Curriculum vitae: Prof. Roy Goodacre (age 58)

Career Prof. Biological Chemistry, ISMIB, Univ. Liverpool (1/11/2018-; HEFCE funded);
Academic Lead for Research & Impact Committee in ISMIB (2020-)
Director of University of Liverpool's Centre for Metabolomics Research (2018-);
Prof. Biological Chemistry, Chemistry, Univ. Manchester (2005-2018);
Reader in Analytical Science, Chemistry, UMIST/University of Manchester (2003-05);
Microbiology Lecturer, University of Wales Aberystwyth (1999-03);
Wellcome Trust Research Career Development Fellow, UWA (1995-99);
PDRA, Biological Sciences, UWA (1992-95).

Degrees PhD, University of Bristol (1992); B.Sc. Hons Microbiology, University of Bristol (1988).

Awards He has featured on *The Analytical Scientist* Power Lists in 2019-2021, 2023. Nils Foss Excellence Prize 2021; FACSS Charles Mann Award for Applied Raman Spectroscopy (2021); RSC Analytical Division Horizon Prize: Robert Boyle Prize for Analytical Science (2021); Fellow of the *Learned Society of Wales* (2017-); Fellow of the *Royal Society of Chemistry* (2017-); Honorary Fellow of the *Metabololomics Society* (2016-); Fellow of the *Society for Applied Spectroscopy* (2015-); RSC Industrially-Sponsored Award in Bioanalytical Chemistry (2005).

Expertise Roy Goodacre is Professor of Biological Chemistry within ISMIB and a codirector of the Centre for Metabolomics Research. He has extensive experience in MS-based metabolomics, Raman spectroscopy and surface-enhanced Raman scattering (SERS), as well as advanced multivariate data analysis. These are being developed for (i) health, disease and ageing; (ii) bacterial detection and AMR; (iii) food security using portable capable guardians; (iv) imaging tissue and single cells. He developed and established long-term metabolomics which allows fusion of GC-MS and LC-MS data collected over 12-24 months. This approach is based on mathematical corrections which effectively removes any (unavoidable) chromatographic and mass spectrometry instrumental drift. This has now been taken up widely by the community, hence why his *Nat. Protoc.* paper from 2011 (6, 1060-1083) is very highly cited (>2500 times), and we have used this for large scale (*n*=2000) metabolic profiling studies (*Nat. Commun.* (2019) 10: 5027). To understand metabolic flux on a single cell level (i.e., with respect to substrate use in bacterial communities), we are also developing high spatial resolution (0.5 µm is typical) photothermal infrared, Raman, SRS and CARS imaging.

Grants PI: ⊗ EPSRC-SFI (EP/V042882/1). Cutting Edge Analytical Solutions for Smart, Integrated, Efficient Biopharmaceutical Production. 2022-25. £442k. ⊗ BBSRC (BB/X511225/1) Impact Acceleration Account. 2022-25. £300k. ⊗ NERC (NE/Y003764/1) Applying multi-omics in environmental research. 2023-24. £58,298. CoI: ⊗ BBSRC Illuminating the dark metabolome: de novo identification of small molecules from their mass spectra using transformer-based deep learning (PI Doug Kell). 2024-2027. ⊗ Leverhulme Trust (RPG-2023-354). Understanding the functional importance of primary metabolism in giant viruses (Lead David Lamb, Swansea). 2024-2027. £289,738. ⊗ MRC (MR/S010483/1). UK Consortium for MetAbolic Phenotyping (MAP UK). Lead ICL. 2019-24. £2.1M (UoL: £413k). ⊗ MRC (MR/X001911/1). Therapeutic potential of targeting bioactive lipids in filariasis. 2022-27. £1.607M. ⊗ NERC Environ. Omics Facility (NEOF). 2024-31 Steve Patterson (PI). £16M. ⊗ BBSRC (BB/Y009258/1). Illuminating the dark metabolome: de novo identification of small molecules from their mass spectra using transformer-based deep learning (PI 2024-27 Doug Kell (PI). £634,113

Group
PDRAs I have supervised 31 postdocs and currently supervise 5.
PhDs Graduated 61 PhD students. As PI have 4 students in years 1-4.
Masters I have successfully supervised 7 MSc and 3 MPhil student(s).

Full details of current group and alumni: www.biospec.net/mems

Alumni have positions as lecturers: UK: Lancaster, Liverpool, LJMU, Manchester, Nottingham, Oxford, Sheffield, Strathclyde. USA: Texas A&M.
Saudi Arabia: King Saud, Princess Nourah Bint Abdulrahman, Umm Al-Qura (x2).

