

Rasayan Labs Inc.

Capability Statement and PoC Pitch Deck

AI-enabled computational drug discovery collaboration for Big Pharma / biopharma PoC studies

Hit discovery

ADMET / tox

Molecular modeling

IP intelligence

Retrosynthesis

Strong recommendation: advance Rasayan Labs to a structured, milestone-driven PoC as a high-conviction collaborator for rapid, decision-ready discovery packages.

Prepared from the PCSK9 allosteric modulator case study and public Rasayan/OCSR capability descriptions.

Executive Recommendation

Why Rasayan should be considered for a Big Pharma PoC collaboration

Recommendation

Rasayan Labs is a strong candidate collaborator for a paid, milestone-gated PoC focused on AI-enabled hit discovery and early lead triage.

Why now

- PCSK9 case study demonstrates an integrated workflow, not a single-point tool
- Big Pharma can validate Rasayan rapidly using prospective assay readouts

What Rasayan brings

- AI/ML discovery engines integrated with medicinal chemistry judgment
- Molecular search, OCSR, docking, ADMET/PK, tox and patent intelligence
- Computational outputs framed as project decisions

What Big Pharma gets

- Prioritized hit packages with rationale and assay plan
- Triage of novelty, tox risk, synthetic feasibility and IP exposure
- A practical path from hypothesis to wet-lab validation

How to engage

- Start with one live target or one buried internal program
- Set pre-agreed success metrics
- Use a joint steering model with rapid data rooms

Rasayan is best positioned as a high-speed computational discovery partner that converts search, modeling and molecular generation into testable PoC packages.

Rasayan Labs: AI Operating System for Drug Discovery

End-to-end chemistry intelligence capabilities

Search & extract

- Chemical search across large molecular space
- OCSR from structures, screenshots and patent figures

Design & prioritize

- Molecular docking and generative design
- Target-aware hit generation and scaffold expansion

Evaluate risk

- ADMET/PK, Ames, Tox21, hERG, DILI and related endpoints
- Multitarget and selectivity triage

Make & defend

- Retrosynthesis and route planning
- Patent search and FTO-oriented intelligence

Platform implication for PoC studies

One connected workflow from target hypothesis to assay-ready molecule lists

Designed to reduce false starts by combining biology, chemistry, safety and IP filters early

Useful for both greenfield discovery and neglected internal programs

Proof-of-Capability: PCSK9 Allosteric Modulators Case Study

The attached deck provides a ready example of Rasayan’s structured discovery thinking

What the case study demonstrates

- Strategic target positioning: oral PCSK9 as modality differentiation on a clinically validated axis
- External benchmark integration: AZD0780 / Iaroprostat and oral PCSK9 competitive context
- Hit and lead criteria covering biology, chemistry, eADME, PK, safety and IP
- Molecular modeling feasibility with PDB-level structural rationale
- Patent and competitor landscape to frame differentiation and FTO risk

Rasayan computational execution described

Input / engine	Role in PoC
Natural products library: 1.09M compounds	Diverse small-molecule starting points
Peptide Mold concept: 160,000 tetrapeptides	Interface-adjacent / motif-inspired hypotheses
DDP Engine + Vina docking	Initial target-pocket fit and binding triage
QVS quantum virtual scoring	Orthogonal re-ranking of computational hits
JANAK Engine	Novel, property-cleared and synthesizable chemotypes

Recommendation: use PCSK9 as a showcase, but pitch Rasayan as a reusable PoC engine for target-to-hit, hit-to-lead and risk-triage workflows.

Rasayan PoC Capability Stack

A Big Pharma PoC should test the complete decision workflow, not only molecule generation



PoC design principle

Measure prospective impact using real compounds and assays: novelty, hit rate, tox-risk reduction, synthesis practicality and decision quality.

Proposed Big Pharma PoC Study Designs

Three modular engagement formats, selectable by partner need

A. Target-to-hit PoC

- Starting point: one target structure or validated biology
- Deliver: 50-200 ranked molecules across 2-4 chemotypes
- Validation: biochemical or cellular assay hit confirmation
- Best for: new target entry or competitive fast-follow

B. Hit-to-lead triage

- Starting point: partner hit series or weak chemical matter
- Deliver: SAR hypotheses, property repair, analog list, tox flags
- Validation: potency/property shift versus baseline
- Best for: stalled internal programs

C. Safety/IP rescue

- Starting point: active molecules with liabilities or crowded IP
- Deliver: safer scaffold hypotheses, alerts, routes and novelty map
- Validation: liability reduction with retained activity
- Best for: candidate-risk mitigation

Preferred first engagement: one high-value live target with clear assay readout, confidential data sharing and pre-agreed success metrics.

Big Pharma Value Proposition

Rasayan addresses the recurring gaps between computational output and discovery decisions

Big Pharma pain point	Rasayan response	PoC evidence to request
Too many AI molecules; too few assayable decisions	Ranked hit packages with rationale, filters and synthesis routes	Top 50 ranked molecules + decision memo
Fragmented tools across search, docking, tox, IP and retrosynthesis	Integrated chemistry intelligence stack	Traceable scoring file and model audit trail
Late discovery tox/IP surprises	Early ADMET, mutagenicity, DILI, hERG and patent filters	Liability map for each proposed chemotype
Slow partner handoffs	Structured milestones and joint review cadence	Data-room-ready package with structure files
Need for novelty without synthetic fantasy	Generative design constrained by synthesizability and IP space	External novelty and route feasibility report

The PoC should prove that Rasayan can improve decision velocity without compromising medicinal chemistry rigor.

