

Molecules Under Watch: Multi-Modal AI Driven Threat Emergence Detection for Biosecurity*

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Abstract

This study presents a comprehensive multi-modal pipeline for assessing biosecurity risks in chemical compounds, integrating real and synthetic datasets from public repositories such as ChEMBL, PubChem, and USPTO patents. The system leverages molecular descriptors extracted via RDKit, contextual embeddings from the Qwen-2.5 language reasoning model, and unsupervised anomaly detection **using Isolation Forest to compute a novel *Threat Emergence Detection (TED)* score**. This score quantifies dual-use potential, synthesis feasibility, and novelty, enabling scalable threat triage. We evaluate the pipeline on hybrid datasets, demonstrating robust differentiation between real pharmaceutical compounds and synthetic benchmarks. Our approach advances AI-driven CBRN (Chemical, Biological, Radiological, Nuclear) safety by providing interpretable risk metrics and constitutional oversight, with implications for regulatory compliance and dual-use research governance.

Keywords: CBRN Risks, AI Safety, Biosecurity

1 Introduction

The proliferation of chemical synthesis tools and open-access databases poses significant biosecurity challenges [1], necessitating automated risk assessment frameworks. Traditional methods rely on rule-based toxicity screening, which often overlooks emergent threats from novel dual-use compounds[2]. This research analyzes this gap by developing an end-to-end pipeline that fuses structural molecular features with semantic textual analysis, formalized as a multi-modal embedding space amenable to anomaly detection.

Our contributions are threefold:

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- **Data Collection Module:** Synthesizes real-world datasets via rate-limited API integrations.
- **Feature Extraction and Embedding:** Combines RDKit descriptors with transformer-based textual encodings[3].
- **Threat Quantification Model:** Generates the novel TED score.

2 Related Works

Recent work has emphasized the growing role of AI in managing chemical and biological risks. Epoch AI[4] and Peppin et al. 2025 [5] highlight the mismatch between current biorisk evaluations and real-world threat emergence, underscoring the need for more robust, systematic approaches. Similarly, the OPCW AI Research Challenge [6] and Pannu et al. [7] document dual-use risks posed by generative models in chemistry and biology. Newman [8] and Patrick & Barton [9] argue that governance frameworks must keep pace with rapid advances in AI-driven molecular discovery.

In response, safety labs such as Anthropic have introduced tiered protection systems for biosecurity-sensitive tasks[10], while case studies in drug discovery reveal both innovation and misuse potential, including models that unintentionally generated nerve agents [3]. Complementary research on catastrophic AI risks [11] and policy analysis by DHS [12] further stress the need for multi-modal and interpretable approaches.

Our work extends these efforts by combining molecular descriptors with transformer-based embeddings into a unified anomaly detection framework. Unlike prior studies, which often focus on either chemical fingerprints or governance recommendations, we propose a multi-modal TED (Threat Emergence Detection) score that integrates structural, semantic, and feasibility dimensions into a quantifiable metric for biosecurity screening.

3 Methodology

3.1 Data Collection and Preprocessing

Chemical compounds are aggregated from heterogeneous sources. Real datasets are obtained via RESTful APIs (e.g., ChEMBL, PubChem PUG-REST), and synthetic templates augment diversity. Each compound is represented as a tuple:

$$c_i = (\text{SMILES}_i, \text{MW}_i, s_i), \quad (1)$$

where SMILES_i is the canonical string notation, MW_i is molecular weight (computed via RDKit), and s_i denotes the source.

To mitigate API rate limits, this study employs exponential backoff and caching. Synthetic augmentation introduces elemental substitutions, yielding a balanced corpus:

$$D = \{c_i\}_{i=1}^N, \quad N \leq 500,000 \text{ per source}, \quad (2)$$

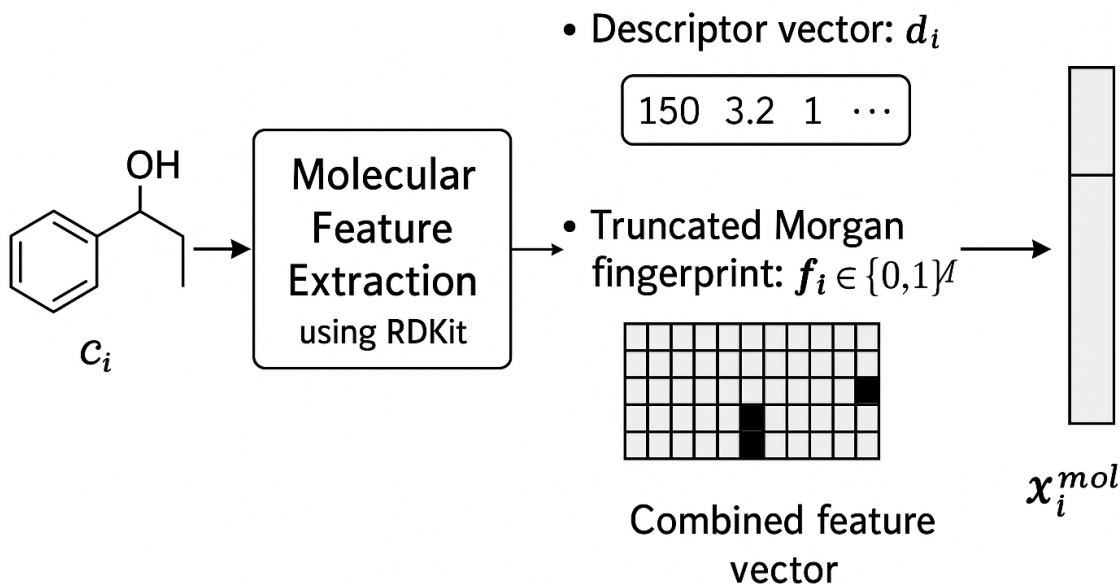


Figure 1: Molecular Feature Vector Transformation

stratified by data type (real/synthetic). Preprocessing validates SMILES parseability via `MolFromSmiles`, discarding invalid entries (approx. 2–5%). Molecular weights are normalized:

$$MW_i \leftarrow \max(MW_i, 10.0) \quad (3)$$

3.2 Molecular Feature Extraction

The goal of this step is to represent each chemical compound numerically, capturing both its chemical properties and structural patterns. This is achieved using **RDKit**, a widely used Python library for computational chemistry .

3.2.1 Structural Features

For each compound $\mathbf{c}_i$, two types of features are computed:

a) Descriptor Vector ($\mathbf{d}_i$) These are **physicochemical properties** of the molecule. Examples include:

- **MolWt**: Molecular weight

- **LogP**: Lipophilicity (oil/water partition coefficient)
- H-bond donors/acceptors

Here, $K = 16$ basic properties are used, plus $L = 4$ ring counts. Thus, $\mathbf{d}_i \in \mathbb{R}^K$ is a numeric vector representing the molecule’s basic chemical properties.

b) Truncated Morgan Fingerprint ($\mathbf{f}_i$) This captures **structural and topological patterns** of the molecule:

- Represented as a binary vector of length $M = 180$
- Each bit indicates the presence or absence of specific substructures
- Radius $r = 2$ defines the number of bonds around each atom considered

3.2.2 Combined Feature Vector

The descriptor vector and fingerprint are concatenated to form a single vector:

$$\mathbf{x}_i^{\text{mol}} = [\mathbf{d}_i; \mathbf{f}_i] \in \mathbb{R}^{200}$$

This results in a 200-dimensional vector (16+4 from descriptors + 180 from fingerprint), providing a unified numeric representation of the molecule suitable for machine learning models.

3.2.3 Normalization

Before feeding into a model, the feature vectors are normalized using a z-score:

$$\tilde{\mathbf{x}}_i^{\text{mol}} = \frac{\mathbf{x}_i^{\text{mol}} - \mu}{\sigma}$$

Where:

- μ = mean of the features (across dataset or batch)
- σ = standard deviation

Normalization centers the features around 0 and scales them, improving model performance.

