

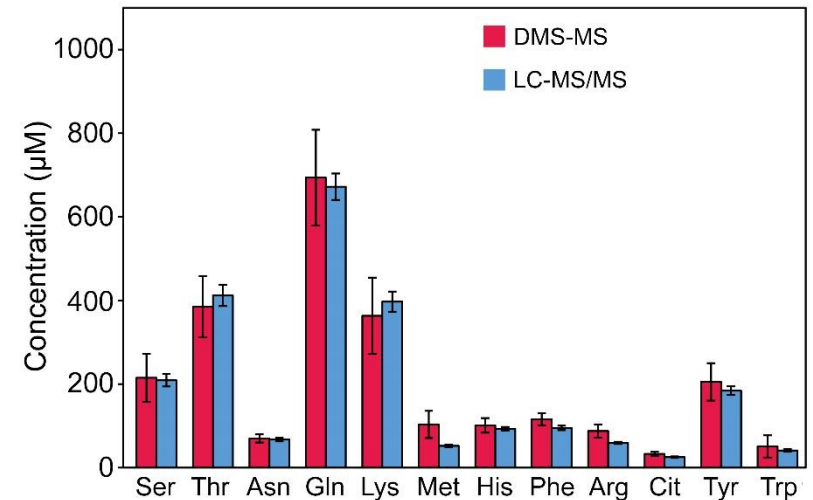
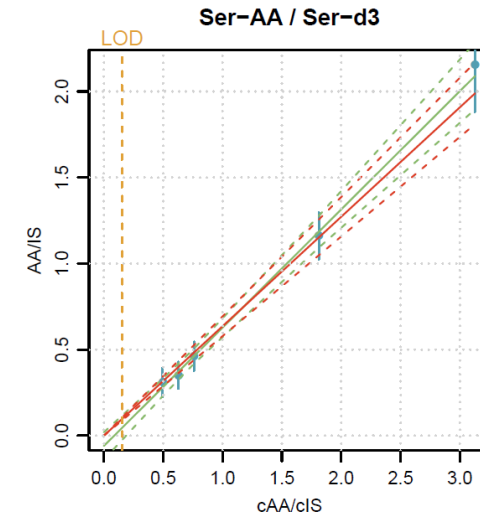
Can we quantify using selected
CV?

Simulation: Fast versus 2D fit

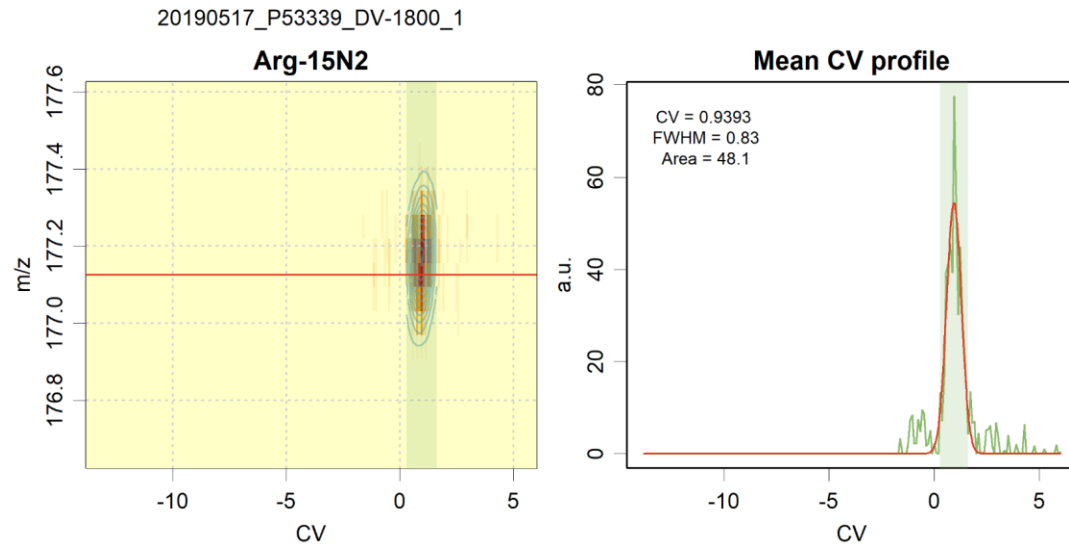
Report on a serie of experiments performed on July 10, 2019

Experiments performed on July 10, 2019

- A series of spiked plasmas (C0, C1000, C500, C100, C50, C10)
 - => Calibration curve
- 6 repeats of a plasma (P53344) quantification

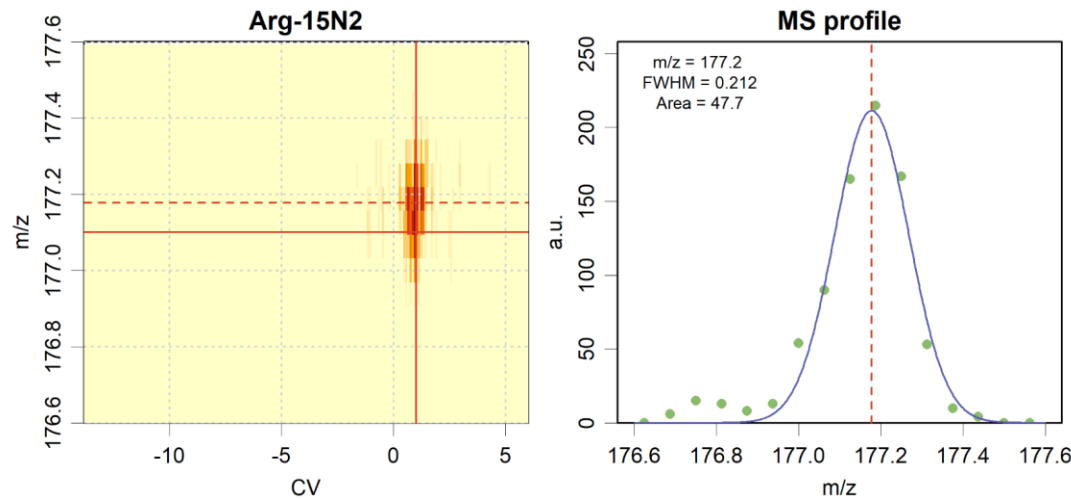


2D fit of the (m/z, CV) peaks



- By default, a 2D fit is performed as illustrated on the left.
- The maximum intensity is search around (dmz, dCV) starting guess values (m/z, Cvref) for each metabolite
- In practice, the fit is performed with a product of two gaussian functions (1 for m/z, 1 for CV)

Fast fit: CV fixed, fit in the m/z dimension



- For each metabolite, the CV is fixed to a value, here corresponding to the average one over a large number of exp.
- A 1D fit is thus performed only in the m/z dimension
- Gaussian fit with 1 gaussian function

