JOURNAL OF APPLIED CRYSTALLOGRAPHY

Volume 48 (2015)

Supporting information for article:

Comparison of silver and molybdenum microfocus X-ray sources for single-crystal structure determination

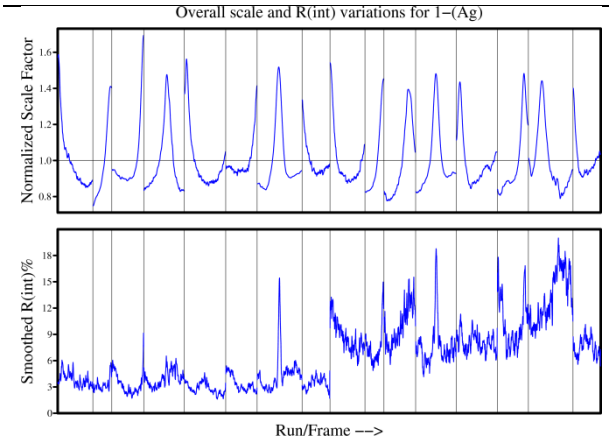
Lennard Krause, Regine Herbst-Irmer, George M. Sheldrick and Dietmar Stalke

S1. *SADABS* Diagnostic plots

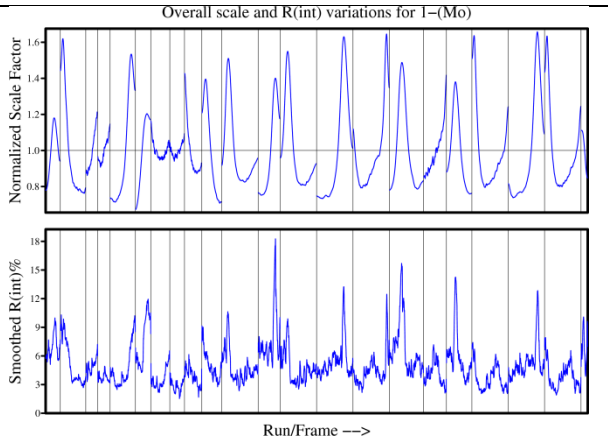
The following plots are generated from *SADABS* and show the variation of the normalized scale factor and smoothed R_{int} as a function of the frame number. It should be noted that the smoothing algorithm for the R(int) plots was changed in *SADABS* 2014/4 to make these plots more informative.

Data of sample 1:

Ag

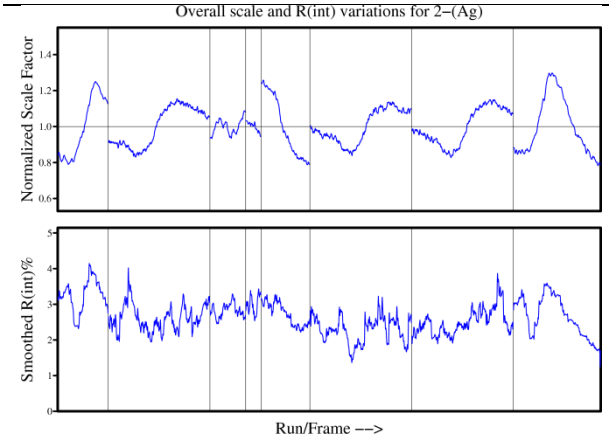


Mo

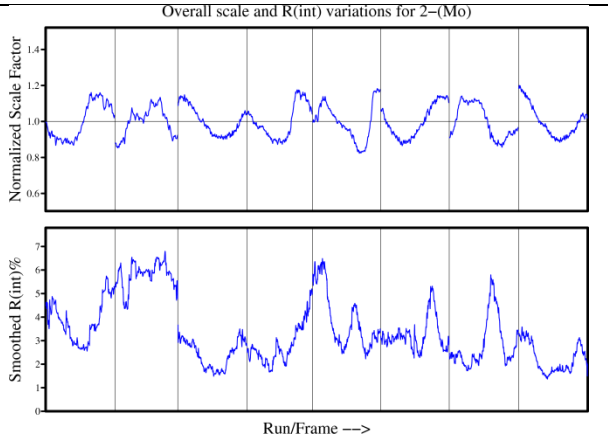


Data of sample 2:

Ag

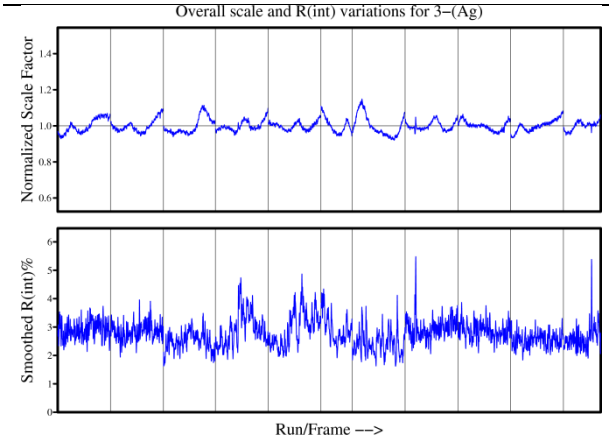


Mo

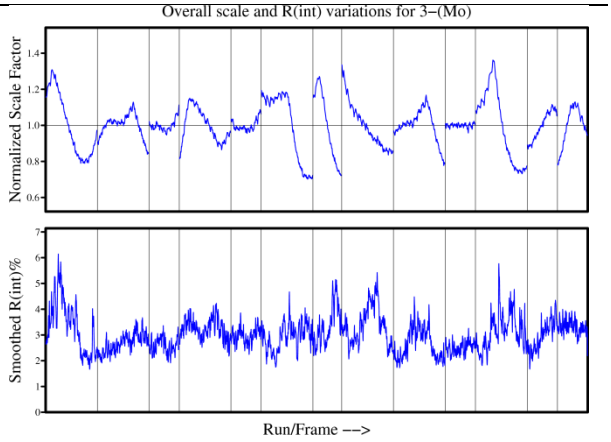


Data of sample 3:

Ag

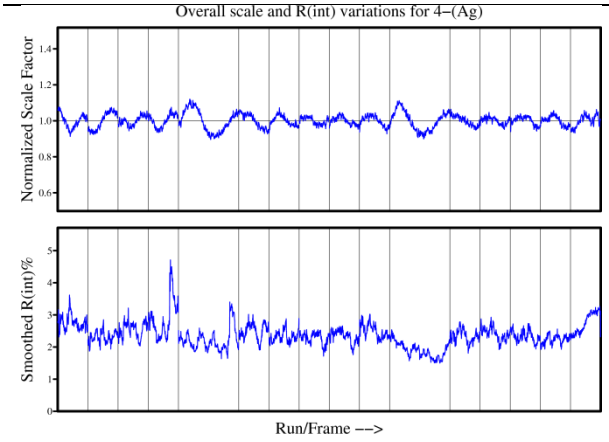


Mo

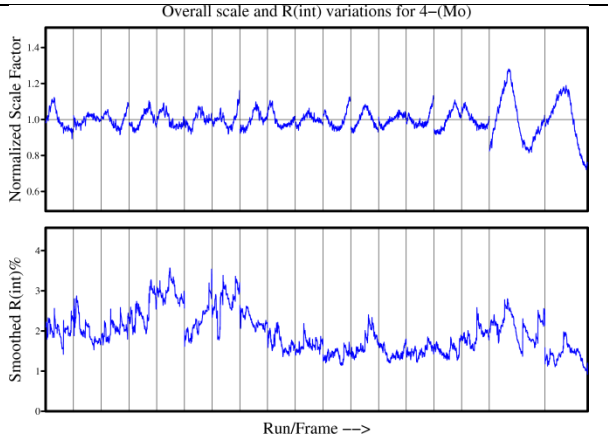


Data of sample 4:

Ag

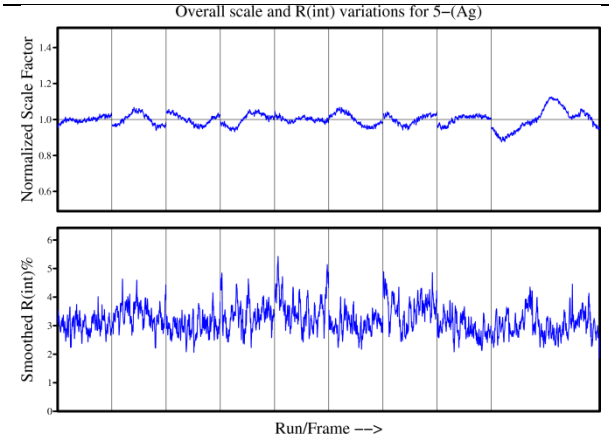


Mo

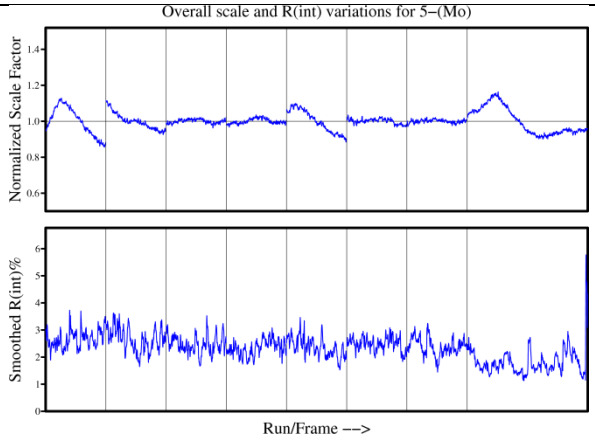


Data of sample 5:

Ag

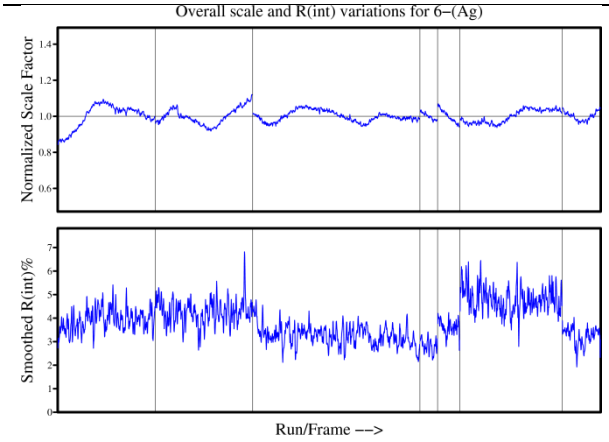


Mo

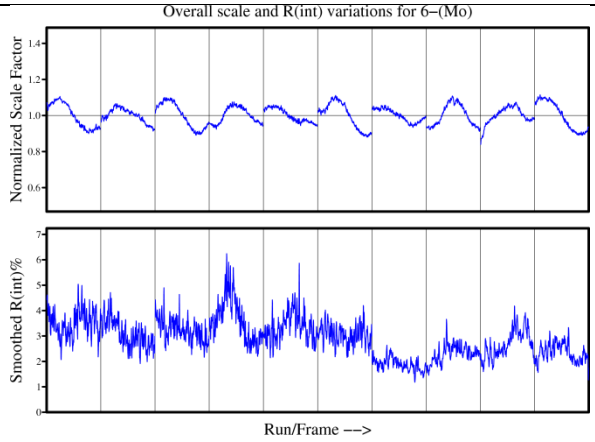


Data of sample 6:

Ag

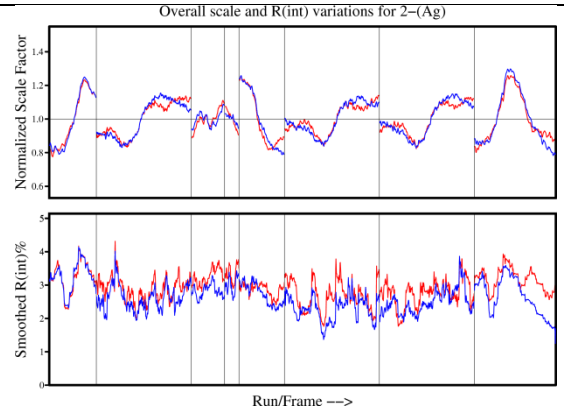
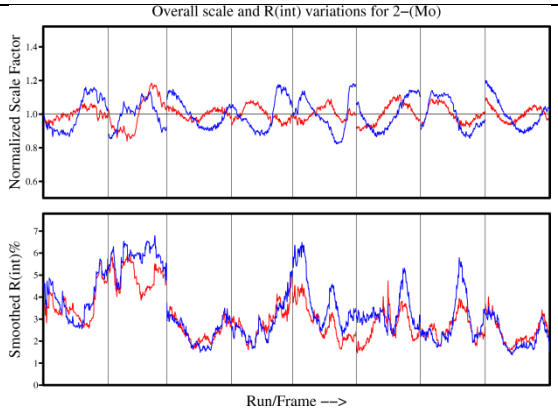


Mo



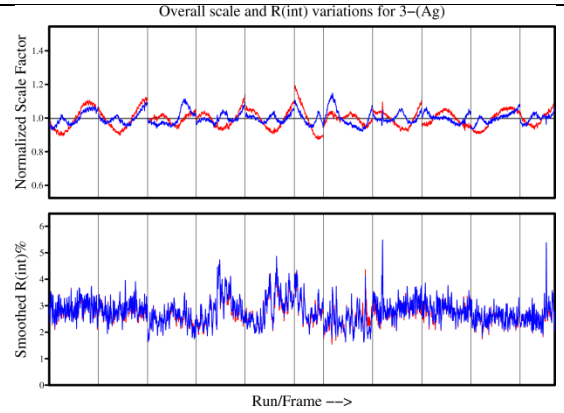
The following Plots are presented as an overlay of the two data sets, one corrected with the numerical (red) and the other with the empirical (blue) absorption correction.

Data of sample 2:

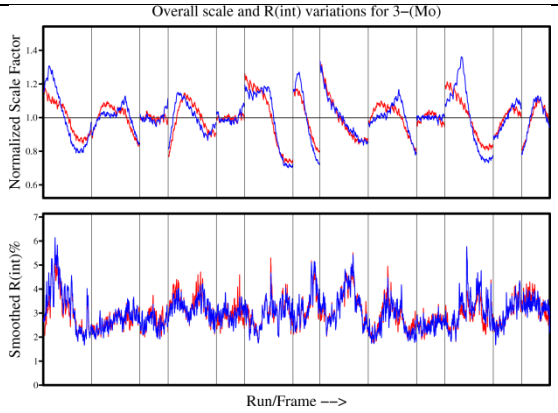
Ag	Mo
	

Data of sample 3:

Ag

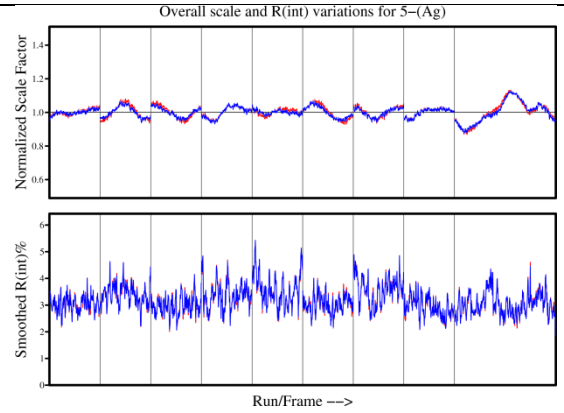


Mo

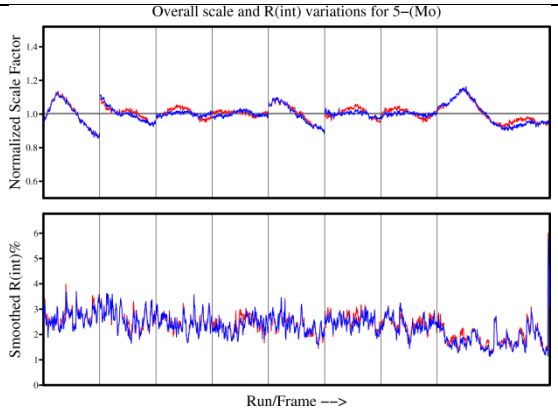


Data of sample 5:

Ag

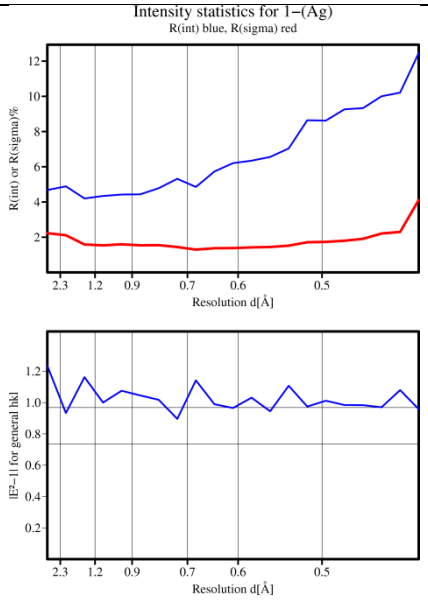
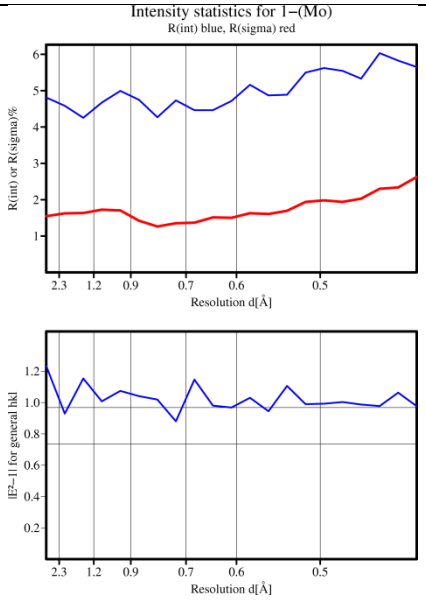


