TargetLynx Auto-Flag v1 – Product Requirements Document (PRD)

Version 1.0 — 2025-08-07

# 1 Background & Pain Points

• Waters LC‑MS/MS (MassLynx + TargetLynx) batches quantify 5–30 steroid hormones.  
• Manual peak review & QC ≈4 h per batch (60‑80 samples).  
• Staffing shortages on off‑hours delay TAT.  
• Rule‑based auto‑flagging can cut review workload to 5–10 %.

# 2 Product Goals & ROI

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| --- | --- |
| Metric | Target |
| Review time | ≤30 min/batch |
| False‑positive rate | ≤5 % |
| False‑negative rate | ≤1 % |
| Deployment cost | No new servers |
| Timeline | ≤5 weeks |
| Annual labour saved | ≈1000 tech hrs/year |

# 3 Key User Stories

* • As a day‑shift tech, I drag‑drop export files to get exceptions in minutes.
* • As a supervisor, I edit thresholds in config.xlsx without coding.
* • As a night‑shift tech, I review only flagged lines to release results fast.

# 4 Scope & Phasing

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| --- | --- | --- |
| Item | Included v1 | Excluded |
| Data source | Waters TargetLynx CSV/TXT | Other vendors |
| Processing | Parse→Rules→Excel | Auto reintegration |
| UI | CSV & Excel | PDF, LIS |
| Deployment | Standalone EXE | Docker/K8s |

# 5 Functional Requirements (Summary)

• Data Input: drag‑drop CSV, column alias mapping.  
• Rule Engine: IS ±25 %, RT hard ±0.20 min, soft window with area/ion‑ratio logic; S/N<10; fit & range; missing.  
• Rule Validation: thresholds from 100 historical batches; weekly tuning.  
• Output: Quant\_Result.csv with Flag; Exception\_List.xlsx (red=hard, yellow=soft); Batch\_Summary.txt stats.  
• Config versioning: MD5 hash logged, timestamped backups.  
• Logging: file list, config hash, rule version, errors.

# 6 Security & Tech Assumptions

Offline; optional AES‑256 output encryption; signed EXE.  
Tech: Python 3.9, pandas, openpyxl, tkinter, PyInstaller.

# 7 Milestones

|  |  |  |
| --- | --- | --- |
| Phase | Week | Deliverables |
| Prototype | 1 | Parser & rule stubs |
| Beta | 3 | Excel output & config UI |
| RC | 4 | Signed EXE + guide |
| Go‑Live | 5 | Stable v1, SOP, training |

# 8 Acceptance

FP≤5 %, FN≤1 % vs consensus gold‑standard; process 3 batches ≤30 min; user completes task after 30 min training.

# 9 Risks & Mitigation

|  |  |  |
| --- | --- | --- |
| Risk | Impact | Mitigation |
| Template change | Parse error | Alias map + tests |

# 10 Glossary

Flag, RT, IS, S/N, TAT