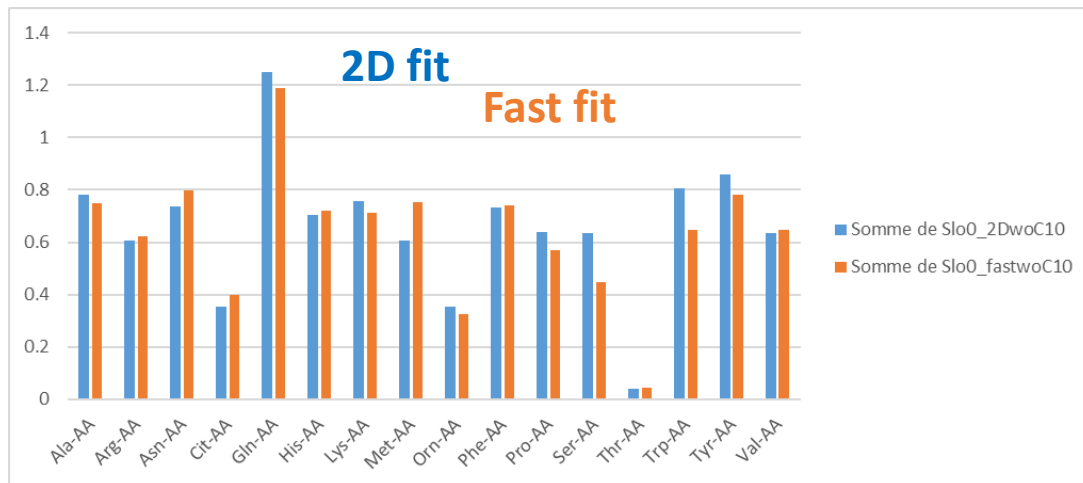
Calibration and derivation of LOD: LOD vs fast

Name	Int	Slo	Slo0	LOD
Ala-AA	-0.65	1.41	0.78	0.14
Ser-AA	-0.06	0.69	0.64	0.15
Pro-AA	-0.08	0.74	0.64	0.15
Val-AA	-0.07	0.71	0.64	0.06
Thr-AA	0.01	0.03	0.04	0.38
Asn-AA	0.16	0.66	0.74	0.57
Gln-AA	0.15	1.04	1.25	0.12
Lys-AA	0.05	0.70	0.76	0.25
Met-AA	0.11	0.52	0.61	0.23
His-AA	0.06	0.64	0.71	0.03
Phe-AA	0.02	0.72	0.73	0.21
Arg-AA	0.06	0.56	0.61	0.21
Cit-AA	0.45	0.30	0.35	9.95
Tyr-AA	-0.04	0.90	0.86	0.63
Trp-AA	-0.03	0.91	0.81	0.05
Orn-AA	0.00	0.35	0.35	0.47

Name	Int	Slo	Slo0	LOD
Ala-AA	-0.27	0.98	0.75	0.33
Ser-AA	0.11	0.35	0.45	0.13
Pro-AA	-0.23	0.89	0.57	0.16
Val-AA	0.06	0.59	0.65	0.46
Thr-AA	0.02	0.03	0.04	1.26
Asn-AA	0.01	0.79	0.80	1.25
Gln-AA	0.08	1.07	1.19	0.23
Lys-AA	0.05	0.67	0.71	0.47
Met-AA	0.09	0.64	0.75	1.18
His-AA	0.01	0.71	0.72	0.28
Phe-AA	-0.12	0.84	0.74	0.18
Arg-AA	0.04	0.59	0.62	0.59
Cit-AA	0.53	0.33	0.40	11.90
Tyr-AA	0.05	0.75	0.78	0.98
Trp-AA	-0.02	0.75	0.65	0.50
Orn-AA	-0.05	0.38	0.33	1.06

The slopes (2D and fast) are very similar

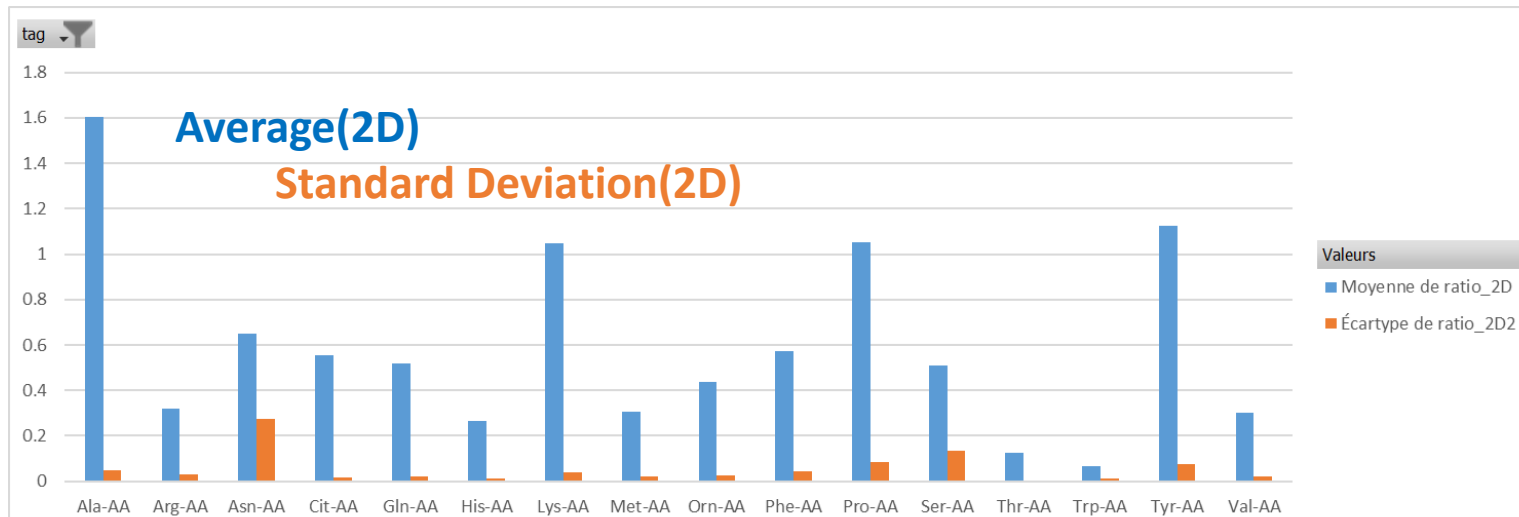
$$\text{Slope0} = (\text{Area}(\text{AA}) / \text{Area}(\text{IS})) / ([\text{AA}] / [\text{IS}])$$



