Smart industrial enzyme engineering

Model the reaction, not just the protein: Our analysis yields the residues that actually change catalysis, providing you with decision-ready mutation shortlists. Each variant comes with risk – opportunity notes, expected trade-offs, and next-step assays, so you commit resources where the likelihood of impact is highest

BACKGROUND

Industrial enzyme programs increasingly rely on computational tools, yet most methods still optimize proxy signals (stability, docking scores, sequence statistics) rather than catalytic performance under process conditions. Static or binding-centric models overlook the reaction pathway and transition-state control, so they miss distal and allosteric residues that govern activity and substrate scope. Limited treatment of dynamics and environmental context (solvent, cofactors, PTMs) makes predictions fragile when substrates, scaffolds, or conditions change. As a result, teams screen large variant sets with low hit rates, timelines stretch, and decisions stall because outputs arrive without a clear, validation-ready plan.

TECHNOLOGY

Our approach analyzes simulations of the catalyzed reaction to rank every residue by a mutability score, turning the full protein into a navigable landscape rather than focusing only on the active site. This lets us pinpoint positions whose mutation is likely to increase activity, including distal and allosteric sites, and has been shown to detect epistasis and shifts in substrate scope while evaluating only a small number of variants.
Compared with methods that rely mainly on global stability or sequence evolution, our workflow includes hybrid quantum mechanics/molecular mechanics (QM/MM) methodologies and explicitly incorporates features of the catalytic process, enzyme dynamics, and environmental factors such as cofactors, post-translational modifications, and solvent. The result is a concise, mechanistically reasoned shortlist that is directly actionable for validation.
We complement our ranking with chemically-intuitive information derived from molecular dynamics simulations under biological conditions, providing atomic-level rationale for recommended mutations and a clear path to experimental testing.
This combination makes the technology a versatile tool for all industrial biocatalysis tasks where improved catalytic efficiency, stability or new activities from existing scaffolds are sought, helping teams focus effort on a reduced, higher-value variant set.

OFFER

Under NDA, we turn your substrate, scaffold, and metric into a mechanistically justified shortlist (6–12 positions) and a ready-to-execute assay plan. All project results, raw data, reports, and experimentally confirmed variants belong to you. On request, the experienced acib team takes over expression, assays, and iterative cycles to move from hypotheses directly to validated hits.

EXPERTS

Prof. Pedro A. Sánchez Murcia
Daniel Platero-Rochart

DEVELOPMENT STATUS:

Technology Readiness Level 4
(Technology validated in lab)

PARTNER:

Medical University of Graz

KEYWORDS

- Computer-aided enzyme activity design
- Advanced protein engineering
- Industrial applications
- Industrial biocatalysis
- QM/MM dynamics
- Molecular dynamics
- Epistasis detection
- Substrate scope expansion
- Activity improvement
- kcat/KM optimization
- Substrate switching
- Temperature robustness
- Solvent tolerance
- Process-relevant conditions

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