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Integrated CADD, Molecular Docking and ADMET Prediction in Anti-Inflammatory Lead Discovery: A Review

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Abstract: *Inflammation involves coordinated activation of vascular, immune, lipid mediator, cytokine, transcriptional and inflammasome pathways. Modern anti-inflammatory lead discovery increasingly uses computer-aided drug design to identify plausible protein-ligand interactions before costly laboratory studies. This review summarizes the rationale for target selection, molecular docking, ADMET prediction, toxicity screening and Quality by Design-based documentation in anti-inflammatory computational pharmacology. The article emphasizes that docking scores are hypothesis-generating outputs and must be interpreted with binding-pose quality, residue relevance, pharmacokinetic feasibility and safety prediction. Selected natural scaffolds such as curcumin, quercetin, luteolin, apigenin, resveratrol, berberine, boswellic acid, andrographolide, withaferin A, gallic acid and ellagic acid are discussed as examples of chemically diverse candidates for pathway-based screening.*

Keywords: inflammation; CADD; ADMET; molecular docking; natural products; cytokines; COX-2; NLRP3; NF-kB

I. INTRODUCTION

Inflammation is a biological defence system rather than a single molecular event. It begins with recognition of harmful stimuli, proceeds through mediator release and leukocyte recruitment, and ideally resolves through tissue repair. When activation persists, the same system contributes to chronic disease, tissue destruction and systemic complications [1-4].

The network character of inflammation explains why anti-inflammatory discovery should consider several target families. Enzymes, cytokines, transcription factors and inflammasome proteins may act together in disease. A compound that affects one target may still fail when pharmacokinetics or toxicity prevents adequate biological exposure.

II. MAJOR INFLAMMATORY TARGET FAMILIES

COX-2 and 5-LOX are central eicosanoid-related targets. COX-2 is associated with prostaglandin-mediated pain, fever and oedema, whereas 5-LOX is linked with leukotriene generation and leukocyte recruitment [16-19]. iNOS contributes to nitric oxide and nitrosative stress, especially in activated immune cells.

Cytokine-linked targets such as TNF-alpha and IL-6-related signalling are clinically important because they amplify immune-cell recruitment and acute-phase responses. NF-kB controls transcription of multiple inflammatory mediators, while NLRP3-associated proteins are relevant to inflammasome activation and cytokine maturation [5-15].

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III. ROLE OF MOLECULAR DOCKING IN ANTI-INFLAMMATORY RESEARCH

Molecular docking predicts possible ligand orientation and binding energy within a selected protein pocket. It is useful for comparing candidates and identifying residue-level hypotheses. However, docking is limited by receptor rigidity, scoring-function error, solvation simplification and uncertainty in ligand protonation or tautomeric state [25-34].

Good docking practice requires suitable protein structure selection, accurate ligand preparation, validated grid selection and careful pose interpretation. Co-crystallized ligand redocking or reference-inhibitor comparison increases confidence before screening novel candidates.

IV. ADMET AND TOXICITY PREDICTION AS DECISION FILTERS

ADMET prediction estimates drug-likeness, solubility, permeability, gastrointestinal absorption, blood-brain barrier penetration, P-gp interaction, CYP inhibition and related pharmacokinetic liabilities. Toxicity tools estimate acute toxicity, mutagenicity, hepatotoxicity, immunotoxicity and hERG-related risk [35-42].

These predictions are not substitutes for experiments, but they prevent overdependence on docking score. Compounds with strong docking but major toxicity or bioavailability problems should be modified, formulated or deprioritized before biological validation.

V. NATURAL COMPOUNDS IN COMPUTATIONAL ANTI-INFLAMMATORY SCREENING

Natural products remain valuable in drug discovery because they provide structural diversity, stereochemical richness and pathway-level biological relevance [53-55]. Curcumin, flavonoids, resveratrol, berberine, boswellic acid, andrographolide and withanolides are frequently discussed in inflammation research because they are linked with mediator modulation, cytokine signalling or oxidative stress mechanisms [56-71].

