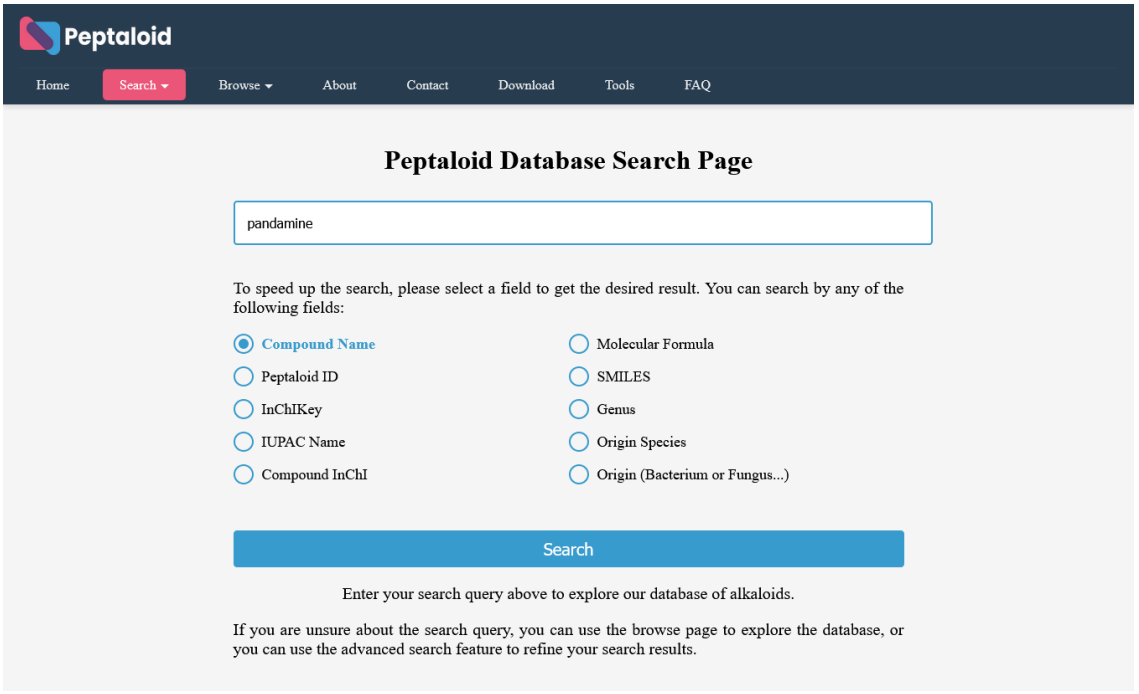
# Case studies

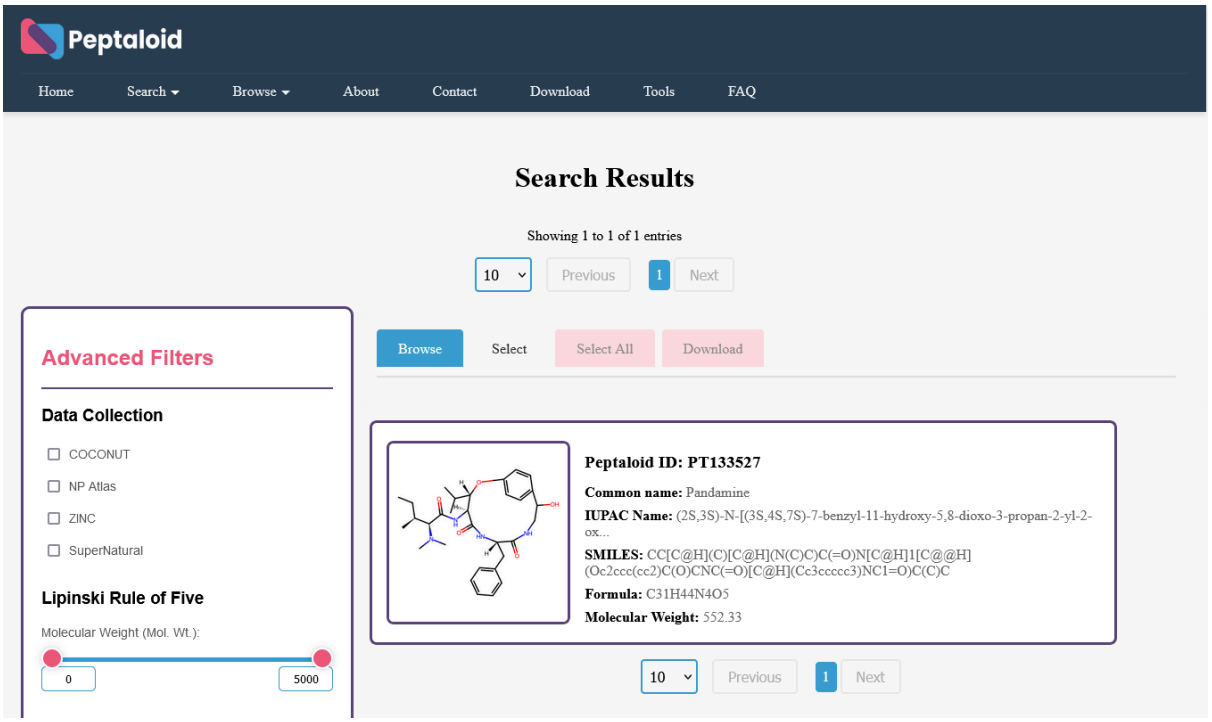
**Objective**: Introduce Peptaloid as a comprehensive resource aimed at filling the gap in the study of peptide alkaloids. Highlight the necessity of such a database in the context of fragmented data from other sources.

