

MedChem Triage Report

Project Summary - 2026-01-29

Total Compounds Processed: 50

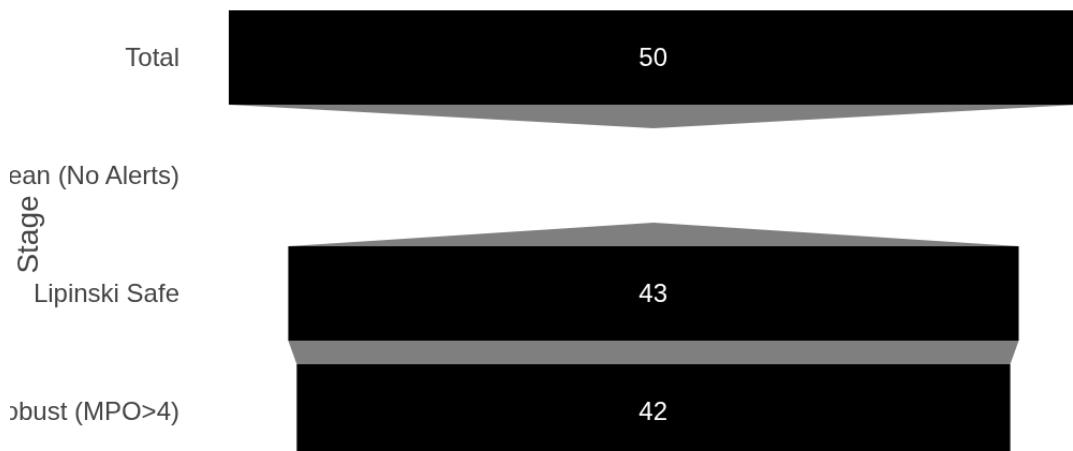
Safe Candidates: 43 (86.0%)

