

Brandye Smith-Goettler

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Current employer: Merck & Co., Inc., West Point, PA

EDUCATION

- Ph.D., Analytical Chemistry (Vibrational Spectroscopy), North Carolina State University, Raleigh, NC — Jan 2003 Thesis: “Application of Single-Pass Attenuated Total Reflectance FT-IR Spectroscopy to Protein Analysis.” Advisor: Stefan Franzen.
- M.S., Analytical Chemistry (Chemometrics), East Carolina University, Greenville, NC — Dec 1997 Thesis: “Application of the Bootstrap and Genetic Algorithm to Pattern Recognition.” Advisor: Paul J. Gemperline.
- B.S., Chemistry; met requirements for B.S.B. in Biochemistry, East Carolina University, Greenville, NC — Dec 1995

PROFESSIONAL EXPERIENCE

- Merck & Co., Inc., West Point, PA (Jul 2008 – Present)
 - Director, Data Science and Applied Mathematics & Modeling (Dec 2021 – Present). Activities: Lead data science support for solid dosage, vaccine, and biologics manufacturing; guide digital transformation across manufacturing sites and labs; build web applications to democratize data and analytics.
 - Principal Scientist, Center for Mathematical Sciences (Nov 2018 – Dec 2021). Activities: Delivered AI/ML and mathematical-modeling solutions for manufacturing and analytical labs; coached cross-functional teams.
 - Associate Principal Scientist, Process Analytical Technologies (Jul 2008 – Nov 2018). Activities: Developed and implemented spectroscopic and chemometric methods for process monitoring, automation, and product release. Supported multiple drug products and two regulatory filings.
- GlaxoSmithKline (GSK), Upper Merion, PA — Investigator, Process Technologies (Nov 2004 – Jun 2008)
 - Provided chemometrics and PAT support to pharmaceutical R&D; supported ~20 products.
- Icoria, Inc. (formerly Paradigm Genetics), RTP, NC — Senior Associate Scientist (Mar 2003 – Oct 2004)
 - Sole chemometrician for metabolomics/LC-MS analyses; worked on systems biology, pathway mapping, data mining, and database/software integration.
- H & A Scientific, Inc., Greenville, NC — Chemometrician (Oct 1997 – Aug 1998)
 - Mathematical support for LIMS and pharmaceutical expiration-dating software; instrumentation consulting and user-acceptance validation.

DIGITAL & TECHNICAL SKILLS

- Programming & tools: Python, R, SQL, Power Apps, Jira, GitHub, Agile Methodology

- Chemometrics/spectroscopy software: SIMCA, Unscrambler, SIPAT, S-BOL
- Other: Design-Expert, SolidWorks
- Instrumentation: FTIR/IR, NIR (including imaging), Raman, HPLC, LC-MS, GC, NMR, UV-Vis, DSC, particle-size analyzers (EyeCon, FBRM, PVM), acoustic emission, capacitance, ultrasound, and OCT

SELECTED TRAINING & CERTIFICATIONS

- Project Management, Merck (2023)
- R&D Leadership Course on Innovation, Merck (2018)
- Merck Sigma — Yellow Belt (MSYB) (2012)
- GSK Pharmaceutical Development Management Training Program (2007)
- SAS Programming Essentials (2003)

SELECTED PROFESSIONAL SERVICE

- Society for Applied Spectroscopy (SAS) — Treasurer (current); Parliamentarian, Executive Committee (2006–2007); Delegate-At-Large to Governing Board (2012–2013); Nominations Committee (2021)
- Coblenz Society — Board Member (2009–2013); President (2017–2019); Craver's Award Nominating Committee (2021)
- Federation of Analytical Chemistry and Spectroscopic Sciences (FACSS) — Workshop Chair (2008–2011); General Chair (2012)
- Eastern Analytical Symposium — Delegate to Governing Board (2007–present); Fundraising Chair (2017); Employment Bureau & Workshops Chair (2019); Exhibition Chair (2021), Short Courses Chair (2023), Program Chair (2025)
- Grace Hopper Celebration — Poster Committee Member (2020–2021)
- Phi Lambda Upsilon (NCSU) — Member (2000–2003)

SELECTED PUBLICATIONS

- Smith, B.M. & Gemperline, P.J., *Analytica Chimica Acta*, 2000, 423, 167–177. "Wavelength Selection and Optimization of Pattern Recognition Methods Using Genetic Algorithm."
- Smith, B.M. & Gemperline, P.J., *Journal of Chemometrics*, 2002, 16, 241–246. "Bootstrap Methods for Assessing the Performance of Near-Infrared Pattern Classification Techniques."
- Smith, B.M. & Franzen, S., *Analytical Chemistry*, 2002, 74, 4076–4080. "Single-Pass Attenuated Total Reflection FT-IR Spectroscopy for the Analysis of Proteins in H₂O Solution."
- Smith, B.M.; Oswald, L.; Franzen, S., *Analytical Chemistry*, 2002, 74, 3386–3391. "Single-Pass ATR FT-IR Spectroscopy for the Prediction of Protein Secondary Structure."

- Smith, B.M. et al., *Langmuir*, 2004, 20, 1184–1188. “Covalent Attachment of a Nickel Nitrilotriacetic Acid Group to a Germanium Attenuated Total Reflectance Element”
- Bakeev, K.A. (Ed.), *Process Analytical Technology*, 2nd ed., Wiley, 2010; (Ch. 13 author).
- Shah, Navnit & Sandhu, Harpreet & Choi, Duk & Chokshi, Hitesh & Malick, Ahmad. (2014). *Amorphous Solid Dispersions: Theory and Practice*. 10.1007/978-1-4939-1598-9.; (contributing author to chapters 5 and 6)
- Liu, H. et al., *Int. J. Pharmaceutics*, 2017, 525, 249–263. “Optimization of critical quality attributes in continuous twin-screw wet granulation via design space validated with pilot scale experimental data.”
- Zaborenko, N. et al., *AAPS J.*, 2019, 21:32. “First-Principles and Empirical Approaches to Predicting *In Vitro* Dissolution for Pharmaceutical Formulation and Process Development and for Product Release Testing.”
- Salami, H.; Smith-Goettler, B.; Yadav, V., *Int. J. Pharmaceutics*, 2025, 669. “How can language models assist with pharmaceuticals manufacturing deviations and investigations?”