At the same time, natural origin does not guarantee safety or drug-like behaviour. Curcumin and boswellic acid may require formulation support; berberine may show transporter-related limitations; withaferin A requires careful toxicity screening because of potent biological activity. Therefore, natural compounds should be evaluated by the same integrated CADD-ADMET standard used for synthetic leads.

VI. QUALITY BY DESIGN FOR COMPUTATIONAL PHARMACOLOGY

Quality by Design principles can be adapted to in silico work by defining target relevance, protein quality, ligand quality, docking validation, ADMET coverage and reporting quality before interpretation. This reduces selective reporting and improves reproducibility.

A computational QbD system records PDB ID, resolution, chain, binding-site selection, ligand identifier, software version, docking parameters, ADMET platform and toxicity output. It also preserves negative findings so that lead ranking remains transparent.

VII. FUTURE PERSPECTIVES

Future anti-inflammatory discovery will benefit from combining docking with molecular dynamics, free-energy methods, multi-target network analysis, machine-learning ADMET prediction and experimental validation. For thesis-level work, however, a transparent and reproducible workflow is more important than excessive computational complexity.

The most reliable shortlists are those that combine target mechanism, predicted binding, residue relevance, ADMET suitability and toxicity caution. Such shortlists can guide enzyme assays, macrophage inflammatory models, cytokine studies and ethics-approved animal experiments.

VIII. CONCLUSION

CADD and ADMET prediction provide a practical early-stage framework for anti-inflammatory lead selection. They are strongest when used as decision-support tools and weakest when docking scores are overstated as proof of efficacy.

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A responsible computational review therefore connects biological mechanism, structural suitability, pharmacokinetic feasibility, toxicity risk and experimental planning.

1. **Table 1. Inflammatory target families for CADD-based review**

Pathway / target family	Representative targets	Reason for computational relevance
Eicosanoid pathway	COX-2, 5-LOX	Links docking output with prostaglandin and leukotriene biology
Nitrosative stress	iNOS	Supports nitric oxide-related inflammatory hypotheses
Cytokine signalling	TNF-alpha, JAK2/IL-6-linked signalling	Represents immune amplification and cell signalling
Transcriptional regulation	IKKbeta/NF-kB pathway	Connects upstream signalling with inflammatory gene expression
Inflammasome biology	NLRP3-associated proteins	Supports inflammasome-inhibition hypotheses

2. **Table 2. Quality checkpoints in computational anti-inflammatory lead discovery**

Computational step	Primary output	Risk if not controlled
Target selection	PDB ID, chain, resolution, active site	Biologically irrelevant docking
Ligand preparation	Verified structure, protonation, minimized geometry	False score due to wrong input ligand
Docking validation	Redocking or reference inhibitor comparison	Unreliable pose interpretation
ADMET prediction	Drug-likeness and pharmacokinetic alerts	Selection of non-developable compounds
Toxicity prediction	Mutagenicity, hepatotoxicity, hERG and acute class	Unsafe candidate prioritization

3. **Table 3. Natural compound classes in anti-inflammatory CADD review**

Compound class	Examples	Key review interpretation
Polyphenols	Curcumin, ellagic acid	Mechanistically attractive but may show solubility or exposure limitations
Flavonoids	Quercetin, luteolin, apigenin	Good polar interaction potential with metabolism considerations
Stilbenes	Resveratrol	Relevant to oxidative/cytokine signalling; rapid metabolism possible
Alkaloids	Berberine	Strong pathway relevance but transporter and interaction risks
Terpenoids/lactones	Boswellic acid, andrographolide, withaferin A	Potent scaffolds requiring careful ADMET and toxicity filtering

IX. STRUCTURE-BASED TARGET SELECTION

Structure-based anti-inflammatory screening begins with evaluating whether a protein structure can reasonably represent the biological target. Resolution, chain completeness, ligand-bound status, mutation state and pocket interpretability must be considered. A protein selected only because it is available in a structural database may not be suitable for docking-based pharmacological interpretation.

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Ligand-bound structures are particularly valuable because they reveal how inhibitors occupy the pocket and which residues are relevant for recognition. For targets linked to protein-protein interactions, such as cytokine systems, docking must be interpreted cautiously because a small-molecule pose may not fully represent pathway inhibition.