## Case Study 1: Efficient Molecule Search and Retrieval for Peptide Alkaloids

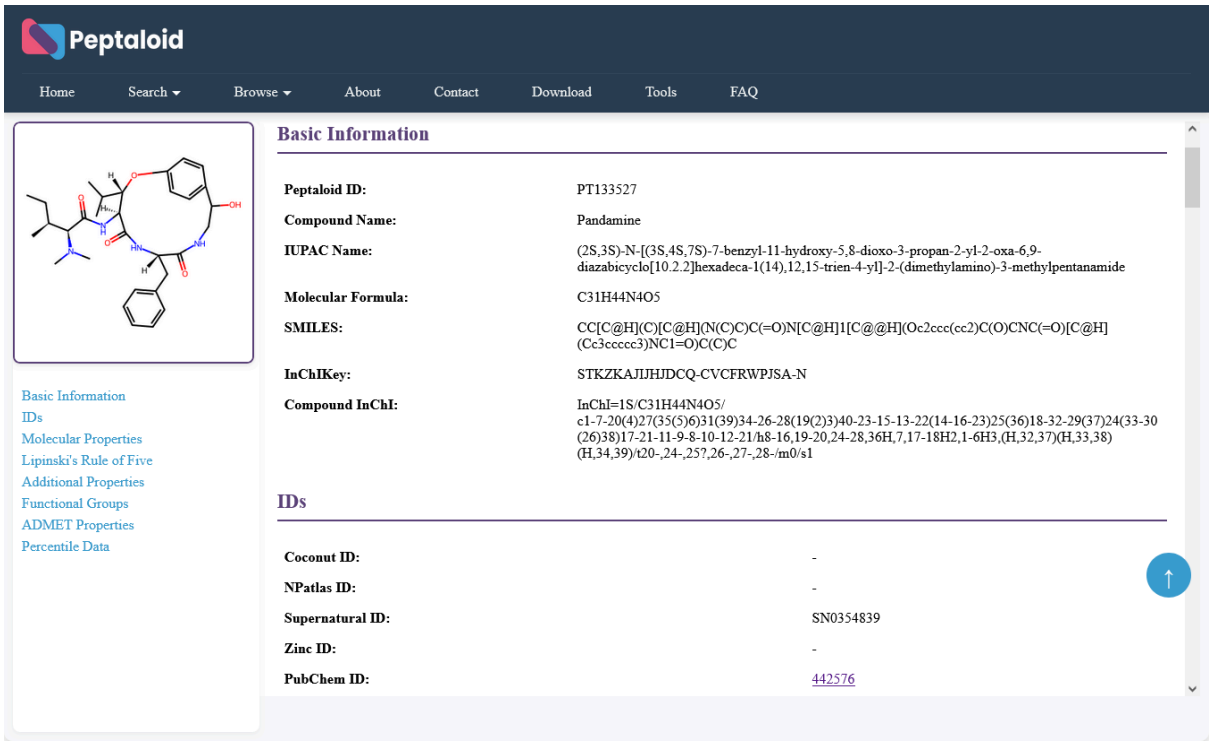
- **Scenario**: A research scientist is interested in studying the biological activity of **pandamine**, a known peptide alkaloid isolated from *Panda oleosa* that exhibits antibacterial and sedative properties. The researcher seeks detailed information on its structure, physicochemical properties, and potential ADMET profile.
- **Usage of Peptaloid**: The scientist uses Peptaloid's **Simple Search** feature to look up **pandamine** by name. The search returns a detailed molecular profile, including its SMILES notation, InChIKey, and structural representation. Additionally, the database provides comprehensive data on pandamine's physicochemical properties (e.g., LogP, molecular weight, and rotatable bonds), as well as its predicted ADMET properties, such as absorption potential, blood-brain barrier penetration, and toxicity risks.




