Dr. Alexander James Porter

Scientific Software & Platform Delivery | R&D Tooling & Adoption | Predictive Modelling Workflows

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PROFESSIONAL PROFILE

Scientific software and platform specialist with strong R&D credibility, practical AI fluency and a track record of building and enabling adoption of predictive modelling, data and digital capabilities across scientific users. Current work spans digital chemical design, predictive modelling platforms, scientific data products, Python engineering and user enablement.

Recent work has moved beyond traditional computational chemistry into reusable scientific software, connected data workflows, AI-enabled tools and shared platforms. Effective where scientific users, data practitioners, platform teams, software developers and digital stakeholders need to turn complex capability into adopted, trusted workflows.

CORE CAPABILITIES

Data & AI Enablement
Predictive models, generative chemistry, batch prediction, data verification, AI-assisted workflows.

Scientific Software Engineering
Python, Dash, Git, client tooling, validation, typing, structured error handling, documentation.

Platform & Product Delivery
Internal model clients, model access tooling, shared framework principles, developer enablement.

Data Products & Connected Data
FAIR-aligned thinking, reusable scientific assets, migration support, audit outputs, evidence products.

Stakeholder Engagement & Change
Bridge across scientists, platform developers, third-party developers, IT/digital stakeholders and leaders.

Training & Community
User guidance, documentation, clear error messages, training, onboarding support and user groups.

SELECTED ACHIEVEMENTS

- **Product owner for a scientific data platform:** delivered Phase 1 of an externally developed platform project on time and on budget, then supported next-phase scope, investment and stakeholder/IT alignment for reusable scientific data foundations.
- **Core contributor to an internal predictive modelling client:** 300+ commits and input into architecture, roadmap, documentation, validation, structured error handling and integration patterns.
- **Enabled predictive modelling and generative chemistry adoption:** Dash/web interfaces, software-evaluation guidance, documentation, best-practice sharing, community support and training for scientific users.
- **Improved platform coherence:** connected predictive modelling capability, scientific users and downstream design tooling through cleaner integration patterns.
- **Enabled developers as well as scientific users:** built centrally maintained client and integration patterns that reduce duplicated integration effort for downstream platforms.
- **Own and enable key scientific software workflows:** go-to technical contact for data access and batch prediction workflows, supporting users, training and practical adoption.
- **Designed resilient batch prediction operations:** manifest-driven execution, retries, reconciliation and delivery/audit outputs across multi-session scientific workflows.
- **De-risked migration decisions:** auditable Python verification workflows, discrepancy clustering and evidence outputs for legacy-to-new scientific data mapping.

PROFESSIONAL EXPERIENCE

Principal Scientist I - Digital Chemical Design

Syngenta, Bracknell | February 2025 - Present

Digitisation of chemical design across methods, software, data products, platform layers, governance and adoption.

- Served as product owner for an externally developed scientific data platform, delivering Phase 1 on time and on budget while supporting next-phase scope, investment and alignment with scientific stakeholders and IT managers.
- Develop internal predictive modelling client tooling as a core contributor, improving user-facing behaviour, typing, validation, structured error handling, documentation and maintainable Python code.
- Own and enable adoption of scientific software workflows including data access and batch prediction, acting as a go-to technical expert for users, training and workflow support.
- Contribute to modelling platform architecture, shared framework principles, roadmap and integration strategy for predictive model access and downstream scientific tools.
- Build centrally maintained client tooling and integration patterns that reduce developer overhead and help downstream teams embed model and data capabilities into their own platforms.
- Coordinate with an external Python developer, aligning implementation, review, feature prioritisation and delivery practices.
- Translate scientific user needs into platform and data-product decisions for project scientists, chemists, expert platform users, computational scientists and wider R&D users.

Principal Scientist I - Digital Chemical Design continued

Syngenta, Bracknell | February 2025 - Present

- Contribute to integration work connecting generative design tools, predictive modelling capabilities, data access layers and scientific workflow platforms.
- Build auditable Python workflows for project definition mapping, data verification and migration support, including structured evidence, plotting, discrepancy clustering and rerun rules.
- Design resilient batch prediction workflows using manifests, job tracking, retries, reconciliation and delivery-versus-audit outputs.
- Apply AI-assisted development and agentic workflows to accelerate Python tooling, data mapping, batch prediction and evidence generation while retaining human review and auditability.

Principal Scientist I - Computational Chemistry

Syngenta, Bracknell | April 2024 - February 2025

- Helped build and deploy the next generation of Syngenta's internal predictive modelling platform, improving stability, performance and access to predictive capability.
- Designed and implemented a web application for seamless access to internal predictive models for chemists and non-expert users.
- Led evaluation and testing of external scientific software against internal requirements, including dataset preparation, user training, community testing and business-value analysis.
- Acted as a generative chemistry champion by sharing best practices, supporting colleagues and creating integrations that increased adoption.

Postdoctoral Researcher - Computational Chemistry

Syngenta, Bracknell | April 2023 - April 2024

- Led multiple research projects as primary computational chemist and organised a global generative chemistry user group meeting.
- Built Python workflows, QSAR models and supported protein preparation, docking, MM/PBSA, MM/GBSA and FEP investigations where relevant to decisions.
- Received a site Chemistry Award for work enabling effective generative chemistry use.

Esports High-Performance Coach & Educational Content Creator

Independent / Team Engagements | July 2018 - Present

- Designed structured team development, communication and performance systems in high-pressure competitive environments.
- Created educational YouTube, course and podcast content focused on performance and improvement, developing experience in audience engagement, structured explanation and self-directed learning resources.
- Developed a Python/Tesseract OCR tool to convert scoreboard screenshots into CSV outputs for analysis workflows.

EDUCATION & AWARDS

PhD, Chemistry

University of Bath | 2019 - March 2023

Research on small molecules in porous materials using molecular dynamics and quasielastic neutron scattering. Four research articles; international conference talks; research-group analysis workflows.

- Site Chemistry Award for generative chemistry contribution.
- SETsquared IKEEP Intrapreneurial Training Award.

TECHNICAL SKILLS

- **Languages & Tools:** Python, Dash, Git, API/client tooling, Tesseract OCR.
- **Engineering:** typing, validation, structured errors, documentation, maintainable code.
- **Data:** mapping, verification, structured outputs, discrepancy clustering, reconciliation, audit outputs.
- **Platforms:** internal model clients, model access tooling, API-oriented components.
- **AI/Science:** generative chemistry, predictive models, batch prediction, QSAR, docking, FEP.