

Application Note 501

Publications citing Markes' TOF MS and software products

Introduction

This Application Note is a compilation of publications and selected presentations that cite Markes' time-of-flight mass spectrometry (TOF MS) and GC-MS software products. The aim is to allow the reader to quickly identify relevant citations in the literature, as well as to demonstrate the versatility of Markes' equipment across the whole range of GC-based analytical applications.

Where available, links to the original sources are provided; if none is given, please contact us (enquiries@markes.com) to check on availability.

Within each subsection, citations are presented in reverse chronological order, and the products covered appear in bold type at the end of each entry. These products are briefly described below – to visit the relevant webpage, please click on the product name.

BenchTOF	Time-of-flight mass spectrometers for GC
Select-eV	Variable-energy ionisation technology for BenchTOF
TargetView	Post-run GC-MS compound-identification software
TOF-DS	Software for BenchTOF (including ChromCompare automated sample comparison algorithm)

Key

-  Book or thesis
-  Peer-reviewed journal article
-  Technical report
-  Magazine article
-  Conference presentation or poster

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T: +34 902 45 6677 F: +34 902 46 6677 E: inf@ingenieria-analitica.com

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General [\(back to Contents\)](#)



Select-eV: Increasing dimensionality in GC×GC–TOF MS, *39th International Symposium of Capillary Chromatography and 12th GC×GC Symposium*, Riva del Garda, Italy, May 2014.

<http://www.markes.com/Resources/Scientific-publications/Conference-posters.aspx>

BenchTOF **Select-eV**



Spot the difference: Novel software developments for comparative analysis of complex mixtures, Pittcon, Chicago, IL, USA, March 2014.

<http://www.markes.com/Resources/Scientific-publications/Conference-posters.aspx>

BenchTOF **Select-eV** **TOF-DS (ChromCompare)**



L. McGregor, N. Bukowski and D. Barden, A new outlook on soft ionisation for GC–MS, *LCGC: Current Trends in Mass Spectrometry*, March 2014, pp. 16–19.

<http://www.markes.com/News/A-New-Outlook-on-Soft-Ionization-for-GCMS.aspx>

BenchTOF **Select-eV**



D. Barden, TOF-MS takes on complex GC analyses, *Chromatography Techniques*, 2012, CT12–CT14.

<http://e-ditionsbyfry.com/Olive/ODE/RLESupp/>

BenchTOF

Environmental monitoring [\(back to Contents\)](#)



Enhanced screening of environmental pollutants in complex matrices by GC×GC–TOF MS with variable-energy electron ionisation, *39th International Symposium of Capillary Chromatography and 12th GC×GC Symposium*, Riva del Garda, Italy, May 2014.

<http://www.markes.com/Resources/Scientific-publications/Conference-posters.aspx>

BenchTOF **Select-eV**



Fast GC–TOF MS with Select-eV ionisation for high-throughput screening of environmental contaminants, *International Network of Environmental Forensics*, Cambridge, UK, August 2014.

<http://www.markes.com/Resources/Scientific-publications/Conference-posters.aspx>

BenchTOF **Select-eV**



Y.-H. Kim, K.-H. Kim, H.-O. Yoon and R.J.C. Brown, The application of gas chromatography-time-of-flight mass spectrometry to the analysis of monomethyl mercury at sub-picogram levels, *Microchemical Journal*, 2013, 110: 107–112.

<http://dx.doi.org/10.1016/j.microc.2013.03.002>

BenchTOF



A. Gravell, P. Kutty, G. Mills, D. Barden and S. Smith, GC×GC–TOF-MS complements passive sampling for the screening of pollutants in water, *LCGC: Current Trends in Mass Spectrometry*, March 2013, pp. 8–14.

<http://www.chromatographyonline.com/lcgc/Articles/GCxGCndashTOF-MS-Complements-Passive-Sampling-for-/ArticleStandard/Article/detail/809050>

BenchTOF



N. Bukowski, G. Roberts, D. Rosser and N. Watson, Identification of trace-level TO-15/TO-17 'air toxics' in complex air samples, *LCGC Applications Notebook*, September 2011.

<http://www.chromatographyonline.com/lcgc/Articles/Identification-of-Trace-Level-TO-15TO-17-Air-Toxic/ArticleStandard/Article/detail/739828>

BenchTOF **TargetView**



N. Watson, S. Davies and D. Wevill, Air monitoring: New advances in sampling and detection, *The Scientific World Journal*, 2011, 11: 2582–2598.

