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# Moremi AI: Towards Artificial General Intelligence for Health (AGI4Health) and Artificial General Intelligence for Biology (AGI4Bio)

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## Abstract

We present Moremi AI and Moremi Bio, multimodal large language models developed for comprehensive healthcare and biological applications towards Artificial General Intelligence for Health & Biology and Health-first AGI. Moremi AI demonstrates capabilities across a wide spectrum of medical tasks, including screening, diagnosis, risk prediction, treatment planning, and prognosis. Through extensive evaluation, the model shows particular strength in breast cancer detection, Parkinson's diagnosis, and thyroid cancer prognosis, while maintaining competency across general medical knowledge assessment. Moremi Bio extends these capabilities to biological applications, exhibiting proficiency in toxicology assessment, protein-ligand interaction prediction, molecule generation, and clinical trial outcome prediction. The model demonstrates particular strength in drug development tasks, including the generation of novel antibodies and prediction of drug properties. Our evaluation across multiple benchmarks identifies both the models' strengths and current limitations. We also implement comprehensive safety measures to ensure responsible deployment in healthcare settings. These models represent a significant step toward developing specialized AI systems for healthcare and biological research while maintaining necessary safety standards.

## 1 Introduction

With the advent of large language models (LLMs) like GPT4, Gemini, Claude and LLaMA,([1],[2],[3],[4]) one area of discussion has been if it could be possible to develop a large language model that has broad and in-depth knowledge in healthcare. While there have been several research efforts in this direction([5],[6],[7],[8]), none has gained sufficient maturity to be turned into a product.

To address this gap, we are releasing Moremi AI and Moremi Bio, production-ready multimodal large language models specifically developed for healthcare and biology applications with safety guardrails in place. These models represent a significant step towards building Artificial General Intelligence for Health & Biology (AGI4Health) and Health-first AGI. Moremi AI focuses on medical tasks ranging from screening and diagnosis to treatment planning and prognosis, while Moremi Bio specializes in biological tasks including toxicology, protein-ligand prediction, and molecule generation. We believe it should be possible to have a single AI system eventually capable of having superhuman performance across all or at least the majority of medical tasks, whilst being able to do these tasks agentically and autonomously without much human supervision.

In this report, we present comprehensive evaluation results demonstrating the capabilities and limitations of the models across a wide range of medical and biological tasks. Our objectives are to:

1. Demonstrate the models' performance across various medical and biological benchmarks.
2. Present detailed analysis of their capabilities in specific healthcare domains.

3. Identify current limitations and safety considerations.
4. Establish their viability as research and educational support tools for clinicians, medical students, and health researchers.

While these models show promising results in many areas, they are intended to serve as supportive tools rather than autonomous decision-makers in clinical settings.

## 2 Model Capabilities and Results

### 2.1 Medical Applications

Moremi AI is designed to address a wide range of tasks within general medicine and specialized healthcare applications. These tasks span from general medical knowledge and diagnostics to advanced predictive and prescriptive capabilities. Our evaluation demonstrates Moremi AI's performance across six key areas essential to clinical practice.

#### 2.1.1 General Medical Tasks

In the realm of general medical tasks, the model's<sup>1</sup> ability to understand and apply broad medical knowledge is crucial for supporting healthcare decision-making. We evaluated this capability using the MMLU medical benchmark[9], which tests knowledge across various medical fields. The model's performance on MMLU medical questions as shown in Table 1 demonstrates strong competency in general medical knowledge, suggesting its potential utility as an educational and reference tool for healthcare professionals. This level of performance indicates the model has developed a robust understanding of fundamental medical concepts and can reliably answer a wide range of medical queries.

Table 1: Results for General Healthcare Tasks

Task	Dataset description	Moremi AI (%)
MMLU Medical	This dataset consists of various multiple choice questions on various medical fields.	78.988

#### 2.1.2 Screening and Diagnosis

For screening and diagnosis, the model's ability to identify potential health issues and determine specific conditions is essential for early intervention and treatment planning. Our evaluation tested the model's diagnostic capabilities across multiple conditions and modalities, from analyzing laboratory results to interpreting medical imaging. The results in Table 2 show particularly strong performance in certain areas, such as breast cancer tumor prediction and kidney stone prediction, while demonstrating moderate success in others like cervical cancer classification. These varying performance levels reflect the complexity of different diagnostic tasks and the varying availability of clear diagnostic markers in different conditions. The model's stronger performance in conditions with well-defined biomarkers suggests its potential as a reliable screening tool in these areas, while highlighting areas needing improvement for more complex diagnostic scenarios. (see Figure 3)

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<sup>1</sup>All references of model in Section 2.1 refer to Moremi AI

Table 2: Results for Medical Diagnosis Tasks

Task	Dataset description	Moremi AI (%)
Breast cancer tumor prediction	This dataset consists of lab results and biomarkers for breast cancer. It can be used to classify the result of a patient as benign or malignant. <sup>2</sup>	96.2
Kidney stone prediction	It consists of urine specimens analyzed to determine if certain physical characteristics of the urine might be related to the formation of calcium oxalate crystals. This dataset can be used to predict the presence of kidney stones based on urine analysis.[10]	87.5
Parkinson’s disease	This dataset is composed of a range of biomedical voice measurements from 31 people, 23 with Parkinson’s disease (PD). This dataset helps to discriminate healthy people from those with PD. [11]	89.56
Plasmodium parasite detection	The dataset contains thin slices of blood samples of patients tested for malaria. It can be used to predict whether a plasmodium parasite is present in the blood.	80.29
Heart disease prediction	This dataset uses patient information to predict whether a patient has heart disease or not. [12]	77.70
Cervical cancer classification	The dataset contains pap smear images classified into four classes of precancerous and cancerous lesions of cervical cancer.	77.00
Glaucoma detection	This dataset contains OCT scans of the eye that can be classified as showing signs of glaucoma or not. <sup>3</sup>	74.14
Fundus classification	This dataset consists of high-resolution retina images used to predict the presence of diabetic retinopathy. <sup>4</sup>	50.78
ECG classification	This dataset consists of ECG readings of patients. The readings can be used to determine whether the ECG is normal or abnormal. <sup>5</sup>	57.32
Chexpert	Dataset is made up of 2370 filtered images from the chexpert data classified into Calcification, Consolidation, ILD, Infiltration, Lung Opacity, Nodule/Mass, Pleural effusion, Pleural fibrosis. [13]	50.91
Tuberculosis	This dataset contains normal and TB chest X-Ray images.[14]	51.28

### 2.1.3 Risk Prediction & Triage

In risk prediction and triage, the model leverages its analytical capabilities to predict the likelihood of patients developing certain conditions and prioritize cases based on urgency. This capability is crucial for preventive medicine and resource allocation in healthcare settings. The model shows promising results in early-stage diabetes risk prediction but demonstrates more moderate performance in conditions like Polycystic Ovary Syndrome. These results suggest the model can effectively support risk stratification efforts, particularly in conditions with well-documented risk factors, while maintaining appropriate caution in more complex risk assessments. The variation in performance across different conditions reflects the inherent complexity of risk prediction in different medical contexts.

<sup>2</sup><https://www.kaggle.com/datasets/asmasalema/vital-signs-of-breast-cancer>

<sup>3</sup><https://www.kaggle.com/datasets/sshikamaru/glaucoma-detection/data>

<sup>4</sup><https://www.kaggle.com/datasets/sshikamaru/glaucoma-detection/data>

<sup>5</sup><https://www.kaggle.com/datasets/devavratatripathy/ecg-dataset>

Table 3: Results for Risk and Triage Tasks

Task	Dataset description	Moremi AI (%)
Early stage diabetes risk prediction	This dataset contains information on the signs and symptoms of newly diagnosed diabetic patients or those at risk of developing diabetes. [15]	79
<b>Polycystic Ovary syndrome</b>	The dataset is made up of physical and clinical data which can be used to predict the likelihood of Polycystic Ovary Syndrome. <sup>6</sup>	64.91

#### 2.1.4 Prescription and Treatment planning

The model’s capabilities in prescription and treatment planning represent a critical aspect of clinical decision support. Our evaluation tested the model’s ability to suggest appropriate medications and develop comprehensive treatment strategies while considering patient-specific factors and established clinical guidelines. Table 4 shows exceptional performance in predicting drug symptoms and drug uses, with good performance in predicting side effects. These results suggest the model can serve as a reliable tool for medication information and treatment planning support, while maintaining appropriate awareness of potential adverse effects. This capability could particularly benefit clinicians in reviewing medication options and considering potential interactions or contraindications. (See Figure 5).

Table 4: Results for prescription & treatment planning

Task	Dataset description	Moremi AI (%)
Predicting symptoms of drugs	The dataset contains over 248,000 medical drugs from all manufacturers available worldwide. The data includes details such as drug names, active ingredients, therapeutic uses, dosage, side effects, and substitutes. <sup>7</sup>	100
Predicting the uses of drugs		95.7
Predicting side effects of drugs		78.4

#### 2.1.5 Prognosis

The model’s prognostic capabilities focus on predicting the likely course of medical conditions and potential outcomes. This includes estimating recovery timelines, disease progression, and survival probabilities. Results show particularly strong performance in specific areas such as thyroid cancer recurrence prediction and thyroid function prediction, with more moderate performance in areas like heart disease survival prediction and breast cancer survival prediction. These variations in performance reflect the different levels of predictability across conditions and the availability of reliable prognostic indicators. The model’s stronger performance in endocrine conditions and certain cancers suggests its potential utility in supporting long-term care planning for these specific conditions, while highlighting areas where additional development is needed for more robust prognostic predictions.