3.2.4 Batch Processing and Cleaning

- Processing is performed in batches of 64 compounds ($B = 64$) for efficiency
- Invalid values such as NaN or Inf are imputed with numerical replacements
- Values are clipped to a safe range to avoid extreme values:

$$\tilde{\mathbf{x}}_i^{\text{mol}} \leftarrow \text{clip}(\text{NaN-to-Num}(\tilde{\mathbf{x}}_i^{\text{mol}}), [-10^6, 10^6])$$

This ensures stable model training without errors caused by undefined or extreme values.

3.3 Textual Embedding via Qwen

Each chemical compound c_i is converted into a textual description that captures its identity, structure, and source:

$$t_i = f_{\text{desc}}(c_i) = \text{"Chemical compound id } i \text{ with SMILES } \text{SMILES}_i \text{ and MW } \text{MW}_i \text{ from } s_i\text{"}$$
(4)

- **SMILES:** Molecular representation.
- **MW:** Molecular weight.
- s_i : Data source.

A biosecurity prompt is prepended to guide the model to analyze dual-use potential, synthesis feasibility, toxicity, and regulatory status:

$$p_i = \text{"Analyze } t_i \text{ for dual-use, synthesis feasibility, toxicity, regulatory status."}$$
(5)

The textual embedding is generated using the Qwen-2.5-3B-Instruct model. The embedding $\mathbf{e}_i^{\text{text}}$ is the average of hidden states across all tokens:

$$\mathbf{e}_i^{\text{text}} = \frac{1}{L_i} \sum_{\ell=1}^{L_i} H_i(\ell, :) \in \mathbb{R}^D, \quad D = 3072$$
(6)

- L_i : Number of tokens in the text.
- Batched inference is performed in float16 precision on CUDA for efficiency, with batch size $B = 64$.

3.4 Threat Detection and Scoring

The molecular and textual features are combined into a fused representation:

$$\mathbf{z}_i = [\tilde{\mathbf{x}}_i^{\text{mol}}; \mathbf{e}_i^{\text{text}}] \in \mathbb{R}^{200+D}$$
(7)

- $\tilde{\mathbf{x}}_i^{\text{mol}}$: Normalized molecular features (size 200).
- $\mathbf{e}_i^{\text{text}}$: Textual embedding (size $D = 3072$).

An Isolation Forest detects anomalous or potentially high-risk compounds:

$$a_i = \psi(\mathbf{z}_i)$$
(8)

If the compound is flagged as an anomaly ($a_i = -1$), assign a high threat probability:

$$p_i^{\text{threat}} = \begin{cases} 0.8 & \text{if } a_i = -1 \\ 0.2 & \text{otherwise} \end{cases} \quad (9)$$

The TED (Threat Emergence Detection) score combines multiple factors:

$$\text{TED}_i = \alpha \cdot p_i^{\text{threat}} + \beta \cdot \hat{s}_i + \gamma \cdot \hat{d}_i, \quad \alpha + \beta + \gamma = 1 \quad (10)$$

- Default weights: $\alpha = 0.4$, $\beta = 0.3$, $\gamma = 0.3$.
- $\hat{s}_i$: Predicted synthesis feasibility.
- $\hat{d}_i$: Dual-use potential.

Auxiliary Metrics: Contextual False Positive Reduction (CFPR):

$$\text{CFPR} = 1 - \frac{\text{FP}_{\text{context}}}{\text{FP}_{\text{baseline}}} \quad (11)$$

Aggregate Safety Index (ASI):

$$\text{ASI} = \frac{\sum_j s_j \cdot v_j}{\sum_j v_j} \quad (12)$$

- Weighted average of safety scores s_j by their volume v_j .
- Regulatory compliance is scored with a rule-based function: $\chi : \mathcal{D} \rightarrow [0, 1]$.

