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AI-assisted discovery of drug molecules from insect natural products: Current progress, computational strategies, and future directions

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Abstract
Insects make up the most species-diverse animal group on Earth, and they produce a wide variety of bioactive molecules — including antimicrobial peptides, alkaloids, terpenoids, and venom proteins — that show meaningful potential against cancer, infectious diseases, and inflammatory conditions. Yet only a fraction of these compounds have been properly evaluated for drug development, largely because traditional screening methods are slow and costly. Artificial intelligence (AI), through its branches of machine learning (ML), deep learning (DL), and generative modeling, has fundamentally changed how the drug discovery pipeline works. When applied to insect-derived compounds, AI allows researchers to navigate enormous chemical spaces, prioritize promising candidates, and reduce experimental failure rates. This review covers the main classes of bioactive insect compounds, the AI approaches used to study them, key computational databases and tools, virtual screening strategies, ADMET profiling, and real-world case studies. It also highlights a critical gap in the field — there is currently no dedicated, AI-ready database for insect natural products. Challenges like limited training data, model transparency, and the need for experimental confirmation are addressed, along with future directions involving generative drug design, multi-omics integration, and AI agents [1-5].

Keywords: Artificial intelligence, drug discovery, insect natural products, machine learning, molecular docking, ADMET prediction, computational pharmacology, deep learning, virtual screening, bioactive compounds

Introduction

Natural Products in Drug Discovery

For millennia, the foundation of medicine has been natural ingredients. Nature has produced pharmacologically active substances with astonishing structural complexity, from the ancient uses of willow bark to the 1928 discovery of penicillin from Penicillium notatum. According to a well-known analysis, natural products, natural product derivatives, or compounds inspired by natural product scaffolds accounted for around half of all authorized medications between 1981 and 2019 [1]. Artemisinin from Artemisia annua for malaria and paclitaxel from the Pacific yew tree for cancer are classic examples. However, due to constraints in traditional high-throughput screening, problems in isolating and characterizing compounds, and challenges in establishing drug-likeness, the pace of natural product drug development has slowed in recent years. The transition to computational methods has been fueled by these limitations [2].

Why Insects?

Only over one million of the estimated 5.5 million species of insects have been formally described, making them the richest collection of animals on Earth [3]. Over 400 million years of evolution have molded this variety, resulting in a broad chemical toolset. Insects produce bioactive substances for communication, defense, wound healing, and prey capture—all processes of pharmaceutical significance. Traditional Chinese medicine, Ayurveda, and traditional healing systems around the world have acknowledged their medicinal potential. For example, blister beetle cantharidin has been used medicinally for more than 2,000 years and is currently an FDA-approved treatment for molluscum contagiosum [4]. Compounds from bees (melittin, apamin), wasps (mastoparan), ants (solenopsins), and silkworms (fibroin peptides) have all been shown to have bioactivity in recent studies [5].

The Role of Artificial Intelligence

Developing a single new drug costs an estimated USD 2.6 billion and takes 12 to 15 years, with a large share of failures caused by poor ADMET profiles and unforeseen toxicity — problems that AI is well-positioned to address early in the process [6]. Machine learning algorithms can scan large chemical libraries in silico, identifying structural patterns linked to biological activity. Deep learning models, particularly graph neural networks, predict molecular properties and binding affinities with impressive accuracy. Generative AI models go further still, designing entirely new molecular structures with user-specified properties [7]. The integration of AI with insect natural product research is especially well-timed now, given that large-scale genome sequencing has revealed biosynthetic gene clusters in insects and their microbiomes that encode many unexplored compounds [8].

Insect-Derived Natural Products as Drug Leads

1. Major Compound Classes

A wide variety of secondary metabolites, including peptides and proteins, alkaloids, terpenoids, polyketides, and fatty acid derivatives, are produced by insects. Each class has unique biological mechanisms and structural characteristics that make them intriguing for pharmacological study [9]. The main classes are shown in Table 1 along with their sources and therapeutic significance.

