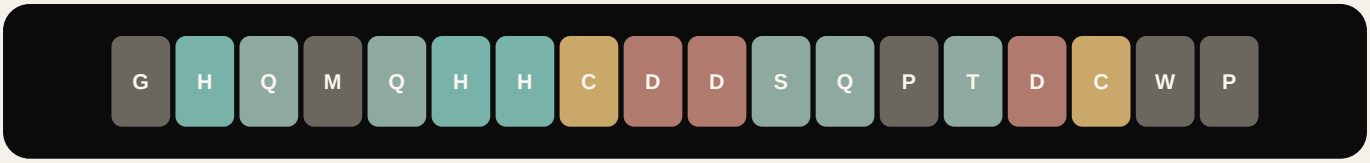
PROTEAN
Computational biology research artifact

REVIEW REQUIRED | NOT SUBMITTED | COMPUTATIONAL

Candidate Wet-Lab Decision Dossier

A concise, review-gated packet for deciding whether this peptide deserves first-pass synthesis and assay spend.



RECOMMENDATION	RANK	SCORE	SUBMISSION
Proceed to review	**#1**	**0.544**	**None**
Small, controlled first-pass packet	Top current candidate	total_constraint_score	No CRO, wallet, or ledger action

FIELD	VALUE
Candidate ID	cycle-20260526T020837Z-02-001
Sequence	GHQMQHHCDDSQPTDCWP
Run ID	cycle-20260526T020837Z-02
Source	data/results/ranked_candidates_latest.csv
Review gate	operator_review_required

Executive Decision Memo

Decision: spend a small, controlled amount on review-gated synthesis and first-pass assays only. The peptide is top-ranked and chemically tractable, but the AMP hypothesis is unproven and the cysteine pair must be handled deliberately.

TEST RATIONALE	NOVELTY	MANUFACTURING	GATE
Moderate	**Review**	**Manageable**	**Closed**
Top-ranked; evidence is computational	No exact public hit; short-region BLAST context	Cys/Met QC required	No external submission

Spend case

- Selected rank 1 with score 0.5436.
- Hydrophilic profile: GRAVY -1.65; pI 5.038.
- Short, standard SPPS length with explicit QC path.
- Testing would quickly falsify activity, toxicity, and handling assumptions.

Primary reasons to hold back

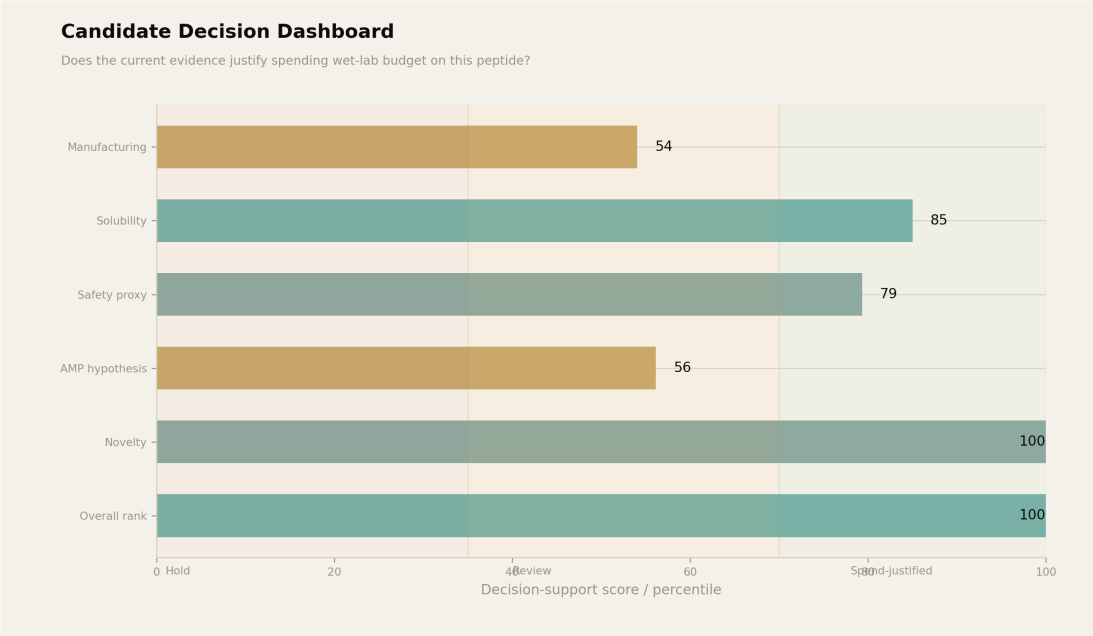
- Net charge is negative near physiological pH, unlike many canonical cationic AMPs.
- Cys and Met require oxidation/disulfide control.
- Similarity and novelty evidence are bounded, not exhaustive.
- No wet-lab outcome, toxicity result, or therapeutic claim exists.