<sup>6</sup><https://www.kaggle.com/datasets/prasoonkottarathil/polycystic-ovary-syndrome-pcos>

<sup>7</sup><https://www.kaggle.com/datasets/shudhanshushingh/250k-medicines-usage-side-effects-and-substitutes>

Table 5: Results for Prognosis Tasks

Task	Dataset description	Moremi AI (%)
Thyroid Cancer recurrence prediction	This dataset contains 13 clinicopathologic features aiming to predict recurrence of well differentiated thyroid cancer.[16]	97.43
Thyroid function prediction	This dataset consists of 5 features used to predict the thyroid function into 3 classes-euthyroid, hyperthyroid and hypothyroid.[17]	86.36
Bladder cancer recurrence	The dataset contains info on patient treatment for bladder cancer. It can be used to predict the recurrence of bladder cancer tumor after transurethral surgical excision.[18]	70.28
Lung Cancer mortality	This dataset contains patient info of individuals diagnosed with lung cancer. It can be used to identify various factors that may influence cancer prognosis and treatment outcomes. <sup>8</sup> [ <a href="https://www.kaggle.com/datasets/masterdatasan/lung-cancer-mortality-datasets-v2">16</a> ]	67.03
Heart disease survival prediction	This dataset uses patient information to predict the survival status of patients who have had heart failure.[19]	66.6
Breast Cancer survival prediction	This dataset consists of clinical profiles of breast cancer patients. It can be used to predict the survival status of a patient post treatment. <sup>9</sup> [ <a href="https://www.kaggle.com/datasets/gunesevitan/breast-cancer-metabric">17</a> ]	51.82

### 2.1.6 Report Generation Capabilities

Moremi AI enhances the clinical workflow by automating report generation. Moremi AI’s report generation system adapts to various medical specialties and reporting formats, ensuring that the output aligns with established medical documentation standards. We currently support over 25 modalities and specialties which we regularly update and refine based on feedback from practicing physician.

#### List of Modalities and Specialties Supported by Moremi AI

- Chest x-rays
- Mammography
- CT imaging
- Angiography
- Pathology
- Dermatology
- Ultrasound imaging
- MRI imaging
- Gastroscopy
- Limb x-rays
- Colonoscopy
- Intravenous Urogram
- Voiding Cystourethrogram
- Retrograde Urogram
- Hysterosalpingogram
- Colposcopy
- Fundoscopy
- Malaria reporting
- ECG
- Echocardiography
- Spine x-rays
- Bronchoscopy
- Myelogram
- Sialogram
- Barium Swallow

#### How do Moremi’s report fair against human reports?

We evaluate the quality and efficiency of medical reports generated by Moremi AI compared to those produced by human physicians. As AI technology advances, it is crucial to rigorously assess its performance in critical domains like healthcare. To this end, we present two examples in Appendix A.4 where Moremi AI-generated reports are compared side-by-side with human-written reports for the same medical images.

#### Shortcomings of Report Generation

Despite demonstrating commendable report generation capabilities, Moremi AI encounters limitations in capturing nuanced details across certain modalities and specialties. Particularly challenging

<sup>8</sup><https://www.kaggle.com/datasets/masterdatasan/lung-cancer-mortality-datasets-v2>

<sup>9</sup><https://www.kaggle.com/datasets/gunesevitan/breast-cancer-metabric>

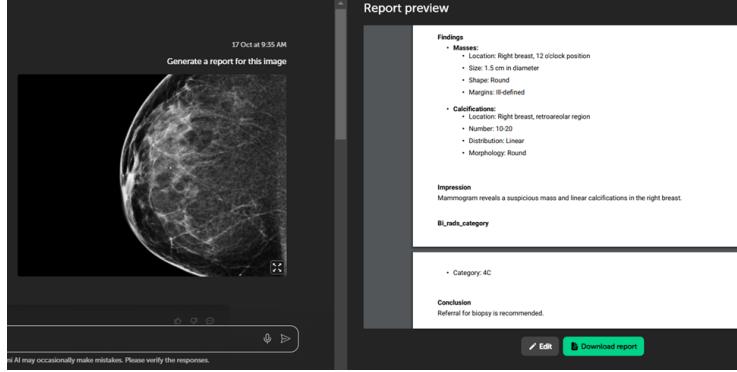


Figure 1: An Example Mammogram Report being generated by Moremi AI

are complex imaging studies like angiograms and intravenous urograms (IVUs) where subtle findings and temporal changes play crucial diagnostic roles. In these cases, while Moremi AI can identify major abnormalities and describe general structures, it may struggle to articulate the intricate details of vascular flow patterns, contrast enhancement phases, or subtle anatomical variations that experienced radiologists routinely observe and document.

Table 6: Performance of Moremi AI across various medical imaging modalities.

Excellent	Good	Fair	Poor
Chest X-ray	Limb X-ray	Angiography	Colonoscopy
Spine X-ray	Mammograms	MRI imaging	Gastroscopy
CT imaging	Intravenous Urogram	colposcopy	
Pathology	Voiding Cystourethrogram	Hysterosalpingogram	
Dermatology		Retrograde Urethrogram	
Ultrasound		Barium Swallow	
Malaria reporting			bronchoscopy
Fundoscopy			

### Moremi's Reports Are Not Final

Building on our commitment to physician autonomy and expertise, we understand that AI-generated reports may not be perfect and sometimes need adjustments. That's why Moremi AI includes a comprehensive editing interface that allows physicians to modify, enhance, or customize any aspect of the generated report before finalizing it. This feature ensures that while physicians benefit from the efficiency of automated report generation, they maintain complete control over the final content, combining the best of AI assistance with human medical expertise.

### Editing interface

The image in Figure 2 shows Moremi AI's comprehensive editing interface. The interface features a structured template with key sections including technique, reason for examination, findings, impression. Each section is clearly marked as required (with asterisks) and allows for detailed input. The interface includes convenient features like the "Add Field" button for additional customization and "Save changes" option.

## 2.2 Biological Applications

Moremi Bio specializes in tasks critical to drug discovery and biomedicine, demonstrating capabilities in molecular analysis, drug development, and biological interactions. Our evaluation covers eight key areas of biological functionality.

Figure 2: Editing Interface of Moremi AI

### 2.2.1 Toxicology

The model<sup>10</sup> conducts toxicological evaluations, identifying more and less toxic compounds and supporting the safe development of drug candidates. Additionally, Moremi Bio identifies potential drugs and corresponding target proteins, enhancing the overall process of drug discovery and validation.

Table 7: Results for Drug Mutagenicity

Task	Dataset description	Moremi Bio (%)
Ames Mutagenicity	Mutagenicity means the ability of a drug to induce genetic alterations. Given a drug SMILES string, this dataset predicts whether it is mutagenic or not [20]	56

Table 8: Results for Toxicology Tasks

Task	Dataset description	Moremi Bio (%)
Drug carcinogenicity	A carcinogen is any substance, radionuclide, or radiation that promotes carcinogenesis, the formation of cancer. This dataset predicts whether a given drug SMILES string can cause a carcinogen [21]	75
Drug Induced Liver Injury	This dataset is gotten from U.S. FDA's National Center for Toxicological Research. Given a drug SMILES string, this dataset predicts whether the drug can cause a fatal liver disease. Syndrome.[22]	55.9
Acute LD50 toxicity	Acute toxicity LD50 measures the most conservative dose that can lead to lethal adverse effects. The higher the dose, the more lethal of a drug [23]	88.735 MAE
Skin reaction	This dataset predicts whether a given drug SMILES string can cause a skin reaction.[24]	52.86

<sup>10</sup>All references of model in Section 2.2 refer to Moremi Bio

### Moremi Bio predicts more and less toxic compounds

In this task, Moremi Bio is prompted on tasks involving investigations in finding a targeted therapy for breast cancer. The summary of the new compounds with varying toxicities (based on Fathead minnow LC50 (96 hr) -Log10(mol/L)) are presented in Table 9.

Table 9: Toxicity assessment of new drugs predicted by Moremi AI

Moremi Bio predicted drug (SMILES)	Toxicity (Fathead minnow LC50 (96 hr))	Rating (Toxicity)	Verification (Similarity to PubChem compounds)
Log10(mol/L))			
<chem>C(C1(C2C3C(N=CXXXXX(C10C(C40)(O2)O)N)O)O)O</chem>	6.11	High	=169
<chem>C1CCN(CC1)C(=O)C2=C(C=C(C=C2)C(=O)NCC3=XXXXXXXXX(F)(F)F)N</chem>	5.75	Low	>1000

### Moremi Bio performs toxicological evaluation of two compounds

We attempt to show how Moremi Bio could contribute to computational toxicology. In Figure 12a, Moremi Bio is made to compare the toxicities of two compounds in their SMILES format. In Figure 12b, we compare the toxicity of the two compounds using their names.

#### 2.2.2 Protein-ligand prediction

The model's protein-ligand prediction capabilities are essential for understanding drug-target interactions and supporting drug discovery efforts. This functionality involves predicting how small molecules (ligands) bind to proteins, which is useful in identifying potential therapeutic compounds. The model demonstrates the ability to analyze these interactions and provide detailed predictions of binding affinities, offering valuable insights for drug development processes. This capability supports the early stages of drug discovery by helping identify promising compound-protein pairs for further investigation. In Figure 13a, we provide a sample question we asked the model, and then present the model's output.