Mo

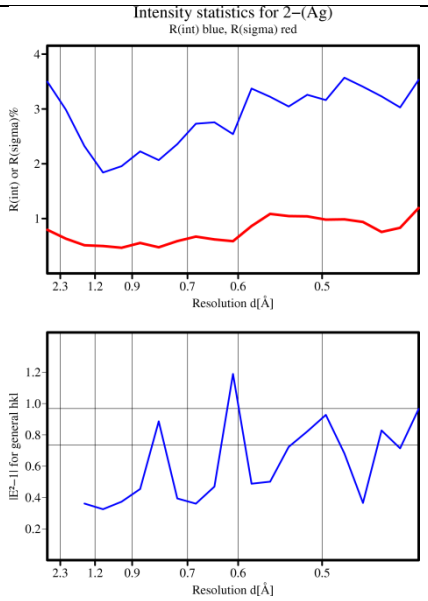
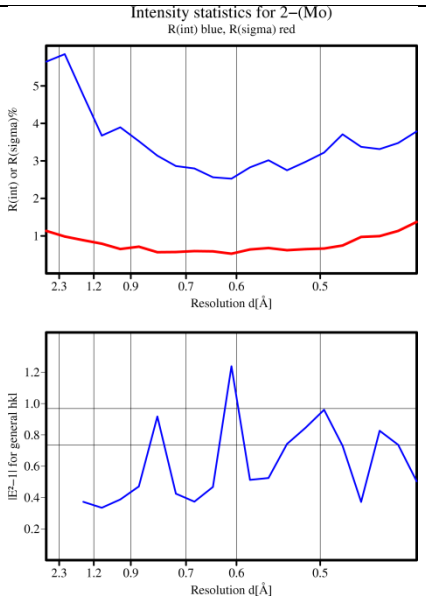


The following plots are generated from *SADABS* and show the variation of R(int), R(sigma) (upper) and $|E^2-1|$ (lower) as a function of resolution.

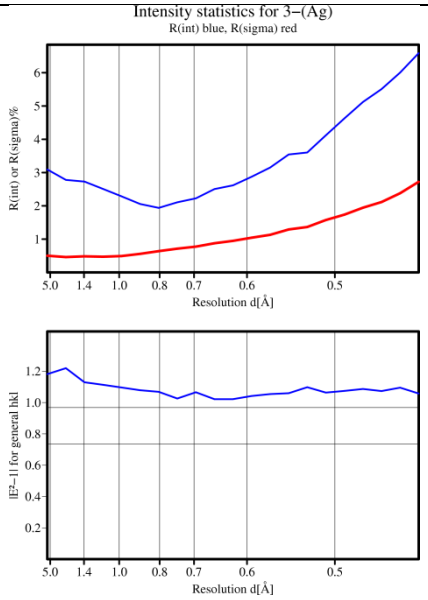
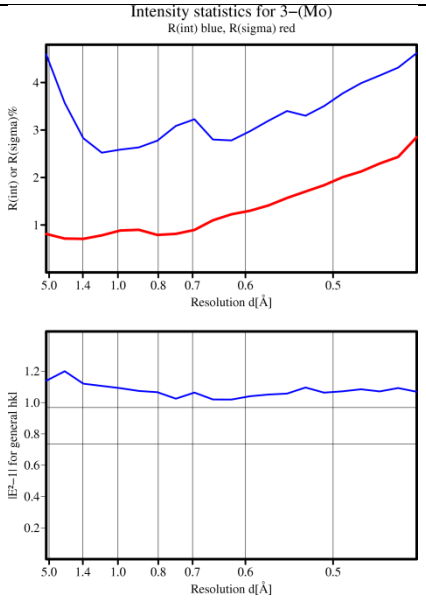
Data of sample 1:

Ag	Mo
	

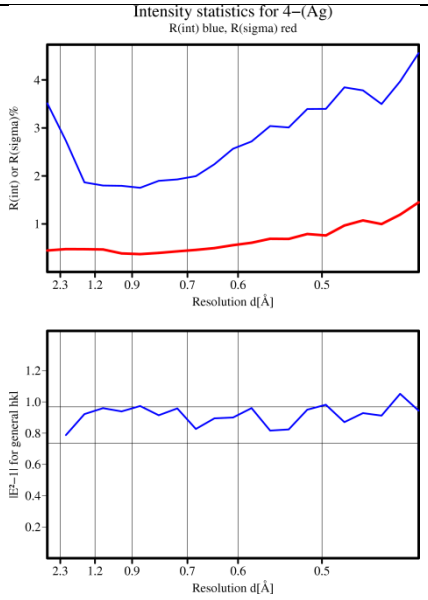
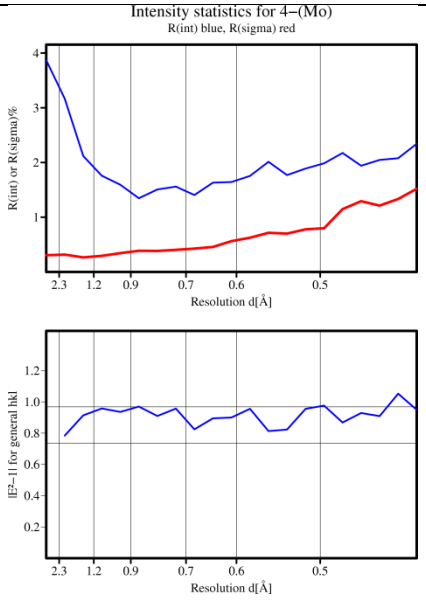
Data of sample 2:

Ag	Mo
	

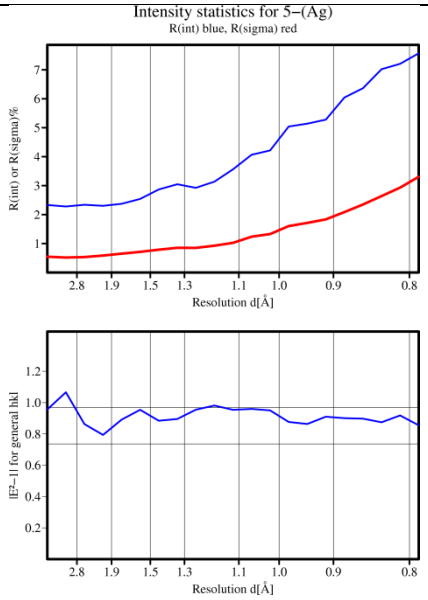
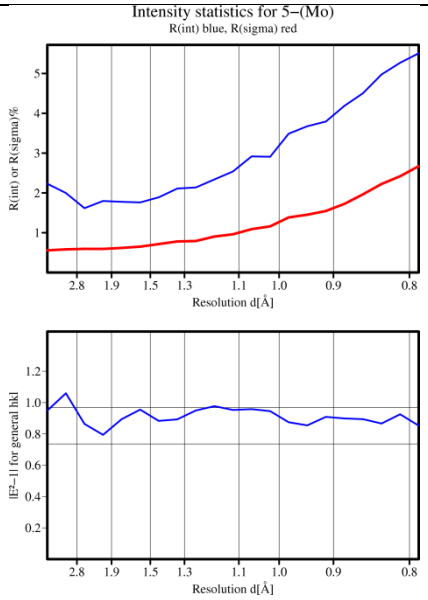
Data of sample 3:

Ag	Mo
	

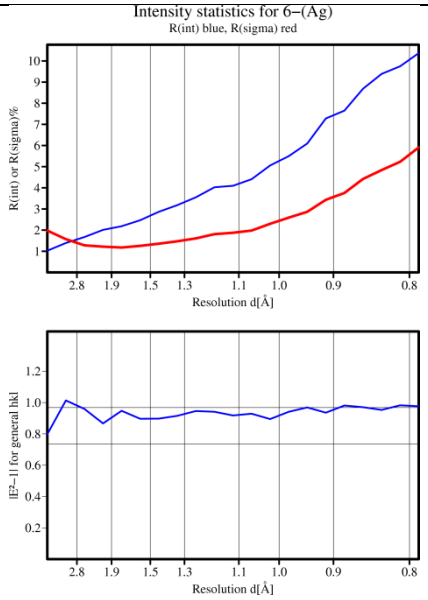
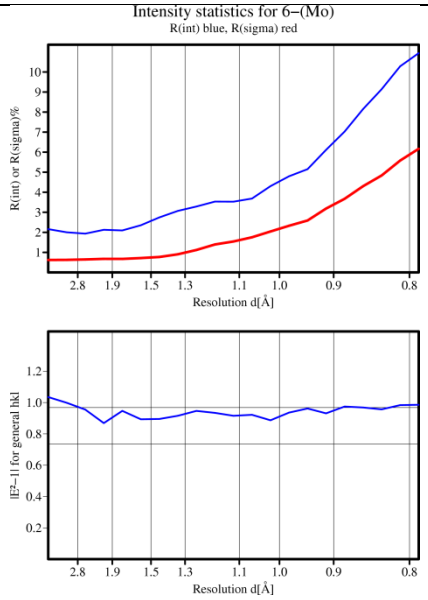
Data of sample 4:

Ag	Mo
	

Data of sample 5:

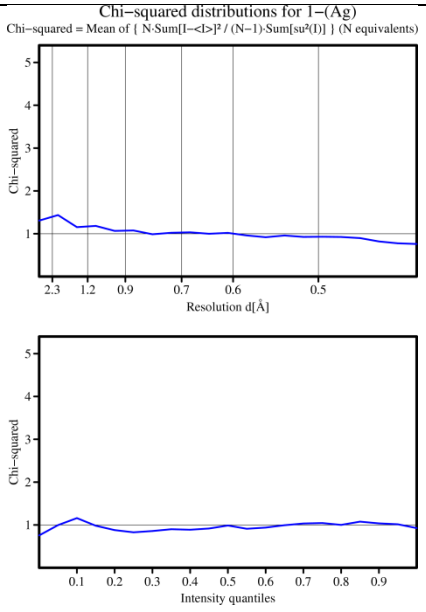
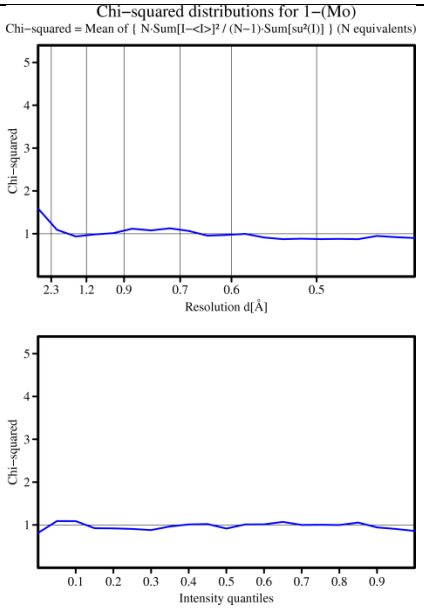
Ag	Mo
	

Data of sample 6:

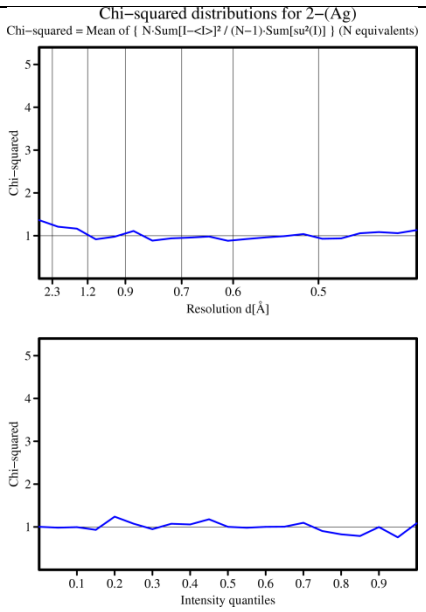
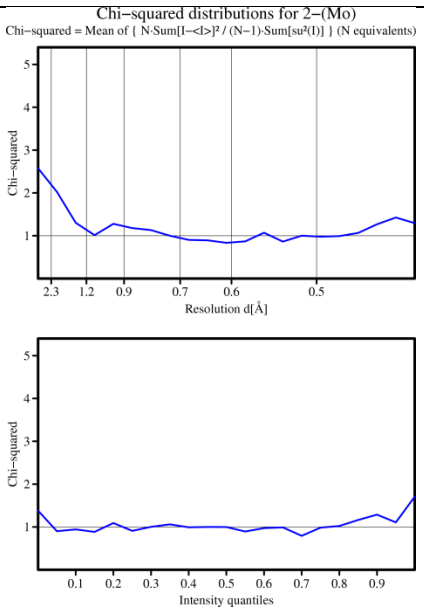
Ag	Mo
	

The following plots are generated from *SADABS* and show the variation of χ^2 as a function of resolution and intensities.

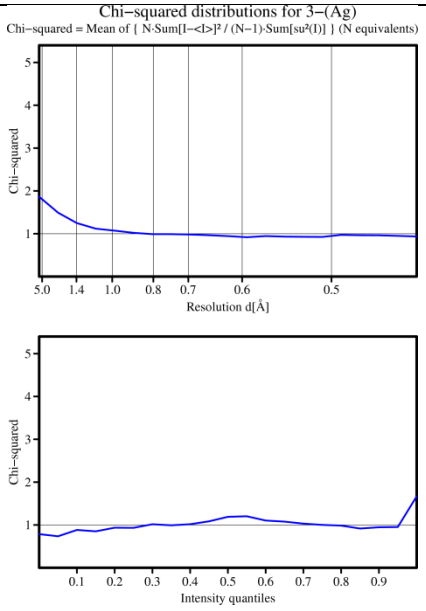
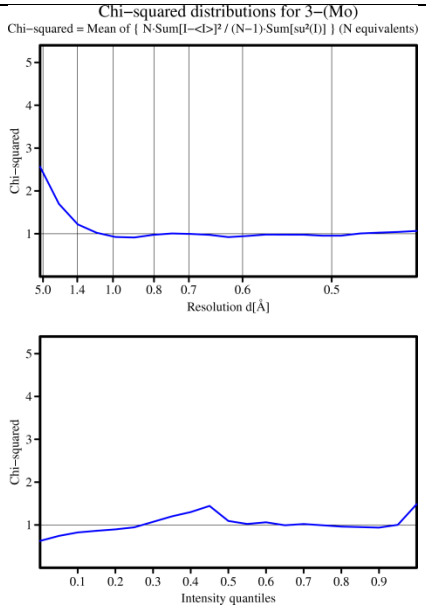
Data of sample 1:

Ag	Mo
	

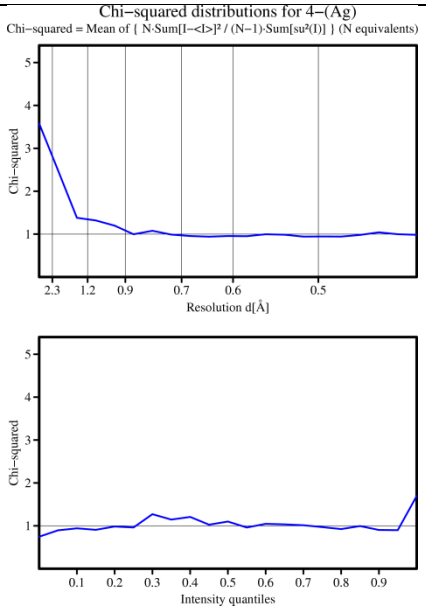
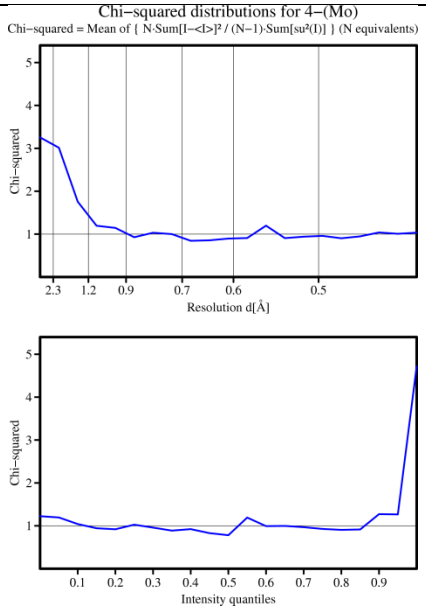
Data of sample 2:

Ag	Mo
	

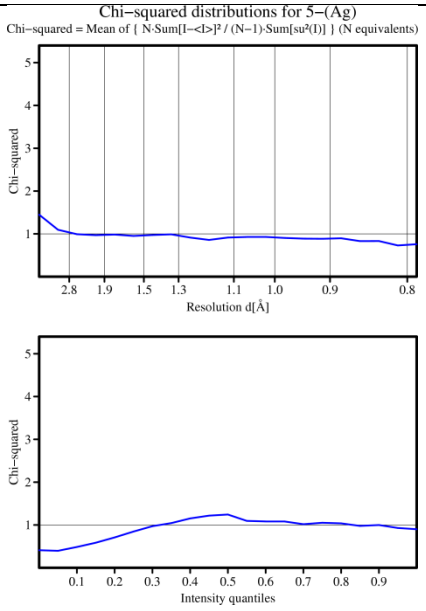
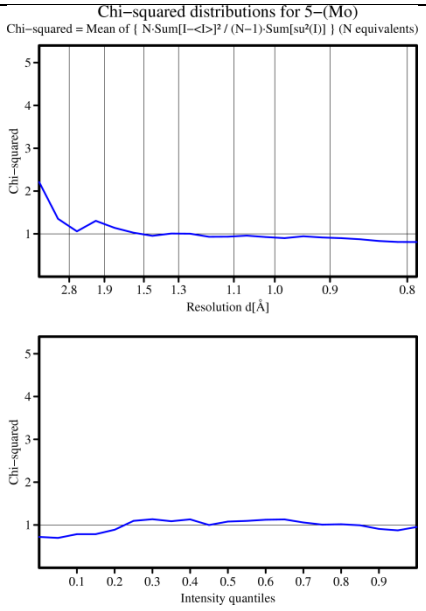
Data of sample 3:

Ag	Mo
	

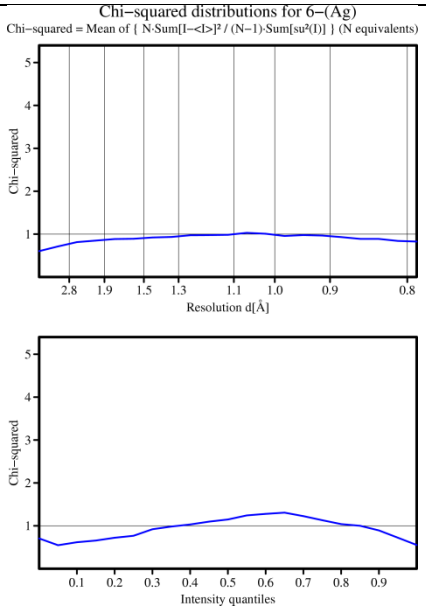
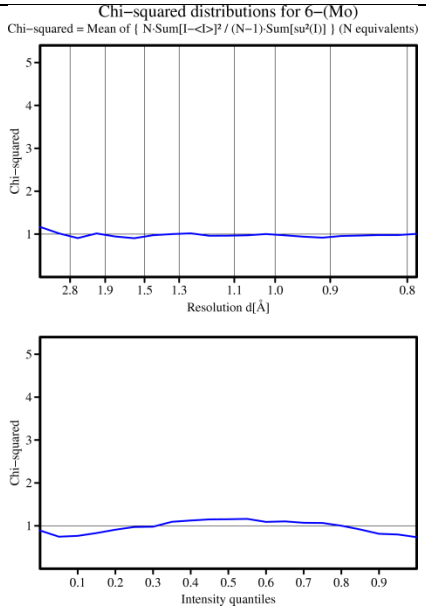
Data of sample 4:

Ag	Mo
	

Data of sample 5:

Ag	Mo
	

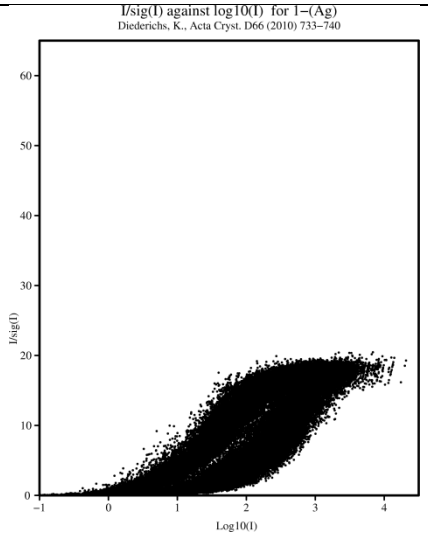
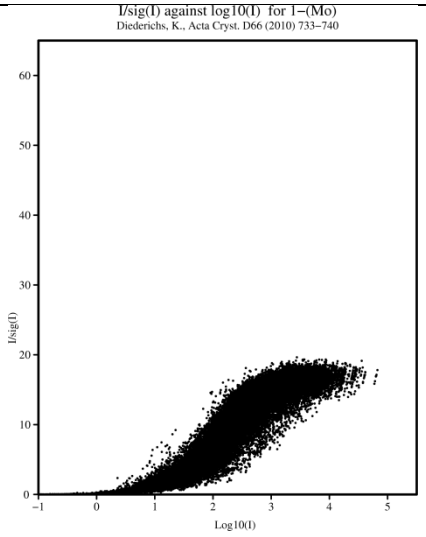
Data of sample 6:

Ag	Mo
	

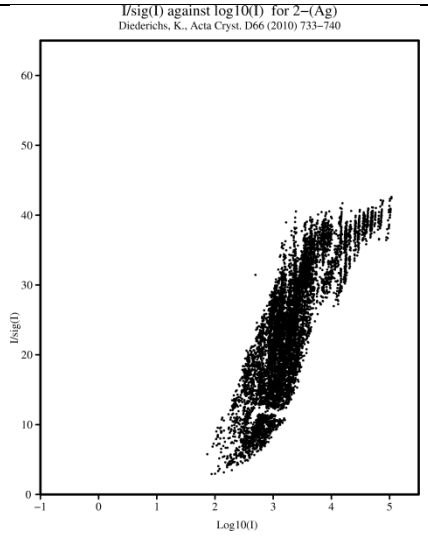
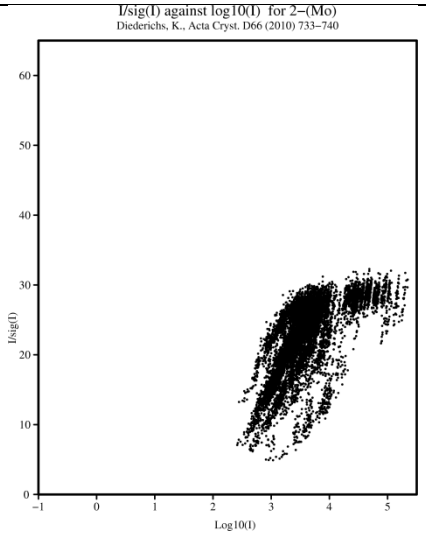
S2. Significance of the data

In 2010, Diederichs suggested an indicator which is calculated after the data reduction to be used to estimate the systematic instrument error of the x-ray source. The value of this indicator is the highest [I/σ(I)] value the given experimental setup can produce.

