RaRaMa — Protein Functionality & Thermal Dossier

July 18, 2026 · 17:27 | Tier 3 · Full dossier | source: **input_protein_beta-lactoglobulin.json** | 1 protein | prepared for: **Hans-Made Research — beta-lactoglobulin single-protein deep-dive (full tier-3 dossier)**

What this report gives you that nothing else does

Reads sequence only	Denaturation T_d, aggregation & colloidal stability — and, for food proteins, gelation, modulus, solubility, emulsification & holding — from the amino-acid sequence, no DSC, no rheometer, no panel.
Zero training data	Nothing to assemble or label first. The same sequence always returns the same numbers.
Fold-gated confidence	A sequence-only fold gate routes every protein to its recognised fold family and states a confidence TIER — **HIGH** on the calibrated cupin core (blind MAE ~2.7 °C), **PROVISIONAL** for other recognised folds (routed to a fold-family anchor, read as a ±band), **LOW/none** for a novel or disordered chain — rather than ever emitting a confident wrong T_d. It refuses only what it genuinely cannot place.
Pre-bench screening estimates	Structure-derived first-pass estimates of DSC / DMA / TGA / solubility behaviour — to help prioritise which candidates to put on the instrument, not to replace the measurement.
Auditable & deterministic	Every number carries its structural reason and is bit-reproducible (SHA-256 + Merkle locked).

Bottom line — the decision in one line per protein

1. beta-lactoglobulin (bovine) — LIPOCALIN fold (PROVISIONAL confidence); predicted T_d ≈ 74 °C; functional profile in the table below · 3 strong bitter culprit(s) → debitter via Pea Legumin (11S).

Protein register — every input, numbered & structurally identified

#	Protein	Len (aa)	Fold	Confidence
1	**beta-lactoglobulin (bovine)**	162	LIPOCALIN	PROVISIONAL

Virtual-instrument method conditions — the settings behind every number (audit-grade)

Virtual instrument	Method conditions (operator controls · defaults where blank)	Reported output
TA DSC (Discovery)	heating rate 10 °C/min · N_2 purge 50 mL/min · Tzero Al hermetic pan · ~5 mg	Td/Tm °C · ΔH · ΔCp · cooperativity
TA rheometer (ARES)	1% strain · 0.1–100 rad/s frequency sweep · 14% w/v · heat-set gel: heat 20→95 °C (gel point at T_gel≈T_d), cool to cure	G′/G″ Pa · gel point °C · K′/n′
TA DMA / TGA	moisture as supplied% · ramp to die temp · N_2 20 °C/min	Tg °C · E′/E″ · decomp onset °C
Wyatt SEC-MALS	calibrated SEC column · dn/dc 0.185 mL/g · 90° + LS detectors	absolute Mw kDa · oligomer · %agg
Wyatt DynaPro DLS	back-scatter · 25 °C · aqueous · cumulants fit (ISO 22412)	Rh nm · PDI · monodispersity
SAXS (BioSAXS)	q 0.1–3.0 nm^{-1} · Guinier + Kratky · buffer-subtracted	Rg nm · Dmax · fold state
UV-PDA (ACQUITY eλ)	190–800 nm · 1.2 nm optical res · 10 mm flow cell · 80 Hz · stray 0.07%	ε280 · A280 · λmax · linearity
LC-MS (ESI, SYNAPT)	BEH C18 1.7 µm · 5→95% B gradient · 0.5 mL/min · ESI+ · cone 30 V · N2 drift gas	intact mass Da · collision cross-section (shape) · tryptic map
Nutrition (DIAAS)	FAO/WHO 2013 reference AA pattern · structural SID digestibility	DIAAS · limiting AA · SID

Every virtual instrument computes from the amino-acid sequence + the panel's line conditions; the method row records the operator controls that shaped each output (scan rate → kinetic Td shift, flow-cell pathlength → absorbance, drift gas → CCS scale). Blank controls fall back to the standard method defaults shown.

Integrity (SHA-256 manifest): 4750cc400ae9ced206d81c7577c52cade6f8571e94a64812d168a9026cfdb20a

Functional readout — every protein, sorted to your tier (the goal: items 2–7)

Protein	T_d ± band °C	tier	pI	Gel kPa	LGC %	EAI	WHC	OHC	ΔH	TGA °C	Tg° C	DIAAS
beta-lactoglobulin (bovine)	74 ±5	PROV	4.6	21.3	6.8	0.99	1.25	0.49	15.8	249	68	0.82

Tier 3 full dossier: + emulsification (EAI), water/oil holding, unfold enthalpy ΔH (DSC), decomposition onset (TGA), glass transition T_g (DMA shelf-life/caking, at the supplied moisture) & predicted DIAAS (composition × structural digestibility — a screen, not a label claim; PDCAAS stays official). **T_d is reported as its disclosed ±band** — the value is deterministic; the ± is the fold-family's characterised uncertainty (so a lower-confidence fold is NOT dressed up as a false-precision point). **tier** = HIGH (calibrated cupin core, ±4 °C) · PROVISIONAL (other recognised fold, wider band) · a novel or disordered chain is **refused** (—), never guessed.

Allergen family screen — sequence-homology pre-bench flag (the EFSA-endorsed first step)

Protein	Allergen family	Cross-reactive with	Heat stability
beta-lactoglobulin (bovine)	milk whey lipocalin	within the lipocalin super-family	heat-stable — largely retained through processing

Sequence-homology allergen FAMILY screen — the pre-bench first step EFSA runs AHEAD of the wet-lab IgE panel. This is a family / cross-reactivity FLAG read from the sequence, not a clinical diagnosis; the certified IgE / oral-food-challenge panel stays official. Heat stability indicates whether cooking is likely to reduce the risk — heat-stable families (cupin storage globulins, 2S albumins) retain allergenicity through processing.

Results & mechanism — read like the methods of a paper, generated per protein

Each paragraph is assembled from this protein's own computed values; the clauses that appear, and the numbers in them, differ for every input.

Results & mechanism — beta-lactoglobulin (bovine)

The assembled particle has a predicted radius of gyration R_g = **2.2 nm** (SAXS observable) and hydrodynamic radius R_h = **2.8 nm** (DLS observable; R_g/R_h 0.78), placing it in a small, stable size range. Aggregation propensity (size-driven): **LOW** (score 0.25) — estimated from the predicted particle size, deterministically and with no molecular-dynamics step. A pre-instrument indicator that complements DLS/SEC-MALS. Predicted denaturation temperature **T_d = 74 ± 5 °C** (recognised LIPOCALIN fold, reported as a band — the value is deterministic, the ± is the fold-family's disclosed uncertainty) — thermolabile for a whey lipocalin. Unfolding enthalpy **ΔH ≈ 15.8 J/g** with $\Delta C_p \approx 9.4$ kJ·mol^{-1}·K^{-1} (the folded→unfolded baseline heat-capacity step, set by the buried-apolar surface). Peak sharpness is set by the cooperativity $\kappa = \Delta H_{vH}/\Delta H_{cal}$ (shown on the DSC thermogram), not by ΔC_p. It forms **a strong, self-supporting gel** (predicted G′ ≈ 21.3 kPa at 14% w/v; least-gelling concentration ≈ 6.8% w/v). Isoelectric point **pI ≈ 4.6**: minimum solubility (and the precipitation pH for purification) sits here, with solubility recovering toward the acid and alkaline extremes. Interfacial and hydration behaviour: surface-activity index 0.99 (emulsification/foaming); water-holding 1.3 / oil-holding 0.5.

Protein bitter-peptide stack — where it turns bitter, and the sequence causing it

From the protein sequence alone — no samples: the in-silico digest, the bitter peptides ranked by liability, and the degree-of-hydrolysis taste arc showing at what stage of processing / digestion the bitterness emerges.

beta-lactoglobulin (bovine) — 162 aa · 235 digest peptides · 122 bitter (51.9% of scanned) · 3 strong culprit(s)

#	Bitter peptide	Liability (0–1)
1	**KYL**	0.824
2	**YL**	0.734
3	**LF**	0.700
4	**YLLFCM**	0.681
5	**IPAVFK**	0.676

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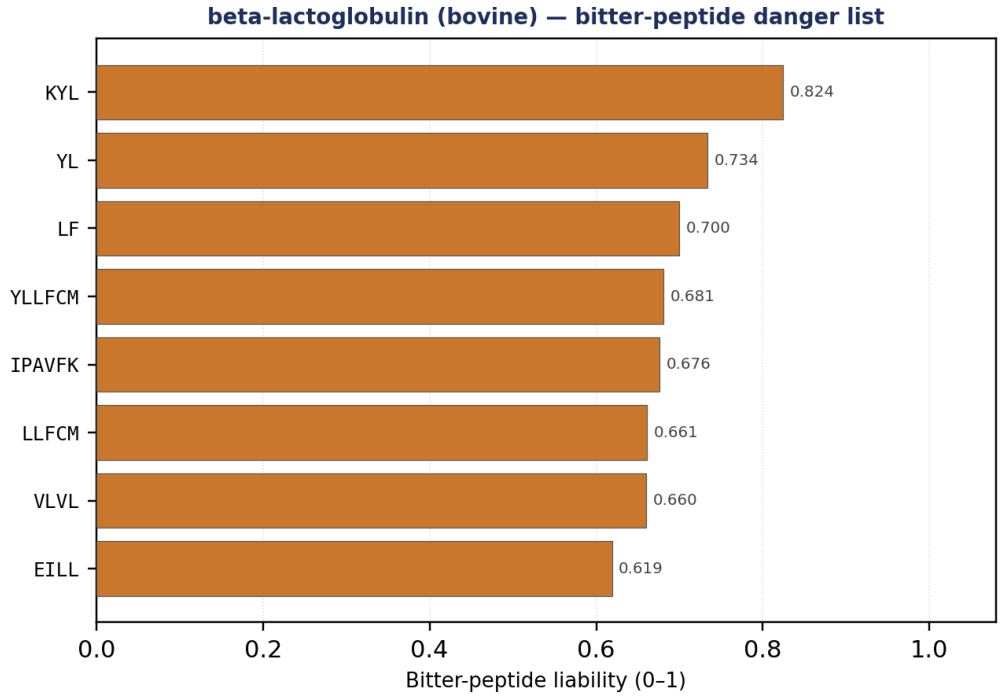
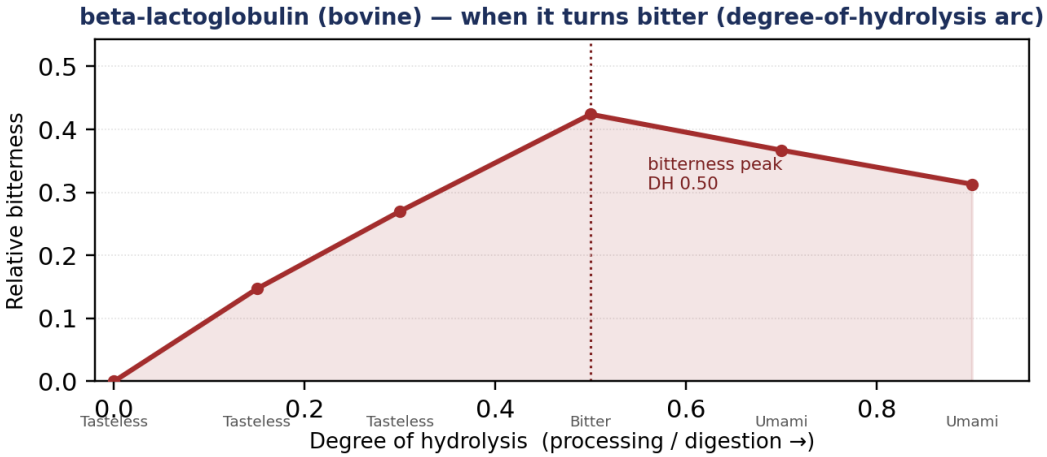
#	Bitter peptide	Liability (0–1)
6	**LLFCM**	0.661
7	**VLVL**	0.660
8	**EILL**	0.619





Degree-of-hydrolysis taste arc: DH 0.00 **Tasteless** → DH 0.15 **Tasteless** → DH 0.30 **Tasteless** → DH 0.50 **Bitter** → DH 0.70 **Umami** → DH 0.90 **Umami**
Predicted denaturation temperature: 74 °C — recognised LIPOCALIN fold — provisional Td (own physics, not cupin) [separation route: wet_iep]
Process conditions (as submitted): feedstock bovine_whey; S-S/protomer 2.0
Debittering route (worst culprit): encapsulate in **Pea Legumin (11S)** — Shell diameter (9.5 nm) > 1.5x payload (0.5 nm) [crosslink: genipin]
Load-bearing coupling & thermal headroom. 29 buried cross-subunit contact pair(s) (10 aromatic + 18 basic residues) that hold the assembly together — the structural grip behind its heat stability (counted from the sequence; a 3-D structure confirms the buried contacts); predicted **failure mode: HYDRATION COLLAPSE** — weakest link is the 18 hydration shell; the lever to move it is moisture / water activity (Flory-Huggins plasticization).