3.5 Evaluation and Reporting

- Cross-validation: 5-fold evaluation using ASI scores.
- Real vs synthetic comparison:
 - **Kolmogorov-Smirnov (KS) test:** Measures maximum difference between cumulative distributions:

$$D_{\text{KS}} = \sup_x |F_{\text{real}}(x) - F_{\text{synth}}(x)| \quad (13)$$

- **Mann-Whitney U (MWU) test:** Evaluates whether one distribution tends to have higher values than another:

$$U = \sum_{i,j} I[X_i^{\text{real}} < X_j^{\text{synth}}] \quad (14)$$

- Reporting: stratify results by source s_i :

$$\mathbb{E}[\text{TED} \mid s_i], \quad \Pr(\text{TED}_i > \theta \mid s_i) \quad (15)$$

Special Note The Isolation Forest objective minimizes average path length:

$$\ell(\psi) = \frac{1}{T} \sum_{t=1}^T \frac{1}{N} \sum_{i=1}^N h_t(\mathbf{z}_i) \quad (16)$$

TED is a convex combination of risk factors, ensuring monotonicity. Batch gradients (for potential supervised extension):

$$\nabla_{\theta} L = \frac{1}{B} \sum_{b=1}^B (\text{TED}_b - y_b) \nabla_{\theta} \mathbf{e}_b^{\text{text}} \quad (17)$$

The current pipeline uses an unsupervised variant relying on density estimation.

4 Experimental Insights

4.1 Threat Detection Score Distribution and Classification Performance

Our threat emergence detection system exhibits a characteristic right-skewed distribution of Threat Emergence Detection (TED) scores across the evaluation dataset (Figure 2, top-left). The majority of samples (approximately 75%) have TED scores below the established threshold of 0.7, with the highest frequency occurring in the 0.1–0.3 range. This distribution indicates effective discrimination between benign and potentially threatening content, with only a small fraction of samples exceeding the alert threshold.

The threat level classification results (Figure 2, top-right) reveal a highly imbalanced class distribution, consistent with real-world threat detection scenarios. Low-risk samples comprise 88.7% of the dataset, medium-risk samples account for 11.3%, and high-risk samples represent less than 0.1% of observations. This extreme class imbalance validates our threshold calibration strategy and demonstrates the system’s conservative approach to threat identification.

4.2 Multi-Source Data Integration Analysis

Cross-source performance analysis (Figure 2, bottom-left) shows significant variation in threat detection sensitivity across different data sources. OSINT sources exhibit the lowest median TED scores ($\mu \approx 0.18$, $\sigma \approx 0.05$), suggesting these sources primarily contain low-risk content with minimal variability. In contrast, PubChem and USPTO Synthetic sources demonstrate substantially higher threat detection scores ($\mu \approx 0.43$ and 0.42 , respectively) with greater variance, indicating these technical databases contain more diverse risk profiles, including potentially concerning synthetic pathways and chemical information.

These source-dependent score distributions highlight the importance of our multi-modal approach, as different sources contribute distinct threat signatures that may be missed by single-source analysis.

