Dr. Prof. Bhushan Bonde, PhD, MTech, BPharm

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Innovating Drug Discovery with GenAI-ML and Quantum Computing

Technical product leader with 20 years in Pharmaceutical IT and In-silico R&D, Bioinformatics /Comp. Biology and platform engineering, building a GenAI platform/product at the intersection of AI and drug discovery. Deep hands-on expertise in agentic AI architectures, RAG pipelines, multi-model orchestration, vector search, and LLM model routing - complemented by a strong computational Informatics and modelling, computational biology science foundation.

Currently leading GenAI Projects: an agentic retrosynthesis platform orchestrating deep learning models, and an AI-driven migration platform converting legacy pharma workflows to Python/open-source tools with LangChain, LangGraph, OpenClaw/BioClaw tools integration as Agentic AI and Bridging deep scientific domain knowledge with platform product thinking, cloud-native architecture, and developer enablement to deliver governed, scalable GenAI capabilities.

CORE COMPETENCIES/SKILLS:

GenAI Platform Strategy	Agentic AI / LangGraph	RAG Pipelines & Vector Search
LLM Model Selection & Routing	Multi-Model Orchestration	Prompt Engineering & Optimization
DevOps / MLOps / CI-CD	Docker/Podman/Apptainer/Kubernetes	Cloud (AWS / Azure) & HPC (on-prem)
Comp Bio-Cheminformatics	Drug Discovery Informatics	Pharma R&D Workflows
IT Product Roadmap & Backlog	Stakeholder Management	Agile Delivery (Jira / Confluence)
API Design & Integration, Testing.	Python / JavaScript / C++	Data Governance & Compliance
Quantum Computing applications		

Key Publications:

- Edge, Fog, and Cloud Against Disease: The Potential of High-Performance Cloud Computing for Pharma Drug Discovery, Bonde B, (2023), In Book Title: High Performance Computing for Drug Discovery and Biomedicine, DOI: 10.1007/978-1-0716-3449-3_8.
- The Future of Drug Development with Quantum Computing, Bonde, B., Patil. P, Choubey B. (2023) In Book Title: High Performance Computing for Drug Discovery and Biomedicine, DOI: 10.1007/978-1-0716-3449-3_7.

PROFESSIONAL WORK EXPERIENCE:

Visiting Honorary Professor of Computational Biology, Uni. of Suffolk. May 2022 - Present

Digital Futures Institute, University of Suffolk Ipswich, England, United Kingdom

- Industry-academic research on Quantum computing-based Drug discovery: 1 PhD student.
- AI-ML and Deep learning-based drug discovery: 3 master's students
- GenAI-Protein Dynamics Model on Physics informed Graph Neural Networks, GenAI based drug discovery, Protein networks, Knowledge Graphs for drug discovery.

Head of Innovation for In-silico R&D, Drug Discovery, Evotec Pharma, UK Oct 2021 – June 2026.

- Designed and built a multi-model deep learning platform for retrosynthetic analysis, orchestrating 6 models (template-based, template-free, diffusion) through an agentic AI architecture with intelligent model routing.
- Defined product vision, roadmap, and go-to-market strategy targeting a market (41% CAGR); conducted customer discovery with medicinal chemistry, process chemistry, and CRO/CDMO stakeholders.
- Architected 6-agent LangGraph orchestration pipeline for prompt orchestration, forward validation, feasibility scoring, literature cross-referencing, and self-improvement—enabling multi-step reasoning and tool use.

- Implemented Cascade of Ensembles routing (3-tier: fast/balanced/powerful) achieving 7× cost reduction through intelligent LLM model selection and query routing.
- Built KnowRAG pipelines integrating reaction databases, supplier catalogues, and scientific literature via embeddings and vector search for context-aware route planning.
- Defined platform governance: model versioning, evaluation frameworks, safety guardrails, and audit trails for GxP-adjacent workflows.
- Scientific application and High-Performance computing for AI-Deep leaning (CPU/GPU) and GPU Molecular Dynamics based compound screening.
- EvoFold/CoFold Protein folding (Chai-1, Boltz2, OpenFold) – Optimise and full stack workflows on GPU/Slurm and In-house development/Fine tuning.
- GenAI driven Antibody discovery (EBiophi, Agentic Antibody discovery workflow tools development)

