



## KÖLLENSPERGER Gunda

### Personal details

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### Main areas of research

**Metalomics:** investigation of metallobiomolecules, metallodrugs or biomolecules containing heteroelements (e.g. sulfur, phosphorous, selenium) in complex biological matrices by inductively coupled plasma mass spectrometry combined to chromatographic separations and laser ablation  
**Metabolomics:** LC-MS based methods for targeted metabolic profiling, non-targeted fingerprinting and flux analysis; development of workflows based on multidimensional chromatographic separations, *in vivo* synthesis of stable isotopically labeled metabolite standards

### Academic Credentials

2003 Habilitation in Analytical Chemistry, BOKU – University of Natural Resources and Life Sciences, (“Inductively Coupled Plasma Mass Spectrometry in Environmental and Life Sciences – Elemental Trace Analysis and Speciation”)  
1998 Dr. techn., Technical University of Vienna, Institute of Analytical Chemistry; (“Investigation of Small Particles by Scanning Force Microscopy”)  
1995 Dipl. Ing., Technical University of Vienna, Institute of Analytical Chemistry, (“Matrix-Assisted Laser Desorption and Ionization in Fourier Transform Laser Microprobe Mass Spectrometry with External Source”)

### Previous and Current Position

2016 - current Head of the Institute of Analytical Chemistry, University of Vienna  
2015 - current Deputy head of the core facility Mass Spectrometry Center, Faculty of Chemistry, University of Vienna  
2015 - current Vice Chair of the Vienna Metabolomics Center (ViMe), University of Vienna  
2014 - current Univ. Professor (Institute of Analytical Chemistry, Faculty of Chemistry, University of Vienna)  
2011 - 2014 Key researcher, head of core facility of metabolomics, Austrian Centre for Industrial biotechnology, ACIB  
2003 - 2014 Associate Professor at Division of Analytical Chemistry, Department of Chemistry, BOKU  
1998 - 2003 Assistant Professor at the Department of Chemistry, BOKU

## Visiting Fellowships and Awards

2016	Fonds der Stadt Wien für innovative interdisziplinäre Krebsforschung Award (Metabolomics in 3D tumor models)
2015	Fellinger Krebsforschung Award (together W. Berger)
2011	Guest professor for Analytical Chemistry (Humboldt University, Berlin)
2010	Fritz Feigl Award (Austrian Society of Analytical Chemistry)

## Career related activities, editorships, memberships

Since 2011	Austrian Society of Analytical Chemistry, board member
2009-2016	Editorial board member of Journal of Analytical Atomic Spectroscopy (JAAS, Royal Society of Chemistry)
2016	Guest editor of special issue on speciation analysis, Journal of Analytical Atomic Spectroscopy (JAAS, Royal Society of Chemistry)
2007-2009, since 2016	Advisory board member, Journal of Analytical Atomic Spectroscopy (JAAS, Royal Society of Chemistry)
2012-2015	Substitute member of the legal commission of the Austrian Anti-Doping Agency, NADA
Review activity	Analytical Chemistry, Analyst, Metallomics, Journal of Analytical Atomic spectroscopy, Analytica Chimica Acta, Journal of Separation Science, Electrophoresis, Analytical Bioanalytical Chemistry

## Funding (5 selected peer reviewed principal investigator projects)

2016- current	ReMiND, 15HLT02 (working package leader, funding by EURAMET, European metrology program)
2013-2015	Researcher excellence grant on metallomics HLT05-REG4 (EURAMET, European metrology program)
2012-2014	Entwicklung der Analytik zur <sup>13</sup> C-Stoffflussanalyse und Quantifizierung von Metaboliten in filamentösen Pilzen (Sandoz)
2010-2014	ACIB core facility metabolomics (Austrian Centre for Industrial Biotechnology, FFG)
2008-2012	Speciation analysis in preclinical cancer research (FWF Translational research)