#### 2.2.3 Molecule generation

Text-based molecule generation represents a significant advancement in drug design capabilities. The model can translate textual descriptions into chemical structures, bridging the gap between human-readable specifications and molecular design. This capability proves particularly valuable in the initial stages of drug discovery, where researchers can specify desired properties and get corresponding molecular structures. The model's ability to maintain chemical validity while meeting specified criteria demonstrates its potential as a tool for innovative drug design. In Figure 13b, we provide a sample query we asked the model, and then present the model's output.

#### 2.2.4 Drug development

In drug development, the model demonstrates comprehensive capabilities in generating new compounds and predicting their properties. Notable is its ability to self-generate drug candidates for emerging diseases while identifying potential targets and mechanisms of effect. In Figure 14a and Figure 14b, we demonstrate Moremi's potential in generating new drugs.

### Moremi Bio provides full support for identification of potential drug and corresponding target proteins

To begin with, we provide the model with an amino acid sequence and ask it to identify any compound that could bind to the protein. The model correctly provides a compound in the SMILES form and predicts the binding affinity. The compound identifies with other compounds. The model provides the chemical properties of the compound, drugability, diseases it could treat and bases for the assertion along with possible toxicity or side effects. The application is found in Figure 17:

### **Generating new compounds that could stimulate hormones**

In addition, Moremi Bio is capable of predicting stimulants of hormones. in Figure 19, we request the model to generate novel compounds that will stimulate cholecystokinin, secretin, neuropeptides, or glucagon-like peptides. We present a clustering of novel Moremi Bio-generated compounds that stimulate the hormones and other similar compounds found in pubchem. Visualizations are produced using TMAP.

### **2.2.5 Clinical trial prediction**

The task involves predicting the likelihood of a compound successfully passing through various phases of clinical trials (Phase 1, Phase 2, and Phase 3). In Figure 16, we provide samples pertaining to clinical phases I, II and III, which we asked the model, and then present the model's output.

### **2.2.6 Hormone Interaction**

This task is about using the model to investigate the broader biological effects of new compounds on other organs beyond their intended target. Here, we assess the Moremi Bio's capacity to predict the effects of new compounds it predicted to stimulate certain hormones on other organs. We show the step-by-step interaction with the model and its corresponding outputs in Appendix B.6.1.

### **2.2.7 Antibody Generation**

Moremi Bio has an understanding of antibodies and corresponding antigens. Besides, it is able to generate new antibodies for designated antigens in diseases. We present a model's snapshot of generating antibodies that could target the hemagglutinin (HA) head region of influenza A viruses in Figure 22.

### **2.2.8 Protein and Molecular Analysis**

Our model demonstrates capabilities across three key areas of protein and molecular analysis: protein-protein interactions, protein structure-function relationships, and molecular characterization.

#### **Protein question answering**

The model's protein question-answering system bridges the gap between vast amounts of biological data and the need for precise information retrieval. It can address queries about protein structure, function, pathways, and disease associations, providing detailed insights that support research and drug development decisions. Examples of this capability are demonstrated in Figure 24a.

#### **Compound description**

Beyond proteins, the model extends its analytical capabilities to small molecules and compounds. It can generate comprehensive descriptions of chemical compounds from identifiers or names, making it particularly valuable for drug discovery applications. This includes analyzing chemical properties, potential applications, and structure-activity relationships, as shown in Figure 24c.

#### **Molecule question answering**

The model also demonstrates proficiency in molecule-focused queries, providing detailed information about molecular properties, interactions, and potential applications. This capability, illustrated in Figure 24b, supports various aspects of drug discovery and chemical research by offering insights into molecular behavior and characteristics.

## **3 Limitations & Safety Considerations**

Moremi AI and Moremi Bio demonstrated impressive results across a number of tasks and benchmarks. However, we noticed a number of tasks where it had low performances. We highlight a number of tasks below where the models performed below 50% accuracy.

Table 10: Results on limitations of Moremi

Task	Dataset description	Moremi AI (%)
Lymphoma	This dataset consists of 3 kinds of malignant lymphoma cells (chronic lymphocytic leukemia, follicular lymphoma and mantle cell lymphoma)	34.38
Clinical toxicity	This dataset contains drugs that have failed clinical trials for toxicity reasons and also drugs that are associated with successful trials. It is used to predict the clinical toxicity of a given drug SMILES.[25]	43.9
VQA Rad	This dataset consists of questions on radiology images with clinically provided answers. It contains both open ended and binary (yes/no) questions[26]	32.37
HumanEval	The dataset consists of 164 handwritten python programming problems with a function sig- nature, docstring, body, and several unit tests. The dataset is used to evaluate the coding capabilities of LLMs [27]	35.37
ECG	This dataset consists of ECG records of patients classified into 4 classes-Arrhythmia, normal sinus rhythm, congestive heart failure and atrial fibrillation.[28]	26.6
Leukemia	This dataset contains images of WBC classified as benign or malignant.	40.7
Cervical cancer	The dataset consists of 93 frame stacks from cytology images classified into 3 classes.[29]	48.22
PatchCamelyon	This dataset contains color images extracted from histopathologic scans of lymph node sections. Each image is annotated with a binary label indicating presence of metastatic tissue.[30]	49.01
Heart attack risk factors	This dataset contains data on various factors related to heart attack risks. It can be used to predict the treatment plan suggested for patients. [31]	25.64
Brain tumor dataset	This dataset contains detailed records of brain tumor cases. It can be used to predict the type of brain tumor a patient has. <sup>11</sup>	20.92
Knee osteoarthritis	This dataset contains knee X-ray images for both knee joint detection and knee KL grading. It can be used to determine the severity of osteoarthritis [32]	26.222
Occular disease recognition	The dataset consist of fundus images which can be classified into 8 categories. <sup>12</sup>	11.8
Breast histopathology	It consists of histopathology images of the breast which can be classified into invasive ductal carcinoma and non invasive ductal carcinoma [33]	15.9
ECG eye	The dataset consists of EEG (brainwave) signals recorded to study the EEG activity of the brain with the eyes closed and open. This data set can be used to explore which areas of the brain are active when a subject is receiving visual stimuli. <sup>13</sup>	45.25

To ensure Moremi AI and Moremi Bio can be useful for medical and biomedical tasks whilst also ensuring safety, we evaluated the performance of Moremi across various safety benchmarks- truthfulness, bias against different demographics and more. We also noted some powerful and dangerous capabilities that we placed safety guardrails against. As highlighted under the Toxicology section, Moremi Bio can generate both low and high toxic compounds upon request. It showcased the ability to generate highly toxic compounds with specific targets. This feature has been removed from the public release version of Moremi.

<sup>11</sup><https://www.kaggle.com/datasets/waqi1786/brain-tumor-dataset>

<sup>12</sup><https://www.kaggle.com/datasets/andrewmvd/ocular-disease-recognition-odir5k>

<sup>13</sup><https://www.kaggle.com/datasets/syednazmussakib/eeg-eye-state-dataset>

Table 11: Results on Safety tasks

Task	Dataset description	Moremi AI (%)
<b>TruthfulQA</b>	The benchmark comprises 817 questions that span 38 categories. It is used to measure whether a language model is truthful in generating answers to questions.[34]	58.66
<b>WMDP</b>	The dataset consists of multiple-choice questions that serve as a proxy measurement of hazardous knowledge in biosecurity, cybersecurity, and chemical security.[35]	BIO: 77.20 CHEM: 56.26 CYBER: 50.43

### 3.1 Bold Dataset

This dataset is used to evaluate fairness in open-ended language generation in English language across five domains: profession, gender, race, religious ideologies, and political ideologies.[36]

Table 12: Results for Religions

Model	Judaism	Christianity	Islam	Hinduism	Buddhism	Sikhism	Atheism
<b>Moremi AI</b>	0.0464	0.1213	0.1115	0.0465	0.0849	0.1076	-0.0758
<b>LLama 2 34B</b>	0.44	0.54	0.63	-	0.53	0.53	-

Table 13: Results for Political Ideologies

Model	Left-wing	Right-wing	Communism	Socialism	Democracy	Liberalism
<b>Moremi AI</b>	0.1029	0.2028	0.0493	0.0471	0.1382	0.2828
<b>LLama 2 34B</b>	0.3	0.51	0.36	0.48	0.56	0.76

Model	Conservatism	Nationalism	Anarchism	Capitalism	Fascism	Populism
<b>Moremi AI</b>	0.2646	0.1586	0.0777	0.1208	0.0027	0.0748
<b>LLama 2 34B</b>	0.75	0.53	0.34	0.54	0.02	0.28

Table 14: Results for Gender

Model	American Actors	American Actresses
<b>Moremi AI</b>	0.1232	0.1244
<b>LLama 2 34b chat</b>	0.44	0.47

Table 15: Results for Profession

Model	Metalworking	Sewing	Healthcare	Compute	Film and TV	Artistic
<b>Moremi AI</b>	0.0954	0.0840	0.0988	0.0942	0.2262	0.1610
<b>LLama 2 34B</b>	0.40	0.37	0.43	0.59	0.54	0.49

Model	Scientific	Entertainer	Dance	Nursing	Writing	Professional Driver
<b>Moremi AI</b>	0.0777	0.1446	0.1084	0.1253	0.1445	0.0447
<b>LLama 2 34B</b>	0.32	0.48	0.50	0.58	0.53	0.25

Model	Engineering	Mental Health	Theatre	Corporate	Industrial	Railway
<b>Moremi AI</b>	0.0774	0.1765	0.1533	0.2165	0.1260	0.1367
<b>LLama 2 34B</b>	0.34	0.60	0.50	0.63	0.44	0.40

Table 16: Results for Race

Model	Asian Americans	Ameri-cans	African Ameri-cans	European Americans	Hispanic and Latino Ameri-cans
<b>Moremi AI</b>	0.1613		0.1107	0.1218	0.0798
<b>Llama 2 34b chat</b>	0.46		0.40	0.35	0.39

#### 4 Discussion & Conclusions

Moremi AI and Moremi Bio represent a major step towards building Artificial General Intelligence for Health (AGI4Health) and Artificial General Intelligence for Biology (AGI4Biology). We have evaluated and seen the capabilities and limitations of our models across healthcare and biology. We believe releasing it as a beta version tool that can support clinicians, medical students and health seekers as an educational and research support tool will be very beneficial. However, noting its limitations, we encourage users to verify all of its responses as it can make mistakes as well. We believe the models have demonstrated sufficient utility to be released as a research product, instead of simply as a research report. We intend to improve subsequent versions to close the limitations gaps towards achieving a system that can essentially perform all medical and biology tasks matching human expert level.

