

# Sanatan Upmanyu

AI for Biomedicine - Hypothesis to Patient | GenAI | LLM-RAG | Knowledge Graphs | Digital Twins

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## SUMMARY

Data-science executive with 18+ years spanning wet-lab biology, AI/ML engineering, and cross-site leadership across pharma, biotech, and consumer health. Architect of the AlphaMeld platform - an end-to-end AI stack that accelerates target triage and indication selection for global drug-makers. Deep experience in clinical-trial design and enrollment prediction, digital-twin modelling, and large-scale knowledge-graph analytics. Known for converting multimodal data into real business value, scaling cross-functional teams, and forging industry partnerships that redefine R&D.

## CORE COMPETENCIES & SKILLS

**Leadership & Strategy:** P&L & site management, Product vision, Agile delivery, Partner & client engagement

**AI/ML & Data Science:** GenAI & LLM-RAG, Agentic workflows, Predictive modelling, Graph analytics, NLP, Causal inference

**Life Sciences & Health:** Clinical-trial optimisation, MOA & target validation, Omics integration, Real-world data, Regulatory intelligence

**Cross-Functional Excellence:** Team mentoring, Stakeholder storytelling, Change management, Regulatory awareness

**Technical Toolset:** Python, R, TypeScript, React, Next.js, LLMs & RAG, Agentic AI, NLP, LangChain, PyTorch, spaCy, Neo4j, PostgreSQL, MongoDB, AWS, Docker, Kubernetes, Git, CI/CD

## EXPERIENCE

### Apxora GmbH

Dec 2024 - Present

Co-Founder & AI/Data Science Head | Basel, Switzerland

- Drives development and deployment of the ResearchNexus and Clinical Navigator platforms.
- Leads strategic AI/ML initiatives for detecting early innovation signals for emerging targets, novel therapeutics, and healthcare solutions.
- Supports the Asset Lifecycle Manager and Portfolio Management platforms.

**Skills:** Python, LLMs, React, AWS, Neo4j

### RenaissThera Pvt Ltd

Sep 2024 - Present

Scientific & AI Advisory Board | Remote

- Advising on AI-driven strategies for early-stage drug discovery and translational research.
- Shaping the future of health through regulatory-aware innovation in digital and data sciences.

**Skills:** AI Strategy, Drug Discovery

### AlphaMeld GmbH (formerly InveniAI GmbH)

Dec 2020 - Present

Head of Data Sciences - Site Head | Basel, Switzerland

- Leads development and deployment of the AlphaMeld Platform.
- Spearheads strategic AI/ML initiatives to enhance AlphaMeld/AlphaCompass capacity.
- Advises pharma/biotech companies on leveraging data science methodologies.
- Applied deep molecular biology expertise for MOA analyses and therapeutic target viability.
- Manages a data science team of 5 members.

**Skills:** Python, Neo4j, AWS, React, LLMs, Knowledge Graphs

## ArtiXio Pvt Ltd

Sep 2017 - Present

Chief Technology Officer | Remote

- Owns technology strategy, architecture, and delivery of ArtiXio's digital product portfolio - from concept to production.
- Conceptualized and built CuriousRI, a secure role-based regulatory intelligence platform covering pharmaceuticals, biologics, biosimilars, and generics across 12+ agencies (FDA, EMA, PMDA, NMPA, Health Canada, MHRA, Swissmedic, and more), with LLM-powered document analysis.
- Architected additional technology applications for the company, including an AI assistant that mines global regulatory updates and auto-drafts submission dossiers - opening a new non-pharma revenue channel.
- Directs enterprise-level data science and AI product development using Agile methodologies, ensuring adherence to global regulatory standards (FDA, EMA, ICH) across the drug development lifecycle.