Table 1: Major Classes of Bioactive Insect-Derived Natural Products

Compound Class	Key Examples	Source Insect	Therapeutic Use
Peptides / AMPs	Melittin, Apamin, Defensins	Honeybee (Apis mellifera)	Anticancer, Antimicrobial
Alkaloids	Solenopsins	Fire ants (Solenopsis invicta)	Antimicrobial, Antifungal
Terpenoids	Cantharidin	Blister beetles (Meloidae)	Dermatology, Antitumor
Polyketides	Pederin	Rove beetles (Paederus sp.)	Anticancer, Antibacterial
Fatty Acid Derivatives	Bombykol, Ceramides	Silkworm (Bombyx mori)	Wound healing, Neuro
Venom Proteins	Phospholipase A2	Wasps, Bees, Ants	Anti-inflammatory, Analgesic

2. Antimicrobial Peptides

One of the most researched bioactives derived from insects is antimicrobial peptides (AMPs). The primary mechanism of action of these brief, amphipathic, cationic peptides is the disruption of bacterial membrane integrity. The 26 amino acids that make up melittin from honeybee venom have been investigated for their antibacterial, antiviral, and anticancer properties. It exhibits some selectivity for tumor over normal cells and activates apoptotic pathways in cancer cells at low concentrations [10]. Insect defensins offer a variety of template libraries for AI-assisted analogue creation because they are effective against fungus, Gram-positive bacteria, and some parasites [11].

3. Alkaloids and Terpenoids

Solenopsins, produced by fire ants, are 2,6-disubstituted piperidine alkaloids with antimicrobial, antifungal, and cytotoxic activities. They inhibit enzymes including PI3K and ceramidase, which are relevant targets in anti-inflammatory and anticancer research [12]. Cantharidin, a terpenoid from blister beetles, is a potent inhibitor of protein phosphatase 2A (PP2A) — an enzyme implicated in cancer cell survival. Computational docking studies have mapped its binding pocket on PP2A and helped design analogues with improved selectivity [4].

4. Therapeutic Applications

Natural insect products have demonstrated potential in a number of disease domains. In oncology, substances including melittin, cantharidin, and pederin cause cell cycle arrest, induce apoptosis, and prevent angiogenesis in cell lines of breast, prostate, liver, and colorectal cancer. As the antimicrobial resistance (AMR) situation worsens, insect AMPs are receiving more interest in the field of infectious illnesses. AMPs are intrinsically less likely to acquire resistance than traditional antibiotics because they function by rupturing membranes rather than interacting with a particular protein target [13]. Bee propolis flavonoids have been shown to have anti-diabetic properties by acting as DPP-4 and alpha-glucosidase inhibitors. Ant alkaloids, wasp phospholipase A2, and bee venom peptides have all been shown to have anti-inflammatory properties [14].

Artificial Intelligence in Drug Discovery

Over the past ten years, the use of AI in drug development has expanded significantly thanks to improvements in computer power, the growth of chemical and biological datasets, and increasingly complex machine learning architectures. The primary methods include explainable AI, generative models, deep learning, and traditional machine learning [7].

1. Classical Machine Learning

Classical ML algorithms work on hand-crafted molecular features called descriptors and have proven highly effective for bioactivity prediction and QSAR modeling. Random Forest is widely used in virtual screening because it handles high-dimensional data well and provides interpretable feature importance scores [15]. Support Vector Machines perform well for classification tasks with small datasets. Gradient boosting frameworks like XGBoost have demonstrated excellent performance in binding affinity prediction and toxicity classification, often outperforming deep learning when training datasets are modest [16].

2. Deep Learning

Deep learning has transformed molecular property prediction by enabling models to learn directly from raw molecular representations — SMILES strings, molecular graphs, or 3D coordinates — without needing engineered features. Graph Neural Networks (GNNs) treat molecules as graphs, with atoms as nodes and bonds as edges, and apply message-passing operations to learn both local and global chemical context [17]. Transformer-based models pretrained on millions of molecular SMILES strings, such as ChemBERTa and MolBERT, have shown strong transfer learning performance for binding affinity prediction, toxicity classification, and property optimization [18].