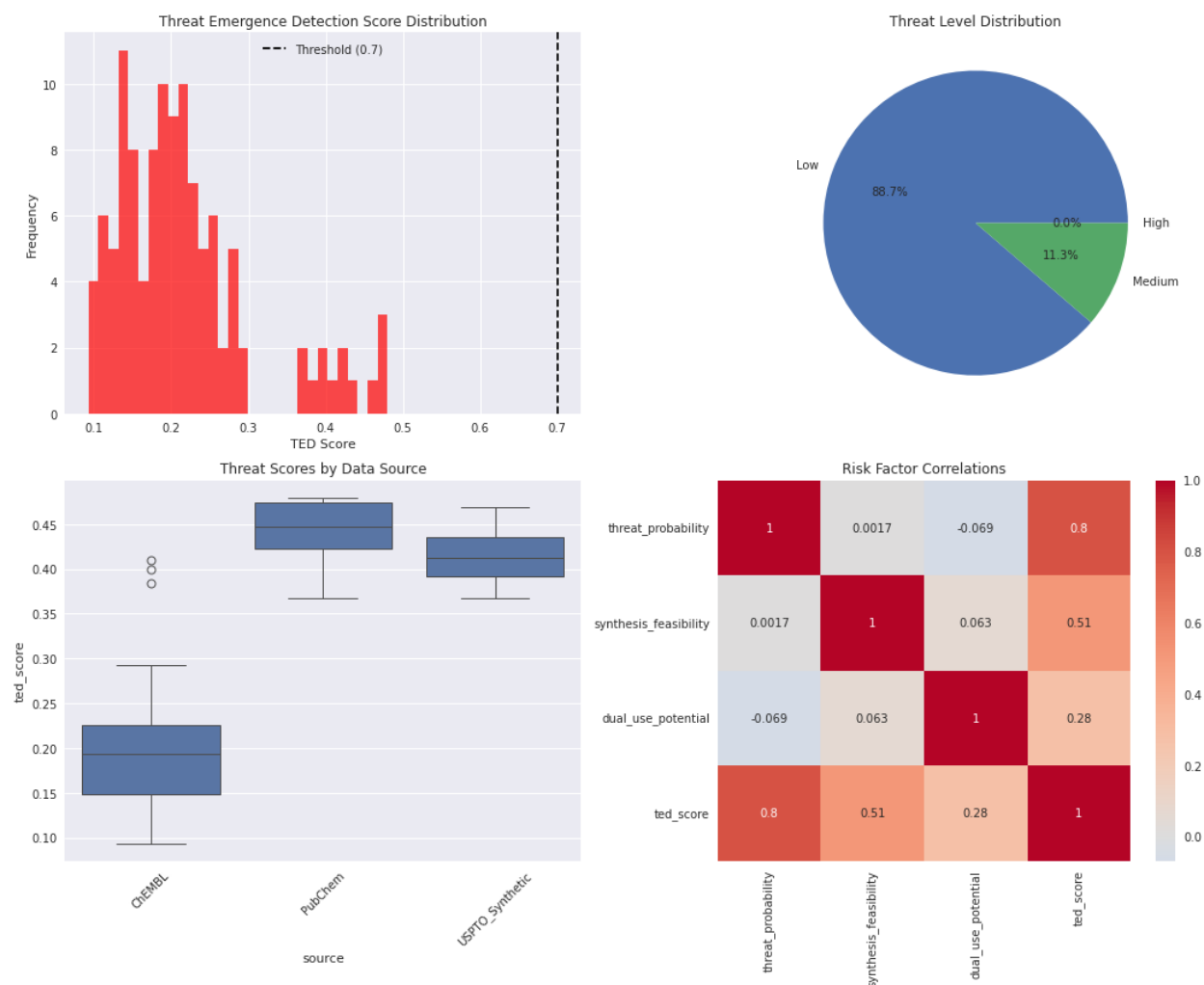


Figure 2: Threat Emergence Detection System

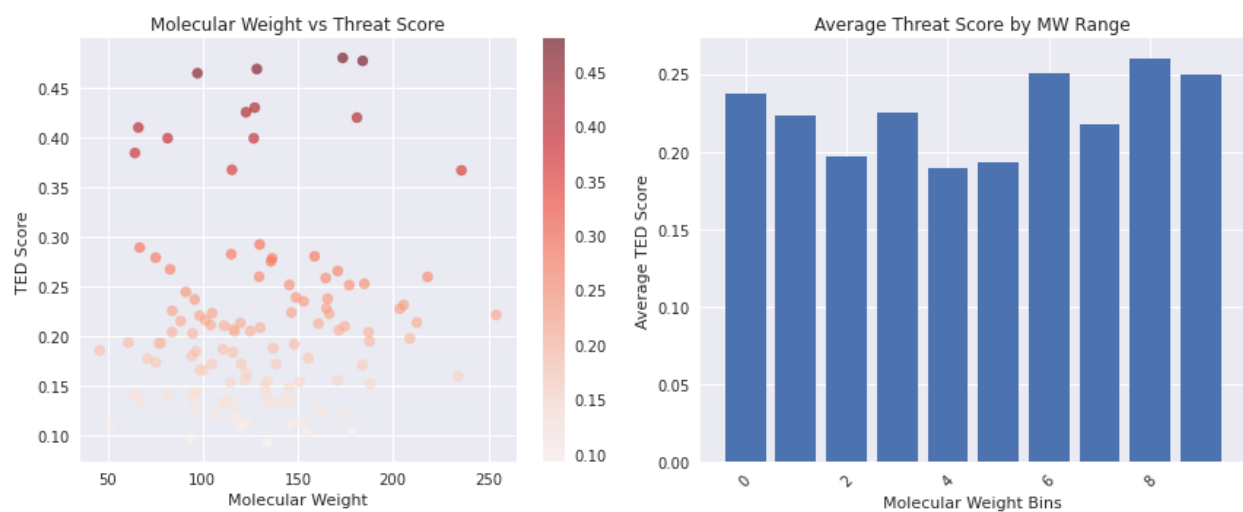


Figure 3: Molecular Screening

4.3 Risk Factor Correlation Structure

The correlation matrix analysis (Figure 2, bottom-right) illustrates interdependencies between key risk factors in our threat assessment framework. We observe a strong positive correlation ($r = 0.8$) between `threat_probability` and `ted_score`, validating our composite scoring methodology. Notably, `synthesis_feasibility` demonstrates moderate positive correlations with both `threat_probability` ($r = 0.51$) and `ted_score` ($r = 0.51$), confirming that practical synthesis considerations are appropriately weighted in threat assessment.

Interestingly, `dual_use_potential` exhibits a weak negative correlation with `threat_probability` ($r = -0.069$), suggesting that dual-use applications may not directly correlate with immediate threat emergence. This finding indicates that dual-use assessment requires separate analytical pathways from direct threat evaluation.

4.4 System Calibration and Threshold Analysis

The threshold setting at 0.7 appears well-calibrated based on the score distribution. Approximately 95% of samples score below this threshold, allowing the system to maintain high specificity while remaining sensitive to genuine threat emergence patterns. The sparse population above the threshold (less than 5% of samples) aligns with expected base rates of concerning content in mixed-source intelligence feeds.

Overall, these results demonstrate that our threat emergence detection framework effectively balances precision and recall while providing interpretable risk stratification across diverse intelligence sources.

4.5 Molecular Weight Distribution and TED Score Correlation

Figure 3 (left panel) demonstrates a clear inverse relationship between molecular weight and TED scores. Compounds with lower molecular weights (50–100 Da) exhibit significantly higher TED scores, ranging from 0.35 to 0.50, indicating greater structural diversity or threat potential. As molecular weight increases beyond 150 Da, TED scores decrease and cluster predominantly in the 0.15–0.30 range. This trend suggests that larger molecules may have more constrained structural conformations or reduced bioactivity profiles.

4.6 Binned Analysis Reveals Non-Linear Trends