<http://dx.doi.org/10.1100/2011/430616>

BenchTOF

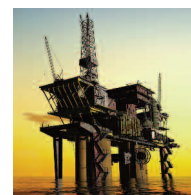
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Oil exploration and petrochemicals [\(back to Contents\)](#)



C.E. West *et al.*, Can two-dimensional gas chromatography/mass spectrometric identification of bicyclic aromatic acids in petroleum fractions help to reveal further details of aromatic hydrocarbon biotransformation pathways?, *Rapid Communications in Mass Spectrometry*, 2014, 28: 1023–1032.

<http://dx.doi.org/10.1002/rcm.6876>

BenchTOF



L. McGregor and D. Barden, Analysing crude oil: Improving compound speciation, *Hydrocarbon Engineering*, 2014, published online.

<http://www.energyglobal.com/news/processing/articles/Crude-oil-markes-analysis.aspx#.U9pAbii-8-g>

BenchTOF Select-eV



D. Jones, Synthesis, fractionation, characterisation and toxicity of naphthenic acids from complex mixtures, 2013, University of Plymouth, UK (Ph.D. thesis).

BenchTOF



R. Reeve and G. Mills, Recent advances in the analysis of complex environmental matrices, *RSC Environmental Chemistry Group Bulletin*, July 2013, pp. 5–9.

<http://www.rsc.org/Membership/Networking/InterestGroups/Environmental/bulletin.asp>

BenchTOF



S. Smith, L. McGregor and D. Barden, Identifying hydrocarbons in petrochemicals, *G.I.T. Laboratory Journal*, May–June 2013, pp. 30–31.

<http://www.laboratory-journal.com/magazine/git-laboratory-journal-europe-5-62013>

BenchTOF



S.J. Rowland, C.E. West, A.G. Scarlett, C. Ho and D. Jones, Differentiation of two industrial oil sands process-affected waters by two-dimensional gas chromatography/mass spectrometry of diamondoid acid profiles, *Rapid Communications in Mass Spectrometry*, 2012, 26: 572–576.

<http://dx.doi.org/10.1002/rcm.6138>

BenchTOF



S.J. Rowland, R. Clough, C.E. West, A.G. Scarlett, D. Jones and S. Thompson, Synthesis and mass spectrometry of some tri- and tetracyclic naphthenic acids, *Rapid Communications in Mass Spectrometry*, 2011, 25: 2573–2578.

<http://dx.doi.org/10.1002/rcm.5153>

BenchTOF



C.E. West, D. Jones, A.G. Scarlett and S.J. Rowland, Compositional heterogeneity may limit the usefulness of some commercial naphthenic acids for toxicity assays, *Science of the Total Environment*, 2011, 409: 4125–4131.

<http://dx.doi.org/10.1016/j.scitotenv.2011.05.061>

BenchTOF



S.J. Rowland, C.E. West, A.G. Scarlett, D. Jones and R.A. Frank, Identification of individual tetra- and pentacyclic naphthenic acids in oil sands process water by comprehensive two-dimensional gas chromatography-mass spectrometry, *Rapid Communications in Mass Spectrometry*, 2011, 25: 1198–1204.

<http://dx.doi.org/10.1002/rcm.4977>

BenchTOF



S.J. Rowland, C.E. West, A.G. Scarlett and D. Jones, Identification of individual acids in a commercial sample of naphthenic acids from petroleum by two dimensional comprehensive gas chromatography/mass spectrometry, *Rapid Communications in Mass Spectrometry*, 2011, 25: 1741–1751.

<http://dx.doi.org/10.1002/rcm.5040>


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 S.J. Rowland, A.G. Scarlett, D. Jones, C.E. West and R.A. Frank, Diamonds in the rough: Identification of individual naphthenic acids in oil sands process water, *Environmental Science & Technology*, 2011, 45: 3154–3159.
<http://dx.doi.org/10.1021/es103721b>


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 S.J. Rowland et al., Monocyclic and monoaromatic naphthenic acids: Synthesis & characterisation, *Environmental Chemistry Letters*, 2011, 9: 525–533.
<http://dx.doi.org/10.1007/s10311-011-0314-6>

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 S.J. Rowland, C.E. West, A.G. Scarlett, D. Jones, R. Frank and L.M. Hewitt, Steroidal aromatic 'naphthenic acids' in oil sands process-affected water: Structural comparisons with environmental estrogens, *Environmental Science & Technology*, 2011, 45: 9806–9815.
<http://dx.doi.org/10.1021/es202606d>