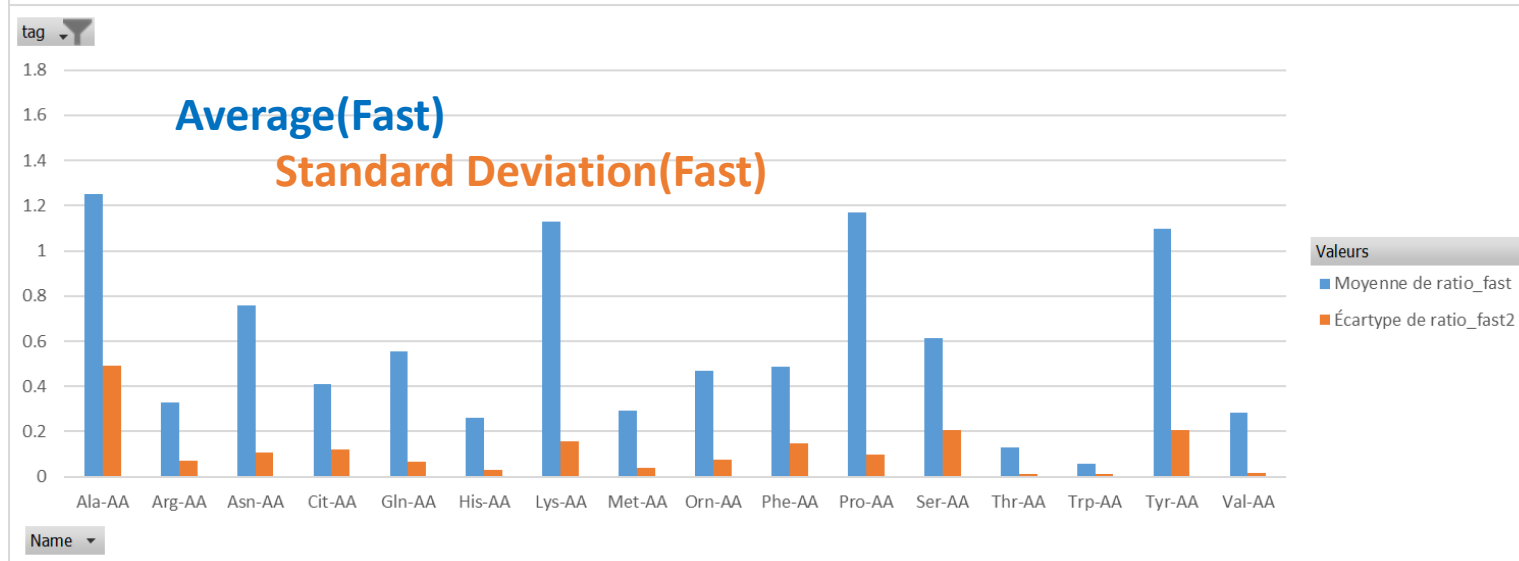
- Slopes (called slo0, intercept=0) are very similar if calculated with the 2D and fast options
- => This means that we can discuss the comparison of RATIOS of the areas in the following

