

John C Lindon

List of Publications by Citations

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332
papers

32,776
citations

85
h-index

175
g-index

353
ext. papers

35,988
ext. citations

6.8
avg, IF

6.84
L-index

| # | Paper | IF | Citations |
|-----|--|------|-----------|
| 332 | Proposed minimum reporting standards for chemical analysis Chemical Analysis Working Group (CAWG) Metabolomics Standards Initiative (MSI). <i>Metabolomics</i> , 2007 , 3, 211-221 | 4.7 | 2472 |
| 331 | Metabolic profiling, metabolomic and metabonomic procedures for NMR spectroscopy of urine, plasma, serum and tissue extracts. <i>Nature Protocols</i> , 2007 , 2, 2692-703 | 18.8 | 1536 |
| 330 | Metabonomics: a platform for studying drug toxicity and gene function. <i>Nature Reviews Drug Discovery</i> , 2002 , 1, 153-61 | 64.1 | 1524 |
| 329 | 750 MHz 1H and 1H-13C NMR spectroscopy of human blood plasma. <i>Analytical Chemistry</i> , 1995 , 67, 793-801 | 9.1 | 890 |
| 328 | Metabolic profiling reveals a contribution of gut microbiota to fatty liver phenotype in insulin-resistant mice. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006 , 103, 12511-6 | 11.5 | 854 |
| 327 | Statistical total correlation spectroscopy: an exploratory approach for latent biomarker identification from metabolic 1H NMR data sets. <i>Analytical Chemistry</i> , 2005 , 77, 1282-9 | 7.8 | 729 |
| 326 | Pharmaco-metabonomic phenotyping and personalized drug treatment. <i>Nature</i> , 2006 , 440, 1073-7 | 50.4 | 689 |
| 325 | Pharmacometabonomic identification of a significant host-microbiome metabolic interaction affecting human drug metabolism. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009 , 106, 14728-33 | 11.5 | 562 |
| 324 | Evaluation of the orthogonal projection on latent structure model limitations caused by chemical shift variability and improved visualization of biomarker changes in 1H NMR spectroscopic metabonomic studies. <i>Analytical Chemistry</i> , 2005 , 77, 517-26 | 7.8 | 508 |
| 323 | Improved WATERGATE Pulse Sequences for Solvent Suppression in NMR Spectroscopy. <i>Journal of Magnetic Resonance</i> , 1998 , 132, 125-129 | 3 | 451 |
| 322 | Metabonomics technologies and their applications in physiological monitoring, drug safety assessment and disease diagnosis. <i>Biomarkers</i> , 2004 , 9, 1-31 | 2.6 | 393 |
| 321 | NMR-based metabonomic approaches for evaluating physiological influences on biofluid composition. <i>NMR in Biomedicine</i> , 2005 , 18, 143-62 | 4.4 | 387 |
| 320 | Scaling and normalization effects in NMR spectroscopic metabonomic data sets. <i>Analytical Chemistry</i> , 2006 , 78, 2262-7 | 7.8 | 383 |
| 319 | A top-down systems biology view of microbiome-mammalian metabolic interactions in a mouse model. <i>Molecular Systems Biology</i> , 2007 , 3, 112 | 12.2 | 374 |
| 318 | Metabolic phenotyping in clinical and surgical environments. <i>Nature</i> , 2012 , 491, 384-92 | 50.4 | 364 |
| 317 | Metabonomics: Metabolic processes studied by NMR spectroscopy of biofluids. <i>Concepts in Magnetic Resonance</i> , 2000 , 12, 289-320 | | 354 |
| 316 | Pattern recognition methods and applications in biomedical magnetic resonance. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2001 , 39, 1-40 | 10.4 | 344 |