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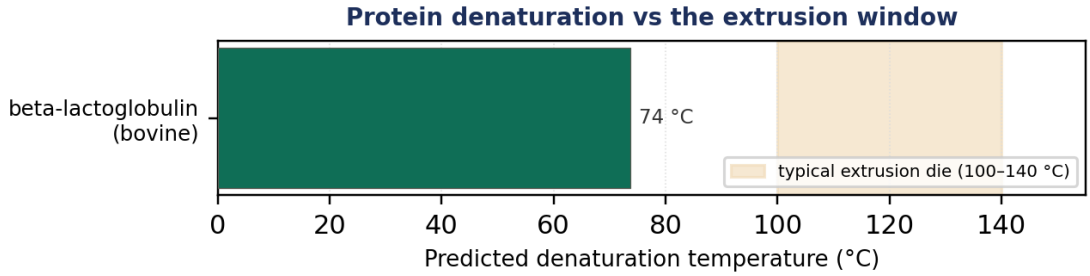
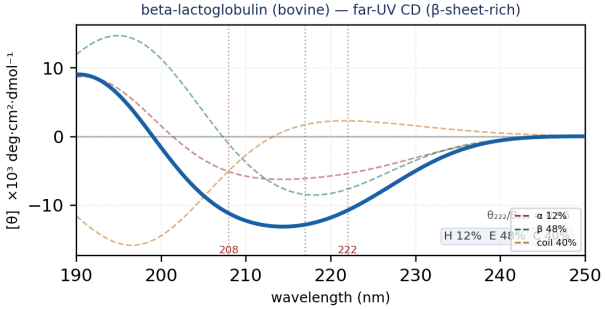
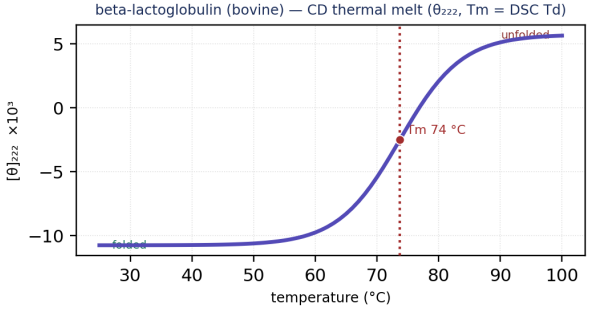
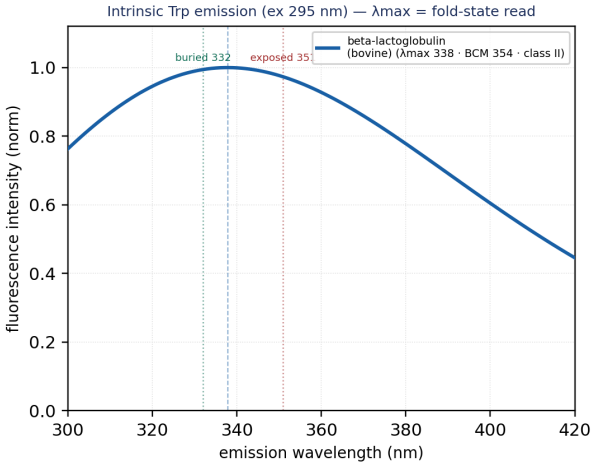


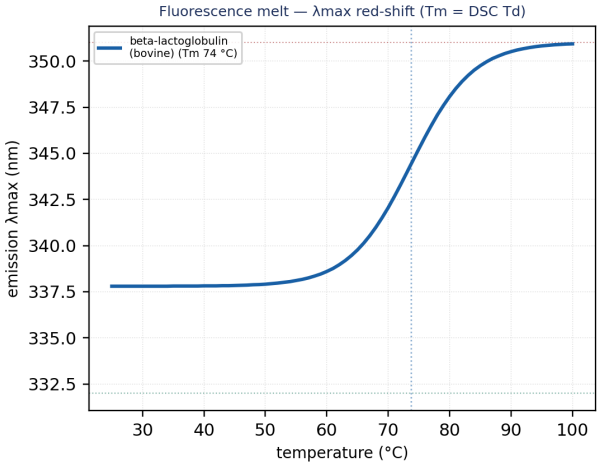
Denaturation temperatures are structure-derived estimates, blind-validated to ±3–5 °C across the storage-globulin core (~84–90 °C). The model saturates at the high end and COMPRESSES genuinely hyperstable globulins (phaseolin, lupin α-conglutin, some faba legumin — really ~95–105 °C) DOWN into the 84–90 °C band, where they can read ~15 °C low. So a predicted T_d in that band may be a true core value OR a compressed hyperstable outlier — confirm any hyperstable-class candidate by DSC before setting a thermal-processing (extrusion / UHT / retort) target.
Predicted far-UV circular dichroism (CD) — the fold-state read (is it folded, and did the process unfold it?). For a RECOGNISED fold the %-secondary-structure is the fold-family canonical signature (every cupin β-barrel reads β-rich, ~11% α / 40% β — the fold DEFINES its secondary structure), so within one fold family the per-protein distinction lives in the MELT (T_d), not the spectrum shape; the CD thermal melt shares the DSC denaturation midpoint. A structure-derived estimate to compare against your CD trace, not a substitute for it.





Predicted intrinsic (tryptophan) fluorescence — the tertiary-structure read: a blue emission maximum means the Trp are buried in a native core, a red-shift means they have become solvent-exposed (unfolded). The thermal melt shares the same denaturation midpoint as the CD and DSC estimates. Compare against your fluorescence trace.





Predicted nanoDSF (F350/F330) thermal shift — the modern label-free way labs read Tm: the intrinsic-fluorescence ratio rises as the core unfolds, and each peak of its first derivative is a melting temperature (the same midpoint as the DSC/CD estimates). A single-domain protein shows one peak; WHERE a bilobal cofactor protein is present, it melts in two transitions — an early cofactor-free lobe (S1) and a late cofactor-bound lobe (S2) — so the S1/S2 areas report the fractional cofactor saturation a single DSC scan cannot (storage globulins are cofactor-free → one transition). Compare against your Prometheus trace.

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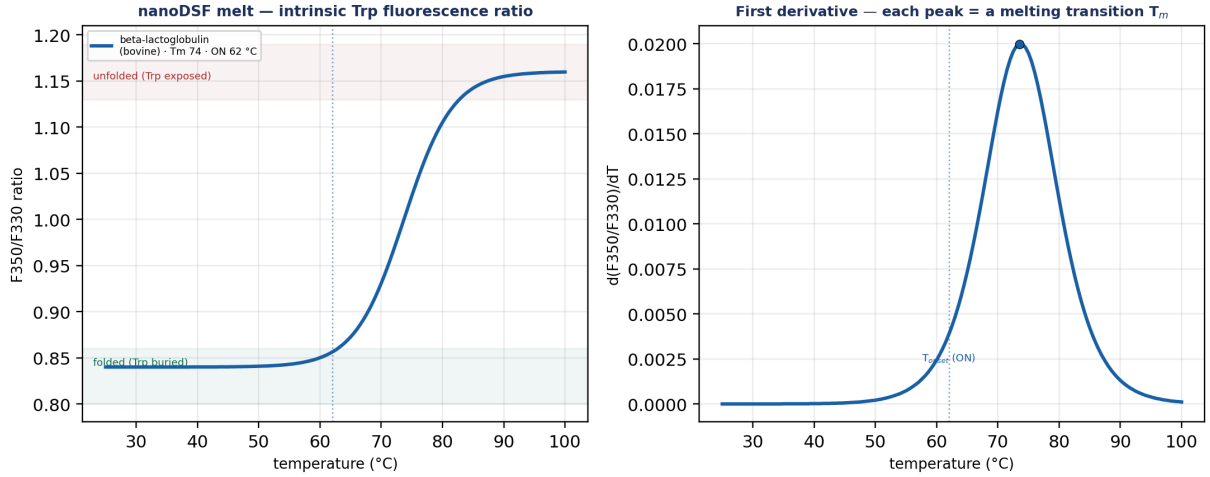
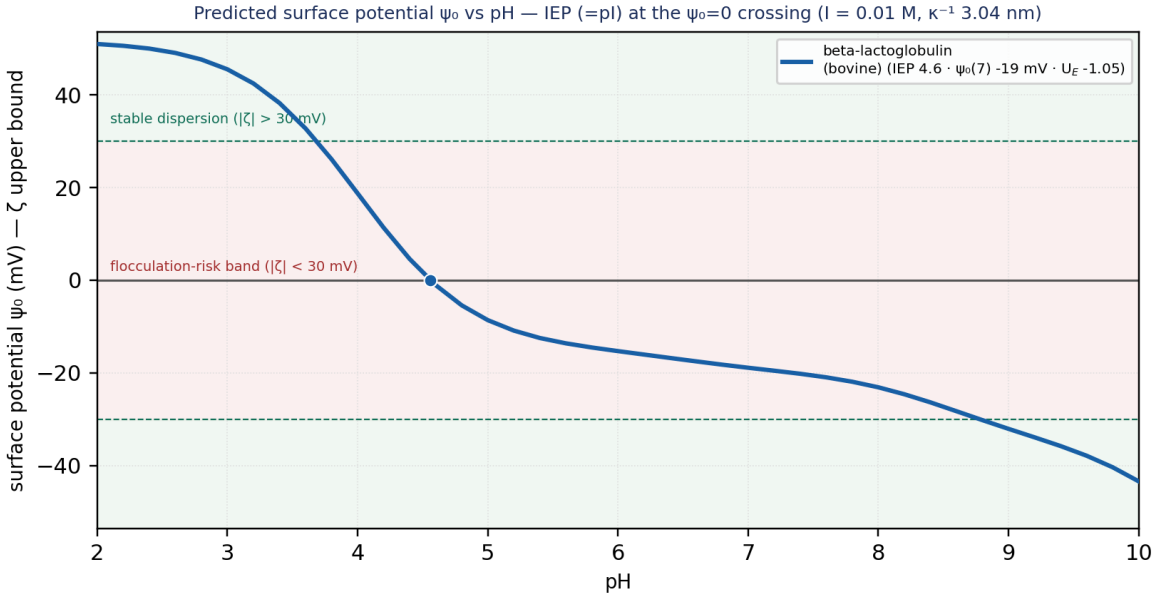
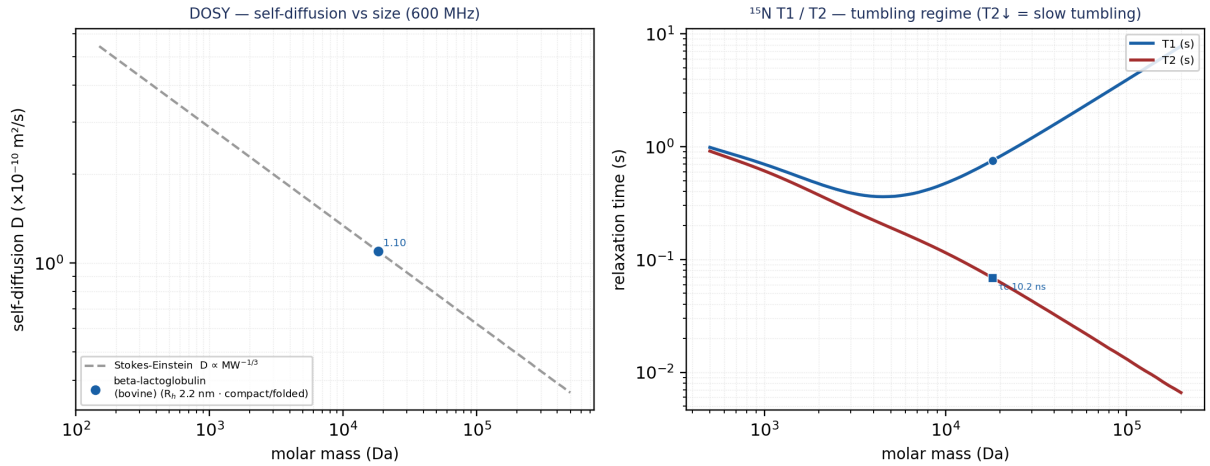


Predicted zeta potential vs pH — the colloidal-stability map: the isoelectric point (ζ = 0) is the pH of least stability (flocculation/precipitation), and |ζ| > 30 mV is the stable-dispersion window. Structure-derived from the charge profile; compare against your Zetasizer trace.



