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## **Literature: Measurements on Body Fluids / Metabonomics**

Some of the articles can be ordered with us. Please indicate (⇒ "☑") which articles you like to receive and return the list to BRUKER.

- A1  *P.J.D. Foxall, M. Spraul, R.D. Farrant, L.C. Lindon, G.H. Neild, J.K. Nicholson.*  
750 MHz <sup>1</sup>H-NMR spectroscopy of human blood plasma.  
*Journal of Pharmaceutical & Biological Analysis*, 11, (1993) 267-276
- A2  *M.J. Lynch, J. Masters, J.P. Pryor, J.C. Lindon, M. Spraul, P.J.D. Foxall, J.K. Nicholson.*  
Ultra high field NMR spectroscopic studies on human seminal fluid, seminal vesicle and prostatic secretions.  
*Journal of Pharmaceutical & Biomedical Analysis*, 12, (1994), 5-19
- A3  *L. Le Moyec, F. Muller, M. Eugene, M. Spraul.*  
Proton Magnetic Resonance Spectroscopy of Human Amniotic Fluids Sampled at 17-18 Weeks of Pregnancy in Cases of Decreased Digestive Enzyme Activities and Detected Cystic Fibrosis.  
*Clinical Biochemistry*, 27, (1994), 475-483
- A4  *M. Spraul, J.K. Nicholson, M.J. Lynch, J.C. Lindon.*  
Application of the one-dimensional TOCSY pulse sequence in 750 MHz <sup>1</sup>H-NMR spectroscopy for assignment of endogenous metabolite resonances in biofluids.  
*Journal of Pharmaceutical & Biomedical Analysis*, 12, (1994), 613-618
- A5 *E. Holmes, P.J.D. Foxall, J.K. Nicholson, G.H. Neild, S.M. Brown, C.R. Bedell, B.C. Sweatman, E.Rahr, J.C. Lindon, M. Spraul, P. Neidig*  
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*Analytical Biochemistry*, 220, (1994) 284-296
- A6 *J.K. Nicholson, P.J.D. Foxall.*  
750 MHz <sup>1</sup>H and <sup>1</sup>H-<sup>13</sup>C NMR Spectroscopy of Human Blood Plasma.  
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- A7  *E. Holmes, P.J.D. Foxall, M. Spraul, R.D. Farrant, J.K. Nicholson, J.C. Lindon.*  
750 MHz <sup>1</sup>H NMR spectroscopy characterisation of the complex metabolic pattern of urine from patients with inborn errors of metabolism: 2-hydroxyglutaric aciduria and maple syrup urine disease  
*Journal of Pharmaceutical and Biomedical Analysis*, 15 (1997) 1647-1659
- A8  *E. Humpfer, M. Spraul, A.W. Nicholls, J.K. Nicholson, J.C. Lindon.*  
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- A9** C. Zuppi, I. Messana, F. Forni, C. Rossi, L. Pennacchiotti, F. Ferrari, B. Giardina  
 $^1\text{H}$  NMR spectra of normal urines: Reference ranges of the major metabolites  
*Clinica Chimica Acta*, 265, (1997) 85-97
- A10**  M. Spraul, M. Hofmann, M. Ackermann, A. W. Nicholls, S. J. P. Damment, J. N. Haselden, J. P. Shockcor, J. K. Nicholson, J.C. Lindon:  
Flow Injection Proton Nuclear Magnetic Resonance Spectroscopy Combined With Pattern Recognition Methods: Implications for Rapid Structural Studies and High Throughput Biochemical Screening.  
*Analytical Communications*, 1997, Vol 34 339-341
- A11**  E. Holmes, A.W. Nicholls, J.C. Lindon, S. Ramos, M. Spraul, P. Neidig, S.C. Connor, J. Connelly, S. J. P. Damment, J. Heselden, J.K. Nicholson:  
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- A16** C.A. Daykin, O. Corcoran, S.H.Hansen, I. Bjørnsdottir, C. Cornett, S.C. Connor, J.C. Lindon, J.K. Nicholson.  