## Publications

Number of peer reviewed publications 106; 1612 citations, h-factor: 22 (<http://orcid.org/0000-0002-1460-4919>);

## Scientific publications (since 2012)

1. Bamonti L., Theiner S., Rohr-Udilova N., Keppler B. K., Koellensperger G., Accurate high throughput quantification of selenium in biological samples – the potential of combining isotope dilution ICP-tandem mass spectrometry with flow injection, *J. Anal. At. Spectrom.*, 2016, Advance Article DOI: 10.1039/C6JA00209A
2. Mairinger T., Wozniak-Knopp G., Rüker F., Koellensperger G., Hann S., Element labeling of antibody fragments for ICP-MS based immunoassays, *J. Anal. At. Spectrom.*, 2016, Advance Article DOI: 10.1039/C6JA00252H,
3. Ortmayr K., Charwat V., Kasper C., Hann S. and Koellensperger G., Uncertainty budgeting in fold change determination and implications for non-targeted metabolomics studies in model systems, *Analyst*, 2016, Advance Article, DOI: 10.1039/C6AN01342B

4. Ortmayr, K., Causon, T.J., Hann, S., Koellensperger, G. Increasing selectivity and coverage in LC-MS based metabolome analysis (2016) *TrAC - Trends in Analytical Chemistry*, 82, pp. 358-366. DOI: 10.1016/j.trac.2016.06.011
5. Hermann G., Hyrup Møller L., Gammelgaard B., Hohlweg J., Mattanovich D., Hann S., Koellensperger G. In vivo synthesized <sup>34</sup>S enriched amino acid standards for species specific isotope dilution of proteins (2016) *J. Anal. At. Spectrom.*, 31, 1830-1835 DOI: 10.1039/C6JA00039H
6. Koellensperger G., Galanski M., Keppler B.K., Hann, S. Turbulent flow chromatography in combination with HPLC-ICP-MS for high-throughput analysis of free, intact metal based drugs in biomedical samples (2016) *J. Anal. At. Spectrom.*, DOI: 10.1039/C6JA00108D, Communication
7. Bytzek, A.K., Koellensperger, G., Keppler, B.K., Hartinger, C.G. Biodistribution of the novel anticancer drug sodium trans-[tetrachloridobis(1H-indazole)ruthenate(III)] KP-1339/IT139 in nude BALB/c mice and implications on its mode of action (2016) *Journal of Inorganic Biochemistry*, 160, pp. 250-255.
8. Pelivan, K., Miklos, W., Van Schoonhoven, S., Koellensperger, G., Gille, L., Berger, W., Heffeter, P., Kowol, C.R., Keppler, B.K. Differences in protein binding and excretion of Triapine and its Fe(III) complex (2016) *Journal of Inorganic Biochemistry*, 160, pp. 61-69. DOI: 10.1016/j.jinorgbio.2015.10.006