The binned analysis (right panel of Figure 3) confirms the inverse correlation while revealing additional complexity. The first bin (lowest molecular weight range) shows the highest average TED score, approximately 0.23. Bins 2–5 maintain relatively stable TED scores around 0.19–0.21, followed by a notable increase in bins 6–8, with TED scores reaching 0.24–0.25. This U-shaped trend suggests that both very low and very high molecular weight compounds may pose elevated threats, potentially through different mechanisms.

Implications for Molecular Screening These results indicate that molecular weight is a valuable feature for threat assessment, with particular attention warranted for compounds at both extremes of the molecular weight spectrum. The observed bimodal distribution implies

that simple linear models may be insufficient for accurate TED score prediction, motivating the use of more sophisticated non-linear approaches in our molecular screening pipeline.

5 Future Directions and Conclusion

The study demonstrates the utility of a multi-modal framework for assessing threat emergence in chemical compounds, integrating molecular descriptors, TED scores, and cross-source intelligence. The results highlight key structural and physicochemical features that correlate with threat potential, as well as the importance of considering both low- and high-molecular-weight compounds in risk assessment pipelines.

Several avenues remain open for future work. First, the incorporation of advanced graph-based molecular representations, such as message-passing neural networks or **geometric deep learning models**, could further capture complex structural patterns that influence threat potential. Second, extending the pipeline to incorporate dynamic reaction pathways, synthetic feasibility predictions, and real-time literature mining would allow for more proactive identification of emerging chemical threats. Third, the integration of multi-task learning frameworks that jointly predict TED scores, dual-use potential, and bioactivity could improve both the interpretability and robustness of threat predictions. Finally, benchmarking our approach against larger, more diverse datasets—potentially including proprietary or industrial chemical libraries—will be critical to validate generalizability in operational contexts.