ψ₀ = Debye-Hückel surface potential (upper bound on shear-plane ζ); electrophoretic mobility U_E via Henry $U_E = 2\varepsilon\varepsilon_0\zeta \cdot f(\kappa a)/3\eta$.
Henry f(κa)=1.07 (Ohshima); κa=2.33

Predicted NMR dossier (600 MHz) — self-diffusion (DOSY) vs size and the ^{15}N T1/T2 tumbling regime, structure-derived from the hydrodynamic radius. Complements DLS/SEC-MALS on aggregation and reports the fold-tumbling timescale; an estimate to compare against your NMR data.



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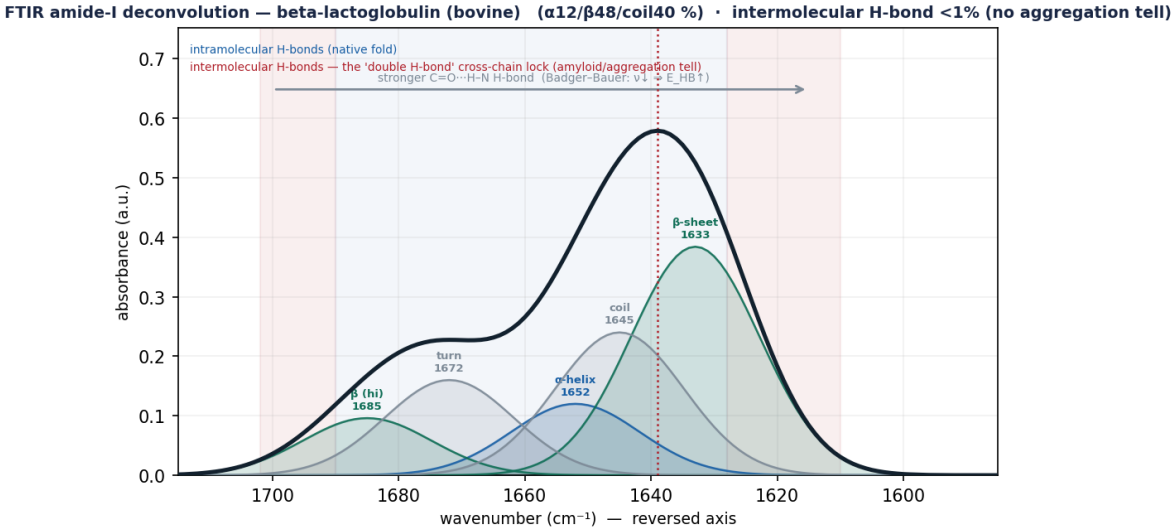
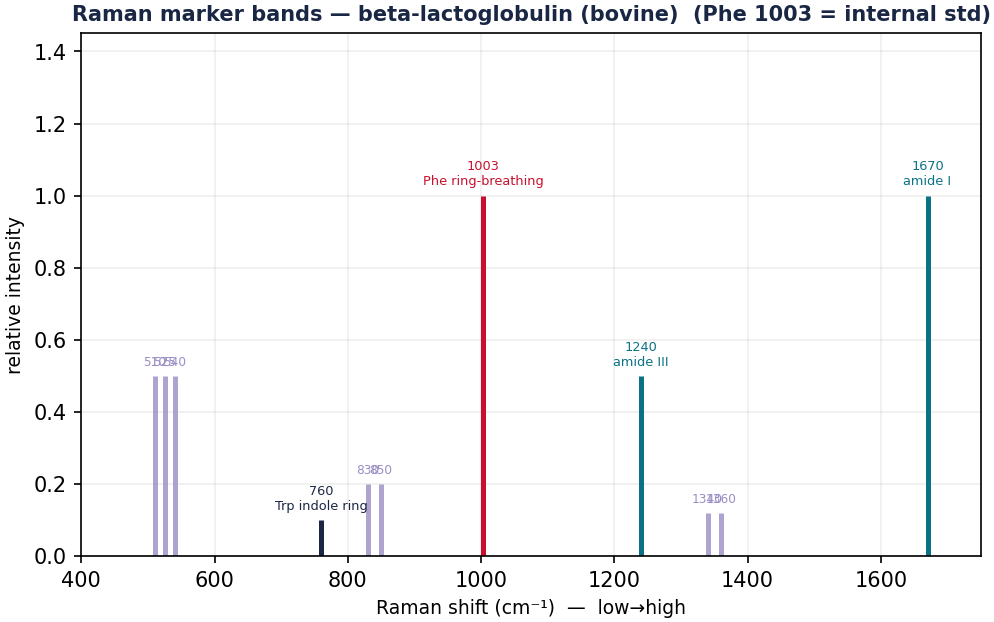
Predicted FTIR amide-I band — a vibrational read of the fold: the amide-I C=O stretch sits at a wavenumber set by the backbone H-bonding, so its position inverts to secondary structure (α-helix ~1652, β-sheet ~1633, intermolecular-β aggregate ~1620 cm⁻¹). Computed from the same fold fractions as the CD and XRD panels — three instruments (far-UV ellipticity · X-ray d-spacing · IR amide-I), one structure, cross-consistent by construction. Reversed wavenumber axis per convention; compare against your ATR-FTIR trace.



Predicted Raman marker-band POSITIONS from the amino-acid composition — the phenylalanine 1003 cm⁻¹ internal standard, the disulfide S–S rotamer triplet (510/525/540), and the tyrosine (850/830) and tryptophan (1360/1340) Fermi doublets. The burial RATIOS (I_{850}/I_{830}, I_{1360}/I_{1340}) and the dominant S–S rotamer are 3-D environment reads and are NOT computed from sequence. Compare positions against your Raman spectrum.



S-S rotamer triplet 510/525/540 · Tyr 850/830 · Trp 1360/1340 shown as POSITIONS (violet); the burial RATIOS I850/I830, I1360/I1340 and the dominant S-S rotamer are 3-D geometry reads — not computed from sequence.

Predicted DSC thermogram (nano-DSC / MicroCal-class) — the excess-heat-capacity C_p unfolding endotherm at the **dilute-buffer** denaturation temperature T_d (the value a dilute DSC / CD / fluorescence run share; the functional table reports T_d at your **submitted moisture** — typically a couple °C lower via plasticisation, so the two differ by the moisture term, not a disagreement), the cooperativity $\kappa = \Delta H_{vH}/\Delta H_{cal}$ (the full-unfolding van't Hoff expectation against the measured calorimetric enthalpy — κ≈1 two-state, κ>1 oligomer dissociation), and the 2nd re-scan that reports reversibility (small disulfide-clamped folds refold; large multi-domain/glyco folds stay denatured). A structure-derived estimate — compare against your DSC C_p trace.

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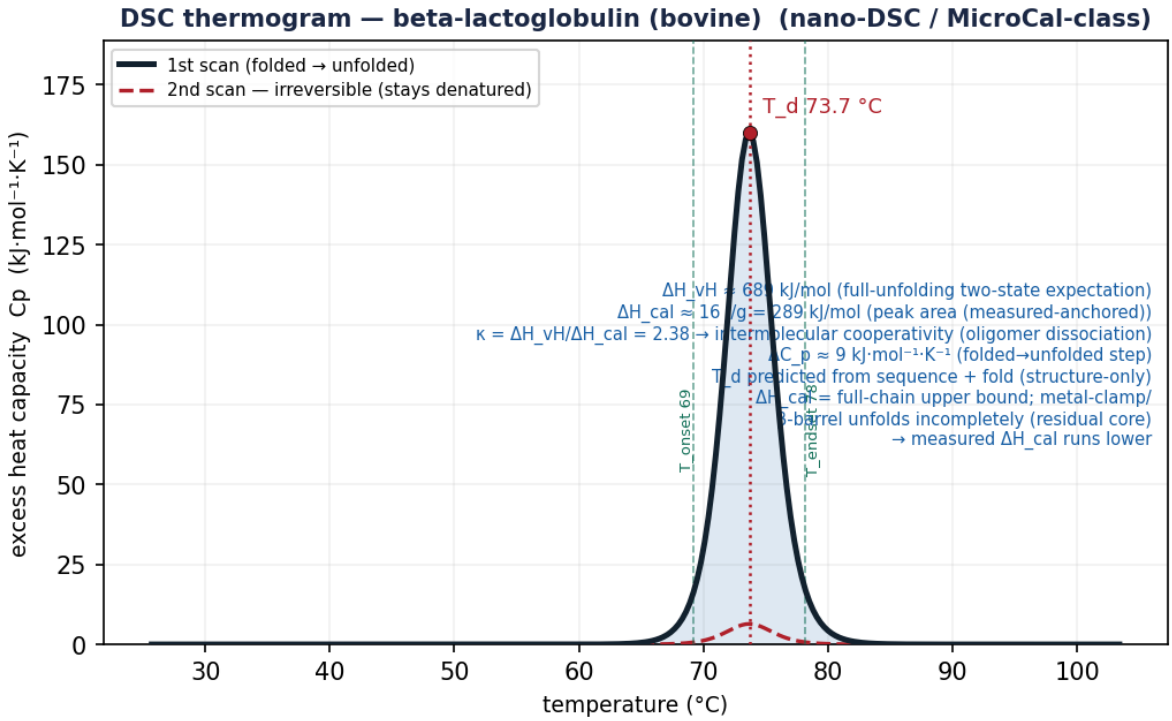
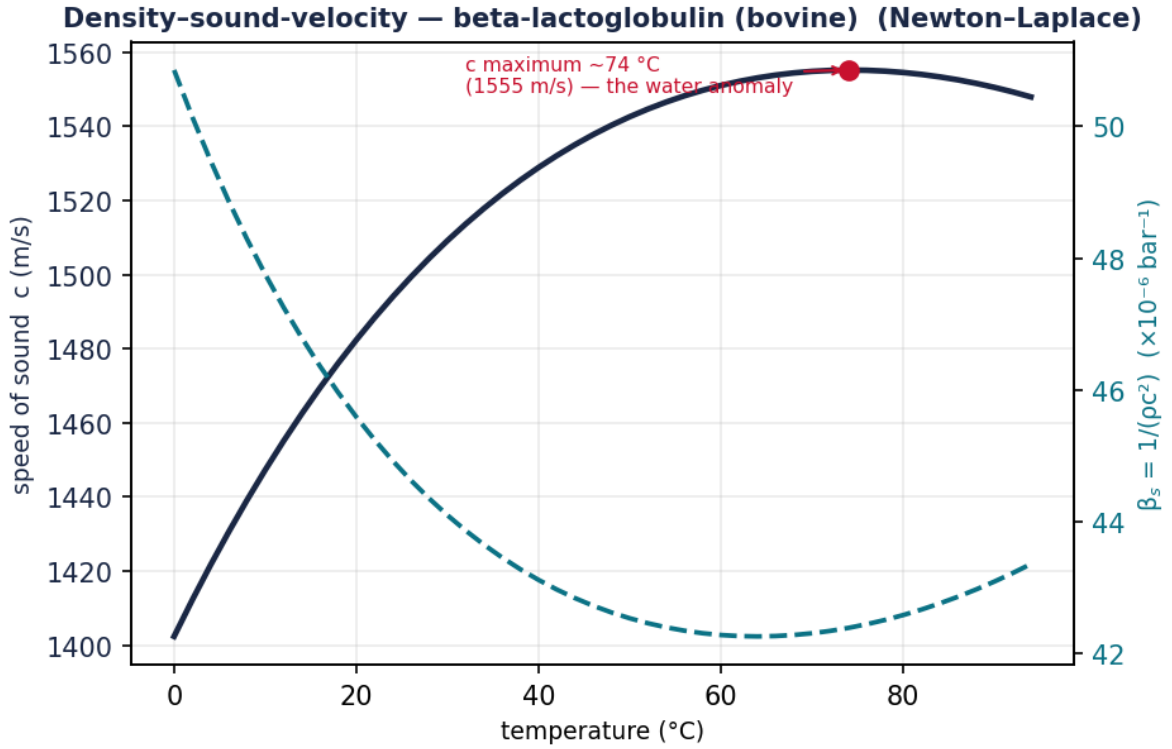


Density–sound-velocity (DSA-5000-class) — the speed-of-sound c(T) signature with its ~74 °C water-anomaly maximum and adiabatic compressibility $\beta_s = 1/(\rho c^2)$, the hydration-structure read the protein's computed partial specific volume $\bar{v}$ and solution density (reported above) are measured against on an oscillating-U-tube densitometer.



