## Roy Goodacre

## List of Publications by Year in descending order

Source: https:/|exaly.com/author-pdf/8249060/publications.pdf
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1 Proposed minimum reporting standards for chemical analysis．Metabolomics，2007，3，211－221．

Procedures for large－scale metabolic profiling of serum and plasma using gas chromatography and liquid chromatography coupled to mass spectrometry．Nature Protocols，2011，6，1060－1083．

4 Metabolomics by numbers：acquiring and understanding global metabolite data．Trends in Biotechnology，2004，22，245－252．

6 Systems level studies of mammalian metabolomes：the roles of mass spectrometry and nuclear magnetic resonance spectroscopy．Chemical Society Reviews，2011，40，387－426．

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7 A tutorial review: Metabolomics and partial least squares-discriminant analysis â€ € a marriage of
7 A tutorial review: Metabolomics and partial least squares-discriminant analysis â
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On Splitting Training and Validation Set：A Comparative Study of Cross－Validation，Bootstrap and
Systematic Sampling for Estimating the Generalization Performance of Supervised Learning．Journal of
Analysis and Testing，2018，2，249－262．
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20 Comparison of five xylan synthesis mutants reveals new insight into the mechanisms of xylan
The role of reporting standards for metabolite annotation and identification in metabolomic studies.
GigaScience, $2013,2,13$.

22 The Metabolomics Standards Initiative. Nature Biotechnology, 2007, 25, 846-848.

| 23 | Global Metabolic Profiling of <i> Escherichia coli</i> Cultures:â€\%o an Evaluation of Methods for Quenching and Extraction of Intracellular Metabolites. Analytical Chemistry, 2008, 80, 2939-2948. | 3.2 | 293 |
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| 24 | Detection of the Dipicolinic Acid Biomarker inBacillusSpores Using Curie-Point Pyrolysis Mass Spectrometry and Fourier Transform Infrared Spectroscopy. Analytical Chemistry, 2000, 72, 119-127. | 3.2 | 292 |
| 25 | The role of metabolites and metabolomics in clinically applicable biomarkers of disease. Archives of Toxicology, 2011, 85, 5-17. | 1.9 | 289 |

A proposed framework for the description of plant metabolomics experiments and their results.
Nature Biotechnology, 2004, 22, 1601-1606.
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29 Mass spectrometry tools and metabolite-specific databases for molecular identification in
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32 Metabolomics of a Superorganism. Journal of Nutrition, 2007, 137, 259S-266S.
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33 Metabolic fingerprinting of salt-stressed tomatoes. Phytochemistry, 2003, 62, 919-928.

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New cofactor supports $\hat{\underline{l}} \pm, \hat{\imath} 2$-unsaturated acid decarboxylation via 1,3-dipolar cycloaddition. Nature, 2015,
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Rapid identification of Streptococcus and Enterococcus species using diffuse reflectance-absorbance
38 Fourier transform infrared spectroscopy and artificial neural networks. FEMS Microbiology Letters,

Point-and-shoot: rapid quantitative detection methods for on-site food fraud analysis â€" moving out of the laboratory and into the food supply chain. Analytical Methods, 2015, 7, 9401-9414.
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Rapid Differentiation of Closely Related <i>Candida</i> Species and Strains by Pyrolysis-Mass
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Exhaled breath analysis: a review of â€~breath-takingâ $€^{T M}$ methods for off-line analysis. Metabolomics, 2017, 13, 110.

| 45 | Ultrasensitive Colorimetric Detection of Murine Norovirus Using NanoZyme Aptasensor. Analyt Chemistry, 2019, 91, 3270-3276. |
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| 46 | Automated workflows for accurate mass-based putative metabolite identification in LC/MS-deriver metabolomic datasets. Bioinformatics, 2011, 27, 1108-1112. |
| 47 | SERS Detection of Multiple Antimicrobial-Resistant Pathogens Using Nanosensors. Analytical Chemistry, 2017, 89, 12666-12673. |

Development and Performance of a Gas Chromatographyâ^Time-of-Flight Mass Spectrometry Analysis
48 for Large-Scale Nontargeted Metabolomic Studies of Human Serum. Analytical Chemistry, 2009, 81,
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173 7038-7046.

