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**Home**

SMAG – Smart Molecules AI-driven Generation.

A patented algorithm with an integrated service portfolio.

Topia AI Validated Models

1. Data Generation
2. QSAR
3. Toxicity
4. Retrosynthesis
5. Drug Repurpose

By leveraging AI, we can accelerate the drug discovery process by swiftly analysing vast datasets, enabling us to identify potential candidates more rapidly than ever.

**Benefit:**

* Enhanced Efficiency
* Increased Accuracy
* Cost-Effective Solutions
* Flexibility and Adaptability
* Predictive Modelling

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**Data Generation:**

The purpose of the Molecule Generation model is to revolutionize the process of molecular design and discovery using advanced deep learning techniques.

The creation of entirely new small molecules for various applications, including drug discovery and materials science. By leveraging, the latest in generative modelling, Topia’s model aims to streamline and accelerate the exploration of chemical space, ultimately leading to the identification of novel compounds with desirable properties. Its applications range from optimizing drug candidates to designing materials with specific characteristics, making it a versatile tool with far-reaching implications across multiple industries.

Key considerations:

Data cleaning and Filtering

Data Standardization and Normalization

Data Fragmentation

Data Encoding

**Topia Life Sciences- Molecule Generation Model:**

* Utilizes Graph Transformer for molecule generation.
* Achieves 100% validity in generated molecules, compared to 87-92% by State-of-the-Art (SOTA) models.
* Achieves 98% uniqueness, 99% accuracy, and 97% novelty in generated molecules, outperforming SOTA models in all these metrics.
* Incorporates parallel processing for enhanced performance.

**QSAR:**

Topia’s Quantitative Structure-Activity Relationship (QSAR) model stands as a pillar of innovation.

Offering a meticulous understanding of how molecular features correlate with biological activity. Our computational tools harness the power of advanced algorithms to decode the intricate relationship between chemical structure and functional behaviour.

Key considerations:

1. Molecular Descriptors
2. Model Building
3. Validation: Calculation of Molecular Fingerprints, Fingerprint Filtering, Data Splitting, Machine Learning Regression, Model Evaluation

**Topia Life Sciences- QSAR Model**

* Predictive Performance
* Flexibility and Customization
* Scalability and Efficiency
* Interpretability and Transparency

**Toxicity:**

Plays a crucial role in ensuring the safety and efficacy of various chemicals and compounds across industries.

Our Toxicity prediction model is a multifaceted endeavour, encompassing various domains such as mutagenicity, carcinogenicity, nephrotoxicity, cardiotoxicity, and hepatotoxicity.

Key considerations:

1. Data Collection and Preprocessing
2. Model Architecture Selection
3. Training and Validation
4. Computational Efficiency and Scalability
5. External Validation and Benchmarking

**Topia Life Sciences- Toxicity Model**

* Our toxicity prediction models consistently outperform existing models.
* Consistently achieve higher true positive and negative rates while minimizing false positives and negatives.
* The ROC curve (AUC) for our in-house models is consistently higher than existing models.
* Our toxicity prediction models cover a range of toxicological endpoints, including mutagenicity, carcinogenicity, nephrotoxicity, cardiotoxicity, and hepatotoxicity.

**Retrosynthesis:** Predicts the synthetic pathway of small organic molecules, empowering chemists to devise efficient synthesis strategies.

The retrosynthesis model developed by Topia Life Sciences incorporates unique methodologies rooted in AI and Chemical Informatics principles.

The model employs a combination of two models wherein the first model is based on Multi-Layer Perceptron that predicts the single step reactions and the second model is based on A\* search algorithm wherein this is used to find the shortest distance between two nodes of a graph.

Key considerations:

* Data Cleaning and Standardization
* Reaction Centre Identification
* Validation and Quality Control

**Topia Life Sciences- Retrosynthesis Model**

* Both run in parallel to search for the commercial availability of the reagents required.
* Predict higher Accuracy for Drug Structures
* Predict higher Accuracy for Modified Structures
* Route Similarity with State-of-the-Art Models
* Feasibility of Predicted Routes

**Drug Repurpose:** Expedite the drug discovery process by repurposing existing drugs for new therapeutic uses.

Our AI model encompasses the development and validation of a Drug Repurposing pipeline, integrating Knowledge Graph embeddings with Machine Learning algorithms.

Key considerations:

1. Knowledge Graph Embeddings (KGE)
2. Machine Learning (ML) Algorithms
3. Novel Approaches and Advancements
4. Data Preprocessing Techniques

**Topia Life Sciences- Repurpose Model**

* Our AI model utilizes a comprehensive biomedical knowledge graph with diverse entities (drugs, diseases, proteins, genes, etc.) and relations, providing a rich source of information, in the form of a fact-based graph which can be used as a reference in drug repurposing.
* Our model can learn complex patterns and relationships, enabling accurate prediction of novel drug-disease associations.
* Overcome some of the issues of Knowledge graphs and Graphs such as sparse and dense subgraphs
* Proprietary Datasets
* With a proven track record of successful projects.

About us:

We are redefining the future of drug discovery with our AI-driven molecular generation technology. Our mission is to empower researchers and pharmaceutical innovators with precise, efficient, and scalable tools to accelerate the identification of novel compounds and therapeutic solutions. By combining patented algorithms with advanced artificial intelligence, we unlock unprecedented opportunities for breakthroughs in drug design and development.

At SMAG, we offer state-of-the-art models, including **Data Generation**, **QSAR**, **Toxicity Prediction**, **Retrosynthesis**, and **Drug Repurposing**, designed to revolutionize molecular research across diverse industries.

**Topia Life Sciences** developed a world-class AI platform that delivers unmatched accuracy and efficiency in molecule generation. From utilizing **Graph Transformers** for designing molecules with superior novelty and uniqueness to deploying cutting-edge predictive models for toxicity and retrosynthesis, our technology consistently outperforms the competition. Through proprietary datasets and advanced processing, SMAG ensures results that lead to impactful discoveries.

*"Through the advancement of our platforms, we will build a fully integrated data economy. At Topia Life Sciences, we are passionate about improving health outcomes for people around the world." -****Kamlesh Patel, Founder***

**Contact**

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First name

UK address

Email Address

Last name

Company

Role

Phone

Email

Message

**Site References:**

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