Failed Candidates: 7

Key Visualizations

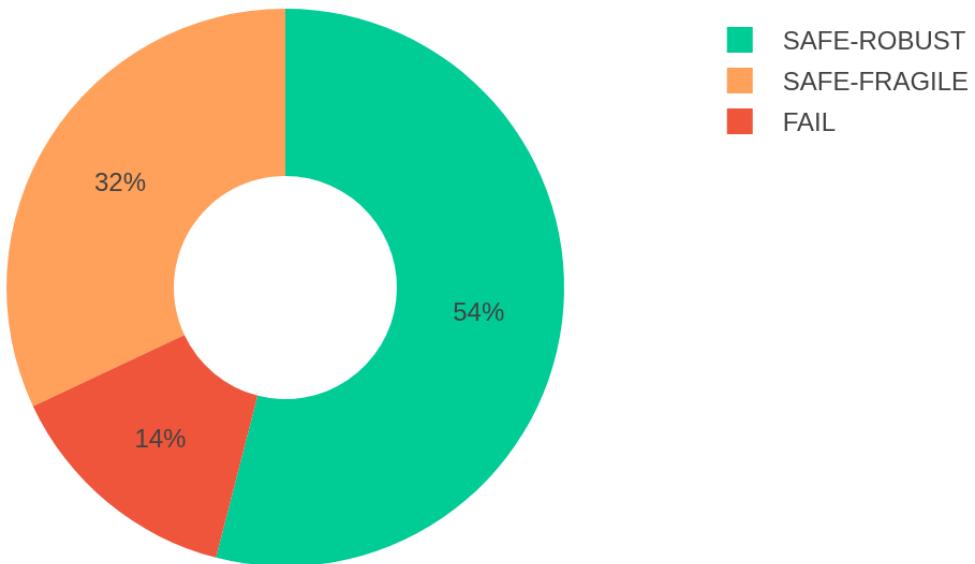
Attrition Funnel

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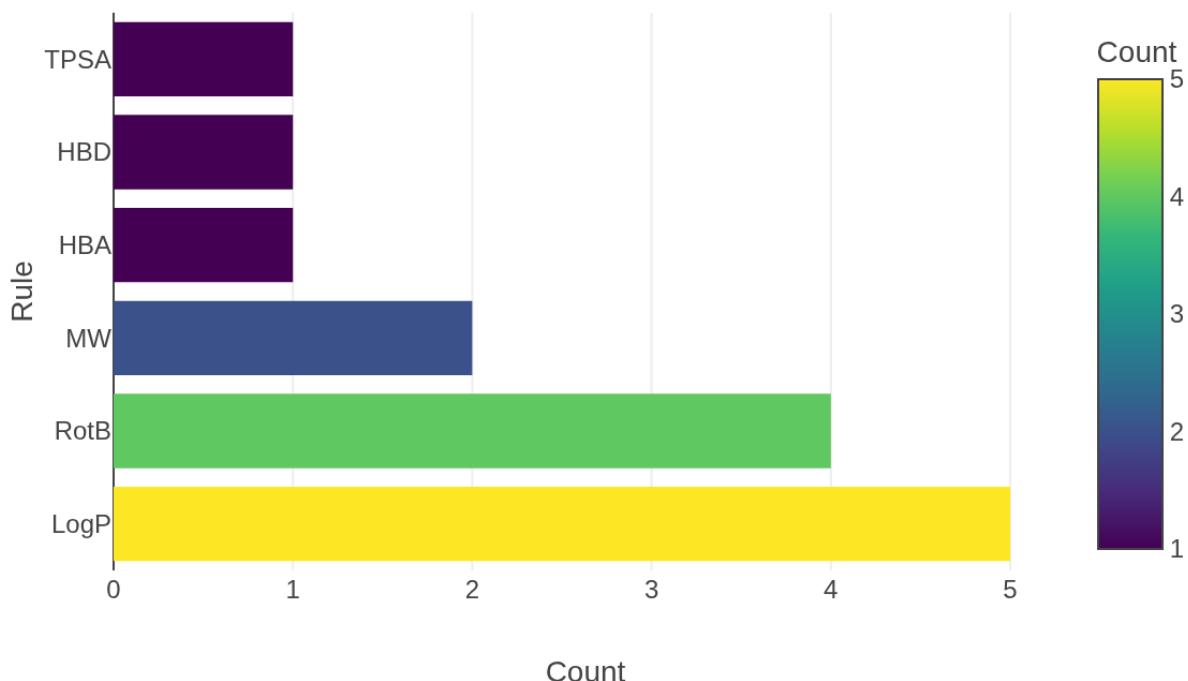


Status Breakdown

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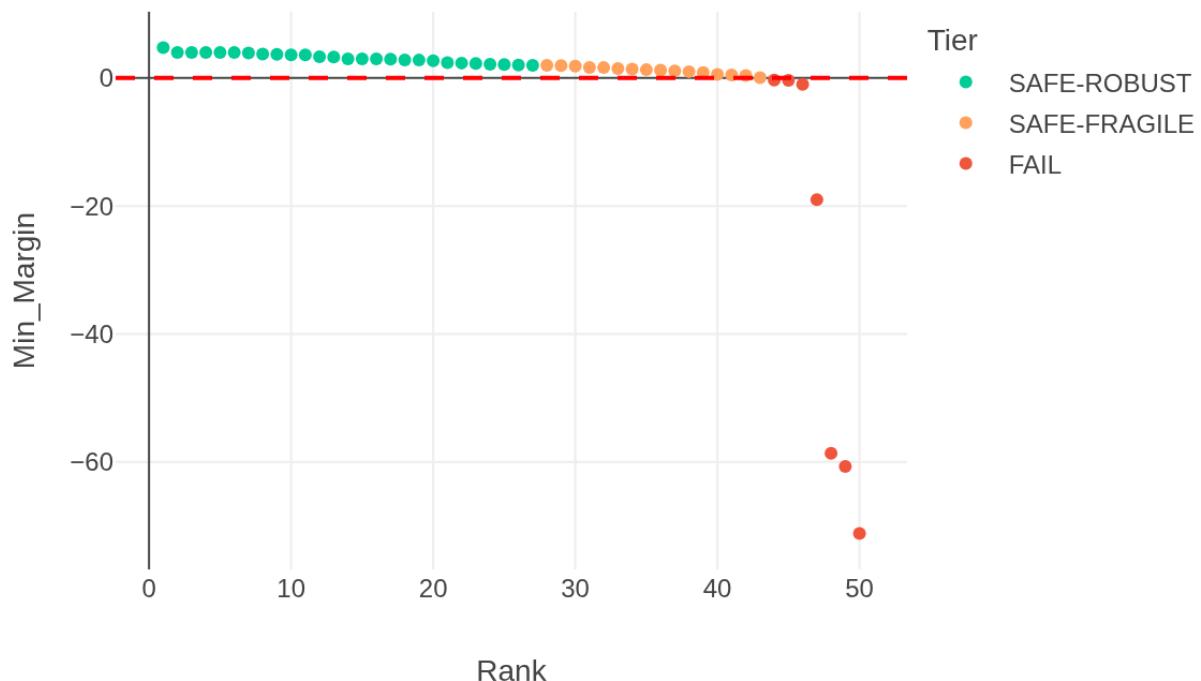