Head of Innovation Development (Early Solutions), UCB-Celltech, UK **Jan 2018 - Oct 2021**

- Provisioning of Docker/Container engineering for Scientific applications
  AI-Deep leaning (CPU/GPU) and GPU Molecular Dynamics based compound screening.
- Retrosynthesis Chemistry and DeepCDR-antibody modelling algorithm development
- Digital Poster App for internal science congress.
- Quantum Computing application to Drug Binding kinetics, metabolic pathway mining.

Data Integration Head, (IT NewMeds), UCB-Celltech, UK **Sept 2014 – Jan 2018**

- Data Integration, Translational/Analytics of Big Data in R&D.
- Omics data management and storage. (Genomics, Proteomics, Metabolomics)
- Preclinical and clinical data standard and integration and Big Bio Data visualization
- Development of Deep Data integration of project for Drug Discovery

High Performance Computing Lead, (IT), UCB-Celltech, UK

- Strategy Management for High-Performance Computing (HP-SuperdomeX and CUP/GPU Cluster) for Drug Discovery, AI and Machine learning for Genetics, statistical teams across UCB
- Deep learning infra provisioning for Early Drug discovery, Job Queue (SLURM) for GPU-Docker-scientific computing.
- Kubernetes and docker provisioning for CADD and Bioinformatics applications

Investigator, (Computational Biology), GSK, UK **June 2009 - Aug 2014**

- Enabled Next Gen Seq (ChIP-Seq/RNA-Seq/DNA-Seq) to metabolic network, Disease network, PK-PD modelling, Synthetic biology and data integration for GSK R&D
- Bioinformatics data analysis for Therapeutic areas: Respiratory, Immune-Inflammation, Oncology, Infectious Disease (Bacterial/Viral), Rare Disease, Synthetic biology and Biologicals,
- Management of small team of Junior Bioinformaticians
- Enabled IT-Technical and Budgeting (Purchase of hardware/software)

Senior Computational Biologist, Sanger Genome Centre, (Hinxton, UK) **Mar 2009 - Jun 2009**

- Worked on Genome wide Single Nucleotide Polymorphism and Copy Number Variation study across large UK population to identify genetic biomarkers for Cardiac and Blood disorders.

Bioinformatics/Systems biology Scientist (GSK, UK) **June 2008 – Dec 2008**

- Work on Respiratory therapeutics and drug discovery, Genomics and Transcriptomics, Microarray data analysis, ChIP-Seq data analysis, *in-house* computational tool development.

Bioinformatics/Systems biology modeller (BBSRC Researcher) **May 2006 – July 2009**

Faculty of Health and Medical Sciences, University of Surrey, Guildford, UK.

- To develop new algorithms, software tools and techniques in understanding the complex biological process for persistent tuberculosis infection.
- ^{13}C labelled metabolic modelling for flux estimation in TB

Research Associate (Computer Aided Drug Discovery) **July 2001 – June 2002**

Molecular Modelling Div., Ranbaxy Research Lab, New Delhi.

- Development of neural network-based drug pharmacophore
- Homology modelling, molecular dynamics for protein-ligand complexes
- Mathematical modelling and software development for new drug discovery.

Research Trainee, Bhabha Atomic Research Centre (BARC), Gov. of India. Jan 2001-Mar 2001

- Isolation, purification & estimation of plasmid DNA from microorganism.
- Genome manipulation for improvement of productivity of plant & microbial products.

Research Assistant, National Chemical Laboratory (NCL), Gov. of India, May 1998 – June 1999

- Synthesis, design & modelling of a new family of biodegradable hydrogels based on Poly (ethylene glycol) and Amino acids for drug delivery.
- Microwave based chemical synthesis of drug derivatives (deprotection of allyl esters) catalysed by montmorillonite K-10 clay.
- Instrumental /analytical data measurement techniques for chemical synthesis.