Thermal transport (Choi–Okos, $\alpha = k/\rho c_p$) — thermal conductivity k and diffusivity α vs temperature computed from THIS ingredient's composition (7% moisture), with the freezing discontinuity where k jumps ~3–4× as water→ice. The process-heat read for drying, pasteurisation and freezing operations.

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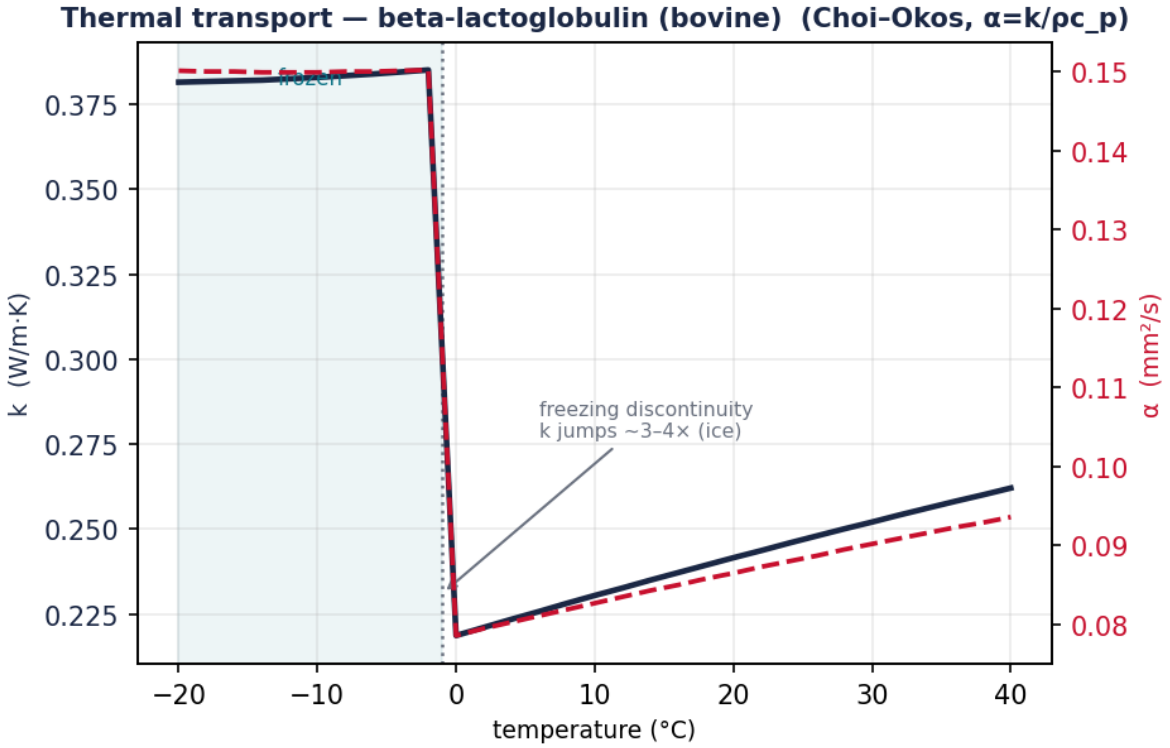
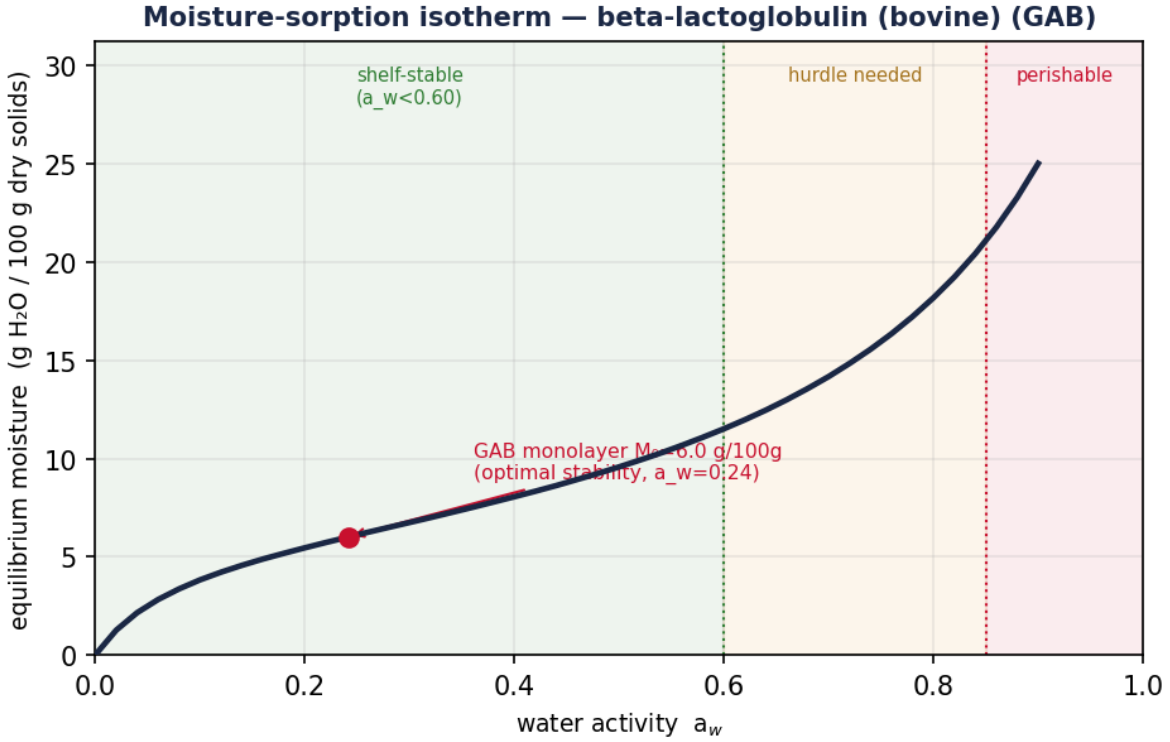


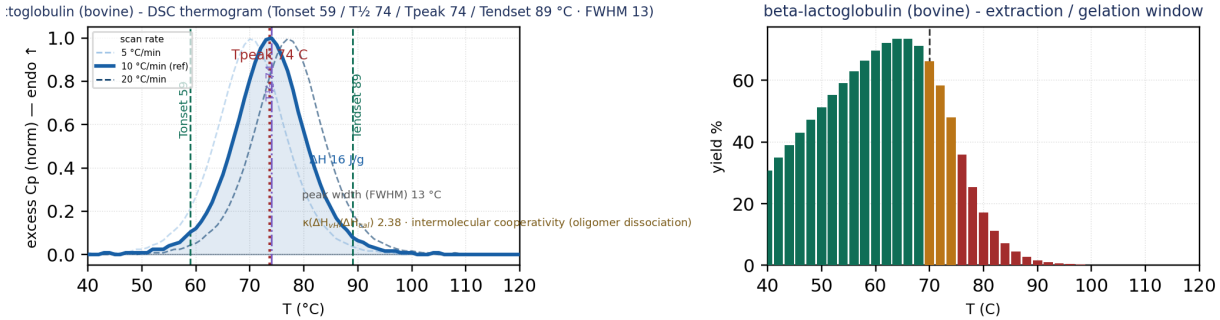
Moisture-sorption isotherm (GAB) — the powder shelf-life reference: equilibrium moisture vs water activity with the GAB monolayer (optimal-stability point) and the microbial hurdle bands (a_w < 0.60 shelf-stable / 0.60–0.85 hurdle needed / > 0.85 perishable) the dried-powder glass-transition and caking read (above) sits on.



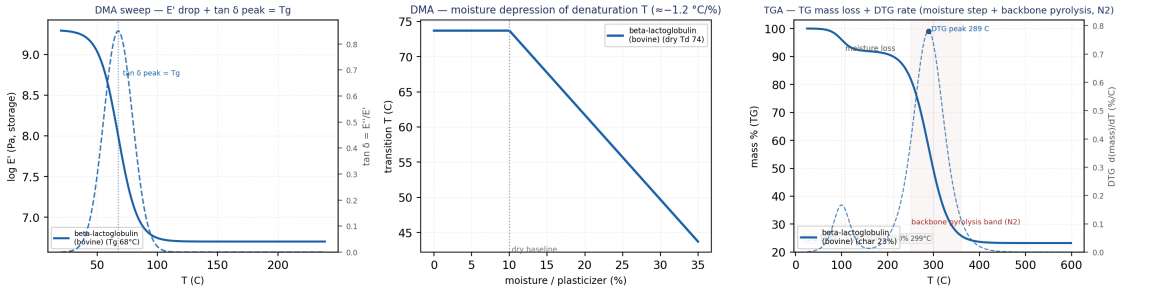
Paired-instrument diagnostics — the cross-machine reads a multi-instrument lab derives by hand, here computed ONCE from the one structure so they are cross-consistent BY CONSTRUCTION (the no-contradiction cascade: a single fold-fraction set and a single T_d drive every read — not independent measurements that happen to agree): **oligomer** n≈2.0 (native 36562.0 / subunit 18281.0 Da, from sequence + oligomer); **2° structure** α 12.0% / β 48.0% (CD far-UV and FTIR amide-I share the one fold-fraction set); **CD-melt midpoint = the DSC T_d** 73.7 °C (one unfolding transition read two ways); **nanoDSF − DSC** Kissinger apparent-T_m gap +6.5 °C (kinetic vs equilibrium); **safe processing window** 68–249 °C (DMA T_g → TGA decomposition onset).

Integrity (SHA-256 manifest): 4750cc400ae9ced206d81c7577c52cade6f8571e94a64812d168a9026cfdb20a

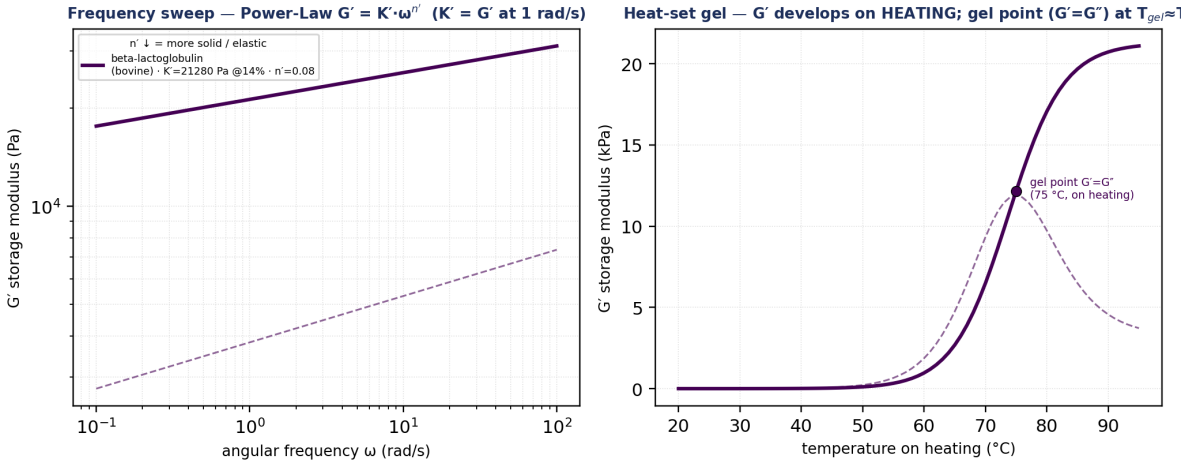
Predicted thermal profile (DSC-style) & extraction/gelation window — per protein, from the structure-derived T_m. An estimate to compare against your DSC trace, not a substitute for it.