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| 315 | Contemporary issues in toxicology the role of metabonomics in toxicology and its evaluation by the COMET project. <i>Toxicology and Applied Pharmacology</i> , 2003 , 187, 137-46 | 4.6 | 342 |
| 314 | The challenges of modeling mammalian biocomplexity. <i>Nature Biotechnology</i> , 2004 , 22, 1268-74 | 44.5 | 321 |
| 313 | Susceptibility of human metabolic phenotypes to dietary modulation. <i>Journal of Proteome Research</i> , 2006 , 5, 2780-8 | 5.6 | 311 |
| 312 | High-resolution magic-angle-spinning NMR spectroscopy for metabolic profiling of intact tissues. <i>Nature Protocols</i> , 2010 , 5, 1019-32 | 18.8 | 309 |
| 311 | Probiotic modulation of symbiotic gut microbial-host metabolic interactions in a humanized microbiome mouse model. <i>Molecular Systems Biology</i> , 2008 , 4, 157 | 12.2 | 304 |
| 310 | The metabolomics standards initiative (MSI). <i>Metabolomics</i> , 2007 , 3, 175-178 | 4.7 | 304 |
| 309 | Statistical heterospectroscopy, an approach to the integrated analysis of NMR and UPLC-MS data sets: application in metabonomic toxicology studies. <i>Analytical Chemistry</i> , 2006 , 78, 363-71 | 7.8 | 304 |
| 308 | Assessment of analytical reproducibility of ¹ H NMR spectroscopy based metabonomics for large-scale epidemiological research: the INTERMAP Study. <i>Analytical Chemistry</i> , 2006 , 78, 2199-208 | 7.8 | 304 |
| 307 | Precision high-throughput proton NMR spectroscopy of human urine, serum, and plasma for large-scale metabolic phenotyping. <i>Analytical Chemistry</i> , 2014 , 86, 9887-94 | 7.8 | 291 |
| 306 | Colonization-induced host-gut microbial metabolic interaction. <i>MBio</i> , 2011 , 2, e00271-10 | 7.8 | 281 |
| 305 | NMR Spectroscopy of Biofluids. <i>Annual Reports on NMR Spectroscopy</i> , 1999 , 38, 1-88 | 1.7 | 275 |
| 304 | NMR-based metabolic profiling and metabonomic approaches to problems in molecular toxicology. <i>Chemical Research in Toxicology</i> , 2008 , 21, 9-27 | 4 | 267 |
| 303 | Chemometric models for toxicity classification based on NMR spectra of biofluids. <i>Chemical Research in Toxicology</i> , 2000 , 13, 471-8 | 4 | 261 |
| 302 | Recursive segment-wise peak alignment of biological (¹ h) NMR spectra for improved metabolic biomarker recovery. <i>Analytical Chemistry</i> , 2009 , 81, 56-66 | 7.8 | 258 |
| 301 | The Consortium for Metabonomic Toxicology (COMET): aims, activities and achievements. <i>Pharmacogenomics</i> , 2005 , 6, 691-9 | 2.6 | 255 |
| 300 | The metabolomics standards initiative. <i>Nature Biotechnology</i> , 2007 , 25, 846-8 | 44.5 | 253 |
| 299 | Spectroscopic and statistical techniques for information recovery in metabonomics and metabolomics. <i>Annual Review of Analytical Chemistry</i> , 2008 , 1, 45-69 | 12.5 | 241 |
| 298 | Analytical reproducibility in (¹ H) NMR-based metabonomic urinalysis. <i>Chemical Research in Toxicology</i> , 2002 , 15, 1380-6 | 4 | 239 |

