

## Vorschau

### Assignment 05

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#### 1. Calibration and LOD (10 Punkte)

Given the following table with detector responses for three samples of a known concentration, create a calibration curve (with linear regression by hand or with a software) and report the following quantities:

Predicted response for a blank sample:

( $R^2$ ) value:

LOD (with 3.3 SD definition):

Given that you take the uncalibrated detector response as a predictor of the real concentration, how big is the systematic error:

Concentration

Measured Intensity

#### 2. Connect the terms(DDA/DIA) (10 Punkte)

SWATH

iTRAQ

SILAC

[Positionen der Definitionen zurücksetzen](#)

- DDA
- DDA
- DIA

### 3. Connect the terms(quantification data) (10 Punkte)

SILAC

iTRAQ

[Positionen der Definitionen zurücksetzen](#)

- MS2 Quantification
- MS1 Quantification

### 4. Connect the terms(quantification strategies) (15 Punkte)

iTRAQ

MRM

SILAC

[Positionen der Definitionen zurücksetzen](#)

- label free
- Chemical labeling
- Metabolic labeling

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## 5. iTRAQ (20 Punkte)

For iTRAQ 8-plex, the reporter group exhibits the same structure as the iTRAQ 4-plex reagent ( $C_6N_2H_{13}$ ). When the nominal mass of the reporter group is 121 dalton, the number of  $(^{13}C)$  in reporter group is . If the isobaric tag has total mass of 315, the nominal mass of the corresponding balance group is .

## 6. Manual quantification (15 Punkte)

You are given a [SILAC pair](#). What is the mass difference (in Da) between the two versions of the peptide?

Manually quantify the peptides. (Note that only one spectrum is present in the file on the website. Therefore, we use the mono-isotopic peak intensity instead of peak areas).

$$c(\text{light}) = \quad * c(\text{heavy})$$

Furthermore, you are given an [MS2 spectrum](#) from an iTRAQ (4 plex) experiment. Manually quantify the four states (using the iTRAQ reporter ions).

$$c(\text{lightest reporter}) = 1$$

$$c(\text{lightest reporter} + 1) =$$

$$c(\text{lightest reporter} + 2) =$$

$$c(\text{lightest reporter} + 3) =$$

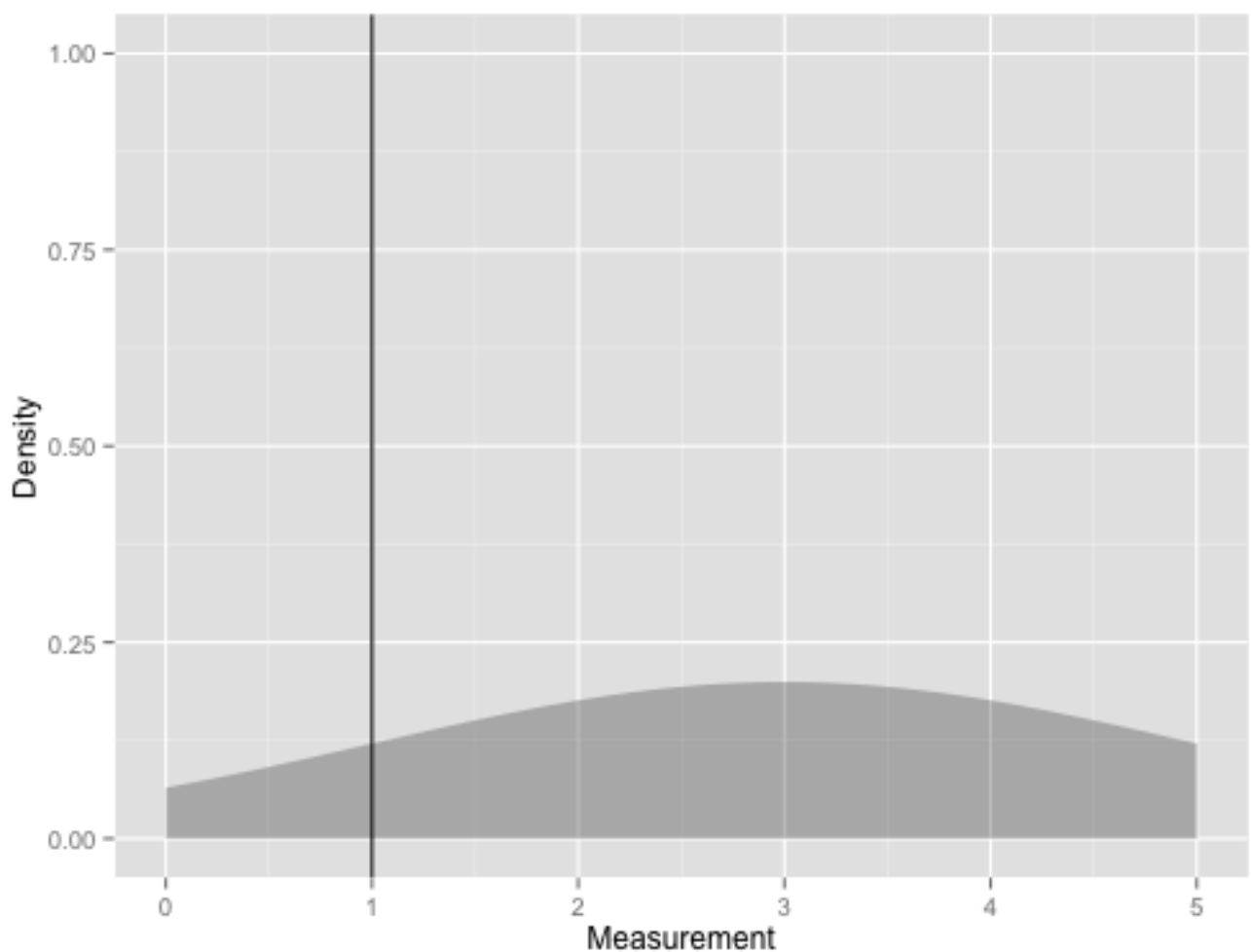
## 7. Mass differences in amino acids (10 Punkte)

You want to analyze a mixture of proteins coming from some usual cells and some cells that

were grown in a medium where all lysines and arginines were replaced by their heavy counterparts (consisting of only  $^{13}\text{C}$ 's and  $^{15}\text{N}$ 's).

In the resulting MS1 scans, what is the difference in Th of the peptide KIRSCHE<sup>(2+)</sup>?

## 8. Precision and Accuracy (10 Punkte)



Given the density of repeated measurements for **one** sample from an analytical method above: Elaborate on its precision and accuracy, given that you know the true value to be measured (1; see vertical line). Would you recommend this method? Why/Why not? How could one improve precision/accuracy?

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