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 N. Bukowski, TOF-MS: A viable solution for crude oil extract analysis, *LCGC: Current Trends in Mass Spectrometry*, May 2010.
<http://www.chromatographyonline.com/lcgc/TOF-MS-A-Viable-Solution-for-Crude-Oil-Extract-Ana/ArticleStandard/Article/detail/667522>


BenchTOF

Food safety and aroma profiling [\(back to Contents\)](#)


 J. Fischer et al., Fast and solvent-free quantitation of boar taint odorants in pig fat by stable isotope dilution analysis–dynamic headspace–thermal desorption–gas chromatography/time-of-flight mass spectrometry, *Food Chemistry*, 2014, 158: 345–350.
<http://dx.doi.org/10.1016/j.foodchem.2014.02.113>

BenchTOF




 P. Morris and D. Barden, Sampling volatile organic compounds released from packaged meat, *International Meat Topics*, 2014, vol. 5, issue 1, p. 11.
<http://www.markes.com/Resources/Scientific-publications/Papers.aspx>

TargetView

 Enhanced aroma profiling by GC–TOF MS with variable-energy electron ionisation, *International Mass Spectrometry Conference*, Geneva, Switzerland, August 2014.
<http://www.markes.com/Resources/Scientific-publications/Conference-posters.aspx>


BenchTOF Select-eV TOF-DS (ChromCompare)

 D. Barden, Analyzing volatile organic chemicals in food: Emerging trends and recent examples, *American Laboratory*, February 2013, pp. 12–16.
<http://www.americanlaboratory.com/913-Technical-Articles/130837-Analyzing-Volatile-Organic-Chemicals-in-Food-Emerging-Trends-and-Recent-Examples/>

BenchTOF TargetView

 P. Morris and D. Barden, Enhancing sensitivity for the GC–TOF-MS detection of strawberry volatiles, *LCGC: The Column*, May 2013.
<http://www.chromatographyonline.com/lcgc/Articles/Enhancing-Sensitivity-for-the-GC-TOF-MS-Detection-/ArticleStandard/Article/detail/812180>

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 L. Pollack, S. Koschinski and D. Barden, Aromastoffe von Erdbeeren Verbesserte Messung mittels TD und TOF MS [Improved measurement of strawberry flavours by TD and TOF MS], *GIT Labor-Fachzeitschrift*, November 2013, pp. 700–702 [in German].
<http://www.git-labor.de/forschung/lebensmittel/aromastoffe-von-erdbeeren-verbesserte-messung-mittels-td-und-tof-ms>

BenchTOF TargetView

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K. Kilcawley and S. Ryan, Application of the Markes UNITY 2 thermal desorption system to access the volatile profiles in cheese, *Environmental Food MS Meeting*, Stansted, UK, September 2012.

TargetView



D. Barden, Milking it – Getting the most out of cheese aroma analysis, *Laboratory News*, July 2012, pp. 28–30.

<http://www.labnews.co.uk/features/milking-%E2%80%93-cheese-aroma-analysis/>

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G. Roberts, Harnessing the power of multi-hyphenation in food flavour and odour analysis, *LCGC: The Column*, March 2012, pp. 11–15.

<http://www.chromatographyonline.com/lcgc/Current+Articles/Harnessing-the-Power-of-Multi-Hyphenation-in-Food-/ArticleStandard/Article/detail/766123>

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N. Bukowski, D. Cooper and K. Thaxton, Comprehensive GC×GC–TOF MS screening for food safety to GC–QQQ regulatory levels without dependence on extensive sample clean-up, *CASSS*, San Diego, CA, USA, May 2011.

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N. Bukowski, D. Cooper and K. Thaxton, Environmental and food safety screening of persistent organic pollutants (POPs) by GC(×GC)/TOF MS without dependence on extensive sample clean-up, *59th ASMS Conference on Mass Spectrometry*, Denver, CO, USA, June 2011.

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P. Gerhards, M. Müller, P. Schanen and G. Horner, Development of a sensitive and reliable method for the measurement of volatile organic compounds migration from food packaging comparing GC/TOF MS vs. GC/quadrupole MS, *59th ASMS Conference on Mass Spectrometry*, Denver, CO, USA, June 2011.

