🧬 Reactome LNP Agent — Ionizable Lipid Reaction Templates
LangGraph + FAISS RAG + AWS Bedrock

User Input

▶ START

Tech Stack

Vector DB: FAISS (local)
Embeddings: Titan Embed v2
LLM: Claude Sonnet 4.5
Framework: LangGraph
Cloud: AWS Bedrock

📝 User Query
"Design a 3-tail ionizable lipid with amine heads…"

RAG Retrieval Layer

🧪 Compound Data
(217K blocks, 293 scores)

⚗ Reaction Templates
(13 SMARTS reactions)

📐 LNP Design Rules
(MCTS, tail constraints)

📄 Research Papers
(4 PDFs, 148 pages)

query

🔍 FAISS Retrieval
(454 vectors, 1024-dim)

context   *context*

Parallel Expert Analysis (Claude Sonnet 4.5 via Bedrock)

⚗ Reaction Expert

- Applicable templates
- Functional group matching
- Reaction conditions
- Known limitations

📐 Design Rules Expert

- Tail config (2-4 tails)
- Symmetry preference
- MCTS compatibility
- Synthesizability check

reaction analysis   *rules check*

Synthesis Planning

🧪 Synthesis Planner

- Step-by-step route
- Reaction ID sequence
- Building block selection
- MCTS action sequence

synthesis plan

Output

📋 Final Answer

- Recommended reactions
- Design rule compliance
- Actionable synthesis route
- Caveats & next steps

🏁 END