**Skills:** React, Next.js, TypeScript, LLMs, Agentic AI, PostgreSQL

## Kstych Pvt Ltd

Jul 2012 - Aug 2023

Co-Founder | Director Data Sciences | Life Science Consultant | Gurgaon, India

- Co-founded and led data sciences, applying statistical, mathematical, and predictive modeling to build algorithms for life-science research questions.
- Advised pharma and biotech firms on de novo, reformulation, repurposing, and drug-rescue strategies using real-world data.
- Built statistical predictive models using NLP and machine learning on RWD; led therapeutic target assessment and MOA analysis.
- Hands-on expertise in Python, R, KNIME, MongoDB, Hadoop, MySQL/MariaDB, Tableau, Gephi, and Cytoscape.

**Skills:** Python, R, NLP, MongoDB, Hadoop, Tableau

## InveniAI LLC

Sep 2017 - Nov 2020

Senior Director of Data Science | Hybrid Gurgaon IN / CT US

- Conceptualized, built, and executed innovative solutions throughout the drug development lifecycle.
- Managed enterprise-level data science products using Agile methodologies.
- Established short- to long-term strategies for Data Science and AI teams.

**Skills:** Python, Agile, Data Science, AI/ML

## BioXcel Corporation

Nov 2010 - Jul 2017

Director Data Sciences | Life Science Consultant | Gurgaon, India

- Directed drug repurposing and novel target hypothesis generation using big data and statistical techniques.
- Advised pharma and biotech firms on diverse scientific strategic projects, surveys, and future opportunity mapping (de novo, reformulation, repurposing, drug rescue) using real-world data.
- Managed and mentored a team of data scientists; partnered closely with US-based pharma and biotech clients.
- Led project management and strategy consulting efforts, providing scientific support to business development.

**Skills:** Data Science, Drug Repurposing, Big Data, Strategy

## Ranbaxy

Jan 2008 - Nov 2010

Research Biologist | Gurgaon, India

- Conducted siRNA targeted gene silencing for target-based drug discovery.
- Cloning, expression, purification, and activity analysis of human kinases, cytochrome P450 proteins, GPCRs, and bacterial enzymes - supporting enzyme- and cell-based NCE screening assays.
- Managed experiments using mammalian, baculovirus, and Dictyostelium expression systems.

**Skills:** Molecular Biology, siRNA, Drug Discovery

## SELECTED PLATFORMS & INITIATIVES

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### AlphaMeld Operating System (Live)

Compresses hypothesis-to-insight cycles from months to weeks, varying by disease area

End-to-end AI stack combining a custom UI layer (Knowledge Graph, ChatAlphaMeld, Bioinformatics, Literature Analysis, AlphaClinMeld) with 12 ML models - including NER, RE, evidence scoring, digital-twin CT predictors and landscape assessment - running on PostgreSQL + Neo4j and self-hosted LLM APIs.

### **Discovery Navigator** (Early access)

Hypothesis landscaping compressed from weeks to hours, with traceable evidence at every step

Guided drug-discovery hypothesis-generation platform built on the AlphaMeld Knowledge Graph. Supports four starting points - disease-first, target-first, indication expansion, and combination therapy - through a step-by-step workflow (project → config → exploration → agent scoring → ranking → hypotheses). A project-aware Discovery Copilot accompanies every step. Multi-tenant SaaS with SSO, RBAC, and audit logging.

### **ChatAlphaMeld Benchmark Suite** (Research)

97.34% accuracy on 188-question ACM benchmark

Two agentic workflow engines fine-tuned on biomedical tasks; outperformed leading general-purpose frontier LLMs; delivered richer step-by-step rationales critical for complex clinical questions.

### **SequenceFlow ResearchNexus & Clinical Navigator** (Live)

6+ integrated modules

End-to-end AI stack combining Knowledge Graph, Clinical Trial Prediction, Literature Analysis, Patient Digital Twin, TPP, TOP with 12 ML models running on PostgreSQL + Neo4j and self-hosted LLM APIs.

### **AlphaCompass Portfolio Intelligence** (Live)

Standardized indication-prioritization across 200 active programs

Clinical-trial-centric SaaS module on AlphaMeld graph analytics; benchmarks pipeline assets and quantifies comparative risk. Adopted by two BD teams within six months, standardizing evidence-based indication-prioritization across 200 active programs.

