IS IT POSSIBLE FOR MY CALCULATED PNOC VALUE TO BE NEGATIVE,

i.e. LESS THAN THE ORIGINAL SAMPLE WEIGHT?

KDOHC LABORATORY

JJ Dekker

17 August 2022

Teams Meeting

CONTENT

- Introduction and Problem Statement
- Accuracy & Precision
- Theoretical / Ideal Calibration Curve for Instrument
- Development of a Calibrations Curve
- Potential Actual Calibrations Curve
- PNOC – Actual Example
- 5 Decimal Balance – Limitation
- Conclusion & Recommendations
- Questions & Comments

INTRODUCTION & PROBLEM STATEMENT

Legislator stipulates that PNOC be calculated as follow:

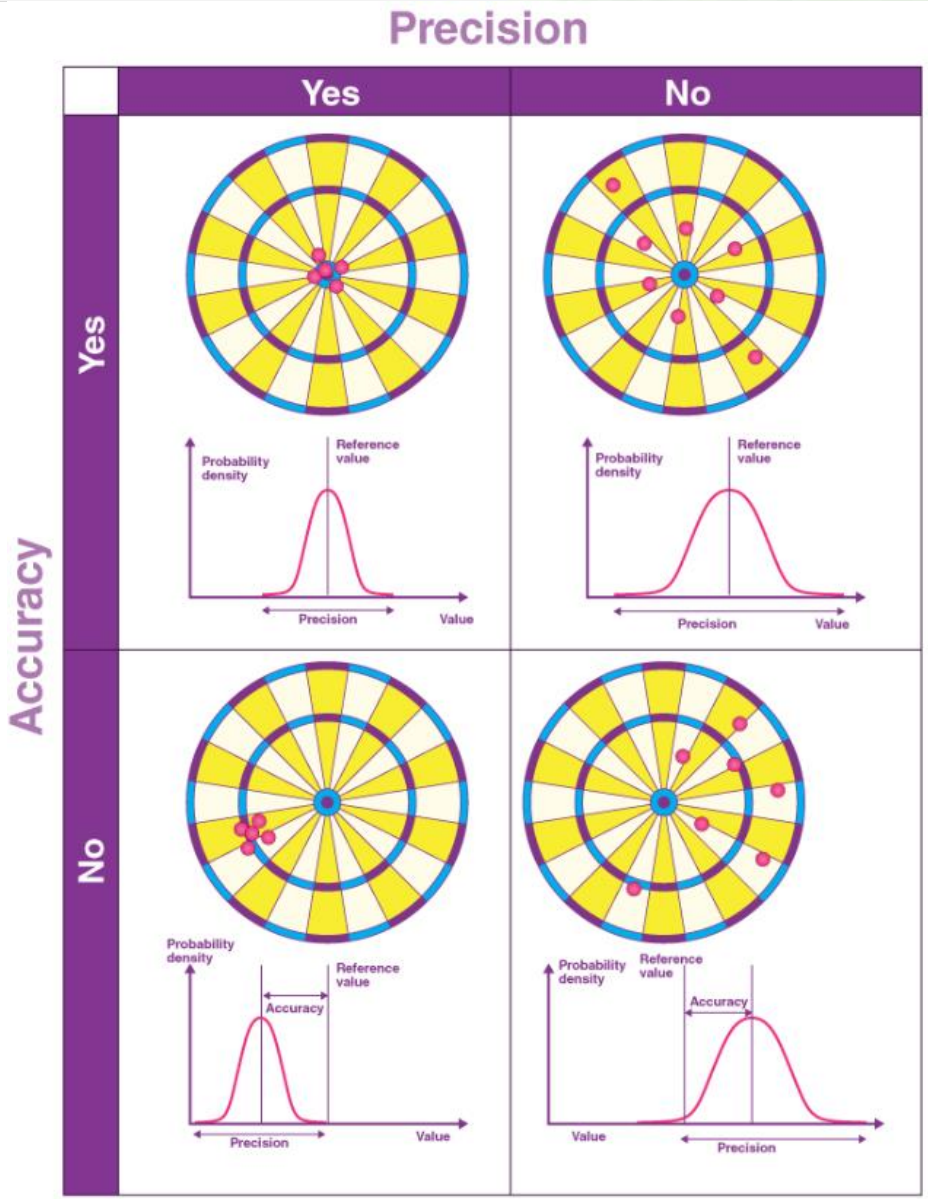
PNOC = Gravimetric weight – Sum of weight of all identified pollutants

In some cases, this result in the PNOC value being NEGATIVE (i.e.: <0).

