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Biosensor and Artificial Intelligence Technologies for the Discovery, Quality Control, And Authentication of Natural Bioactive Compounds: A Biomedical Engineering and Biophysics Perspective

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ABSTRACT: The discovery, quality control, and clinical translation of bioactive compounds derived from medicinal plants and other natural resources increasingly depend not on botany or pharmacology alone, but on the convergence of biomedical engineering, biophysical sensing, and computational informatics. Biosensors, analytical devices that couple a biological recognition element with a physical or electrochemical transducer, and artificial intelligence, which increasingly assists compound identification, extraction optimization, and bioactivity prediction, together constitute a rapidly advancing methodological toolkit for natural-product research. This review examines recent evidence on biosensor platforms applied to natural medicine research, including electrochemical, optical, and piezoelectric quartz crystal microbalance sensors, and on the current applications and limitations of artificial intelligence across the medicinal plant drug discovery pipeline. The reviewed literature indicates that nanomaterial-enhanced biosensors can achieve femtomolar-to-picogram sensitivity for herb authentication, active-compound screening, and quality-control contaminant detection, that quartz crystal microbalance platforms in particular offer a direct, label-free route to real-time monitoring of natural-compound binding events, and that artificial intelligence tools, while not yet delivering a fully AI-derived approved botanical drug, meaningfully accelerate compound identification, extraction optimization, and virtual screening. These findings position biomedical engineering, biophysics, and informatics as indispensable, integrative disciplines for advancing natural resources toward validated human health applications, while also highlighting substantial translational and standardization challenges that remain.

1. INTRODUCTION

Natural resources, principally medicinal plants but also fungi, algae, and other biological sources, remain one of the most productive wellsprings of bioactive compounds for human health, yet translating a promising plant extract into a validated, standardized, and clinically usable product depends heavily on analytical and computational capabilities that lie outside traditional botany and pharmacognosy. Two disciplines in particular, biomedical engineering and its associated biophysical sensing technologies, and biomedical informatics through artificial intelligence and machine learning, have become central to this translation process over the past several years. Biosensors provide the physical means to detect, quantify, and authenticate natural bioactive compounds and the biological targets they act upon with a sensitivity and speed that conventional

chromatographic and spectroscopic methods often cannot match in field or point-of-care settings, while artificial intelligence provides the computational means to make sense of the vast and structurally complex chemical space that natural products occupy.

This review brings these two strands together, examining how biosensor platforms, including electrochemical, optical, and piezoelectric quartz crystal microbalance sensors, are currently applied to the discovery, quality control, and authentication of natural bioactive compounds, and how artificial intelligence is being integrated across the medicinal plant drug discovery pipeline from species identification through virtual screening. Because both strands directly serve the goal of converting natural resources into validated human health applications, they represent a natural and increasingly necessary extension of natural-product research into biomedical engineering, biophysics, and informatics.

1.1. Why an Engineering and Informatics Perspective Is Needed

Traditional natural-product workflows have long relied on solvent extraction followed by chromatographic separation and mass spectrometric or nuclear magnetic resonance identification, a sequence that is accurate but slow, equipment-intensive, and poorly suited to point-of-care, field-based, or high-throughput screening contexts. Biosensors close this gap by embedding a biological or biochemical recognition step directly onto a physical transducer, so that binding, hybridization, or catalytic events are converted immediately into an electrical, optical, or mechanical signal without the sample-preparation burden of conventional analytical chemistry. Artificial intelligence closes a complementary gap: even when analytical data are generated efficiently, the sheer combinatorial diversity of plant secondary metabolites, several hundred thousand structurally distinct compounds are estimated to exist across the plant kingdom, exceeds what manual literature review and structure-activity reasoning can process. Positioning these two toolkits as core competencies of a combined biomedical engineering, informatics, and biophysics department, rather than as occasional collaborations with outside laboratories, is what allows natural-product research to scale from single-compound case studies to systematic, reproducible discovery and quality-control pipelines.

