

A wide-angle photograph of a large, modern server room. The room is filled with rows of server racks, some of which are illuminated with blue light. The ceiling is high and features a complex network of pipes and structural beams. The floor is made of large, light-colored tiles. The overall atmosphere is one of a high-tech, industrial environment.

New metrics for XRF data quality

Presentation to IMPROVE Steering Committee at Lake Tahoe, October 2012, by Crocker Air Quality Group

dreamed

IMPROVE Reported Detection Limits and Uncertainty Estimates

IMPROVE Steering Committee Meeting
October 2008

Nicole Hyslop and Warren White

http://vista.cira.colostate.edu/improve/Activities/Meetings/2008Pres/White_ISC_unc_and_mdL_NPH.pdf

realized

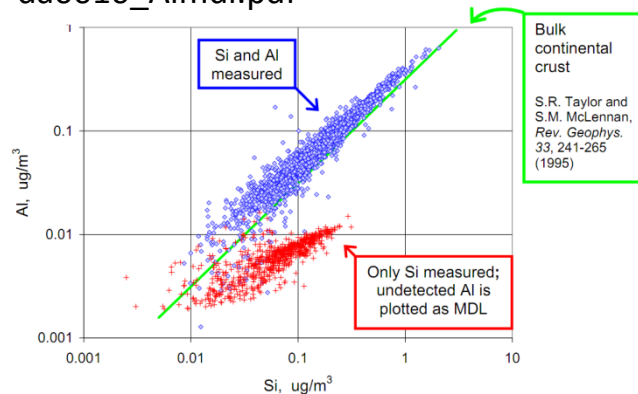
Dataset	SiteCode	Date	CLf:Value	CLf:Unc	CLf:MDL
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IMPFSPED	ACAD1	12/19/2010	0	0	0.00034
IMPFSPED	ACAD1	12/22/2010	0.05468	0.00283	0.0003
IMPFSPED	ACAD1	12/25/2010	0	0	0.00025
IMPFSPED	ACAD1	12/28/2010	0.00369	0.00029	0.00024
IMPFSPED	ACAD1	12/31/2010	0	0	0.00032
IMPFSPED	ACAD1	1/3/2011	0.00028	0.00011	0.00017
IMPFSPED	ACAD1	1/6/2011	0.00382	0.00055	0.00017
IMPFSPED	ACAD1	1/9/2011	0.00972	0.00137	0.00017
IMPFSPED	ACAD1	1/12/2011	0.04249	0.00597	0.00017
IMPFSPED	ACAD1	1/15/2011	0.0007	0.00014	0.00017

Detection Limit (DL)

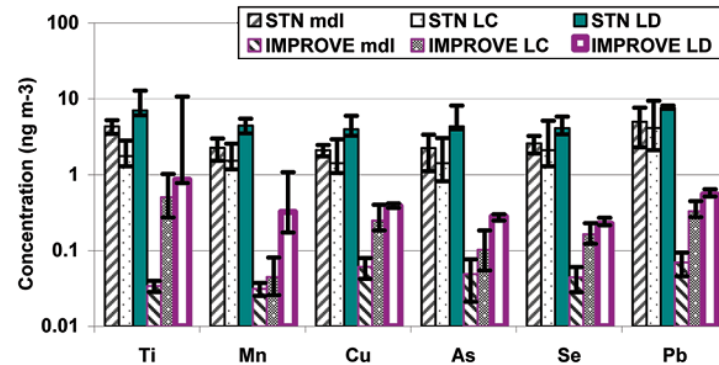
Legacy: Theoretical, based on RACE estimate of spectral background.

<http://vista.cira.colostate.edu/...>

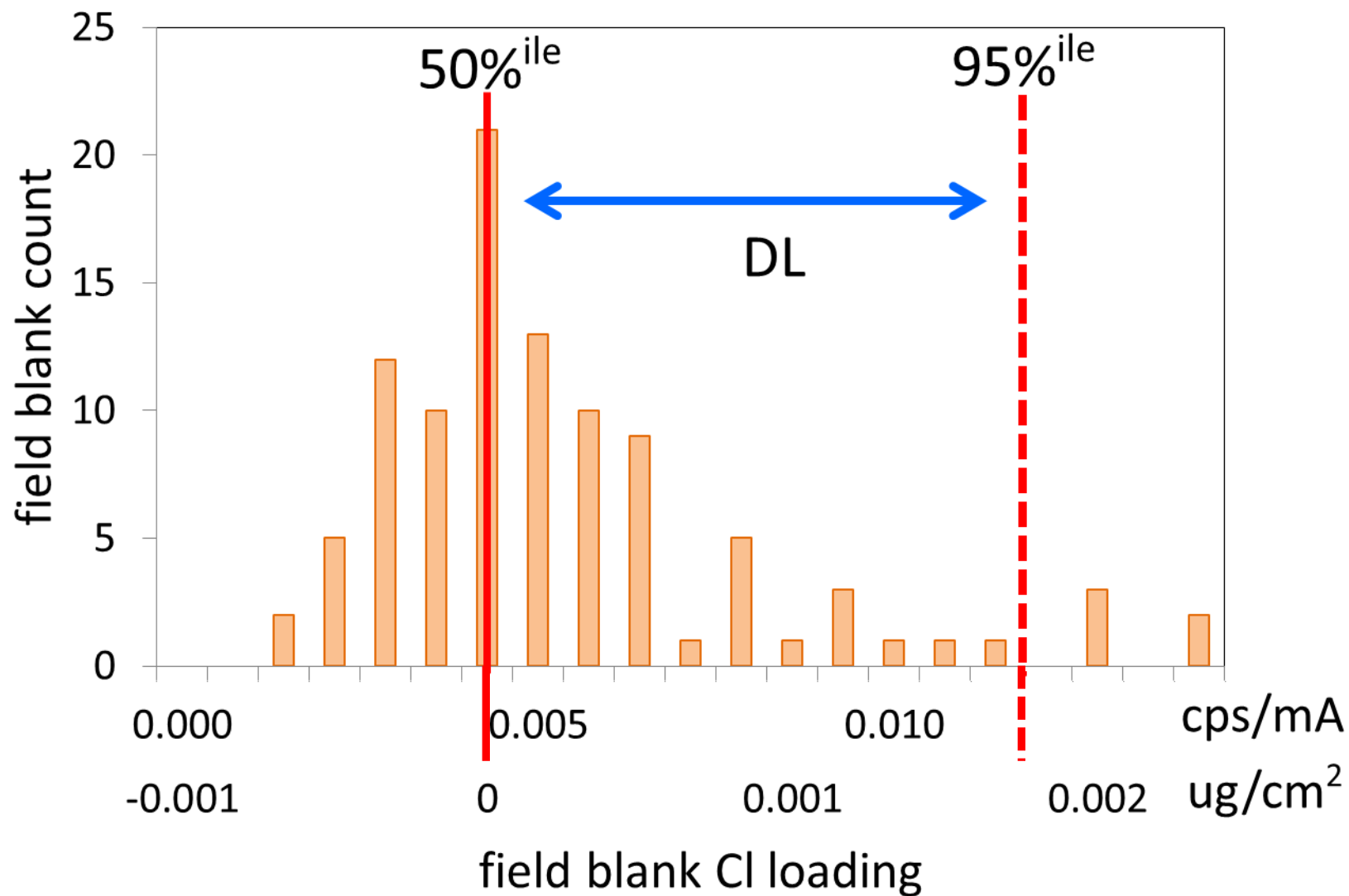
da0010_Almdl.pdf



Environ. Sci. Technol. 2008, 42, 5235–5240



New: Empirical, based on observed distribution of field blank loadings.



Error ↔ Uncertainty

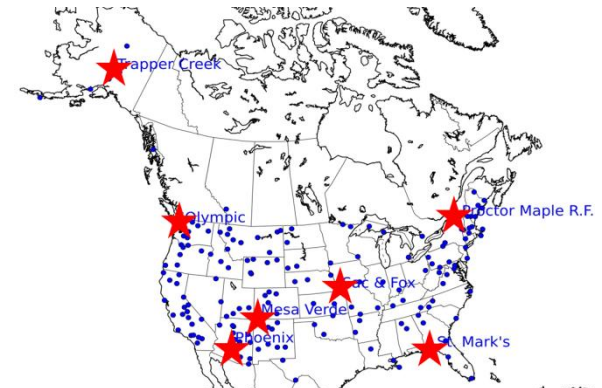
Legacy: Based on quality of spectral peak, and estimates of uncertainty in analytical calibration and sample volume determination.

N.P. Hyslop, W.H. White / Atmospheric Environment 42 (2008) 2691–2705

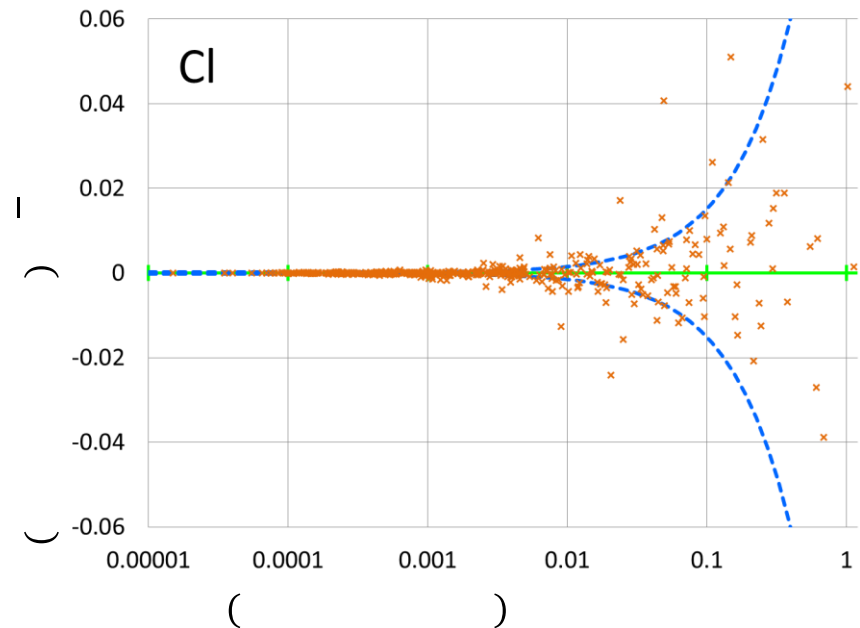
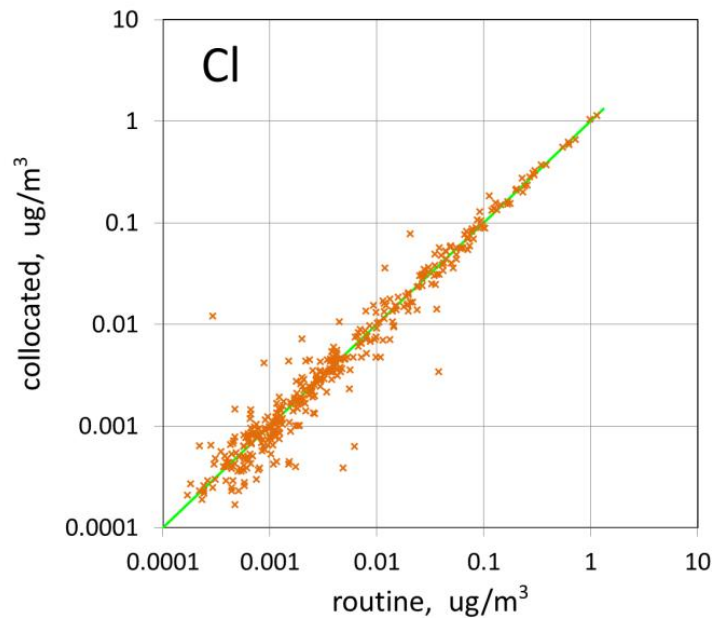
statistics

Analytical method	Species	Collocated precision (%)	Predicted precision (%)	Ratio collocated/predicted
Cu-anode XRF	Na	$n < 10$	—	—
	Mg	$n < 10$	—	—
	Al	69 (46–94)	14 (9–18)	5.0 (4.4–5.5)
	Si	41 (19–61)	11 (6–14)	3.7 (2.4–4.5)
	P	$n < 10$	—	—
	S	8 (7–10)	5 (5–6)	1.6 (1.4–1.7)
	Cl	68 (60–67)	12 (9–11)	5.6 (5.8–6.5)
	K	13 (10–19)	6 (5–8)	2.3 (1.8–3.3)
	Ca	19 (12–32)	6 (5–9)	3.0 (1.8–5.9)
	Ti	30 (19–60)	11 (6–17)	2.6 (1.9–3.6)
	V	21 (11–29)	18 (9–26)	1.2 (1–1.4)
	Cr	56 (26–79)	28 (19–43)	2.0 (1.3–3.2)
	Mn	24 (16–41)	12 (6–17)	2.0 (1.7–2.8)
	Fe	18 (12–27)	5 (5–6)	3.3 (2.1–5.2)
Mo-anode	Ni	32 (13–111)	12 (10–13)	2.8 (1.1–10.2)

New: Empirical, based on observed differences between collocated measurements.