Predicted DMA (moisture plasticization) & TGA (mass-loss) — structure-derived estimates, consistent with the same T_d

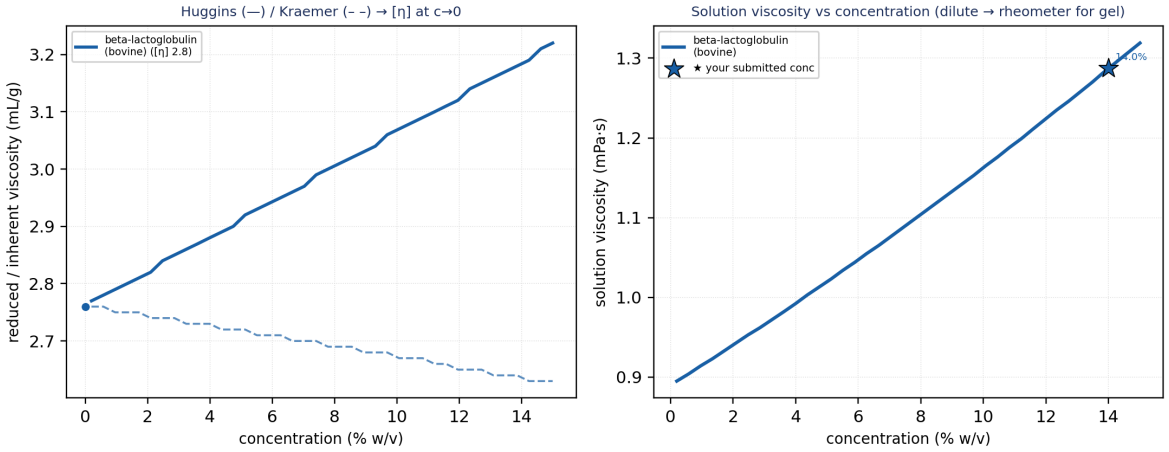


Predicted rheology — structure-derived G′ frequency sweep (Power-Law $K'\cdot\omega^{n'}$) & heat-set gel point (on heating, $T_{gel}\approx T_d$)

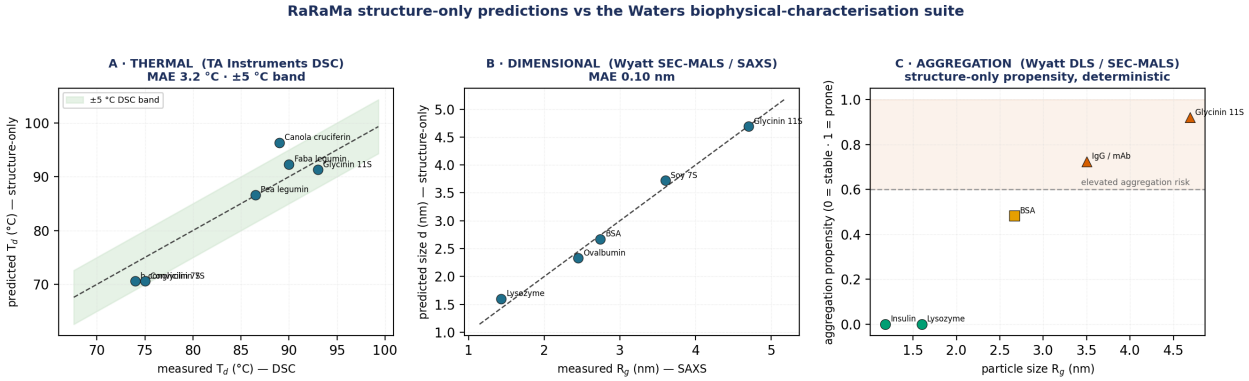


Predicted small-amplitude oscillatory G′ from the structure-derived gel modulus + T_d (heat-set globulin: the network forms on HEATING at $T_{gel}\approx T_d$; cooling cures it further). Absolute scale is rank-valid — supply a measured G′ to calibrate it.

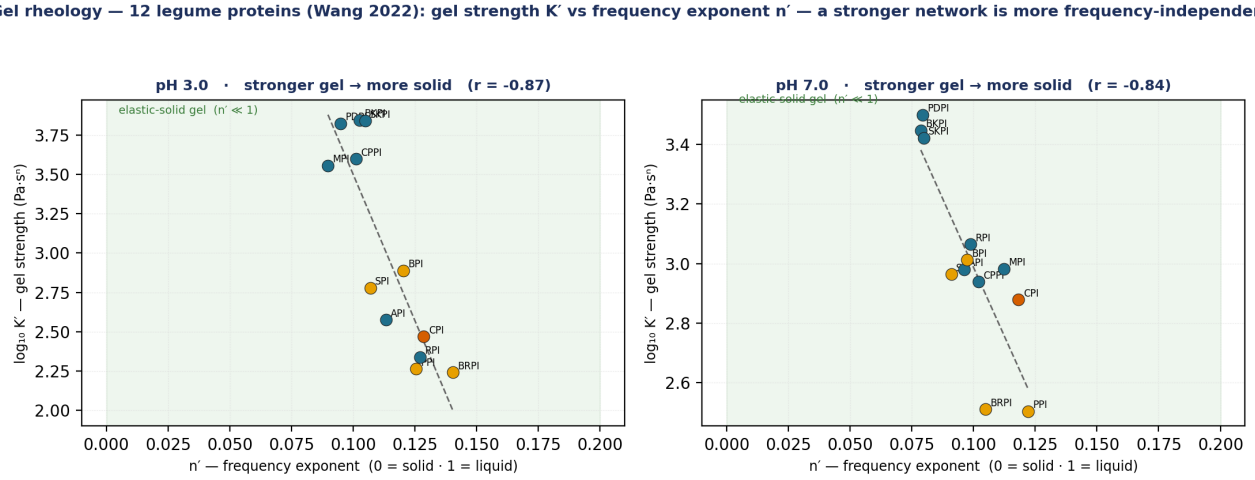
Predicted solution viscosity — the intrinsic viscosity [η] (Huggins/Kraemer double extrapolation) and the dilute-to-semi-dilute viscosity vs concentration for beverage/RTD processing. Accurate for compact globular proteins; the concentrated/gel regime is covered by the rheometer above. Compare against your capillary/rotational viscometer.



Instrument correlation — how these structure-only predictions line up with the Waters / TA-Instruments / Wyatt biophysical-characterisation suite: one engine across three instruments (DSC thermal · SAXS/SEC-MALS dimensional · DLS aggregation), each shown predicted-vs-measured on a reference set. This is the validation context beneath every prediction in this dossier.

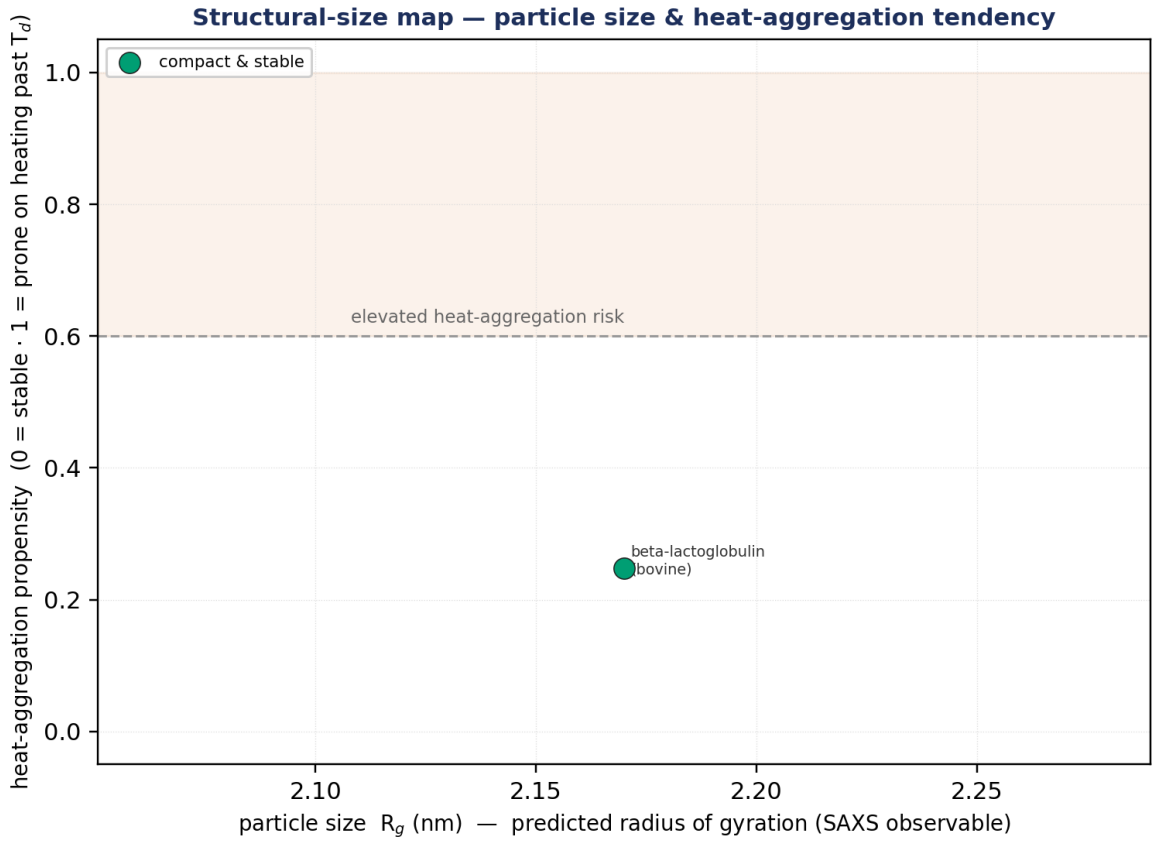


Rheometer correlation (external study) — Wang et al. 2022 measured the gel strength K′ and frequency exponent n′ of 12 legume-protein gels. A stronger network is more frequency-independent, so K′ and n′ move opposite — confirmed at both pH (r ≈ −0.85), and every gel sits in the elastic-solid band. This is the rheometer half of the biophysical suite, validated against an independent study.



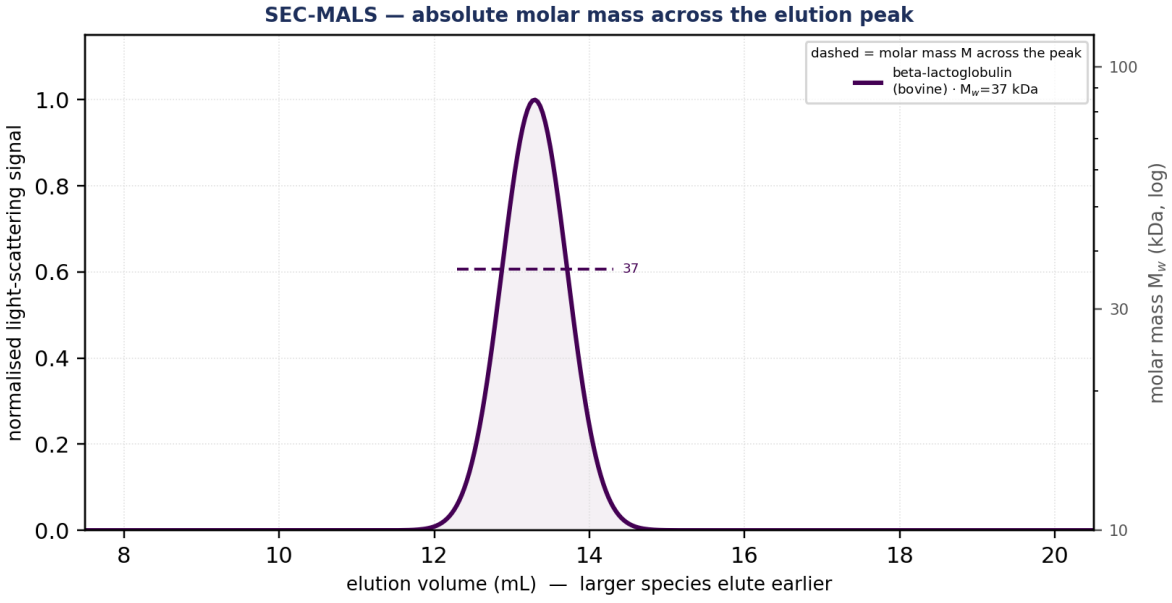
Integrity (SHA-256 manifest): 4750cc400ae9ced206d81c7577c52cade6f8571e94a64812d168a9026cfdb20a

Structural-size map — particle size and aggregation tendency



RSIBLY on heating past T_d (the gelation route) — larger particles are more prone; the scale discriminates (small compact monomers read LOW, not all-high). The NATIVE folded-oligomer size is s