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*Clin Chem Lab Med*, 41, (2003) 1642-1658
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- A30**  M.A. Constantinou, E. Papakonstantinou, D. Benaki, M. Spraul, K. Shulpis, M.A. Koupparis, E. Mikros:  
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*Analytica Chimica Acta* 511 (2004) 303-312
- A31**  U.F.H. Engelke, M.L.F. Liebrand-van Sambeek, J. G.N. de Jong, J. G. Leroy, E. Morava, J. A. M. Smeitink, R. A. Wevers:  
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- A34** *R. A. Wevers, U.F. Engelke:*  
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*Ned Tijdschr Klin Chem Labgeneesk* (2005) vol. 30 No. 4, 272-275
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- A37** *C.L. Gavaghan McKee, I.D. Wilson, J.K. Nicholson:*  
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*J. of Proteome Res.* (2006), 5, 378-384
- A38** *Y. Wang, E. Holmes, H. Tang, J.C. Lindon, N. Sprenger, M.E. Turini, G. Bergonzelli, L. B. Fay, S. Kochhar, J.K. Nicholson:*  
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*J. of Proteome Res.* (2006), 5, 2642-2655
- A41** *YC. Stella, B. Beckwith-Hall, O. Cloarec, E. Holmes, J.C. Lindon, J. Powell, F. van der Ouderaa, S. Bingham, A. J. Cross, J.K. Nicholson:*  
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- A42** *M.E. Dumas, R. H. Barton, A. Toye, O. Cloarec, C. Blancher, A., Rothwell, J. Fearnside, R. Tatoud, V. Blanc, John C. Lindon, S. C. Mitchell, E. Holmes, M. I. MacCarthy, J. Scott, D. Gauguier, J.K. Nicholson:*  
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*Anal. Chem.* 2007, 79, 1181-1186
- A44** □ *M. Assfalg, I. Bertini, D. Colangiuli, C. Luchinat, H. Schäfer, B. Schütz, M. Spraul:*  
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- A46**  *J. L. Ward, J. M. Baker, S. J. Miller, C. Deborde, M. Maucourt B. Biais, D. Rolin, A. Moing, S. Moco, J. Vervoort, A. Lommen, H. Schäfer, E. Humpfer, M. H. Beale:*  
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- A47** *J.K. Nicholson, E. Holmes, J. M. Kinross, A. W. Darzi, Z. Takats, J. Lindon:*  
Metabolic phenotyping in clinical and surgical environments  
*Nature*, Vol 491, Nov. **2012**, 384 – 392
- A48**  *L. Tritten, J. Keiser, M. Godejohann, J. Utzinger, M. Vargas, O. Beckonert, E. Holmes, J. Saric:*  
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- A49**  *C. Seger, H. Stuppner:*  
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- A50**  *L. Da Silva, M. Godejohann, F.-P. J. Martin, S. Collino, A. Bürkle, M. Moreno-Villanueva, J. Bernhardt, O. Toussaint, B. Grubeck-Loebenstein, E. S. Gonos, E. Sikora, T. Grune, N. Breusing, C. Franceschi, A. Hervonen, M. Spraul, S. Moco:*  
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- A51**  *S. Aygen, U. Dürr, P. Hegele, J. Kunig, M. Spraul, H. Schäfer, D. Krings, C. Cannet, F. Fang, B. Schütz, S. F.H.Bülbul, H.I. Aydin, S. Ü. Sarici, M. Yalaz, R. Örs, R. Atalan, O. Tuncer:*  
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#### Bruker Information

- B1**  *M. Spraul:*  
High-Resolution NMR and Mixture Analysis: Medical Applications.  