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| 297 | Urinary metabolic phenotyping differentiates children with autism from their unaffected siblings and age-matched controls. <i>Journal of Proteome Research</i> , 2010 , 9, 2996-3004 | 5.6 | 237 |
| 296 | Metabonomics techniques and applications to pharmaceutical research & development. <i>Pharmaceutical Research</i> , 2006 , 23, 1075-88 | 4.5 | 236 |
| 295 | Summary recommendations for standardization and reporting of metabolic analyses. <i>Nature Biotechnology</i> , 2005 , 23, 833-8 | 44.5 | 233 |
| 294 | Metabonomics in pharmaceutical R&D. <i>FEBS Journal</i> , 2007 , 274, 1140-51 | 5.7 | 229 |
| 293 | An integrated metabonomic investigation of acetaminophen toxicity in the mouse using NMR spectroscopy. <i>Chemical Research in Toxicology</i> , 2003 , 16, 295-303 | 4 | 224 |
| 292 | Optimized preprocessing of ultra-performance liquid chromatography/mass spectrometry urinary metabolic profiles for improved information recovery. <i>Analytical Chemistry</i> , 2011 , 83, 5864-72 | 7.8 | 201 |
| 291 | Use of relaxation-edited one-dimensional and two dimensional nuclear magnetic resonance spectroscopy to improve detection of small metabolites in blood plasma. <i>Analytical Biochemistry</i> , 2004 , 325, 260-72 | 3.1 | 186 |
| 290 | Cryogenic probe ¹³ C NMR spectroscopy of urine for metabonomic studies. <i>Analytical Chemistry</i> , 2002 , 74, 4588-93 | 7.8 | 174 |
| 289 | Metabonomic investigations into hydrazine toxicity in the rat. <i>Chemical Research in Toxicology</i> , 2001 , 14, 975-87 | 4 | 170 |
| 288 | So what's the deal with metabonomics?. <i>Analytical Chemistry</i> , 2003 , 75, 384A-391A | 7.8 | 165 |
| 287 | Species variation in the fecal metabolome gives insight into differential gastrointestinal function. <i>Journal of Proteome Research</i> , 2008 , 7, 352-60 | 5.6 | 156 |
| 286 | Directly coupled HPLC-NMR and HPLC-NMR-MS in pharmaceutical research and development. <i>Biomedical Applications</i> , 2000 , 748, 233-58 | | 154 |
| 285 | Integrated application of transcriptomics and metabonomics yields new insight into the toxicity due to paracetamol in the mouse. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2004 , 35, 93-105 | 3.5 | 151 |
| 284 | Improved analysis of multivariate data by variable stability scaling: application to NMR-based metabolic profiling. <i>Analytica Chimica Acta</i> , 2003 , 490, 265-276 | 6.6 | 149 |
| 283 | Metabonomics and its role in drug development and disease diagnosis. <i>Expert Review of Molecular Diagnostics</i> , 2004 , 4, 189-99 | 3.8 | 149 |
| 282 | Combined HPLC, NMR spectroscopy, and ion-trap mass spectrometry with application to the detection and characterization of xenobiotic and endogenous metabolites in human urine. <i>Analytical Chemistry</i> , 1996 , 68, 4431-5 | 7.8 | 149 |
| 281 | Prediction and classification of drug toxicity using probabilistic modeling of temporal metabolic data: the consortium on metabonomic toxicology screening approach. <i>Journal of Proteome Research</i> , 2007 , 6, 4407-22 | 5.6 | 146 |
| 280 | Human metabolic phenotypes link directly to specific dietary preferences in healthy individuals. <i>Journal of Proteome Research</i> , 2007 , 6, 4469-77 | 5.6 | 145 |