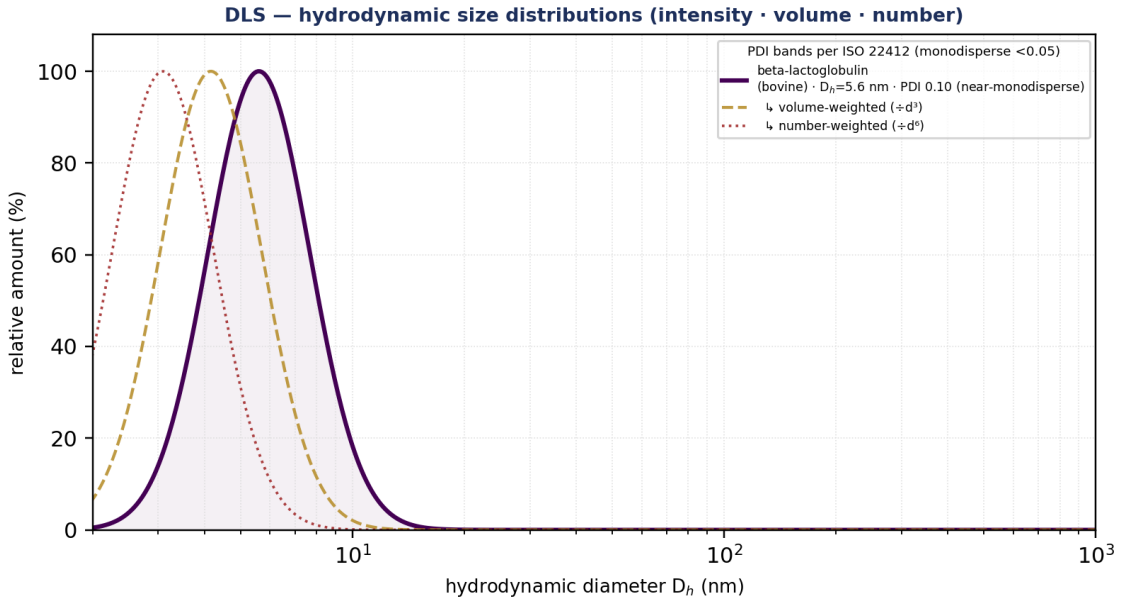
SEC-MALS — absolute molar mass & oligomeric state (computed from sequence + oligomer)



M_w computed from sequence + oligomer (structure-only). A flat M across each peak = a single monodisperse species (no aggregate/fragment); elution volume from a calibrated-column model.

Integrity (SHA-256 manifest): 4750cc400ae9ced206d81c7577c52cade6f8571e94a64812d168a9026cfdb20a

DLS — hydrodynamic size distribution (R_h, monodispersity)

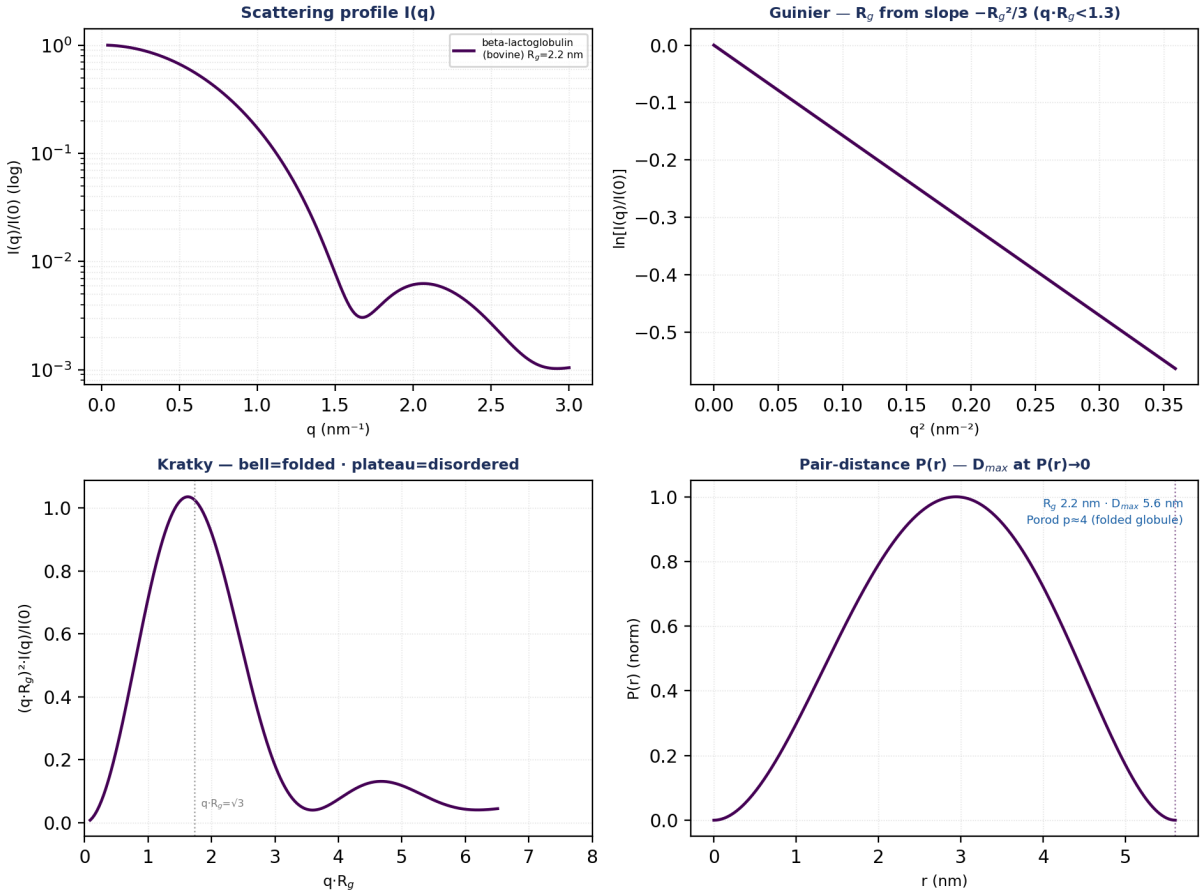


/→volume→number shifts the peak smaller (÷d³ each); PDI at the ~0.1 monodisperse floor. This is the NATIVE-state read (folded oligomer, monodisperse); on heating past T_d the size-driven mode aggre

What a DLS run measures is a rate, not a size: the scattered-light autocorrelation decays as the particles diffuse, the instrument fits that decay to the translational self-diffusion coefficient D, then inverts the Stokes–Einstein relation ($R_h = k_B T / 6\pi\eta D$) to the hydrodynamic radius — the size is read out of a dynamical measurement at the length scale set by the 633 nm laser and back-scatter geometry. Predicted self-diffusion for your proteins (25 °C, water): beta-lactoglobul D=88 µm²/s. This is the NATIVE-state read: a single narrow peak = monodisperse folded oligomer. On heating past T_d the size-driven mode aggregates irreversibly (the gelation route, mapped separately) → a second large-size population which, being intensity-weighted ∝ R_h^6, dominates the reported Z-average even at trace levels.

Integrity (SHA-256 manifest): 4750cc400ae9ced206d81c7577c52cade6f8571e94a64812d168a9026cfdb20a

SAXS — scattering profile & Kratky fold state (R_g, compact vs disordered)



Structure-derived: R_g (Guinier), $D_{max} = 2{\cdot}R_g{\cdot}\sqrt{(5/3)}$ sphere estimate (elongated particles read higher), Porod exponent 4 = smooth folded sphere / 2 = disordered coil. Compare against your ATSAS/SASBDB analysis.

XRD / WAXS — fold order & amorphous halos (Bragg d-spacings)

A diffractometer records the angle 2θ at which the probe X-ray (Cu-Kα, 1.54 Å) constructively interferes, then inverts Bragg's law (nλ = 2d·sinθ → d = nλ/2·sinθ) to the backbone d-spacings the solid shows — the β-strand H-bond spacing (~4.7 Å, 2θ≈18.9°), inter-sheet/inter-helix packing (~9–10 Å), and the amorphous halo (~4.4 Å, 2θ≈20°). Predicted from your proteins' secondary structure (the same %helix/%sheet the CD panel reports): beta-lactoglobul 60% ordered SS, main halo 4.7 Å at 2θ=18.9° (β-strand H-bond spacing). Note a dried globular protein is X-ray amorphous — these are broad halos, not sharp crystalline reflections; the ordered-SS fraction is a solid-state fold-order read that complements solution SAXS.
AUC — c(s) sedimentation distribution ($s_{20,w}$ in Svedberg, structure-derived from the exact molar mass and hydrodynamic radius; a calibration ruler marks lysozyme 1.9 · BSA 4.3 · IgG 6.5 · catalase 11.3 S). Resolves oligomeric state and shape — accurate for compact globulars, ~15–20% high for elongated folds. Compare against your Beckman Optima c(s) trace.

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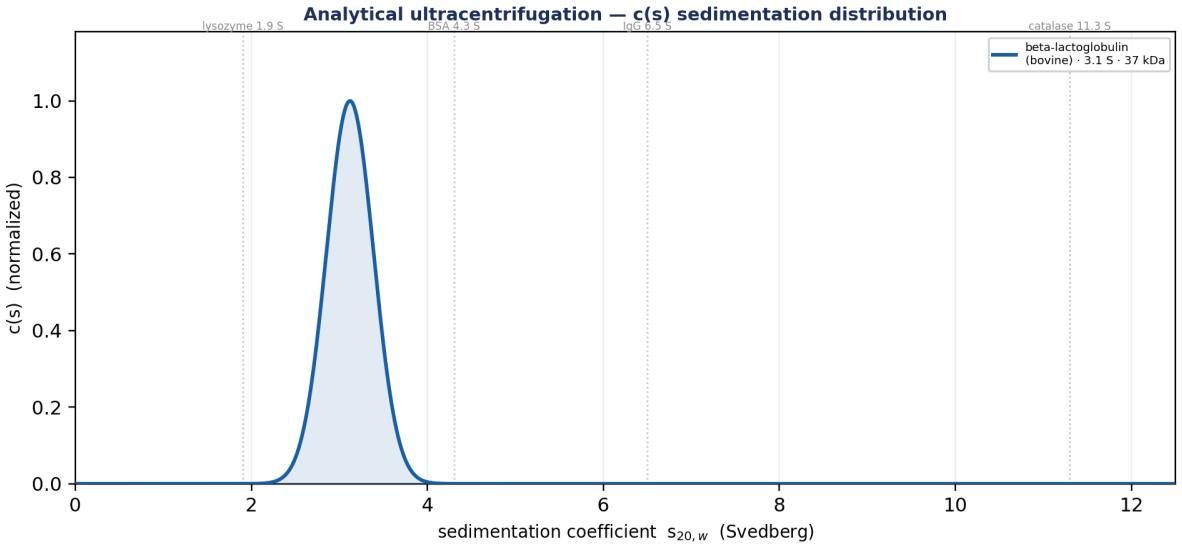


Density / sound-velocity (DSA) — compressibility & hydration

A density–sound-velocity analyser measures the solution density and the speed of sound c in one cycle, and inverts the Newton–Laplace relation (β = 1/ρc²) to the adiabatic compressibility — a direct probe of interior packing and hydration. The partial specific volume v̄ is exact from the amino-acid composition; the sign of the apparent specific adiabatic compressibility follows from the fold — a compact globular interior with interior packing voids reads positive (void-dominated), an extended or disordered chain reads negative (hydration-dominated). beta-lactoglobul v̄=0.737 cm³/g, apparent adiabatic compressibility predicted positive (packing-void-dominated). A measured sound-velocity increment fixes the magnitude and the hydration number (Gekko–Hasegawa; Kharakoz–Sarvazyan).