FIELD	VALUE
Recommendation	Proceed to operator review; do not submit externally from Galen.
Wet-lab spend	Justified only as a small first-pass screen with identity/QC confirmation.
Decision-changing data	MIC signal, hemolysis/cytotoxicity window, solubility, serum/protease stability, LC-MS/HPLC identity.
Hard boundary	No biological activity, selectivity, toxicity, or therapeutic promise is claimed.
Current gate state	not_submitted; external_submission_allowed=False; ledger_tx=False

Selection and Population Context

Figure 1. Candidate Decision Dashboard

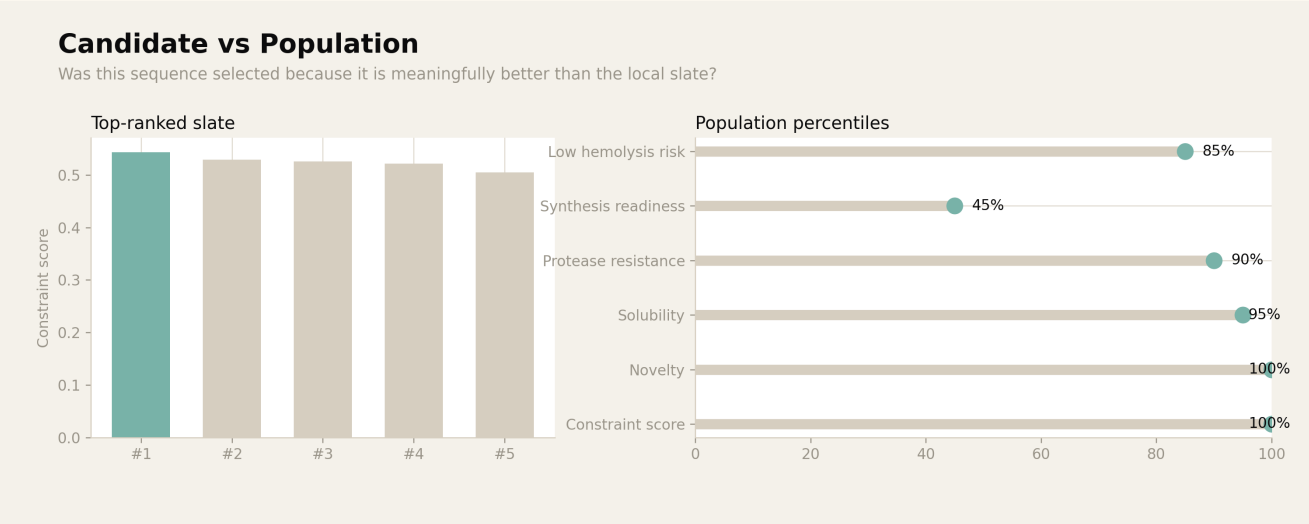
Does the evidence justify first-pass wet-lab spend?



The candidate earns a review-gated test because rank, handling, and solubility are reasonable; biology and selectivity remain experimental questions.

Figure 2. Candidate vs Population

Was this peptide selected for a real slate-level advantage?