X. DOCKING VALIDATION AND SCORING LIMITATIONS

Docking validation reduces methodological uncertainty. Redocking a co-crystallized ligand, comparing pose overlap and assessing RMSD give evidence that the grid and preparation protocol can reproduce a known binding orientation. When redocking is not possible, a reference ligand or literature-defined site provides only supportive evidence and should be described accordingly.

Scoring functions estimate binding affinity through simplified energy terms. They may fail to fully capture solvent effects, entropy, induced fit, allosteric dynamics or cellular exposure. Therefore, docking scores are best used for prioritization inside a controlled workflow rather than as direct measures of biological potency.

XI. ADMET PLATFORMS AND DRUG-LIKENESS RULES

SwissADME, pkCSM, ADMETlab and related tools estimate physicochemical and pharmacokinetic properties that influence lead development. Molecular weight, polarity, lipophilicity, hydrogen-bonding pattern and rotatable bonds influence solubility and permeability. Prediction of P-gp and CYP interaction helps identify potential absorption and metabolism risks.

Drug-likeness rules are not strict pass-or-fail laws; rather, they flag compounds requiring caution. Natural products may violate some rules while still being biologically useful, but such violations should trigger deeper formulation, delivery or safety evaluation.

XII. TOXICITY PREDICTION IN EARLY SCREENING

Early toxicity prediction identifies candidates that may be unsuitable despite promising docking. Alerts for mutagenicity, hepatotoxicity, immunotoxicity, hERG risk or high acute-toxicity class should be reported transparently. The purpose is not to eliminate every molecule with an alert, but to prevent uncritical lead promotion.

In natural compound research, safety language should be especially careful. Natural origin does not imply absence of toxicity. Potent scaffolds such as steroidal lactones or alkaloids require the same level of toxicity scrutiny as synthetic candidates.

XIII. EXPERIMENTAL VALIDATION AFTER COMPUTATIONAL RANKING

Computational shortlisting should be followed by target-specific assays. COX-2 and 5-LOX hits may be evaluated using enzyme inhibition tests. iNOS-related hypotheses may be studied in macrophage nitric oxide models. Cytokine and NF-kB-linked hypotheses require cell-based models with biomarker measurement.

Animal studies should be proposed only after in vitro evidence and institutional approval. This staged validation pathway protects scientific integrity and ensures that computational predictions remain connected with real biological endpoints.

XIV. REVIEW CONCLUSION

The reviewed thesis framework shows that CADD, molecular docking, ADMET prediction and toxicity screening are complementary components of early anti-inflammatory lead discovery. The strongest computational evidence emerges when target biology, structure suitability, ligand preparation, docking validation and safety prediction are combined.

Future studies should integrate molecular dynamics, free-energy refinement, experimental enzyme assays, inflammatory cell models and formulation approaches for candidates limited by solubility or permeability. Such development will strengthen the transition from in silico ranking to biologically validated anti-inflammatory leads.