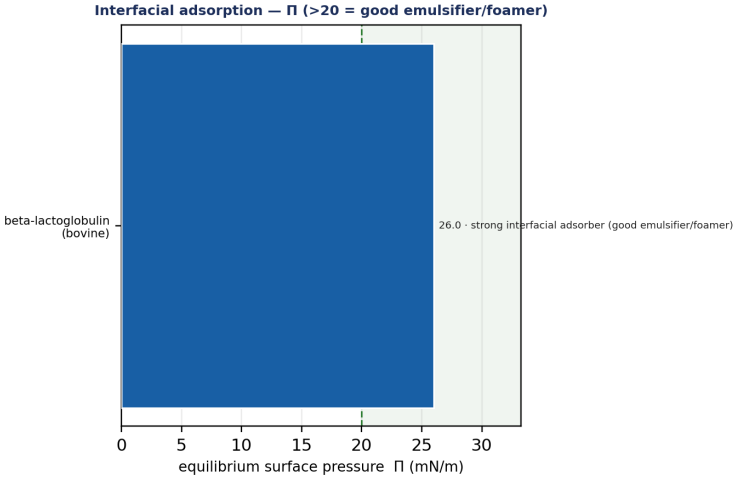
Thermal transport — conductivity, diffusivity & heat capacity (processing)

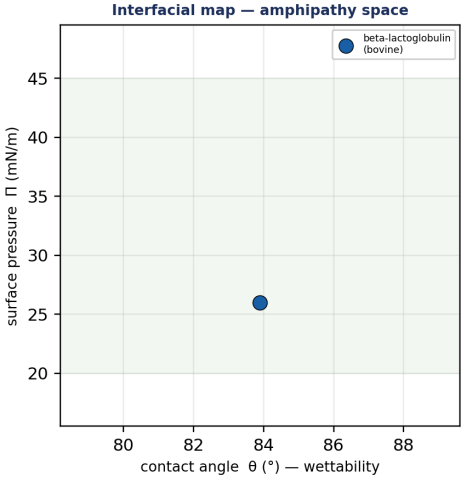
For process design (heating, cooling, drying, freezing): a laser-flash run measures the rear-face half-rise time after a light pulse and inverts Parker's relation (α = 0.1388·L²/t½) to the thermal diffusivity; the conductivity k, specific heat c_p and diffusivity α follow from the composition (Choi–Okos). For a protein food across moisture — 10% moisture: k=0.26 W/m·K, cp=2.3 kJ/kg·K, α=0.090 mm²/s · 50% moisture: k=0.44 W/m·K, cp=3.1 kJ/kg·K, α=0.124 mm²/s · 80% moisture: k=0.55 W/m·K, cp=3.7 kJ/kg·K, α=0.139 mm²/s. On freezing, the conductivity rises ≈4.0× (ice conducts ~4× water) and the diffusivity ≈8.1× — why a frozen product cools faster than it thawed. A held-out LFA or hot-wire run refines these.

Water activity (a_w) — shelf-stability & food safety

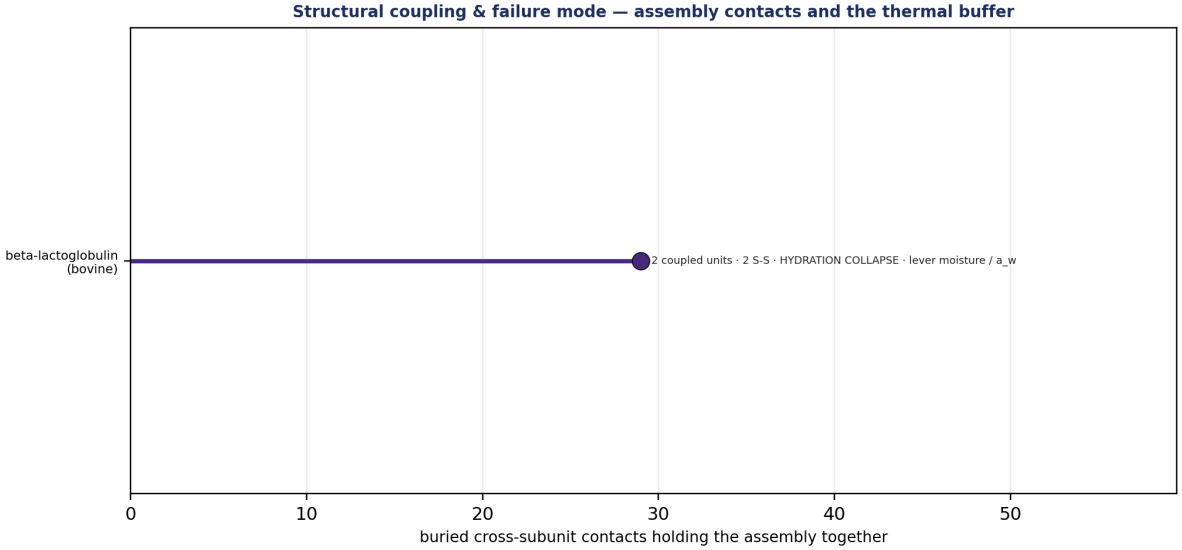
A water-activity meter reads the equilibrium relative humidity a_w = p/p₀ and inverts the moisture-sorption isotherm (GAB) to the water-binding state — the single best predictor of microbial and chemical shelf-life. The monolayer M₀ (the maximum-stability moisture, at the lipid-oxidation minimum) is structure-estimated from the polar-residue content: beta-lactoglobul M₀=0.069 g/g (stability optimum a_w≈0.24); at 10% moisture a_w≈0.45. Safety ladder: no microbial growth below a_w 0.60, molds below 0.70, FDA shelf-stable at ≤ 0.85, bacterial pathogens need > 0.90 (S. aureus the exception at 0.86). A measured sorption isotherm refines M₀ (ICMSF / Beuchat / FDA thresholds).
Predicted interfacial behaviour (pendant-drop / tensiometer) — the equilibrium surface pressure Π each protein develops at the air–water interface (Π > ~20 mN/m marks a strong adsorber → a good emulsifier/foamer), and the contact-angle (wettability) vs Π map placing each protein in amphipathy space. Structure-derived from the hydrophobic-moment profile; compare against your tensiometer.

Integrity (SHA-256 manifest): 4750cc400ae9ced206d81c7577c52cade6f8571e94a64812d168a9026cfdb20a



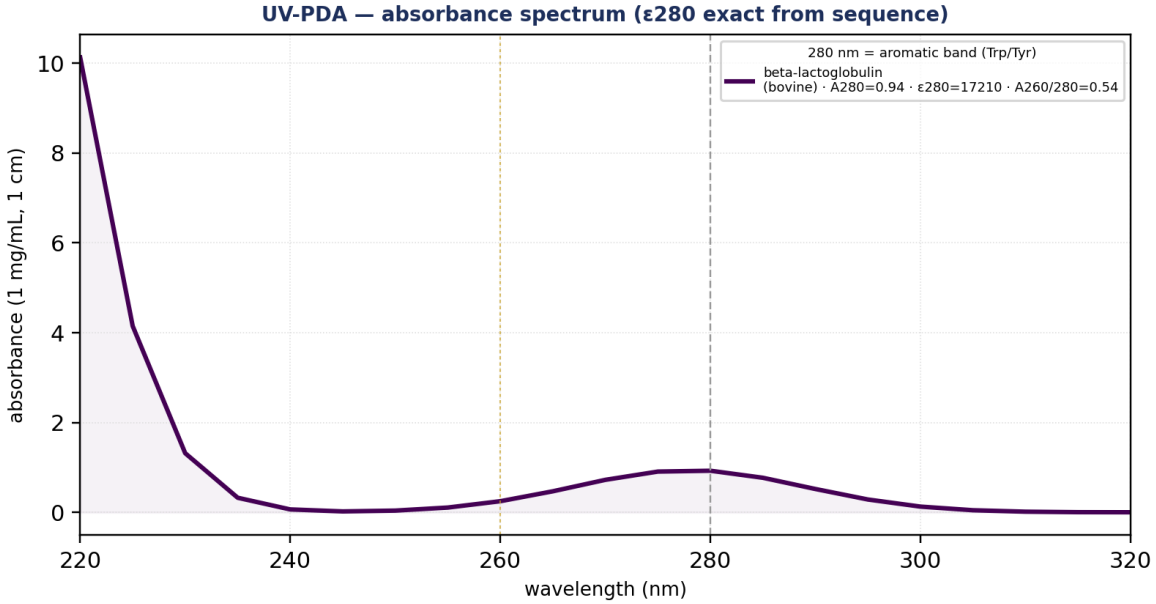


Predicted structural coupling & failure mode — the buried cross-subunit contacts that hold each assembly together, with its assembly cooperativity (set by how many subunits and disulfide links share the load) and the mechanism it fails by when pushed past its limit (the subunits pulling apart vs. hydration collapse) plus the formulation lever to counter it. A structure-derived stability-mechanism read, not a wet measurement.



Integrity (SHA-256 manifest): 4750cc400ae9ced206d81c7577c52cade6f8571e94a64812d168a9026cfdb20a

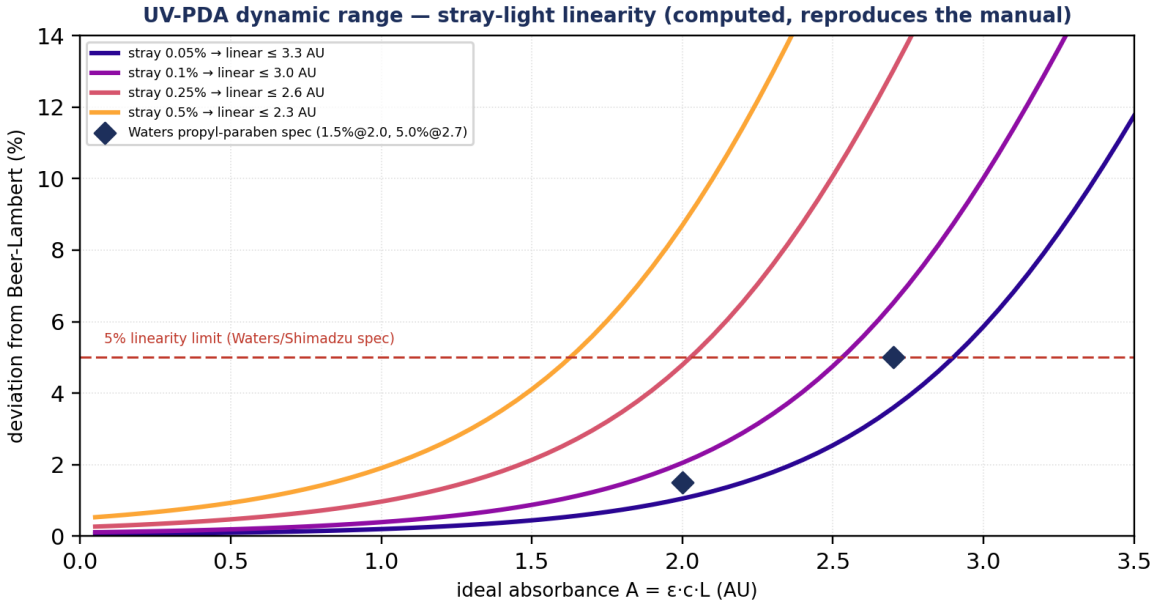
UV-PDA detector — absorbance spectrum & $\varepsilon_{280}/A_{280}$ (exact from sequence; converts a UV peak to concentration)



00·Trp + 1490·Tyr + 125·disulfide (Pace) — EXACT from sequence (matches ProtParam: lysozyme 37,970 / A280 2.65). A280(0.1%) = ε280/MW converts the UV peak to concentration; peptide band

Concentration by Beer–Lambert: a UV detector measures absorbance A and inverts A = ε·c·l (ε the molar extinction, l the 1 cm path length) to concentration — c = A / (ε·l). Because ε_{280} is exact from the Trp/Tyr/disulfide content (Pace), a measured A_{280} reads straight to mg/mL for your proteins: beta-lactoglobul ε_{280}=17210 $M^{-1}cm^{-1}$, A_{280}(1 mg/mL)=0.94. The law is linear over A≈0.1–1.5; above that (a concentrated stock) dilute to bring the reading back into range.

