

Peptaloid: A Comprehensive Database for Exploring Peptide Alkaloid

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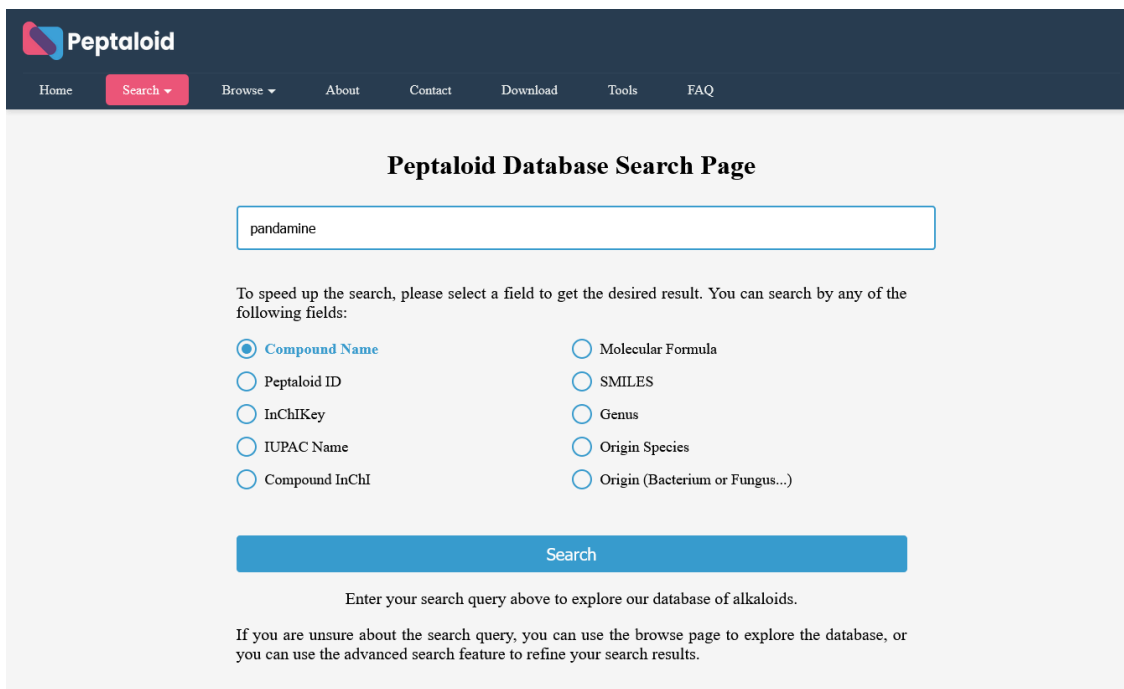
Case studies

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



The screenshot displays the Peptaloid website's search interface. At the top is a dark blue navigation bar with the Peptaloid logo and links for Home, Search, Browse, About, Contact, Download, Tools, and FAQ. The main content area is titled 'Peptaloid Database Search Page'. It features a search input field containing the text 'pandamine'. Below the input field, a message states: 'To speed up the search, please select a field to get the desired result. You can search by any of the following fields:'. There are two columns of radio button options: 'Compound Name' (selected), 'Peptaloid ID', 'InChIKey', 'IUPAC Name', 'Compound InChI', 'Molecular Formula', 'SMILES', 'Genus', 'Origin Species', and 'Origin (Bacterium or Fungus...)'. A large blue 'Search' button is positioned below the options. At the bottom, there is a prompt: 'Enter your search query above to explore our database of alkaloids.' followed by a note: 'If you are unsure about the search query, you can use the browse page to explore the database, or you can use the advanced search feature to refine your search results.'

2. Results Page



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Search Results

Showing 1 to 1 of 1 entries

10

Previous

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Advanced Filters

Data Collection

☐ COCONUT

☐ NP Atlas

☐ ZINC

☐ SuperNatural

Lipinski Rule of Five

Molecular Weight (Mol. Wt.):

0

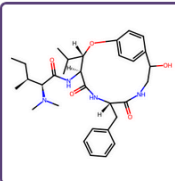
5000

Browse

Select

Select All

Download



Peptaloid ID: PT133527

Common name: Pandamine

IUPAC Name: (2S,3S)-N-[(3S,4S,7S)-7-benzyl-11-hydroxy-5,8-dioxo-3-propan-2-yl-2-oxo-...]