Area ratios: Average and standard deviations

2D /
6 experiments

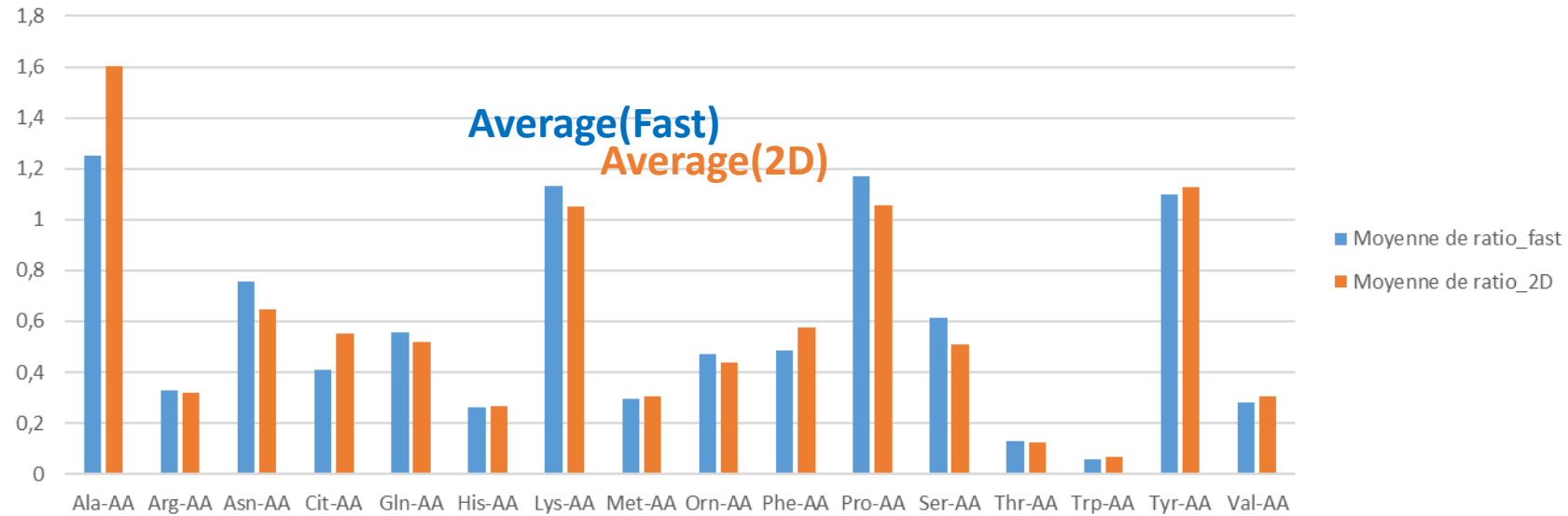


Fast/
6 experiments

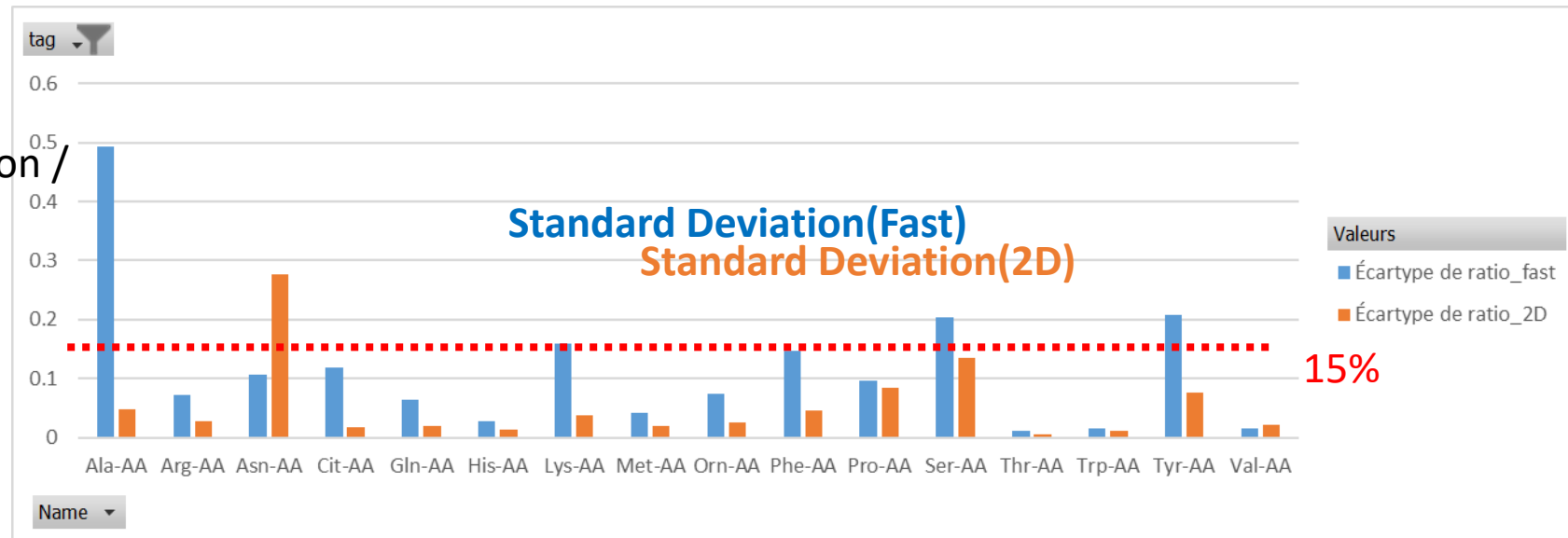


Area ratios: Average and standard deviations

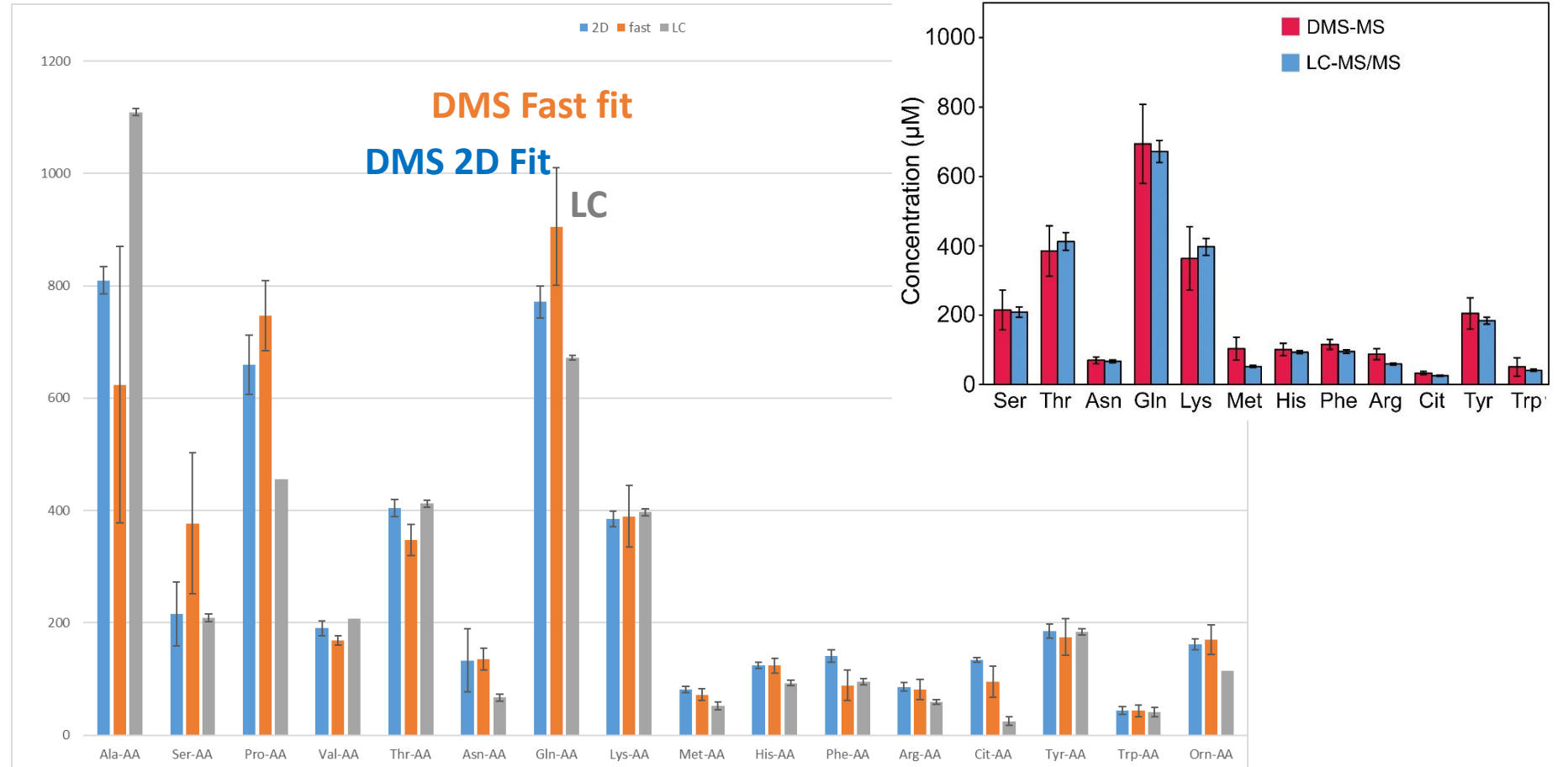
Average /
6 experiments



Standard deviation /
6 experiments