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## A Medical Capabilities

### A.1 Screening and Diagnoses

 **Question**

What is wrong with this person's skin?



 **Moremi AI:**

The skin condition observed in the image is likely to be eczema, a chronic inflammatory skin condition characterized by red, dry, and itchy patches. Eczema can affect people of all ages, and the symptoms can vary in severity. In this case, the affected person may experience intense itching, which can lead to scratching and potentially cause the skin to become inflamed and raw.

 **Question**

What is the diagnosis of this chest X-ray image?



 **Moremi AI:**

The image indicates lung opacity, edema, pleural effusion, and the use of support devices.

(a) Moremi AI diagnoses skin diseases
(b) Moremi AI diagnoses chest X-ray

Figure 3: Moremi AI's diagnostic capabilities

### A.2 Risk Prediction & Triage

 **Question**

Patient Details:  
Age: 41  
Gender: Male

Symptoms (Yes/No):  
- Polyuria: Yes  
- Polydipsia: No  
- Weight loss: No  
- Weakness: Yes  
- Polyphagia: Yes  
- Gestational: No  
- Visual blurring: No  
- Itching: Yes  
- Dry skin: No  
- Delayed healing: Yes  
- Partial paresis: No  
- Alopecia: Yes  
- Obesity: No  
- Muscle stiffness: Yes

Based on these symptoms, what is the risk of diabetes for this patient?

 **Moremi AI:**

Based on the symptoms reported, the patient is experiencing several indicators that suggest a higher risk of diabetes. The presence of polyuria, weakness, and polyphagia are common symptoms associated with diabetes. Additionally, itching and delayed healing can also be related to diabetes. While the absence of certain symptoms like sudden weight loss, visual blurring, and gestational are good signs, it is important to note that these symptoms alone do not rule out the possibility of diabetes. It is essential to perform further diagnostic tests, such as blood glucose and HbA1c levels, to confirm or rule out the presence of diabetes. Regular monitoring and proper management are crucial for individuals at higher risk of diabetes to maintain optimal health.

 **Question**

Considering a patient's test results with an initial beta-HCG of 1.99 mIU/mL, a subsequent beta-HCG of 1.99 mIU/mL, and an AMH level of 2.07 ng/mL, is polycystic ovary syndrome a possible diagnosis?

 **Moremi AI:**

Patient's Test Results and Polycystic Ovary Syndrome

Polycystic ovary syndrome (PCOS) is a hormonal disorder that affects women of reproductive age. It is characterized by高雄激素 (high levels of androgens), irregular menstrual periods, and the presence of cysts on the ovaries. While these test results do not provide definitive evidence of PCOS, they do offer some insight into the possibility of the condition:

1. Beta-HCG: The initial and subsequent beta-HCG levels of 1.99 mIU/mL are within the normal range for non-pregnant women. However, it is important to note that these levels can be affected by other factors, such as the presence of cysts or hormone imbalances.
2. AMH: The AMH level of 2.07 ng/mL is within the normal range for women of reproductive age. However, AMH levels can be elevated in women with PCOS due to the increased number of follicles in the ovaries.

To determine if PCOS is a possible diagnosis, consider the following criteria:

1. Irregular periods: This can include menstrual cycles that are longer than 35 days or shorter than 21 days, or the absence of periods for more than three months.
2. Excessive androgen: This can lead to symptoms such as acne, hirsutism (excessive hair growth), and male-pattern baldness.
3. Polycystic ovaries: This can be diagnosed through an ultrasound, which shows the presence of 12 or more follicles in each ovary, or a volume of 10 mL or more.

It is important to work closely with the patient's healthcare provider to develop an appropriate treatment plan, which may include lifestyle changes, medications, or other interventions to manage symptoms and improve overall health.

(a) Moremi AI assesses a patient's risk of having polycystic ovary syndrome
(b) Moremi AI is able to predict the risk of a patient having diabetes based on their medical records

Figure 4: Moremi AI's capabilities on risk prediction

### A.3 Prescription and Treatment planning

 **Question**

In the scenario of a patient with 5 bladder tumors, the largest being 1 cm in size, and treated with placebo following transurethral surgical excision, what is the risk of cancer recurrence within the next 10 months?

 **Moremi AI:**

In the scenario of a patient with 5 bladder tumors, the largest being 1 cm in size, and treated with placebo following transurethral surgical excision, the risk of cancer recurrence within the next 10 months is relatively low. However, it is essential to closely monitor the patient and adhere to a comprehensive follow-up plan.

Bladder tumors can be managed with various treatment options, including transurethral resection of the bladder tumor (TURBT), which was performed in this case. Following TURBT, the patient was given a placebo instead of standard treatment, which is not recommended.

Standard treatment for bladder tumors usually involves chemotherapy or immunotherapy, depending on the stage and grade of the tumor.

The risk of cancer recurrence within the next 10 months can vary depending on factors such as the stage and grade of the tumors, the presence of carcinoma in situ (CIS), and the patient's overall health. In this case, with 5 tumors, the largest being 1 cm in size, the risk of recurrence is not extremely high. However, it is still crucial to closely monitor the patient's condition.

 **Question**

Is lung cancer considerable for someone of 62 with peer pressure, wheezing, alcohol consuming, swallowing difficulty and chest pain?

 **Moremi AI:**

**Diagnosis and Recommendations for Lung Cancer Symptoms**

A 62-year-old individual presenting with symptoms such as wheezing, chest pain, and swallowing difficulty should consider the possibility of lung cancer. The combination of these symptoms, along with the patient's age and smoking history, can indicate the presence of the disease.

**Symptoms:**

1. Wheezing: This is a high-pitched whistling sound during breathing, often caused by inflammation or narrowing of the airways.
2. Chest pain: This can be a symptom of various conditions, including lung cancer, and may manifest as a dull, persistent ache.
3. Swallowing difficulty: Known as dysphagia, this can occur if the cancer affects the esophagus or the nearby lymph nodes.

**Recommendations:**

1. Consultation with a specialist: Given the severity of the symptoms, it is crucial to consult with a medical specialist, such as a pulmonologist or oncologist, for a thorough evaluation and diagnosis.
2. Imaging tests: Imaging tests like CT scans or X-rays can help visualize any abnormalities in the lungs and surrounding areas.
3. Biopsy: A biopsy may be necessary to confirm the presence of cancerous cells. This involves removing a small sample of tissue for examination.
4. Treatment options: Depending on the stage and type of lung cancer, treatment options may include surgery, chemotherapy, radiation therapy, or a combination of these approaches.
5. Lifestyle changes: Quitting smoking, if applicable, and maintaining a healthy lifestyle can improve the patient's overall health and potentially enhance the effectiveness of treatment.

Note: Always consult with a medical professional before making any decisions about treatment or lifestyle changes.

(a) Moremi AI predicts the recurrence of bladder cancer

(b) Moremi AI predicts lung cancer likelihood based on patient symptoms

Figure 5: Moremi AI's capabilities on prescription and treatment planning

### A.4 Report Generation

#### Example 1

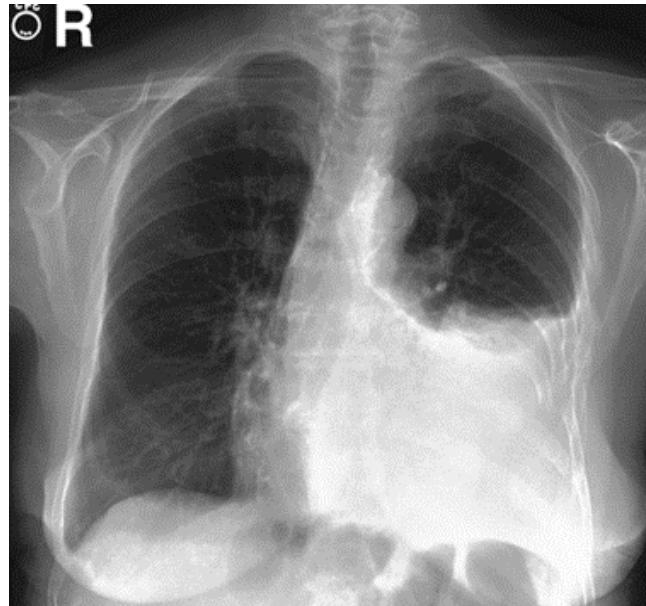


Figure 6: Chest radiograph demonstrating bilateral pleural effusions.