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N. Bukowski and D. Cooper, Detecting pesticides in an apple matrix using GC×GC–TOF-MS without complex sample preparation, *LCGC Applications Notebook*, October 2011.

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T. Haas, P. Boeker, A. Cole and G. Horner, High-definition screening for boar taint in fatback samples using GC–MS, *LCGC North America*, July 2011.

<http://www.chromatographyonline.com/lcgc/article/articleDetail.jsp?id=735430&sk=&date=&pageID=4>

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T. Studt, Global food safety relies on testing, *Laboratory Equipment*, March 2011.

<http://www.laboratoryequipment.com/articles/2011/10/global-food-safety-relies-testing>

BenchTOF



N. Bukowski, Accurate and reliable analysis of beer using time-of-flight technology for gas chromatography, *American Laboratory*, April 2010.

<http://www.americanlaboratory.com/913-Technical-Articles/484-Accurate-and-Reliable-Analysis-of-Beer-Using-Time-of-Flight-Technology-for-Gas-Chromatography/>

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Fragrance [\(back to Contents\)](#)



F. Van Opstaele, T. Praet, G. Aerts and L. De Cooman, Characterization of novel single-variety oxygenated sesquiterpenoid hop oil fractions via headspace solid-phase microextraction and gas chromatography–mass spectrometry/olfactometry, *Journal of Agricultural and Food Chemistry*, 2014, 61: 10555–10564.

<http://dx.doi.org/10.1021/jf402496t>

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S. Smith, L. McGregor and D. Barden, Characterization of allergens in cosmetics by GC×GC–TOF-MS with variable-energy electron ionization, *LCGC: The Column*, February 2014, pp. 13–17.

<http://www.markes.com/Resources/Scientific-publications/Papers.aspx>

BenchTOF Select-eV



L. Kelly and G. Roberts, The analysis of complex fragrance samples using a new high-sensitivity bench-top time-of-flight mass spectrometer, incorporating on-line dynamic background compensation, *12th International Flavor Conference*, 2009, Skiathos, Greece

BenchTOF

Homeland security [\(back to Contents\)](#)



M.R. Gravett, F.B. Hopkins, A.J. Self, A.J. Webb, C.M. Timperley and J.R. Riches, Fate of the chemical warfare agent O-ethyl S-2-diisopropylaminoethyl methylphosphonothiolate (VX) on soil following accelerant-based fire and liquid decontamination, *Analytical and Bioanalytical Chemistry*, 2014, 406: 5121–5135.

<http://dx.doi.org/10.1007/s00216-014-7963-9>

BenchTOF



F.B. Hopkins *et al.*, Chemical analysis of bleach and hydroxide-based solutions after decontamination of the chemical warfare agent O-ethyl S-2-diisopropylaminoethyl methylphosphonothiolate (VX), *Analytical and Bioanalytical Chemistry*, 2014, 406: 5111–5119.

<http://dx.doi.org/10.1007/s00216-014-7674-2>

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J. Leppert, G. Horner, F. Rietz, J. Ringer, P. Schulze Lammers and P. Boeker, Near real time detection of hazardous airborne substances, *Talanta*, 2012, 101: 440–446.

<http://dx.doi.org/10.1016/j.talanta.2012.09.056>

BenchTOF TargetView



G.M. Roberts *et al.*, The detection and identification of trace level CW compounds and explosives using an online thermal desorption (TD) system with a high-sensitivity GC-based time-of-flight (TOF) mass spectrometer, *Hyphenated Techniques for Chromatography (HTC-12)*, Bruges, Belgium, January/February 2012.

BenchTOF TargetView



G. Bunte *et al.*, Near real time trace analysis of airborne chemical warfare agents and explosives, *EXAKT – Joint BMBF Research Project*, 2009.

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Forensic [\(back to Contents\)](#)



M. Statheropoulos et al., Combined chemical and optical methods for monitoring the early decay stages of surrogate human models, *Forensic Science International*, 2011, 210: 154–163.

<http://dx.doi.org/10.1016/j.forsciint.2011.02.023>

BenchTOF



P. Gerhards, P. Schanen and G. Horner, Using novel TOF-MS to increase sensitivity and confidently detect drugs of abuse in urine, *LCGC: Current Trends in Mass Spectrometry*, October 2010.