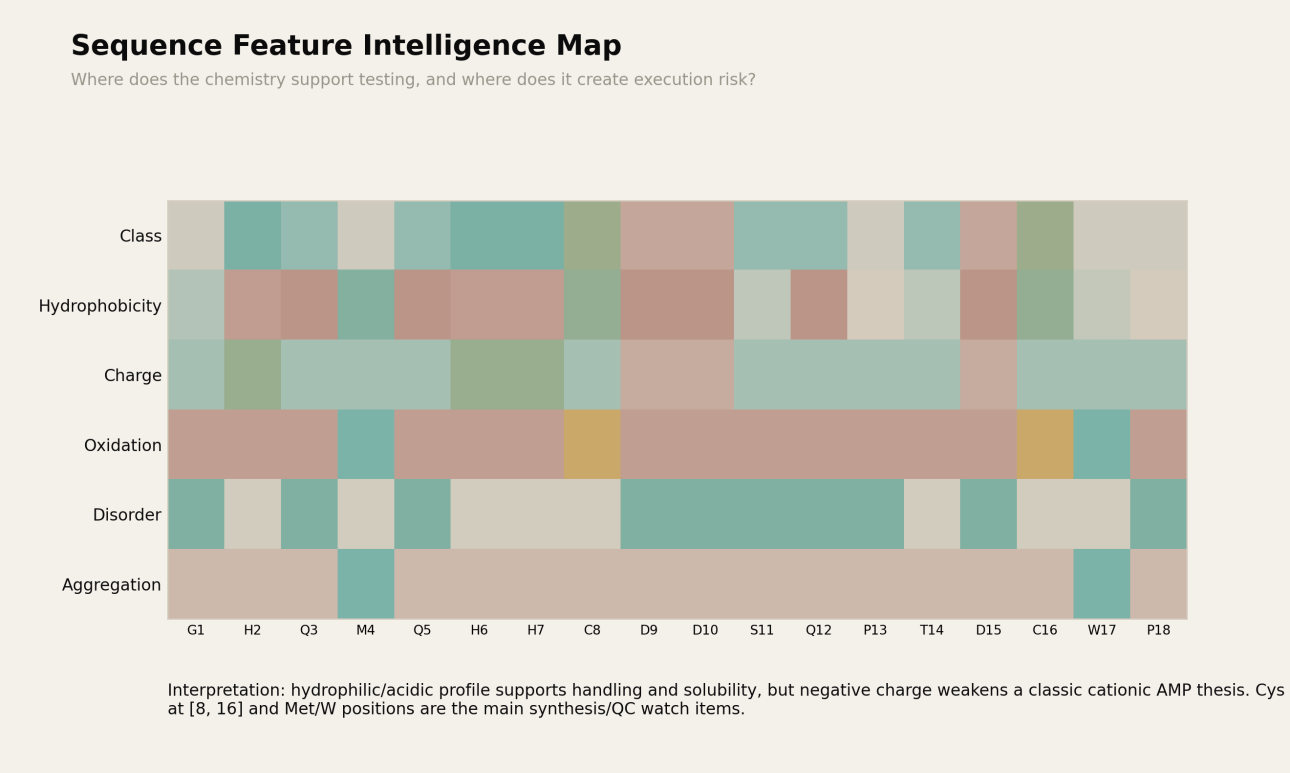


Support view: the selected peptide leads the slate by configured score and remains strong across available percentiles.

Sequence Intelligence

Figure 3. Sequence Feature Intelligence Map

What chemistry supports testing, and what chemistry creates risk?



