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Mini Review

Assessment of Potential Nutraceuticals for Cancer Treatment Through Computational Method

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Abstract

Nutraceuticals such as curcumin, resveratrol, and epigallocat- echin gallate (EGCG) have emerged as promising bioactive compounds with anticancer potential through the modulation of molecular signaling pathways. Recent advances in com- putational biology, particularly molecular docking and virtual screening, have accelerated the discovery of nutraceutical pro- tein interactions that underlie therapeutic efficacy. This summarizes key computational strategies focusing on AutoDock Vina for assessing the binding affinity and structural comple- mentarity of nutraceuticals against major oncogenic targets, and outlines current challenges in translating in silico results into clinically meaningful interventions.

Keywords: Nutraceuticals; Cancer; Molecular Docking; AutoDock Vina; Computational Biology

Introduction

Cancer remains one of the leading causes of mortality worldwide, necessitating the continuous search for safer and more effective therapeutic agents. In this context, nutraceuticals naturally occurring dietary compounds with pharmacological activity offer a viable complementary approach to conventional chemotherapy. Several studies have highlighted that compounds such as curcumin, EGCG, quercetin, and lycopene ex- ert antiproliferative, pro-apoptotic, and anti-angiogenic effects by modulating signaling cascades including PI3K/AKT, NF- κB, and Wnt/β-catenin [1–3]. Despite strong experimental ev- idence, the molecular basis of their selectivity and affinity to- ward cancer related proteins remains incompletely understood. Computational docking has therefore become an indispensable tool for visualizing and quantifying these interactions at the atomic level Figure 1.

Computational Methods and AutoDock Vina Framework

Molecular docking allows the prediction of the most energetically favorable orientation of a ligand within a target binding pocket, estimating the binding free energy and identifying key stabilizing interactions. AutoDock Vina, developed by Trott and Olson [4], is one of the most widely used open-source engines due to its balance between computational efficiency and prediction accuracy. The docking process generally be- gins with ligand and receptor preparation: three-dimensional structures of nutraceuticals are optimized and protonated at physiological pH, while crystallographic protein structures re- trieved from the Protein Data Bank are refined by removing water molecules and adding polar hydrogens. Search grids are defined to encompass

the active site, followed by automated exploration of binding poses using stochastic optimization al-gorithms. The binding affinities, expressed in kcal/mol, pro- vide a comparative measure of interaction strength and com- plement experimental prioritization.

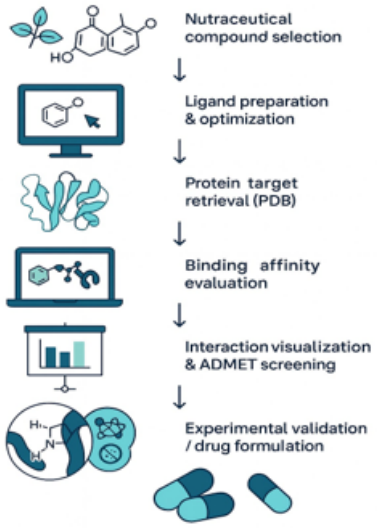

Figure 1: Computational pipeline for nutraceutical assessment using molecular docking and AutoDock Vina.

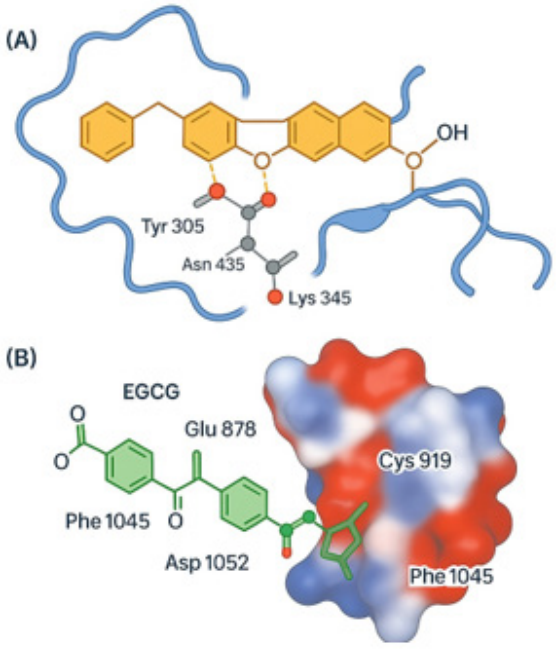

Figure 2: Representative docking poses showing (A) Cur- cumin binding to -catenin and (B) EGCG interaction within VEGF receptor active site. Hydrogen bonds are highlighted in yellow.