1.2. Scope and Organization of This Review

Section 2 reviews biosensor platforms currently applied to natural medicine research, drawing on two recent systematic reviews of the field. Section 3 examines the piezoelectric quartz crystal microbalance in particular detail, both because of its distinctive biophysical operating principle and because it connects directly to synthetic piezoelectric quartz materials research. Section 4 reviews the current state and limitations of artificial intelligence across the medicinal plant drug discovery pipeline. Section 5 proposes an integrated framework linking biosensor and artificial intelligence contributions stage by stage, and Sections 6 and 7 discuss remaining limitations, translational challenges, and concluding perspectives.

2. BIOSENSOR PLATFORMS FOR NATURAL MEDICINE RESEARCH

A systematic review of biosensor applications in traditional medicine research identifies several converging use cases in which biosensors, devices that integrate a biological recognition element with a physicochemical signal transducer, provide direct and often more rapid alternatives to conventional wet-chemistry analysis [1]. For herb identification and authentication, electrochemical DNA biosensors targeting species-specific genetic sequences have achieved femtomolar sensitivity in distinguishing closely related medicinal plant species, directly addressing the long-standing problem of botanical misidentification and adulteration in herbal product supply chains [1]. For active-component analysis, surface plasmon resonance biosensors have been used to screen flavonoids and other phytochemical classes directly from herbal extracts, quantifying their binding affinities to therapeutic protein targets and thereby connecting chemical composition to biological function in a single measurement [1].

The same review documents biosensor applications in quality control and safety testing, where sensor platforms have detected pesticide residues, heavy metals, and mycotoxins in medicinal raw materials at trace levels, complementing rather than replacing conventional pharmacopeial testing methods [1]. A broader review of biosensor technologies for natural medicine discovery similarly categorizes the field into optical biosensors, including surface plasmon resonance, bio-layer interferometry, and fluorescence-based systems enabling label-free detection; electrochemical biosensors offering rapid response and amenability to miniaturization; and microfluidic-integrated platforms that combine multiple detection modalities for higher-throughput screening of antiviral, anti-inflammatory, anticancer, neuroprotective, and nucleic-acid-targeting natural compounds [2]. Both reviews converge on a common set of limitations that must be addressed before wider clinical and industrial adoption, namely

matrix interference from the chemically complex background of natural extracts, biological recognition element instability, and the absence of standardized validation protocols across regulatory frameworks [1, 2].

2.1. Electrochemical Biosensors

Electrochemical biosensors detect a target analyte through a change in current, potential, or impedance at an electrode surface functionalized with a recognition element such as a DNA probe, aptamer, or enzyme. Their principal advantages for natural-product applications include low cost, amenability to miniaturization into handheld or point-of-care devices, and compatibility with the aqueous, often optically turbid extracts typical of plant material, which can interfere with purely optical detection methods [1]. The femtomolar-sensitivity DNA biosensors used for medicinal plant species authentication described above are a representative electrochemical application, exploiting hybridization of a target genomic sequence to a complementary probe immobilized on the electrode surface, with hybridization producing a measurable change in electrode impedance or redox current.

2.2. Optical Biosensors

Optical biosensors, including surface plasmon resonance, bio-layer interferometry, and fluorescence-based platforms, detect binding events through changes in refractive index, interference patterns, or emitted light intensity at or near a sensor surface, without requiring a secondary labeling step in many configurations [2]. Their principal strength for natural-product research lies in real-time, label-free measurement of binding kinetics and affinity between a candidate phytochemical and a therapeutic target protein, information that is difficult to obtain efficiently through conventional biochemical assays and that directly supports structure-activity and target-validation studies [1, 2].