### **Digital Twins for Systemic Sclerosis (EUSTAR)** (Research)

In-silico control arms over a 23,000+ patient, 200+ center systemic sclerosis registry

Outcome-focused digital-twin framework built on the EUSTAR systemic sclerosis registry - longitudinal records for 23,000+ patients across 200+ centers. A PyTorch deep/generative stack (a mask- and time-aware GRU-D sequence forecaster plus a conditional sequence-VAE twin generator) produces prognostic scores and synthetic placebo trajectories for organ-specific and composite clinical outcomes. Designed as an ML-generated digital control arm - a PROCOVA/ANCOVA covariate that lifts trial power and cuts sample size - aligned with FDA digital-twin and EMA/ICH MIDD guidance.

### **Clinical-Trial Digital Twins** (Research)

In-silico placebo arms demonstrated for Phase II Type 2 Diabetes trials

Conditional variational auto-encoder (CVAE) pipeline that synthesizes patient-level digital twins for Phase II Type 2 Diabetes trials. Generated matched placebo trajectories and predicted drug-response curves - proving feasibility of in-silico arms for protocol optimization and hypothesis testing.

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## **EDUCATION**

### **University of Rajasthan**

Bachelor's Degree, Biotechnology | 2008

### **Bioinformatics Institute of India**

Diploma, Bioinformatics | 2004

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## **PUBLICATIONS**

- DeAngelis, M., Wilkinson, E., Anant, M., Sharma, S., Vijayadamodar, G., Upmanyu, S., Ganjoo, A., Alesci, S., Kant, A., & Nandabalan, K. (2022). AI-based deconvolution of the gut-brain axis (GBA) and its therapeutic implications. *Gastroenterology*, 162(7-S), 760.
- Rastelli, L., Gupta, S., Dahiya, A., Jagga, Z., Nandabalan, K., & Upmanyu, S. (2017). The synergy between BXCL701, a DPP inhibitor, and immune checkpoint inhibitors discovered using AI and Big Data analytics. *AACR; Cancer Res*, 77(13 Suppl), Washington, DC.
- Sheetal, K., Upmanyu, S., Sharma, H., & Nandabalan, K. (2015). Targeting immune checkpoints: using a big data approach for their identification, prioritization and application. *AACR 106th Annual Meeting*, Philadelphia, PA.
- Tiwari, P., Saini, S., Upmanyu, S., Benjamin, B., Tandon, R., Saini, K. S., & Sahdev, S. (2010). Enhanced expression of recombinant proteins utilizing a modified baculovirus expression vector. *Molecular Biotechnology*, 46, 80-89.
- Tiwari, P., Saini, S., Upmanyu, S., Saini, K. S., & Sahdev, S. (2009). Enhanced expression of kinases and cyp-450 enzymes through a modified Baculovirus expression vector for oncology research. Poster, *International Symposium on Cancer Chemoprevention*, JNU, New Delhi.

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## **PATENTS**

- Novel Immunomodulatory Therapeutic Strategies Targeting Tumors in Cancer (US20180134771, United States Patent and Trademark Office)
- Immunomodulation Therapies for Cancer (US20190008918, United States Patent and Trademark Office)

## **SELECTED SPEAKING & PANELS**

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- NLP for Life Sciences - Speaker: NLP in Healthcare: From Patient Records to Research & Education (Delhi (Virtual), 14 Nov 2025)
- Web Summit 2025 - Startup Showcase: Agentic AI for Asset and Portfolio Lifecycle Decisions (Lisbon, 14 Nov 2025)
- Microsoft AI Tour - Startup Pitch Presenter: Agentic AI for Portfolio & Product Lifecycle Decisions (Lausanne, 18 Jun 2025)
- Basel Data Science & AI Meetup - Invited Speaker: Effects & Impact of Knowledge Graphs in Drug Discovery (Basel, 11 Dec 2024)
- GlobalBioIndia 2024 - Panelist: AI for Next-Generation Therapeutics (New Delhi, 13 Sep 2024)
- AI for Pharma & Biotech - Workshop Presenter: Quantum Leap in Drug Discovery: LLMs & Deep Learning for Material Sciences (Virtual, 2024)