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\begin{aligned}
& 49 \text { UbiX is a flavin prenyltransferase required for bacterial ubiquinone biosynthesis. Nature, 2015, } 522 \text {, } \\
& 502-506 .
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50 Systems biology guided by XCMS Online metabolomics. Nature Methods, 2017, 14, 461-462.
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Clinical applications of infrared and Raman spectroscopy: state of play and future challenges. Analyst,

An automated Design-Build-Test-Learn pipeline for enhanced microbial production of fine chemicals.
Communications Biology, 2018, 1, 66.

| 55 | Rapid Quantitative Assessment of the Adulteration of Virgin Olive Oils with Hazelnut Oils Using Raman Spectroscopy and Chemometrics. Journal of Agricultural and Food Chemistry, 2003, 51, 6145-6150. | 2.4 | 153 |
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| 56 | A metabolome pipeline: from concept to data to knowledge. Metabolomics, 2005, 1, 39-51. | 1.4 | 152 |
| 57 | Genetic algorithm optimization for pre-processing and variable selection of spectroscopic data. Bioinformatics, 2005, 21, 860-868. | 1.8 | 149 |
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| 59 | Metabolomics and systems pharmacology: why and how to model the human metabolic network for drug discovery. Drug Discovery Today, 2014, 19, 171-182. | 3.2 | 140 |
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| 66 | Characterization of Microorganisms Using UV Resonance Raman Spectroscopy and Chemometrics. Analytical Chemistry, 2004, 76, 585-591. | 3.2 | 131 |
| 67 | Portable, Quantitative Detection of <i>Bacillus<\|i> Bacterial Spores Using Surface-Enhanced Raman Scattering. Analytical Chemistry, 2013, 85, 3297-3302. | 3.2 | 130 |

68 Metabolic profiling using direct infusion electrospray ionisation mass spectrometry for the characterisation of olive oils. Analyst, The, 2002, 127, 1457-1462.

Chemometric discrimination of unfractionated plant extracts analyzed by electrospray mass
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& \text { Multivariate Chemometrics. Journal of Physical Chemistry C, 2010, 114, 7285-7290. }
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| 79 | Non-invasive metabolomic analysis of breath using differential mobility spectrometry in patients with chronic obstructive pulmonary disease and healthy smokers. Analyst, The, 2010, 135, 315. | 1.7 | 119 |
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| 80 | Is Serum or Plasma More Appropriate for Intersubject Comparisons in Metabolomic Studies? An Assessment in Patients with Small-Cell Lung Cancer. Analytical Chemistry, 2011, 83, 6689-6697. | 3.2 | 119 |
| 81 | Electronic cigarette exposure triggers neutrophil inflammatory responses. Respiratory Research, 2016, 17, 56. | 1.4 | 117 |
| 82 | Metabolomic approaches reveal that phosphatidic and phosphatidyl glycerol phospholipids are major discriminatory nonâ€polar metabolites in responses by Brachypodium distachyon to challenge by Magnaporthe grisea. Plant Journal, 2006, 46, 351-368. | 2.8 | 115 |
| 83 | A comparison of Raman and FT-IR spectroscopy for the prediction of meat spoilage. Food Control, 2013, 29, 461-470. | 2.8 | 115 |
| 84 | Surface-Enhanced Raman Scattering from Intracellular and Extracellular Bacterial Locations. Analytical Chemistry, 2008, 80, 6741-6746. | 3.2 | 114 |
| 85 | Untargeted Metabolic Profiling Identifies Altered Serum Metabolites of Type 2 Diabetes Mellitus in a Prospective, Nested Case Control Study. Clinical Chemistry, 2015, 61, 487-497. | 1.5 | 113 |

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