PoC Deliverables: Decision-Ready Package

Recommended deliverables for a milestone-gated collaboration

Deliverable	Description	Decision enabled
Target dossier	Biology, structural data, ligandability, competitor and patent context	Is target / pocket worth pursuing?
Hit package	Ranked molecules by score convergence, novelty, chemistry and property profile	Which compounds should be assayed first?
ADMET / tox file	Ames, Tox21, hERG, DILI, clearance, solubility, permeability and structural alerts	Which hits are developability-compatible?
Synthesis package	Route feasibility, building blocks and risk flagging	Can chemistry move quickly?
IP / novelty scan	Patent-aware scaffold landscape and white-space analysis	Can the series be defended?
Validation plan	Assay cascade, controls, go/no-go metrics and resynthesis priorities	How is the PoC judged objectively?

Governance, Data and IP Model

A collaboration framework compatible with pharmaceutical diligence

Governance

- Joint steering team: computational chemistry, medchem, biology, DMPK and IP
- Predefined success metrics and stop/go gates
- Weekly data review during active PoC

Data room

- Structure files, scoring tables, provenance and model outputs
- Assay-ready ranked lists and rationale
- Reusable templates for audit and scientific review

IP / confidentiality

- Partner owns confidential starting data and agreed project outputs
- Rasayan can operate under CDA/MSA/SOW
- FTO is a legal workstream; Rasayan supports prior-art intelligence

Recommendation: start with a CDA-protected technical diligence package, then move rapidly to one paid PoC with prospective wet-lab validation.

Success Metrics for the PoC

Define objective metrics before launch so Big Pharma can make a fast expansion decision

Novelty: non-obvious chemotypes versus known actives and patents
Assay hit rate: experimentally confirmed activity above baseline screen expectation
Developability: reduced ADMET/tox alerts and acceptable chemical properties
Synthesis practicality: feasible routes and building blocks
Decision quality: clear go/no-go recommendation with rationale

Suggested acceptance criteria

- ✓ 2-4 distinct chemotypes
- ✓ 50-200 high-priority candidates
- ✓ orthogonal scoring convergence
- ✓ early tox and IP flags removed
- ✓ assay-ready structures + synthesis logic

The right PoC output is not a “model demo”; it is a validated discovery decision package.

Why Rasayan Is a Strong Collaborator for Big Pharma

Positioning against common alternatives

Alternative	Typical limitation	Rasayan advantage
Point docking vendors	Often rank binders without downstream developability	Integrates docking with tox, ADME, novelty and synthesis
Generic AI molecule generators	Can create attractive but impractical compounds	Generative design constrained by project criteria and chemical feasibility
Database-only tools	Find what is known, but do not create differentiated hypotheses	Search + de novo design + patent-aware expansion
Traditional CRO-only workflows	Wet-lab cycles can start before computational triage is mature	Computationally enriches the funnel before spend-heavy experiments
Internal overloaded teams	Hard to rapidly run parallel exploratory hypotheses	External swarm capacity with structured deliverables

Recommendation: treat Rasayan as a strategic computational discovery partner, not a commodity modeling vendor.

Recommended First PoC: Target-to-Hit Package

Best first proof point for a biopharma partner

Proposed scope

- One partner-selected target with structure or validated homology model
- One agreed chemical-space strategy: internal library, external purchasable set, patent-derived structures, or de novo generation
- Partner provides assay format and activity threshold before computational launch
- Rasayan delivers ranked molecules plus rationale, risks and synthesis plan

Work products

- Target and pocket assessment
- Primary and orthogonal computational screens
- ADMET/tox/IP triage
- Top compound list with confidence tiers
- Assay plan and go/no-go memo

Governed by milestones

Gate	Decision
Gate 1	Target/pocket feasibility accepted
Gate 2	Computational hit list accepted for assay
Gate 3	Experimental data reviewed and next program decision made

This format gives Big Pharma a clean diligence path and gives Rasayan a fair opportunity to prove prospective impact.

Closing Recommendation

A high-conviction, low-friction way to evaluate Rasayan

Advance Rasayan Labs to a structured PoC collaboration.

The PCSK9 allosteric modulator case study demonstrates the right strategic architecture for pharma-grade discovery: target rationale, competitive positioning, molecular modeling, hit/lead criteria, safety gates, patent landscape and an assay-forward plan.

Rasayan's public platform capabilities cover the critical early-discovery stack: search, OCSR, docking, ADMET/PK, tox, retrosynthesis and patent intelligence.

The PoC should be designed prospectively with real wet-lab readouts and predefined success metrics so expansion decisions are evidence-based.

Recommended next step: NDA/CDA → target selection → PoC SOW → computational package → experimental validation → expansion decision

Sources and Basis of Preparation

For discussion use; factual claims should be revalidated before external circulation

Attached file: 2026_PCSK9_Allosteric_Modulators_CASE_Study.pptx, Rasayan Labs PCSK9 project deck.

Rasayan public website: AI operating system for pharmaceutical R&D; platform areas include retrosynthesis, impurity prediction, ADMET/PK, patent search, molecular docking and OCSR.

OCSR.ai public website/about/terms: chemical intelligence engine by Rasayan Labs Inc.; search and OCSR capabilities; toxicity and safety predictions including Ames, Tox21, DILI, hERG and cardiotoxicity.

Recommended Big Pharma PoC materials should be supplemented with confidential technical validation, benchmarking and legal/IP review before commercial use.

This deck intentionally recommends a structured PoC, not unqualified adoption. Experimental validation remains the decision gate.