*Bruker Report 1/1991*, NMR Applications, 28-32
- B2**  *E. Humpfer, H. Schäfer, M. Spraul:*  
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- B3**  *L.-H. Tseng, M. Spraul, U. Braumann, M. Godejohann, M. Hofmann:*  
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- B5**  *M. Spraul, H. Schäfer, D. Langhans, R. Rabelo-Schefer, D. Moka:*  
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- B6**  *E. Humpfer:*  
Mixture Analysis: Hardware, Software and Applications  
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- B7**  *M. Spraul:*  
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(powerpoint presentation) Lomonosov Moscow University, March **2006**
- B8**  *M. Spraul, H. Schäfer:*  
Integrated NMR and LC-MS Analysis in Metabolic Profiling and Fingerprinting.  
(powerpoint presentation) ISC'06 Conference, Copenhagen, August **2006**
- B9**  *Ulrich Braumann, Markus Godejohann:*  
Metabolic Profiler: Completely integrated system.  
(powerpoint presentation) Bruker BioSpin NMR Users Meeting, November **2006**
- B10**  *M. Spraul:*  
The Use of a Reference Compound Spectral Base for NMR based Metabonomics.  
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- B11**  *U. Braumann, M. Godejohann, H. Schäfer, M. Spraul:*  
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SpinReport 157/158, December **2006**
- B12**  *M. Spraul:*  
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(powerpoint presentation) ENC Conference, April **2007**
- B13**  *M. Spraul:*  
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- B14**  *U. Braumann, M. Godejohann, E. Humpfer, H. Schäfer, P. Rinke, G. Zurek, C. Baessmann, M. Spraul:*  
Metabolic Profiling and Fingerprinting of Beverages using LC-MS and NMR.  
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- B15**  *U. Braumann, M. Godejohann, S. Keller, H. Schäfer, C. Fischer, P. Neidig G. Zurek, C. Baessmann, M. Spraul:*  
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- B16**  *H. Schäfer:*  
Optimization of Metabonomics Experiments.  
(powerpoint presentation) Bruker Users' Meeting, SMASH, September **2007**
- B17**  *M. Spraul, H. Schäfer:*  
Important Considerations for all Metabonomics and Epidemiological Studies.  
(powerpoint presentation) Bruker Users' Meeting, Stockholm, October **2008**
- B18**  *M. Spraul, H. Schäfer, B. Schütz:*  
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(powerpoint presentation) Bruker Users' Meeting, Singapore, **2008**
- B19**  *M. Spraul, H. Schäfer, B. Schütz:*  
Nutritional Influences on the Metabolic Profile, Chances and Pitfalls.  
(ppt presentation) SMASH Chamonix, September **2009**
- B20**  *M. Spraul, H. Schäfer:*  
NMR-based Tools for Metabonomics.  
(ppt presentation) Imperial College London, October **2009**
- B21**  *M. Spraul, B. Schütz, C. Daolio, P. Rinke, S. Koswig, E. Humpfer, H. Schäfer, M. Mörtter:*  
NMR-based Quality Control of Fruit Juices.  
(poster) RAFA Conference Prague, November **2009**

- B22** ☐ *S. Keller, U. Braumann, B. Schütz, H. Schäfer, G. Hofmann, R. Kerssebaum, M. Spraul:*  
Validierung der quantitativen Probenvorbereitung in der Automation.  
(poster) *Users' Meeting Ettlingen, November 2009*
- B23** ☐ *Metabolic Profiler – A Fully-Integrated Solution for Metabolic Analysis.*  
(brochure) **2009**
- B24** ☐ *M. Spraul, S. Aygen:*  
Urine-based Newborn Screening Project applying High Resolution NMR-Spectroscopy.  
(flyer) *SSIEM, September 2010*
- B25** ☐ *M. Spraul, H. Schäfer, B. Schütz, F. Fang, D. Krings:*  
NMR in the Screening of Newborn Children.  
(ppt presentation) *SSIEM Conference, September 2011*
- B26** ☐ *E. Humpfer, H. Schäfer, B. Schütz, M. Spraul:*  
Combination of targeted and non-targeted screening in biofluids by NMR.  
(ppt presentation) *NMR in Life Sciences Symposium, Lübeck December 2011*
- B27** ☐ *D. Krings, C. Cannet, B. Schütz, H. Schäfer, M. Spraul, F. Fang:*  
NMR-based Metabolomics in Clinical Studies of Human Population: Quantification.  