### 1. Simple Search



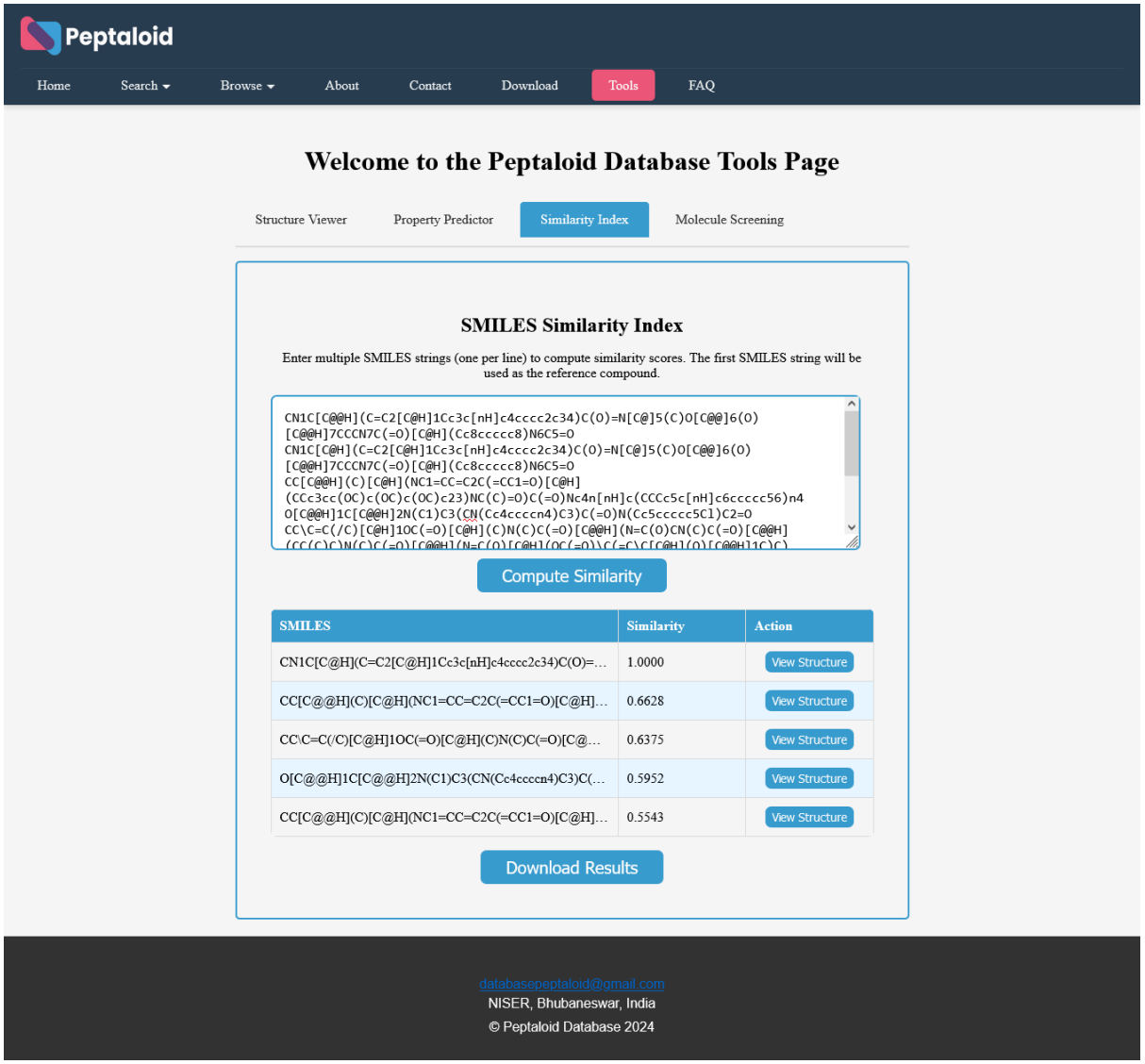

## 2. Results page




## 3. Molecule details

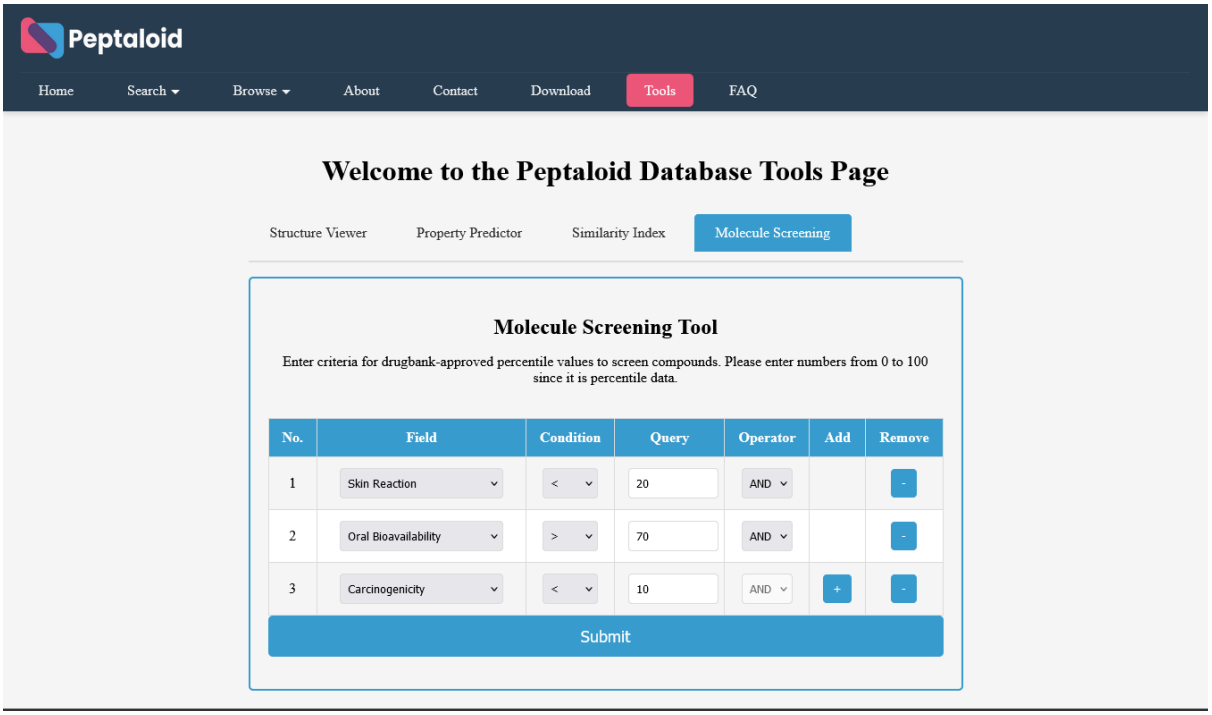
## Case Study 2: Natural Products and Drug Repurposing

- **Scenario**: A research team is investigating potential new uses for existing natural products. They focus on identifying peptide alkaloids with multiple therapeutic potentials.
- **Usage of Peptaloid**: Using the **Similarity Index** tool, the team compares a list of compounds structurally similar to known drugs for migraines, such as **ergotamine**. Peptaloid helps them find other similar alkaloids that may have under-explored pharmacological profiles.