2.3. Microfluidic-Integrated and Multiplexed Platforms

Microfluidic integration allows several detection modalities, or several parallel assays against the same natural extract, to be combined on a single miniaturized platform, substantially increasing throughput relative to sequential single-assay testing [2]. For natural-product screening, in which a single plant extract may need to be evaluated for antiviral, anti-inflammatory, anticancer, and neuroprotective activity simultaneously, this multiplexing capability is particularly valuable, and the reviewed literature identifies microfluidic-integrated biosensing as one of the fastest-growing sub-areas within natural medicine biosensor research [2].

Figure 1. Integrated biosensor-informatics pipeline for natural bioactive compound research

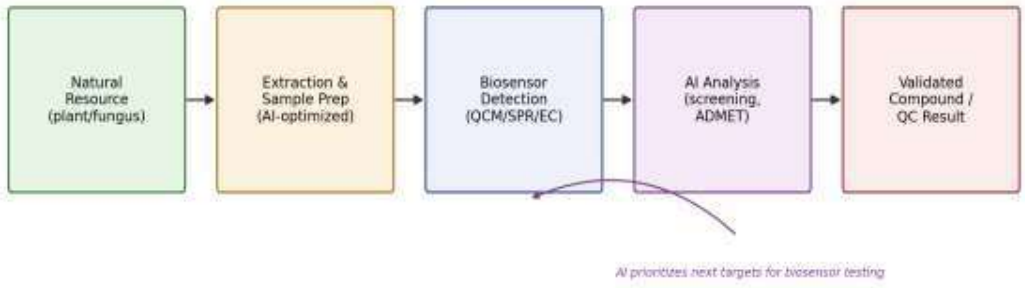


Figure 1. Integrated biosensor-informatics pipeline linking natural resource sourcing, extraction, biosensor detection, and AI-guided analysis, with AI outputs feeding back to prioritize the next round of biosensor testing.

3. PIEZOELECTRIC QUARTZ CRYSTAL MICROBALANCE SENSING: A BIOPHYSICAL BRIDGE

Among the biosensor architectures relevant to natural-product research, the quartz crystal microbalance occupies a distinctive position because it is fundamentally a biophysical device, translating a mass or viscoelastic change at the sensor surface into a measurable shift in the resonant frequency of a piezoelectric quartz crystal, the same physical property that underlies synthetic

piezoelectric quartz growth and characterization work in materials physics [3]. A recent comprehensive review of nanostructured quartz crystal microbalance biosensors demonstrates that integrating nanomaterials such as gold nanoparticles, magnetic beads, and two-dimensional composites at the sensor surface substantially amplifies detection sensitivity by increasing effective surface area and mass-loading efficiency, enabling detection of low-abundance biomarkers including cancer antigens, inflammatory markers, and pathogens at picogram-per-milliliter concentrations in several documented cases [4].

Figure 2. Working principle of the quartz crystal microbalance (QCM) biosensor

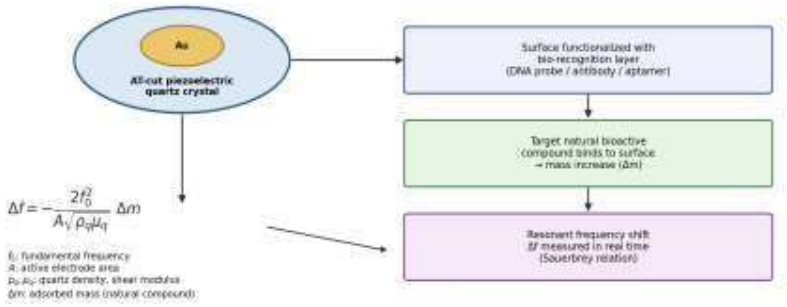


Figure 2. Working principle of the quartz crystal microbalance biosensor: surface functionalization, target binding, and Sauerbrey-relation-based conversion of mass loading into a measurable frequency shift.