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| 279 | 750 MHz ¹ 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. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1997 , 15, 1647-59 | 3.5 | 143 |
| 278 | Panorganismal gut microbiome-host metabolic crosstalk. <i>Journal of Proteome Research</i> , 2009 , 8, 2090-1056 | 3.5 | 137 |
| 277 | Spectral editing and pattern recognition methods applied to high-resolution magic-angle spinning ¹ H nuclear magnetic resonance spectroscopy of liver tissues. <i>Analytical Biochemistry</i> , 2003 , 323, 26-32 | 3.1 | 134 |
| 276 | Geometric trajectory analysis of metabolic responses to toxicity can define treatment specific profiles. <i>Chemical Research in Toxicology</i> , 2004 , 17, 579-87 | 4 | 131 |
| 275 | High-resolution diffusion and relaxation edited one- and two-dimensional ¹ H NMR spectroscopy of biological fluids. <i>Analytical Chemistry</i> , 1996 , 68, 3370-6 | 7.8 | 131 |
| 274 | HILIC-UPLC-MS for exploratory urinary metabolic profiling in toxicological studies. <i>Analytical Chemistry</i> , 2011 , 83, 382-90 | 7.8 | 128 |
| 273 | The identification of novel biomarkers of renal toxicity using automatic data reduction techniques and PCA of proton NMR spectra of urine. <i>Chemometrics and Intelligent Laboratory Systems</i> , 1998 , 44, 245-255 | 3.8 | 127 |
| 272 | NMR-based metabonomic toxicity classification: hierarchical cluster analysis and k-nearest-neighbour approaches. <i>Analytica Chimica Acta</i> , 2003 , 490, 3-15 | 6.6 | 127 |
| 271 | The comparison of plasma deproteinization methods for the detection of low-molecular-weight metabolites by (¹ H) nuclear magnetic resonance spectroscopy. <i>Analytical Biochemistry</i> , 2002 , 304, 220-30 | 3.1 | 126 |
| 270 | Direct coupling of chromatographic separations to NMR spectroscopy. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 1996 , 29, 1-49 | 10.4 | 126 |
| 269 | Biochemical classification of kidney carcinoma biopsy samples using magic-angle-spinning ¹ H nuclear magnetic resonance spectroscopy. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1998 , 17, 125-32 | 3.5 | 122 |
| 268 | Human metabolic profiles are stably controlled by genetic and environmental variation. <i>Molecular Systems Biology</i> , 2011 , 7, 525 | 12.2 | 119 |
| 267 | Pharmacometabonomics as an effector for personalized medicine. <i>Pharmacogenomics</i> , 2011 , 12, 103-11 | 2.6 | 118 |
| 266 | Environmental metabonomics: applying combination biomarker analysis in earthworms at a metal contaminated site. <i>Ecotoxicology</i> , 2004 , 13, 797-806 | 2.9 | 117 |
| 265 | Analytical technologies for metabonomics and metabolomics, and multi-omic information recovery. <i>TrAC - Trends in Analytical Chemistry</i> , 2008 , 27, 194-204 | 14.6 | 114 |
| 264 | A genome-wide metabolic QTL analysis in Europeans implicates two loci shaped by recent positive selection. <i>PLoS Genetics</i> , 2011 , 7, e1002270 | 6 | 109 |
| 263 | Detection of urinary drug metabolite (xenometabolome) signatures in molecular epidemiology studies via statistical total correlation (NMR) spectroscopy. <i>Analytical Chemistry</i> , 2007 , 79, 2629-40 | 7.8 | 108 |
| 262 | Robust data processing and normalization strategy for MALDI mass spectrometric imaging. <i>Analytical Chemistry</i> , 2012 , 84, 1310-9 | 7.8 | 107 |