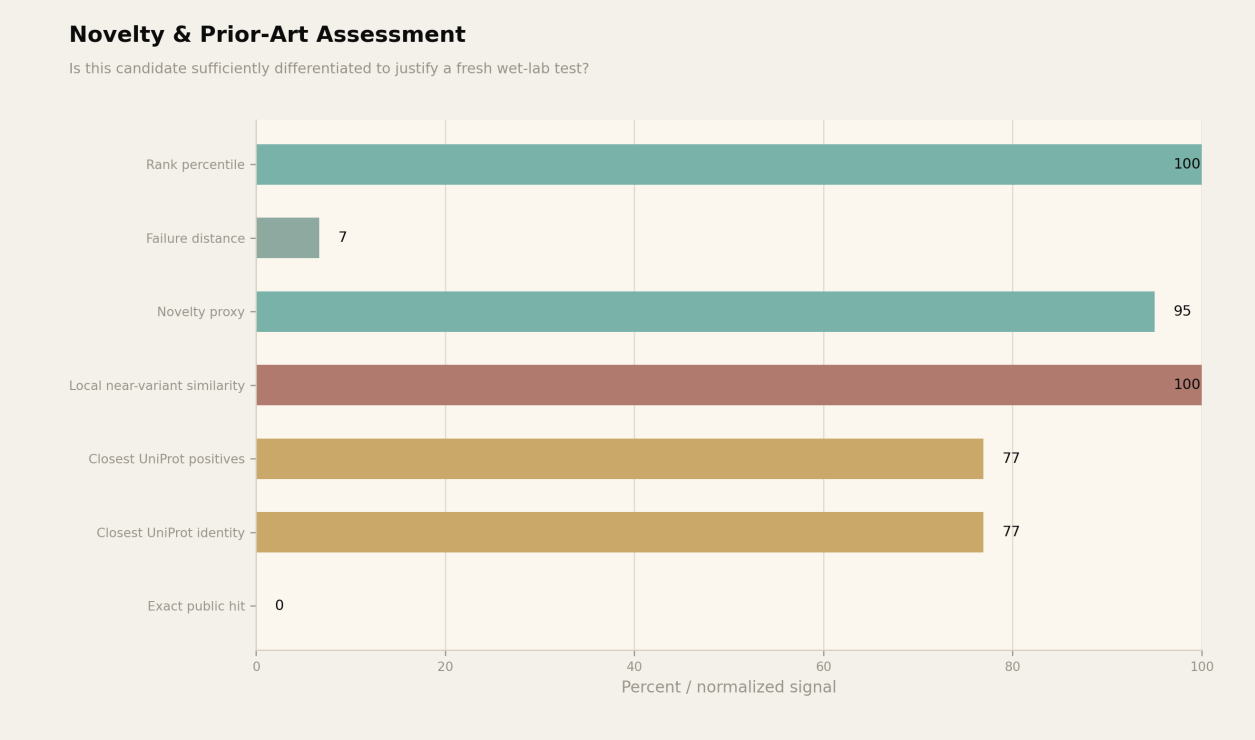
This figure replaces raw residue-class, charge, polarity, hydrophobicity, and oxidation widgets with one integrated sequence-level decision view.

FIELD	VALUE
Length	18
Molecular weight	2122.238
Estimated pI	5.038
Net charge at pH 7.4	-3.38
GRAVY	-1.65
Hydrophobic moment	0.5558
Cys positions	[8, 16]
Decision implication	Soluble/tractable chemistry, but negative physiological charge weakens a classic cationic AMP...

Novelty and Similarity Landscape

Figure 4. Novelty & Prior-Art Assessment

What makes this peptide different, and what similarity risks remain?