3. Generative AI for Molecular Design

Generative models represent a fundamental shift from screening existing libraries to designing entirely new molecules with desired properties. Variational autoencoders, generative adversarial networks, and diffusion models have all been applied to molecular generation with impressive results [19]. Reinforcement learning has been combined with generative architectures to optimize molecules toward specific goals such as binding affinity, synthetic accessibility, and ADMET profiles. Applied to insect natural product scaffolds, these approaches could produce novel analogues with better drug-likeness while preserving the core pharmacophoric features responsible for biological activity [20].

4. Explainable AI

The black-box nature of many deep learning models has been a real barrier to adoption in regulatory settings where mechanistic understanding is required. Explainable AI (XAI) methods — including SHAP, LIME, attention mechanisms, and gradient attribution — provide interpretable insights into model predictions [21]. In natural product research, XAI has been used to identify which structural features most strongly predict bioactivity, enabling medicinal chemists to make targeted modifications to natural product scaffolds. Regulatory agencies like the FDA and EMA have increasingly emphasized interpretability, making XAI capabilities essential for the clinical adoption of AI-driven candidates.

AI Workflow for Insect Natural Product Discovery

A systematic AI-driven pipeline for insect natural product discovery integrates multiple computational and experimental stages, moving from insect collection through compound isolation, database curation, AI screening, molecular docking, ADMET profiling, lead optimization, and experimental validation.

Stage 1 — Insect Collection and Species Authentication: Targeted collection is guided by ethnopharmacological data, phylogenetic proximity to bioactive species, and ecological observations. DNA barcoding using the COI gene enables rapid species authentication [22].

Stage 2 — Compound Isolation and Structural Elucidation: LC-MS/MS metabolomics and NMR spectroscopy enable comprehensive profiling of insect metabolomes. Mass spectrometry molecular networking via platforms like GNPS facilitates identification of novel scaffolds [8].

Stage 3 — Database Curation: Identified compounds are curated into structured databases with SMILES representations, descriptors, and bioactivity data, cross-referenced with PubChem, ChEMBL, and COCONUT [23].

Stage 4 — AI-Based Virtual Screening: Trained ML/DL models screen the compound library against target proteins, generating ranked lists based on predicted binding affinity and bioactivity scores [7].

Stage 5 — Molecular Docking: Top-ranked candidates are docked using AutoDock Vina, Glide, or GOLD to characterize binding poses, key interactions, and estimated binding energies [24].

Stage 6 — ADMET Prediction: Candidates are filtered through in silico ADMET profiling for drug-likeness, metabolic stability, blood-brain barrier permeability, hERG cardiotoxicity, and mutagenicity [25].

Stage 7 — Lead Optimization and Validation: Optimized candidates are synthesized or isolated and tested *in vitro* through cell viability assays, enzyme inhibition assays, and antimicrobial susceptibility testing [6].

Computational Databases and Resources

The success of AI-driven drug discovery depends fundamentally on the quality of the underlying databases. Key resources include PubChem (compound structures and properties), ChEMBL (bioactivity data), DrugBank (drug-target interactions), UniProt (protein sequences), AlphaFold DB (3D protein structures), COCONUT and LOTUS (natural product structures and organism links), and SwissTargetPrediction (target prediction for small molecules) [23, 26, 27].

A critical gap exists in the current database landscape: there is no dedicated, comprehensive, AI-ready database specifically curated for insect-derived natural products. While COCONUT and LOTUS contain many insect-derived entries, they lack systematic annotation for insect species of origin, biosynthetic pathway data, and associated bioactivity from insect-specific literature. Developing such a resource — an InsectNatProd database integrating structural, bioactivity, taxonomic, and omics data — would substantially accelerate AI-driven insect natural product discovery [23].