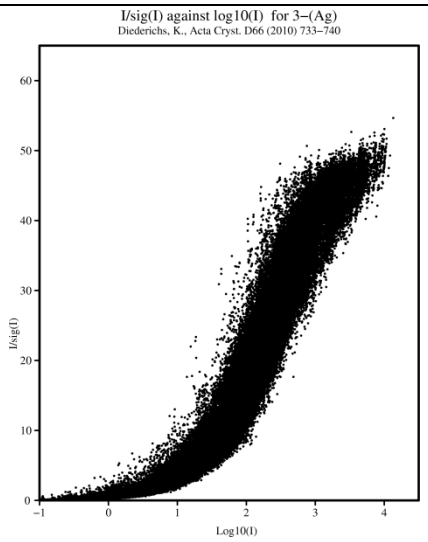
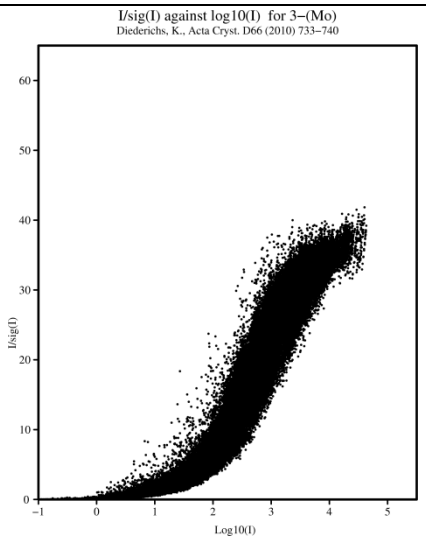
Data of sample 1:

Ag	Mo
	

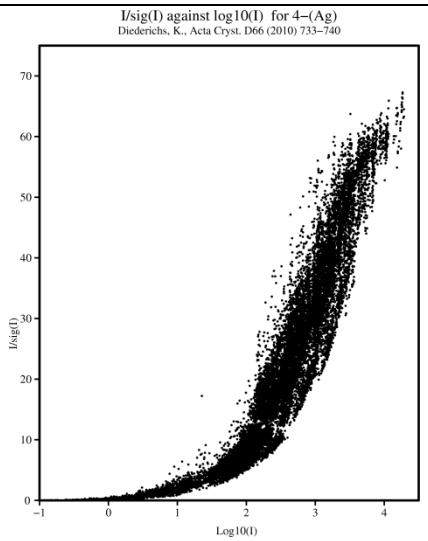
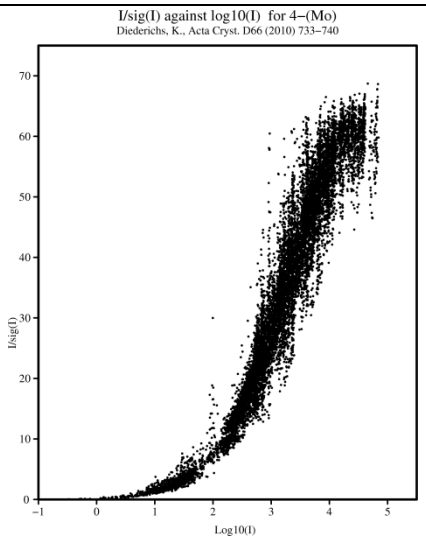
Data of sample 2:

Ag	Mo
	

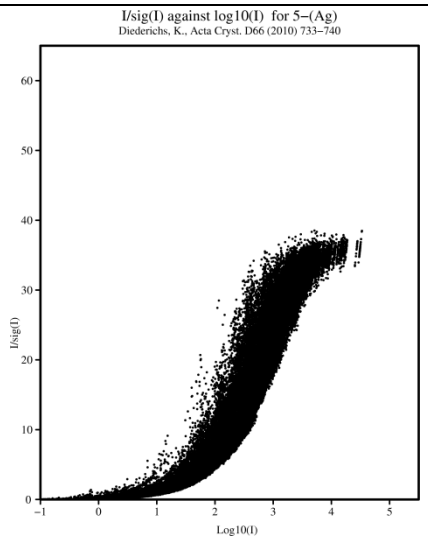
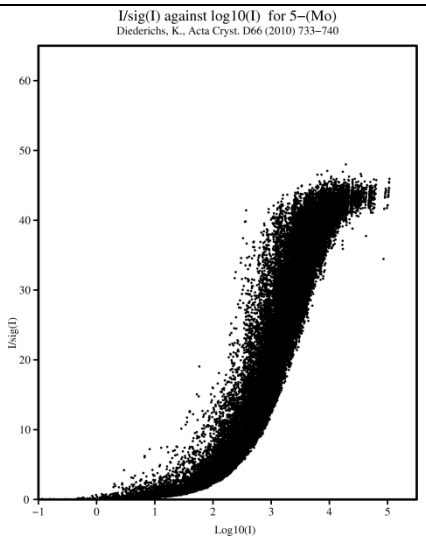
Data of sample 3:

Ag	Mo
	

Data of sample 4:

Ag	Mo
	

Data of sample 5:

Ag	Mo
	

Data of sample 6:

Ag	Mo