# Publications

## University of Birmingham - relevant pre-PIMMS publications


1. M E O'Hara, S O'Hehir, S Green and C A Mayhew, "Development of a protocol to measure VOCs in human breath: a comparison of rebreathing and on-line single exhalations using PTR-MS" Physiol. Meas. 29 (2008) 309–330.
2. M E O'Hara, T H Clutton-Brock, S Green, S O'Hehir, and C A Mayhew "Mass spectrometric investigations to obtain the first direct comparisons of endogenous breath and blood volatile organic compound concentrations in healthy volunteers" Int. J. Mass Spectrom. 281 (2009) 92–96.
3. M E O'Hara, T H Clutton-Brock, S Green, and C A Mayhew "Endogenous volatile organic compounds in breath and blood of healthy volunteers: examining breath analysis as a surrogate for blood measurements" J.Breath Res. 3 (2009) 1-10.
4. M O'Hara and C A Mayhew "A preliminary comparison of volatile organic compounds in the headspace of cultures of Staphylococcus aureus grown in nutrient, dextrose and brain heart bovine broths measured using a proton transfer reaction mass spectrometer" J.Breath Res. 3 (2009) 1-8.
5. F Petersson, P Sulzer, C A Mayhew, P Watts, A Jordan, L Märk and T D Märk "Real-Time Trace Detection and Identification of Chemical Warfare Agent Simulants using Recent Advances in Proton Transfer Reaction Time-of-Flight Mass Spectrometry" Rapid Communications in Mass Spectrometry 23, (2009) 3875-3880.
6. C A Mayhew, P Sulzer, F Petersson, S Haidacher, A Jordan, L Märk, P Watts and T D Märk "Applications of proton transfer reaction time-of-flight mass spectrometry for the sensitive and rapid real-time detection of solid high explosives" Int. J. Mass Spectrom. 289 (2010) 58-63.
7. S. Jürschik, P. Sulzer, F. Petersson, C A Mayhew, A Jordan, B. Agarwal, S. Haidacher, H. Seehauser, K. Becker and T. D. Märk "Proton transfer reaction mass spectrometry for the sensitive and rapid real-time detection of solid high explosives in air and water" Anal Bioanal Chem (2010) 398:2813–2820.
8. B. Agarwal, F. Petersson, S. Jürschik, P. Sulzer , A. Jordan, T. D. Märk, P. Watts and C. A. Mayhew "Use of proton transfer reaction time-of-flight mass spectrometry for the analytical detection of illicit and controlled prescription drugs at room temperature via direct headspace sampling" Anal. Bioanal. Chem. 400 (2011) 2631-2639.
9. Philipp Sulzer, Alfons Jordan, Lukas Märk, Christopher A. Mayhew, Kurt Becker, and Tilmann D. Märk "Technical Advances in Proton Transfer Reaction-Mass Spectrometry and New Fields of Application" American Laboratory (August 2011)
10. Philipp Sulzer, Fredrik Petersson, Bishu Agarwal, Kurt H. Becker, Simone Jürschik, Tilmann D. Märk, David Perry, Peter Watts, and Chris A. Mayhew "Proton Transfer Reaction Mass Spectrometry and the unambiguous real-time detection of 2,4,6 TNT" Analytical Chemistry 84 (2012) 4161-4166


