B.I.QUANT-PS 2.0™ Bruker IVDr Quantification in Plasma/Serum (for research use only)

The Bruker IVDr platform is optimized towards supporting the analysis of epidemiological studies with large scale, dedicated clinical and translational trials, and high throughput Biobank quality control. Based on nuclear magnetic resonance (NMR) spectroscopy, the standardized Bruker IVDr Methods module (B.I.Methods) guarantees high reproducibility and transferability under full automation at anytime and anywhere what is not achievable by any other analytical tool.

This standardized platform allows to combine different solutions. For plasma/serum, it means Bruker IVDr Lipoprotein Subclass Analysis (B.I.LISA™) and automated quantification of small molecule metabolites (B.I.QUANT-PS™) using the same experiment. Now we upgrade the quantification from 26 metabolites up to 41 metabolites in B.I.QUANT-PS 2.0.

Benefits of B.I.QUANT-PS 2.0

- Ease of use, simple and rapid sample preparation
- Fully automated quantification of 41 metabolites
- Different analytes classes can be quantified simultaneously in a single run
- Absolute concentration for each metabolite is given due to the calibration with one Quantification Reference sample (B.I.Methods™)
- Validation of all LODs has been done following ISO 17025 guidelines for wet spiking
- Raw concentration and additional
- quantification result assessment information (correlation and residue) for each metabolite is given even below LOD
- Interactive PDF report allowing visual fit ambiguity assessement
- Rapid analysis: daily 120 samples can be prepared, measured and analyzed
- Retrospective analysis possible if the sample was prepared and measured using B.I.Methods module
- Works on plasma or serum sample

Requirements for B.I.QUANT-PS 2.0

- Bruker IVDr platform or compatible AVANCE™ III HD or AVANCE NEO 600 MHz systems
- Use of B.I.Methods module and SOPs for plasma/serum for sample preparation and measurement
- Regular quality control of the absolute temperature, solvent suppression and quantification reference sample (preferably daily using automated quality control tool including in B.I.Methods)
- Access to Bruker Data Analysis server for fully automated remote analysis (transfer of spectra after measurement to Bruker server via private ftp, back-transfer of result PDF report and XML file)

Deliverables B.I.QUANT-PS 2.0

- Includes 41 metabolites (free metabolites, no protein denaturing done) with concentration ranges, occurring in most human plasma/serum samples
- Includes matrix identity test, differentiation between EDTA plasma and heparin plasma or serum
- In the analysis report, the metabolites are grouped according to their chemical class
  - Alcohols and derivatives
  - Amines and derivatives
  - Amino acids and derivatives
  - Carboxylic acids
  - Essential nutrient
  - Keto acids and derivatives
  - Sugars and derivatives
  - Sulfones
  - Technical additives

The methods and solutions described here are for research use only and not for use in clinical diagnostic procedures.

In table 1 an extract of the report automatically generated by B.I.QUANT-PS 2.0 is shown. Metabolites are sorted into chemical classes. Absolute quantification values are given, LODs are listed as well as a 95% concentration range derived from the validation spectra set. The actual sample is shown as a black bar in the concentration range, if the corresponding metabolite is detected.

Figure 1

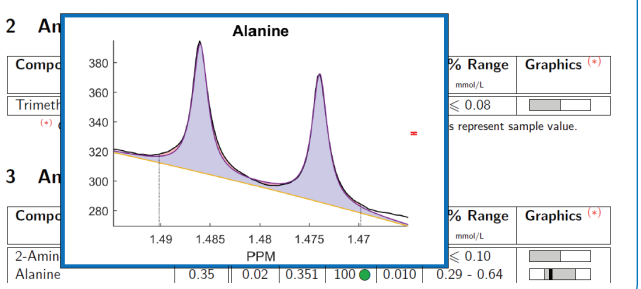

Figure 1 shows the interactive graphics of Alanine on a B.I.QUANT-PS 2.0 PDF report. It is an ideal situation, where the fit corresponds fully to the metabolite signal well above LOD, the raw concentration (r) is close to the result concentration and the correlation (ρ) is > 95% and the residue (Δ) is close to zero mmol/L.