SMILES: CC[C@H](C)[C@H](N(C)C)C(=O)N[C@H]1[C@@H](Oc2ccc(cc2)C(O)CNC(=O)[C@H](Cc3ccccc3)NC1=O)C(C)C

Formula: C31H44N4O5

Molecular Weight: 552.33


10

Previous

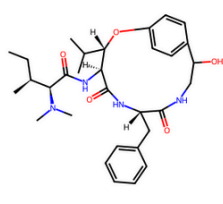
1

Next

3. Molecule Details



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Basic Information

IDs

Molecular Properties

Lipinski's Rule of Five

Additional Properties

Functional Groups

ADMET Properties

Percentile Data

Basic Information

| | |
|---------------------------|---|
| Peptaloid ID: | PT133527 |
| Compound Name: | Pandamine |
| IUPAC Name: | (2S,3S)-N-[(3S,4S,7S)-7-benzyl-11-hydroxy-5,8-dioxo-3-propan-2-yl-2-oxa-6,9-diazabicyclo[10.2.2]hexadeca-1(14),12,15-trien-4-yl]-2-(dimethylamino)-3-methylpentanamide |
| Molecular Formula: | C31H44N4O5 |
| SMILES: | CC[C@H](C)[C@H](N(C)C)C(=O)N[C@H]1[C@@H](Oc2ccc(cc2)C(O)CNC(=O)[C@H](Cc3ccccc3)NC1=O)C(C)C |
| InChIKey: | STKZKAJJHJDCQ-CVCFRWPJSA-N |
| Compound InChI: | InChI=1S/C31H44N4O5/c1-7-20(4)27(35(5)6)31(39)34-26-28(19(2)3)40-23-15-13-22(14-16-23)25(36)18-32-29(37)24(33-30(26)38)17-21-11-9-8-10-12-21/h8-16,19-20,24-28,36H,7,17-18H2,1-6H3,(H,32,37)(H,33,38)(H,34,39)/t20-,24-,25?,26-,27-,28-/m0/s1 |


IDs

| | |
|-------------------------|------------------------|
| Coconut ID: | - |
| NPAtlas ID: | - |
| Supernatural ID: | SN0354839 |
| Zinc ID: | - |
| PubChem ID: | 442576 |

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.

1. Using Similarity Index



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Welcome to the Peptaloïd Database Tools Page

Structure Viewer

Property Predictor

Similarity Index

Molecule Screening

SMILES Similarity Index

Enter multiple SMILES strings (one per line) to compute similarity scores. The first SMILES string will be used as the reference compound.

CN1C[C@@H](C=C2[C@H]1Cc3c[nH]c4cccc2c34)C(O)=N[C@]5(C)O[C@@]6(O)[C@@H]7CCCN7C(=O)[C@H](Cc8ccccc8)N6C5=O
CN1C[C@H](C=C2[C@H]1Cc3c[nH]c4cccc2c34)C(O)=N[C@]5(C)O[C@@]6(O)[C@@H]7CCCN7C(=O)[C@H](Cc8ccccc8)N6C5=O
CC[C@@H](C)[C@H](NC1=CC=C2C(=CC1=O)[C@H](CCc3cc(OC)c(OC)c(OC)c23)NC(C)=O)C(=O)Nc4n[nH]c(CCCc5c[nH]c6ccccc56)n4O[C@@H]1C[C@@H]2N(C1)C3(CN(Cc4ccccc4)C3)C(=O)N(Cc5ccccc5C1)C2=O
CC\C=C(/C)[C@H]1OC(=O)[C@H](C)N(C)C(=O)[C@H](N=C(O)CN(C)C(=O)[C@H](CC(C)C)N(C)C(=O)[C@H](N=C(O)[C@H]1OC(=O)\C(=C)C[C@H]1(O)[C@H]1C)C

Compute Similarity

| SMILES | Similarity | Action |
|---|------------|--------------------------------|
| CN1C[C@H](C=C2[C@H]1Cc3c[nH]c4cccc2c34)C(O)=... | 1.0000 | View Structure |
| CC[C@H](C)[C@H](NC1=CC=C2C(=CC1=O)[C@H]... | 0.6628 | View Structure |
| CC\C=C(/C)[C@H]1OC(=O)[C@H](C)N(C)C(=O)[C@... | 0.6375 | View Structure |
| O[C@H]1C[C@H]2N(C1)C3(CN(Cc4ccccc4)C3)C(... | 0.5952 | View Structure |
| CC[C@H](C)[C@H](NC1=CC=C2C(=CC1=O)[C@H]... | 0.5543 | View Structure |

Download Results

databasepeptaloïd@gmail.com


NISER, Bhubaneswar, India

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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.