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REFERENCES

1. Aderem A, Ulevitch RJ. Toll-like receptors in the induction of the innate immune response. Nature. 2000;406(6797):782-787.
2. Banerjee P, Eckert AO, Schrey AK, Preissner R. ProTox-II: a webserver for the prediction of toxicity of chemicals. Nucleic Acids Res. 2018;46(W1):W257-W263.
3. Barton GM. A calculated response: control of inflammation by the innate immune system. J Clin Invest. 2008;118(2):413-420.
4. Chakote VR, Dhembre GN, Rajguru JR, Joshi DA. In-Situ Gel for Nasal Drug Delivery. *International Journal of Development Research*. 2018;8(2):18763–18769.
5. Cronstein BN, Aune TM. Methotrexate and its mechanisms of action in inflammatory arthritis. Nat Rev Rheumatol. 2020;16(3):145-154.
6. Daina A, Michielin O, Zoete V. SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness. Sci Rep. 2017;7:42717.
7. DeLano WL. The PyMOL Molecular Graphics System. San Carlos: DeLano Scientific; 2002.
8. Desai RS, Rajguru JR, Gawari PB, Isal AA. Overview of Intrauterine Drug Delivery System. *International Journal of Creative Research Thoughts (IJCRT)*. 2024;12(1)–D316.
9. Dhamale GR, Shinde PB, Rajguru JR. A Review: Gastroretentive Drug Delivery Systems. *International Journal of Pharmaceutical Sciences*. pp.1825–1840. doi:10.5281/zenodo.12818744.
10. Dinarello CA. Proinflammatory cytokines. Chest. 2000;118(2):503-508.
11. Doke R, Rajguru J, Vinchurkar K. Personalized Medicine Through AI-Driven Imaging. In: *Springer Nature*. doi:10.1007/978-3-032-02963-8_7.
12. Eberhardt J, Santos-Martins D, Tillack AF, Forli S. AutoDock Vina 1.2.0: new docking methods, expanded force field, and Python bindings. J Chem Inf Model. 2021;61(8):3891-3898.
13. Egan WJ, Merz KM, Baldwin JJ. Prediction of drug absorption using multivariate statistics. J Med Chem. 2000;43(21):3867-3877.
14. Fu L, Shi S, Yi J, et al. ADMETlab 3.0: an updated comprehensive online ADMET prediction platform. Nucleic Acids Res. 2024;52(W1):W422-W431.
15. Fullerton JN, Gilroy DW. Resolution of inflammation: a new therapeutic frontier. Nat Rev Drug Discov. 2016;15(8):551-567.
16. Furman D, Campisi J, Verdin E, et al. Chronic inflammation in the etiology of disease across the life span. Nat Med. 2019;25(12):1822-1832.
17. Gabay C, Kushner I. Acute-phase proteins and other systemic responses to inflammation. N Engl J Med. 1999;340(6):448-454.
18. Gadekar SN, Rajguru JR, Biyani KR. Review on Solid Dispersion for Suitable Drug. *World Journal of Pharmaceutical Sciences*. 2021;9(9):230–235.
19. Gawai NM, Jadhav RR, Modak A, Sawarkar HS, Rajguru JR. Advancements in Nanogel Technology for Drug Delivery: Current Innovations and Future Perspectives. *African Journal of Biomedical Research*. 2024;27(3S):3200–3212. doi:10.53555/AJBR.v27i3S.2905.
20. Gawari PB, Rajguru JR. Confronting the Nipah Virus: Critical Insights and Practical Recommendations. *International Journal of Creative Research Thoughts (IJCRT)*. 2026;14(2). ISSN: 2320-2882.
21. Gordon S. Alternative activation of macrophages. Nat Rev Immunol. 2003;3(1):23-35.
22. Ingole RD, Gawai NM, Rajguru JR. Nanoformulation of Vitamin D Derivatives and Metabolites. *African Journal of Biomedical Research*. 2024;27(4S). doi:10.53555/AJBR.v27i4S.4897.
23. JRajguru R. Development and Validation of RP-HPLC and UV Spectrophotometric Absorptivity Method for Simultaneous Estimation of Cyclobenzaprine Hydrochloride and Aceclofenac in Pharmaceutical Dosage Form. *International Journal of Science & Engineering Development Research*. 2020;5(4):320–329.