3.1. From Materials Physics to Biosensing: A Shared Physical Principle

The quartz crystal microbalance operates on the Sauerbrey relation illustrated in Figure 2, in which the frequency shift produced by a small added mass at the crystal surface is proportional to that mass and inversely proportional to the square of the crystal's fundamental resonant frequency, with the crystal's intrinsic density and shear modulus entering as material constants. These are precisely the physical parameters that govern the growth, cut orientation, and resonant behavior of synthetic piezoelectric quartz produced and characterized for other applications, including the AT-cut piezoelectric quartz materials described in recent work on synthetic quartz growth technology [3]. This shared physical foundation means that expertise in piezoelectric quartz materials characterization, resonant frequency measurement, and crystal-cut optimization, developed originally for materials-physics or sensing-device applications, transfers directly to the design and calibration of quartz crystal microbalance biosensors for natural-compound detection, illustrating a concrete, mechanistic link between biophysics and natural-product analytical chemistry rather than a merely thematic one.

3.2. Applications and Current Translational Status

This capacity for label-free, real-time detection of binding events at a quartz crystal surface makes the quartz crystal microbalance particularly well suited to monitoring interactions between natural bioactive compounds and their protein or nucleic acid targets, extending the same piezoelectric quartz platform used in physical and materials characterization work directly into biosensing applications for natural-product research [3, 4]. The reviewed evidence also identifies a significant translational gap common to this class of device: despite favorable analytical performance in controlled laboratory conditions, most nanostructured quartz crystal microbalance biosensor prototypes remain at low technology readiness levels, with long-term stability, performance in authentic biological matrices, and manufacturing scalability identified as the principal barriers to clinical and industrial deployment [4].

Table 1. Comparison of biosensor platforms applied to natural bioactive compound research.

Platform	Transduction Principle	Typical Sensitivity	Best-Suited Application
Electrochemical (DNA)	Impedance / redox current change on hybridization	Femtomolar range [1]	Species authentication, adulteration detection

Surface Plasmon Resonance (SPR)	Refractive-index shift on surface binding	Sub-nanomolar range [1, 2]	Binding-affinity screening, target validation
Nanostructured QCM	Resonant frequency shift on mass loading (Sauerbrey)	Picogram/mL range [4]	Real-time binding kinetics, label-free monitoring
Microfluidic multiplexed	Parallel optical/electrochemical modules on one chip	Platform-dependent [2]	High-throughput multi-activity extract screening

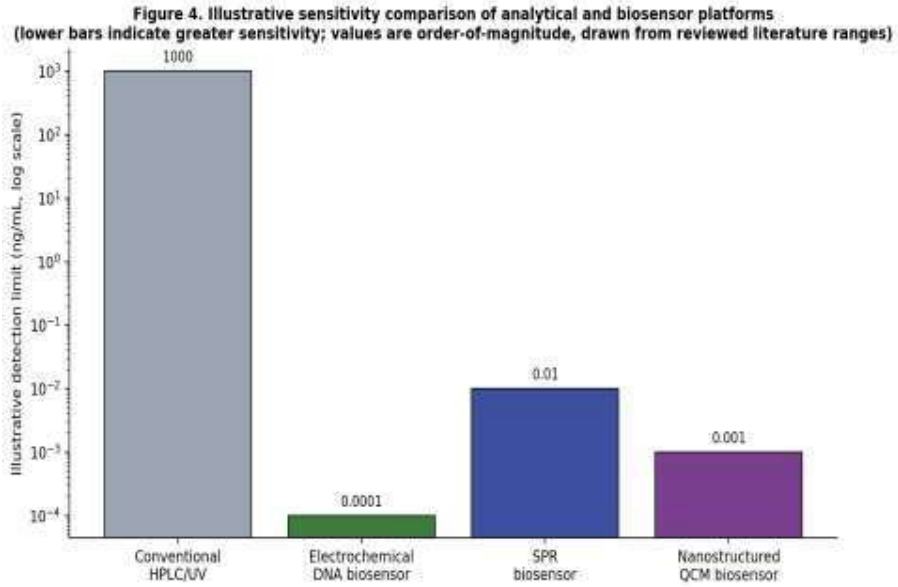


Figure 3. Illustrative order-of-magnitude sensitivity comparison across conventional chromatographic analysis and the three principal biosensor categories reviewed, based on ranges reported in [1], [2], and [4].