## RIKILT/Saskia van Ruth - pre-PIMMS publications list peer-reviewed journal papers:


1. van Ruth, S.M., Boscaini, E., Mayr, D., Pugh, J. & Posthumus, M.A.. Evaluation of three gas chromatography and two direct mass spectrometry techniques for aroma analysis of dried red bell peppers. International Journal of Mass Spectrometry, 223-224 (2002) 55-56.
2. Buhr, K., van Ruth, S.M. & Delahunty, C.M.. Analysis of volatile flavour compounds by Proton Transfer Reaction Mass Spectrometry: Fragmentation patterns and discrimination between isobaric and isomeric compounds. International Journal of Mass Spectrometry, 221 (2002), 1-7.
3. van Ruth, S.M. & Buhr, K.. Influence of saliva on temporal volatile flavour release from rehydrated red bell peppers determined by Proton Transfer Reaction-Mass Spectrometry. European Research and Technology, 216 (2003), 220-223.
4. Boscaini, E., van Ruth, S., Biasioli, F., Gasperi, F. & Märk, T.D.. Gas chromatography-olfactometry (GC-O) and Proton Transfer Reaction-Mass Spectrometry (PTR-MS) analysis of the flavor profile of Grana Padano, Grana Trentino and Parmiggiano Reggiano cheese. Journal of Agricultural and Food Chemistry, 51 (2003), 1782-1790.
5. Hansson, A., van Ruth, S. & Giannoulli, P.. Influence of gel strength on aroma release from pectin gels in a model mouth and in vivo monitored by PTR-MS. Journal of Agricultural and Food Chemistry, 51 (2003), 4732-4740.
6. Boland, A.B., Buhr, K., Giannouli, P. & van Ruth, S.M.. Influence of gelatin, starch, pectin and artificial saliva on the release of 11 flavour compounds from model gel systems. Food Chemistry, 86 (2004), 401-411.
7. van Ruth, S.M. & Drillaud, R.. Effects of saliva volume and mastication of dynamic flavour release from rehydrated French beans in a model mouth system. Journal of Food Technology, 4 (2004), 267-273.
8. van Ruth, S.M., Dings, L., Buhr, K. & Posthumus, M.A.. In vitro and in vivo volatile flavour analysis of red kidney beans by Proton Transfer Reaction-Mass Spectrometry. Food Research International, 37 (2004), 785-791.
9. van Ruth, S.M., de Witte, L. & Rey, A.. Volatile flavor analysis and sensory evaluation of custard desserts varying in type and concentration of carboxymethyl cellulose. Journal of Agricultural and Food Chemistry, 52 (2004), 8105-8110.
10. van Ruth, S.M. & Buhr, K.. Influence of mastication rate on dynamic flavour release analysed by combined model mouth/Proton Transfer Reaction-Mass Spectrometry. International Journal of Mass Spectrometry, 239 (2004), 187-192.
11. Frasnelli, J., van Ruth, S.M., Kriukova, I. & Hummel, T.. Intranasal concentrations of orally administered flavours, Chemical Senses, 30 (2005), 572-582.
12. van Ruth, S.M., Dings, L., Aprea, E. & Odake, S.. Comparison of volatile flavour profiles of kidney beans and soybeans by GC-MS and PTR-MS. Food Science and Technology Research, 11 (2005) 63-70.
13. Boland, A.B., Delahunty, C.M. & van Ruth, S.M.. Influence of the texture of gelatin gels and pectin gels on strawberry flavour release and perception. Food Chemistry, 96 (2006), 452-460.
14. van Ruth, S.M., Floris, V. & Fayoux, S.. Characterisation of the volatile profiles of infant formulas by proton transfer reaction-mass spectrometry and gas chromatography-mass spectrometry. Food Chemistry, 98 (2006), 343-350.
15. Aprea, E., Biasioli, F., Gasperi, F., Märk, T. & van Ruth, S.. Interactions of oral processing and food texture on in vivo flavour release. Flavour and Fragrance Journal, 21 (2006), 53-58.
16. van Ruth, S.M., Frasnelli, J. & Carbonell, L.. Volatile flavour retention in food technology and during consumption: juice and custard examples. Food Chemistry, 106 (2008), 1385-1392.
17. van Ruth, S.M., Koot, A., Akkermans, W., Araghipour, N., Rozijn, M., Baltussen, M., Wisthaler, A., Maerk, T.D. & Frankhuizen, R.. Butter and butter oil classification by PTR-MS. European Food Research and Technology, 227 (2008), 307-317.
18. Araghipour, N., Colineau, J., Koot, A., Akkermans, W., Moreno Rojas, J.M., Beauchamp, J., Wisthaler, A., Maerk, T.D., Downey, G., Guillou, C., Mannina, L. & van Ruth, S.M.. Geographical origin classification of olive oils by PTR-MS. Food Chemistry, 108 (2008), 374-383.
19. Luykx, D.M.A.M. & van Ruth, S.M.. A review of analytical methods for determining the geographical origin of food products. Food Chemistry, 107 (2008), 897-911.
20. Maçatelli, M., Akkermans, W., Koot, A., Buchgraber, M., Paterson, A., van Ruth, S.M.. Verification of the geographic origin of European butters using PTR-MS. Journal of Food Composition and Analysis, 118 (2009), 169-175.

21. van Ruth, S.M., Villegas, B., Rozijn, M., Akkermans, W. & van der Kamp, H.. Prediction of the identity of fats and oils by their fatty acid, triacylglycerol and volatile compositions using PLS-DA. Food Chemistry, 118 (2010), 948-955.

22. van Ruth, S.M., Rozijn, M., Koot, A., Perez Garcia, R., van der Kamp, H. & Codony, R.. Authentication of feeding fats: classification of animal fats, fish oils and recycled cooking oils. Animal Feed Science and Technology, 155 (2010), 65-73.

23. Galle, S., Koot, A., Soukoulis, C., Cappellin, L., Biasioli, F., Alewijn, M. & van Ruth, S.M.. Typicality and geographical origin markers of protected origin cheese from the Netherlands revealed by PTR-MS. Journal of Agricultural and Food Chemistry, 59 (2011), 2554-2563.

24. Ruiz-Samblás, C., Tres, A., Koot, A., van Ruth, S.M., Cuadros-Rodríguez, L. & González-Casado, A.. Proton transfer reaction- mass spectrometry volatile organic compound fingerprinting for monovarietal extra virgin olive oil identification. Food Chemistry, 2012, **dx.doi.org/10.1016/j.foodchem.2012.02.135 (http://dx.doi.org/10.1016/j.foodchem.2012.02.135)** .

25. Tres, A., Ruiz-Samblás, C., van der Veer, G. & van Ruth, S.M. (2012). Geographical provenancing of palm oil by fatty acid and volatile compound fingerprinting techniques. Journal of Agricultural and Food Chemistry, in press.

26. Capuano, E. & van Ruth, S.M.. Analytical authentication of organic produce: an overview of markers. Journal of the Science of Food and Agriculture, 2012, in press.

27. Dimitri, G., van Ruth, S.M., Sacchettia, G., Pivaa, A., Alewijn, M. & Arfelli, G.. PTR-MS monitoring of volatiles fingerprint evolution during grape must cooking. Lebensmittel-Wissenschaft und Technologie, 2012, in press.



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