EDUCATION:

Ph. D. in Computational Biology (Oxford Brookes University, Oxford) **Oct 2002 – May 2006**

School of Biological & Molecular Science, Oxford Brookes University, Oxford, UK

Title: Bioinformatics and Metabolism: The relationship between metabolism and genome structure.

M.S. Tech in Bioprocess Technology (Engineering) **Jun 1999 – May 2001**

Institute of Chemical Technology (UICT), University of Mumbai, India

Junior Research Fellowship (JRF: DBT award 1999)

Title: Application of Computer Modelling in Biocatalysis. (Application of neural networks for development of ANN based pharmacophore for new drug discovery)

Grade: First Class

Bachelor of Pharmacy (University of Pune, India) **Jun 1994 – May 1998**

AWARDS:

- Honoured to be selected on the top 75 scientist : Scientific Computing World 75 (SCW75) people across the globe for achievement in the filed of AI, ML and Quantum Computing for year 2026.
- UCB-Microsoft Covid-19 Moonshot: Internal award for the work on Covid-19 Azure Fragment based Drug Discovery (Sept-2020), Belgium IT Project of the year award (Oct-20).
- Multiple impact awards for work on HPC computing and Bio/Chem informatics projects, UCB.
- GSK CEO's Sustainability award for project on Amigal production, Synthetic Biology data analysis, Mar 2014
- GSK Coronation festival award for Multiverse GSEA software design May 2013
- GSK Bronze impact award for MetabolomDB database design and implementation Oct 2013.
- Silver Impact award, Comp. Biology, GSK, Systems Pharmacology GeneGo2SBML model conversion, 2012.
- Bronze Impact award, Comp Biology, GSK, Rare disease/Orpha-net data analysis, 2012.
- Bronze Impact Award, Comp Biology, GSK. Two awards for work on ChIP-Seq/RNA-Seq analysis workflow development 2010, 2011.

- Post-Doctoral Fellowship (June 2006 – Nov 2008) from Biotechnology and Biological Sciences Research Council, (BBSRC) at University of Surrey.
- University research fellowship for Doctoral research in Computational biology and metabolic modelling, Oxford Brookes University (Oct 2002 – Nov 2005).
- Junior research fellowship for Masters in Bioprocess Technology from Dept. of Biotechnology (DBT), Government of India (Jun 1999 – Mar 2001).
- Summer research fellowship from Indian Academy of Sciences, Bangalore (1998).
- National Scholarship at school level from state government (1984 -1987).
- State and National level awards for various project in Science exhibition at school level (1987-1990).

PROFESSIONAL CERTIFICATIONS:

- UCB Accelerate Leadership program – Year 2017
- Internet of Things (IoT): Business Transformation: 2016
- RNA-Seq/NGS data analysis, EMBL-EBI, UK 2010.
- Project Management/Networking for Researchers, Univ. of Surrey, Feb-2007.
- Transcriptomics (Microarray Data Analysis), Ensembl from EMBL-EBI-UK, July 2008
- Systems Biology Dynamics: From Genes to Organisms, 17 – 28 May 2004, the Centre for Nonlinear Dynamics in Physiology and Medicine, McGill University, Montreal, Canada.
- Statistical analysis using SPSS, Jan 2004, Oxford, UK.
- Genomics, Proteomics and Beyond, 9-12 Dec 2003, University of Oxford, UK.
- Molecular Modelling and Pharm informatics, 22-26 July 2002, NIPER, India.

CONFERENCE PRESENTATIONS / INVITED TALKS:

- B. Bonde, Technology Practice - The Age of Quantum Computing: discover how it will change the world, 27 June 2019. UCB Next Gen Tech Foundation UCB Belgium.
- B. Bonde, Applications of Artificial Intelligence in Pharmaceutical Industry, AI in Pharma R&D meeting, London, Nov 2016.
- B. Bonde, Post NGS-Drug Discovery Based Data Integration, 13 Nov 2015, 7th Annual Next Gen Seq Congress. London, Nov 15.
- B. Bonde, Challenges of omics data management: Integration and data analysis in the post genomic NGS era, 15 June 2015, Next Gen Seq Data Congress, London 2015.
- B.Bonde, Integrating and analysing NGS data: Applications to Drug Discovery. NGS Pharma Conference, Frankfurt, Jan 2013.
- B. Bonde, Application of NGS to Microbial strain improvement**,** NGS Conference, Oxford Global, London Nov 2012.
- B. Bonde, Applications of Systems Biology in Drug Discovery: From Target to Toxicity Prediction using Genome Scale Metabolic Network modelling, Indian Pharmaceutical Congress 2009.
- B.Bonde, WebFBA-Tools for genome scale metabolic modelling of *M. tuberculosis*. Workshop on Systems Biology at Univ of Iceland, Reykjavik (25 Oct 2007)
- Fell D. A., Bonde B., Poolman M. G, The substructure of large metabolic networks, 2005, *FEBS Journal* **272** (s1), [H4-003] at FEBS conference.
- Bonde, B., Structural Modelling of *E.coli* metabolic network, 2004, at Systems Biology Dynamics: from Genes to Organisms, organised by Centre for Nonlinear Dynamics, McGill University, Montreal, Canada.
- Bonde, B., *In-silico* structural modelling of metabolic network, 2004, at Postgraduate Research Students Seminar, Oxford Brookes University, Oxford.
- Bonde, B., Poolman, M., Fell, D., Structural Analysis of Genomic Scale Metabolic Models, 2004 at Young-BTK workshop 2004, Oxford.
- Bonde, B., Modelling of large genomic scale metabolic networks, 2003, at School of Biological and Molecular Sciences Research Symposium, Oxford.
- Bhushan K. Bonde**,** Applications of Neural Networks in Pharmacy, 2000 at International Symposium on Strategies and Prospective in Drug Development, Design and Molecular Modelling, Indian Institute of Chemical Biology, Calcutta.

- Bina Ningu, Bhushan Bonde, Sunil Bhagwat. Development of Mathematical model for OSMAT (Osmotical drug delivery tablet), 2000, Indian Pharmaceutical Congress, Hyderabad, 1-3 Dec. 2000.

PUBLICATIONS & RESEARCH SUPERVISIONS:

- Edge, Fog, and Cloud Against Disease: The Potential of High-Performance Cloud Computing for Pharma Drug Discovery, Bonde B, (2023), In Book Title: High Performance Computing for Drug Discovery and Biomedicine (ISBN: 978-1-0716-3448-6), DOI: 10.1007/978-1-0716-3449-3_8 .
- The Future of Drug Development with Quantum Computing, Bonde, B., Patil. P, Choubey B. (2023) In Book Title: High Performance Computing for Drug Discovery and Biomedicine (ISBN: 978-1-0716-3448-6), DOI: 10.1007/978-1-0716-3449-3_7 .
- Simulation of Small molecules on Quantum Computers, Oxford Uni. DPhil Project, Maranga Mokaya, DPhil candidate in Sustainable Approaches to Biomedical Science, Supervised by: Prof. Philip Biggin and Industry Supervisors Dr. Bhushan Bonde and Jiye She, UCB, September 2020.
- Borah K, Kearney J-L, Banerjee R, Vats P, Wu H, Dahale S, Bonde B *et.al* (2020) GSMN-ML- a genome scale metabolic network reconstruction of the obligate human pathogen Mycobacterium leprae. PLoS Negl Trop Dis 14(7): e0007871. https://doi.org/10.1371/journal.pntd.0007871
- Nicolaas C Kist, Robert A Power, Andrew Skelton, Seth D Seegobin, Moira Verbelen, Bhushan Bonde, Karim Malki, RNASeq_similarity_matrix: visually identify sample mix-ups in RNASeq data using a 'genomic' sequence similarity matrix, *Bioinformatics*, Volume 36, Issue 6, 15 March 2020, Pages 1940–1941, https://doi.org/10.1093/bioinformatics/btz821
- Application of Causal Reasoning to Yeast Molecular Interaction Networks,
  Thesis: Effrosyni Karakitsou, Surrey Uni. MSc Systems Biology, Supervisors: Dr Emma Laing, Professor Andre Gerber, Industry Supervisor: Dr Bhushan Bonde, Sept 2015.
- Network analysis plays diverse roles in drug discovery,
  Samiul Hasan, Bhushan K Bonde, Natalie S Buchan, Matthew D Hall, *Drug Discov Today*. 2012 Aug;17(15-16):869-74.
- ^{13}C metabolic flux analysis identifies an unusual route for pyruvate dissimilation in mycobacteria which requires isocitrate lyase and carbon dioxide fixation.
  Beste DJ, Bonde B, Hawkins N, Ward JL, Beale MH, Noack S, Nöh K, Kruger NJ, Ratcliffe RG, McFadden J. *PLoS Pathog*. 2011 Jul;7(7).
- The application of next-generation sequencing technologies to drug discovery and development. Woollard PM, Mehta NA, Vamathevan JJ, Van Horn S, Bonde BK, Dow DJ. *Drug Discov Today*. 2011 Jun;16(11-12):512-9.
- Differential Producibility Analysis (DPA) of transcriptomic data in the context of genome scale metabolic reaction networks: Deconstructing the metabolic response of M. tuberculosis to the host environment. Bhushan Bonde, Dany Beste , Emma Laing, Andrzej Kierzek, Johnjoe McFadden. Bonde BK, Beste DJ, Laing E, Kierzek AM, McFadden J. *PLoS Comput Biol*. 2011 Jun;7(6):e1002060. Epub 2011 Jun 30.
- Selection of objective function in genome scale flux balance analysis for process feed development in antibiotic production. Chiraphan Khannapho, Hongjuan Zhao, Bhushan K Bonde, Andrzej M Kierzek, Claudio A Avignone-Rossa, Michael E Bushell, *Metab Eng*. 2008 Sep;10(5):227-33.
- The Genetic Requirements for Fast and Slow Growth in Mycobacteria. Dany J. V. Beste, Mateus Espasa, Bhushan Bonde, Andrzej M. Kierzek, Graham R. Stewart, and Johnjoe McFadden, *PLoS ONE*. 2009; 4(4): e5349.
- GSMN-TB: a web-based genome scale network model of *Mycobacterium tuberculosis* metabolism. Dany Beste, Tracy Hooper, UBhushan BondeU, Graham Stewart, Claudio Avignone-Rossa, Michael Bushell, Paul Wheeler, Steffen Klamt, Andrzej Kierzek and Johnjoe McFadden, *Genome Biology*, 2007, 8:R89
- Transcriptomic analysis identifies growth rate modulation as a component of the adaptation of mycobacteria to survival inside the macrophage, Dany Beste, Emma Laing, Bhushan Bonde, Claudio Avignone-Rossa, Michael Bushell and Johnjoe McFadden *J. Bacteriology*, 2007, 189(11), 3969-3976.
- Challenges to Be Faced in the Reconstruction of Metabolic Networks from Public Databases, Poolman, M. G., Bonde, B. K., Gevorgyan, A., Patel, H. H. and Fell, D. A. (2006), *IEE Proc. Syst. Biol.* 153, 379-384

- Microwave accelerated selective and facile deprotection of allyl esters catalyzed by montmorillonite K-10., A. S. Gajare, N. Shaikh, B. K. Bonde, V. H. Deshpande. *JCS Perkin Trans. I*, 2000, 639-640.
- Patents in Pharmacy: The Indian Scenario, Bhushan K. Bonde and V. M. Aurangabadkar. *The Eastern Pharmacists*, 1999, Vol. XLII (501), 21-27.

VOLUNTEER EXPERIENCE:

- **UK STEM Ambassador (STEMNET) UK** **Jan 2010 - till Present**
- STEMNET (http://www.stemnet.org.uk) creates opportunities to inspire young people in Science, Technology, Engineering and Mathematics (STEM), STEM Ambassadors are an invaluable and free resource for teachers and schools. They offer their time voluntarily to enthuse and inspire students within schools about STEM subjects. They can do this through a variety of activities such as clubs, careers talks, helping with school events, lessons and competitions, and much more.