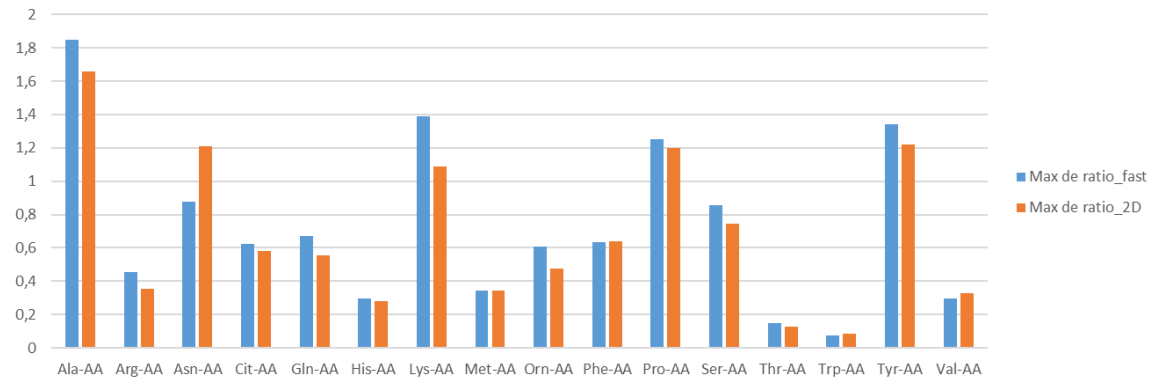


Quantification / Plasma P53344

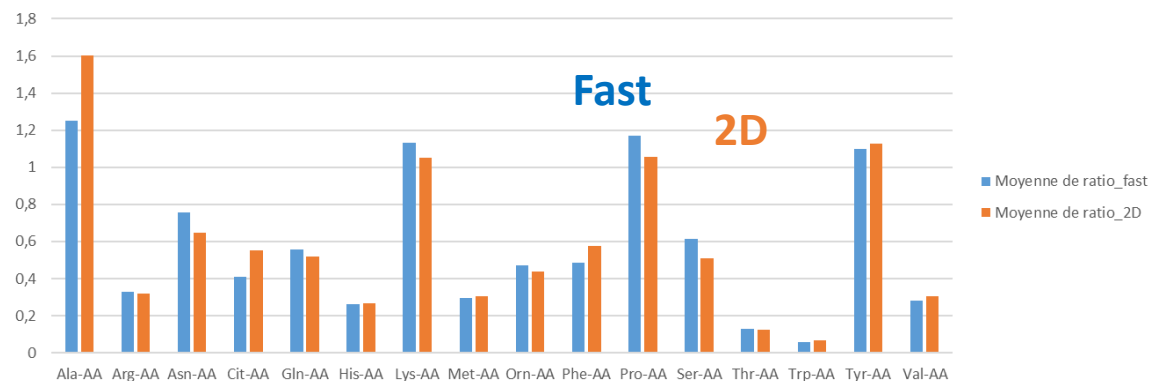


Area ratio: 2D versus fast

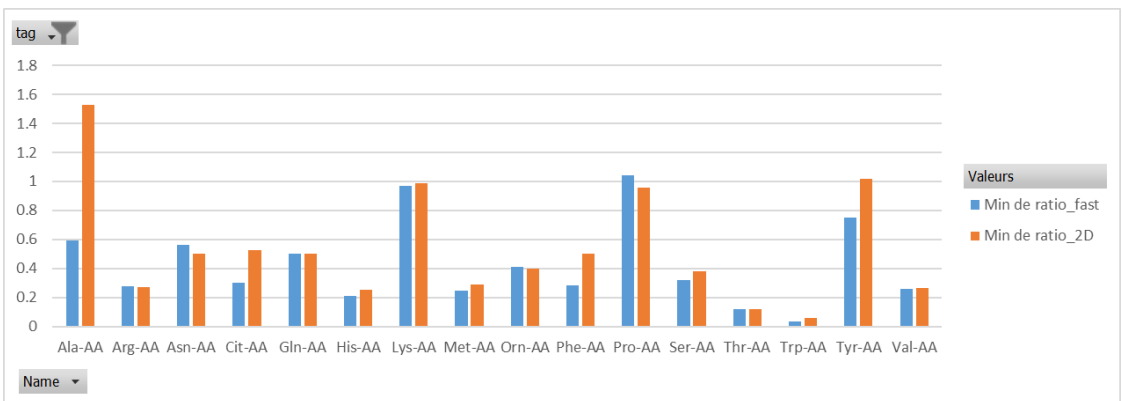
Max /
6 experiments



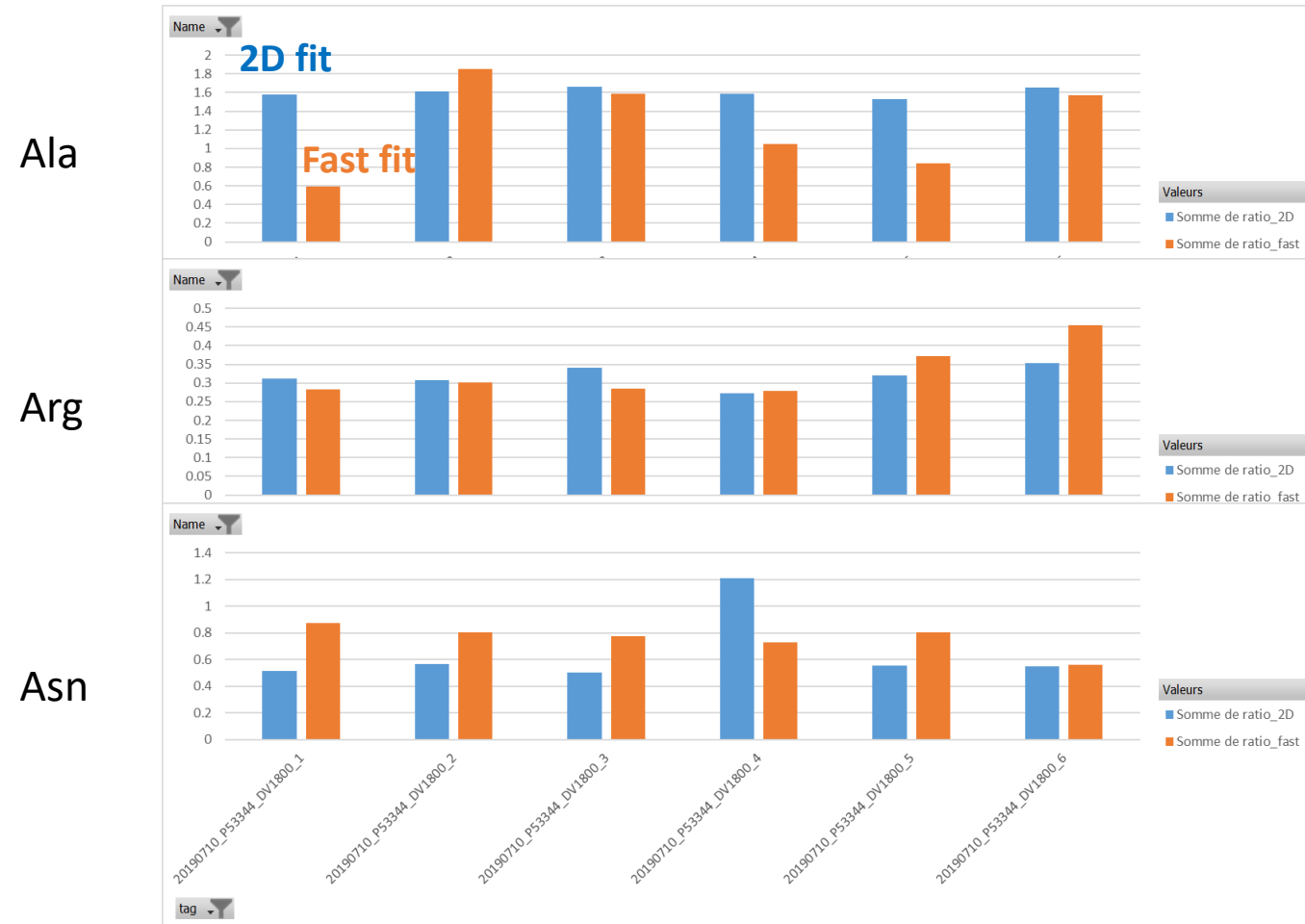
Average /
6 experiments



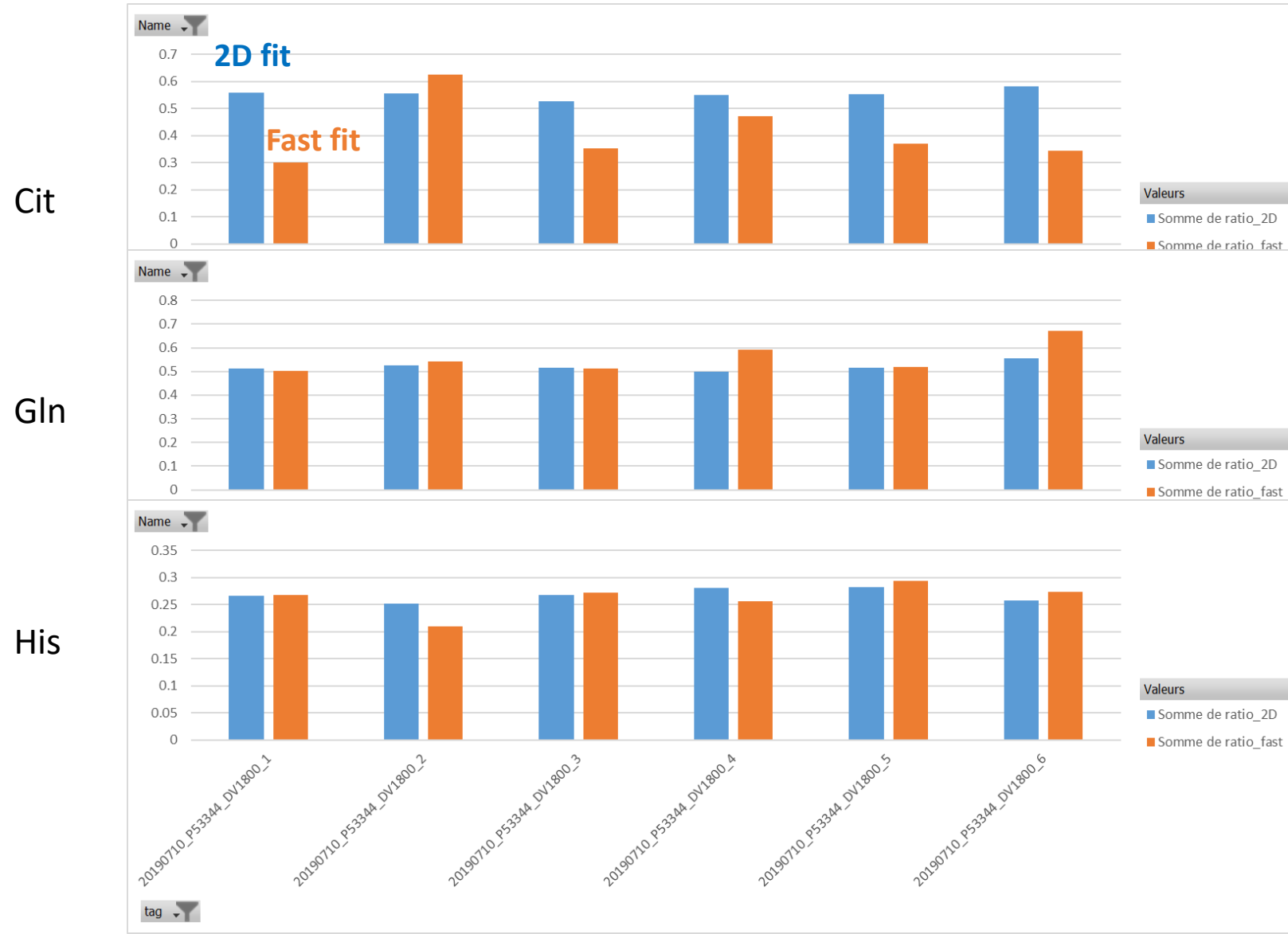
Min /