Figure 2

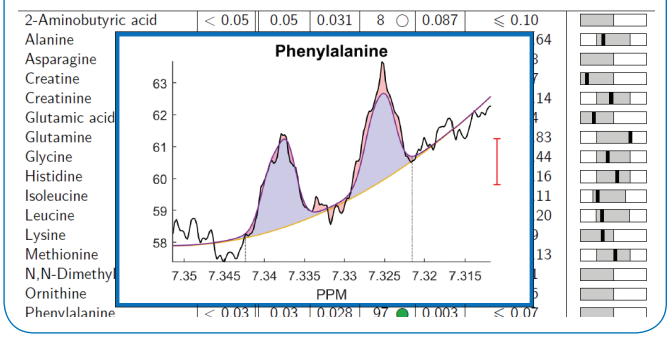

Figure 2 shows the interactive graphics of phenylalanine, where the raw concentration is below LOD. Using the graphical figure displayed, the fit signal can be clearly discriminated from the rest of the spectrum and the correlation is > 95%. The raw concentration can be used as approximative concentration estimate.

The results are provided twice, in PDF format as well as in XML format, which allows easier transfer into other programs for statistical analysis.

Table 1

3 Amino acids and derivatives

Compound	Conc. mmol/L	LOD mmol/L	r mmol/L	ρ %	Δ mmol/L	95% Range mmol/L	Graphics (*)
2-Aminobutyric acid	< 0.05	0.05	0.031	8 ○	0.087	⩽ 0.10	
Alanine	0.35	0.02	0.351	100 ●	0.010	0.29 - 0.64	
Asparagine	< 0.05	0.05	0.000	0 ○	5.082	⩽ 0.08	
Creatine	0.01	0.01	0.014	100 ●	0.002	⩽ 0.07	
Creatinine	0.09	0.01	0.091	100 ●	0.002	0.06 - 0.14	
Glutamic acid	0.10	0.05	0.099	87 ○	0.025	⩽ 0.24	
Glutamine	0.83	0.02	0.832	99 ●	0.023	0.30 - 0.83	
Glycine	0.26	0.01	0.257	100 ●	0.006	0.17 - 0.44	
Histidine	0.13	0.02	0.127	100 ●	0.002	0.07 - 0.16	
Isoleucine	0.04	0.03	0.043	93 ○	0.010	0.03 - 0.11	
Leucine	0.09	0.01	0.090	95 ●	0.013	0.07 - 0.20	
Lysine	0.19	0.04	0.194	66 ○	0.073	⩽ 0.29	
Methionine	0.09	0.05	0.093	97 ●	0.009	0.05 - 0.13	
N,N-Dimethylglycine	< 0.01	0.01	0.001	88 ○	0.000	⩽ 0.01	
Ornithine	< 0.02	0.02	0.000	0 ○	2.497	⩽ 0.16	
Phenylalanine	< 0.03	0.03	0.028	97 ●	0.003	⩽ 0.07	
Proline	0.29	0.05	0.293	24 ○	3.267	⩽ 0.59	
Sarcosine	< 0.01	0.01	0.004	80 ○	0.001	⩽ 0.01	
Threonine	< 0.04	0.04	0.000	0 ○	3.053	⩽ 0.24	
Tyrosine	0.04	0.03	0.038	97 ●	0.003	⩽ 0.08	
Valine	0.23	0.03	0.233	100 ●	0.005	0.15 - 0.35	

(*) Gray horizontal boxes represent 95% concentration range, black vertical lines represent sample value.

Extract of B.I.QUANT-PS 2.0 of a serum

Validation of Plasma/Serum Quantification Method

To test the validity of the results, the following measures were taken and continuously followed:

- Test reproducibility of measurement and analysis
- Test transferability of measurement and analysis (participation of multi-laboratory trial)
- Recovery rate (wet spiking)
- Comparison to conventional methods
- Traceability tests on some metabolites

For detailed metabolite lists and more technical information, please contact manfred.spraul@bruker.com and for sales information your local sales representative.
B.I.QUANT-PS 2.0 module is offered as flat rate for 1 year, 3 years with remote result generation and as pay per use transferring datasets to be analyzed by email or other means.

Disclaimer

The B.I.QUANT-PS 2.0 module is for research use only and is not released for clinical diagnostics.

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