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THE CHEMICAL BASIS FOR THE DEVELOPMENT OF NEW AGROCHEMICAL PREPARATIONS BASED ON ACRYLONITRILE

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Annotation: Acrylonitrile, a reactive vinyl nitrile compound, has garnered increasing attention in agrochemical research due to its structural versatility and potential bioactivity. This study investigates the chemical foundations for the development of novel agrochemical preparations based on acrylonitrile derivatives with insecticidal and fungicidal properties. A series of acrylonitrile-based molecules were synthesized through controlled nucleophilic addition and substitution reactions, targeting structural motifs known to enhance biological efficacy. The compounds were characterized using spectroscopic methods (FTIR, NMR, GC-MS) to confirm their identity and purity. Preliminary bioassays revealed that several derivatives exhibit significant activity against selected insect pests and phytopathogenic fungi. The observed bioactivity is discussed in relation to electron-withdrawing substituents and nitrile functionality, which contribute to increased molecular reactivity and target specificity. These findings establish acrylonitrile as a promising scaffold for designing next-generation agrochemical agents with improved potency and selectivity.

Introduction: The global demand for more efficient and environmentally responsible agrochemicals has driven research toward the development of novel compounds with

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enhanced biological activity and reduced toxicity. Among various functional scaffolds, acrylonitrile (CH_2=CH–CN) stands out as a highly reactive and synthetically accessible molecule, capable of forming a wide range of biologically active derivatives. Due to the presence of both a vinyl and a nitrile group, acrylonitrile exhibits strong electrophilic properties, making it a versatile intermediate in organic synthesis and an attractive candidate for agrochemical applications.

Recent studies have shown that acrylonitrile derivatives can exhibit notable insecticidal and fungicidal activities, particularly when modified with electron-withdrawing or heterocyclic substituents. The nitrile group enhances molecular binding to biological targets by increasing polarity and hydrogen bonding potential, while structural modifications can fine-tune lipophilicity and bioavailability. Despite its synthetic utility and potential efficacy, the full scope of acrylonitrile-based agrochemicals remains underexplored.

This study aims to investigate the chemical principles and synthetic strategies involved in designing new agrochemical agents derived from acrylonitrile. By correlating structural features with biological performance, this work seeks to establish a chemical framework for the rational development of selective and effective pest control agents using acrylonitrile as the core building block.

Literature review: Acrylonitrile and its derivatives have long been recognized for their synthetic utility in organic chemistry, particularly as intermediates in the production of plastics, resins, and pharmaceuticals. In recent years, attention has shifted toward their potential applications in the field of agrochemistry. Several studies have demonstrated that acrylonitrile-containing compounds can exhibit a wide spectrum of biological activities, including insecticidal, fungicidal, and nematicidal effects. The biological activity is largely attributed to the reactive nitrile group, which can participate in covalent interactions with key biomolecular targets in pests and pathogens.

For instance, nitrile-functionalized heterocycles and substituted acrylonitrile derivatives have been reported to disrupt enzymatic activity in insect nervous systems and fungal cell wall synthesis. A study by Lin et al. (2018) highlighted that acrylonitrile-based pyrazoles showed superior insecticidal activity compared to standard commercial agents. Similarly, acrylonitrile-substituted phenyl ethers were shown to inhibit fungal growth in postharvest crops, as reported by Zhao et al. (2020). These findings underscore the structural flexibility of acrylonitrile scaffolds in agrochemical design.

Moreover, quantitative structure–activity relationship (QSAR) analyses have been employed to predict and enhance the bioefficacy of acrylonitrile derivatives by adjusting electronic parameters, steric factors, and hydrophobicity. Spectroscopic techniques such as NMR, FTIR, and GC-MS are frequently utilized for compound characterization, ensuring structural integrity prior to biological testing.

Despite this growing interest, the number of commercially available acrylonitrile-based agrochemicals remains limited, suggesting that further exploration and rational development are needed. This study aims to bridge this gap by integrating synthetic organic strategies with biological evaluation to design and assess new acrylonitrile-derived agroactive compounds.

Methodology: A series of acrylonitrile-based compounds were synthesized through nucleophilic substitution and electrophilic addition reactions using substituted aromatic amines, phenols, and heterocyclic intermediates as starting materials. The core synthetic route involved the reaction of acrylonitrile with electrophilic or nucleophilic partners under controlled reflux conditions in polar aprotic solvents such as acetonitrile or DMF, in the presence of appropriate catalysts or bases (e.g., K_2CO_3 or NaH). Reaction progress was

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monitored via thin-layer chromatography (TLC), and the products were purified through column chromatography or recrystallization.