<http://www.chromatographyonline.com/lcgc/article/articleDetail.jsp?id=691435&sk=&date=&pageID=3>

BenchTOF



Material emissions [\(back to Contents\)](#)



M. Biedermann, R. Castillo, A.-M. Riquet and K. Grob, Comprehensive two-dimensional gas chromatography for determining the effect of electron beam treatment of polypropylene used for food packaging, *Polymer Degradation and Stability*, 2014, 99: 262–273.

<http://dx.doi.org/10.1016/j.polymdegradstab.2013.10.021>

BenchTOF



K.-H. Kim, S.K. Pandey, Y.-H. Kim, J.R. Sohn and J.-M. Oh, Emissions of amides (N, N-dimethylformamide and formamide) and other obnoxious volatile organic compounds from different mattress textile products, *Ecotoxicology and Environmental Safety*, 2014, published online.

<http://dx.doi.org/10.1016/j.ecoenv.2014.07.008>

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M. Biedermann and K. Grob, Assurance of safety of recycled paperboard for food packaging through comprehensive analysis of potential migrants is unrealistic, *Journal of Chromatography A*, 2013, 1293: 107–119.

<http://dx.doi.org/10.1016/j.chroma.2013.04.009>

BenchTOF



V.M. Brown and D.R. Crump, An investigation into the performance of a multi-sorbent sampling tube for the measurement of VVOC and VOC emissions from products used indoors, *Analytical Methods*, 2013, 5: 2746–2756.

<http://dx.doi.org/10.1039/c3ay40224j>

TargetView



V.M. Brown, Development of improved methods for the characterisation of organic chemicals emitted into indoor air by building and furnishing products, Cranfield University, UK, 2013.

BenchTOF



V. Brown and D. Crump, Improved methods for the screening of building and furnishing materials for VOC emissions, *10th International Healthy Buildings Conference*, Brisbane, Queensland, Australia, July 2012.

TargetView



M. Statheropoulos et al., A preliminary study of combining mass spectrometric data with audio and video signals for real-time monitoring of controlled lab-scale fires, *Sensors and Actuators B*, 2011, 159: 193–200.

<http://dx.doi.org/10.1016/j.snb.2011.06.071>

BenchTOF



V. Brown and D. Crump, The use of screening tests to determine emissions of VOCs from building and furnishing materials, *Proceedings of Indoor Air*, Austin, TX, USA, June 2011.

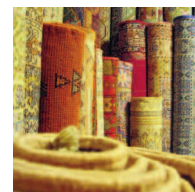
TargetView



G. Davies, Emission testing a burden?, *Quality Manufacturing Today*, January 2010, pp. 32–35.

http://www.qmtmag.com/display_edcs.cfm?edno=7572943

TargetView



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Human health [\(back to Contents\)](#)



M. Biedermann *et al.*, Mineral oil in human tissues, Part II: Characterization of the accumulated hydrocarbons by comprehensive two-dimensional gas chromatography, *Science of the Total Environment*, 2014, published online.

<http://dx.doi.org/10.1016/j.scitotenv.2014.07.038>

BenchTOF



D.C. Mueller, C. Degen, G. Scherer, G. Jahreis, R. Niessner and M. Scherer, Metabolomics using GC-TOF-MS followed by subsequent GC-FID and HILIC-MS/MS analysis revealed significantly altered fatty acid and phospholipid species profiles in plasma of smokers, *Journal of Chromatography A*, 2014, 966: 117–126.

<http://dx.doi.org/10.1016/j.chromb.2014.02.044>

BenchTOF



D.C. Mueller, M. Piller, R. Niessner, M. Scherer and G. Scherer, Untargeted metabolomic profiling in saliva of smokers and nonsmokers by a validated GC-TOF-MS method, *Journal of Proteome Research*, 2013, 13: 1602–1613.

<http://dx.doi.org/10.1021/pr401099r>

BenchTOF

Metabolomics [\(back to Contents\)](#)



P.A. Sutton, M.J. Wilde, S.J. Martin, J. Cvačka, V. Vrkoslav and S.J. Rowland, Studies of long chain lipids in insects by high temperature gas chromatography and high temperature gas chromatography-mass spectrometry, *Journal of Chromatography A*, 2013, 1297: 236–240.

<http://dx.doi.org/10.1016/j.chroma.2013.05.006>

BenchTOF



C. Degen, J. Ecker, S. Piegholdt, G. Liebisch, G. Schmitz and G. Jahreis, Metabolic and growth inhibitory effects of conjugated fatty acids in the cell line HT-29 with special regard to the conversion of t11,t13-CLA, *Biochimica et Biophysica Acta*, 2011, 1811: 1070–1080.