Significant external duties

1997 - Editorial Advisory Board *Journal of Analytical and Applied Pyrolysis*
2005-15 Founder and Director of the Metabolomics Society
2005 - Founder and Editor-in-Chief of *Metabolomics*
2007 Conference Chair of *Metabolomics 2007*, Manchester, UK 11-14 June
2007-13 Expert member of Marie Curie fellowship evaluations for life sciences (IEF, IIF, IOF)
2008 Editor: Special Edition on SERS in *Chemical Society Reviews* 37(5), 873-1076
2008 - Director of the Metabolic Profiling Forum
2012-15 BBSRC core member committee D
2013 Editor: topical issue on Metabolomics in *Anal. Bioanal. Chem*. 450(15), 5003-5169
2014 - Editorial Advisory Board *Analyst*
2014-23 Founder and Company Director of spinout *Spectromics*: http://www.spectromics.com
2015-16 Editor: Food Authenticity & Integrity themed collection in *Analyst* and *Anal. Methods*
2015 - International Scientific Committee for the French National Infrastructure – MetaboHUB
2015-17 Senior Editor *New Horizons in Translational Medicine*.
2016 - EAB *Spectrochimica Acta A: Molecular and Biomolecular Spectroscopy*
2016 - Intern. Advisory Board for National Center for Genetic Engineering & Biotech, Thailand.
2017-21 External Examiner for Imperial: MRes Biomed Research for the Data Science stream.
2017-18 Scientific Advisory Board for Nestlé Research Center, Lausanne, Switzerland.
2019-22 Committee member of Royal Society of Chemistry's Analytical Division Council (ADC)
2019 - Trustee of Royal Society of Chemistry's Analytical Chemistry Trust Fund (ACTF)
2020 - Director of the *Metabolomics Society* (2 terms) and current President (2022-2024).
2022 Conference co-Chair of *Spring SciX 2022*, Liverpool, UK.
2023 - International Advisory Board for *International Joint Research Center on Food Security (IJC-FOODSEC)* based in Thailand.
2024 - Scientific Advisory Board for *Singapore Lipidomics Incubator* based in the National University of Singapore.
2024 Conference co-Chair of *MetaboMeeting 2025*, Liverpool, UK.

Publications

Goodacre has authored two international patents, published >480 peer-reviewed research articles, has an H-index of 118 (Google Scholar: https://goo.gl/B3yWRC), and edited two books on metabolomics [ISBN 978-1-4615-0333-0; ISBN 978-0-387-25240-7].

Raman and imaging Spectroscopy

- *Lima, C., *Ahmed, S., Xu, Y., Muhamadali, H., Parry, C., McGalliard, R.J., Carrol, E.D. & **Goodacre, R.** (2022) Simultaneous Raman and Infrared spectroscopy: a novel combination for studying bacterial infections at the single cell level. *Chemical Science* **13**, 8171-8179.
- Lima, C.A., Muhamadali, H., Yun Xu, Y., Kansiz, M. & **Goodacre, R.** (2021) Imaging isotopically labeled bacteria at the single cell level using optical PT-IR. *Anal Chem* **93**, 3082-88.
- Subaihi, A., Trivedi, D.K., Hollywood, K.A., Bluett, M.A., Xu, Y., Muhamadali, H., Ellis, D.I. & **Goodacre, R.** (2017) Quantitative on-line liquid chromatography-surface-enhanced Raman scattering (LC-SERS) of methotrexate and its major metabolites. *Anal. Chem.* **89**, 6702-6709.
- Westley, C., Xu, Y., Thilaganathan, B., Carnell, A.J., Turner, N.J. & **Goodacre, R.** (2017) Absolute quantification of uric acid in human urine using SERS. *Analytical Chem* **89**, 2471-77.
- *Westley, C., *Fisk, H., Xu, Y., Hollywood, K.A., Carnell, A.J., Micklefield, J., Turner, N.J. & **Goodacre, R.** (2017) Real-time monitoring of enzyme-catalysed reactions using deep UV resonance Raman spectroscopy. *Chemistry - A European Journal* **23**, 6983-6987.
- Gracie, K., Correa, E., Mabbott, S., Dougan, J.A., Graham, D., **Goodacre, R**. & Faulds, K. (2014) Simultaneous detection and quantification of three bacterial meningitis pathogens by SERS. *Chemical Science* **5**, 1030-1040.
- Jarvis, R.M. & **Goodacre, R**. (2004) Rapid discrimination of bacteria using surface enhanced Raman spectroscopy. *Analytical Chemistry* **76**, 40-47.