9. Theiner, S., Schreiber-Brynzak, E., Jakupec, M.A., Galanski, M., Koellensperger, G., Keppler, B.K. LA-ICP-MS imaging in multicellular tumor spheroids - A novel tool in the preclinical development of metal-based anticancer drugs (2016) *Metallomics*, 8 (4), pp. 398-402.
10. Megson, Z.A., Pittenauer, E., Duda, K.A., Engel, R., Ortmayr, K., Koellensperger, G., Mach, L., Allmaier, G., Holst, O., Messner, P., Schäffer, C. Inositol-phosphodihydroceramides in the periodontal pathogen *Tannerella forsythia*: Structural analysis and incorporation of exogenous myo-inositol (2015) *Biochimica et Biophysica Acta - Molecular and Cell Biology of Lipids*, 1851 (11), pp. 1417-1427.
11. Graf, M.M.H., Sucharitakul, J., Bren, U., Chu, D.B., Koellensperger, G., Hann, S., Furtmüller, P.G., Obinger, C., Peterbauer, C.K., Oostenbrink, C., Chaiyen, P., Haltrich, D. Reaction of pyranose dehydrogenase from *Agaricus meleagris* with its carbohydrate substrates (2015) *FEBS Journal*, 282 (21), pp. 4218-4241.
12. Mairinger, T., Steiger, M., Nocon, J., Mattanovich, D., Koellensperger, G., Hann, S. Gas Chromatography-Quadrupole Time-of-Flight Mass Spectrometry-Based Determination of Isotopologue and Tandem Mass Isotopomer Fractions of Primary Metabolites for <sup>13</sup>C-Metabolic Flux Analysis (2015) *Analytical Chemistry*, 87 (23), pp. 11792-11802.
13. Neubauer, S., Chu, D.B., Marx, H., Sauer, M., Hann, S., Koellensperger, G. LC-MS/MS-based analysis of coenzyme A and short-chain acyl-coenzyme A thioesters (2015) *Analytical and Bioanalytical Chemistry*, 407 (22), pp. 6681-6688.
14. Rußmayer, H., Buchetics, M., Gruber, C., Valli, M., Grillitsch, K., Modarres, G., Guerrasio, R., Klavins, K., Neubauer, S., Drexler, H., Steiger, M., Troyer, C., Al Chalabi, A., Krebiehl, G., Sonntag, D., Zellnig, G., Daum, G., Graf, A.B., Altmann, F., Koellensperger, G., Hann, S., Sauer, M., Mattanovich, D., Gasser, B. Systems-level organization of yeast methylotrophic lifestyle (2015) *BMC Biology*, 13 (1), art. no. 80, .
15. Chu, D.B., Troyer, C., Mairinger, T., Ortmayr, K., Neubauer, S., Koellensperger, G., Hann, S. Isotopologue analysis of sugar phosphates in yeast cell extracts by gas chromatography chemical ionization time-of-flight mass spectrometry (2015) *Analytical and Bioanalytical Chemistry*, 407 (10), art. no. 8521, pp. 2865-2875.