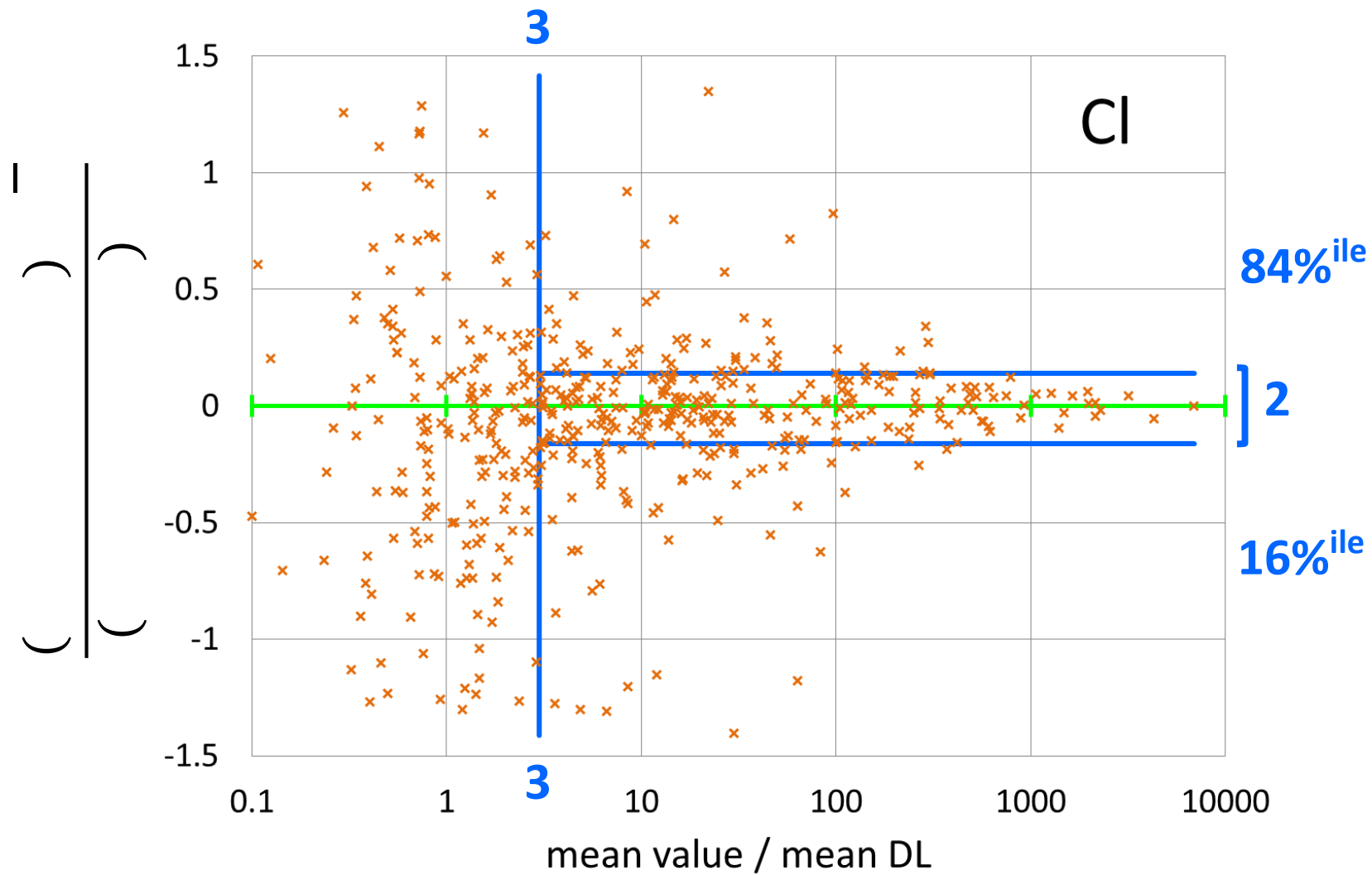


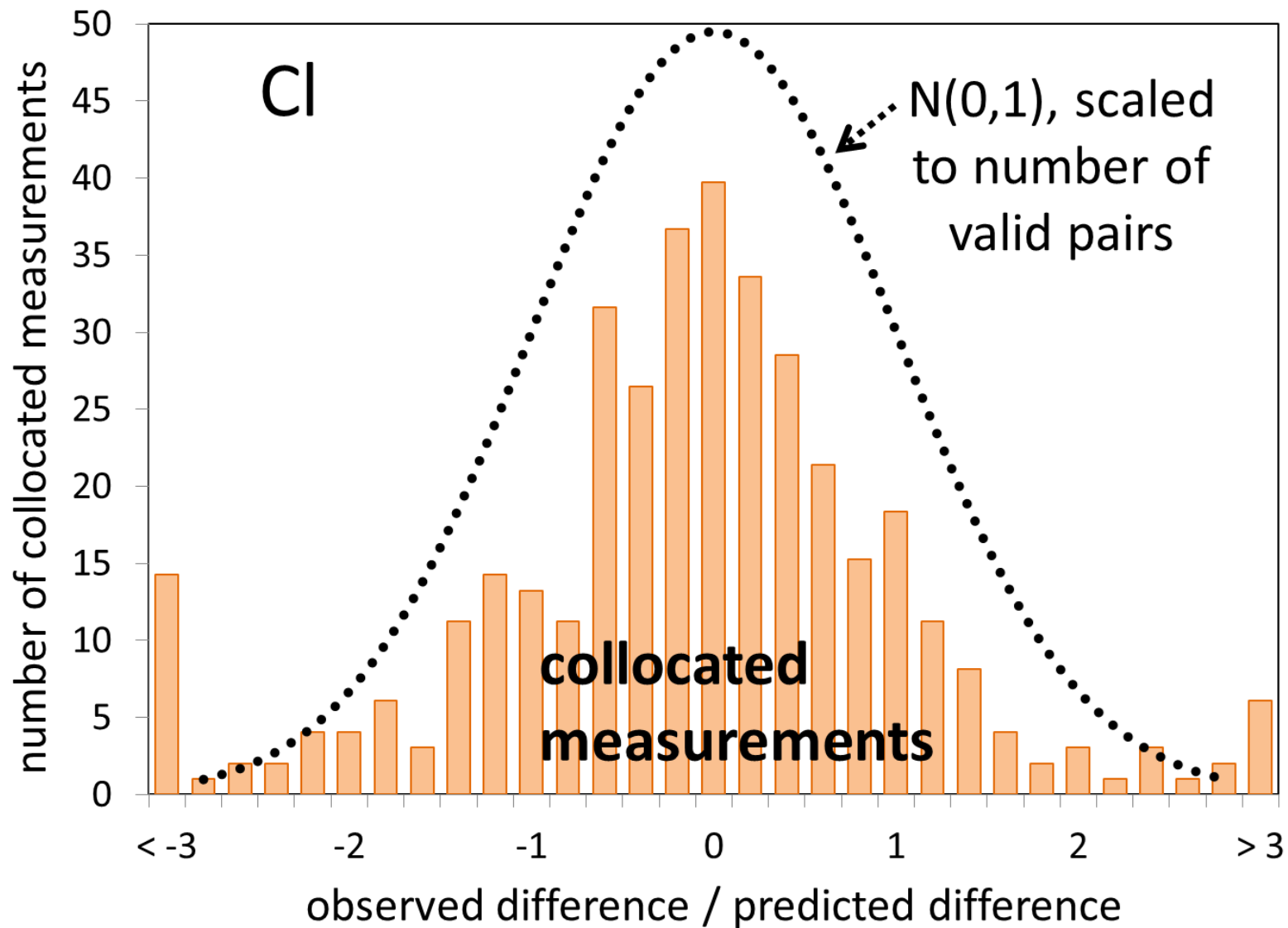
Uncertainty in concentration X: $\left(\right) \sqrt{\left(\right)}$



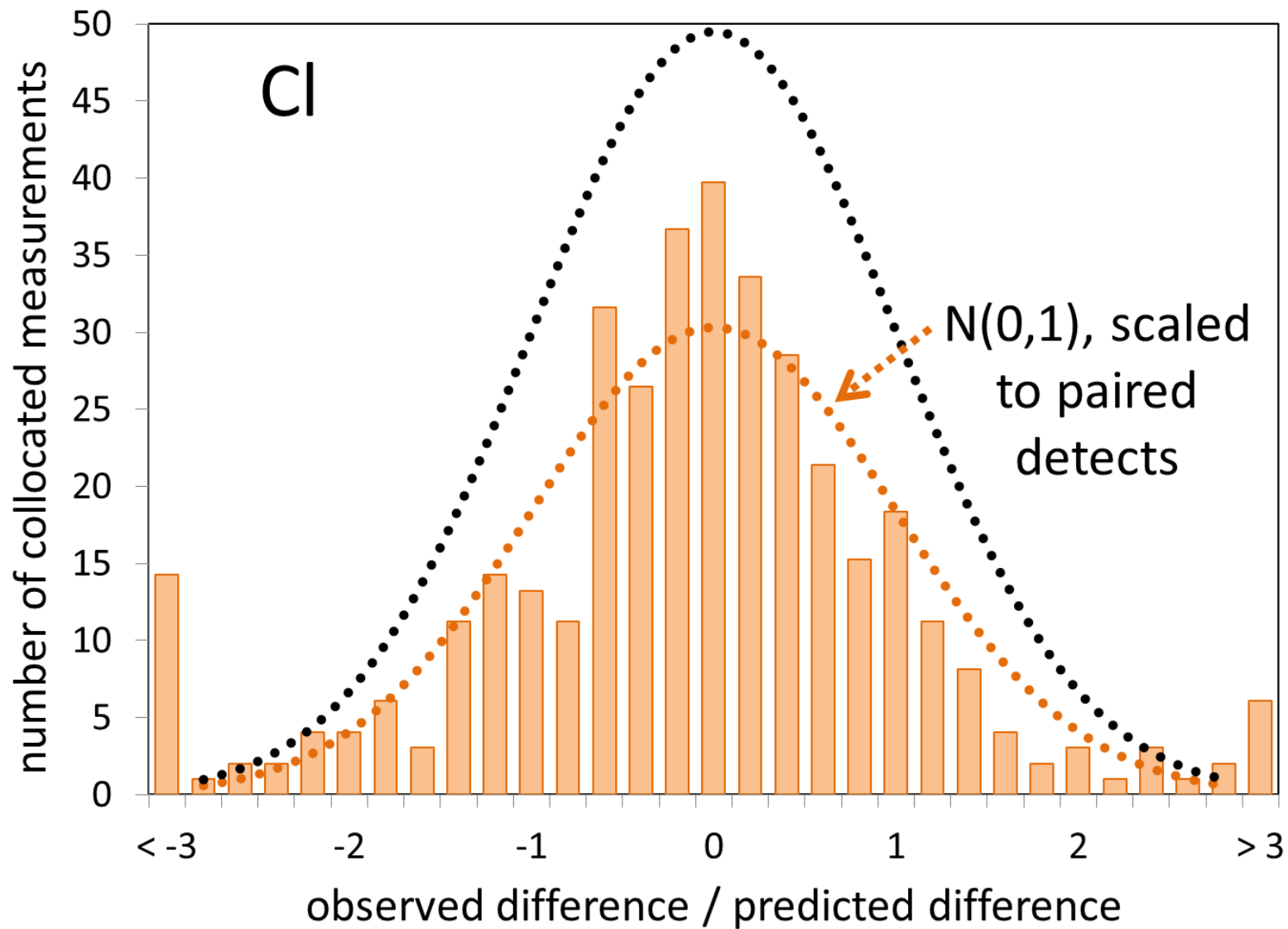
is based on field blank data.

is based on collocated data [next slide]:

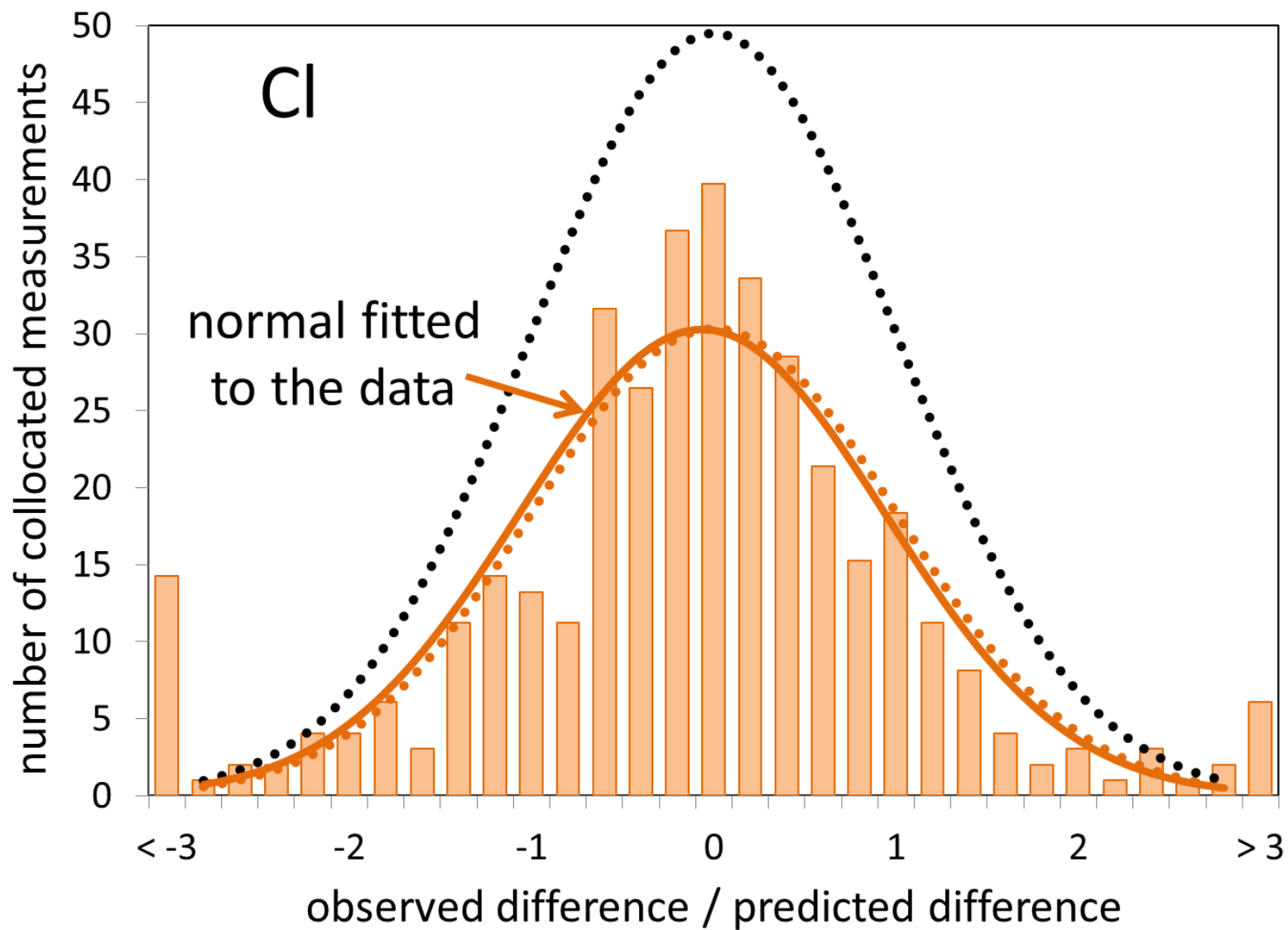




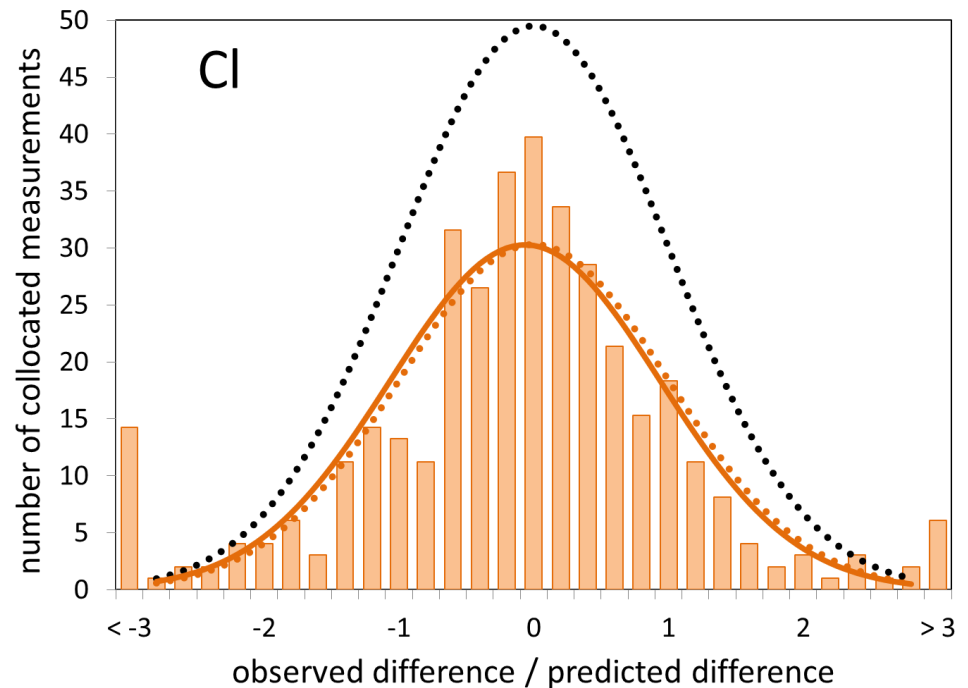
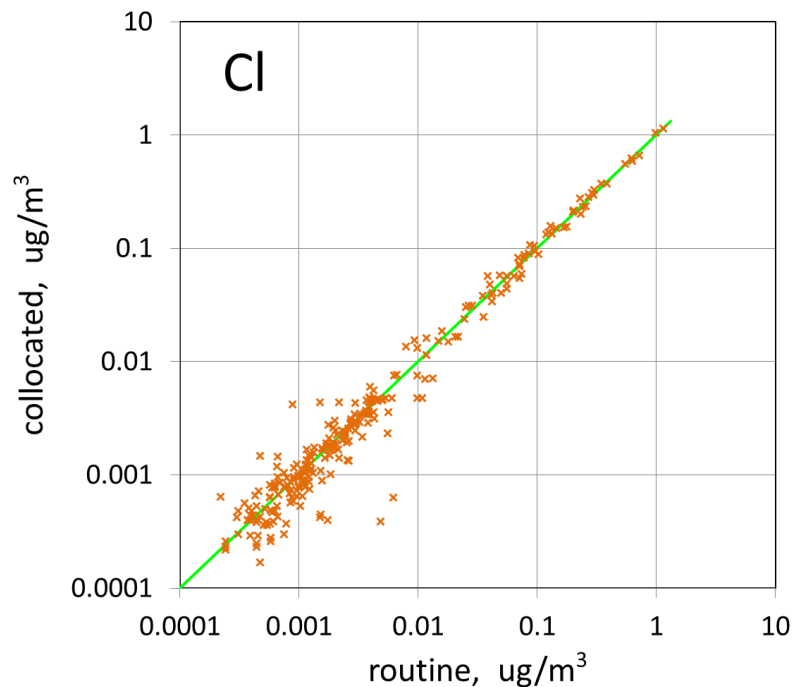
$\sqrt{\quad}$



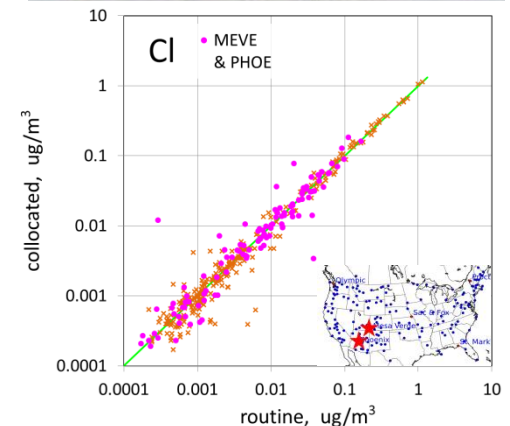
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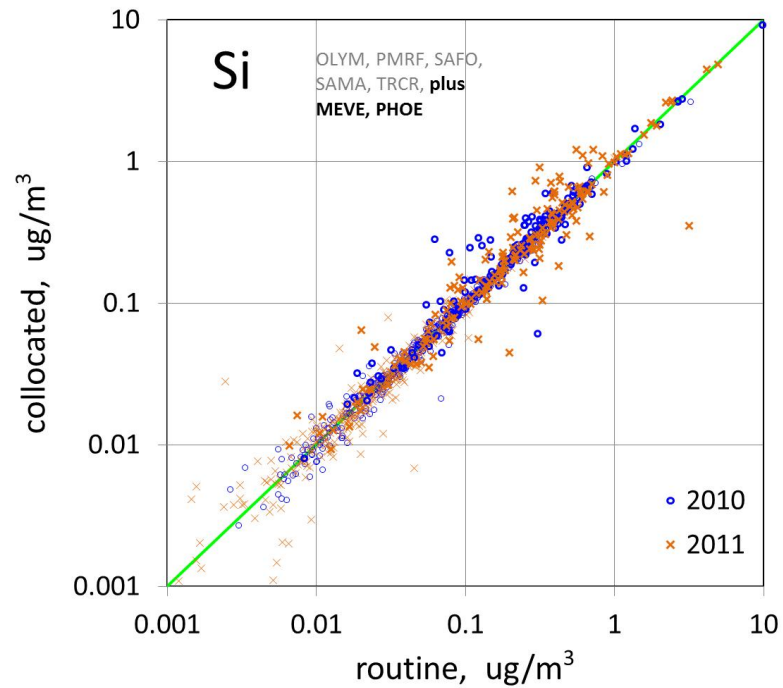
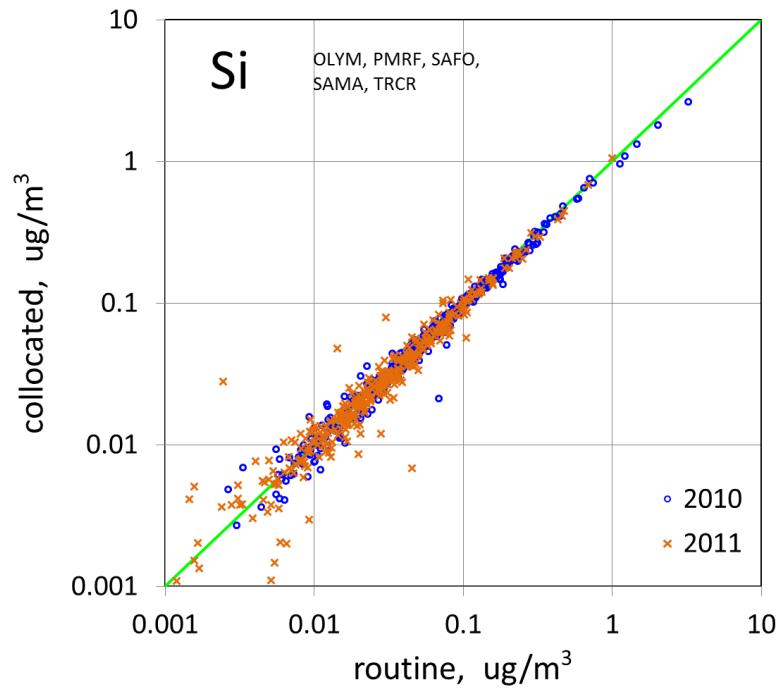
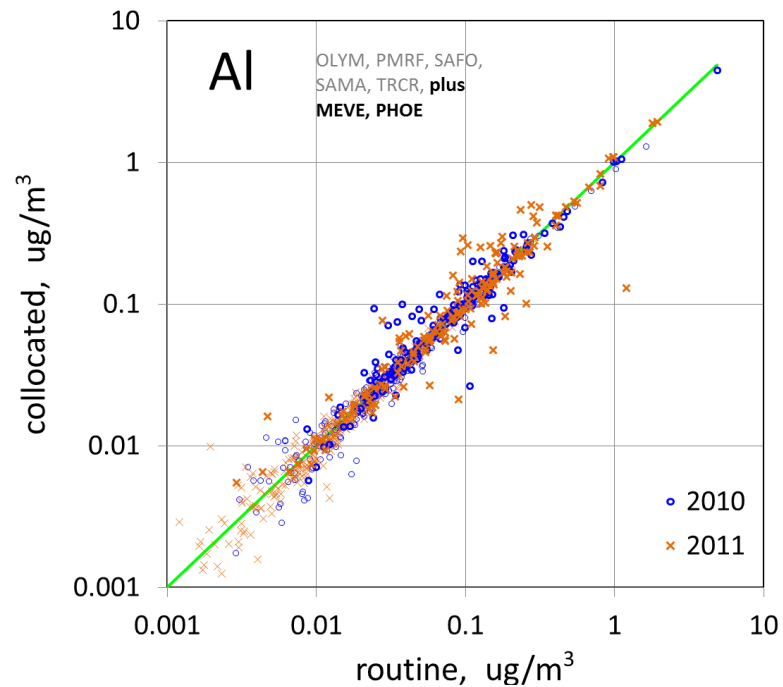
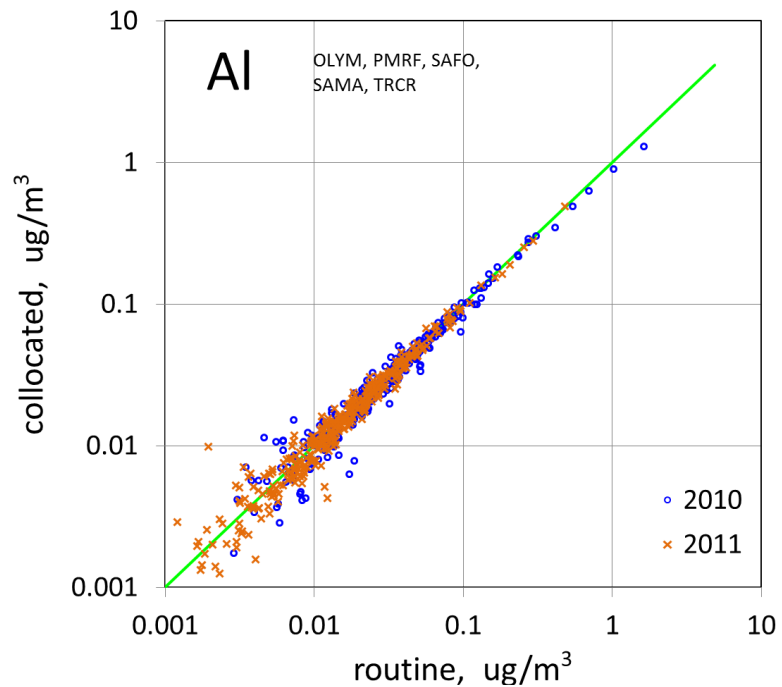