AI-Assisted Virtual Screening and Target Identification

1. Structure-Based and Ligand-Based Screening

Structure-based virtual screening (SBVS) uses the 3D structure of a target protein to computationally evaluate how well candidate molecules fit the binding site. The availability of AlphaFold2-predicted structures for nearly all human proteins has dramatically expanded the target space accessible to SBVS. AI has enhanced this process through deep learning models for binding pose prediction — such as DiffDock — ML-based scoring functions, and active learning strategies that reduce computational cost while maintaining screening quality [28]. Ligand-based virtual screening (LBVS) is applicable when a reliable target structure is unavailable, relying on structural similarity to known active compounds. For insect natural products, LBVS is particularly valuable when targeting poorly characterized enzymes from insect-associated pathogens [29].

2. Network Pharmacology and Multi-Target Discovery

Network pharmacology integrates compound-target interaction data with protein-protein interaction networks, disease gene networks, and pathway databases to reveal the polypharmacological landscape of natural products [30]. This systems-level approach suits insect natural products well, since many exhibit pleiotropic effects by simultaneously engaging multiple targets. A typical workflow involves identifying active constituents, constructing a compound-target network, intersecting targets with disease-associated genes, performing GO and KEGG pathway enrichment, and identifying hub genes using topological metrics. Multi-target drug discovery has revealed dual-target profiles for several insect-derived scaffolds, including solenopsins (PI3K and ceramidase inhibition) and cantharidin (PP2A and HDAC inhibition) [12].

ADMET Prediction Using AI

Approximately 40 to 50 percent of drug failures in clinical development are attributable to poor pharmacokinetic and toxicological profiles — which is why in silico ADMET prediction has become a cornerstone of modern drug discovery. AI models trained on experimental data can assess oral bioavailability, P-glycoprotein substrate status, blood-brain barrier penetration, CYP450 enzyme interactions, hERG cardiotoxicity, hepatotoxicity, and mutagenicity [25]. Key freely accessible tools for insect natural product ADMET profiling include SwissADME, pkCSM, ADMETlab 2.0, and ProTox-II, collectively covering more than 50 ADMET endpoints [31]. Deep learning models — particularly directed message-passing neural networks — have achieved competitive performance on the Tox21 and ToxCast benchmark datasets, enabling reliable toxicity profiling of novel insect-derived scaffolds [32].

Case Studies

1. Cantharidin Derivatives as Anticancer Agents

Cantharidin, isolated from blister beetles, is a potent PP2A inhibitor with significant cytotoxicity against multiple cancer cell lines. Its clinical use is limited by nephrotoxicity and mucosal damage, so researchers have applied AI-driven approaches to design safer analogues. A library of over 500

cantharidin analogues was screened computationally using AutoDock Vina against the PP2A crystal structure, and top-ranked candidates were filtered by ADMET profiles. QSAR models trained on experimental IC50 data from 89 analogues using Random Forest and XGBoost achieved cross-validation R-squared values of 0.81 and 0.84, respectively. Three synthesized analogues showed reduced toxicity in normal cells while maintaining cytotoxicity against hepatocellular carcinoma cells, representing a genuine improvement in therapeutic index [4, 33].

2. Melittin-Based Anticancer Lead Optimization

Melittin, the principal toxic component of honeybee venom, is a 26-amino acid peptide with broad-spectrum anticancer activity working through membrane disruption, phospholipase A2 activation, apoptosis induction, and NF-kB inhibition. Non-selective membrane disruption and rapid degradation by serum proteases have hindered its direct clinical use. Deep learning-assisted peptide design using recurrent neural networks trained on databases of AMPs generated novel peptide sequences sharing key structural features with melittin while incorporating modifications predicted to improve cancer cell selectivity. Molecular dynamics simulations confirmed that the generated analogues preferentially disrupted cancer cell membrane models over normal cell models, consistent with observed experimental selectivity [10, 34].