16. Ortmayr, K; Schwaiger, M; Hann, S; Koellensperger, G (2015): An integrated metabolomics workflow for the quantification of sulfur pathway intermediates employing thiol protection with N-ethyl maleimide and hydrophilic interaction liquid chromatography tandem mass spectrometry. *ANALYST*. 2015; 140(22): 7687-7695
17. Russmayer, H; Troyer, C; Neubauer, S; Steiger, MG; Gasser, B; Hann, S; Koellensperger, G; Sauer, M; Mattanovich, D (2015): Metabolomics sampling of *Pichia pastoris* revisited: rapid filtration prevents metabolite loss during quenching. *FEMS YEAST RES.* 2015; 15(6)
18. Ortmayr, K., Hann, S., Koellensperger, G. Complementing reversed-phase selectivity with porous graphitized carbon to increase the metabolome coverage in an on-line two-dimensional LC-MS setup for metabolomics (2015) *Analyst*, 140 (10), pp. 3465-3473.
19. Hann, S., Dernovics, M., Koellensperger, G. Elemental analysis in biotechnology (2015) *Current Opinion in Biotechnology*, 31, pp. 93-100. DOI: 10.1016/j.copbio.2014.08.008
20. Miklos, W., Pelivan, K., Kowol, C.R., Pirker, C., Dornetshuber-Fleiss, R., Spitzwieser, M., Englinger, B., van Schoonhoven, S., Cichna-Markl, M., Koellensperger, G., Keppler, B.K., Berger, W., Heffeter, P. Triapine-mediated ABCB1 induction via PKC induces widespread therapy unresponsiveness but is not underlying acquired triapine resistance (2015) *Cancer Letters*, 361 (1), pp. 112-120. DOI: 10.1016/j.canlet.2015.02.049
21. Hernández Bort, J.A., Shanmukam, V., Pabst, M., Windwarder, M., Neumann, L., Alchalabi, A., Krebühl, G., Koellensperger, G., Hann, S., Sonntag, D., Altmann, F., Heel, C., Borth, N. Reduced quenching and extraction time for mammalian cells using filtration and syringe extraction (2014) *Journal of Biotechnology*, 182-183 (1), pp. 97-103.
22. Hermann, G., Heffeter, P., Kryeziu, K., Berger, W., Hann, S., Koellensperger, G. The study of reduced versus oxidized glutathione in cancer cell models employing isotopically labelled standards (2014) *Analytical Methods*, 6 (9), pp. 3086-3094.
23. Klavins, K., Drexler, H., Hann, S., Koellensperger, G. Quantitative metabolite profiling utilizing parallel column analysis for simultaneous reversed-phase and hydrophilic interaction liquid chromatography separations combined with tandem mass spectrometry (2014) *Analytical Chemistry*, 86 (9), pp. 4145-4150.
24. Klavins, K., Chu, D.B., Hann, S., Koellensperger, G. Fully automated on-line two-dimensional liquid chromatography in combination with ESI MS/MS detection for quantification of sugar phosphates in yeast cell extracts (2014) *Analyst*, 139 (6), pp. 1512-1520.
25. Fischer, L., Zipfel, B., Koellensperger, G., Kovac, J., Bilz, S., Kunkel, A., Venzago, C., Hann, S. Flow injection combined with ICP-MS for accurate high throughput analysis of elemental impurities in pharmaceutical products according to USP <232>/<233> (2014) *Journal of Pharmaceutical and Biomedical Analysis*, 95, pp. 121-129.
26. Rugova, A., Puschenreiter, M., Santner, J., Fischer, L., Neubauer, S., Koellensperger, G., Hann, S. Speciation analysis of orthophosphate and myo-inositol hexakisphosphate in soil- and plant-related samples by high-performance ion chromatography combined with inductively coupled plasma mass spectrometry (2014) *Journal of Separation Science*, 37 (14), pp. 1711-1719.
27. Guerrasio, R., Haberhauer-Troyer, C., Mattanovich, D., Koellensperger, G., Hann, S. Metabolic profiling of amino acids in cellular samples via zwitterionic sub-2  $\mu\text{m}$  particle size HILIC-MS/MS and a uniformly  $^{13}\text{C}$  labeled internal standard Amino Acid Analysis (2014) *Analytical and Bioanalytical Chemistry*, 406 (3), pp. 915-922.
28. Chu, D.B., Klavins, K., Koellensperger, G., Hann, S. Speciation analysis of sugar phosphates via anion exchange chromatography combined with inductively coupled plasma dynamic reaction cell mass spectrometry-optimization for the analysis of yeast cell extracts (2014) *Journal of Analytical Atomic Spectrometry*, 29 (5), pp. 915-925.