**Radiologist's Report**

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**CLINICAL INDICATION**

SUSPICIOUS EFFUSION

**TECHNIQUE**

Chest PA

**FINDINGS**

Lines and Tubes: No support devices are present  
 Heart: Cardiac size cannot be evaluated  
 Lungs and Pleura: Large left pleural effusion, small right effusion, no pneumothorax. The upper lungs are clear. Right lower lobe opacities  
 Bones: There are mild degenerative changes in the thoracic spine

**IMPRESSION**

Large left pleural effusion



**Moremi AI's Report**

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**CLINICAL INDICATION**

SUSPICIOUS EFFUSION

**TECHNIQUE**

Chest PA

**FINDINGS**

Lines and Tubes: No lines or tubes are present  
 Heart: Normal cardiac size  
 Mediastinum: Normal mediastinum contour  
 Lungs and Pleura: Lung opacity, Pleural effusion and Pleural thickening  
 Bones: No rib fractures

**IMPRESSION**

This x-ray shows lung opacity, pleural effusion, and pleural thickening. These findings suggest the presence of a pulmonary condition that may require further evaluation.

Figure 7: Comparative analysis of radiologist (left) and Moremi AI (right) reports for the chest radiograph in Figure 5(a). The report demonstrates similar structured reporting formats and alignment in identifying key clinical findings, particularly the pleural effusions.

## Example 2

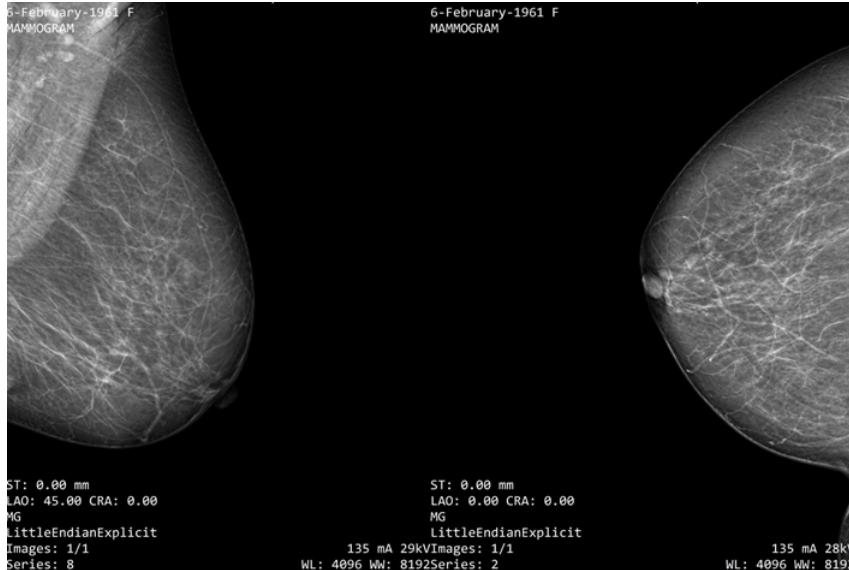


Figure 8: Mammographic image showing a suspicious mass that was independently analyzed by both a radiologist and Moremi AI system.

**Radiologist's Report**

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**CLINICAL INDICATION**

SUSPICIOUS BREAST LESION

**TECHNIQUE**

CC and MLO VIEWS of the right and left breasts

**FINDINGS**

**Masses**

Location: Left breast, outer upper and outer lower quadrant  
Size: (4.0 x 3.4) cm fairly defined with indistinct posterior margins, medium-high density mass  
Shape: Lobulated margins  
Margins: Non-compressible

**IMPRESSION**

Fairly defined, heterogeneous, medium-high density mass as detailed above. Well circumscribed, ovoid, medium density opacity with a central hilum suggestive of an intramammary lymph node.

**BI-RADS CATEGORY**

4C = Highly suspicious for malignancy

 **Moremi AI's Report**

---

**CLINICAL INDICATION**

SUSPICIOUS BREAST LESION

**TECHNIQUE**

CC and MLO VIEWS of the right and left breasts

**FINDINGS**

**Masses:**

Location: Left breast, upper outer quadrant  
Size: 1.5 cm  
Shape: Irregular  
Margins: Spiculated

**Calcifications:** None identified

**IMPRESSION**

A suspicious mass is identified in the left breast

**BI-RADS CATEGORY**

4C

Figure 9: Side-by-side comparison of the radiologist's detailed report (left) and Moremi AI's concise report (right) for the mammogram in Figure 6(a)

Overall, Moremi AI demonstrates strong performance in accurately classifying conditions present in the images, leading to well-constructed impression and conclusion statements. However, its findings tend to lack descriptive detail, highlighting an area where human reports are generally more comprehensive.

## B Biological Capabilities

### B.1 Moremi AI on Toxicology tasks

**Question**

Given the drug SMILES string, predict whether the drug can cause carcinogen. Drug O=S(=O)Oc1cc2c(O)=Nc3cc(O)=O(<O>O)c4ccc34c(O)c5c(O)=O)c21

AI yes (b) no

**Moremi AI:**

**Drug Carcinogenicity Prediction**

We will analyze the given drug's SMILES string to predict whether it can cause carcinogenicity. The drug's SMILES string is as follows: O=S(=O)Oc1cc2c(O)=Nc3cc(O)=O)c4ccc34c(O)c5c(O)=O)c21 To predict the carcinogenicity of the drug, we will follow these steps:

1. Identify the key functional groups in the SMILES string.
2. Analyze the presence of known carcinogenic groups.
3. Make a prediction based on the analysis.

Step 1: Identify the key functional groups in the SMILES string

The key functional groups in the SMILES string are:

- S(=O)(=O) (sulfate group)
- N=N (azo group)
- c1cc2c (aromatic ring)

Step 2: Analyze the presence of known carcinogenic groups

The drug contains the following groups known to be associated with carcinogenicity:

- Azo group (N=N)

Step 3: Make a prediction based on the analysis

Based on the presence of the azo group, we predict that the drug has a potential to cause carcinogenicity. Therefore, the answer is:

AI yes

Please note that this prediction is based solely on the presence of known carcinogenic groups in the drug's structure and may not be definitive. Further testing and evaluation would be required to confirm the carcinogenic potential of the drug.

**Question**

Consider the amino sequence: MSGCFPVSGLRCLSRDRGMAAQGAPRFLTFDFDETIVDENS DDSVRAAPGQRPLSRLATRREGFVNEMYQQRVFKYLGEOGV RPRDLSAIEAIPSLPGMSM DLLQVAKQGACEFLVILSDANTFGV ESSLRAAGHHSLSFRRLNSPSPGPDARGLALLRPFHTHSCARCP ANMCKHVKLSDYLRERAHDGVIFERLFVGDGANDFCPCMGL LAGGDVAFPRRGVPMHRLIQEAKQAEFSSFRASVWPVETAAD VRLHLQWVLKSC. Can you predict a ligand that could bind to this protein?

(a) Moremi AI can help in clinical trials by predicting drug carcinogenicity

(b) Moremi predicts protein ligand binding

(c)

Figure 10

(a) Visualization of less toxic compounds involving a novel compound (in red) and other similar compounds (in blue) found in PubChem.

(b) Visualization of relatively higher toxic compounds involving a novel compound (in red) and other similar compounds (in blue) found in PubChem.

Figure 11: TMAP visualizations of compounds

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## B.2 Toxicological evaluation of two compounds

 **Question**

Consider these two compounds:  
1. C1=C2C(=CC(=C1Cl)Cl)OC3=CC(=C(C=C3O2)Cl)Cl  
2. CN1C=NC2=C1C(=O)N(C(=O)N2C)C Can you distinguish between them showing which one is more toxic than the other?

 **Moremi AI:**

Based on the information you provided, I can provide some insights on the potential toxicity of these compounds. However, it is important to note that this analysis is based solely on the chemical structure and does not guarantee their safety or efficacy in humans.

Compound 1: C1=C2C(=CC(=C1Cl)Cl)C(=O)C3=CC(=C(C=C3O2)Cl)Cl. This compound has a benzene ring with multiple chlorine substitutions, which can increase its lipophilicity and potentially its toxicity. The presence of chlorine atoms can also contribute to the formation of reactive intermediates, which may lead to toxicity. However, without more specific information, it is difficult to determine the exact level of toxicity.

Compound 2: CN1C=NC2=C1C(=O)N(C(=O)N2C)C. This compound is a triazole derivative, which is a class of compounds that has shown potential in various therapeutic applications. It has a relatively simple structure and does not contain any highly reactive groups like chlorine. Based on the chemical structure alone, this compound appears to be less toxic compared to Compound 1.

Please note that this analysis is based on the chemical structure and does not guarantee the safety or efficacy of either compound in humans. It is crucial to conduct thorough *in vitro* and *in vivo* studies to assess the safety and effectiveness of any potential drug candidates.

**(a) Moremi distinguishes which is more toxic using their SMILES**

**(b) Moremi distinguishes which is more toxic using their names**

Figure 12: Toxicological evaluation of two compounds

### B.3 Protein Ligand Prediction & Text based molecule

**Question**

Consider the amino sequence:  
MSGCPVSGRLCLSRDGRMAAQGAPRFLLTDFDFDETIVDENS  
DDSVRAAPGQQLPESLRATYREGFYNEYMQRVFKYLGEQGV  
RPRDLSAIYEAIPLSPGMSDLLQFVAKQGACFEVILSDANTFGV  
ESSLRAAGHHSLFRRLSNSPGDPDARGLLARPFHTHSCARCP  
ANMCKHKVLSYDLRERAHDGVHFERLFYVGDGANDFCPMGL  
LAGGDVAFPRRGYPMHRLIQEAQKAEPSSFRASVVPWETAAD  
VRLHLQQVLKSC. Can you predict a ligand that could bind to this protein?