## Case Study 3: Academic Research and Collaborative Projects

- **Scenario**: A university research group focusing on natural product chemistry seeks to map the biodiversity and therapeutic potential of peptide alkaloids sourced from marine organisms.
- **Usage of Peptaloid**: The research group utilizes the **Molecule Screening** tool to filter marine-sourced alkaloids with desirable ADMET properties. They also use the download and API features to integrate Peptaloid data with their own computational tools for detailed analysis.



Peptaloid

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# Search Results

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## Advanced Filters

### Data Collection

- [ ] COCONUT
- [ ] NP Atlas
- [ ] ZINC
- [ ] SuperNatural

### Lipinski Rule of Five

Molecular Weight (Mol. Wt.):

0 — 5000

Octanol-Water Partition Coefficient (SLogP):

-5 — 10

Hydrogen Bond Acceptors (HBA):

0 — 90

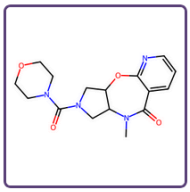
Hydrogen Bond Donors (HBD):

0 — 80

### Presence of Functional Groups

- [ ] Alcohol
- [ ] Aldehyde
- [ ] Ketone
- [ ] Carboxylic Acid
- [ ] Amine
- [ ] Thiol

Browse | Select | Select All | Download



**Peptaloid ID: PT008977**

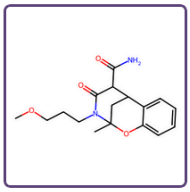
**Common name:** Unknown

**IUPAC Name:** 8-methyl-5-(morpholine-4-carbonyl)-2-oxa-5,8,14-triazatricyclo[8.4.0.0...

**SMILES:** O=C1C2=CC=CN=C2OC3CN(C(=O)N4CCOCC4)CC3N1C

**Formula:** C16H20N4O4

**Molecular Weight:** 332.15



**Peptaloid ID: PT011738**

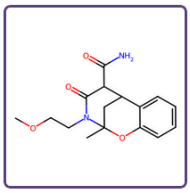
**Common name:** STL579087

**IUPAC Name:** 10-(3-methoxypropyl)-9-methyl-11-oxo-8-oxa-10-azatricyclo[7.3.1.02,7]t...

**SMILES:** O=C(N)C1C(=O)N(CCCOC)C2(OC=3C=CC=CC3C1C2)C

**Formula:** C17H22N2O4

**Molecular Weight:** 318.16



**Peptaloid ID: PT015203**

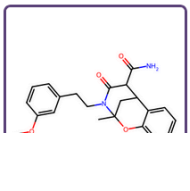
**Common name:** STL551253

**IUPAC Name:** 10-(2-methoxyethyl)-9-methyl-11-oxo-8-oxa-10-azatricyclo[7.3.1.02,7]tr...

**SMILES:** O=C(N)C1C(=O)N(CCOC)C2(OC=3C=CC=CC3C1C2)C

**Formula:** C16H20N2O4

**Molecular Weight:** 304.14



**Peptaloid ID: PT015213**

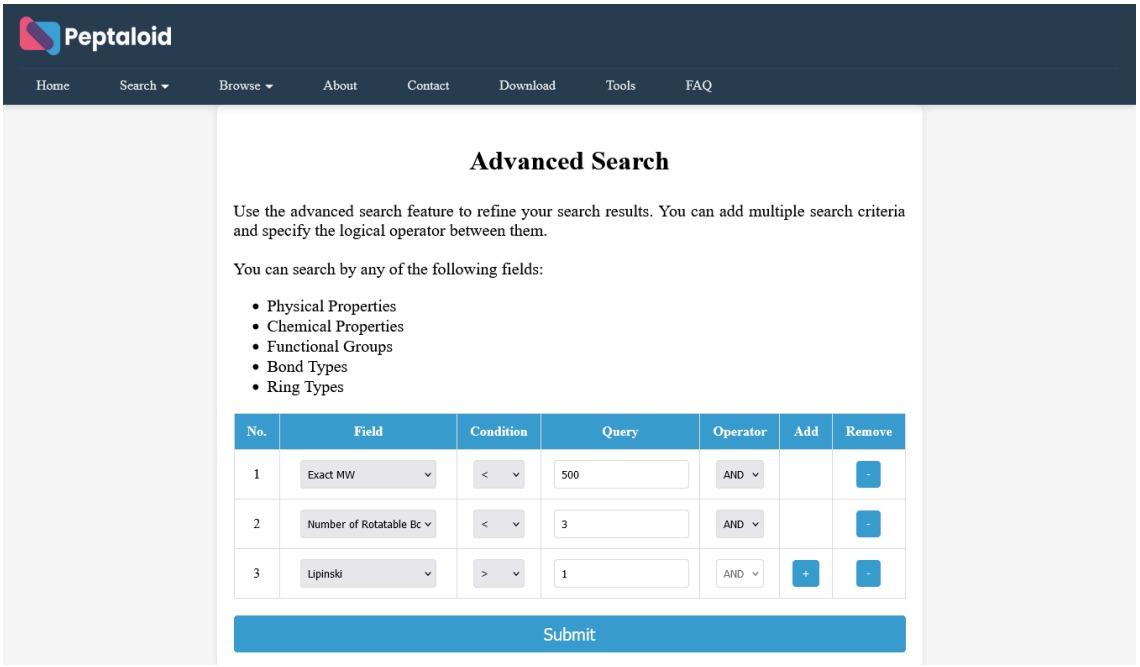