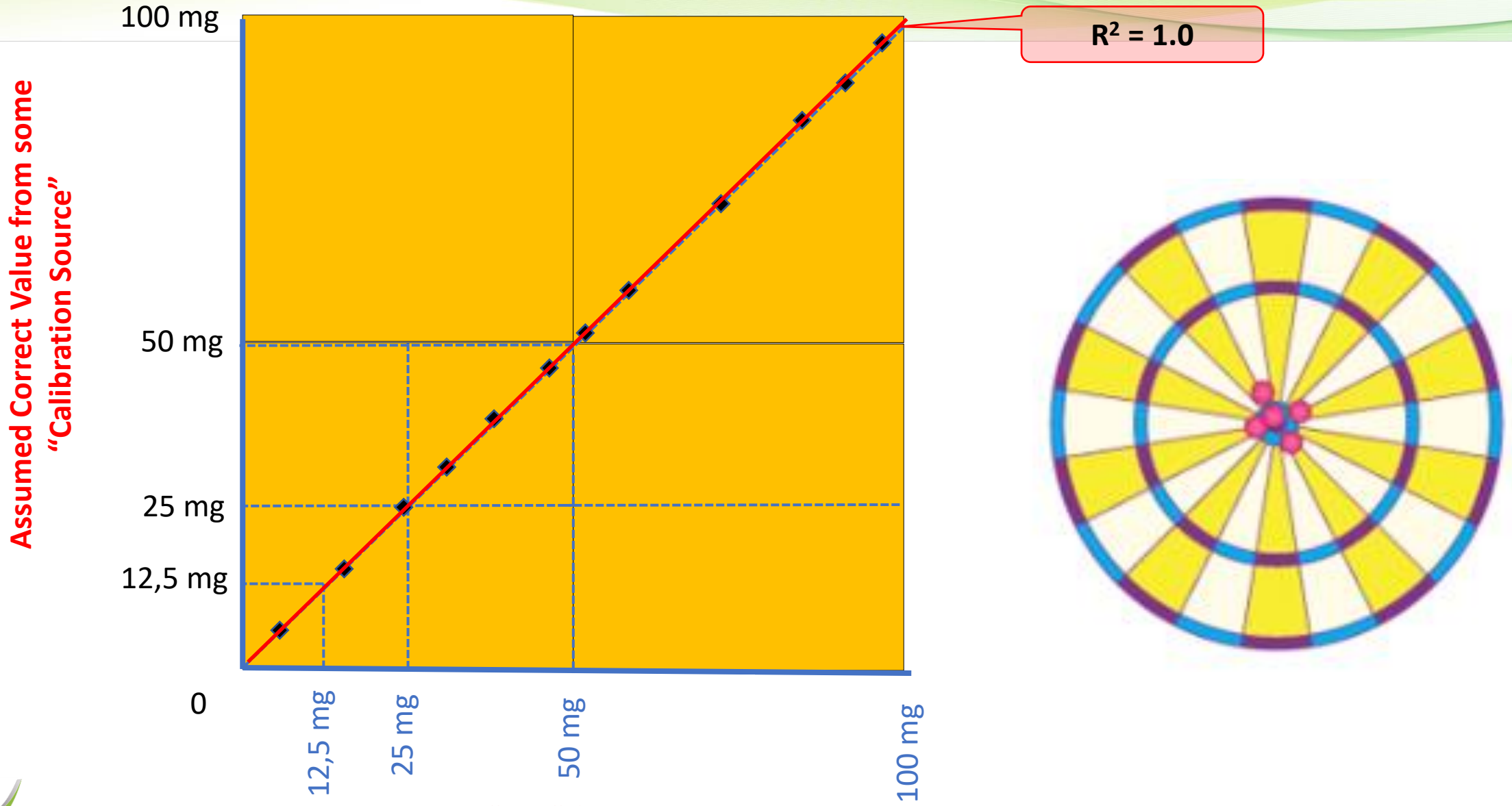
How is this possible?