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| 261 | Comparative metabonomics of differential hydrazine toxicity in the rat and mouse. <i>Toxicology and Applied Pharmacology</i> , 2005 , 204, 135-51 | 4.6 | 107 |
| 260 | NMR spectroscopy as a novel approach to the monitoring of renal transplant function. <i>Kidney International</i> , 1993 , 43, 234-45 | 9.9 | 106 |
| 259 | High resolution magic angle spinning 1H nuclear magnetic resonance analysis of intact prostatic hyperplastic and tumour tissues. <i>Analytical Communications</i> , 1998 , 35, 113-115 | | 105 |
| 258 | Acyl glucuronides: biological activity, chemical reactivity, and chemical synthesis. <i>Journal of Medicinal Chemistry</i> , 2006 , 49, 6931-45 | 8.3 | 105 |
| 257 | Metabonomic assessment of toxicity of 4-fluoroaniline, 3,5-difluoroaniline and 2-fluoro-4-methylaniline to the earthworm <i>Eisenia veneta</i> (rosa): Identification of new endogenous biomarkers. <i>Environmental Toxicology and Chemistry</i> , 2002 , 21, 1966-1972 | 3.8 | 104 |
| 256 | Stability and robustness of human metabolic phenotypes in response to sequential food challenges. <i>Journal of Proteome Research</i> , 2012 , 11, 643-55 | 5.6 | 103 |
| 255 | Metabonomic studies on the physiological effects of acute and chronic psychological stress in Sprague-Dawley rats. <i>Journal of Proteome Research</i> , 2007 , 6, 2080-93 | 5.6 | 96 |
| 254 | Directly coupled HPLC-NMR and its application to drug metabolism. <i>Drug Metabolism Reviews</i> , 1997 , 29, 705-46 | 7 | 94 |
| 253 | Metabolic assessment of human liver transplants from biopsy samples at the donor and recipient stages using high-resolution magic angle spinning 1H NMR spectroscopy. <i>Analytical Chemistry</i> , 2005 , 77, 5570-8 | 7.8 | 94 |
| 252 | High-resolution magic angle spinning NMR spectroscopy: Application to biomedical studies. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2009 , 55, 79-100 | 10.4 | 93 |
| 251 | Identification of human urinary biomarkers of cruciferous vegetable consumption by metabonomic profiling. <i>Journal of Proteome Research</i> , 2011 , 10, 4513-21 | 5.6 | 89 |
| 250 | A metabolic system-wide characterisation of the pig: a model for human physiology. <i>Molecular BioSystems</i> , 2011 , 7, 2577-88 | | 89 |
| 249 | An integrated metabonomic approach to describe temporal metabolic dysregulation induced in the rat by the model hepatotoxin allyl formate. <i>Journal of Proteome Research</i> , 2006 , 5, 2675-84 | 5.6 | 87 |
| 248 | Distinction between normal and renal cell carcinoma kidney cortical biopsy samples using pattern recognition of (1)H magic angle spinning (MAS) NMR spectra. <i>NMR in Biomedicine</i> , 2000 , 13, 64-71 | 4.4 | 85 |
| 247 | Top-down systems biology integration of conditional probiotic modulated transgenomic interactions in a humanized microbiome mouse model. <i>Molecular Systems Biology</i> , 2008 , 4, 205 | 12.2 | 84 |
| 246 | Evaluation of full-resolution J-resolved 1H NMR projections of biofluids for metabonomics information retrieval and biomarker identification. <i>Analytical Chemistry</i> , 2010 , 82, 1811-21 | 7.8 | 83 |
| 245 | Effects of probiotic <i>Lactobacillus paracasei</i> treatment on the host gut tissue metabolic profiles probed via magic-angle-spinning NMR spectroscopy. <i>Journal of Proteome Research</i> , 2007 , 6, 1471-81 | 5.6 | 83 |
| 244 | Quantitative Lipoprotein Subclass and Low Molecular Weight Metabolite Analysis in Human Serum and Plasma by H NMR Spectroscopy in a Multilaboratory Trial. <i>Analytical Chemistry</i> , 2018 , 90, 11962-11971 | 7.8 | 83 |