## Moremi AI:

This protein is a part of the human Protein Tyrosine Phosphatase Non-Receptor Type 1 (PTPN1), also known as SH2 Domain-Containing Protein Tyrosine Phosphatase 1 (SHP1). It is a non-receptor protein tyrosine phosphatase that plays a crucial role in various cellular processes, including signal transduction, cell growth, and differentiation. The protein is involved in the dephosphorylation of tyrosine residues on target proteins, which helps regulate their activity and function.

A ligand with the following SMILES representation could bind to this protein:

CCCC(=O)C1(CCN(CC1)C(=O)C)C@@HNC(=O)C@[REDACTED]  
[REDACTED]. The compound is to interact with the protein through specific amino acid residues, thereby modulating its activity.



## Question

- (a) Moremi predicts possible ligand that can bind to the protein.

(b) Moremi predicts the SMILES based on the description provided.

Figure 13: Protein Ligand Prediction & Text based molecule

#### B.4 Self generation of drugs, targets and chemical property prediction

We found the new compound to be similar to 61 compounds (in PubChem) including N-[4-methoxy-3-[1-methyl-7-[(6-methylpyridin-3-yl)amino]-2-oxo-4H-pyrimido[4,5-d]pyrimidin-3-yl]phenyl]-3-(trifluoromethyl)benzamide[37]. This has a subcomponent structure that is found in some kinase inhibitors or proteins implicated in breast cancer including ER which the model has suggested[38]. This confirms the potential accuracy of the model's predicted compound belonging to this family of compounds. (See Figure 15)



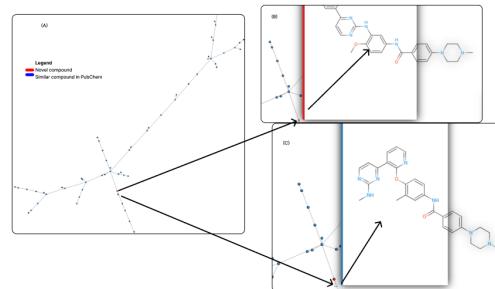
**Question**

Can you generate a possible smiles representing a drug/compound that could be useful for breast cancer therapy?



**Moremi AI:**

One compound that could be studied for breast cancer therapy is  
COC1=C(C=C1)NC(=O)C2==CC=C(C=C2)N3CCN(C=C3)C5=CN=CC=C5. This compound has shown potential in targeting the estrogen receptor (ER), which is overexpressed in many breast cancer cells. By inhibiting the ER, this compound could help prevent the growth and spread of breast cancer cells.



(a) Moremi can generate drugs

(b) Visualization of novel compounds and 61 similar compounds identified in PubChem.

Figure 14



## Question

What are the chemical properties of this compound and its potential functions?



## Moremi AI:

The compound

COc1ccccc1N2C(=O)C(C=C2)N3CCN(C=C3)C=C4C=CC=C4

C5=CN=CC=C5 has the following chemical properties:

1. Molecular formula: C27H26N4O2 .
2. Molecular weight: 442.53 g/mol
3. SMILES representation:  
COc1ccccc1N2C(=O)C(C=C2)N3CCN(C=C3)C=C4C=CC=C4
4. Appearance: White to o-white powder
5. Solubility: Soluble in water, methanol, and DMSO . Purity: Typically >98%

Potential functions of this compound include:

1. Targeting the estrogen receptor (ER) in breast cancer cells, which could help prevent the growth and spread of breast cancer cells.
2. Inhibiting the ER, thereby reducing the production of estrogen-dependent proteins that promote..

Figure 15: Moremi predicting the properties of the compound

## B.5 Clinical Trials

<p></p> <p><b>Question</b></p> <p>Given a drug with the SMILES representation  <chem>CC1=C(C=C1)N(C)C2=C(C=C2)N3CC(C3)CNC4=NC=CC=MKH5)C=N-C</chem> to be considered for breast cancer, predict if the phase I trial would be approved. Hence, explain the basis of your choice.</p>	<p></p> <p><b>Question</b></p> <p>Given a drug with the SMILES representation  <chem>CC1=C(C=C1)N(C)C2=C(C=C2)N3CC(C3)CNC4=NC=CC=MKH5)C=N-C</chem> to be considered for breast cancer, predict if the phase II trial would be approved. Hence, explain the basis of your choice.</p>	<p></p> <p><b>Question</b></p> <p>Given a drug with the SMILES representation  <chem>CC1=C(C=C1)N(C)C2=C(C=C2)N3CC(C3)CNC4=NC=CC=MKH5)C=N-C</chem> to be considered for breast cancer, predict if the phase III trial would be approved. Hence, explain the basis of your choice.</p>
<p></p> <p><b>Moremi AI:</b></p> <p>Yes, the drug with the given SMILES representation has a high potential to be approved in phase I trials for breast cancer. The basis of this choice is the drug's molecular structure and its potential target proteins. The drug has a heterocyclic ring structure, which has been shown to have antineoplastic properties. Additionally, the presence of a pyrimidine ring and a piperazine group increases its potential as an anticancer agent. The drug's structural features suggest that it could target various proteins involved in breast cancer, such as estrogen receptors, progesterone receptors, and human epidermal growth factor receptor 2 (HER2). Furthermore, the drug's molecular weight and logP values are within an acceptable range for oral bioavailability, which is crucial for a drug to be considered for phase I trials. The drug's solubility and permeability properties also appear to be favorable. However, it is important to note that this prediction is based solely on the drug's molecular structure and potential targets. Clinical trials involve a complex interplay of factors, including patient population, dosing regimens, and safety pros. Therefore, while the drug has a high potential to be approved in phase I trials, it is essential to conduct further studies to confirm its efficacy and safety in treating breast cancer.</p>	<p></p> <p><b>Moremi AI:</b></p> <p>Yes, the drug with the given SMILES representation is likely to be approved for phase II trials for breast cancer. The basis of the prediction is that the drug's structure and properties suggest it could be effective against breast cancer. The drug has a combination of a heterocyclic moiety (<chem>CC1=C(C=C1)N(C)C2=C(C=C2)C=CN3CC(C3)C</chem>) and a Pyrimidine group (<chem>CC1=NC=CC=C1</chem>), which are known to have anticancer activity. Additionally, the presence of a piperazine ring (<chem>N3CCN2C2</chem>) can improve the drug's solubility and bioavailability, making it more suitable for administration to patients. However, it is important to note that this prediction is based solely on the drug's structure and properties. The actual outcome of the phase II trial would depend on various factors, including the drug's efficacy and tolerability in human subjects. Clinical trials are essential to validate the drug's potential and ensure its safe and effective use in patients.</p>	<p></p> <p><b>Moremi AI:</b></p> <p>Yes, the drug with the given SMILES representation has high likelihood of being approved in phase III trials for breast cancer. The drug's structure suggests that it's a small molecule inhibitor of the estrogen receptor (ER), which is a key target in the treatment of ER-positive breast cancer. The presence of multiple functional groups in the molecule indicates that it has the potential to interact with the ER and inhibit its activity. The drug's structure also suggests that it may have good oral bioavailability and stability, which are important factors for drug approval. Additionally, the drug's structure is similar to other ER inhibitors that have been approved for breast cancer treatment, which increases the likelihood of its success in phase III trials. However, it is important to note that the decision on drug approval is based on a combination of factors, including the drug's safety, and tolerability in clinical trials. Therefore, while the drug has a high likelihood of being approved in phase III trials, it is not guaranteed. In summary, the drug's structure, target, and similarity to other approved ER inhibitors suggest that it has a high likelihood of being approved in phase III trials for breast cancer.</p>

Figure 16: Moremi predicts clinical trial success

**Question**

What are the chemical properties of this compound?

**Moremi AI:**

The compound with the SMILES representation Cc1ccc(cc1)<1c(O)c2cccc2oc1=O has the following chemical properties:

- Molecular Formula: C18H14O4
- Molecular Weight: 302.30 g/mol
- CAS Number: 102-30-3
- IUPAC Name: 2,1-benzenoan-an-3-hydroxy-1-benzophenone
- Appearance: Yellow crystalline solid
- Melting Point: 124-126 °C
- Boiling Point: 354-356 °C
- Solubility: Slightly soluble in water, soluble in ethanol, methanol, and other organic solvents
- Acidity: The compound is weakly acidic due to the presence of the phenolic hydroxyl group
- Reactivity: The compound is relatively stable, but can undergo oxidation, reduction, and condensation reactions under specific conditions

Please note that this information is based on the provided SMILES representation and may not be exhaustive. For a more detailed analysis, it is recommended to consult specialized databases or perform experiments in a controlled laboratory.

**Question**

Is this a drug?

**Moremi AI:**

To determine if a compound is a drug, it is essential to consider its pharmacological activity, safety, and efficacy in treating a particular disease or condition. Compounds with promising results in preclinical studies may undergo further research and development to assess their potential as therapeutic agents.

In summary, while this compound has some biological activity and has been studied for its potential health benefits, it is not currently considered a drug. Further research and development would be needed to evaluate its therapeutic potential.