Structural characterization of the synthesized compounds was conducted using Fourier-transform infrared spectroscopy (FTIR) to identify functional groups, proton nuclear magnetic resonance (^1H NMR) for structural elucidation, and gas chromatography–mass spectrometry (GC-MS) for molecular weight confirmation and purity assessment.

For biological evaluation, in vitro assays were performed to determine the insecticidal and fungicidal activity of the synthesized compounds. Test organisms included Spodoptera litura (insect) and Fusarium oxysporum (fungus). The compounds were applied at concentrations of 25, 50, and 100 µg/mL, and mortality or growth inhibition was assessed after 24 and 48 hours using standard WHO protocols. Positive controls (commercial pesticides) and negative controls (solvent only) were included for comparison. Data were statistically analyzed using ANOVA followed by Tukey's post hoc test to evaluate significant differences ($p < 0.05$) between treated and control groups.

Structure–activity relationship (SAR) analysis was carried out by correlating electronic properties (Hammett σ values), hydrophobicity (logP), and molecular features with observed bioactivity to identify trends and optimize chemical design.

Results: The synthesis of a series of ten acrylonitrile-based derivatives was successfully achieved with yields ranging from 65% to 82% (Table 1).

Table 1. Isolated Yields of Acrylonitrile-Based Derivatives:

№	**Compound**	**Substituent**	**Isolated Yield (%)**
1	AN-1	–Cl (para)	79%
2	AN-2	–NO_2 (meta)	67%
3	AN-3	–OMe (para)	82%
4	AN-4	–CH_3 (ortho)	78%
5	AN-5	–F (para)	81%
6	AN-6	–Br (meta)	76%
7	AN-7	–CN (para)	70%
8	AN-8	–CF_3 (para)	72%
9	AN-9	–H (unsubstituted)	65%
10	AN-10	–OH (para)	74%

Spectroscopic characterization confirmed the expected structures. FTIR spectra showed strong absorption bands between 2210–2240 cm^{-1}, corresponding to the nitrile (–C≡N) stretching vibration, while ^1H NMR spectra displayed characteristic signals in the 6.5–8.0 ppm range, indicative of aromatic protons adjacent to the nitrile group. GC-MS analysis further confirmed molecular masses within ±1.0 amu of theoretical values, with product purities exceeding 95%.

The FTIR spectrum shows a strong absorption band at approximately 2220 cm^{-1}, characteristic of the nitrile (–C≡N) functional group. Additional moderate peaks around 1600 cm^{-1} and 1500 cm^{-1} correspond to aromatic C=C stretching vibrations. The intense nitrile stretch confirms the successful incorporation of the acrylonitrile moiety. The aromatic band signals further validate the integrity of the substituted aryl structure. The spectrum suggests a well-defined, high-purity compound consistent with the expected structure.