1. Molecule Screening

 **Peptaloid**

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Welcome to the Peptaloid Database Tools Page

Structure ViewerProperty PredictorSimilarity IndexMolecule Screening


Molecule Screening Tool

Enter criteria for drugbank-approved percentile values to screen compounds. Please enter numbers from 0 to 100 since it is percentile data.

| No. | Field | Condition | Query | Operator | Add | Remove |
|-----|------------------------|-----------|-------|----------|-----|--------|
| 1 | Skin Reaction ▾ | < ▾ | 20 | AND ▾ | | - |
| 2 | Oral Bioavailability ▾ | > ▾ | 70 | AND ▾ | | - |
| 3 | Carcinogenicity ▾ | < ▾ | 10 | AND ▾ | + | - |

Submit

2. Results Page



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Search Results

Showing 1 to 10 of 123 entries

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1

2

3

4

5

...

13

Next

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

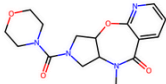
☐ Aldehyde

☐ Ketone

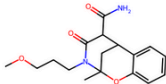
☐ Carboxylic Acid

☐ Amine

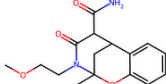
☐ Thiol



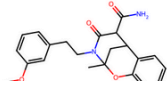
Peptaloid ID: PT008977
Common name: Unknown
IUPAC Name: 8-methyl-5-(morpholine-4-carbonyl)-2-oxa-5,8,14-triazatricyclo[8.4.0.0...
SMILES: O=C1C2=CC=CN=C2OC3CN(C(=O)N4CCOCC4)CC3N1C
Formula: C16H20N4O4
Molecular Weight: 332.15



Peptaloid ID: PT011738
Common name: STL579087
IUPAC Name: 10-(3-methoxypropyl)-9-methyl-11-oxo-8-oxa-10-azatricyclo[7.3.1.02,7]tr...
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.

1. Advanced Search

 **Peptaloid**





Home Search ▾ Browse ▾ About Contact Download Tools FAQ

Advanced Search

Use the advanced search feature to refine your search results. You can add multiple search criteria and specify the logical operator between them.


You can search by any of the following fields:

- Physical Properties
- Chemical Properties
- Functional Groups
- Bond Types
- Ring Types

| No. | Field | Condition | Query | Operator | Add | Remove |
|-----|--------------------------|-----------|-------|----------|---|---|
| 1 | Exact MW ▾ | < ▾ | 500 | AND ▾ | |  |
| 2 | Number of Rotatable Bc ▾ | < ▾ | 3 | AND ▾ | |  |
| 3 | Lipinski ▾ | > ▾ | 1 | AND ▾ |  |  |

Submit

2. Results Page

 **Peptaloid**

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Search Results

Showing 1 to 10 of 300 entries

10

Previous

1

2

3

4

5

...

30

Next

Browse

Select

Select All

Download

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

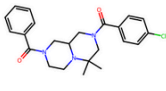
Presence of Functional Groups

☐ Alcohol

☐ Aldehyde

☐ Ketone

☐ Carboxylic Acid



Peptaloid ID: PT000003

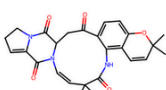
Common name: Unknown

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(=C=CC1)N2CCN3C(C2)CN(C(=O)C4=CC=C(C1)C=C4)CC3(C)C

Formula: C23H26ClN3O2

Molecular Weight: 411.17



Peptaloid ID: PT000026

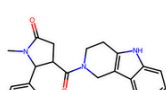
Common name: Unknown

IUPAC Name: 15,15,22,22-tetramethyl-23-oxa-6,12,17-triazapentacyclo[16.8.0.0.04,12.0...

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=C2CC=CC2)C(C(=O)N3CC=4C=5C=CC=CC5NC4CC3)C1

Formula: C23H23N3O2

Molecular Weight: 373.18



Peptaloid ID: PT000047

Note: These case studies illustrate just a few of the diverse ways the Peptaloid database can be employed to advance research in peptide alkaloids, from molecular search and property retrieval to drug repurposing and ADMET screening. However, the scope of Peptaloid is not confined to these examples alone. The database offers an expansive platform with numerous tools and features that enable users to explore, analyze, and apply its data in innovative ways. We encourage researchers to explore the full breadth of the Peptaloid database and discover novel approaches to harnessing its capabilities for their specific scientific inquiries.