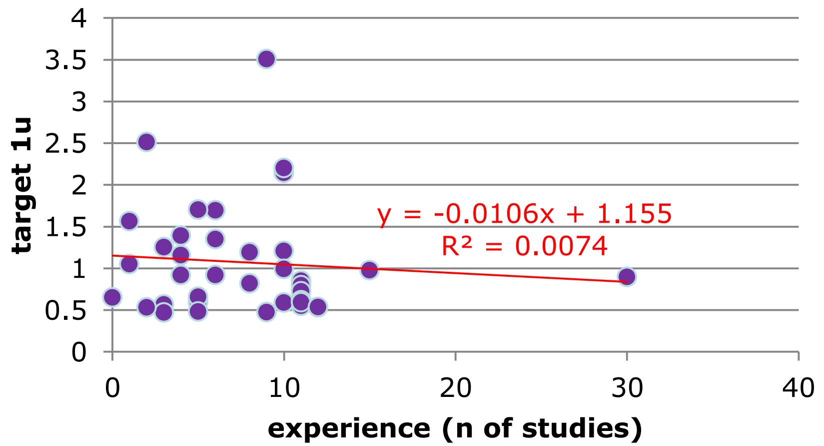
Coherence between the sum of the mass of the sources (sce provided by participants, red bars) and the average mass of the sce time series (blue dots)

Problems for *E, J and Q

RM analysis
Practitioner experience

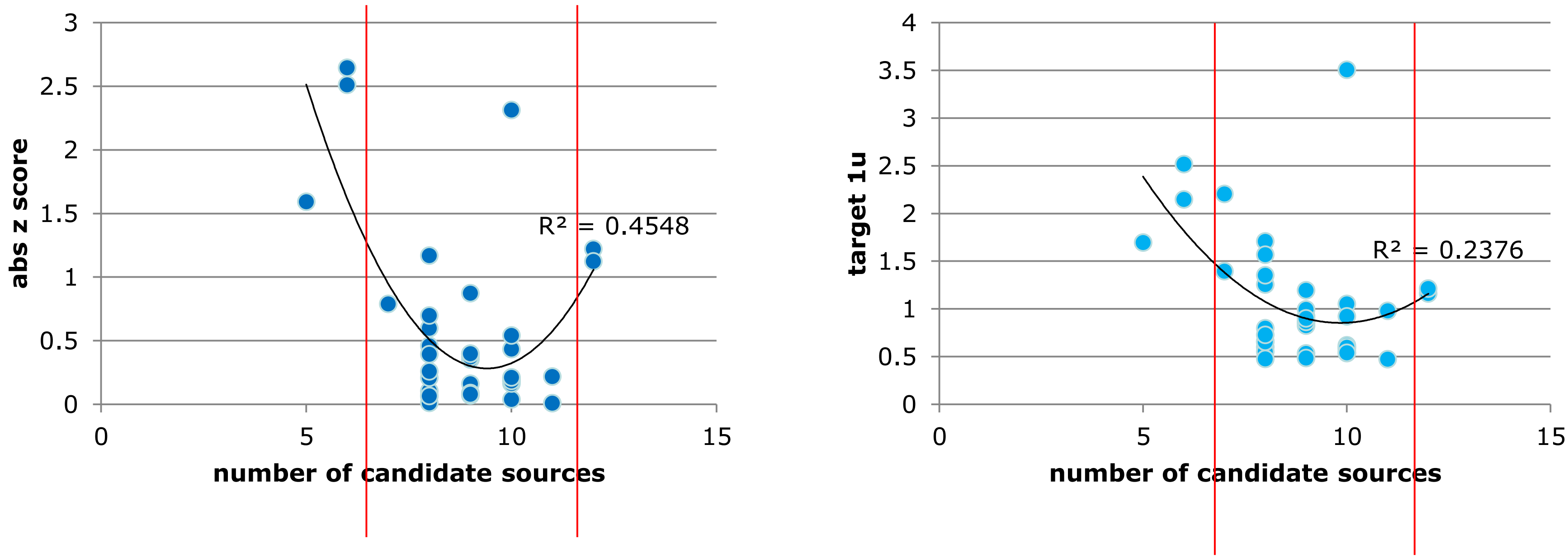
European Commission





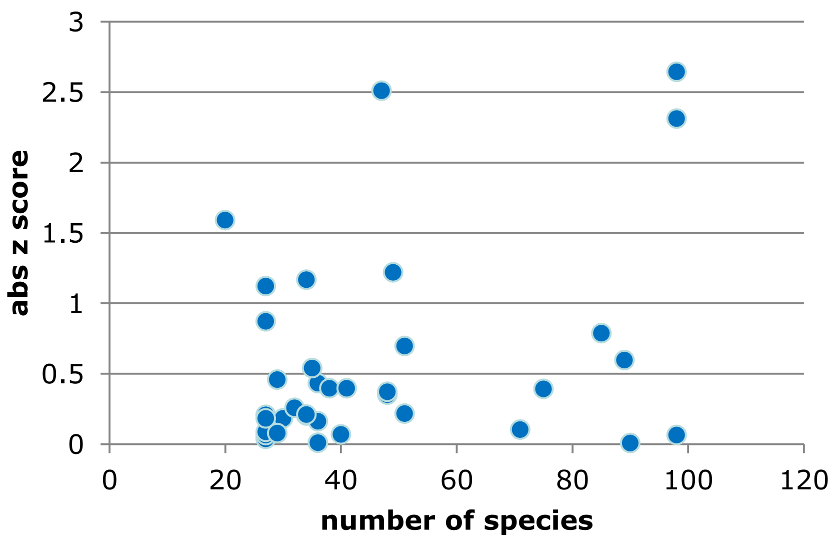
The performance for practitiones that have conducted 10 or less studies is quite variable. Practitioners declaring to have conducted more than 10 studies have always good performances (low scores).

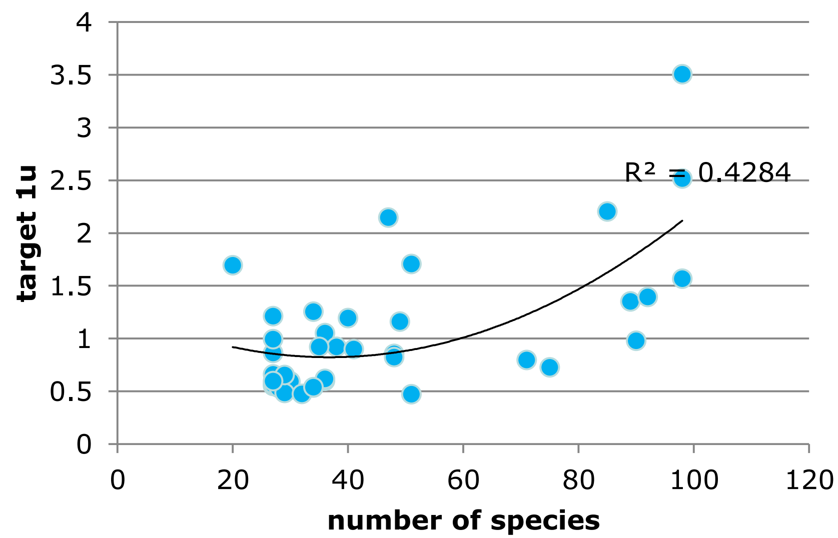
RM analysis



Results (solutions) with a number of candidate sources (factors) near to the average (9±2) present better performance than those with a difference of 3 or more sources from the average.

RM analysis





No clear relationship between number of species and performance is observed

Thank you for your attention