What can be done to correct the situation?

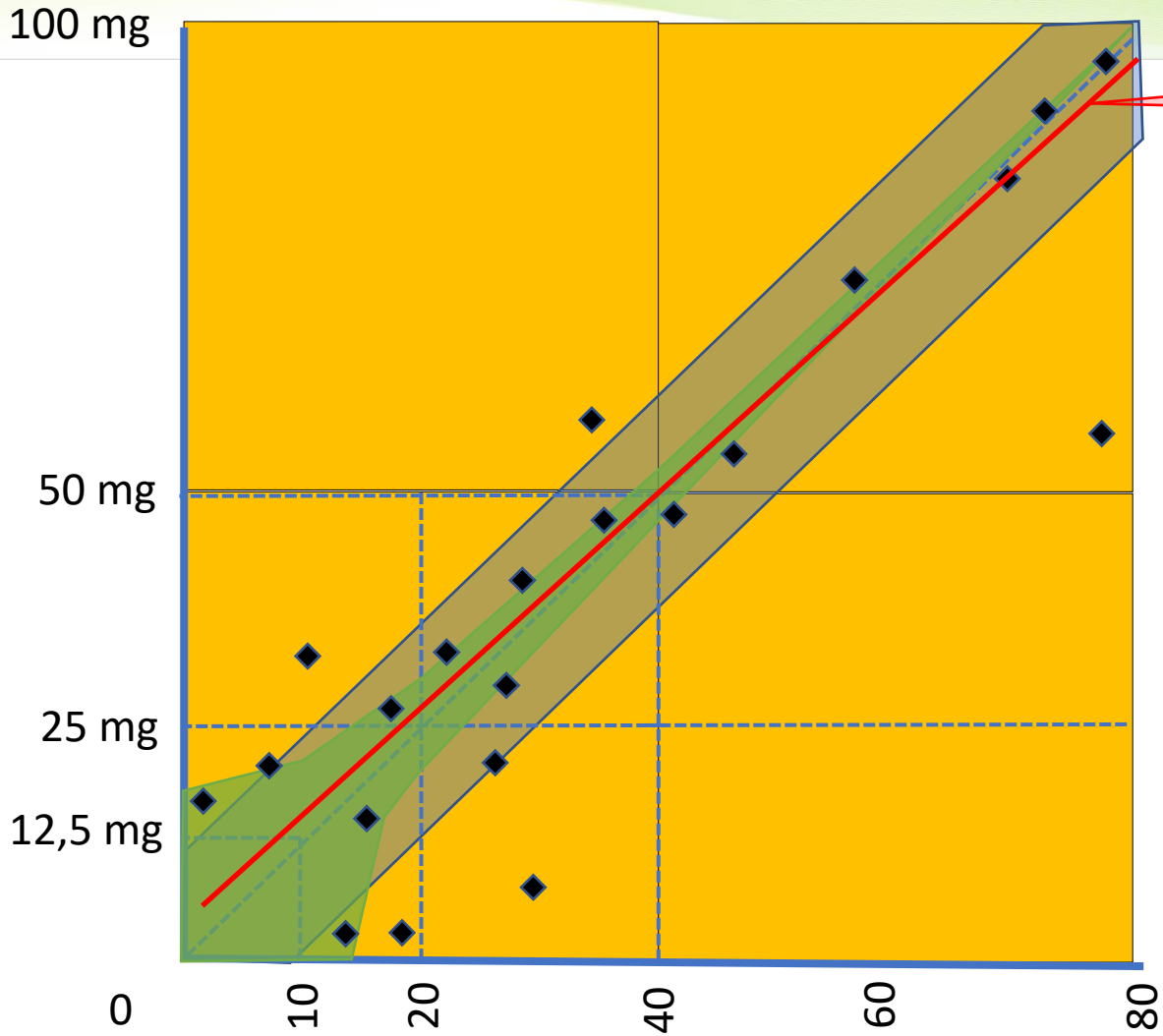
ACCURACY & PRECISION

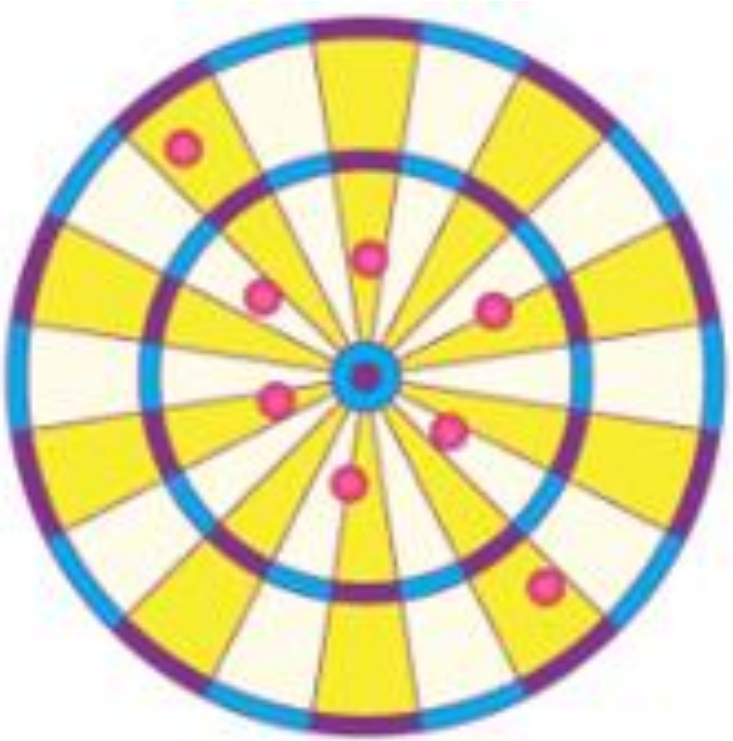


THEORETICAL / IDEAL CALIBRATION CURVE FOR INSTRUMENT

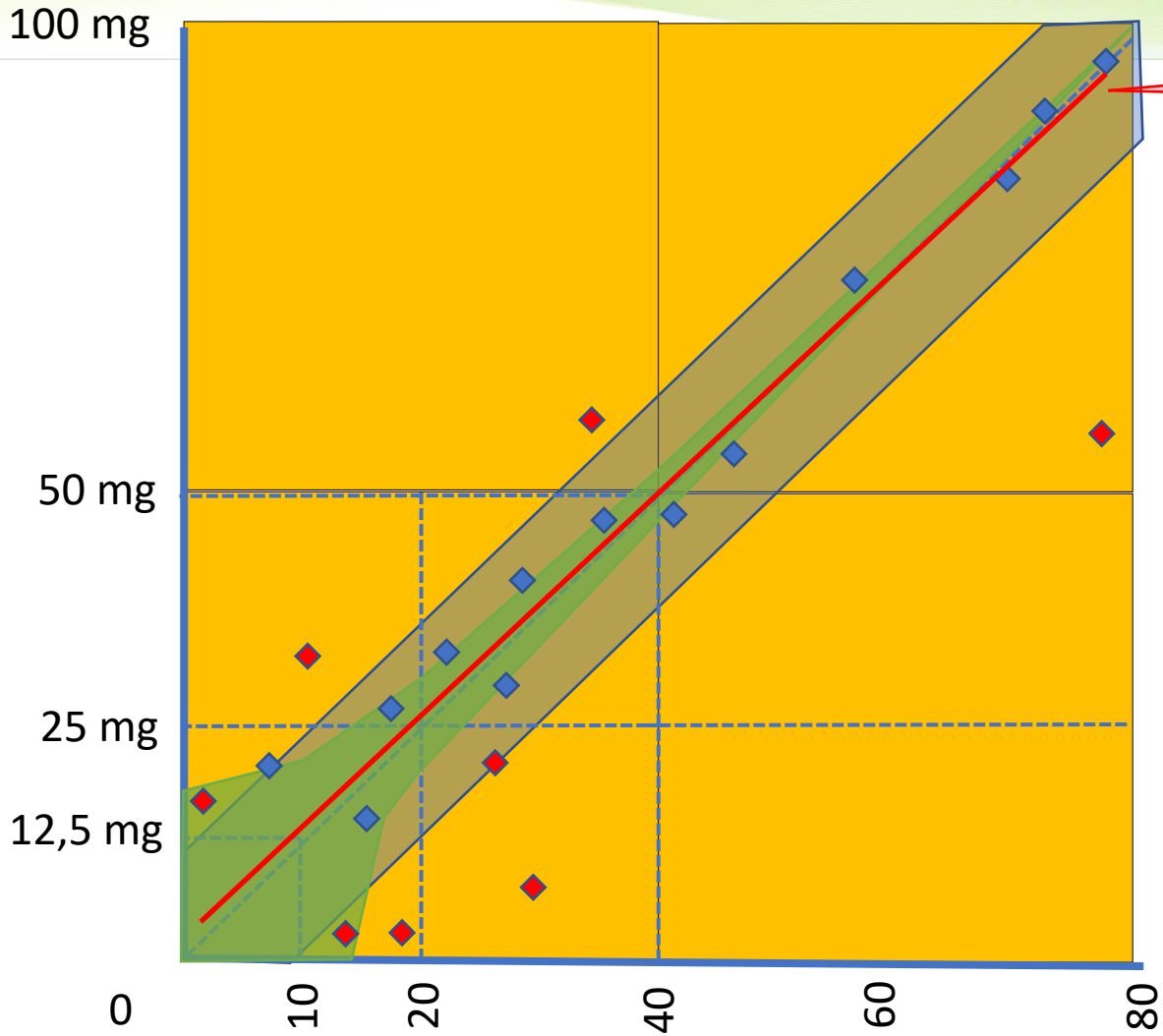


DEVELOPMENT OF A CALIBRATIONS CURVE