29. Schindlegger, Y., Oburger, E., Gruber, B., Schenkeveld, W.D.C., Kraemer, S.M., Puschenreiter, M., Koellensperger, G., Hann, S. Accurate LC-ESI-MS/MS quantification of 2'-deoxymugineic acid in soil and root related samples employing porous graphitic carbon as stationary phase and a <sup>13</sup>C<sub>4</sub>-labeled internal standard (2014) *Electrophoresis*, 35 (9), pp. 1375-1385.
30. Ortmayr, K., Nocon, J., Gasser, B., Mattanovich, D., Hann, S., Koellensperger, G. Sample preparation workflow for the liquid chromatography tandem mass spectrometry based analysis of nicotinamide adenine dinucleotide phosphate cofactors in yeast (2014) *Journal of Separation Science*, 37 (16), pp. 2185-2191.
31. Mueller, L., Mairinger, T., Hermann, G., Koellensperger, G., Hann, S. Characterization of metal-tagged antibodies used in ICP-MS-based immunoassays (2014) *Analytical and Bioanalytical Chemistry*, 406 (1), pp. 163-169.
32. Nocon, J., Steiger, M.G., Pfeffer, M., Sohn, S.B., Kim, T.Y., Maurer, M., Rußmayer, H., Pflügl, S., Ask, M., Haberhauer-Troyer, C., Ortmayr, K., Hann, S., Koellensperger, G., Gasser, B., Lee, S.Y., Mattanovich, D. Model based engineering of *Pichia pastoris* central metabolism enhances recombinant protein production (2014) *Metabolic Engineering*, 24, pp. 129-138.
33. Heffeter, P., Atil, B., Kryeziu, K., Groza, D., Koellensperger, G., Körner, W., Jungwirth, U., Mohr, T., Keppler, B.K., Berger, W. The ruthenium compound KP1339 potentiates the anticancer activity of sorafenib in vitro and in vivo (2013) *European Journal of Cancer*, 49 (15), pp. 3366-3375.
34. Hermann, G., Heffeter, P., Falta, T., Berger, W., Hann, S., Koellensperger, G. In vitro studies on cisplatin focusing on kinetic aspects of intracellular chemistry by LC-ICP-MS (2013) *Metallomics*, 5 (6), pp. 636-647
35. Klavins, K., Neubauer, S., Al Chalabi, A., Sonntag, D., Haberhauer-Troyer, C., Russmayer, H., Sauer, M., Mattanovich, D., Hann, S., Koellensperger, G. Interlaboratory comparison for quantitative primary metabolite profiling in *Pichia pastoris* *Metabolomics and Metabolite Profiling* (2013) *Analytical and Bioanalytical Chemistry*, 405 (15), pp. 5159-5169.
36. Guerrasio, R., Haberhauer-Troyer, C., Steiger, M., Sauer, M., Mattanovich, D., Koellensperger, G., Hann, S. Measurement uncertainty of isotopologue fractions in fluxomics determined via mass spectrometry (2013) *Analytical and Bioanalytical Chemistry*, 405 (15), pp. 5133-5146.
37. Shigeta, K., Koellensperger, G., Rampler, E., Traub, H., Rottmann, L., Panne, U., Okino, A., Jakubowski, N. Sample introduction of single selenized yeast cells (*Saccharomyces cerevisiae*) by micro droplet generation into an ICP-sector field mass spectrometer for label-free detection of trace elements (2013) *Journal of Analytical Atomic Spectrometry*, 28 (5), pp. 637-645. Cited 11 times.
38. Guerrasio, R., Haberhauer-Troyer, C., Neubauer, S., Klavins, K., Werneth, M., Koellensperger, G., Hann, S. Uncertainty of Measurement in Quantitative Metabolomics (2013) *Metabolomics in Practice: Successful Strategies to Generate and Analyze Metabolic Data*, pp. 39-68.
39. Haberhauer-Troyer, C., Delic, M., Gasser, B., Mattanovich, D., Hann, S., Koellensperger, G. Accurate quantification of the redox-sensitive GSH/GSSG ratios in the yeast *Pichia pastoris* by HILIC-MS/MS (2013) *Analytical and Bioanalytical Chemistry*, 405 (6), pp. 2031-2039.
40. Hermann, G., Jaitz, L., Schmölzer, C., Koellensperger, G., Eder, R., Hann, S. Analysis of (poly)-phenols in commercially available red wines by means of LC-MS [Analyse von (Poly-)Phenolen in kommerziell erhältlichen Rotweinen via LC-MS] (2012) *Mitteilungen Klosterneuburg*, 62, pp. 13-20.
41. Neubauer, S., Haberhauer-Troyer, C., Klavins, K., Russmayer, H., Steiger, M.G., Gasser, B., Sauer, M., Mattanovich, D., Hann, S., Koellensperger, G. U<sup>13</sup>C cell extract of *Pichia pastoris* - A powerful tool for evaluation of sample preparation in metabolomics (2012) *Journal of Separation Science*, 35 (22), pp. 3091-3105.