3. AI-Predicted Antimicrobial Peptides Against Drug-Resistant Pathogens

A landmark study applied machine learning to predict antimicrobial activity and selectivity across over 1,000 insect-derived AMP sequences from genomic and transcriptomic datasets. A gradient boosting classifier trained on 2,470 AMPs with experimental MIC data achieved AUC above 0.90 on held-out test sets. Ten top-ranked predicted AMPs were synthesized and experimentally validated, with 7 of 10 showing MIC below 8 micrograms per milliliter against Staphylococcus aureus and Escherichia coli — an AI prediction-to-validation success rate of 70%, which is highly encouraging for the field [35].

4. Insect Microbiome-Derived Compounds

The insect gut microbiome is an underexplored reservoir of biosynthetic diversity. Genomic mining of microbiomes from termites, bark beetles, and social insects has revealed biosynthetic gene clusters encoding non-ribosomal peptide synthetases and polyketide synthases — the same types of pathways responsible for many clinical antibiotics. AI tools including antiSMASH, BiG-SCAPE, and PRISM have been applied to insect microbiome metagenomes. A study of leafcutter ant microbiomes identified 14 previously unknown biosynthetic gene clusters, several encoding products with structural similarity to known antibiotics, with network pharmacology analysis pointing to potential activity against Mycobacterium tuberculosis targets [8, 36].

Challenges, Gaps, and Future Directions

1. Data and Model Challenges

The performance of any machine learning model is bounded by the quality and quantity of training data. Insect natural product research faces small experimental datasets, class imbalance between active and inactive compounds, inconsistent reporting of assay conditions, and publication bias toward positive results [37]. The chemical space of insect natural products also differs substantially from the synthetic compound space on which most AI drug discovery models are trained — insect compounds frequently feature unusual bicyclic ring systems and non-proteinogenic amino acids that may be poorly represented in training data, leading to unreliable predictions [38]. Transfer learning, semi-supervised learning, and active learning protocols offer promising strategies to partially overcome the small data problem.

2. Critical Research Gaps

Several interconnected gaps explain why the integration of AI with insect natural product research remains underdeveloped relative to its potential. No comprehensive AI-ready database exists specifically for insect-derived natural products; most bioactivity data sits locked in PDF journal articles rather than structured databases; the overwhelming majority of research has focused on bees, ants, and beetles, leaving vast insect orders like Diptera and Orthoptera largely unexplored; and interdisciplinary collaboration between entomologists, natural product chemists, and computational biologists remains limited [3, 38]. Addressing these gaps — particularly through the creation of a dedicated insect natural product database — is a high priority for the field.

3. Future Perspectives

Several emerging technologies are positioned to transform insect natural product drug discovery over the next decade. AI agents — autonomous systems capable of planning and executing multi-step research workflows, including literature mining, hypothesis generation, virtual screening, and experimental design — represent a step-change in research throughput [20]. Multi-omics integration, combining genomics, transcriptomics, proteomics, and metabolomics data from insect species and their microbiomes, will enable a far more complete picture of biosynthetic potential. Generative models built on equivariant diffusion and structure-based design principles are increasingly capable of producing novel molecular scaffolds with desired binding profiles. Federated learning approaches could enable collaboration across research groups without requiring sensitive data sharing, helping to address the fragmented data landscape that currently limits model performance [39].

Conclusion

Insects represent one of the most underexplored frontiers in natural product drug discovery. Their extraordinary chemical diversity — spanning antimicrobial peptides, alkaloids, terpenoids, polyketides, and venom proteins — holds genuine promise for addressing some of medicine's most pressing challenges, from antimicrobial resistance to treatment-resistant cancers. The convergence of this chemical diversity with modern AI methodologies creates a powerful opportunity that the research community is only beginning to realize. Virtual screening, ADMET prediction, generative design, and network pharmacology have all demonstrated their value in insect natural product research, as illustrated by the case studies in this review. Moving this field forward will require dedicated infrastructure — particularly a comprehensive, AI-compatible insect natural product database — along with stronger interdisciplinary collaboration and more systematic experimental validation of computational predictions. The integration of AI with entomological natural product research is not just timely; it is arguably essential if this rich but neglected chemical

space is to be translated into the next generation of medicines.

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