

¹H-NMR Spectroscopy of biological fluids

Requirements for biological samples

Our operating experience contains NMR measurement of metabolite profiles from **human urine**, just as **human and rat EDTA-plasma/serum** samples. So far we have no NMR experience working with saliva and cerebrospinal fluid.

Many studies have demonstrated that bacterial contamination of urine samples significantly alters the metabolite profile. We recommend the screening of urine samples for significant bacteriuria and exclude them from NMR analysis.

Immediately after collection the biological sample should be stored at -80°C and shipped on dry ice (address see below). It should be noted that every freeze-thaw cycle may induce any changes in the metabolic profile of the biological sample!

For one NMR measurement a volume of **500µl urine** and **270µl EDTA-plasma/serum** is required!

NMR Techniques

¹H-NMR spectra of **urine samples** were acquired on a Bruker DRX-400 NMR spectrometer (Bruker BioSpin GmbH, Rheinstetten, Germany) operating at 400.13 MHz ¹H frequency. Samples were measured at 300 K.

¹H-NMR spectra of **EDTA-plasma** and **serum** were obtained at 600.27 MHz on a Bruker AVANCE-II 600 (Bruker BioSpin GmbH, Rheinstetten, Germany). Samples were measured at 309.2 K.

Metabolites

We use the potential of ¹H-NMR spectroscopy as a tool to identify and quantify metabolites in urine and plasma. So far we focus on investigations of following compounds.

Acetate	Alanine	Arginine	Asparagine
Betaine	Carnitine	Choline	Citrate
Creatinine	Creatine	Dimethylamine	Ethanolamine
Formate	Glucose	Glutamine	Glycine
Glycolate	Hippurate	Histidine	Hypoxanthine
Isopropanol	Lactate	Lysine	Methylamine
Mannitol	Methanol	N,N-Dimethylglycine	O-Acetylcarnitine
O-Phosphocholine	Propylene glycol	Pyroglutamate	Succinate
Taurine	Threonine	Trimethylamine N-oxide	Trigonelline
Trimethylamine	Tyrosine	Uracil	Urea
Valine	1-Methylnicotinamide	2-Hydroxyisobutyrate	3-Aminoisobutyrate
3-Hydroxyisovalerate	3-Hydroxymandelate	3-Indoxylsulfate	cis-Aconitate
Methylhistidine	trans-Aconitate	tau-Methylhistidine	
1,6-Anhydro-beta-D-glucose		4-Hydroxyphenylacetate	

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