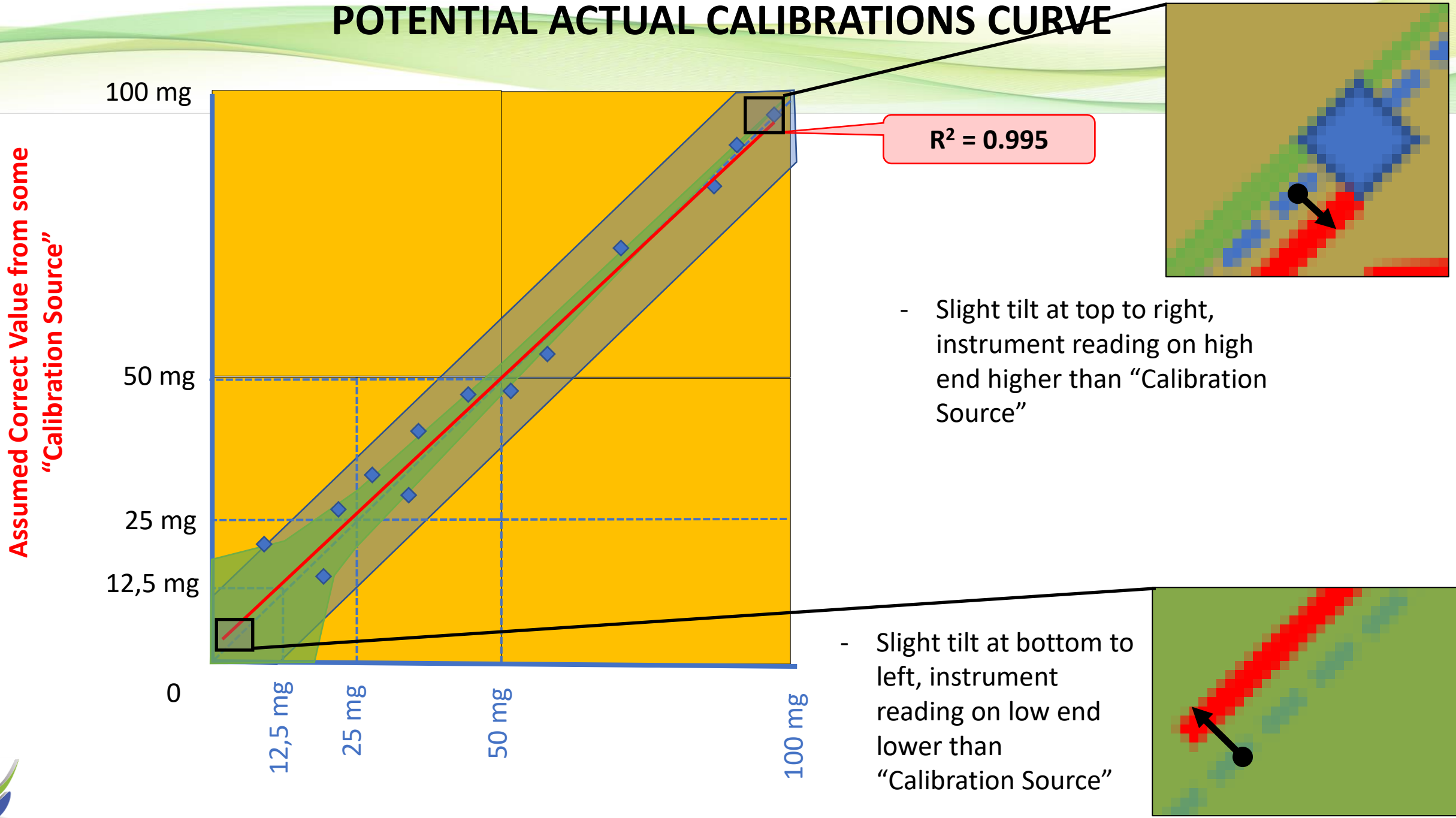
DEVELOPMENT OF CALIBRATIONS CURVE



$R^2 = 0.995$

- R2 not equal to 1

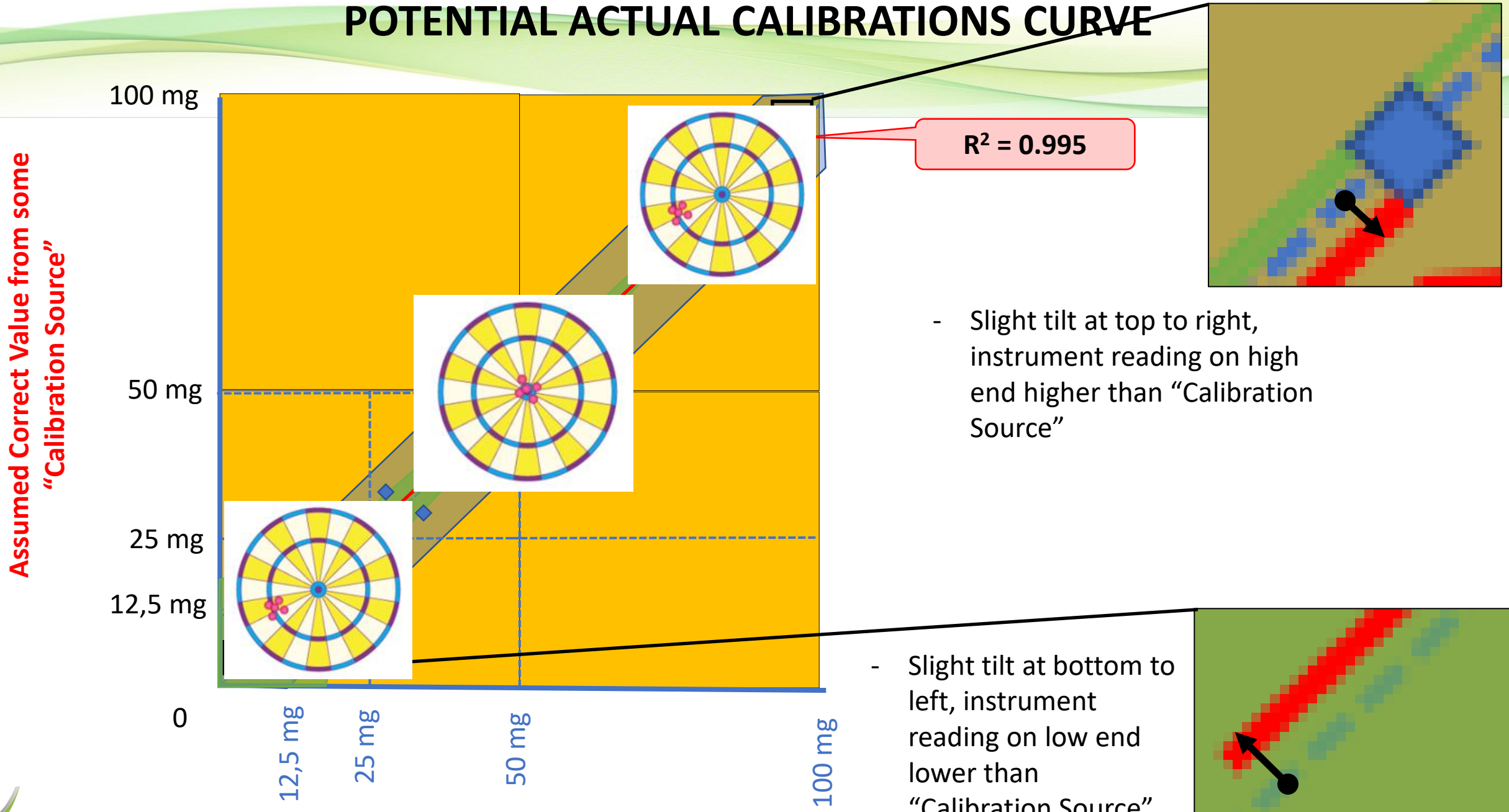
POTENTIAL ACTUAL CALIBRATIONS CURVE



- Slight tilt at top to right, instrument reading on high end higher than "Calibration Source"

- Slight tilt at bottom to left, instrument reading on low end lower than "Calibration Source"

POTENTIAL ACTUAL CALIBRATIONS CURVE



- Slight tilt at top to right, instrument reading on high end higher than "Calibration Source"

- Slight tilt at bottom to left, instrument reading on low end lower than "Calibration Source"

PNOC – ACTUAL EXAMPLE

Filter No:	Sample Mass (mg)	Pollutant Analysis Mass (mg)					PNOC (mg)
		Cr	Cu	Fe	Ni	Total Pollutant	
T134	0.007	0.0005	0.0005	0.0188	0.0005	0.0203	0.007 – 0.0203 = - 0.0133 mg
T144	0.007	0.0005	0.0005	0.0098	0.0005	0.0113	0.007 – 0.0113 = - 0.0043 mg
T162	0.003	0.0011	0.0005	0.0081	0.0056	0.0142	0.003 – 0.0142 = - 0.0112 mg
BDL	?	0.0005	0.0005	0.0006	0.0005	?	?
	None SANAS Results	SANAS Results				None SANAS Results	None SANAS Results