4. ARTIFICIAL INTELLIGENCE ACROSS THE MEDICINAL PLANT DRUG DISCOVERY PIPELINE

Parallel to the biophysical sensing advances discussed above, artificial intelligence has been integrated across nearly every stage of the medicinal plant drug discovery pipeline. A recent review identifies applications spanning automated plant species identification through deep learning and computer vision, machine learning-guided optimization of extraction solvent, temperature, and pressure conditions to maximize bioactive compound yield, AI-assisted dereplication of metabolites using mass spectrometry and nuclear magnetic resonance data to avoid redundant rediscovery of known compounds, predictive virtual screening and absorption-distribution-metabolism-excretion-toxicity modeling to prioritize phytochemicals before costly experimental testing, network pharmacology approaches using graph neural networks to map the multi-component, multi-target interactions characteristic of herbal formulations, and generative artificial intelligence for the de novo design of pseudo-natural product derivatives with improved synthesizability [5].

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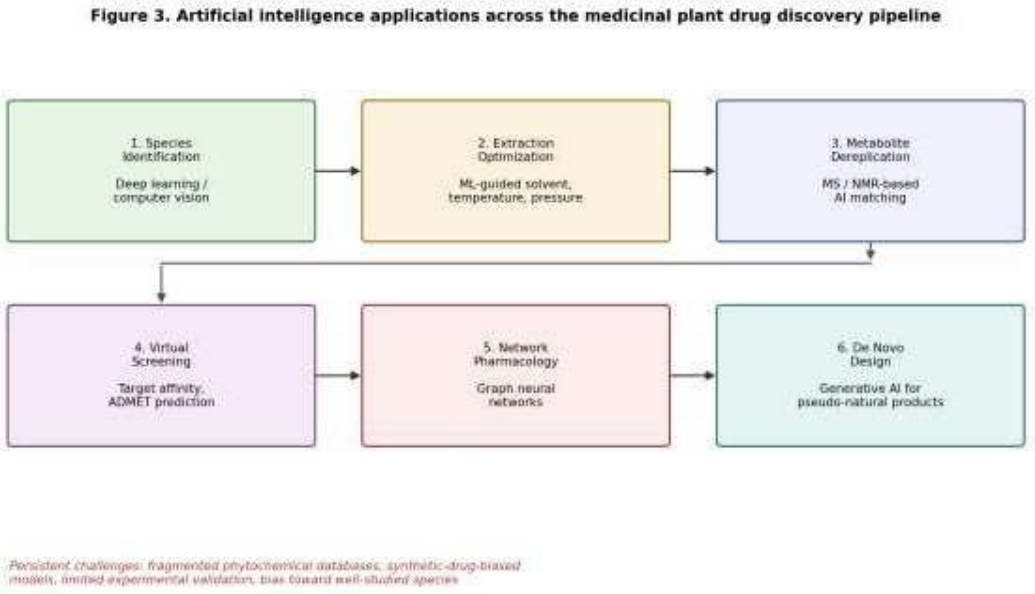


Figure 4. Artificial intelligence applications mapped across six stages of the medicinal plant drug discovery pipeline, from species identification through de novo compound design, with persistent cross-cutting challenges noted below.

4.1. Compound Identification and Extraction Optimization

At the earliest pipeline stages, deep learning-based computer vision models now support automated botanical species identification from leaf, flower, or whole-plant images, reducing dependence on scarce taxonomic expertise and bypassing morphological ambiguity between closely related species [5]. Once a species is confirmed, machine learning models trained on prior extraction datasets can predict the solvent composition, temperature, and pressure conditions expected to maximize yield of a target bioactive compound class, shortening the empirical optimization process that traditionally required extensive trial-and-error experimentation [5].