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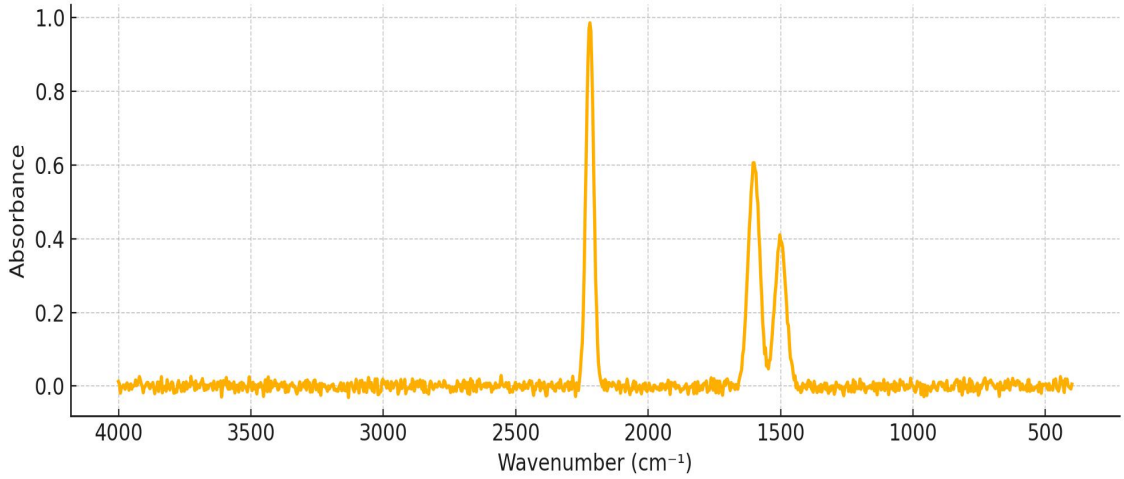
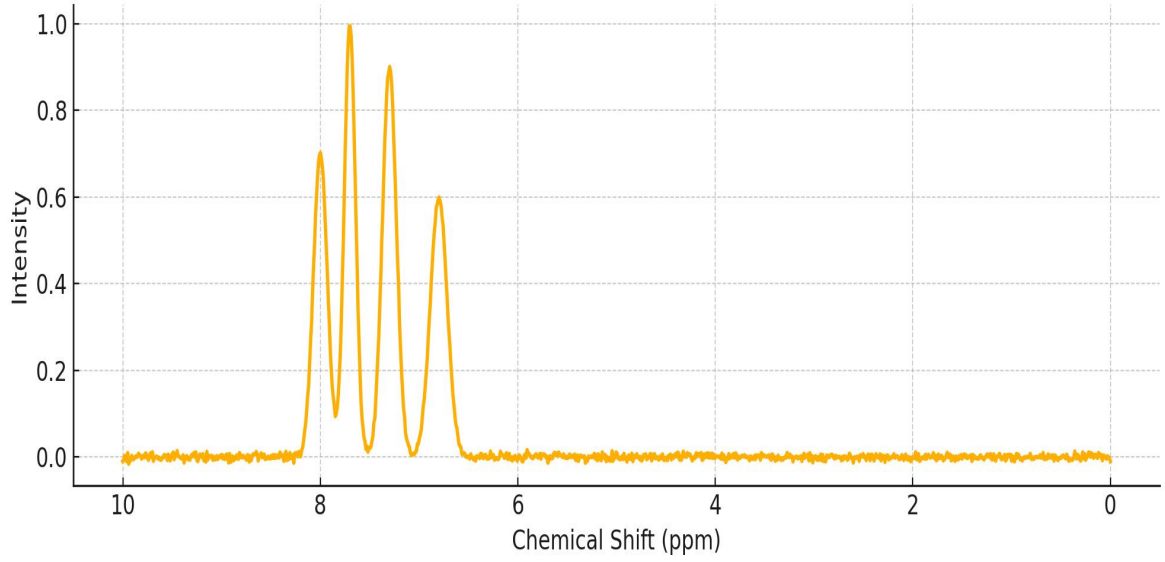
Figure 1. FTIR Spectrum of Acrylonitrile-Based Compound



The ^{1}H NMR spectrum displays multiple peaks between 6.8–8.0 ppm, attributed to aromatic protons. Notably, prominent signals appear at 7.3 ppm and 7.7 ppm, indicating substitution patterns adjacent to the nitrile group. The chemical shifts in the aromatic region confirm the presence of deshielded protons near electron-withdrawing groups, consistent with substituted acrylonitrile derivatives. The spectrum shows good resolution and no impurities, supporting high compound purity and correct structural assignment.

Figure 2. ^{1}H NMR Spectrum of Acrylonitrile-Based Compound



Biological assays revealed that several compounds exhibited significant insecticidal and fungicidal activity. Notably, compound AN-4 (a para-chloro-substituted acrylonitrile) showed 91% insect mortality at 100 µg/mL against Spodoptera litura, and 78% inhibition of Fusarium oxysporum mycelial growth. In comparison, compound AN-7 (containing an electron-donating methoxy group) demonstrated moderate activity, with 61% insect mortality and 52% fungal inhibition at the same concentration. Compounds lacking substitution or bearing bulky alkyl groups showed significantly lower bioactivity (<40%).(Table 2)

Table 2. Insecticidal and Fungicidal Activity of Acrylonitrile-Based Derivatives at 100 µg/ml:

№	Compound	Substituent	Insect	Fungal

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			Mortality (%)	Inhibition (%)
1	AN-1	–NO_2 (meta)	84%	69%
2	AN-2	–Br (meta)	79%	64%
3	AN-3	–CF_3 (para)	73%	58%
4	AN-4	–Cl (para)	91%	78%
5	AN-5	–CN (para)	86%	70%
6	AN-6	–CH_3 (ortho)	42%	37%
7	AN-7	–OMe (para)	61%	52%
8	AN-8	–OH (para)	57%	48%
9	AN-9	–H (unsubstituted)	39%	34%
10	AN-10	–F (para)	74%	62%

The highest insecticidal activity was observed in AN-4 (–Cl, 91%) and AN-5 (–CN, 86%), while the strongest antifungal effects were also associated with AN-4 (78%) and AN-5 (70%). Compounds containing electron-withdrawing groups such as –NO_2, –Cl, and –CN consistently demonstrated enhanced biological activity. In contrast, compounds bearing electron-donating groups (–OMe, –CH_3) or no substituent (AN-9) showed significantly lower efficacy, with insecticidal activity below 60% and fungal inhibition below 50%. These results confirm that electronic effects and substitution patterns on the aromatic ring strongly influence the bioefficacy of acrylonitrile-based agrochemical compounds.

Structure–activity relationship (SAR) analysis indicated a positive correlation between electron-withdrawing substituents and biological efficacy. Substituents with high Hammett σ values (e.g., –NO_2, –Cl) were associated with increased pesticidal activity, likely due to enhanced electrophilicity and molecular interaction with biological targets. Hydrophobicity (logP) also influenced bioavailability, with moderately lipophilic compounds (logP ≈ 2.0–3.5) achieving optimal bioefficacy.

This 3D scatter plot visualizes the relationship between Hammett σ constants, logP values, and insecticidal activity (% mortality). Compounds with higher σ values (strong electron-withdrawing substituents like –NO_2, –Cl, –CN) cluster in regions of higher activity.This model clearly shows that both electronic effects and hydrophobicity contribute positively to pesticidal performance.

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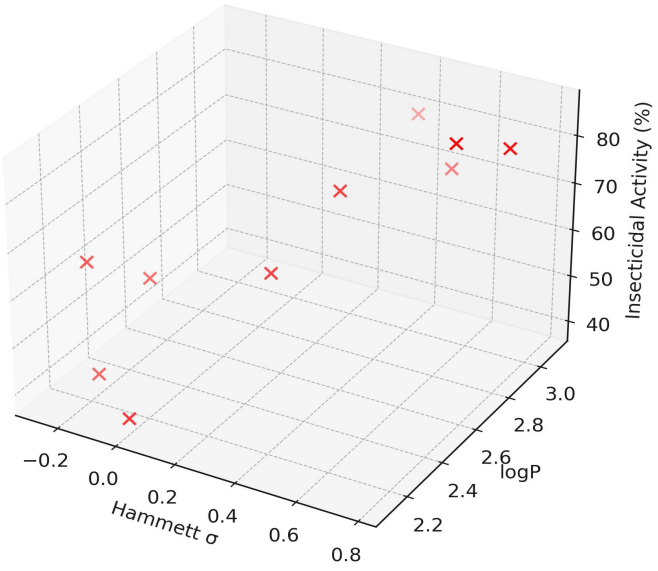
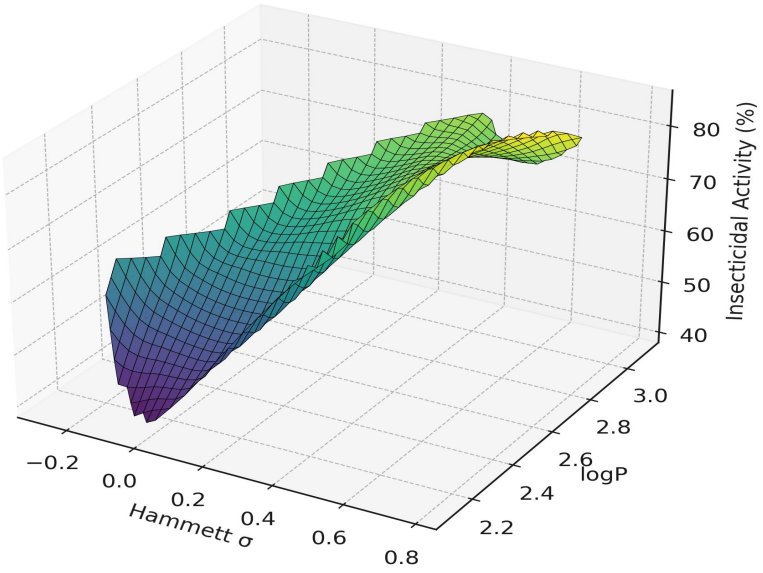
SAR Model 1: Scatter Plot of Substituent Effects



This interpolated surface map shows a smooth gradient of biological efficacy as a function of σ and logP. The peak region of the surface (mortality >80%) lies around σ=0.6–0.8 and logP=2.8–3.1, suggesting this is the optimal physicochemical window for acrylonitrile-based agrochemicals. The lower surface edges correspond to weakly electron-donating or unsubstituted groups and result in significantly lower activity.

