AI Lab Transition Strategy — Detailed Overview

Three Pillars Per Phase: Technology · Organisation & Culture · Data Supply

PHASE	TECHNOLOGY	ORGANISATION & CULTURE	DATA SUPPLY	KEY METRICS
Phase 0 Data Readiness Human decides Digital records	**Instrument data capture** Machine-readable formats **Metadata standardisation** Assay, project, site consistency **Experiment-result linkage** Done → outcome → meaning **Ontology adoption** BAO, ChEBI, OBI mapping LIMS · ELN · Integration	**Leadership sponsors data as priority** Not delegated to IT **Lab champions (2–3 per group)** Peer-credible senior scientists **Data quality ownership defined** Scientist vs. manager vs. steward ■ Data Practices & Attitudes Survey ■ Expect passive non-compliance on data entry	**Audit captured vs. generated data** 30–60% of instrument output typically lost **Prospective capture design** Env, reagent lot, calibration data **External ontology mapping** Lightweight, high interop impact **Data quality baseline** Error rates, completeness, consistency	**>90% structured** data capture **Cross-team** query volume ↑ **Metadata** completeness % **Survey Δ** vs. baseline
Phase 1 Predictive Intelligence Human decides ML recommends	**Assay performance prediction** Yield, variability, failure probability **Instrument drift detection** Predictive maintenance **Compound-property prediction** ADMET, solubility, stability **Experiment prioritisation / DoE** XGBoost · TxGemma · Local models · SPC	**"Trust but verify" posture** Leadership endorses, doesn't mandate **ML literacy training** Evaluate outputs, not build models **Accountability framework** Who owns a bad ML-informed decision? ■ AI Readiness & Trust Survey (quarterly) ■ "The model is wrong" — handle constructively	**Labelled training data (bottleneck)** Retrospective + prospective labelling **New data streams required** Env monitoring, reagent lots, operator **External datasets** ChEMBL, PubChem, BindingDB **Volume reality check** Small n → classical ML, not deep learning	**Model accuracy** vs. actuals per model **Adoption %** predictions consulted **Downtime ↓** unplanned instrument **Trust Δ** quarterly survey trend
Phase 2 Augmented Workflows Human approves LLM agents draft	**Protocol & document drafting** SOPs, deviations, stability reports **Literature-informed design (RAG)** Internal + external corpus **NL query over lab databases** Cross-system data access **Equipment troubleshooting** Frontier LLMs · Fine-tuned SLMs · RAG · MCP	**Explicit AI authority boundaries** Documented by leadership **AI Review Board established** Science, quality, IT, regulatory **AI output review skills training** Agent errors ≠ human errors ■ Workflow Impact & Autonomy (quarterly) ■ Approval fatigue + "It'll take my job" fears	**Curated RAG corpus** SOPs, protocols, records — kept current **Agent interaction logs** Prompt, output, review, edits **External literature access** PubMed, bioRxiv, regulatory guidance **IP governance framework** Which models see which data	**>70% draft** acceptance rate **Hallucination** rate tracked **Review time** ↓ may = fatigue ■ **Role Δ** autonomy survey
Phase 3 Bounded Autonomy AI decides within guardrails	**Automated parameter adjustment** Within validated ranges **Dynamic experiment scheduling** Resource + priority optimisation **Automated QC triage** Flag / hold / release by criteria **Predictive inventory ordering** Orchestrated agents · Validated decision engines	**Delegated decision authority** Leadership accepts AI outcome liability **Role redesign** Scientist → exception handler & auditor **QA/Regulatory co-design** Architects of guardrails, not reviewers ■ Post-Autonomy Impact (per use case) ■ QA/Reg resistance: "How do we audit this?"	**Real-time data feeds (not batch)** Live instrument, inventory, scheduling **High-volume decision logs** Trigger → input → output → outcome **External operational feeds** Supplier lead times, regulatory calendar **Closed-loop feedback data** Continuous validation & drift detection	**>95% decision** accuracy **Zero scope** creep incidents **Intervention** rate monitored **Confidence Δ** post-autonomy survey

■ **Technology alone does not deliver AI transitions. Every phase requires parallel investment in culture, leadership behaviour, and data supply.**