4.2. Metabolite Dereplication and Virtual Screening

Dereplication, the process of rapidly recognizing already-known compounds within a complex extract before committing resources to their full structural elucidation, has been substantially accelerated by AI-assisted matching of mass spectrometry and nuclear magnetic resonance data against reference spectral libraries, allowing research effort to be redirected toward genuinely novel constituents [5]. Downstream of dereplication, virtual screening and computational absorption-distribution-metabolism-excretion-toxicity prediction allow candidate phytochemicals to be ranked by predicted target affinity and pharmacokinetic suitability before any wet-laboratory testing occurs, in principle reducing the number of compounds that must be experimentally evaluated to identify a promising lead [5].

4.3. Network Pharmacology and Generative Design

Because herbal formulations typically contain many bioactive constituents acting on multiple molecular targets simultaneously, rather than a single compound acting on a single target as in conventional pharmacology, graph neural network-based network pharmacology approaches have been developed specifically to map these multi-component, multi-target interaction networks, offering a more mechanistically complete picture of how a traditional formulation might produce its observed therapeutic effect [5]. At the most computationally advanced end of the pipeline, generative artificial intelligence models have begun to design de novo pseudo-natural product derivatives, structures inspired by natural product scaffolds but computationally optimized for improved synthesizability or bioavailability relative to the parent natural compound [5].

4.4. Persistent Challenges

Despite this breadth of application, the same review is explicit that substantial barriers currently limit the translational impact of artificial intelligence in this domain, noting directly that fully AI-driven, clinically approved botanical drugs have yet to emerge [5]. Identified obstacles include fragmented and inconsistently annotated phytochemical databases, algorithmic models trained predominantly on synthetic small-molecule drug datasets that may underperform on structurally complex and stereochemically diverse phytochemicals, a persistent translational gap in which computational predictions frequently fail during biological validation because isolated compounds do not replicate the synergistic effects observed in whole extracts, and an overrepresentation of well-studied plant species that introduces systematic bias toward already-established therapeutic leads [5]. The authors call for foundational reforms, including metadata harmonization, dataset balancing, and development of phytochemistry-specific foundation models, before large-scale artificial intelligence deployment can be expected to yield validated clinical outcomes [5].

Table 2. Artificial intelligence methods mapped to medicinal plant drug discovery pipeline stages.

Pipeline Stage	AI/ML Method	Primary Benefit
Species identification	Deep learning, computer vision	Bypasses taxonomic ambiguity, reduces expert dependence
Extraction optimization	Supervised machine learning regression	Predicts optimal solvent, temperature, pressure
Metabolite dereplication	AI-assisted MS/NMR spectral matching	Avoids redundant rediscovery of known compounds
Virtual screening	Predictive target-affinity and ADMET models	Prioritizes candidates before wet-lab testing
Network pharmacology	Graph neural networks	Maps multi-component, multi-target interactions
De novo design	Generative AI models	Designs synthesizable pseudo-natural product derivatives

5. AN INTEGRATED BIOMEDICAL ENGINEERING PERSPECTIVE

Table 3. Complementary roles of biosensor and artificial intelligence technologies across the natural-product research pipeline.

Pipeline Stage	Biosensor / Biophysical Contribution	Artificial Intelligence / Informatics Contribution
Species identification & authentication	Electrochemical DNA biosensors, femtomolar sensitivity [1]	Deep learning / computer vision species recognition [5]
Extraction & sample preparation	Real-time monitoring of extraction/binding via QCM [3, 4]	ML-guided optimization of solvent, temperature, pressure [5]
Bioactive compound screening	SPR / QCM binding-affinity screening against targets [1, 2, 4]	Virtual screening, ADMET prediction, dereplication [5]
Quality control & safety	Trace detection of pesticides, heavy metals, mycotoxins [1]	Automated data analysis, anomaly/adulteration flagging [1, 2]
Translational readiness	Mostly low technology readiness level (TRL 3-4) [4]	No fully AI-derived approved botanical drug yet [5]