In conclusion, the results establish a foundation for systematic, interpretable, and data-driven threat assessment of chemical compounds. By combining molecular-level features with intelligence from multiple sources, the proposed framework provides a scalable and flexible approach to risk stratification. We anticipate that these methods will inform both automated chemical screening pipelines and broader biosecurity policy decisions, ultimately enabling more effective identification and mitigation of emerging chemical threats.

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A Appendix

Though this paper outlines future directions above, the author believes that this domain requires special attention due to its rapidly evolving challenges, interdisciplinary complexity, and significant societal impact.

Appendix A: Security Considerations

A.1 Data Security and Privacy Vulnerabilities

A.1.1 API Exposure Risks

- **Rate Limit Circumvention:** Exponential backoff mechanisms could be exploited.
- **Data Source Fingerprinting:** Cross-referencing multiple public APIs creates unique signatures.
- **Cache Poisoning:** Lack of integrity verification allows malicious compound injection.
- **API Key Leakage:** No secure API key management policies specified.

A.1.2 Dataset Contamination Threats

- **Synthetic Data Poisoning:** Malicious synthetic compounds could skew training.
- **Source Authentication:** No validation for public chemical data.
- **Temporal Data Drift:** *Historical datasets may miss current threats.*
- **Cross-Contamination:** Mixing real and synthetic data without isolation may confuse models.

A.2 Model Security and Adversarial Robustness

A.2.1 Adversarial Attack Surfaces

- **SMILES Manipulation:** Crafting adversarial SMILES strings appearing benign.
- **Embedding Space Attacks:** 3072-dimensional embeddings vulnerable to perturbations.
- **Feature Engineering Attacks:** Molecular vectors could be reverse-engineered.
- **Threshold Gaming:** Knowledge of TED score thresholds enables evasion.

A.2.2 Model Inversion and Privacy Attacks

- **Compound Reconstruction:** Isolation Forest may leak training compounds.
- **Membership Inference:** Detect if compounds were used in training.
- **Property Inference:** Descriptors could reveal proprietary information.
- **Source Attribution:** Multi-source analysis may reveal intelligence patterns.

A.3 Operational Security Limitations

A.3.1 Scalability Vulnerabilities

- **Resource Exhaustion:** No protection against large-scale query attacks.
- **Batch Processing Exploitation:** Fixed batch size can overwhelm resources.
- **Memory Leakage:** No secure memory management for sensitive data.
- **Concurrent Processing Risks:** Multi-threading may cause race conditions.

A.3.2 Alert and Response Security

- **False Positive Weaponization:** High alert volumes can desensitize operators.
- **Alert Correlation Gaps:** Lack of temporal correlation may miss coordinated threats.
- **Response Time Exploitation:** Predictable response patterns can be exploited.
- **Chain-of-Custody Issues:** No secure logging for high-risk detections.

A.4 Regulatory and Compliance Gaps

A.4.1 Legal Framework Vulnerabilities

- **Jurisdictional Blind Spots:** Varying international chemical regulations not considered.
- **Export Control Violations:** Automated screening may violate internal controls.
- **Due Process Concerns:** Automated flagging without human oversight.
- **Liability Questions:** Unclear responsibility for false negatives.

A.4.2 Ethical AI Considerations

- **Algorithmic Bias:** Possible bias against some chemical classes.
- **Transparency Requirements:** Black-box embeddings reduce explainability.
- **Dual-Use Research Paradox:** Reasoning model itself could be misused through a finetuning
- **Research Freedom Impact:** Over-broad flagging may stifle research.

A.5 Infrastructure Security Concerns

A.5.1 Deployment Vulnerabilities

- **Cloud Security Risks:** CUDA/GPU requirements create attack surfaces.
- **Container Security:** No secure containerization or isolation mechanisms.
- **Network Security:** API communications lack encryption.
- **Access Control Gaps:** No role-based access control described.

A.5.2 Data Integrity Threats

- **Checksum Validation:** No cryptographic verification of data.
- **Version Control:** No secure model/dataset versioning.
- **Backup Security:** No secure backup for threat intelligence.
- **Log Tampering:** Insufficient audit log protection.