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| 243 | Ultra performance liquid chromatography-mass spectrometry profiling of bile acid metabolites in biofluids: application to experimental toxicology studies. <i>Analytical Chemistry</i> , 2010 , 82, 5282-9 | 7.8 | 79 |
| 242 | Statistical correlation and projection methods for improved information recovery from diffusion-edited NMR spectra of biological samples. <i>Analytical Chemistry</i> , 2007 , 79, 5682-9 | 7.8 | 79 |
| 241 | Automatic alignment of individual peaks in large high-resolution spectral data sets. <i>Journal of Magnetic Resonance</i> , 2004 , 170, 329-35 | 3 | 79 |
| 240 | UPLC-MS metabolic profiling of second trimester amniotic fluid and maternal urine and comparison with NMR spectral profiling for the identification of pregnancy disorder biomarkers. <i>Molecular BioSystems</i> , 2012 , 8, 1243-54 | | 78 |
| 239 | Directly Coupled 800 MHz HPLC-NMR Spectroscopy of Urine and Its Application to the Identification of the Major Phase II Metabolites of Tolfenamic Acid. <i>Analytical Chemistry</i> , 1997 , 69, 607-612 | 7.8 | 76 |
| 238 | Earthworm species of the genus <i>Eisenia</i> can be phenotypically differentiated by metabolic profiling. <i>FEBS Letters</i> , 2002 , 521, 115-20 | 3.8 | 76 |
| 237 | ¹ H NMR spectroscopy-based interventional metabolic phenotyping: a cohort study of rheumatoid arthritis patients. <i>Journal of Proteome Research</i> , 2010 , 9, 4545-53 | 5.6 | 75 |
| 236 | 600 MHz ¹ H-NMR spectroscopy of human cerebrospinal fluid: effects of sample manipulation and assignment of resonances. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1993 , 11, 651-64 | 3.5 | 74 |
| 235 | Hyperspectral visualization of mass spectrometry imaging data. <i>Analytical Chemistry</i> , 2013 , 85, 1415-23 | 7.8 | 73 |
| 234 | Transgenomic metabolic interactions in a mouse disease model: interactions of <i>Trichinella spiralis</i> infection with dietary <i>Lactobacillus paracasei</i> supplementation. <i>Journal of Proteome Research</i> , 2006 , 5, 2185-93 | 5.6 | 72 |
| 233 | Development and Application of Ultra-Performance Liquid Chromatography-TOF MS for Precision Large Scale Urinary Metabolic Phenotyping. <i>Analytical Chemistry</i> , 2016 , 88, 9004-13 | 7.8 | 71 |
| 232 | Statistical spectroscopic tools for biomarker discovery and systems medicine. <i>Analytical Chemistry</i> , 2013 , 85, 5297-303 | 7.8 | 70 |
| 231 | Experimental metabonomic model of dietary variation and stress interactions. <i>Journal of Proteome Research</i> , 2006 , 5, 1535-42 | 5.6 | 70 |
| 230 | Measurement of biomolecular diffusion coefficients in blood plasma using two-dimensional ¹ H- ¹ H diffusion-edited total-correlation NMR spectroscopy. <i>Analytical Chemistry</i> , 1997 , 69, 1504-9 | 7.8 | 69 |
| 229 | Toxicity classification from metabonomic data using a density superposition approach: [CLOUDS] <i>Analytica Chimica Acta</i> , 2003 , 490, 109-122 | 6.6 | 69 |
| 228 | NMR-based metabolic profiling identifies biomarkers of liver regeneration following partial hepatectomy in the rat. <i>Journal of Proteome Research</i> , 2010 , 9, 59-69 | 5.6 | 68 |
| 227 | Metabolomics Standards Workshop and the development of international standards for reporting metabolomics experimental results. <i>Briefings in Bioinformatics</i> , 2006 , 7, 159-65 | 13.4 | 68 |
| 226 | Topographical variation in metabolic signatures of human gastrointestinal biopsies revealed by high-resolution magic-angle spinning ¹ H NMR spectroscopy. <i>Journal of Proteome Research</i> , 2007 , 6, 3944-51 | 5.6 | 67 |