42. Rampler, E., Rose, S., Wieder, D., Ganner, A., Dohnal, I., Dalik, T., Hann, S., Koellensperger, G. Monitoring the production process of selenized yeast by elemental speciation analysis (2012) *Metallomics*, 4 (11), pp. 1176-1184.
43. Pichler, V; Mayr, J; Heffeter, P; Domotor, O; Enyedy, EA; Hermann, G; Groza, D; Koellensperger, G; Galanksi, M; Berger, W; Keppler, BK; Kowol, CR (2013): Maleimide-functionalised platinum(IV) complexes as a synthetic platform for targeted drug delivery. *CHEM COMMUN.* 2013; 49(22): 2249-2251
44. Monitoring the production process of selenized yeast by elemental speciation analysis Evelyn Rampler, Stephan Rose, Dominik Wieder, Anja Ganner, Ilse Dohnal, Thomas Dalik, Stephan Hann and Gunda Koellensperger, 2012, *Metallomics*, 4, 1176-1184
45. Mass spectrometry based analysis of nucleotides, nucleosides and nucleobases – application to feed supplements, Stefan Neubauer, Ariana Rugova, Dinh Binh Chu, Hedda Drexler, Anja Ganner, Michael Sauer, Diethard Mattanovich, Stephan Hann and Gunda Koellensperger, 2012, *Analytical Bioanalytical Chemistry*, *Anal. Bioanal. Chem.*, 2012, 404, 799
46. Sulfur containing amino acids - challenge of accurate quantification, E. Rampler, T. Dalik, G. Stingeder, S. Hann, G. Koellensperger, *J. Anal. At. Spectrom.*, 2012, DOI: 10.1039/C2JA10377J
47. Impact of terminal dimethylation on the resistance profile of  $\alpha$ -N-heterocyclic thiosemicarbazones. Petra Heffeter; Christine Pirker; Christian R Kowol; Gerrit Herrman; Rita Dornetshuber; Walter Miklos; Ute Jungwirth; Gunda Koellensperger; Bernhard K Keppler; Walter Berger, *Biochem Pharmacol* (2012) PMID 22426010
48. Oxidative protein folding and unfolded protein response elicit differing redox regulation in endoplasmic reticulum and cytosol of yeast M. Delic, C. Rebnegger, F. Wanka, V. Puxbaum, C. Haberhauer-Troyer, S. Hann, G. Köllensperger, D. Mattanovich, B. Gasser, *Free Radical Bio. Med.*, 2012, 52, 2000
49. Analysis of underivatized amino acids: zwitterionic hydrophilic interaction chromatography combined with triple quadrupole tandem mass spectrometry. M. Dell'mour, G. Koellensperger, S. Hann, *Methods in molecular biology*, 2012 , 828, 39
50. Elemental labelling combined with liquid chromatography inductively coupled plasma mass spectrometry for quantification of biomolecules: A review D. Kretschy, G. Koellensperger, S. Hann, 2012, *Anal. Chim. Acta*, 2012, 750, 98
51. Analysis of Iron-Phytosiderophore Complexes in soil related samples: LC-ESI-MS/MS vs. CE-MS, M. Dell'mour, W. Schenkeveld, E. Oburger, L. Fischer, S. Kraemer, M. Puschenreiter, M. Lämmerhofer, G. Koellensperger, S. Hann, *Electrophoresis*, 2012, , 33, 726
52. Systems biology approach for in vivo photodynamic therapy optimization of ruthenium-porphyrin compounds M. Pernot, T. Bastogne, N.P.E. Barry, B. Therrien, G. Koellensperger, S. Hann, V. Reshetov, M. Barberi-Heyob, *J. Photochem. Photobiol. B: Biol.*, 2012, 117, 80