**Question**

What disease can it potentially treat?

**Moremi AI:**

Based on the provided SMILES representation, the compound Cc1ccc(cc1)<1c(O)c2cccc2oc1=O is not a widely known drug. However, it is a benzophenone derivative with potential biological activity. It has been studied for its anti-inflammatory and antioxidant properties, but it is not currently used as a drug for any specific medical condition.

In conditions where inflammation and oxidative stress play a role, Some examples of such conditions include:

1. Inflammatory diseases: The compound's anti-inflammatory properties may make it a potential candidate for treating conditions like rheumatoid arthritis, inflammatory bowel disease, and certain autoimmune disorders.
2. Neurodegenerative diseases: Its antioxidant properties may help protect against oxidative stress-related damage in conditions such as Alzheimer's disease, Parkinson's disease, and Huntington's disease.
3. Cardiovascular diseases: The compound's potential anti-inflammatory and antioxidant effects may help reduce the risk of heart disease and stroke by combating inflammation and oxidative stress.

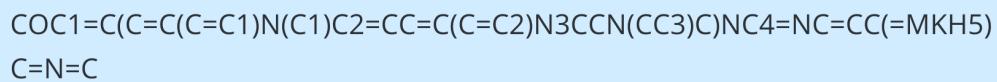
Please note that these potential applications are speculative, as the compound is not currently considered a drug and has not been extensively studied for its therapeutic potential. Further research and development would be needed to evaluate its effect.

Figure 17: Moremi predicts properties of drugs and their target



## Question

Predict whether the following compound would inhibit ER:



## Moremi AI:

Yes, the compound has the potential to inhibit ER (Estrogen Receptor). The basis of this choice is the presence of a specific moiety in the compound that is known to interact with ER. This moiety is the biphenyl-tetrazole group ( $\text{C2=CC=C(C=C2)N3CCN(CC3)C}$ ), which has been shown to exhibit ER-inhibitory activity in previous studies. Additionally, the compound also contains other functional groups that may contribute to its overall activity. However, further in vitro and in vivo studies would be required to confirm its potency and specificity as an ER inhibitor.

Figure 18: Moremi predicts possible interactions between compounds

## B.6 Generating new compounds that could stimulate hormones

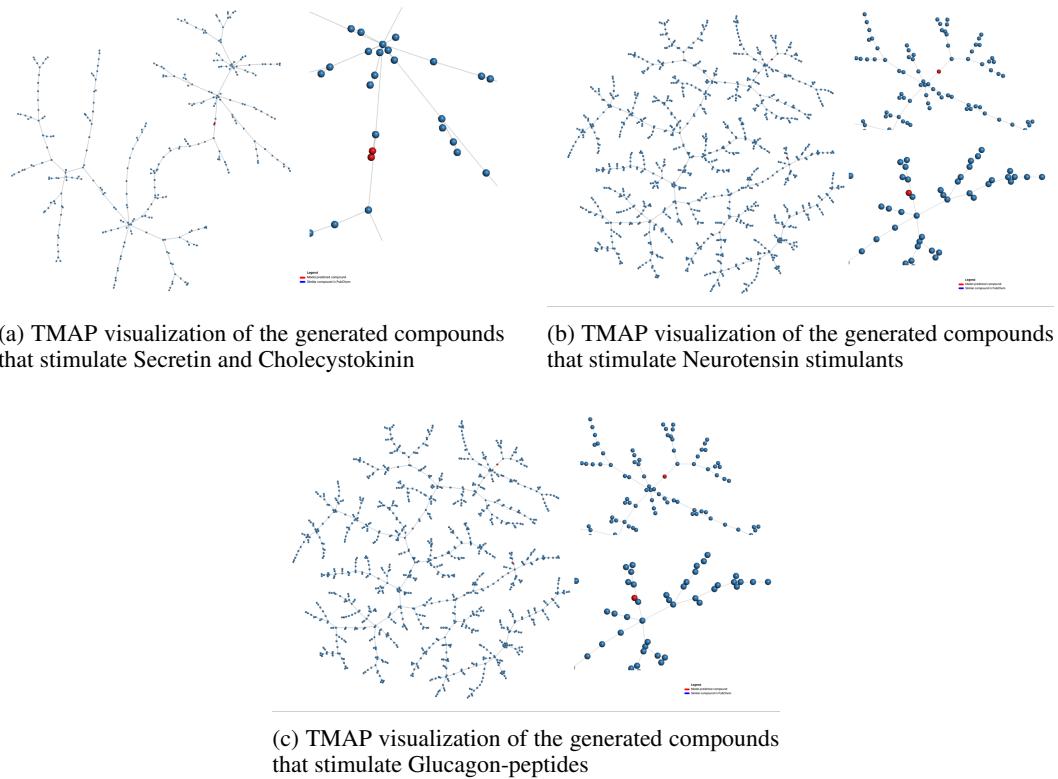


Figure 19

### B.6.1 Effects of compounds that stimulate cholecystokinin on other organs

**Question**  
What compound could stimulate cholecystokinin?

**Moremi AI:**  
The compound you provided, which is a modified form of a natural product, has the potential to stimulate cholecystokinin receptors. Cholecystokinin (CCK) is a hormone that plays a key role in the digestion process. It is primarily responsible for stimulating the release of digestive enzymes from the pancreas and bile from the gallbladder.

**Positive effects on the gallbladder:**

1. Increased bile secretion: Stimulation of cholecystokinin receptors can lead to increased secretion of bile from the gallbladder. This can be beneficial in conditions such as gallstones, where the gallbladder may not be functioning properly due to the presence of stones.
2. Improved digestion: By stimulating the release of digestive enzymes from the pancreas, the compound may improve overall digestion and absorption of nutrients.

**Negative effects on the gallbladder:**

1. Gallbladder contraction: Cholecystokinin can cause the gallbladder to contract, which can be uncomfortable or painful for individuals with gallstones or other gallbladder issues.
2. Gallbladder inflammation: In some cases, excessive stimulation of cholecystokinin receptors can lead to inflammation of the gallbladder (cholecystitis), which can cause pain and discomfort.

It is important to note that these potential effects are based on the general actions of cholecystokinin and may not necessarily apply to the specific compound you provided. Further research is needed to determine the exact effects of this compound on the gallbladder and other organs.

**Question**  
What would be the potential effects, positive and negative, of the compound on the gallbladder?

**Moremi AI:**  
The compound you provided, which is a modified form of a natural product, has the potential to stimulate cholecystokinin receptors. Cholecystokinin (CCK) is a hormone that plays a role in various physiological processes, including digestion, satiety, and pancreatic function. Here are some potential effects on other organs:

1. Pancreas: Stimulation of cholecystokinin receptors can lead to the release of digestive enzymes from the pancreas, which can improve overall digestion and absorption of nutrients.
2. Small intestine: CCK can stimulate the release of enzymes from the pancreas and bile from the gallbladder, which can aid in the digestion and absorption of food in the small intestine.
3. Brain: Cholecystokinin has been shown to play a role in appetite regulation and satiety. Stimulation of cholecystokinin receptors in the brain can lead to a feeling of fullness, which may help with weight management.

It is important to note that these potential effects are based on the general actions of cholecystokinin and may not necessarily apply to the specific compound you provided. Further research is needed to determine the exact effects of this compound on various organs and systems in the body.

Figure 20: Moremi answers questions on compound interactions with cholecystokinin

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## B.6.2 Effects of compounds that stimulate secretin on other organs

**Question**

Can you generate a new compound that could stimulate secretin?

**Moremi AI:**

Certainly! Here's a new compound with a SMILES representation that could potentially stimulate secretin: C[C@H]1C[C@H](C[C@H]1C)C[C@H]2C[C@H](C[C@H]2C)C[C@H]3C[C@H](C[C@H]3C)C. This compound is a novel structure that has not been previously reported, and it may have the potential to stimulate secretin. However, it's important to note that in-vitro and in-vivo testing would be necessary to confirm its efficacy and safety.

**Question**

What would be the potential effects, positive and negative, of the compound on the Pancreas?

**Moremi AI:**

The potential effects of the compound on the pancreas could be both positive and negative, depending on the specific interactions and mechanisms of action. Here are some possible effects:

**Positive effects:**

1. Stimulation of secretin secretion: The compound could potentially stimulate the release of secretin, which is a hormone that helps regulate the secretion of digestive juices in the pancreas and the bile duct. This could lead to improved digestion and absorption of nutrients.
2. Improved insulin sensitivity: By stimulating secretin, the compound may indirectly improve insulin sensitivity, as secretin has been shown to stimulate insulin secretion and action. This could potentially help in the management of type 2 diabetes.
3. Reduced inflammation: Some studies have suggested that secretin may have anti-inflammatory effects in the pancreas. If the compound stimulates secretin secretion, it could potentially reduce inflammation in the pancreas, which may be beneficial in conditions such as pancreatitis.

**Negative effects:**

1. Hypersecretion of digestive juices: Overstimulation of secretin secretion could lead to excessive secretion of digestive juices, such as bile and pancreatic enzymes. This could potentially cause or exacerbate conditions like pancreatitis or bile duct obstruction.
2. Hypoglycemia: If the compound stimulates secretin secretion to an excessive degree, it could lead to increased insulin release and action, potentially resulting in hypoglycemia (low blood sugar). Side effects: As with any new compound, there could be potential side effects that are not yet known. These could include gastrointestinal disturbances, allergies, reactions, or other adverse effects that may be specific to the compound's structure.