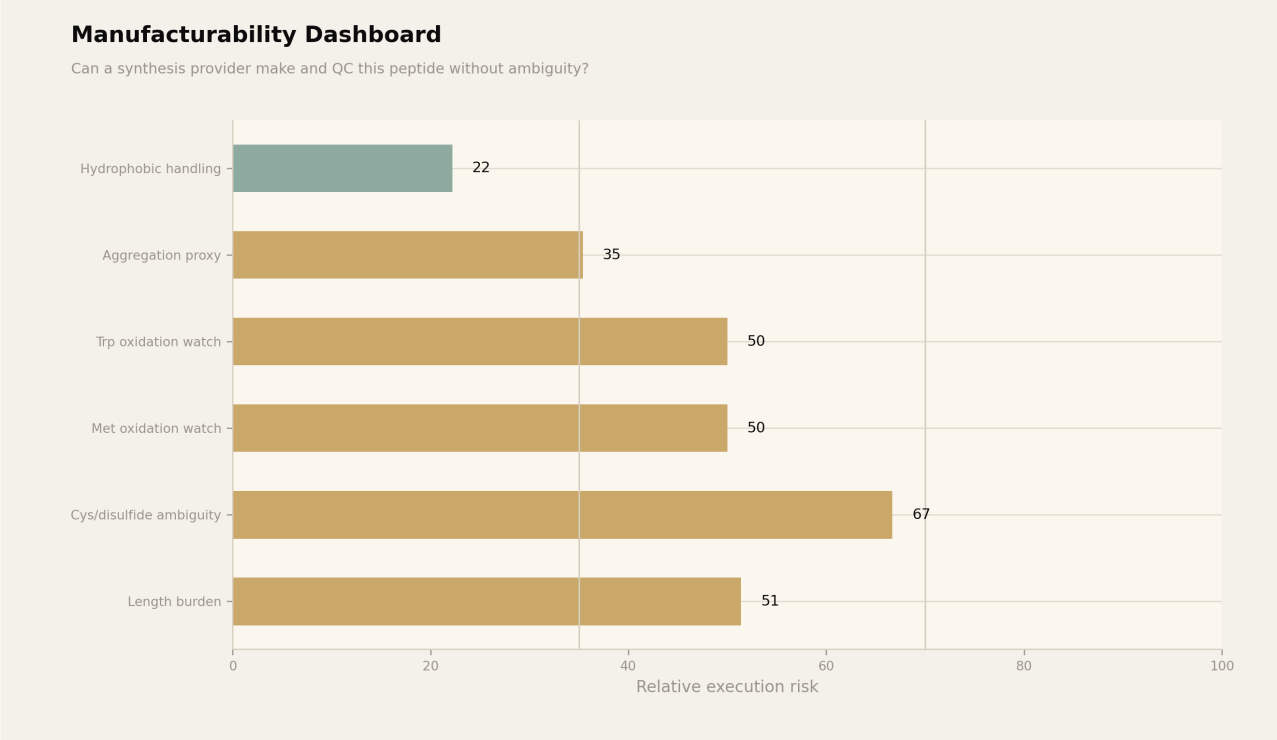
UniProtKB BLAST and local dedup are interpreted as context. A short-region hit inside a longer protein is not equivalent to a tested peptide.

FIELD	VALUE
Dedup gate result	unblocked
Exact local mentions before generation	65
Near variants retained for review	11
Closest UniProtKB BLAST hit	A0A0J1EFS7
Closest hit identity	76.9%
Nearest AMP in top hits	not_found_in_top_hits
Blocked reason	none

Manufacturability and Failure Risk

Figure 5. Manufacturability Dashboard

Can a CRO synthesize and QC this peptide without ambiguity?