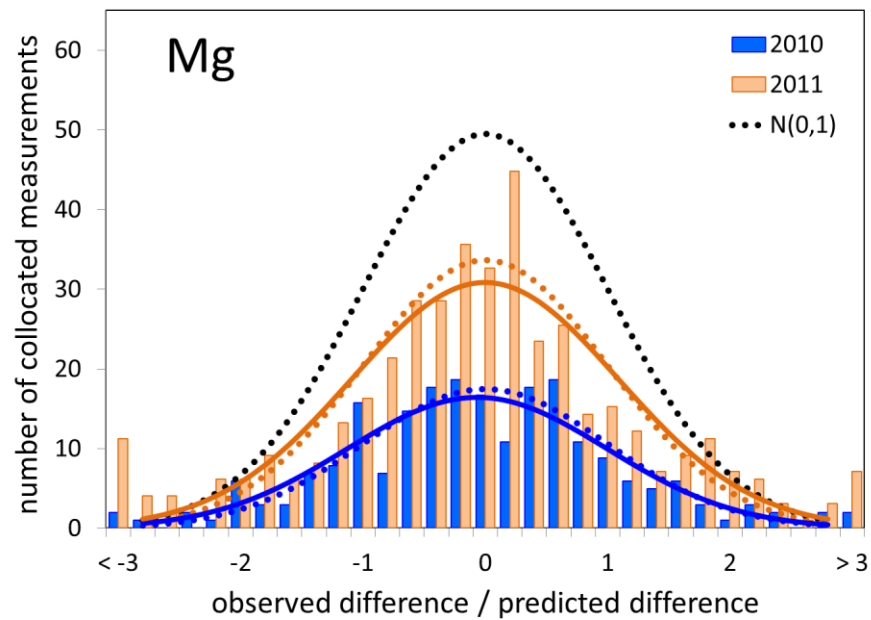
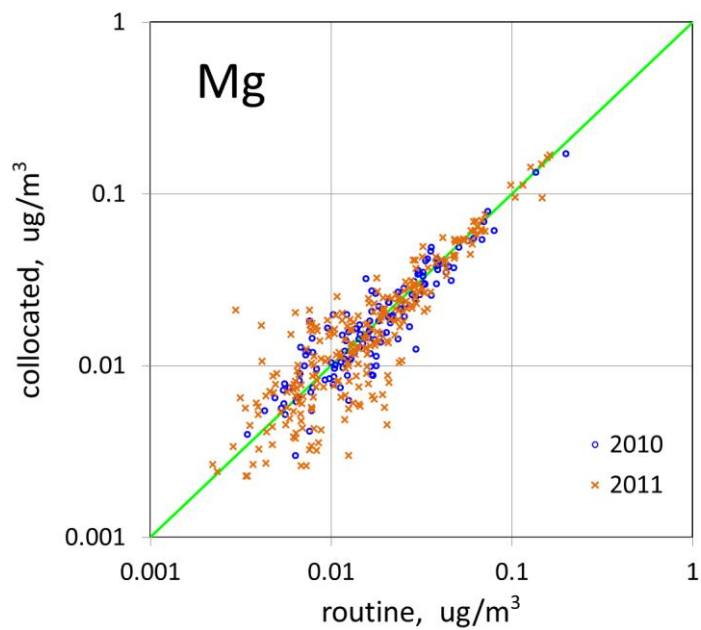
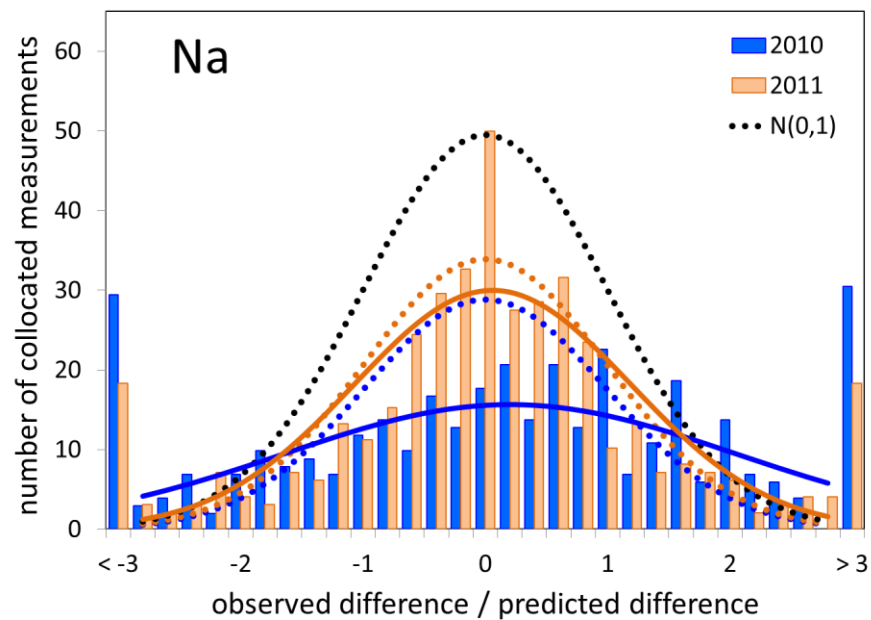
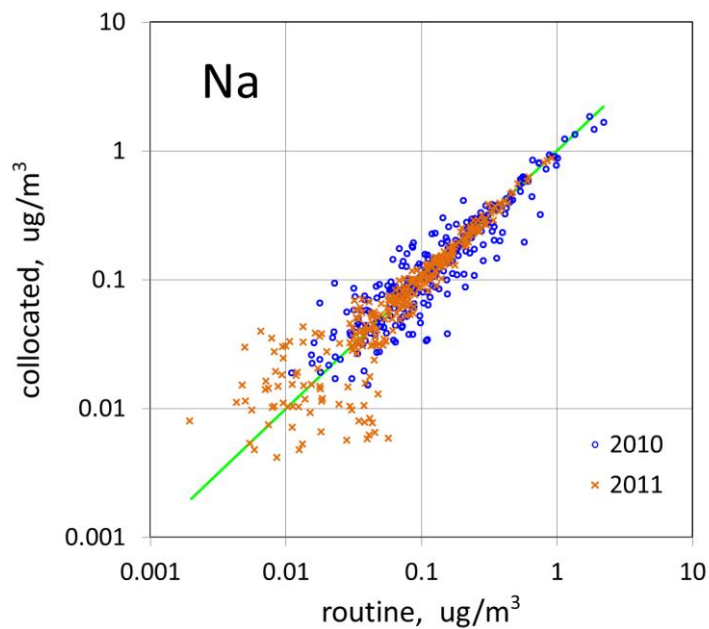
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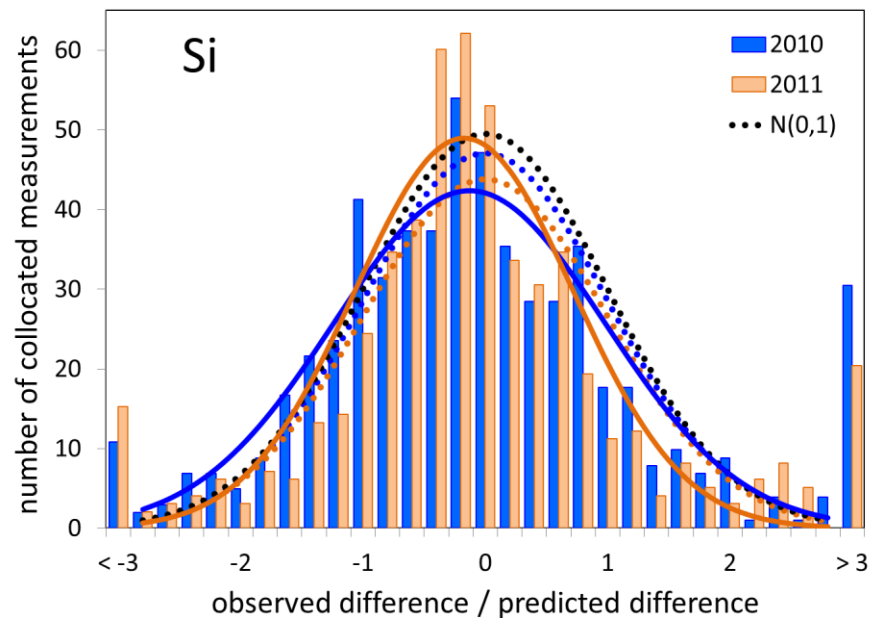
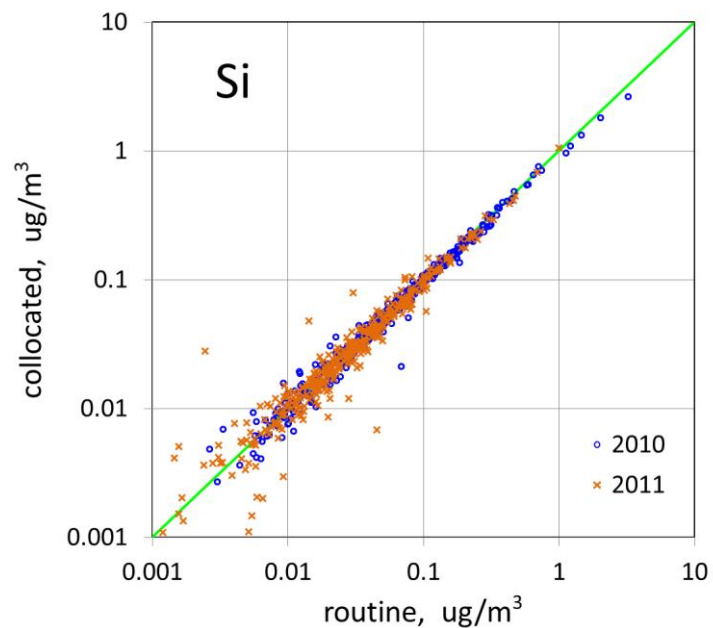
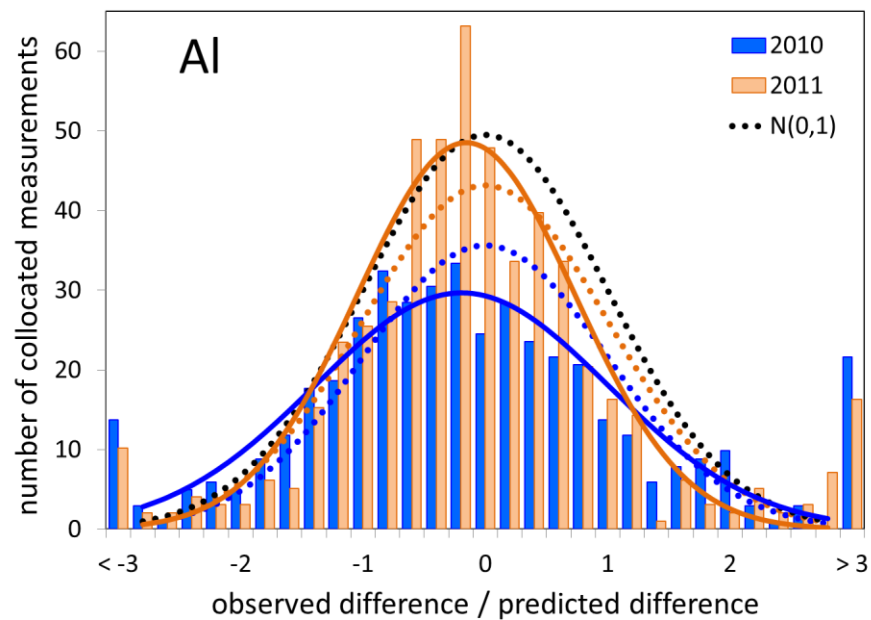
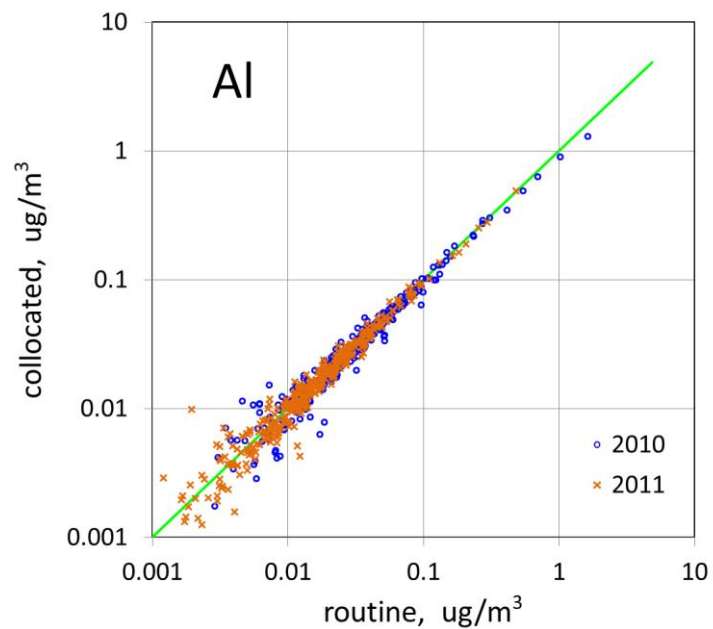


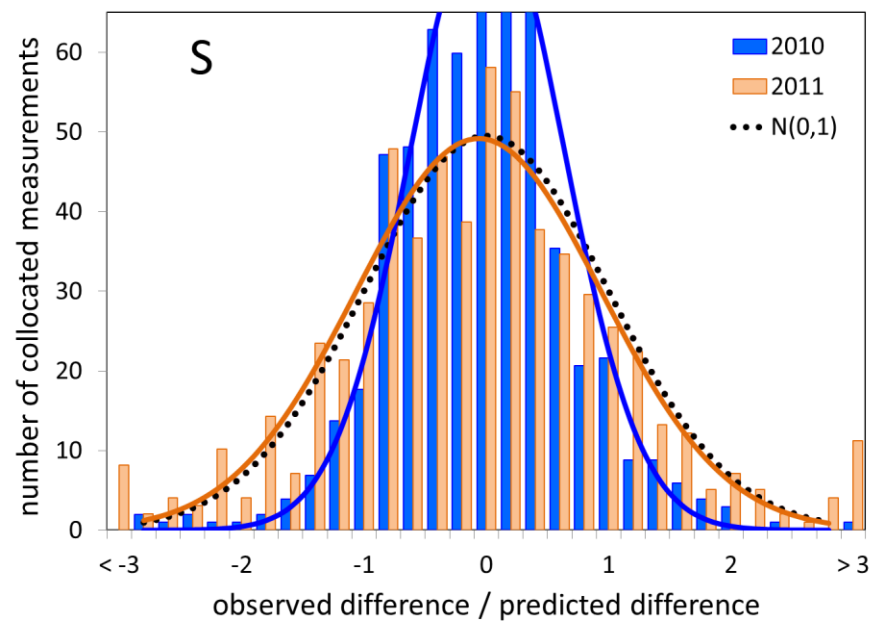
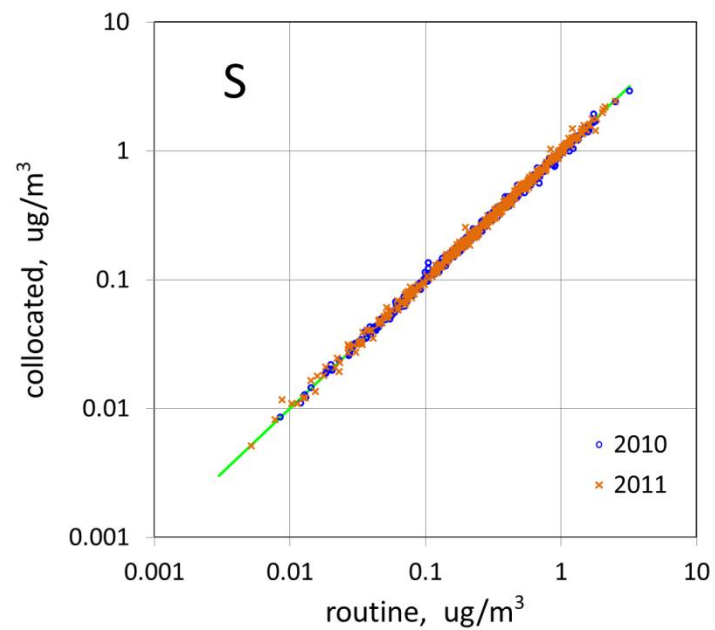
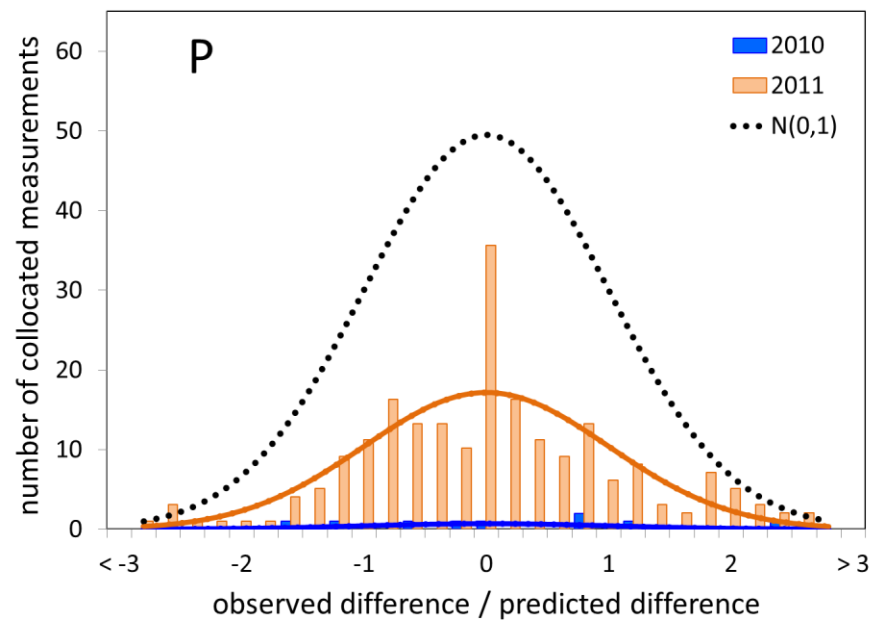
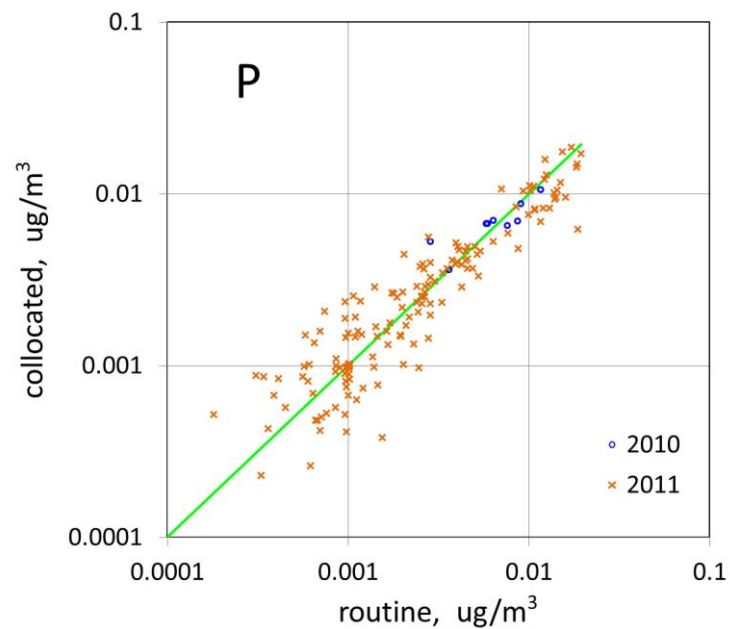
We are now ready for our parade of the elements!
 We use all collocated data from January through Oct, in 2010 (legacy) and 2011 (new). [Jan-Jun at SAFO in both years.] The cross-plots (above left) will exclude data from MEVE and PHOE, as coarse-particle sampling errors create outliers there [shown next slide] that impede comparisons of the legacy and new XRF. MEVE and PHOE data are included in the error distributions (above right).