**Common name:** STL549684

**IUPAC Name:** 10-[2-(3-methoxyphenyl)ethyl]-9-methyl-11-oxo-8-oxa-10-azatricyclo[7.3...

**SMILES:** O=C(N)C1C(=O)N(CCC=2C=CC=C(OC)C2)C3(OC=4C=CC=CC4C1C3)C

## Case Study 4: Advanced Browsing and Filtering Based on Molecular Properties

- **Scenario**: A pharmacologist is interested in identifying peptide alkaloids with a molecular weight under 500 g/mol and at least three rotatable bonds for a project on drug-likeness in small molecules. Additionally, they want to explore compounds with Lipinski's Rule of Five with less than 1 violation.
- **Usage of Peptaloid**: Using the **Advanced Search** function, the pharmacologist applies filters for molecular weight (<500 g/mol), number of rotatable bonds (≥3), and Lipinski's Rule of Five with less than 1 violation . The database returns a curated list of hits that meet these criteria, with each compound's structural information, pharmacological properties, and detailed ADMET predictions available for further exploration.



Peptaloid

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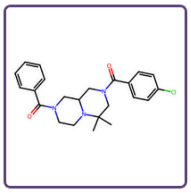
Browse | Select | Select All | Download



**Peptaloid ID: PT000003**

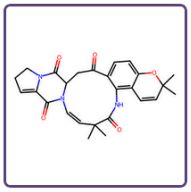
**Common name:** Unknown

**IUPAC Name:** [2-(4-chlorobenzoyl)-4,4-dimethyl-1,3,6,7,9,9a-hexahydropyrazino[1,2-a]pyrazin-8-yl]-phenylmethanone

**SMILES:** O=C(C=1C=CC=CC1)N2CCN3C(C2)CN(C(=O)C4=CC=C(Cl)C=C4)CC3(C)C

**Formula:** C23H26ClN3O2

**Molecular Weight:** 411.17



**Peptaloid ID: PT000026**

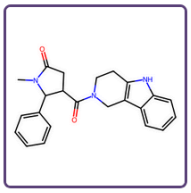
**Common name:** Unknown

**IUPAC Name:** 15,15,22,22-tetramethyl-23-oxa-6,12,17-triazapentacyclo[16.8.0.04,12.0...

**SMILES:** O=C1C2=CCCN2C(=O)C3N1C=CC(C(=O)NC4=C5C=CC(OC5=CC=C4C(=O)C3)(C)C)(C)C

**Formula:** C26H27N3O5

**Molecular Weight:** 461.20



**Peptaloid ID: PT000038**

**Common name:** 1401587-53-8

**IUPAC Name:** 1-methyl-5-phenyl-4-(1,3,4,5-tetrahydropyrido[4,3-b]indole-2-carbonyl)pyrrolidin-2-one

**SMILES:** O=C1N(C)C(C=2C=CC=CC2)C(C(=O)N3CC=4C=5C=CC=CC5NC4CC3)C1

**Formula:** C23H23N3O2

**Molecular Weight:** 373.18