

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.

The screenshot displays the Peptaloid website's search interface. At the top is a dark 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 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.'

1. Simple Search

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Search Results

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Select All

Download

Advanced Filters

Data Collection

☐ COCONUT
 ☐ NP Atlas
 ☐ ZINC
 ☐ SuperNatural

Lipinski Rule of Five

Molecular Weight (Mol. Wt.):

0

5000

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-6,9-diazabicyclo[10.2.2]hexadeca-1(14),12,15-trien-4-yl]-2-(dimethylamino)-3-methylpentanamide
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

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2. Results page

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[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-oxo-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-m/s1


IDs

Coconut ID: -
NPAtlas ID: -
Supernatural ID: SN0354839
Zinc ID: -
PubChem ID: [442576](#)

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.



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Welcome to the Peptaloid Database Tools Page

Structure ViewerProperty PredictorSimilarity IndexMolecule 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)c23)NC(C)=O)C(=O)Nc4n[nH]c(CCCc5c[nH]c6ccccc56)n4

O[C@@H]1C[C@@H]2N(C1)C3(CN(Cc4ccccc4)C3)C(=O)N(Cc5ccccc5)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]1N=C(O)[C@H]1OC(=O)\C=C(\C[C@H](O)C[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

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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.

 **Peptaloid**

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Welcome to the Peptaloid Database Tools Page

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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

Search Results

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[Browse](#) [Select](#) [Select All](#) [Download](#)

Advanced Filters

Data Collection

- ☐ COCONUT
☐ NP Atlas
☐ ZINC
☐ SuperNatural

Lipinski Rule of Five

Molecular Weight (Mol. WT.):



Octanol-Water Partition Coefficient (SLogP):



Hydrogen Bond Acceptors (HBA):

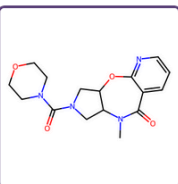


Hydrogen Bond Donors (HBD):



Presence of Functional Groups

- ☐ Alcohol
☐ Aldehyde
☐ Ketone
☐ Carboxylic Acid
☐ Amine
☐ Thiol



Peptaloid ID: PT008977

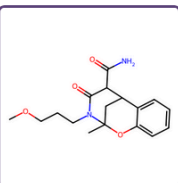
Common name: Unknown

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

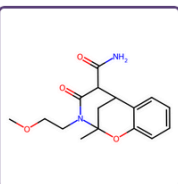
Common name: STL579087

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

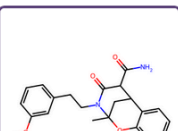
Common name: STL551253

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(CCCOC)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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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

Search Results

Showing 1 to 10 of 300 entries

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Advanced Filters

Data Collection

- ☐ COCONUT
- ☐ NP Atlas
- ☐ ZINC
- ☐ SuperNatural

Lipinski Rule of Five

Molecular Weight (Mol. Wt.):



Octanol-Water Partition Coefficient (SLogP):



Hydrogen Bond Acceptors (HBA):

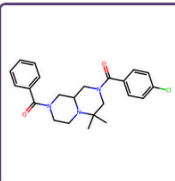


Hydrogen Bond Donors (HBD):



Presence of Functional Groups

- ☐ Alcohol
- ☐ Aldehyde
- ☐ Ketone
- ☐ Carboxylic Acid



Peptaloid ID: PT000003

Common name: Unknown

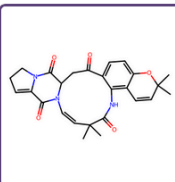
IUPAC Name: [2-(4-chlorobenzoyl)-4,4-dimethyl-1,3,6,7,9,9a-hexahydropyrazino[1,2-a]pyrazin-8-yl]-phenylmethanone

SMILES:

O=C(C=C1C=CC=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

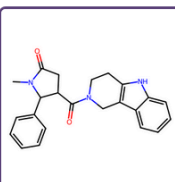
IUPAC Name: 15,15,22,22-tetramethyl-23-oxa-6,12,17-triazapentacyclo[16.8.0.0.4.12.0...

SMILES:

O=C1C2=CCCN2C(=O)C3N1C=CC(C(=O)NC4=C5C=CC(OC5=CC=C4C(=O)C3)(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(=O)C2=CC=CC2)C(C(=O)N3CC=CC(=O)C=C3N4CC3)C1

Formula: C23H23N3O2

Molecular Weight: 373.18

Peptaloid ID: PT000047