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24. Jeevan Rajguru R. Magnetic and pH Sensitive Nanoparticles for Cancer Drug Delivery. *Asian Journal of Pharmaceutical Research and Development*. 2019;7(4).
25. Jorgensen WL. The many roles of computation in drug discovery. Science. 2004;303(5665):1813-1818.
26. JR.Rajguru Biomarkers and Diagnostics. *International Journal of Scientific Development and Research*. 2020;5(4).
27. JR.Rajguru Development and Evaluation of Nasal Mucoadhesive In-Situ Gel Formulations of Carbamazepine Using In-Vitro, Ex-Vivo and In-Vivo Methods. *International Research Journal of Pharmacy and Medical Sciences*. 2018;1(6).
28. Kelley N, Jeltema D, Duan Y, He Y. The NLRP3 inflammasome: an overview of mechanisms of activation and regulation. Int J Mol Sci. 2019;20(13):3328.
29. Kitchen DB, Decornez H, Furr JR, Bajorath J. Docking and scoring in virtual screening for drug discovery. Nat Rev Drug Discov. 2004;3(11):935-949.
30. Kushwah P, Rajguru JR, Jain G, Patidar A, Tomar PS. A Review of Classic Cures for Contemporary Marvels: Unveiling the Medicinal Secrets of *Piper betle* Linn. Leaves and *Nyctanthesarbor-tristis*. *International Journal of Creative Research Thoughts (IJCRT)*. 2024;12(1)–D747.
31. Laskowski RA, Swindells MB. LigPlot+: multiple ligand-protein interaction diagrams for drug discovery. J Chem Inf Model. 2011;51(10):2778-2786.
32. Lawrence T. The nuclear factor NF-kappaB pathway in inflammation. Cold Spring Harb Perspect Biol. 2009;1(6):a001651.
33. Lipinski CA, Lombardo F, Dominy BW, Feeney PJ. Experimental and computational approaches to estimate solubility and permeability in drug discovery. Adv Drug Deliv Rev. 2001;46(1-3):3-26.
34. Liu T, Zhang L, Joo D, Sun SC. NF-kappaB signaling in inflammation. Signal Transduct Target Ther. 2017;2:17023.
35. Mangan MSJ, Olhava EJ, Roush WR, Seidel HM, Glick GD, Latz E. Targeting the NLRP3 inflammasome in inflammatory diseases. Nat Rev Drug Discov. 2018;17(9):688.
36. McInnes IB, Schett G. Pathogenetic insights from the treatment of rheumatoid arthritis. Lancet. 2017;389(10086):2328-2337.
37. Medzhitov R. Origin and physiological roles of inflammation. Nature. 2008;454(7203):428-435.
38. Mitchell JA, Warner TD. Cyclo-oxygenase-2: pharmacology, physiology, biochemistry and relevance to NSAID therapy. Br J Pharmacol. 1999;128(6):1121-1132.
39. Morris GM, Huey R, Lindstrom W, et al. AutoDock4 and AutoDockTools4: automated docking with selective receptor flexibility. J Comput Chem. 2009;30(16):2785-2791.
40. Motr PR, Wayal SR, Darekar SM, Jalindar AS, Gawai NM, Bodake PL, Barke SA, Dongare AB, Rajguru JR. Development of a Validated HPTLC Method for the Simultaneous Estimation of Curcumin and Berberine in DashamoolaKvatha. *International Journal of Environmental Sciences*. doi:10.64252/kq9rtn45.
41. Nathan C. Points of control in inflammation. Nature. 2002;420(6917):846-852.
42. Pawar A, Zade A, Shastri A, Ingole R, Kharde S, Rajguru J. Gold Nanoparticles: Innovative Supramolecular Platforms for Targeted Drug Delivery and Bioorthogonal Catalysis. *Indian Journal of Pharmaceutical Education and Research*. 2026;60(3S)–S905. doi:10.5530/ijper.20261157.
43. Pawar PP, Rajguru JR, Navghare AB, Shinde SP, Lokhande PB. An Overview of Implantable Drug Delivery Systems. *International Journal of Creative Research Thoughts (IJCRT)*. 2024;12(1)–F958.
44. Pettersen EF, Goddard TD, Huang CC, et al. UCSF ChimeraX: structure visualization for researchers, educators, and developers. Protein Sci. 2021;30(1):70-82.
45. RRajguru J. Gene Therapy – Challenges & Success. *International Journal of Trend in Scientific Research and Development*. 2020;4(3).