KDOHC

PNOC – ACTUAL EXAMPLE

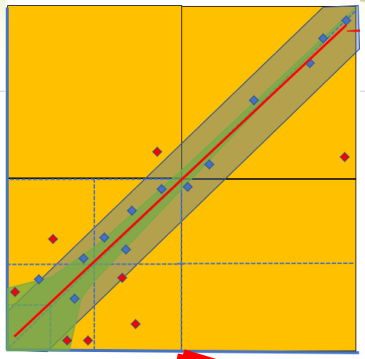
Filter No:	Sample Mass (mg)	Pollutant Analysis Mass (mg)					PNOC (mg)
		Cr	Cu	Fe	Ni	Total Pollutant	
T134	0.007	0.0005	0.0005	0.0188	0.0005	0.0203	0.007 – 0.0203 = - 0.0133 mg
T144	0.007	0.0005	0.0005	0.0098	0.0005	0.0113	0.007 – 0.0113 = - 0.0043 mg
T162	0.003	0.0011	0.0005	0.0081	0.0056	0.0142	0.003 – 0.0142 = - 0.0112 mg

If "BDL" = 0

Filter No:	Sample Mass (mg)	Pollutant Analysis Mass (mg)					PNOC (mg)
		Cr	Cu	Fe	Ni	Total Pollutant	
T134	0.007	**0**	**0**	0.0188	**0**	0.0188	0.007 – 0.0188 = **- 0.0118** mg
T144	0.007	**0**	**0**	0.0098	**0**	0.0098	0.007 – 0.0098 = **- 0.0028** mg
T162	0.003	0.0011	**0**	0.0081	0.0056	0.0148	0.003 – 0.0148 = **- 0.0118** mg

KDOHC

PNOC – ACTUAL EXAMPLE



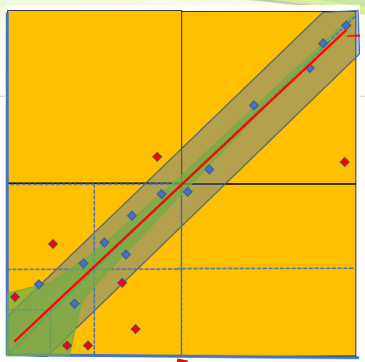
BUT,
Negative PNOC results always possible, especially with very low results.

If "BDL" = 0

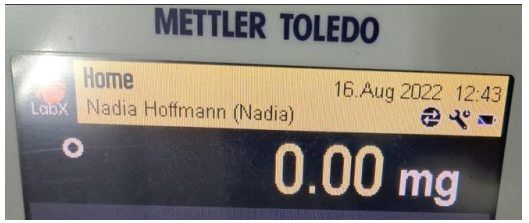
Filter No:	Sample Mass (mg)	Pollutant Analysis Mass (mg)					PNOC (mg)
		Cr	Cu	Fe	Ni	Total Pollutant	
T134	0.007	**0**	**0**	0.0188	**0**	0.0188	0.007 – 0.0188 = **- 0.0118** mg
T144	0.007	**0**	**0**	0.0098	**0**	0.0098	0.007 – 0.0098 = **- 0.0028** mg
T162	0.003	0.0011	**0**	0.0081	0.0056	0.0148	0.003 – 0.0148 = **- 0.0118** mg

KDOHC

5 DECIMAL BALANCE – LIMITATION



= 0,00001g
= 0,01mg
= The smallest weight that could potentially be weighed by the balance.
i.e. any weigh smaller than 0,01 mg results purely from calculations



	None SANAS Results
BDL	3

Filter No:	Sample Mass (mg)
T134	0.007
T144	0.007
T162	0.003

The following for the balance must still be determined:

- Accuracy (proficiency testing / inter laboratory tests
- Uncertainty of measurement
- Linearity for working range
- LoD

e.g. Silver filter 25mm = 0.088mg
MCE 25mm = 0.104mg
MCE 37mm = 0.055mg

KDOHC

CONCLUSION & RECOMMENDATIONS

Conclusion:

Negative PNOC results always possible,
especially with very low results.

Recommendation, if calculated PNOC value is negative:

a) Report calculated Negative PNOC as 0 (Zero) as there is no current BDL value for PNOC. PNOC is always a calculated value and does not result from any chemical analytical process.

OR

b) Reject and repeat the sample

OR

c) Ask Legislator to advise

Thank you for your time

Questions / Comments ?