

Supplementary Materials Index

ASMD/Xenpozyme QSP v2.0 — IQANOVA ATLAS Master Pipeline

S1. SBML model files

- ASMD_Xenpozyme_QSP_v2_0_adult.xml — adult population model (libSBML L3v2, 0 errors)
- ASMD_Xenpozyme_QSP_v2_0_paediatric.xml — paediatric population model (libSBML L3v2, 0 errors)
- ASMD_Xenpozyme_QSP_v2_0_build_summary.json — structural metadata

S2. Synthetic data

- ASMD_Xenpozyme_QSP_v2_0_synthetic_data.csv — 370 rows (64 reliability-A + 306 reliability-B)
- ASMD_Xenpozyme_QSP_v2_0_data_provenance.xlsx — 4 sheets documenting all 6 source classes
- ASMD_Xenpozyme_QSP_v2_0_synthetic_data.json — machine-readable index

S3. Calibration

- ASMD_Xenpozyme_QSP_v2_0_parameters.csv — final calibrated parameter values (adult + paediatric)
- ASMD_Xenpozyme_QSP_v2_0_predictions.csv — predicted vs observed for every data row
- ASMD_Xenpozyme_QSP_v2_0_rmse_summary.csv — per-(population, endpoint) RMSE and PASS/CHECK
- calibrate_v2.py — full reproducible calibration script

S4. V&V

- ASMD_Xenpozyme_QSP_v2_0_VV_report.csv / .json — 21 V&V checks (20 PASS, 1 borderline)

S5. GSA

- gsa_results.json — full Spearman matrix for both populations
- gsa_spearman_*.csv, gsa_pvalues_*.csv — analysis outputs

- GSA_heatmap.png, GSA_barchart.png — 300 DPI publication figures

S6. Identifiability

- rse_adult.csv, rse_paediatric.csv — per-parameter RSE and class
- identifiability_summary.json — high-corr pairs, mean/median RSE
- RSE_bars_*.png, FIM_corr_*.png, profile_likelihood_*.png — 300 DPI figures

S7. Bayesian meta-analysis

- meta_results.json — full posterior summary
- meta_diagnostics.csv — \hat{R} , ESS, QC pass/fail per endpoint
- posterior_*.csv — per-study θ_i , posterior means and 94 % HDI
- forest_plots.png, posterior_distributions.png — 300 DPI figures

S8. Combination/regimen optimisation

- ASMD_Xenpozyme_QSP_v2_0_combination_outcomes.csv — W52/W104 outcomes per regimen \times population
- ASMD_Xenpozyme_QSP_v2_0_decision_table.csv — sorted by composite score
- ASMD_Xenpozyme_QSP_v2_0_benefit_risk_table.csv — categorical benefit/risk/recommendation
- Figure4_Combination_Outcomes.png — 300 DPI publication figure

S9. Master figures

- Figure1_Architecture.png — five-layer model schematic
- Figure2_Calibration.png — predicted vs observed time-courses
- Figure3_BiomarkerTrajectories.png — six-panel mechanistic trajectories
- Figure4_Combination_Outcomes.png — eight-panel regimen comparison
- FigureS1-S10 — supplementary figures (GSA, identifiability, Bayesian)

S10. Regulatory artefacts

- Parameter table.xlsx (3 sheets, colour-coded)

- Model equations document (DOCX + PDF)
- References table landscape (DOCX + PDF, 39 refs)
- Bayesian meta-analysis report (DOCX + PDF)
- Identifiability report (DOCX + PDF)
- Regulatory report R1–R14 (DOCX + PDF)

S11. Reproducibility

- All Python scripts run end-to-end on a Linux container with python-libsaml, scipy, pymc, arviz, openpyxl, python-docx, reportlab installed.
- Random seeds fixed at 42 throughout for full bitwise reproducibility.
- Version-controlled archive: <https://iqanova.org/atlas/asmd-xenpozyme-v2>