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46. Rajguru JR, Shirsat MK. Development of the Formulation and Evaluation of the Anti-Arthritic Activity of *Vitex negundo* Gel and Latex. *International Journal of Drug Delivery Technology*. 2023;13(1).
47. Rajguru JR. A Review – Corona Virus (COVID-19). *International Journal of Science and Engineering Development Research*. 2020;5(4):1–6.
48. Rajguru JR. A Review on: Mucormycosis. *International Journal of Innovative Research in Technology*. 2021;8(1):323–330.
49. Rajguru JR. Cancer Chemotherapy with Peptides and Peptidomimetics Drug and Peptide-Based Vaccines. *International Research Journal of Pharmacy and Medical Sciences*. 2019;2(2).
50. Rajguru JR. Novel Drug Delivery System in Recent Trends as Carrier. *World Journal of Pharmacy and Pharmaceutical Sciences*. 2020;9(5):193–205. doi:10.20959/wjpps20205-15995.
51. Rhen T, Cidlowski JA. Antiinflammatory action of glucocorticoids: new mechanisms for old drugs. N Engl J Med. 2005;353(16):1711-1723.
52. Ricciotti E, FitzGerald GA. Prostaglandins and inflammation. ArteriosclerThrombVasc Biol. 2011;31(5):986-1000.
53. Samuelsson B. Leukotrienes: mediators of immediate hypersensitivity reactions and inflammation. Science. 1983;220(4597):568-575.
54. Serhan CN. Pro-resolving lipid mediators are leads for resolution physiology. Nature. 2014;510(7503):92-101.
55. Shinde PB, Rajguru JR, Shinde SP, Humbe KA, Pawar PP. Nasal Routes of Drug Delivery: A Creative Approach. *International Journal of Creative Research Thoughts (IJCRT)*. 2024;12(1)–E477.
56. Shirsat MK. Rajguru JR, Development of the Formulation and Evaluation of the Anti-Inflammatory Activity of *Vitex negundo* Gel and Latex. *International Journal of Pharmaceutical Quality Assurance*. 2023;14(1).
57. Shoichet BK. Virtual screening of chemical libraries. Nature. 2004;432(7019):862-865.
58. Sitaphale GR, Tathe PR, Laddha PR, Charhate KB, Rajguru JR. Phytochemical Screening, Isolation, and Characterization of Extract from Various Parts of *Phoenix sylvestris*. *African Journal of Biomedical Research*. 2024;27(3S):3368–3374. doi:10.53555/AJBR.v27i3S.2938.
59. Sliwoski G, Kothiwale S, Meiler J, Lowe EW. Computational methods in drug discovery. Pharmacol Rev. 2014;66(1):334-395.
60. Smith WL, Urade Y, Jakobsson PJ. Enzymes of the cyclooxygenase pathways of prostanoid biosynthesis. Chem Rev. 2011;111(10):5821-5865.
61. Smolen JS, Aletaha D, McInnes IB. Rheumatoid arthritis. Lancet. 2016;388(10055):2023-2038.
62. Tathe PR, Laddha PR, Sitaphale GR, Charhate KB, Pimple UA, Jadhao YD, Alhat RM, Rajguru JR. Studies in Preparation and Evaluation of Nanoparticles for Controlled Drug Delivery of Peptide-Based Drugs. *African Journal of Biomedical Research*. 2024;27(3S):3179–3190. doi:10.53555/AJBR.v27i3S.2894.
63. Trott O, Olson AJ. AutoDock Vina: improving the speed and accuracy of docking. J Comput Chem. 2010;31(2):455-461.
64. Turner MD, Nedjai B, Hurst T, Pennington DJ. Cytokines and chemokines: at the crossroads of cell signalling and inflammatory disease. BiochimBiophys Acta. 2014;1843(11):2563-2582.
65. Vane JR, Botting RM. Mechanism of action of nonsteroidal anti-inflammatory drugs. Am J Med. 1998;104(3A):2S-8S.
66. Veber DF, Johnson SR, Cheng HY, Smith BR, Ward KW, Kopple KD. Molecular properties that influence oral bioavailability. J Med Chem. 2002;45(12):2615-2623.
67. Wayal SR, Barke SA, Darekar SM, Jalindar AS, Gawai NM, Wankhede HR, Bathe RS, Rajguru JR. Development of Currant-Loaded Nanoparticles and Phytosomes for Enhanced Antioxidant Delivery. *International Journal of Environmental Sciences*. 2025;11(22S):4067–4071. doi:10.64252/p2tecx31.
68. Wayal SR, Rajguru JR, Bhise MR. A Systematic Review on the Effective Teaching Strategies and Methods for Cancer Patient Education. *Journal of Cancer Education*. 2025. doi:10.1007/s13187-025-02759-z.