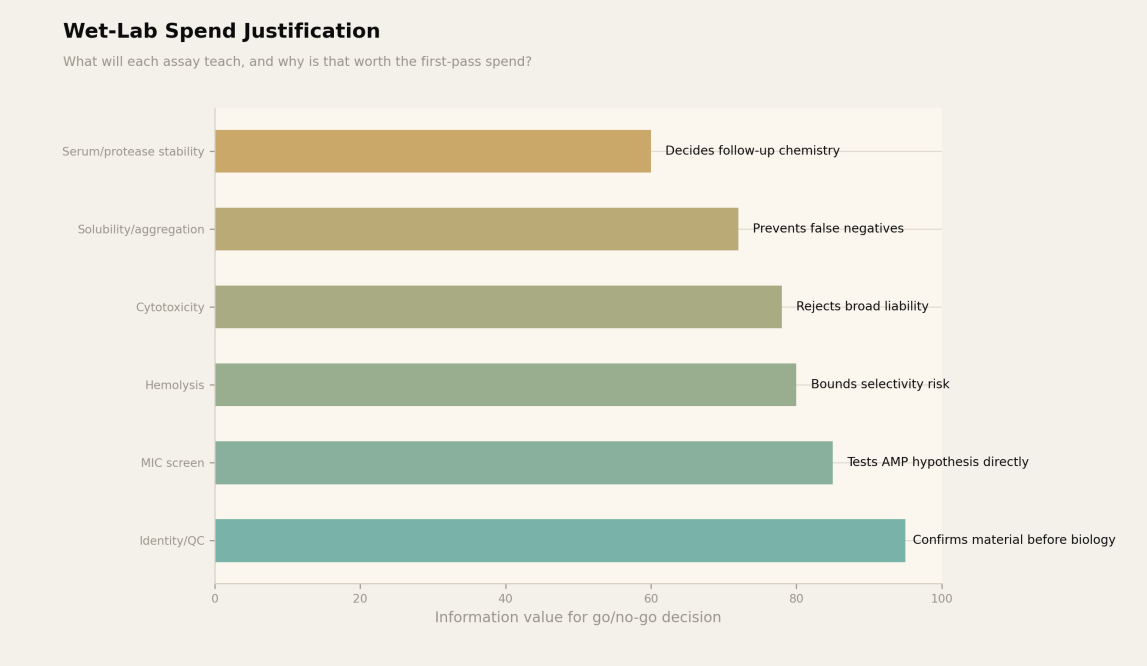
The principal risk is not length; it is cysteine/disulfide state control and oxidation monitoring.

FIELD	VALUE
Aggregation	low_to_moderate
Solubility estimate	good_by_charge_and_hydrophilicity
Synthesis difficulty	moderate: cysteine_oxidation_control, methionine_oxidation_monitoring, local_repetition
Cys/disulfide ambiguity	two cysteines can form intramolecular disulfide or intermolecular dimer; request reduced linear materi...
HPLC/MS QC	LC-MS, analytical HPLC, purity trace, CoA, oxidation/disulfide status.

Wet-Lab Spend and Assay Plan

Figure 6. Wet-Lab Spend Justification

What will each first-pass assay teach?



The assay plan is designed to falsify the candidate cheaply and honestly before any stronger biological claim is made.

FIELD	VALUE
MIC screen	Question: antimicrobial signal? Gate: reproducible activity against selected Gram-positive/negative panel.
Hemolysis	Question: membrane selectivity? Gate: acceptable RBC liability at active-range concentrations.
Cytotoxicity	Question: mammalian safety window? Gate: no broad toxicity near candidate MIC range.
Solubility/aggregation	Question: false-negative risk? Gate: soluble test article under assay conditions.
Stability	Question: is follow-up chemistry needed? Gate: serum/protease trend supports next-cycle design.
Controls	Known AMP positive, scrambled peptide, vehicle, inactive/negative peptide.

CRO Packet and Appendix

CRO-ready order specification

FIELD	VALUE
Sequence	GHQMQHHCDDSQPTDCWP
Form	Linear peptide exactly as generated; no terminal modifications for first pass.
Termini	Free N-terminus and free acid C-terminus unless operator revises.
Purity	Prefer >95% for screening; document tradeoff if lower purity is selected.
Amount	Small first-pass quantity sufficient for QC plus MIC, hemolysis, cytotoxicity, solubility, and stability screens.
QC required	LC-MS, analytical HPLC trace, CoA, peptide content/net peptide if available.
Cys handling	Request reduced/linear material first; vendor must report oxidation/disulfide status.

Go / No-Go matrix

FIELD	VALUE
Advance	Confirmed identity/purity plus reproducible antimicrobial signal and acceptable hemolysis/cytotoxicity window.
Redesign	Weak activity but clean handling/safety; use assay results to guide next sequence iteration.
Stop	No activity, poor solubility/aggregation, failed QC identity, or unacceptable mammalian toxicity.
Escalate	Any vendor ambiguity, unexpected oxidation species, or dedup/provenance conflict requires operator review.

Provenance boundary

Full references, query strings, BLAST job metadata, chart hashes, commands, and tool versions live in provenance.json. Manifest hash: sha256:42f5e6ca773c1f6779e7a... Source CSV hash: sha256:fac526e6d5aaa10e858a6...

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