AutoDock Vina 1.2.0 introduced expanded scoring func- tions, flexible residue handling, and Python bindings that facil- itate high-throughput virtual screening [5]. For reproducibil- ity, best practices include multiple docking runs with var- ied random seeds, pose clustering within an RMSD thresh- old of 2 A˚, and redocking of co-crystallized ligands to val- idate pocket selection. Combining Vina with deep-learning- assisted rescoring engines such as GNINA can further improve binding-pose discrimination [6]. The integration of ADMET prediction and molecular dynamics simulation provides addi- tional refinement to evaluate pharmacokinetic feasibility Figure 2.

Applications to Nutraceuticals in Cancer Research

Curcumin, a polyphenolic compound derived from Curcuma longa, has been computationally and experimentally validated as an inhibitor of multiple oncogenic pathways. Docking stud- ies have demonstrated favorable binding (–6 to –9 kcal/mol) toward kinases and transcriptional regulators such as EGFR, BCL-2, and β-catenin, supporting its role in apoptosis in- duction and metastasis suppression [2, 7]. Similarly, EGCG, the major catechin in green tea, exhibits high binding affinity with VEGF receptors, matrix metalloproteinases, and topoiso- merases, rationalizing its anti-angiogenic and cytostatic effects [3, 8]. Other nutraceuticals such as resveratrol and quercetin also show multi-target binding patterns that correlate with an- tioxidant and anti-inflammatory properties. While docking energies and hydrogen-bond patterns pro- vide mechanistic hypotheses, bioavailability and metabolic stability remain key bottlenecks. Many nutraceuticals suffer from poor aqueous solubility and rapid metabolism; thus, the design of nanoparticle or phytosome based formulations has become a parallel computational target. In silico docking can also assess drug–excipient interactions, ensuring the retention of pharmacophoric integrity in delivery systems [9, 10] Figure 3.

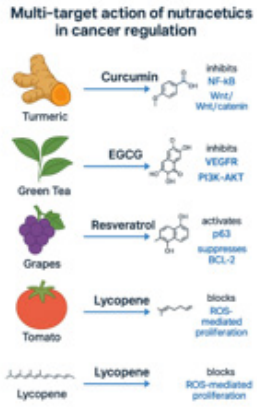

Figure 3: Nutraceutical sources and their corresponding molecular pathways implicated in anticancer activity.

Challenges and Future Perspectives

Although docking offers rapid screening and hypothesis gen- eration, the accuracy of predicted affinities depends on the scoring function and the quality of the receptor structure. Flexible binding pockets, allosteric sites, and solvent effects are often simplified in classical docking, potentially leading to false positives or overestimated affinities. Moreover, nu- traceuticals typically exert polypharmacological effects that challenge single-target assumptions. Future computational pipelines should integrate molecular dynamics, quantum me- chanics/molecular mechanics (QM/MM) refinement, and net- work pharmacology approaches to capture the systemic im- pact of nutraceuticals on interconnected pathways. The in- creasing incorporation of machine-learning-based scoring and large-scale datasets is expected to further enhance predictive reliability and guide experimental validation [11].

Conclusion

Computational methods such as molecular docking and AutoDock Vina have transformed the early-stage evaluation of nutraceuticals for cancer therapy. By revealing the structural determinants of binding and providing rapid screening capa- bility, these tools bridge the gap between traditional natural- product research and precision oncology. However, successful translation from virtual hits to clinical outcomes will require multidisciplinary integration of computational chemistry, for- mulation science, and experimental pharmacology. Continued methodological advances promise to accelerate the rational de- sign of nutraceutical-based anticancer therapeutics.

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