Peptaloid: A Comprehensive Database for Exploring Peptide Alkaloid

Bibhu Prasad Behera, Hemangini Naik, V. Badireenath Konkimalla*

[1] School of Biological Sciences, National Institute of Science Education and Research, HBNI, Jatni, Odisha 752050, India; Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai 400094, India,

[2] Department of Biotechnology and Bioinformatics, Sambalpur University, Jyoti Bihar, Burla, 768019, Odisha, India

* The correspondence should be addressed to V. Badireenath Konkimalla, Email: badireenath@niser.ac.in

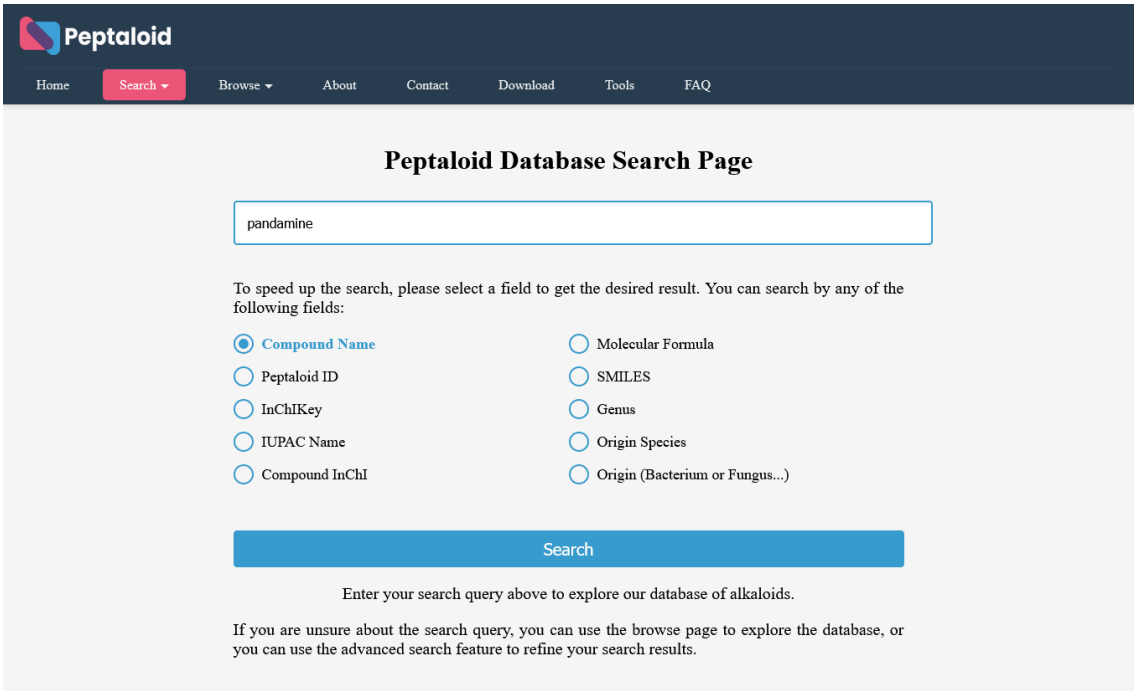
Case studies

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.