<http://dx.doi.org/10.1016/j.bbaliip.2011.08.005>

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Methodology [\(back to Contents\)](#)



M. Statheropoulos *et al.*, Dynamic vapor generator that simulates transient odor emissions of victims entrapped in the voids of collapsed buildings, *Analytical Chemistry*, 2014, 86: 3887–3894.

<http://dx.doi.org/10.1021/ac404175e>

BenchTOF



Y.-H. Kim, K.-H. Kim, J.E. Szulejko, M.-S. Bae and R.J.C. Brown, Experimental validation of an effective carbon number-based approach for the gas chromatography-mass spectrometry quantification of 'compounds lacking authentic standards or surrogates', *Analytica Chimica Acta*, 2014, 830: 32–41.

<http://dx.doi.org/10.1016/j.aca.2014.04.052>

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P. Boeker, T. Haas and P. Schulze Lammers, Theory and practice of a variable dome splitter for gas chromatography-olfactometry, *Journal of Chromatography A*, 2013, 1286: 200–207.

<http://dx.doi.org/10.1016/j.chroma.2013.02.057>

BenchTOF



P. Boeker, J. Leppert, B. Mysliwicz and P.S. Lammers, Comprehensive theory of the Deans' switch as a variable flow splitter: Fluid mechanics, mass balance, and system behavior, *Analytical Chemistry*, 2013, 85: 9021–9030.

<http://dx.doi.org/10.1021/ac401419j>


BenchTOF

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 Y.-H. Kim and K.-H. Kim, Generation of sub-part-per-billion gaseous volatile organic compounds at ambient temperature by headspace diffusion of aqueous standards through decoupling between ideal and nonideal Henry's law behavior, *Analytical Chemistry*, 2013, 85: 5087–5094.


<http://dx.doi.org/10.1021/ac4004425>

BenchTOF

 Y.-H. Kim and K.-H. Kim, Extent of sample loss on the sampling device and the resulting experimental biases when collecting volatile fatty acids (VFAs) in air using sorbent tubes, *Analytical Chemistry*, 2013, 85: 7818–7825.


<http://dx.doi.org/10.1021/ac401385m>

BenchTOF

 Y.-H. Kim and K.-H. Kim, An accurate and reliable analysis of trimethylamine using thermal desorption and gas chromatography–time of flight mass spectrometry, *Analytica Chimica Acta*, 2013, 780: 46–54.

<http://dx.doi.org/10.1016/j.aca.2013.03.069>

BenchTOF

 L. Pollack and D. Barden, Vielseitig und empfindlich Flugzeit-Massenspektrometer für die Gaschromatographie [Versatile and sensitive time-of-flight mass spectrometers for gas chromatography], *GIT Labor-Fachzeitschrift*, June 2013, pp. 380–383 [in German].


<http://www.git-labor.de/printausgabe/git-labor-fachzeitschrift-62013>

BenchTOF

 P.A. Sutton and S.J. Rowland, High temperature gas chromatography–time-of-flight-mass spectrometry (HTGC–ToF-MS) for high-boiling compounds, *Journal of Chromatography A*, 2012, 1243: 69–80.

<http://dx.doi.org/10.1016/j.chroma.2012.04.044>


BenchTOF TargetView

 Y.-H. Kim and K.-H. Kim, Ultimate detectability of volatile organic compounds: How much further can we reduce their ambient air sample volumes for analysis?, *Analytical Chemistry*, 2012, 84: 8284–8293.

<http://dx.doi.org/10.1021/ac301792x>

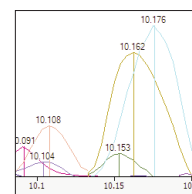
BenchTOF


Data processing [\(back to Contents\)](#)

 G.M. Roberts, Identifying trace compounds in complex mixtures with MS data-processing software, *American Laboratory*, September 2010, pp. 13–15.

<http://www.americanlaboratory.com/914-Application-Notes/511-Identifying-Trace-Compounds-in-Complex-Mixtures-With-MS-Data-Processing-Software/>

TargetView



 L. Kelly and N. Bukowski, A novel software package for identification of trace-level target compounds in clinical breath investigations using GC/MS, *Breath 2009 – International Conference on Breath and Breath Odor Research*, 2009, Dortmund, Germany.

TargetView

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T: +34 902 45 6677

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