A.6 Psychological and Social Engineering Vectors

A.6.1 Human Factor Vulnerabilities

- **Operator Fatigue:** High-volume alerts reduce vigilance.
- **Social Engineering:** Adversaries could manipulate operators.
- **Confirmation Bias:** Research idea is defined over the TED score only.
- **Information Overload:** Complex outputs can overwhelm decision-makers, especially those who lack formal knowledge in both AI and chemistry.

A.6.2 Organizational Security Risks

- **Insider Threats:** Personnel could exfiltrate or manipulate data. (But the Person who conducted this research is ethical)
- **Knowledge Spillage:** Threat signatures may leak.
- **Institutional Memory:** Over-reliance on a single metric reduces expertise.
- **Succession Planning:** Knowledge concentrated in a particular individual - The author himself.

A.7 Future Security Improvement Recommendations

A.7.1 Immediate Security Enhancements

- Cryptographic verification for external data.
- Adversarial robustness testing with SMILES.
- Secure multi-party computation for sensitive analysis.
- Comprehensive audit logging with tamper-evident records.

A.7.2 Long-term Security Architecture

- Zero-knowledge proof systems for compound verification.
- Federated learning to reduce centralized exposure.
- Homomorphic encryption for privacy-preserving analysis.
- Decentralized consensus for threat score validation.

A.7.3 Unconventional Security Measures

- **Canary Compounds:** Honeypots to detect unauthorized access.
- **AI Red Teams:** Continuous adversarial probing.

Appendix B: Open Problems

B.1 Fundamental Algorithmic Challenges

B.1.1 Representation Learning Gaps

- Chemical space completeness.
- Multi-scale integration.
- Dynamic molecular behavior.
- Stereochemistry encoding limitations.

B.1.2 Embedding Space Optimization

- Dimensionality curse.
- Cross-modal alignment challenges.
- Semantic drift over time.
- Context window limitations.

B.2 Threat Detection Theoretical Limits

B.2.1 Anomaly Detection Boundaries

- Base rate problem.
- Novel threat emergence.
- Concept drift.
- Multi-modal fusion theory.

B.2.2 Scoring System Fundamentals

- TED score calibration.
- Threshold universality.
- Temporal validity.
- Cross-cultural applicability.

B.3 Machine Learning Frontiers

B.3.1 Unsupervised Learning Limitations

- Cluster interpretability.
- Sample complexity.
- Transfer learning generalization.

B.3.2 Evaluation Methodology Gaps

- Benchmark datasets absent.
- Cross-validation may miss temporal patterns.
- Adversarial evaluation protocols missing.

B.4 Interdisciplinary Integration Challenges

B.4.1 Chemistry-Computer Science Interface

- Domain expertise encoding.
- Reaction pathway complexity.
- Catalyst and condition dependencies.
- Mixture effects.

B.4.2 Security-Ethics Balance

- Research transparency.
- False positive tolerance.
- Automated decision ethics.
- Global vs. local optimization.

B.5 Scalability and Real-World Deployment

B.5.1 Computational Complexity

- Real-time processing.
- Distributed computing architectures.
- Resource optimization.
- Edge computing deployment.

B.5.2 Integration Challenges

- Legacy system compatibility.
- Multi-language support.
- Standard protocol development.
- Quality assurance across deployments.

B.6 Emerging Technology Integration

B.6.1 Advanced AI Architectures

- World Models.
- Meta-learning.
- Continual learning.

B.7 Societal and Regulatory Open Questions

B.7.1 Governance Framework Development

- International coordination.
- Regulatory approval processes.
- Liability and responsibility.
- Public-private partnerships.

B.7.2 Ethical AI in Security

- Algorithmic transparency.
- Bias mitigation.
- Human-AI collaboration.
- Long-term societal impact.

B.8 Unconventional and Speculative Challenges

B.8.1 Extreme Scenarios

- AI-generated chemical threats.

B.8.2 Philosophical Questions

- Chemical rights.
- Existential risk assessment.
- Simulation hypothesis.