6 experiments



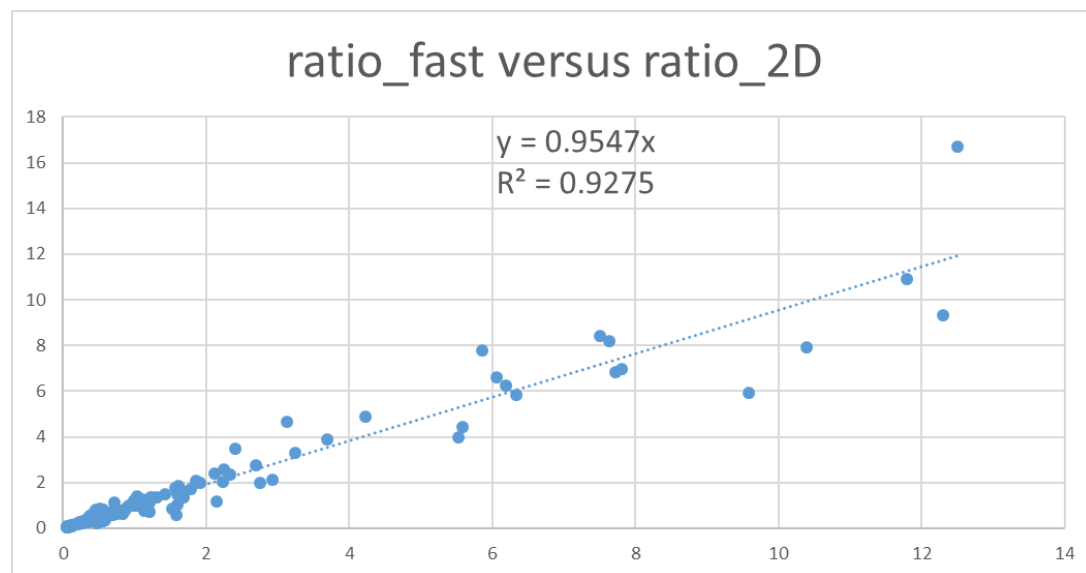
For each AA, as a function of the exp



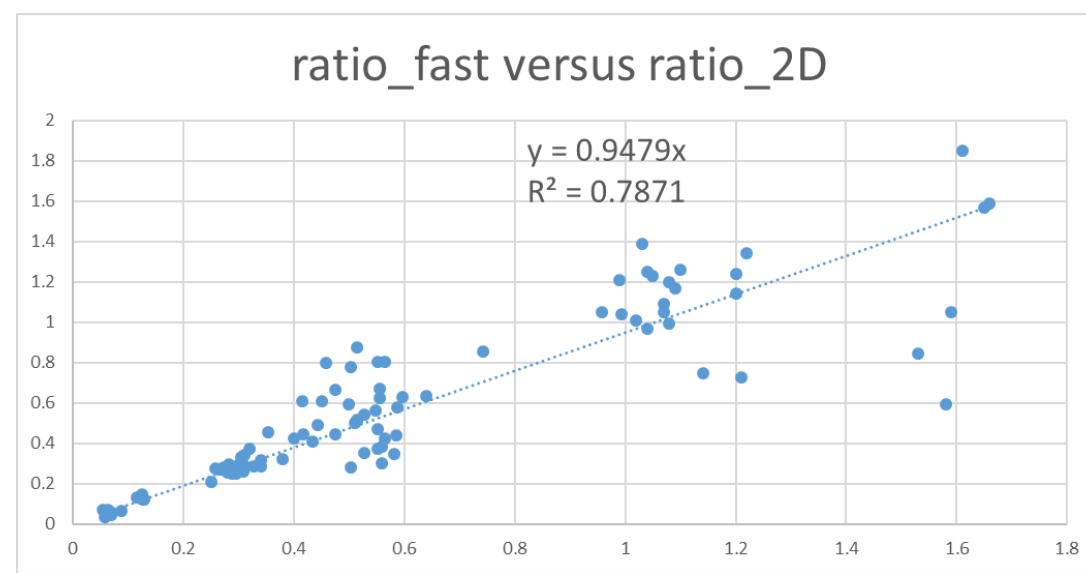
For each AA, as a function of the exp



Ratio(Area(AA)/Area(IS)): Fast versus 2D



All data (6 calibration pts + 6 plasma repeats)



Only 6 plasma repeats

Can we quantify using selected
CV?