Top Failures

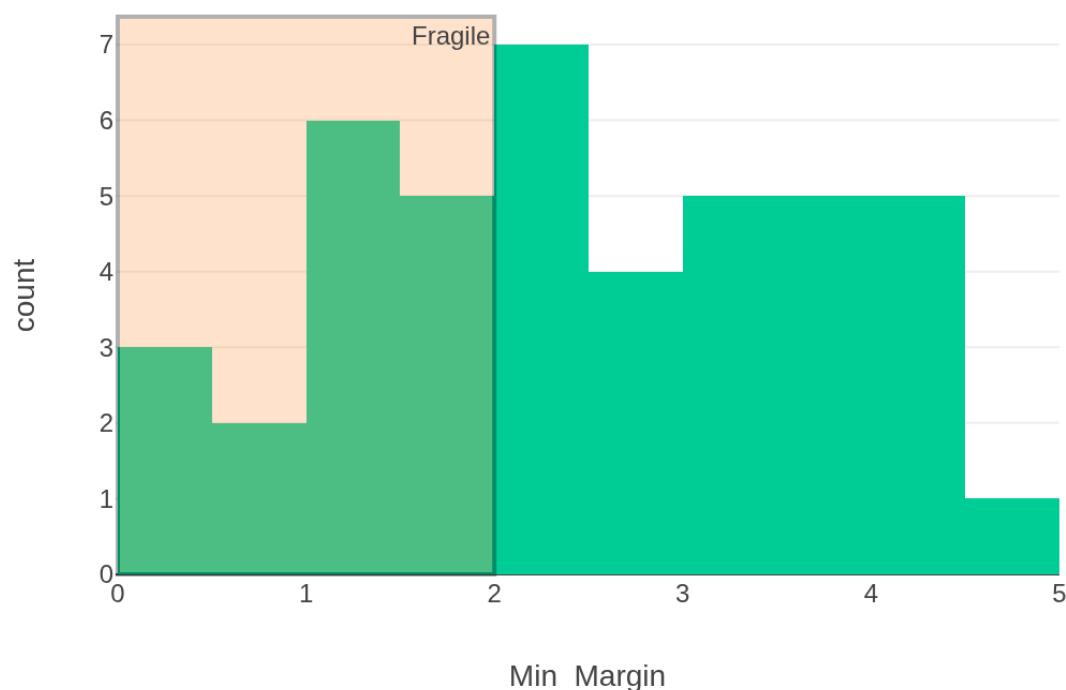


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Risk Landscape

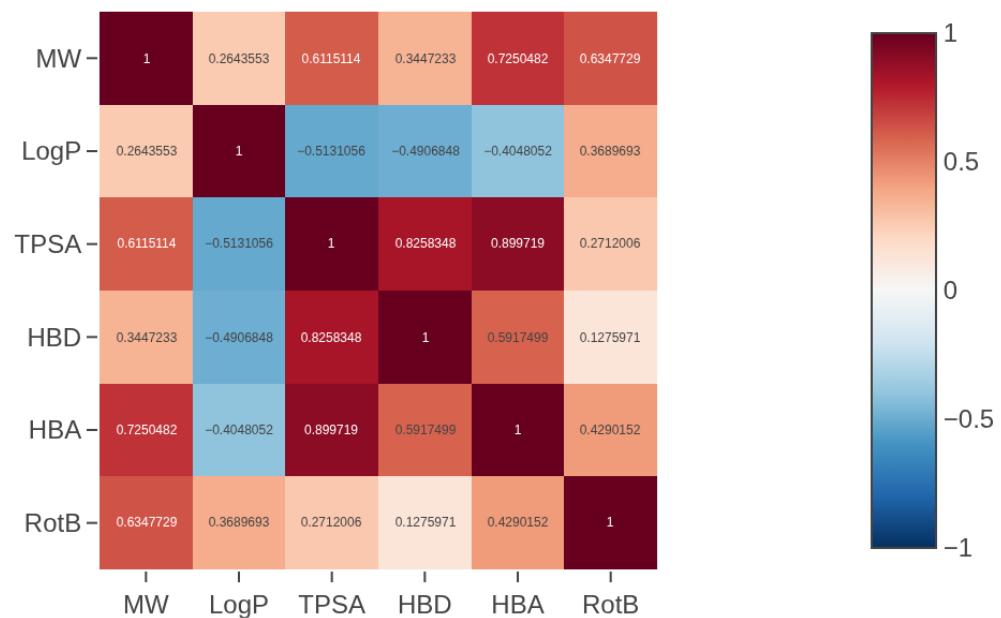


Robustness



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Correlation Matrix



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Top 10 SAFE Candidates

Compound_ID	Tier	MPO_Score	MW	LogP
Sulfa_1	SAFE-ROBUST	6.0	157.19	0.33
Sulfa_3	SAFE-ROBUST	6.0	191.64	0.99
Sulfa_2	SAFE-ROBUST	6.0	171.22	0.64
Sulfa_5	SAFE-ROBUST	6.0	199.23	0.51
Aspirin	SAFE-ROBUST	6.0	180.16	1.31
Indole_3	SAFE-ROBUST	6.0	175.19	1.73
Caffeine	SAFE-ROBUST	5.5	194.19	-1.03
Frag_Pyridine	SAFE-ROBUST	5.5	79.1	1.08
Frag_Aniline	SAFE-ROBUST	5.5	93.13	1.27
Frag_Acid	SAFE-ROBUST	5.5	122.12	1.38

Top Failure Rules

- LogP: 5 violations
- RotB: 4 violations
- MW: 2 violations
- HBA: 1 violations
- HBD: 1 violations