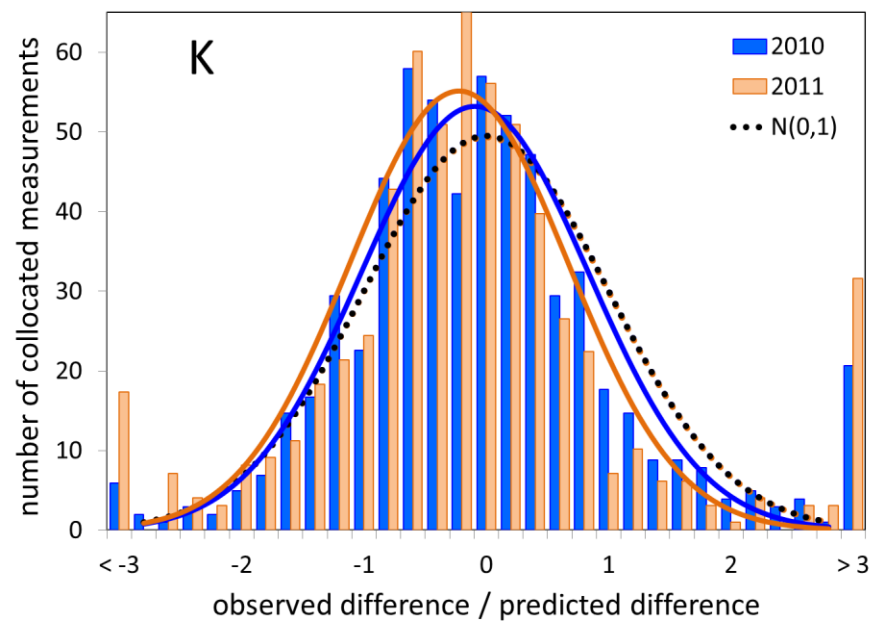
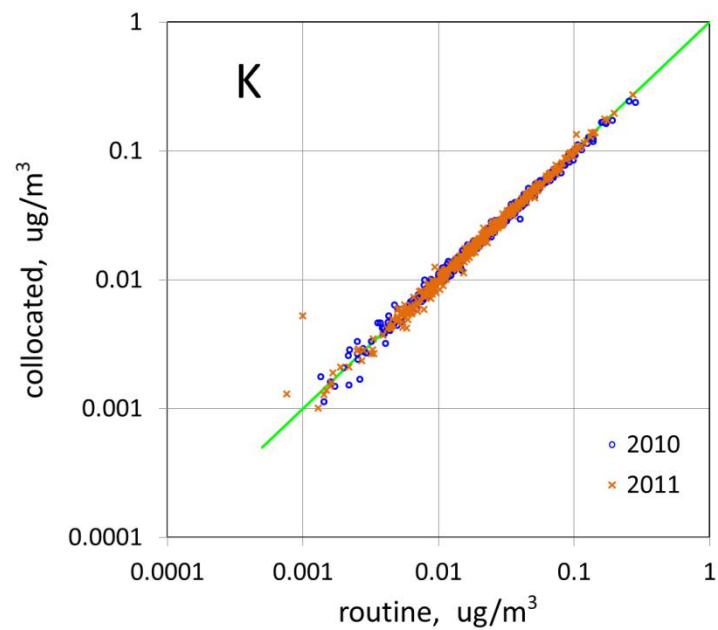
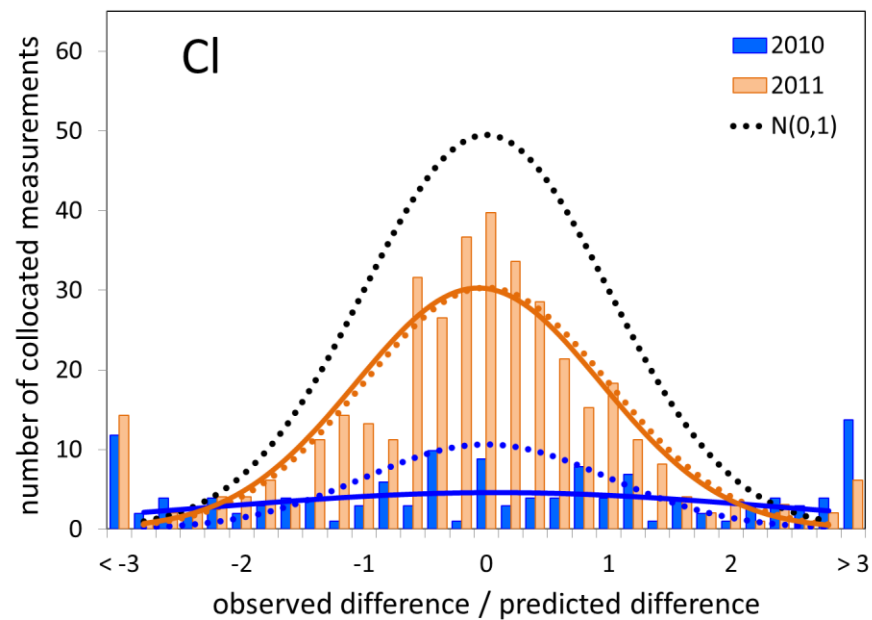
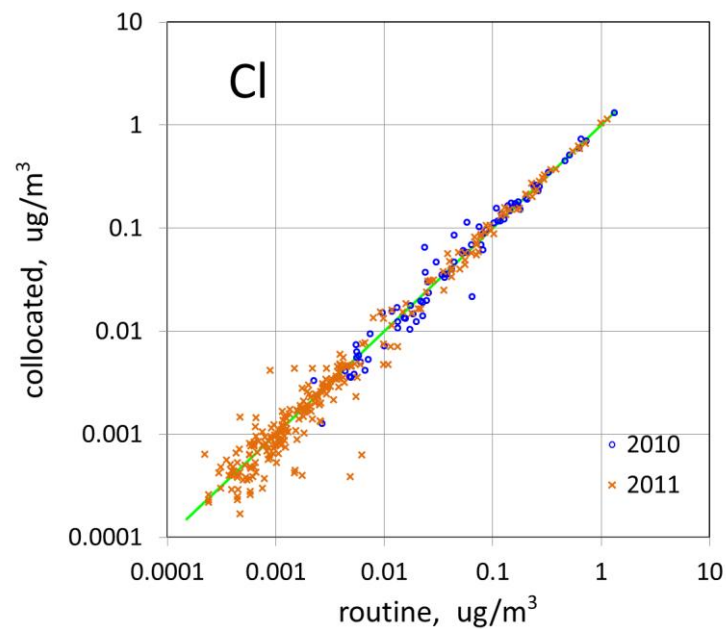


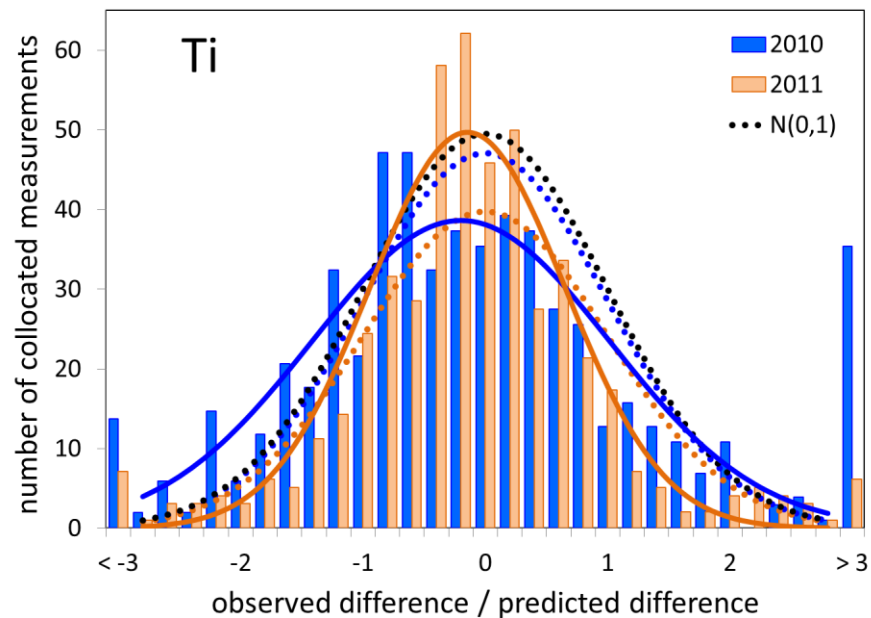
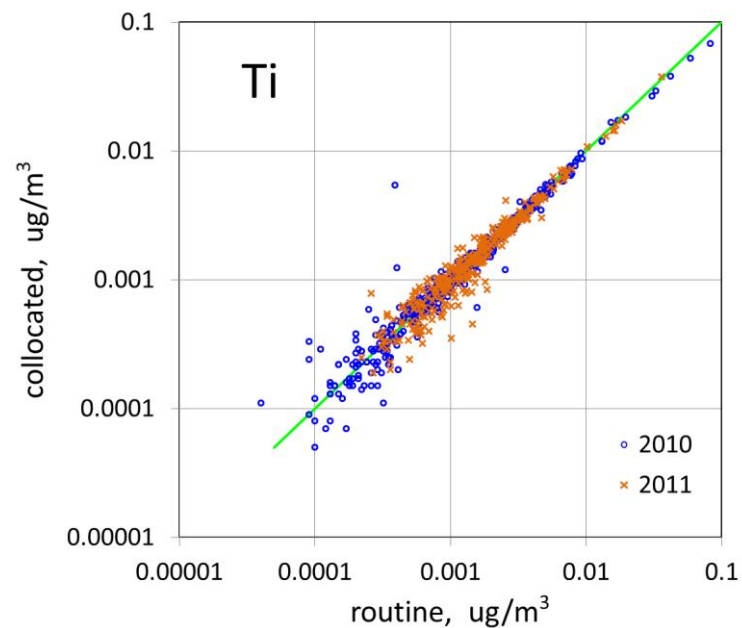
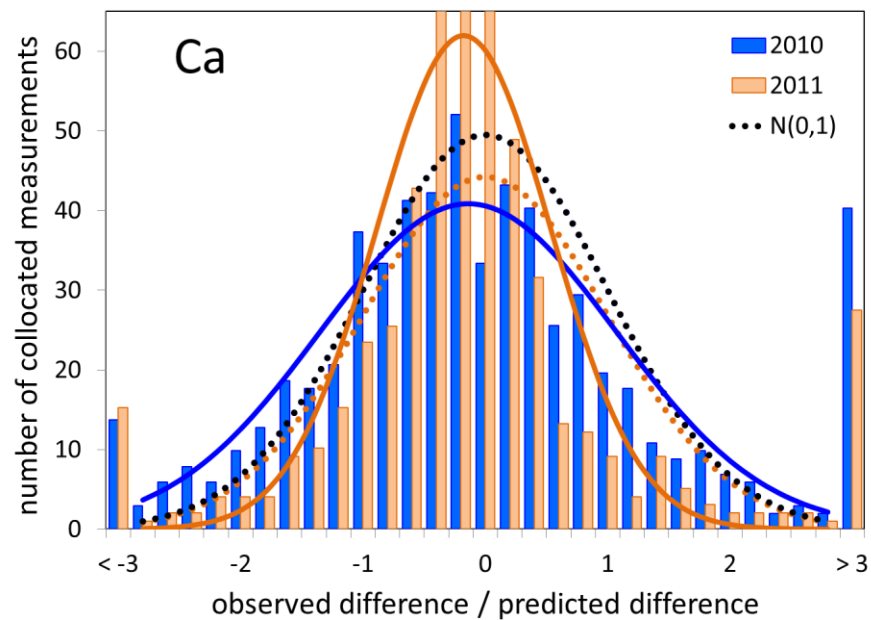
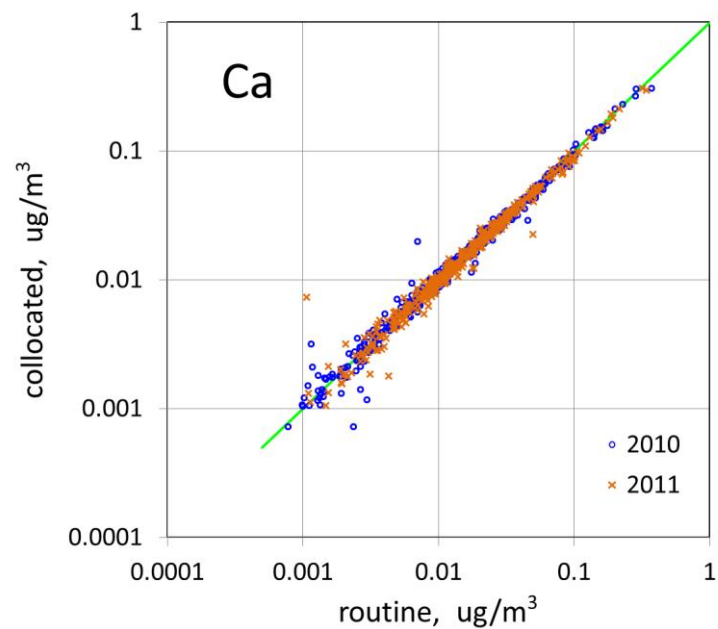