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| 225 | Subset optimization by reference matching (STORM): an optimized statistical approach for recovery of metabolic biomarker structural information from ¹ H NMR spectra of biofluids. <i>Analytical Chemistry</i> , 2012 , 84, 10694-701 | 7.8 | 64 |
| 224 | Biochemical characterization of rat intestine development using high-resolution magic-angle-spinning ¹ H NMR spectroscopy and multivariate data analysis. <i>Journal of Proteome Research</i> , 2005 , 4, 1324-9 | 5.6 | 61 |
| 223 | Classification of toxin-induced changes in ¹ H NMR spectra of urine using an artificial neural network. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1995 , 13, 205-11 | 3.5 | 61 |
| 222 | Topographical variation in murine intestinal metabolic profiles in relation to microbiome speciation and functional ecological activity. <i>Journal of Proteome Research</i> , 2009 , 8, 3464-74 | 5.6 | 59 |
| 221 | NMR-based metabonomic studies on the biochemical effects of commonly used drug carrier vehicles in the rat. <i>Chemical Research in Toxicology</i> , 2002 , 15, 1136-41 | 4 | 59 |
| 220 | Serum metabolic signatures of coronary and carotid atherosclerosis and subsequent cardiovascular disease. <i>European Heart Journal</i> , 2019 , 40, 2883-2896 | 9.5 | 58 |
| 219 | The influence of EDTA and citrate anticoagulant addition to human plasma on information recovery from NMR-based metabolic profiling studies. <i>Molecular BioSystems</i> , 2010 , 6, 215-24 | | 58 |
| 218 | Magic Angle Spinning Proton Nuclear Magnetic Resonance Spectroscopic Analysis of Intact Kidney Tissue Samples. <i>Analytical Communications</i> , 1997 , 34, 107-109 | | 58 |
| 217 | NMR-based metabonomic studies on the biochemical effects of epicatechin in the rat. <i>Journal of Agricultural and Food Chemistry</i> , 2003 , 51, 4139-45 | 5.7 | 58 |
| 216 | Statistical experimental design and partial least squares regression analysis of biofluid metabonomic NMR and clinical chemistry data for screening of adverse drug effects. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2004 , 73, 139-149 | 3.8 | 57 |
| 215 | Detection of in vivo biomarkers of phospholipidosis using NMR-based metabonomic approaches. <i>Magnetic Resonance in Chemistry</i> , 2001 , 39, 559-565 | 2.1 | 57 |
| 214 | Heteronuclear ¹ H- ³¹ P statistical total correlation NMR spectroscopy of intact liver for metabolic biomarker assignment: application to galactosamine-induced hepatotoxicity. <i>Analytical Chemistry</i> , 2007 , 79, 8956-66 | 7.8 | 56 |
| 213 | High performance liquid chromatography coupled to nuclear magnetic resonance spectroscopy and mass spectrometry applied to plant products: Identification of ecdysteroids from <i>Silene otites</i> . <i>Chromatographia</i> , 1999 , 49, 374-378 | 2.1 | 55 |
| 212 | Metabonomics: systems biology in pharmaceutical research and development. <i>Current Opinion in Molecular Therapeutics</i> , 2004 , 6, 265-72 | | 55 |
| 211 | An hypothesis for a mechanism underlying hepatotoxin-induced hypercreatinuria. <i>Archives of Toxicology</i> , 2003 , 77, 208-17 | 5.8 | 53 |
| 210 | Identification of metabolites in human hepatic bile using 800 MHz ¹ H NMR spectroscopy, HPLC-NMR/MS and UPLC-MS. <i>Molecular BioSystems</i> , 2009 , 5, 180-90 | | 52 |
| 209 | Robust algorithms for automated chemical shift calibration of 1D ¹ H NMR spectra of blood serum. <i>Analytical Chemistry</i> , 2008 , 80, 7158-62 | 7.8 | 52 |
| 208 | Directly coupled HPLC-NMR and HPLC-MS approaches for the rapid characterisation of drug metabolites in urine: application to the human metabolism of naproxen. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2001 , 24, 569-79 | 3.5 | 52 |

