Nanoparticle Toxicity Classification Model Card

Transparent AI Documentation

Model Card: Nanoparticle Toxicity Classifier

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Version: 1.0

Model Type: Stacked Ensemble (LightGBM + Random Forest)

1. Model Details

This is a machine learning model for classifying nanoparticle toxicity into four categories based on physicochemical properties and biological response metrics. The model employs a stacked ensemble approach combining LightGBM and Random Forest classifiers for robust performance across imbalanced toxicity classes.

ARCHITECTURE:

- Base Models: LightGBM and Random Forest
- Meta-Learner: Logistic Regression
- Training Data: 90 nanoparticle samples
- Features: 20+ physicochemical and biological variables

2. Intended Use

PRIMARY USE CASES:

- Early-stage nanoparticle toxicity screening
- Research and development of safer nanomaterials
- Prioritization of nanoparticles for further testing
- Educational purposes in nanotoxicology

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INTENDED USERS:

- Materials scientists and nanotechnologists
- Toxicology researchers
- Regulatory science professionals
- Academic researchers

OUT-OF-SCOPE USES:

- Clinical decision making for human health
- Regulatory approval without experimental validation
- High-stakes safety assessments
- Replacement for in-vivo testing

3. Performance Metrics

Model performance evaluated on held-out test set:

Metric	Class 0	Class 1	Class 2	
F1-Score	0.903	0.727	0.857	
Precision	0.875	0.800	0.857	
Recall	0.933	0.667	0.857	
Support	15	3	7	

4. Factors and Limitations

KEY FACTORS INFLUENCING PREDICTIONS:

- Cell viability and membrane damage metrics
- Nanoparticle size and surface properties
- Exposure dosage and duration

- Oxidative stress indicators

KNOWN LIMITATIONS:

- Limited dataset size (n=90 samples)
- Class imbalance in toxicity labels
- Trained on in-vitro data only
- Limited representation of novel nanoparticle types

DATA DEPENDENCIES:

- Requires complete physicochemical characterization
- Dependent on standardized biological assays
- Assumes consistent experimental protocols

5. Ethical Considerations

TRANSPARENCY: This model card provides full disclosure of model capabilities and limitations.

SAFETY: Predictions should be verified with experimental testing before safety decisions.

BIAS MITIGATION: Model uses balanced accuracy metrics and class weights to address imbalance.

ACCOUNTABILITY: Users are responsible for appropriate application and validation of predictions.

ENVIRONMENTAL IMPACT: Supports development of safer nanomaterials, reducing environmental risks.