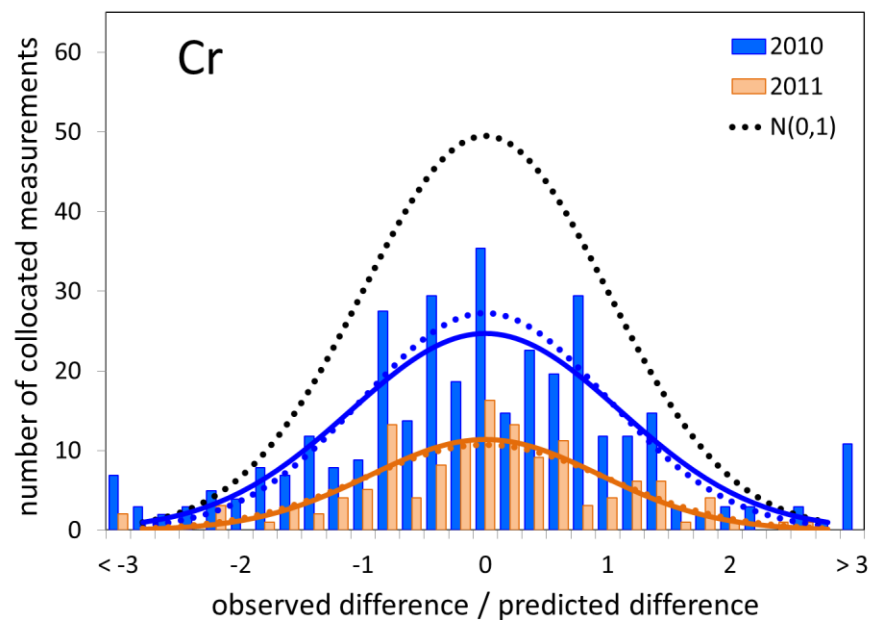
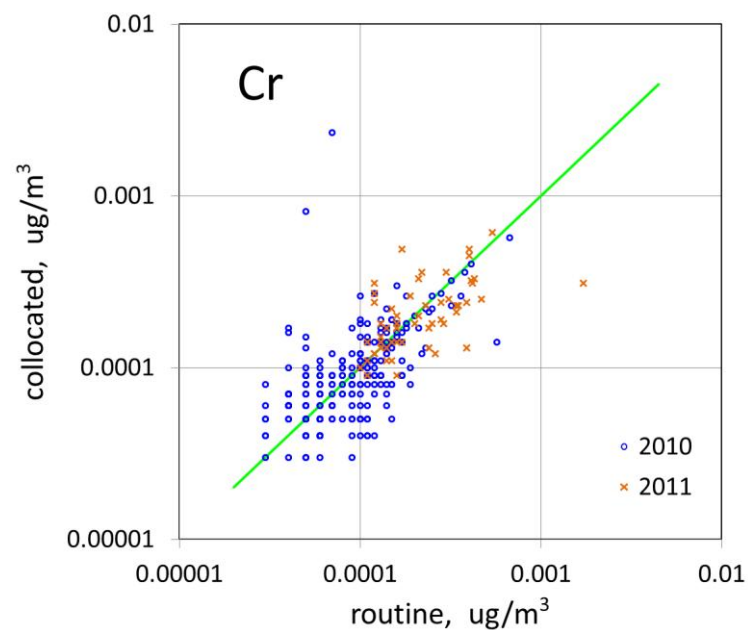
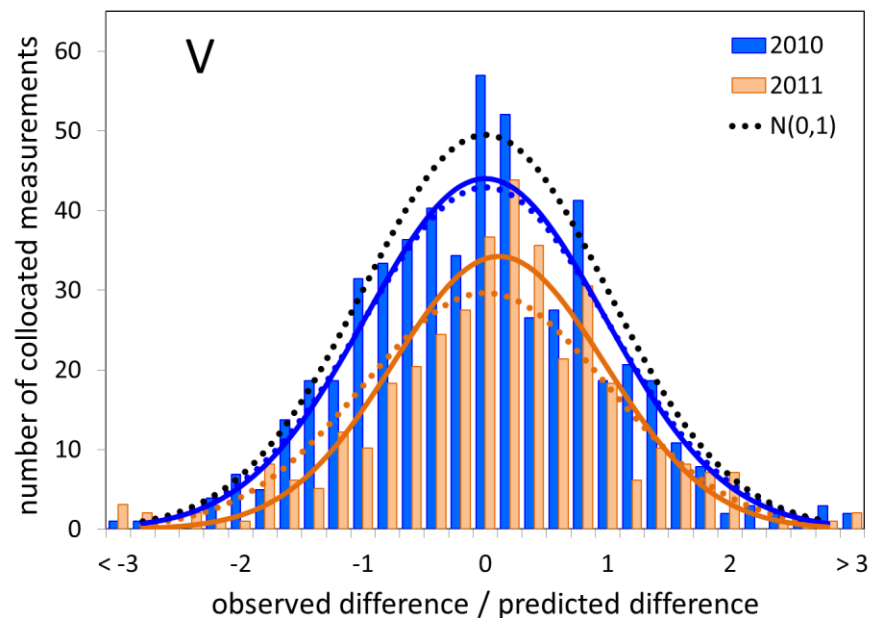
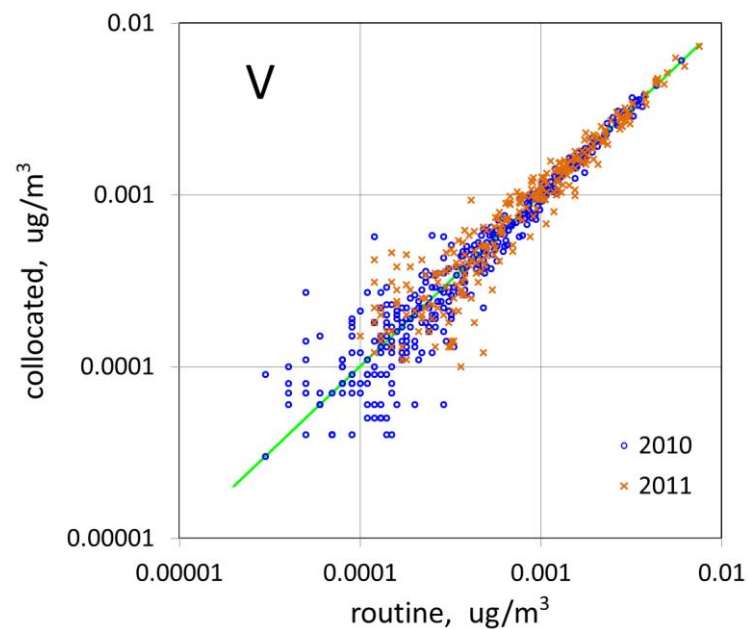


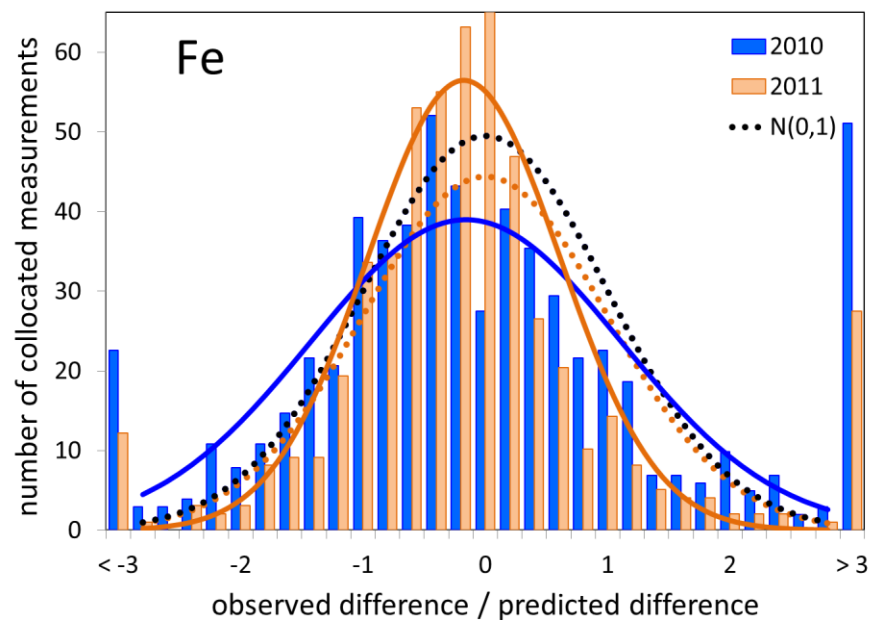
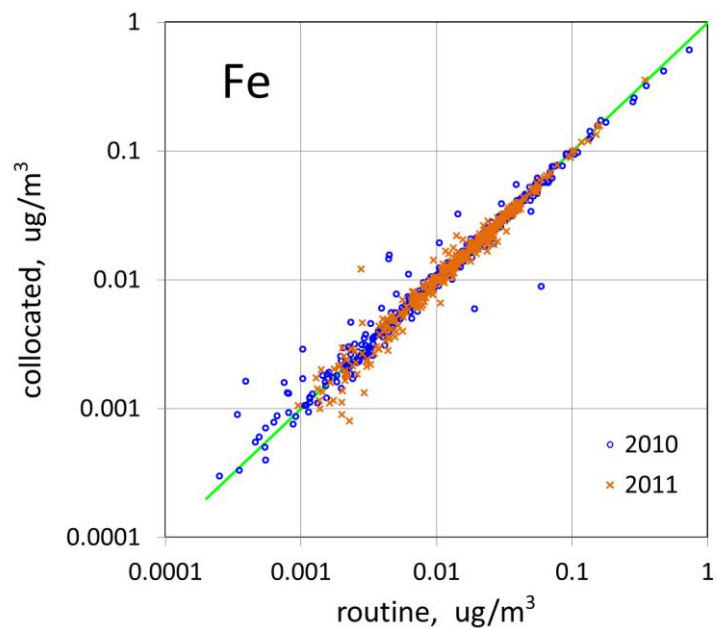
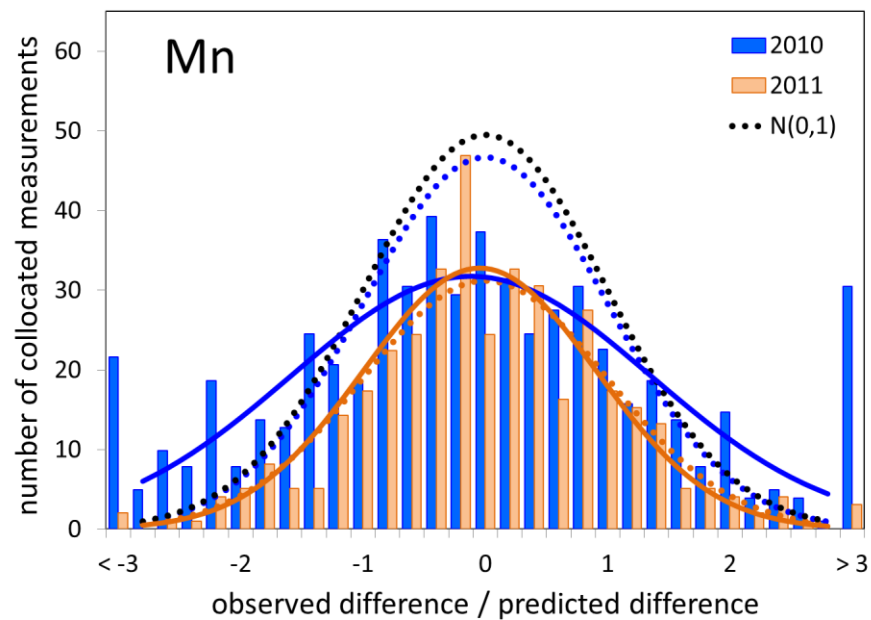
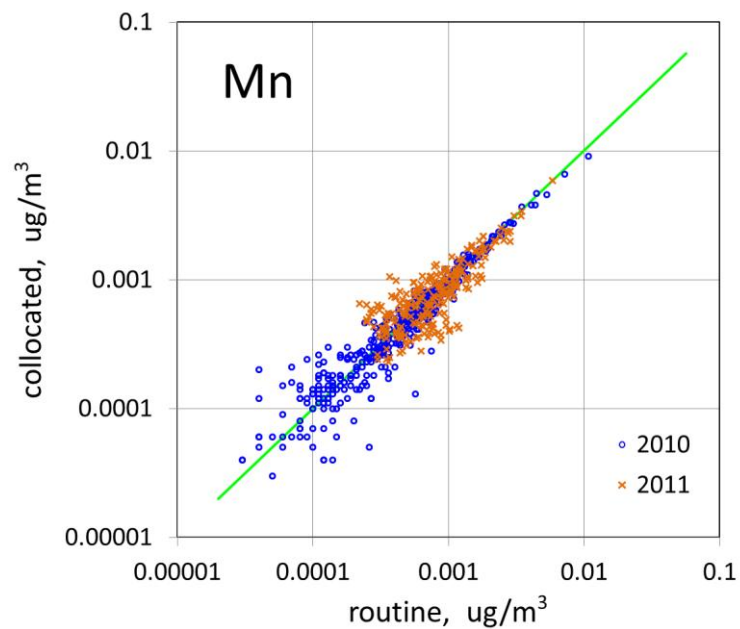


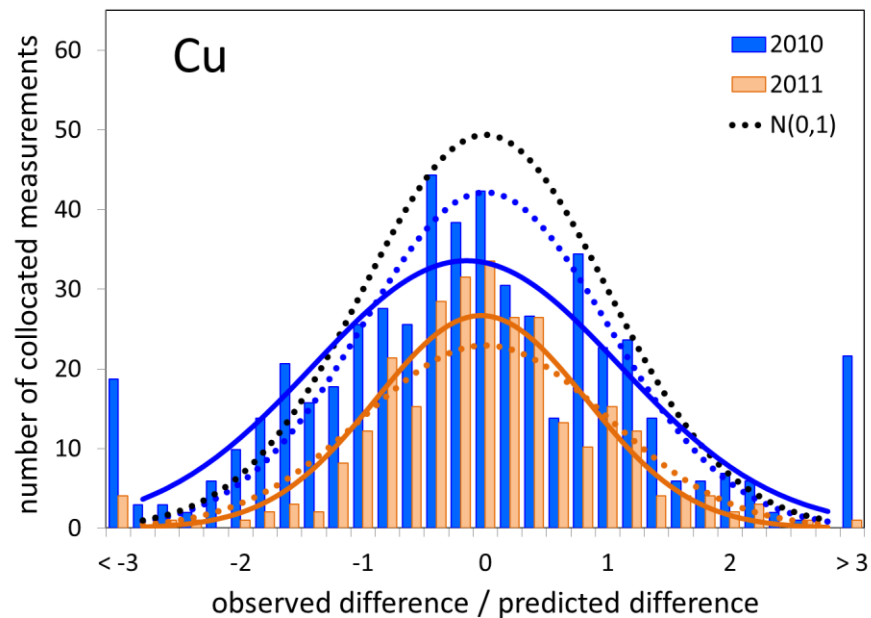
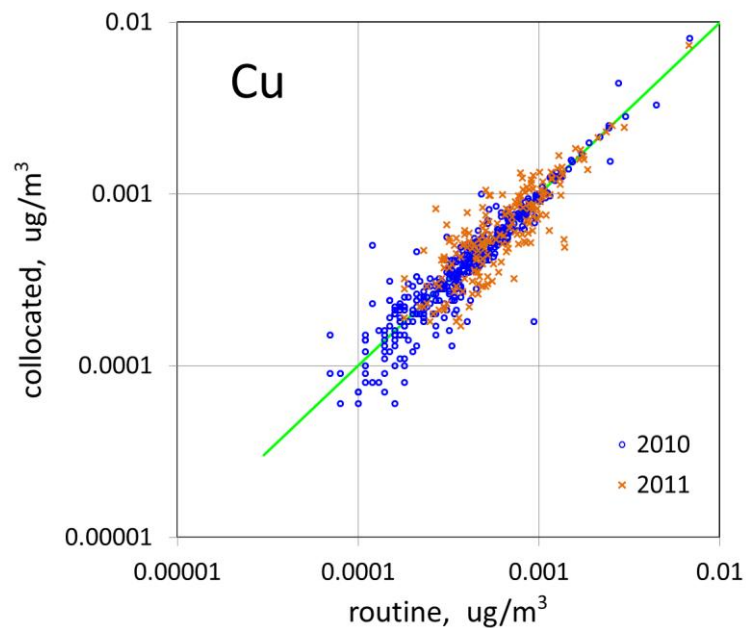
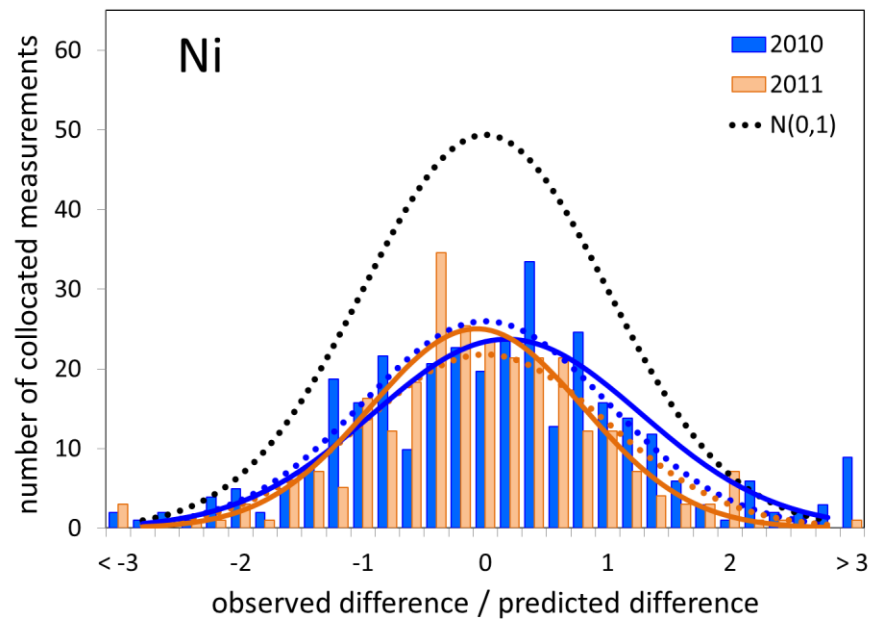
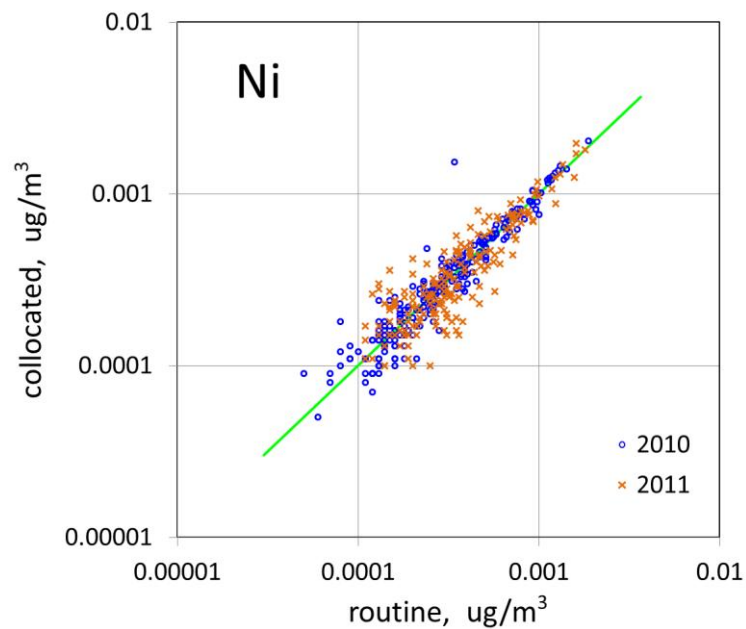