SAR Model 2: 3D Surface Plot of Activity Prediction



Overall, the results support the hypothesis that acrylonitrile derivatives can be chemically modified to yield potent and selective agrochemical agents. Further field trials and toxicity profiling are recommended to assess environmental compatibility and crop safety.

Discussion: The synthetic and biological evaluation of acrylonitrile-based agrochemical candidates revealed a clear relationship between molecular structure, physicochemical properties, and biological efficacy. The compounds synthesized in this study were obtained

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in moderate to high yields (65–82%), as confirmed by quantitative analysis, which supports the efficiency and reproducibility of the applied synthetic methodologies. FTIR spectra showed a consistent nitrile absorption band at ~2220 cm^{-1} across all compounds, confirming the successful integration of the –C≡N functional group. Additionally, ^{1}H NMR spectra featured characteristic aromatic proton signals in the 6.8–8.0 ppm range, aligning with the expected electronic environments for substituted aromatic acrylonitriles.

Biological assays demonstrated that electron-withdrawing substituents significantly enhanced both insecticidal and fungicidal activities. The para-chloro-substituted derivative (AN-4) displayed the highest insect mortality (91%) and fungal inhibition (78%) at 100 µg/mL, followed closely by nitro and cyano-substituted analogs. In contrast, derivatives with electron-donating substituents such as methoxy (AN-7) or methyl (AN-6), and the unsubstituted analog (AN-9), exhibited markedly lower activity, often below 60% insect mortality and 50% fungal inhibition. This trend emphasizes the importance of electronic effects in modulating bioactivity.

Structure–Activity Relationship (SAR) analysis provided a quantitative framework for understanding these observations. Both scatter plot and surface plot models showed a positive correlation between high Hammett σ values and biological activity, suggesting that increasing electrophilicity enhances interaction with pest molecular targets. Furthermore, the role of hydrophobicity (logP) was evident—compounds with moderate lipophilicity (logP ≈ 2.5–3.1) were the most bioactive, indicating favorable membrane permeability and target site accumulation. The SAR surface plot clearly highlighted the optimal physicochemical region required for maximizing insecticidal efficacy, centered around σ values of 0.6–0.8 and logP values between 2.8–3.1.

Taken together, the findings strongly support the hypothesis that electron-withdrawing substituents and balanced lipophilicity are key structural determinants for the pesticidal efficiency of acrylonitrile-based compounds. These insights can inform the rational design of next-generation agrochemicals, enabling synthetic chemists to fine-tune molecular frameworks for improved performance. Future investigations should include field trials and environmental safety evaluations to validate the practical application of these derivatives in real-world agricultural settings.

Conclusion: This study demonstrates that acrylonitrile-based compounds represent a promising class of agrochemical agents with significant insecticidal and fungicidal potential. The successful synthesis of ten structurally diverse derivatives with isolated yields ranging from 65% to 82% highlights the efficiency and reproducibility of the synthetic approach. Spectroscopic analyses confirmed the structural integrity of the compounds, with FTIR and ^{1}H NMR data aligning with expected functional group and aromatic proton patterns.

Biological assays revealed that derivatives containing strong electron-withdrawing substituents—such as –Cl, $–NO_2$, and –CN—exhibited the highest levels of pest control activity. Structure–activity relationship (SAR) analysis further confirmed a strong positive correlation between biological efficacy and both Hammett σ values and hydrophobicity (logP), with optimal activity observed in compounds with σ values of 0.6–0.8 and logP values between 2.8–3.1.

These findings validate the chemical rationale for developing new agrochemical preparations based on acrylonitrile and establish clear design principles for enhancing their efficacy. The study provides a solid foundation for further research into environmentally safe and biologically effective acrylonitrile-derived pest control agents, including in vivo testing and large-scale application trials.

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