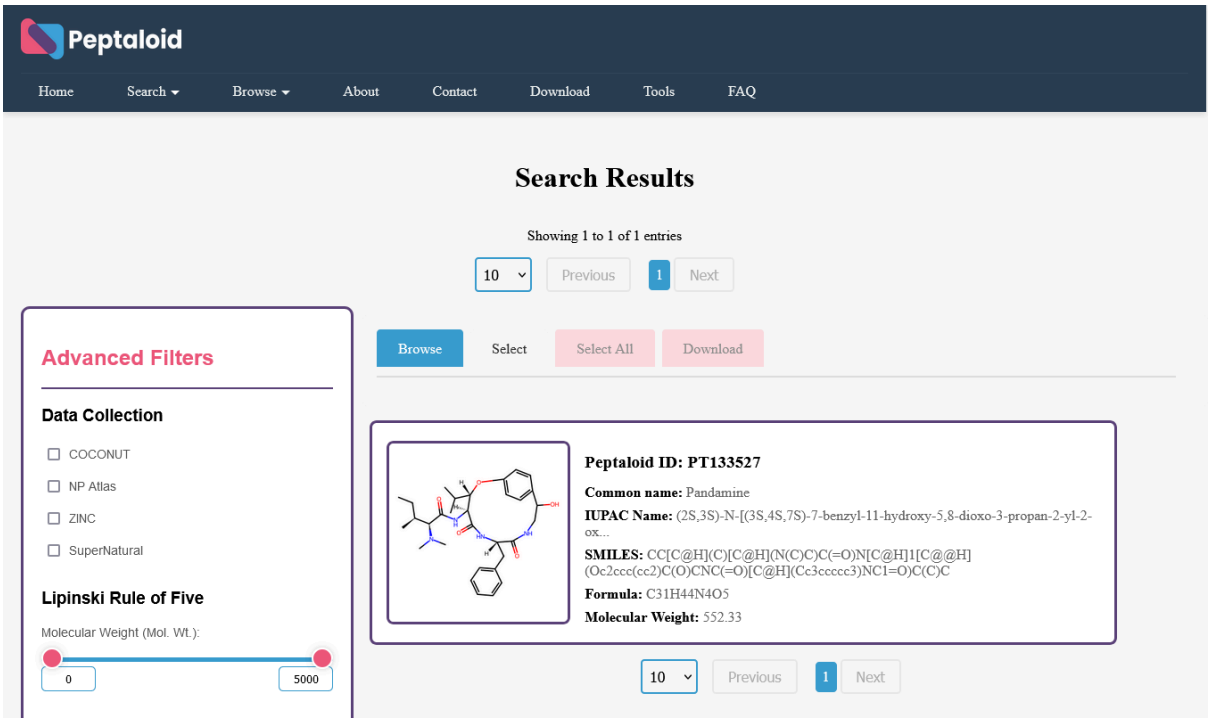
Case Study 1: Efficient Molecule Search and Retrieval for Peptide Alkaloids

- **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.