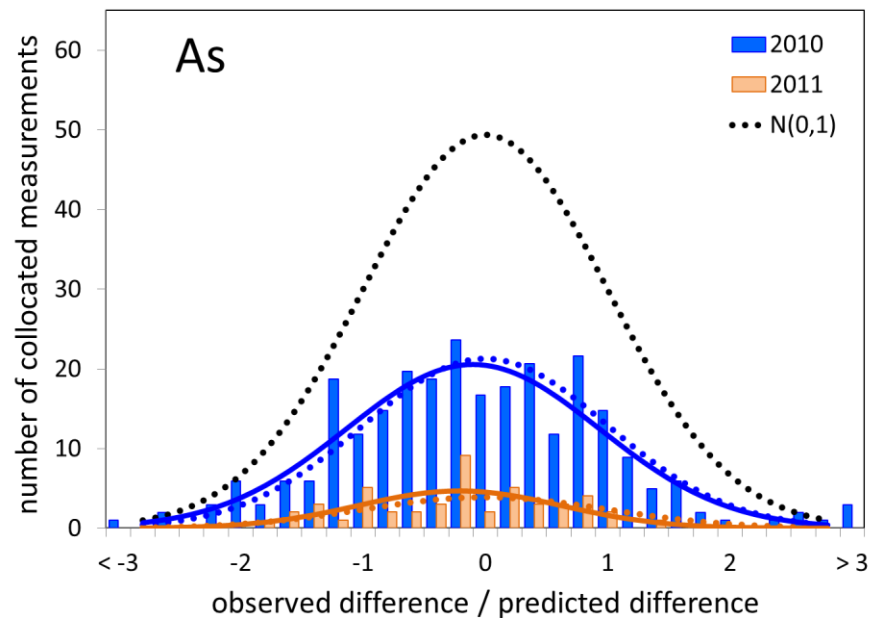
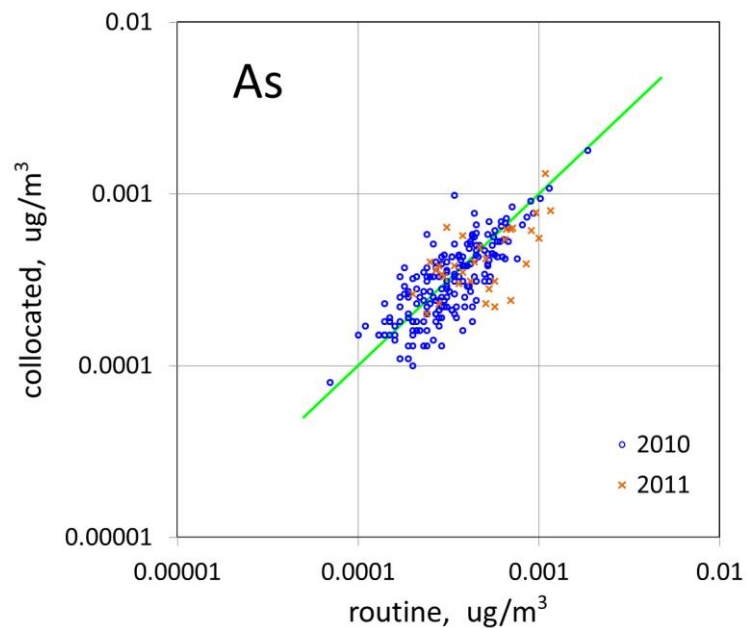
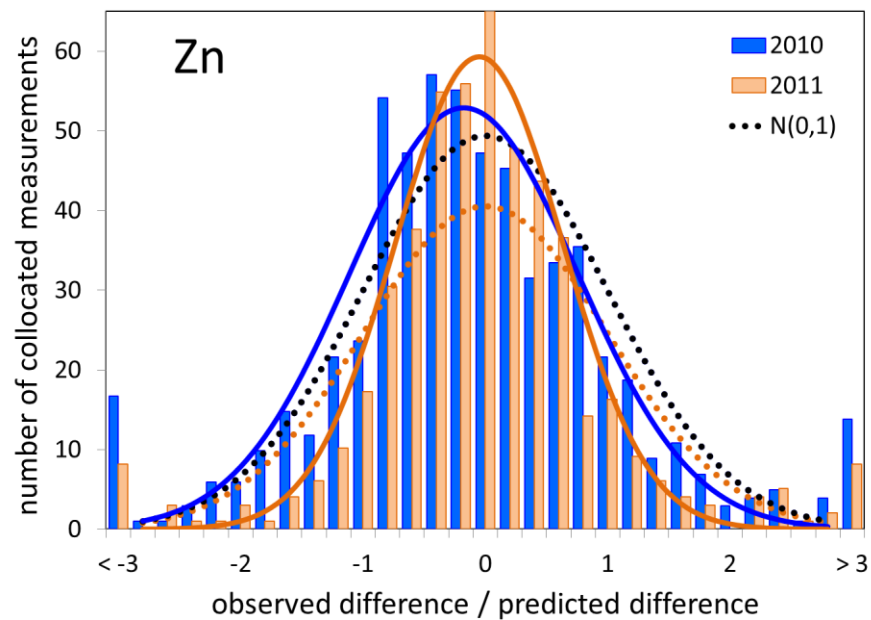
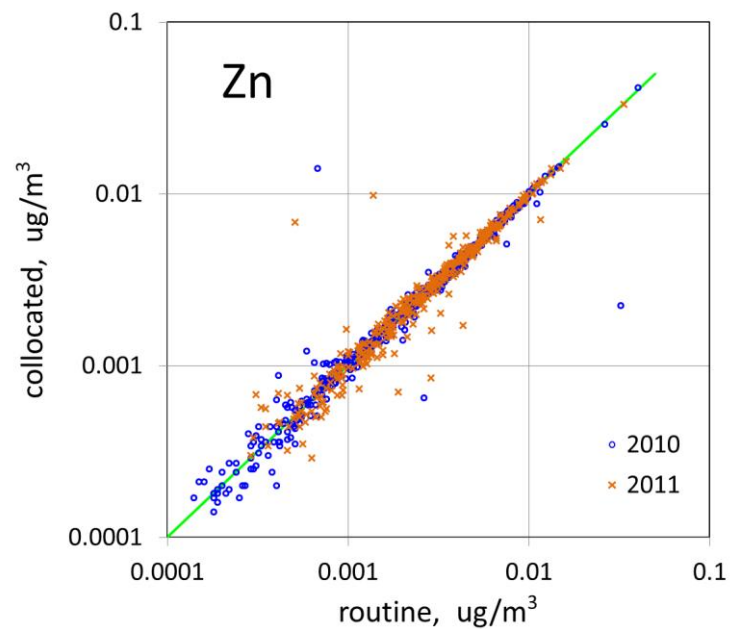


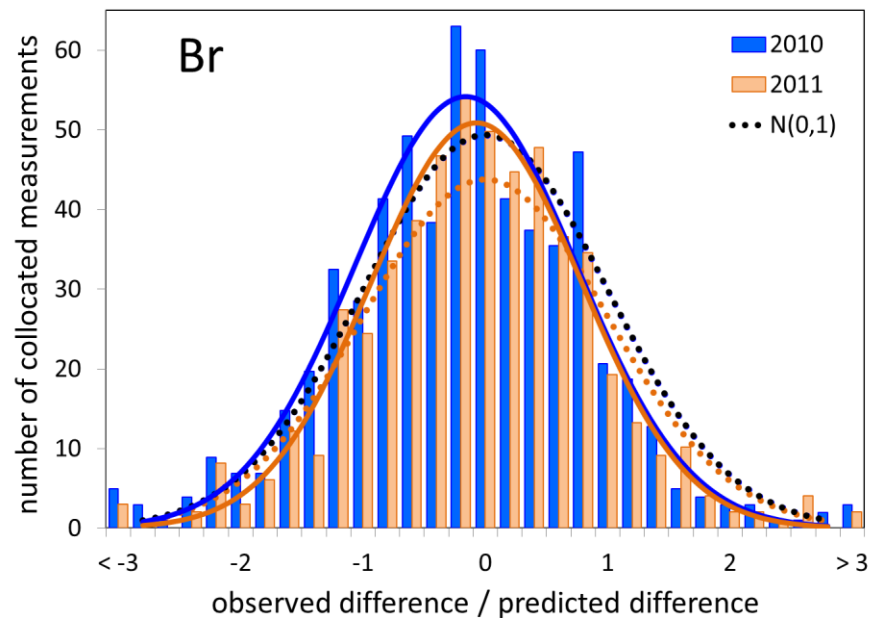
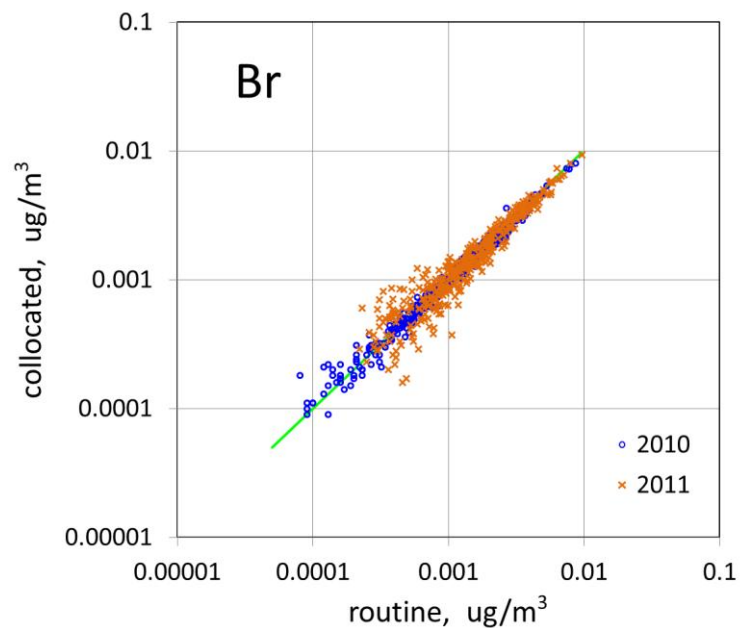
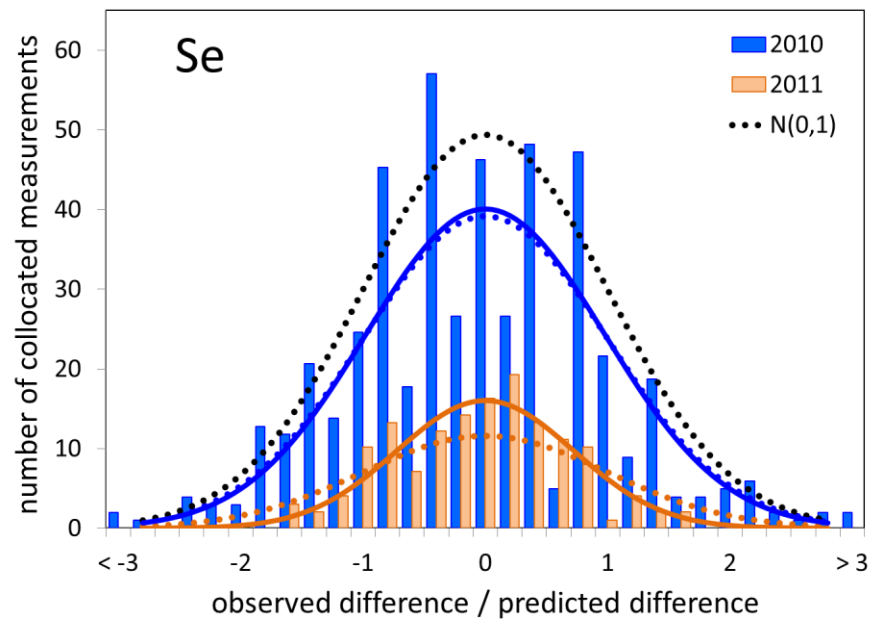
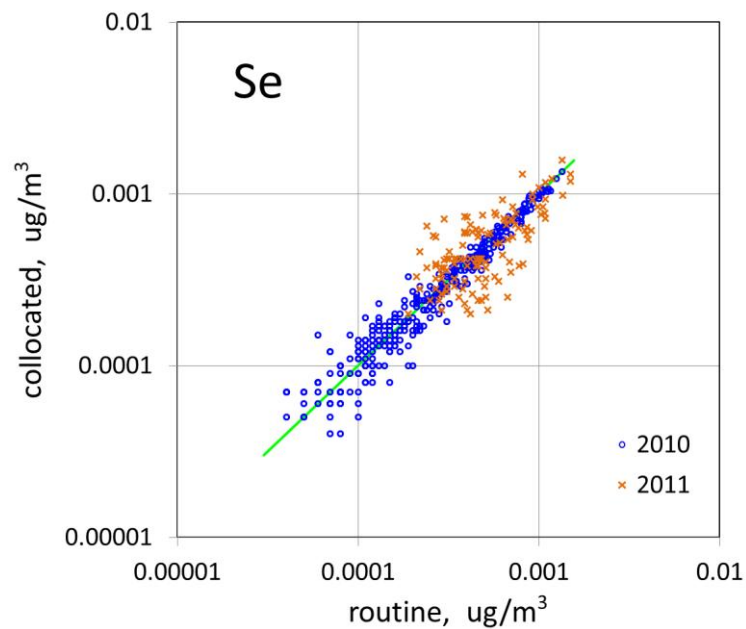