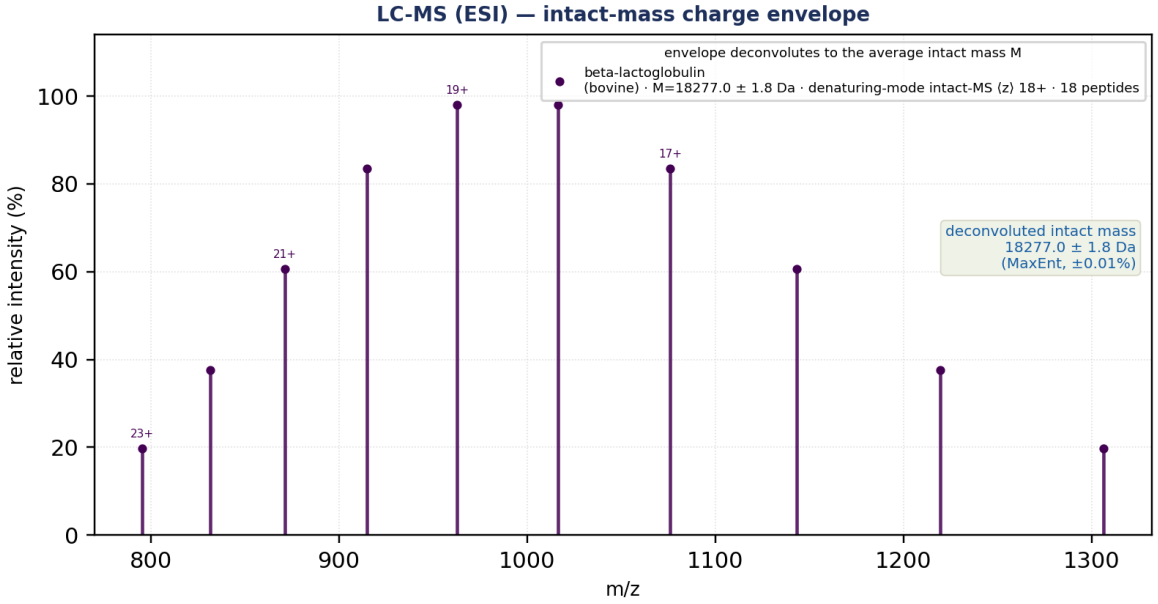
UV-PDA dynamic range — stray-light linearity (computed transfer function; reproduces the Waters/Shimadzu spec)



ction (the detector transfer function). Ceiling = −log10(s); above ~2 AU dilute or use a shorter (10 mm) flow cell. Our curve passes through the Waters propyl-paraben spec points — the framework ε280 i

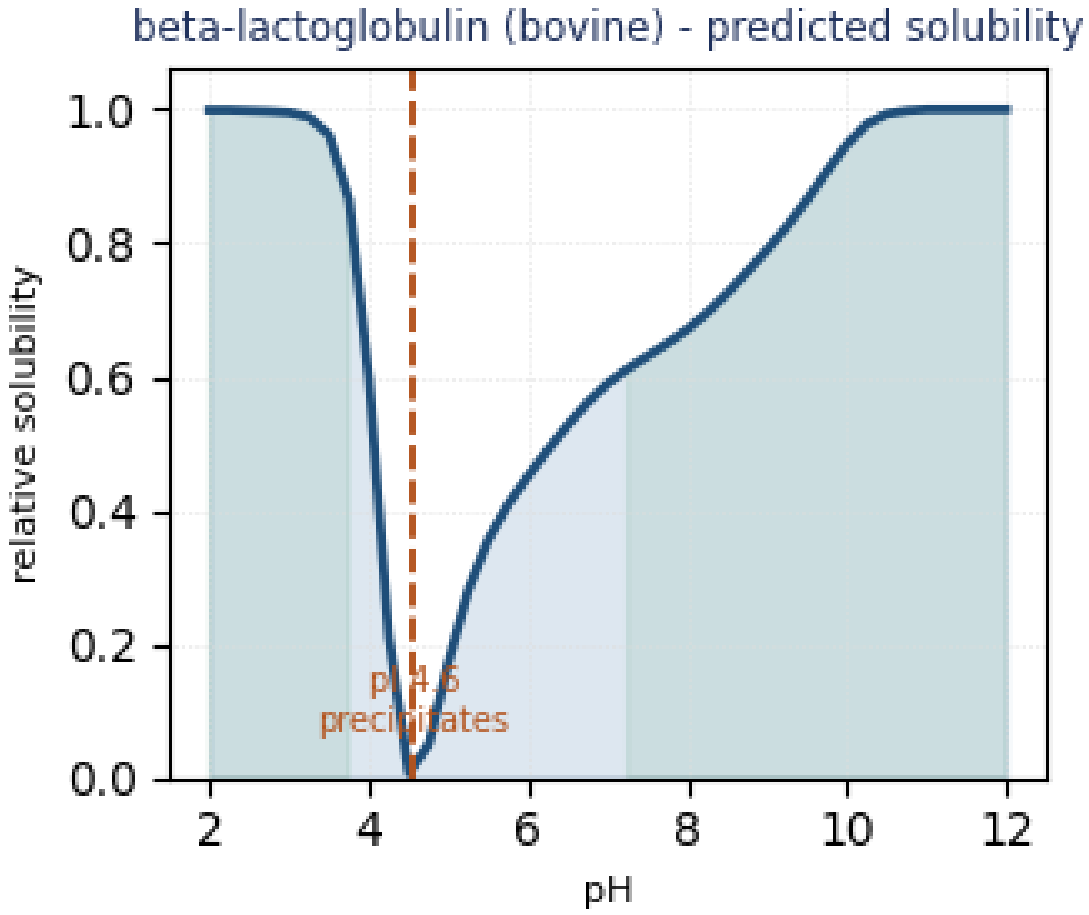
Integrity (SHA-256 manifest): 4750cc400ae9ced206d81c7577c52cade6f8571e94a64812d168a9026cfdb20a

LC-MS (ESI) — intact-mass charge envelope (the exact atomic-sum mass) & tryptic peptide-mass fingerprint



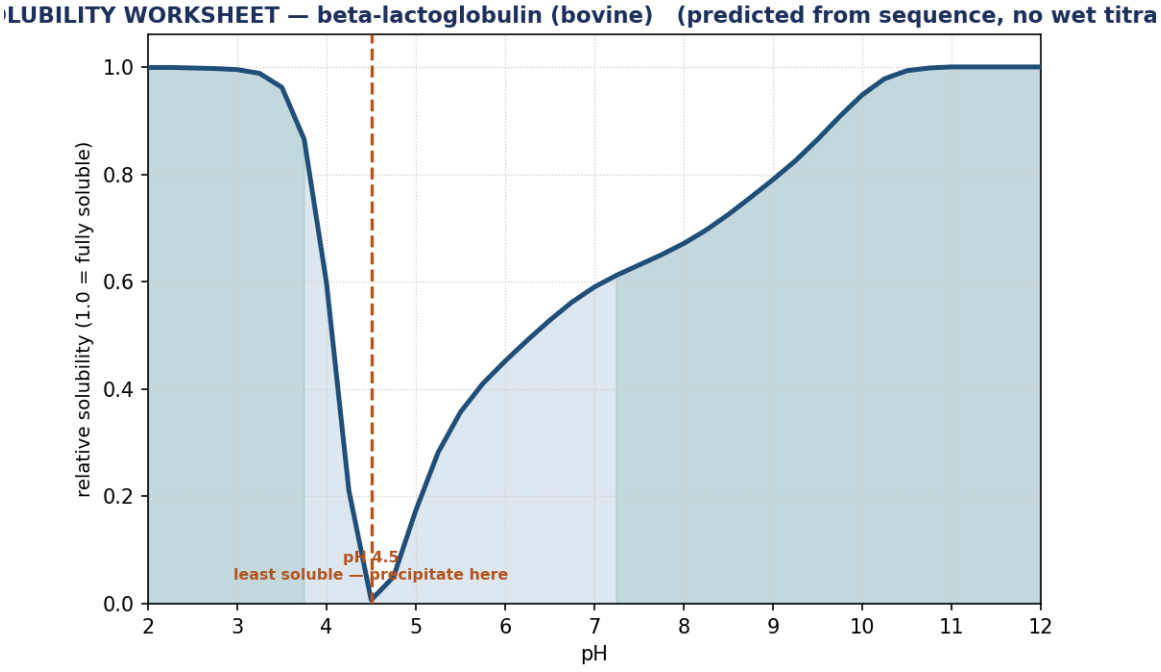
the AVERAGE (isotope-abundance-weighted) intact mass from sequence; the monoisotopic mass and its 0-mDa standard check are on the stick-spectrum panel. The envelope spacing deconvolute:

Predicted solubility vs pH & isoelectric point — the functionality bottleneck for plant protein, predicted from sequence (the pH to avoid for solubility, the pH to precipitate for purification)

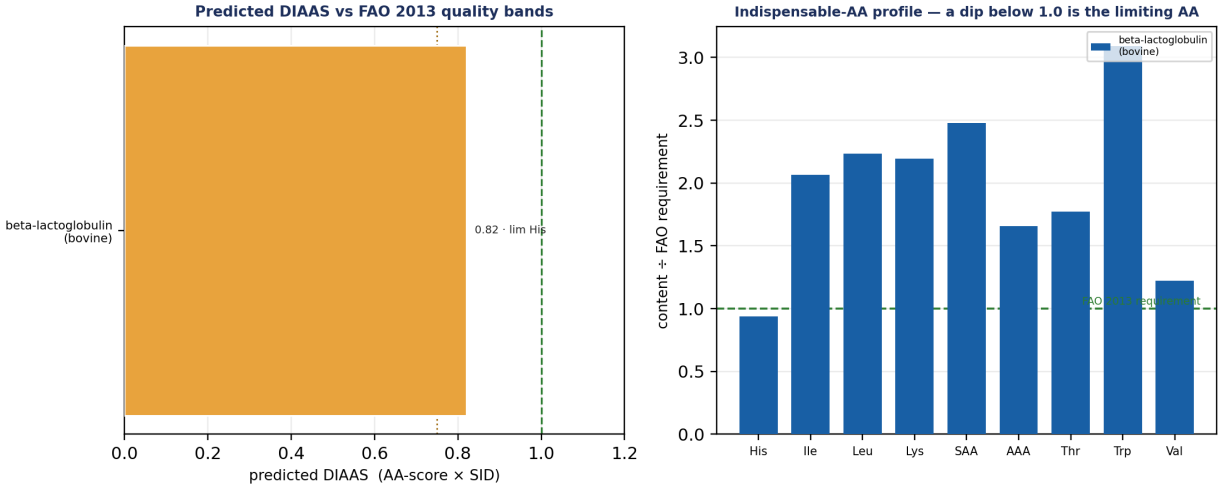


Integrity (SHA-256 manifest): 4750cc400ae9ced206d81c7577c52cade6f8571e94a64812d168a9026cfdb20a

Solubility worksheet — read the predicted solubility at any pH straight off the sheet (graphical calculation aid; no software needed).



Predicted DIAAS (protein nutrition) — the amino-acid-analyzer read: each protein's predicted DIAAS (composition AA-score × structure-derived digestibility SID) against the FAO 2013 quality bands, labelled with its limiting amino acid, plus the indispensable-amino-acid profile showing which AA dips below the requirement and caps the score. A composition + structural SCREEN — official DIAAS needs an in-vivo ileal-digestibility assay.



Integrity (SHA-256 manifest): 4750cc400ae9ced206d81c7577c52cade6f8571e94a64812d168a9026cfdb20a

Method & scope

Every value is computed live from the submitted structure by one fixed, deterministic physical model (zero training data — the same structure always returns the same result), with the structural mechanism named on each call. Where you supply measured labels the report scores itself against them above (with a label-shuffle control). This is a pre-bench shortlist / decision-support layer — it shows where to look first; it does not replace your panel or assays.

Appendix — input / output JSON (machine-readable)

Input (as evaluated):


```
{ "options": { "tier": 3 }, "proteins": [ { "id": "beta-lactoglobulin (bovine)", "name": "beta-lactoglobulin (bovine)" } ]
}
```


Output (the read returned):


```
[ { "name": "beta-lactoglobulin (bovine)", "denaturation_C": 73.7, "pI": 4.56, "fold_class": "LIPOCALIN" }
]
```


Provenance & integrity

This report is cryptographically bound to the exact compounds submitted and the engine version. Re-running the same inputs on the same engine reproduces the identical hash; any change in transit — an input or a computed result — changes it. Reproducible and tamper-evident from the hash alone.

Field	Value
Prepared for	Hans-Made Research — beta-lactoglobulin single-protein deep-dive (full tier-3 dossier)
Source file	input_protein_beta-lactoglobulin.json
Compounds bound	1
Engine version (SHA-256)	0e0e0386b9a08aa3f3861449891d210fad17b68daa79f5aa
Merkle root — all results	a2db356f4adad709c254729dcc3dc1bd9f506f8cc5d6a97c
Manifest hash (the seal)	4750cc400ae9ced206d81c7577c52cade6f8571e94a64812d168a9026cfdb20a
Spec	RaRaMa-merkle-v1 (sha256, dup-last)

Verify: recompute the Merkle root from the per-compound leaves in the sidecar (RaRaMa_report_<name>_merkle.json) and confirm it matches the manifest hash above — no access to the engine is needed to check integrity.