(poster) *Metabolomics 2012 Washington; June 2012*
- B28** ☐ *C. Cannet, D. Krings, M. Spraul, H. Schäfer, B. Schütz, F. Fang, S. Aygen, U. Dürr, P. Tremmel:*  
NMR-based Screening of neonate urines.  
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- B29** ☐ *M. Spraul, H. Schäfer, B. Schütz, E. Humpfer, C. Cannet, D. Krings, A. Grote, F. Fang, L.-H. Tseng:*  
NMR in Clinical Environment and Epidemiology.  
(ppt presentation) *Bangkok, June 2013*
- B30** ☐ *A. Steck, C. Fischer, K.-P. Neidig, H. Schäfer, B. Schütz, M. Spraul, L.-H. Tseng:*  
BBIORFCODE – A NMR Database for Biofluid Metabolites  
(poster) *Euroanalysis Warsaw, August 2013*
- B31** ☐ *M. Spraul, C. Cannet, F. Fang, D. Krings, H. Schäfer, B. Schütz:*  
A New Standard for NMR based Screening  
(ppt presentation) *ICIEM Barcelona, September 2013*
- B32** ☐ *C. Cannet, F. Fang, D. Krings, H. Schäfer, B. Schütz, M. Spraul:*  
Results of Newborn Screening Obtained in Germany and Turkey  
(ppt presentation) *ICIEM Barcelona, September 2013*
- B33** ☐ *M. Spraul, C. Cannet, D. Krings, H. Schäfer, B. Schütz, A. Grote, F. Fang, L.-H. Tseng, E. Humpfer:*  
IVDr – A Spectrometer for Clinical Research  
(ppt presentation) *Users' Meeting, Coventry, November 2013*
- B34** ☐ *Avance™-IVDr – NMR Screening solution for Translational Metabonomics Research*  
(flyer), *January 2014*
- B35** ☐ *M. Spraul, H. Schäfer, B. Schütz, C. Cannet, D. Krings, F. Fang, E. Humpfer, M. Mörtter:*  
Mixture Analysis & Metabonomics  
(ppt presentation) *Pre-ENC Users' Meeting, Boston, April 2014*
- B36** ☐ *M. Spraul, H. Schäfer, B. Schütz, C. Cannet, D. Krings, F. Fang, E. Humpfer, M. Mörtter:*  
Tools and Technologies used for NMR based Metabolic Profiling and Fingerprinting  
(ppt presentation) *Lima, May 2014*
- B37** ☐ *M. Spraul, H. Schäfer, B. Schütz, C. Cannet, D. Krings, F. Fang, E. Humpfer, M. Mörtter:*  
NMR Based Screening in Metabolic Profiling and Fingerprinting  
(ppt presentation) *Lima, May 2014*

- B38**  *M. Spraul, H. Schäfer, B. Schütz, F. Fang, E. Humpfer, A. Steck, C. Cannet, A. Grote, M. Mörtter, L.-H. Tseng, S. Schmidt:*  
Latest Metabolomics Applications in Food-, Agricultural Screening and Molecular Diagnostics Research  
(ppt presentation) *NMR Users Meetings, 2014*
- B39**  *M. Spraul, H. Schäfer, B. Schütz, E. Humpfer, C. Cannet, D. Krings, A. Grote, F. Fang, L-H. Tseng:*  
NMR in Neonatal Health, Inborn Error Screening and general clinical research.  
(ppt presentation) *Vilnius, December 2014*
- B40**  *M. Spraul, H. Schäfer, B. Schütz, E. Humpfer, C. Cannet, D. Krings, A. Grote, F. Fang, L-H. Tseng:*  
Metabonomics Screening by NMR for Clinical and Translational Research.  
(ppt presentation) *May 2016*
- B41**  IVDr Research by NMR – An Innovative Analytical Solution for Biobanking.  
(brochure) *May 2016*