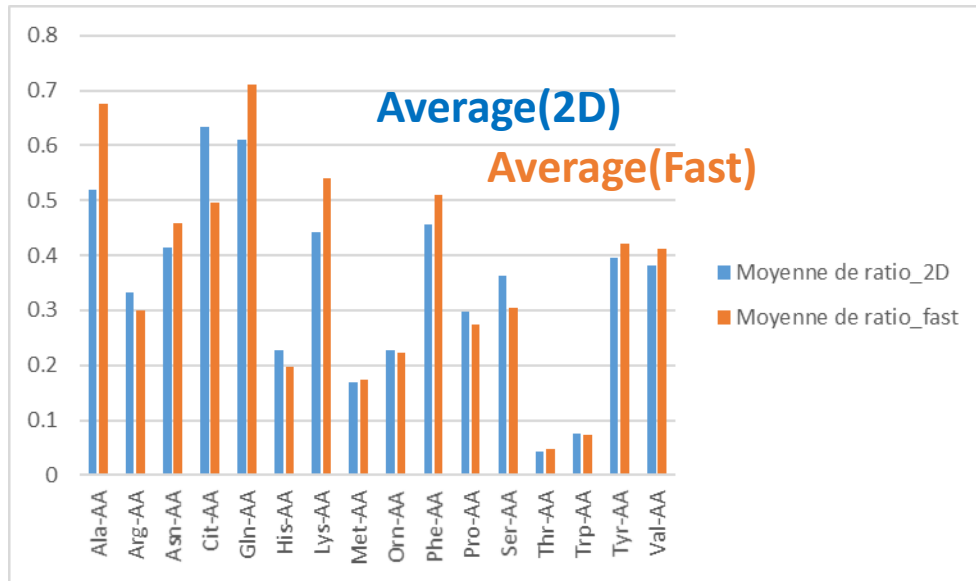
Simulation: Fast versus 2D fit

Exp from May through July 2019

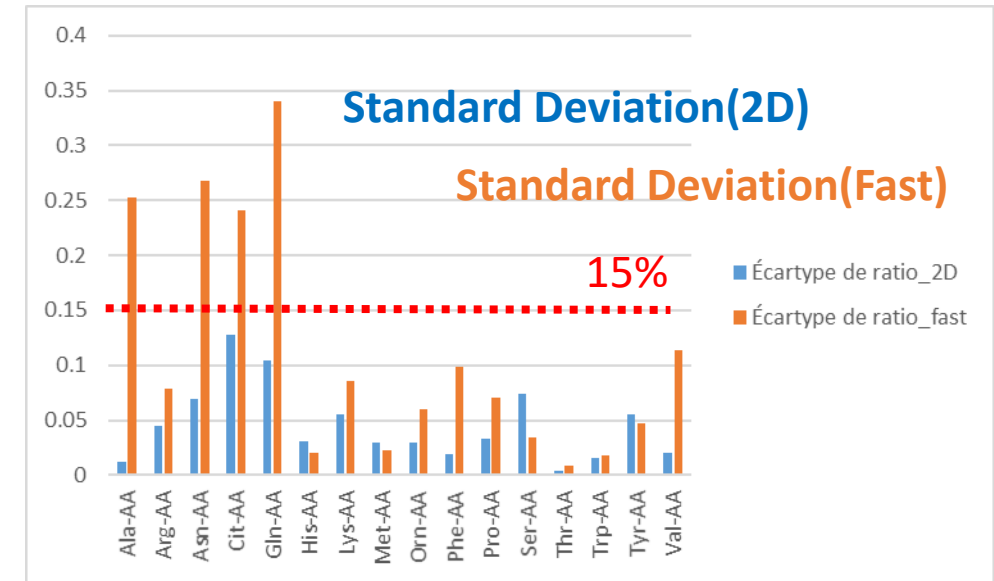
Interday experiments on the pool of plasmas

Pool of plasma (C0 experiments)

Average /
5 experiments



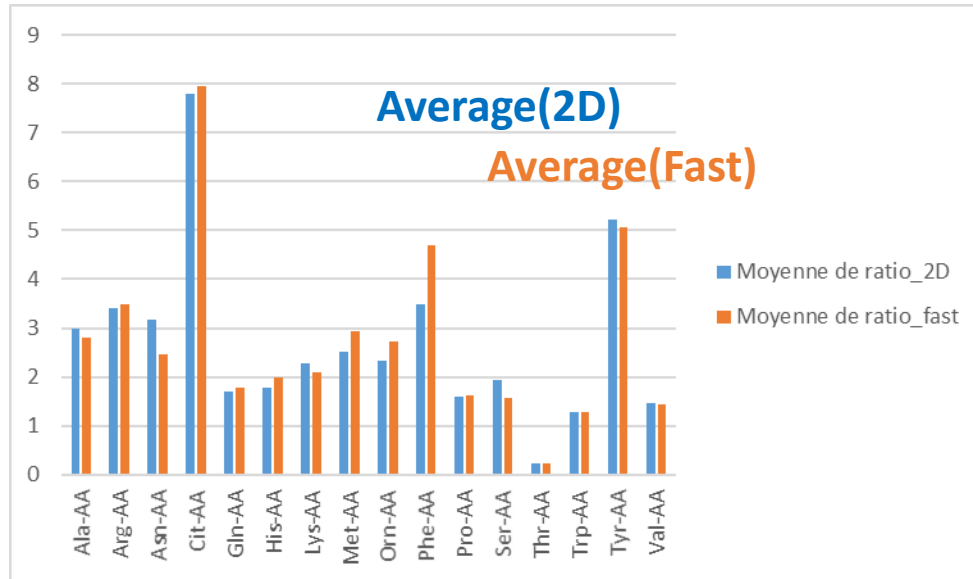
Standard deviation /
5 experiments



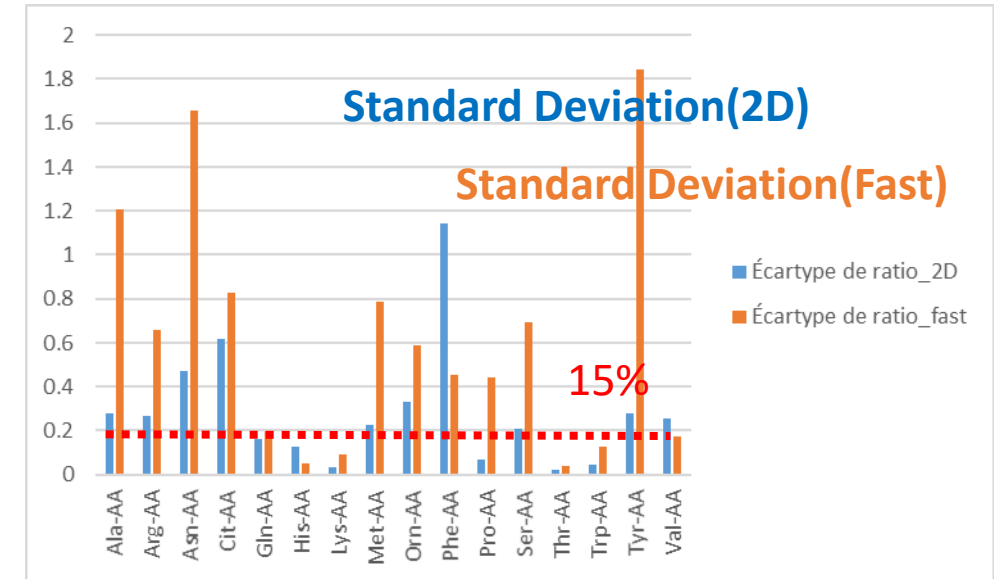
Interday experiments on the pool of plasmas

Pool of plasma (C50 experiments)