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| 207 | Characterisation of impurities in bulk drug batches of fluticasone propionate using directly coupled HPLC-NMR spectroscopy and HPLC-MS. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 1997 , 16, 697-705 | 3.5 | 51 |
| 206 | Use of ¹ H NMR-determined diffusion coefficients to characterize lipoprotein fractions in human blood plasma. <i>Magnetic Resonance in Chemistry</i> , 2002 , 40, S83-S88 | 2.1 | 51 |
| 205 | Omics and its potential impact on R&D and regulation of complex herbal products. <i>Journal of Ethnopharmacology</i> , 2012 , 140, 587-93 | 5 | 50 |
| 204 | Genetic algorithms for simultaneous variable and sample selection in metabonomics. <i>Bioinformatics</i> , 2009 , 25, 112-8 | 7.2 | 50 |
| 203 | Heteronuclear ¹⁹ F- ¹ H statistical total correlation spectroscopy as a tool in drug metabolism: study of flucloxacillin biotransformation. <i>Analytical Chemistry</i> , 2008 , 80, 1073-9 | 7.8 | 50 |
| 202 | Magic angle spinning NMR and ¹ H- ³¹ P heteronuclear statistical total correlation spectroscopy of intact human gut biopsies. <i>Analytical Chemistry</i> , 2008 , 80, 1058-66 | 7.8 | 50 |
| 201 | Statistical search space reduction and two-dimensional data display approaches for UPLC-MS in biomarker discovery and pathway analysis. <i>Analytical Chemistry</i> , 2006 , 78, 4398-408 | 7.8 | 50 |
| 200 | Targeting the human genome-microbiome axis for drug discovery: inspirations from global systems biology and traditional Chinese medicine. <i>Journal of Proteome Research</i> , 2012 , 11, 3509-19 | 5.6 | 49 |
| 199 | Flow Injection Proton Nuclear Magnetic Resonance Spectroscopy Combined With Pattern Recognition Methods: Implications for Rapid Structural Studies and High Throughput Biochemical Screening. <i>Analytical Communications</i> , 1997 , 34, 339-341 | | 49 |
| 198 | Temporal metabonomic modeling of l-arginine-induced exocrine pancreatitis. <i>Journal of Proteome Research</i> , 2008 , 7, 4435-45 | 5.6 | 49 |
| 197 | Optimization of human plasma ¹ H NMR spectroscopic data processing for high-throughput metabolic phenotyping studies and detection of insulin resistance related to type 2 diabetes. <i>Analytical Chemistry</i> , 2008 , 80, 7354-62 | 7.8 | 48 |
| 196 | A metabonomic investigation of hepatotoxicity using diffusion-edited ¹ H NMR spectroscopy of blood serum. <i>Analyst, The</i> , 2003 , 128, 814-8 | 5 | 47 |
| 195 | NMR spectroscopy of human post mortem cerebrospinal fluid: distinction of Alzheimer's disease from control using pattern recognition and statistics. <i>NMR in Biomedicine</i> , 1993 , 6, 163-7 | 4.4 | 47 |
| 194 | High-performance liquid chromatography linked to inductively coupled plasma mass spectrometry and orthogonal acceleration time-of-flight mass spectrometry for the simultaneous detection and identification of metabolites of 2-bromo-4-trifluoromethyl. <i>Analytical Chemistry</i> , 2001 , 73, 1491-4 | 7.8 | 46 |
| 193 | On-flow identification of metabolites of paracetamol from human urine using directly coupled CZE-NMR and CEC-NMR spectroscopy. <i>Analytical Communications</i> , 1998 , 35, 213-215 | | 45 |
| 192 | Analysis of Drug-Protein Binding Using Nuclear Magnetic Resonance Based Molecular Diffusion Measurements. <i>Analytical Communications</i> , 1997 , 34, 225-228 | | 43 |
| 191 | Directly coupled CZE-NMR and CEC-NMR spectroscopy for metabolite analysis: paracetamol metabolites in human urine. <i>Analyst, The</i> , 1998 , 123, 2835-7 | 5 | 43 |
| 190 | Identification of the Positional Isomers of 2-Fluorobenzoic acid 1-O-Acyl Glucuronide by Directly Coupled HPLC-NMR. <i>Analytical Chemistry</i> , 1995 , 67, 3401-3404 | 7.8 | 43 |

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| 189 | Hepatotoxin-induced hypercreatininaemia and hypercreatinuria: their relationship to one another, to liver damage and to weakened nutritional status. <i>Archives of Toxicology</i> , 2004 , 78, 86-96 | 5.8 | 41 |
| 188 | Quantitative structure-metabolism relationships for substituted benzoic acids in the rat. Computational chemistry, NMR spectroscopy and pattern recognition studies. <i>Biochemical Pharmacology</i> , 1992 , 44, 1935-46 | 6 | 41 |
| 187 | Application of directly coupled LC-NMR-MS to the structural elucidation of metabolites of the HIV-1 reverse-transcriptase inhibitor BW935U83. <i>Biomedical Applications</i> , 2000 , 748, 269-79 | | 40 |
| 186 | A rapid and facile method for the dereplication of purified natural products. <i>Journal of Natural Products</i> , 2001 , 64, 1541-4 | 4.9 | 40 |
| 185 | NMR spectroscopic studies on the in vitro acyl glucuronide migration kinetics of Ibuprofen ((+/-)-(R,S)-2-(4-isobutylphenyl) propanoic acid), its metabolites, and analogues. <i>Analytical Chemistry</i> , 2007 , 79, 8720-7 | 7.8 | 39 |
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