Table 3 summarizes how biosensor and biophysical technologies on one hand, and artificial intelligence and informatics tools on the other, offer complementary rather than competing contributions at nearly every stage of the natural-product research pipeline, from initial species authentication through to quality-control testing of finished products. A department combining biomedical engineering, informatics, and biophysics expertise is therefore uniquely positioned to advance natural-resource-derived human health research: biophysical sensing platforms such as the piezoelectric quartz crystal microbalance directly generate the quantitative binding and mass-loading data that machine learning models require for training and validation, while artificial intelligence tools in turn guide which natural compounds and extraction conditions are prioritized for biosensor-based experimental confirmation, creating a genuinely integrative, closed-loop research workflow rather than two separately operating toolkits [1-5], as illustrated by the feedback arrow in Figure 1.

5.1. A Worked Example of the Closed-Loop Workflow

Consider a hypothetical but representative workflow that concretely illustrates this integration. An extract from a candidate medicinal plant species, first confirmed by computer-vision-assisted taxonomic identification, is fractionated under machine learning-optimized extraction conditions. Each fraction is then screened by an electrochemical or quartz crystal microbalance biosensor functionalized with a disease-relevant protein target, generating real-time binding-affinity data. These experimental binding measurements are fed back into a virtual screening or network pharmacology model, which re-ranks the remaining untested fractions and proposes the next set of candidates for biosensor confirmation, progressively narrowing a large initia l extract library down to a small set of experimentally validated leads with substantially fewer total biosensor assays than an unguided, exhaustive screening campaign would require. This kind of iterative, AI-guided experimental design is precisely the capability that a combined biomedical engineering, biophysics, and informatics department is positioned to develop and refine.

6. LIMITATIONS AND FUTURE DIRECTIONS

Several limitations temper the current state of this integrated field. Biosensor platforms, and quartz crystal microbalance devices in particular, remain predominantly at early technology readiness levels, with long-term operational stability and reliable performance in complex, unprocessed biological or botanical matrices still requiring substantial engineering development before routine field or clinical deployment [4]. Artificial intelligence tools, meanwhile, are constrained by fragmented phytochemical data infrastructure and a validation gap between computational prediction and biological confirmation that has so far prevented any fully AI-derived botanical drug from reaching clinical approval [5]. Addressing both sets of limitations in tandem, rather than in isolation, through standardized biosensor validation protocols paired with phytochemistry-specific, well-curated training datasets, represents the most promising path toward reliable, scalable, and clinically translatable natural-product research.

A further limitation specific to this review is that the sensitivity figures compared in Figure 3 are order-of-magnitude illustrations drawn from ranges reported across different studies, extracts, and target analytes rather than a single head-to-head comparative study; direct, matched comparisons of electrochemical, optical, and quartz crystal microbalance platforms against the same natural-compound panel remain comparatively rare in the literature and would strengthen future quantitative benchmarking in this field.

7. CONCLUSION

Biomedical engineering, biophysics, and informatics have become indispensable partners to natural-product science, providing the sensing and computational infrastructure required to discover, validate, and quality-control bioactive compounds derived from natural resources. Biosensor platforms, spanning electrochemical, optical, and piezoelectric quartz crystal microbalance architectures, already achieve high analytical sensitivity for herb authentication, target-binding screening, and contaminant detection, while artificial intelligence tools increasingly accelerate species identification, extraction optimization, and virtual screening across the medicinal plant drug discovery pipeline. Realizing the full translational potential of this convergence will require closing the technology-readiness and data-standardization gaps identified in the current literature, but the trajectory of recent research indicates that integrated biosensor-informatics workflows are set to become a defining methodological pillar of natural-resource-for-human-health research in the coming years.

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