Average /
5 experiments



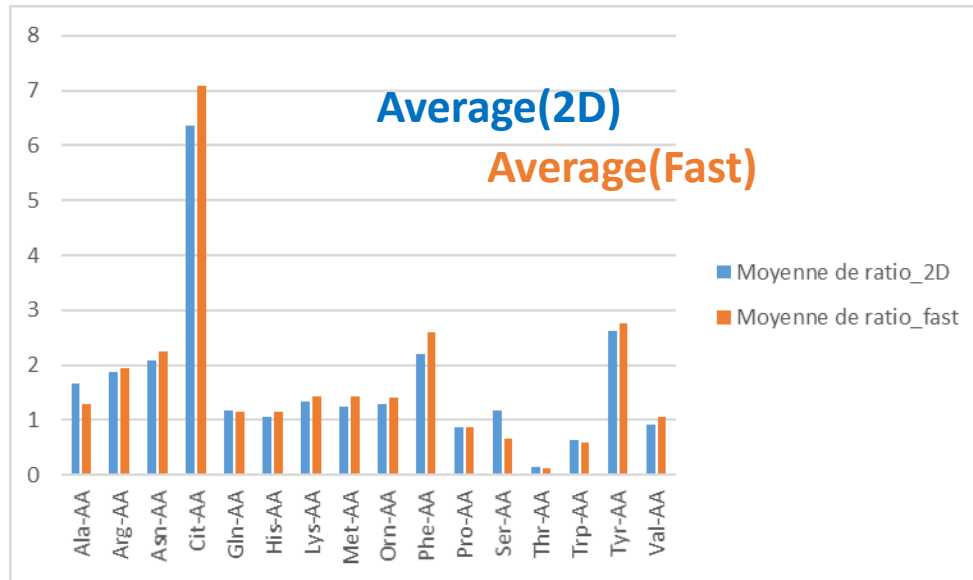
Standard deviation /
5 experiments



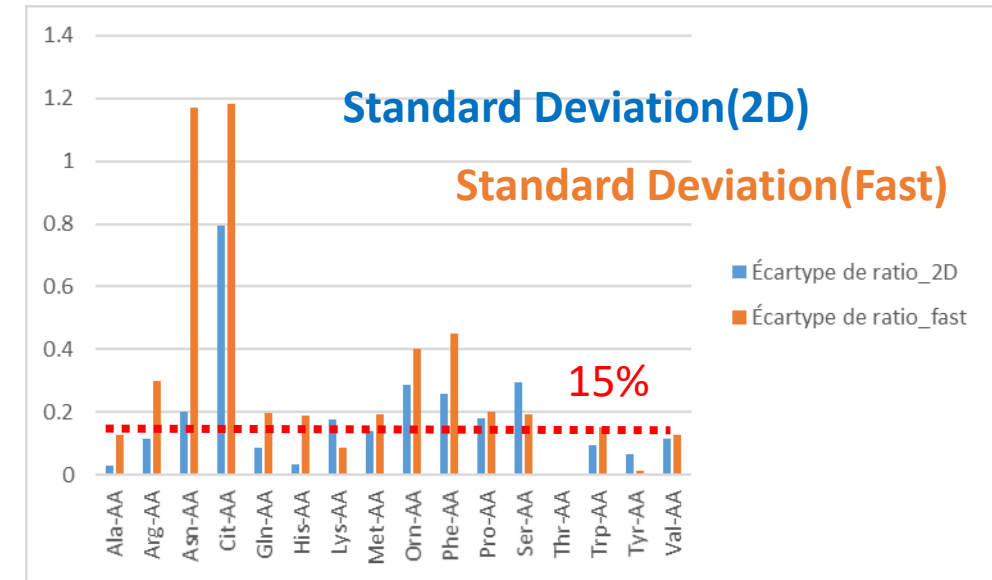
Interday experiments on the pool of plasmas

Pool of plasma (C100 experiments)

Average /
5 experiments



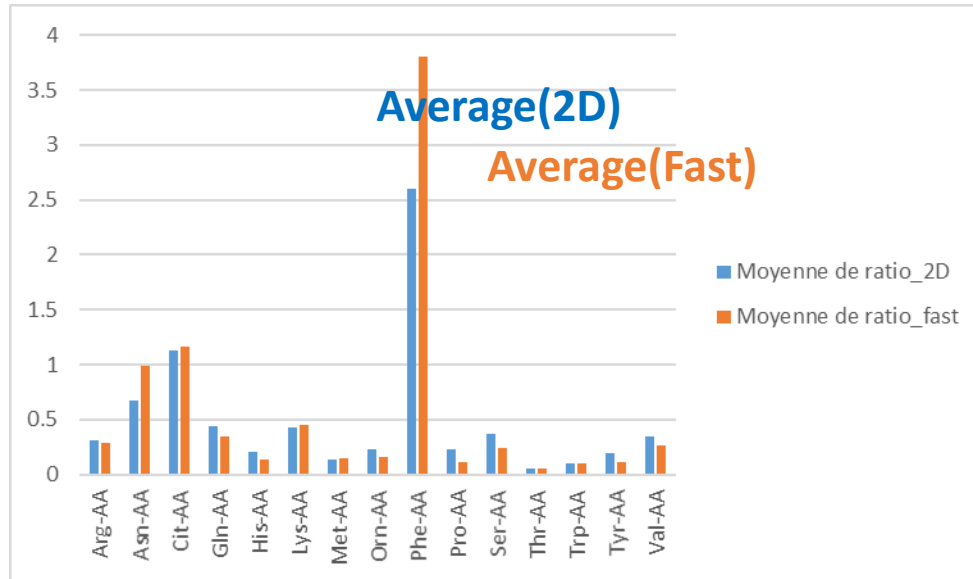
Standard deviation /
5 experiments



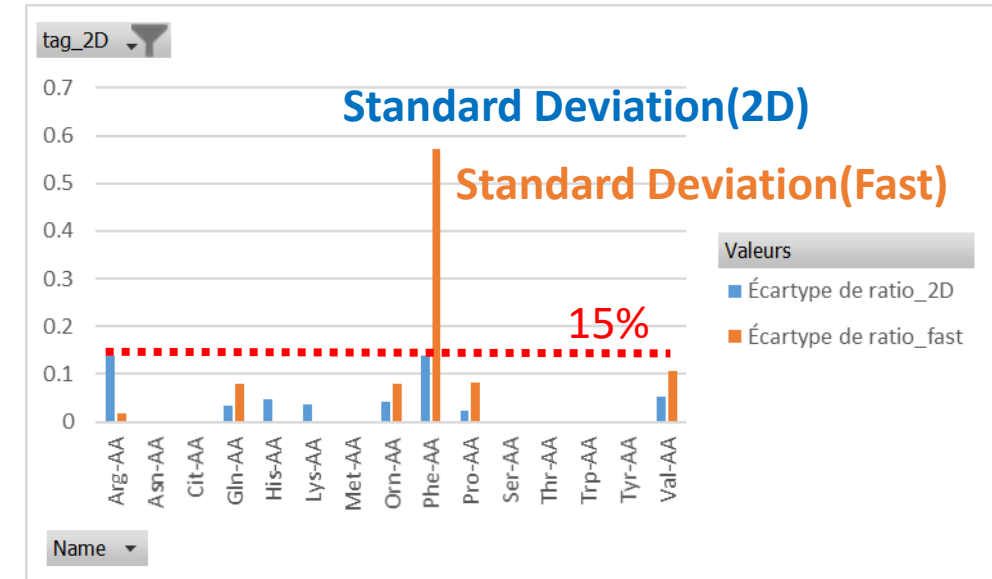
Interday experiments on the pool of plasmas

P53339 (Phenylkeuniria)

Average /
5 experiments



Standard deviation /
5 experiments



DOE (plan d'expérience)

Samples / Targets

- Only one set of samples
 - Blank
 - Three levels (L, M, H)
 - 3 plasmas
- Set of 10 different AA (CV)
- Control
 - 10 AA in H₂O/MeOH

Every day

- Cleaning
 - Standardized procedure
- Control (concentration)
- Calibration (L, M, H)
 - CV
 - LOD, LOQ, slopes
- $3 \times 3 \times 10 = 90$ (Single CV) experiments