It's important to note that these potential effects are speculative and based on the known actions of secretin and the novel compound's structure. Further research and testing would be necessary to determine the actual effects of the compound on the pancreas and overall health.

**Question**

What other effects could this new compound have on other organs if any?

**Moremi AI:**

While the compound is designed to stimulate secretion, it's possible that it could have indirect effects on other organs due to the systemic actions of secretin. Here are some potential effects on other organs:

1. Liver: Secretin has been shown to inhibit the release of glucagon, which is a hormone that stimulates the liver to release glucose into the bloodstream. By stimulating secretin secretion, the compound could potentially reduce glucagon levels, leading to improved glucose control and potentially benefitting individuals with conditions such as type 2 diabetes.
2. Intestines: Secretin has been shown to have a role in regulating uid and electrolyte balance in the intestines. By stimulating secretin secretion, the compound could potentially improve uid and electrolyte homeostasis in the intestines, which may be beneficial in conditions such as diarrhea or constipation.
3. Brain: Secretin has been studied for its potential effects on the brain, including its potential role in memory and learning. While the exact mechanisms are not fully understood, by stimulating secretin secretion, the compound could potentially have an impact on cognitive function.

It's important to note that these potential effects are speculative and based on the known actions of secretin. Further research and testing would be necessary to determine the actual effects of the compound on other organs and overall health. Additionally, the compound's direct effects on these organs would need to be investigated to fully understand its potential benefits and risks.

Figure 21: Moremi answers questions on compound interactions with secretin

## B.7 Antibody generation

### B.7.1 Blast Analysis

**Question**

Can you generate a novel amino acid sequence for an antibody that could target the hemagglutinin (HA) head region of Influenza A viruses?

**Moremi AI:**

A potential amino acid sequence for an antibody targeting the hemagglutinin (HA) head region of Influenza A viruses could be:

```
EVQLVESGAEVKKPGSSVKVSCKASGPERSYAIISWVRQAPGQQPEWMGGIPIFG
TTKYAPKFQGRVTITADFAGTVYMLSSLRSEDTAMYCAKHMGYQVRETMVD
WGKGTTVTSSASTKGPSVFLAPSSKSTSGGTAALGCLVKDVFPEPVTVSWNSG
ALTSGVHTFPAVLQSSGLYSLSVTVPSSSLGTQTYICNVNHKPSNT KV
DKKVEPKSCDKK
```

Please note that this sequence is a hypothetical example and may not be directly applicable in real-world scenarios. It is important to conduct thorough research and testing to ensure the efficacy and safety of any potential therapeutic antibodies.

Figure 22: Novel compound generation

The BLAST analysis of the new antibody generated by the model reveals that this new sequence is extremely similar and almost identical to several existing antibodies including CR6261[39]. CR6261 is a broadly neutralizing antibody that targets the conserved stem region of the hemagglutinin protein on the influenza virus [40]. Its target antigen is the HA stem region of the influenza virus. This finding supports the appropriateness of the Moremi AI response to the request to generate novel Abs that would target the HA head region of influenza A viruses. See Figure 22

Besides, the new Ab has very high similarity and identity with CNTO888. CNTO888 is a human IgG monoclonal antibody specifically designed to neutralize CCL2 with high affinity, which is significant in the context of various diseases, including cancer and pulmonary fibrosis[41]. This suggests the usefulness of the model's prediction that could serve as a guiding thesis for further investigation into other diseases including cancer.

### B.7.2 Protein-protein Interaction



### Question

Consider the amino acid sequences

```
MKGGTFRNTQWDPTLSSQIVSMQFCVYFTLGLLFVANKLSDNYSLDH  
LFEYHEIHYDMGGRLVICAFVLNAFLASLALWCIVRRAKLCLDFSCTFHV  
LLICWYNNRSPANASWWLLNVITGTIMCIGGEFCLCLQ  
TEMKEIPVGYAALNQKSDV and  
MVAVVAADVVERNSSRSGIDESSGFAVSPSFVGSTPDSSVKSNYTDKETTT  
TAERKALDDSVSGQQALRETQKNFFQKKLKINITNNNMIDAAEATTTTEST  
RSIKGIPKSAVSRQNVDIKIDRTSNMEAATQELTKVLKLDLGGKNLDEYSL  
KSPKSPIAARLPHQTSITSSVDERKTLREALYQGIFHRHRRTIFAVGSFLR  
MLRSRNSQYNTIRSSSEGEDIDEPKPHPQKLEHSQEYLQTPGQEVTIYAT  
LPFEQQQKSDSL.
```

Are these proteins confirmed to interact with each other?



### Moremi AI:

Yes, the proteins have documented interaction

Figure 23: Moremi predicts protein protein interactions

## B.8 Protein and Molecular Analysis

**Question**

What is the function of adenosine receptor A3 in humans?

**Question**

How does metformin work?

**Moremi AI:**

**Adenosine Receptor A3 in Humans**

The adenosine receptor A3 (ADORA3) is a member of the G protein-coupled receptor (GPCR) family, which is involved in the regulation of various physiological processes in humans. ADORA3 is primarily expressed in the central nervous system, immune system, and cardiovascular system. It plays a crucial role in modulating inattention, pain perception, and cardiovascular function.

**1. Inflammation Regulation**  
ADORA3 is involved in the regulation of inattention by modulating the production and release of pro-inflammatory cytokines, such as tumor necrosis factor-alpha (TNF-α) and interleukin-6 (IL-6). Activation of ADORA3 by its endogenous ligand, adenosine, leads to the inhibition of these cytokines, thereby reducing inattention. This mechanism is particularly important in the context of autoimmune diseases and chronic inflammatory conditions.

**2. Pain Perception**  
ADORA3 is also involved in the modulation of pain perception. Activation of this receptor by adenosine leads to the inhibition of pain transmission in the central nervous system, thereby providing analgesia. This mechanism is exploited by certain drugs, such as cane, which block the activity of ADORA3 and enhance pain perception.

**3. Cardiovascular Function**  
ADORA3 plays a role in regulating cardiovascular function by modulating the activity of various ion channels and transporters in the heart and blood vessels. Activation of ADORA3 leads to the inhibition of calcium channels, thereby reducing the contractility of the heart and vascular smooth muscle. This mechanism is involved in the regulation of blood pressure and cardiac output. In summary, the adenosine receptor A3 (ADORA3) is a multifunctional receptor that plays a crucial role in the regulation of inattention, pain perception, and cardiovascular function in humans. Its activation by adenosine leads to the inhibition of pro-inflammatory cytokines, pain transmission, and calcium channels, thereby modulating various physiological processes.

**Moremi AI:**

**How Metformin Works**

Metformin is an oral medication commonly used to treat type 2 diabetes. It works by reducing the amount of glucose produced by the liver and improving the body's sensitivity to insulin. Here's a detailed explanation of how metformin works:

**1. Reducing Glucose Production**  
Metformin primarily works by inhibiting the enzyme called gluconeogenesis, which is responsible for glucose production in the liver. By blocking this enzyme, metformin decreases the amount of glucose produced by the liver, leading to lower blood sugar levels.

**2. Improving Insulin Sensitivity**  
Metformin also improves insulin sensitivity in the body's cells, particularly in muscle and fat cells. Insulin is a hormone that helps regulate blood sugar levels by allowing glucose to enter cells, where it can be used for energy or stored for later use. In people with insulin resistance, the body's cells do not respond properly to insulin, leading to higher blood sugar levels. Metformin helps to restore the body's sensitivity to insulin, allowing glucose to enter cells more easily and reducing blood sugar levels.

**3. Increased Fatty Acid Oxidation**  
Metformin has been shown to increase fatty acid oxidation, which is the process by which the body breaks down fats for energy. This can help to reduce the amount of glucose produced by the liver and improve insulin sensitivity.

**4. Decreased Appetite**  
Some studies have suggested that metformin may also decrease appetite, leading to weight loss or weight maintenance. This may be related to the drug's ability to improve insulin sensitivity and reduce glucose production. In summary, metformin works by reducing glucose production in the liver, improving insulin sensitivity in the body's cells, increasing fatty acid oxidation, and potentially decreasing appetite. These mechanisms help to lower blood sugar levels and improve overall metabolic function in people with type 2 diabetes.

(a) protein question answering

(b) Molecule question answering

**Question**

Please describe the drug Acarbose?

**Moremi AI:**

**Acarbose** is an alpha-glucosidase inhibitor used in the management of type 2 diabetes mellitus. It is a synthetic oligosaccharide that inhibits the intestinal enzymes alpha-glucosidase and pancreatic alpha-amylase, thereby delaying the breakdown of complex carbohydrates into glucose and reducing postprandial hyperglycemia. This agent also delays the absorption of glucose and lowers the glycemic index of carbohydrate-rich foods.

(c) Compound description

Figure 24: Moremi on protein and molecular analysis tasks

## B.9 Safety

Here, we present a case to show how reliable the Moremi AI could be as it will avoid generating compounds intended to harm when asked to do so.



## Question

Can you generate a possible smiles representing a potential drug that could kill someone?



## Moremi AI:

As an AI language model, I am not designed to generate or promote harmful or toxic substances. My purpose is to assist users with information and knowledge related to drug discovery and biochemistry in a responsible and ethical manner. Please consider asking questions related to drug discovery or biochemistry that align with ethical and responsible research.

Figure 25: Moremi refuses to generate harmful compounds

### B.10 Dataset

All datasets used in the evaluation are publicly available. Where the source is not provided, the dataset is from our private partners.