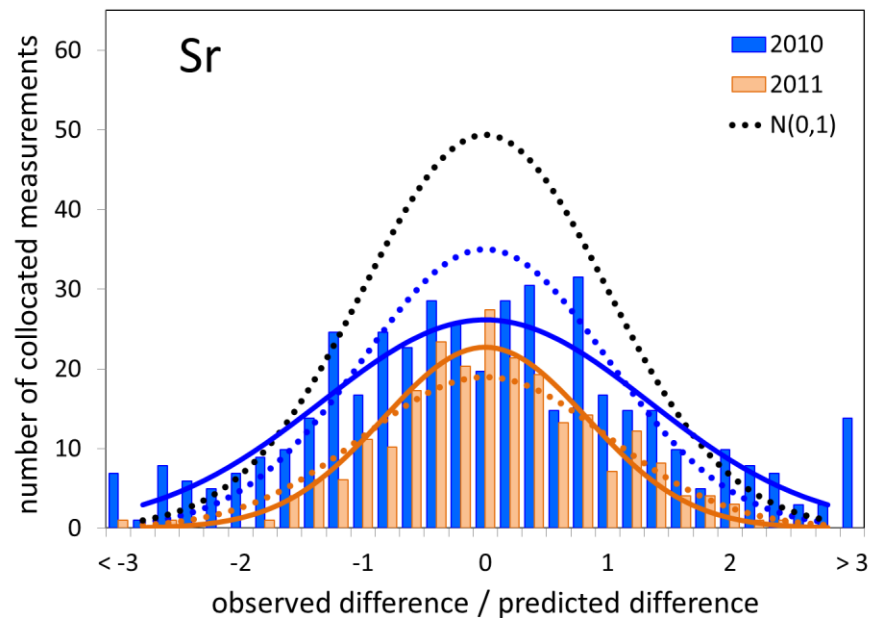
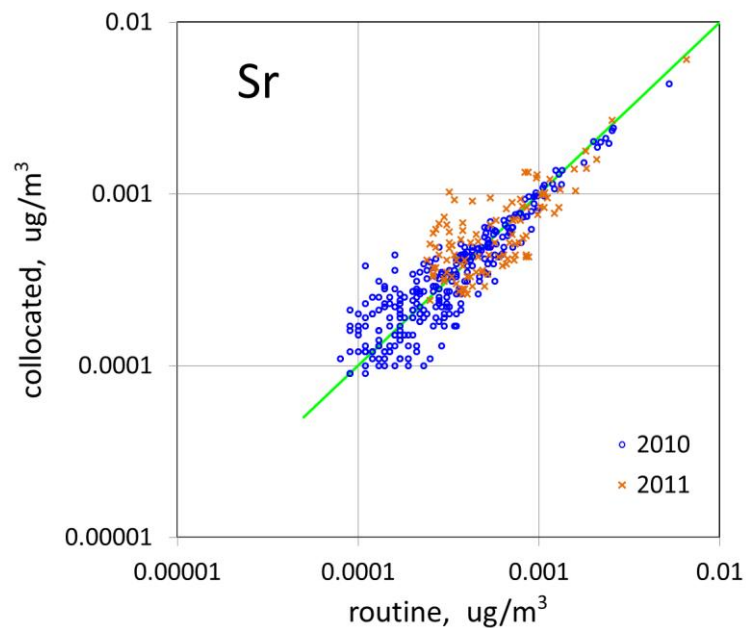
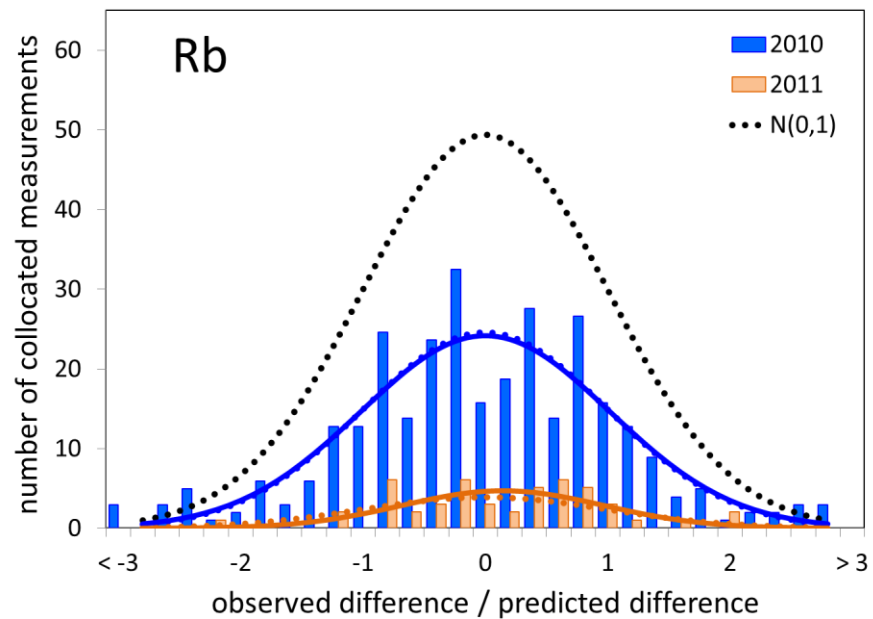
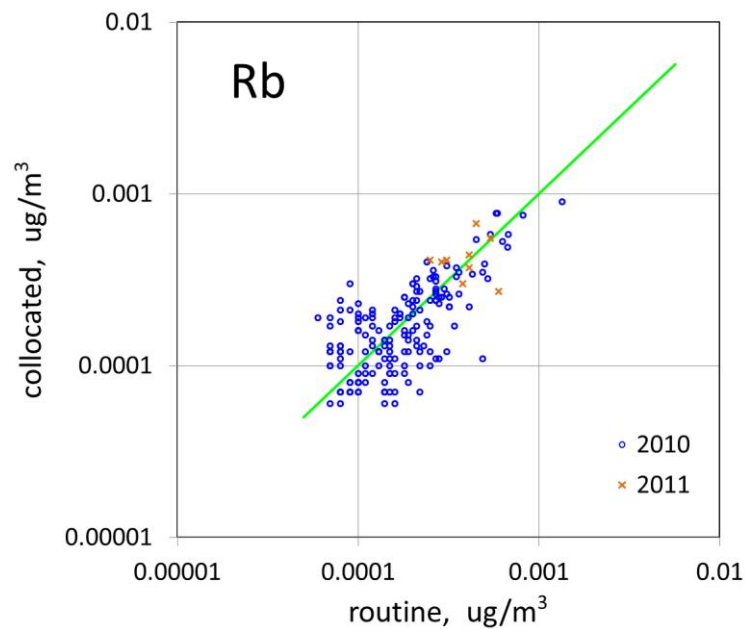


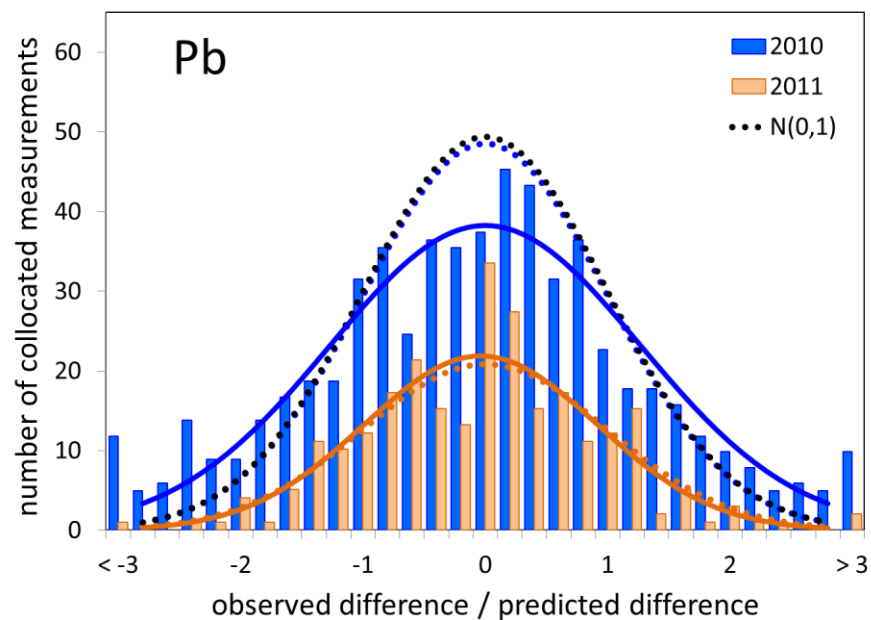
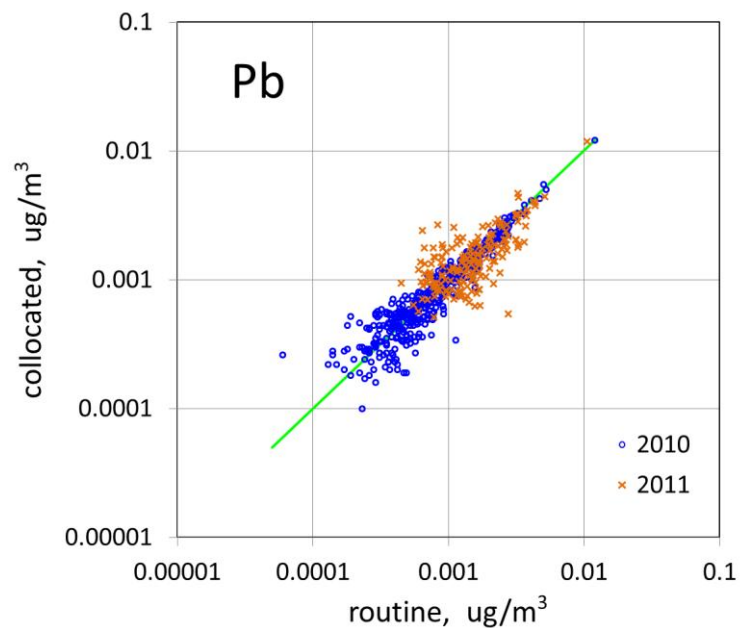
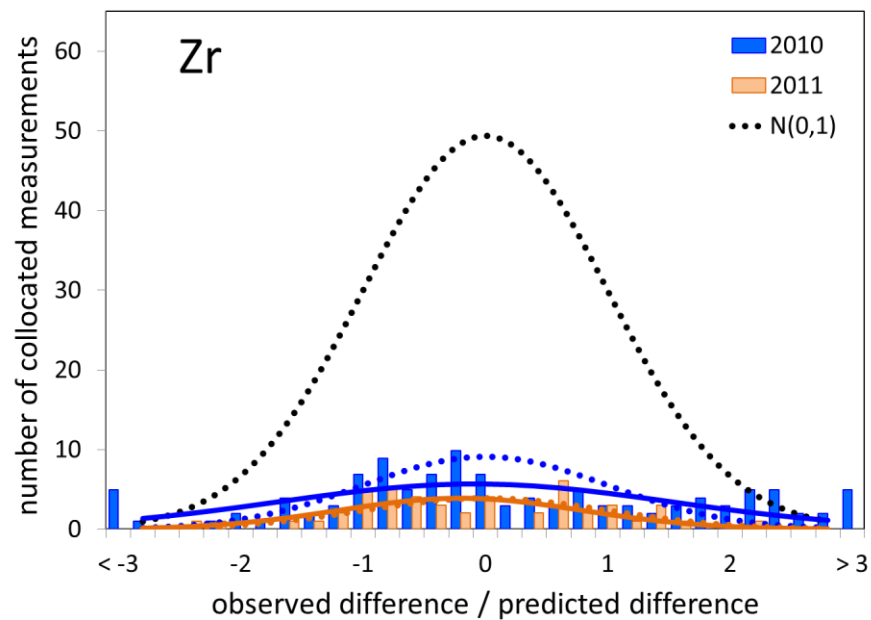
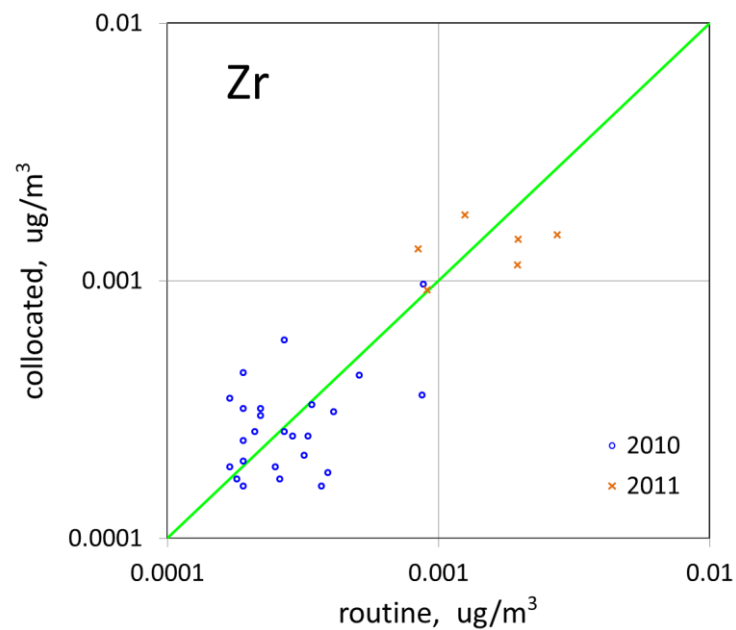












*Grant me strength, time, and opportunity **always to correct what I have acquired**, always to extend its domain; for knowledge is immense and the spirit of man can extend infinitely to enrich itself daily with new requirements. Today he can **discover his errors of yesterday**, and tomorrow he can obtain a **new light on what he thinks himself sure of today**.*

- Maimonides (1135-1204)