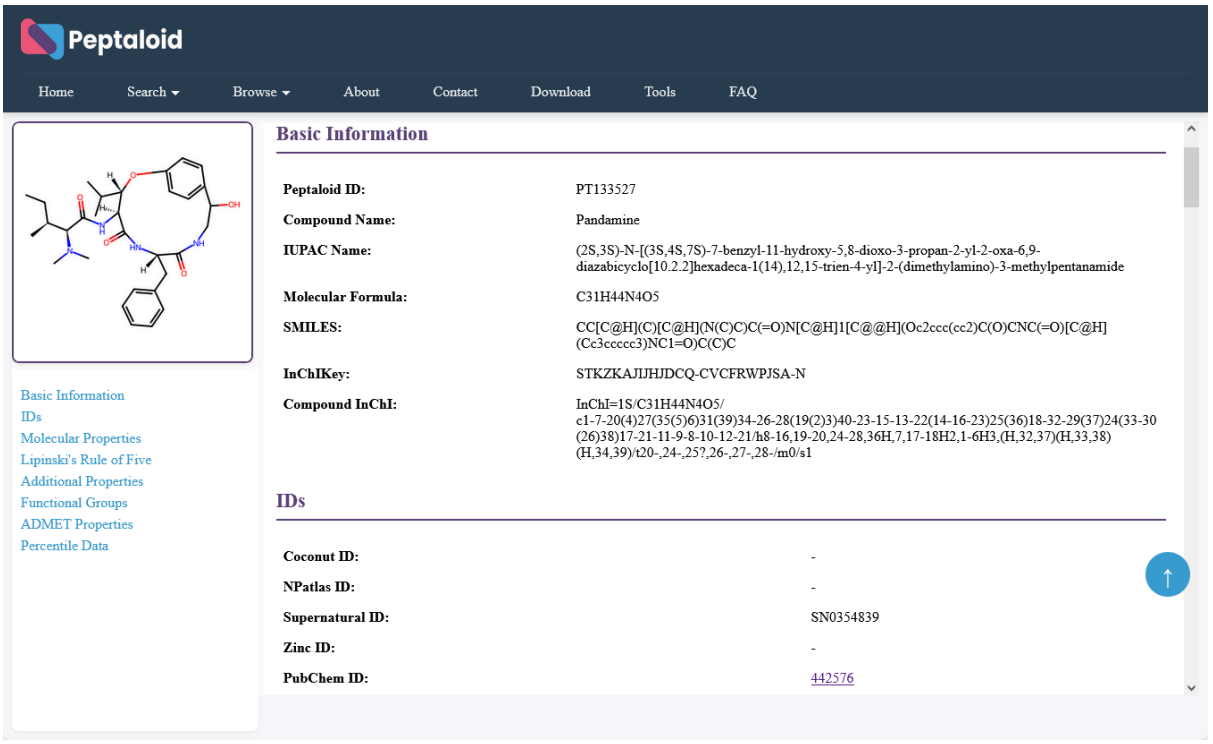
1. Simple Search



2. Results Page



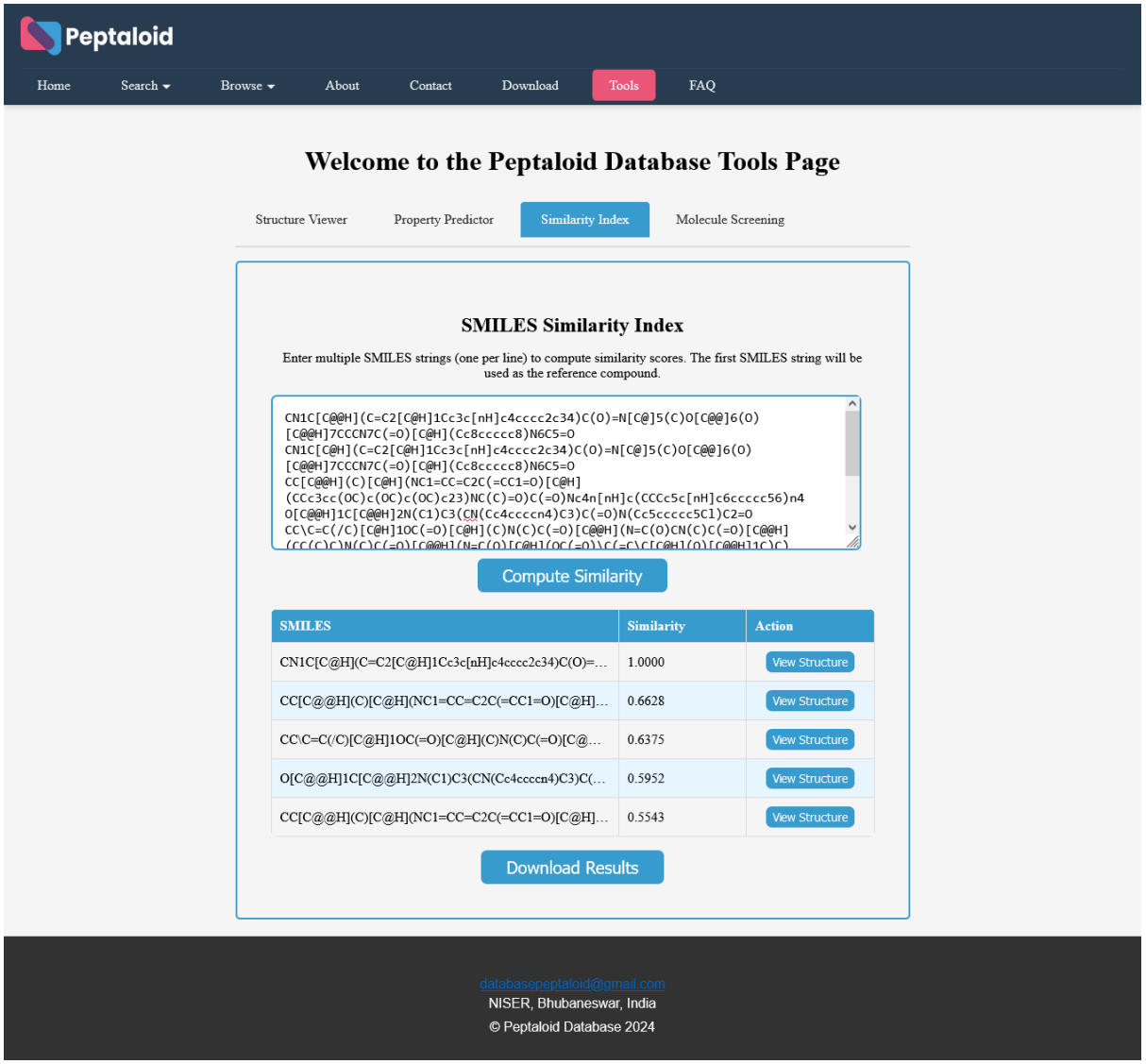
3. Molecule Details



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.

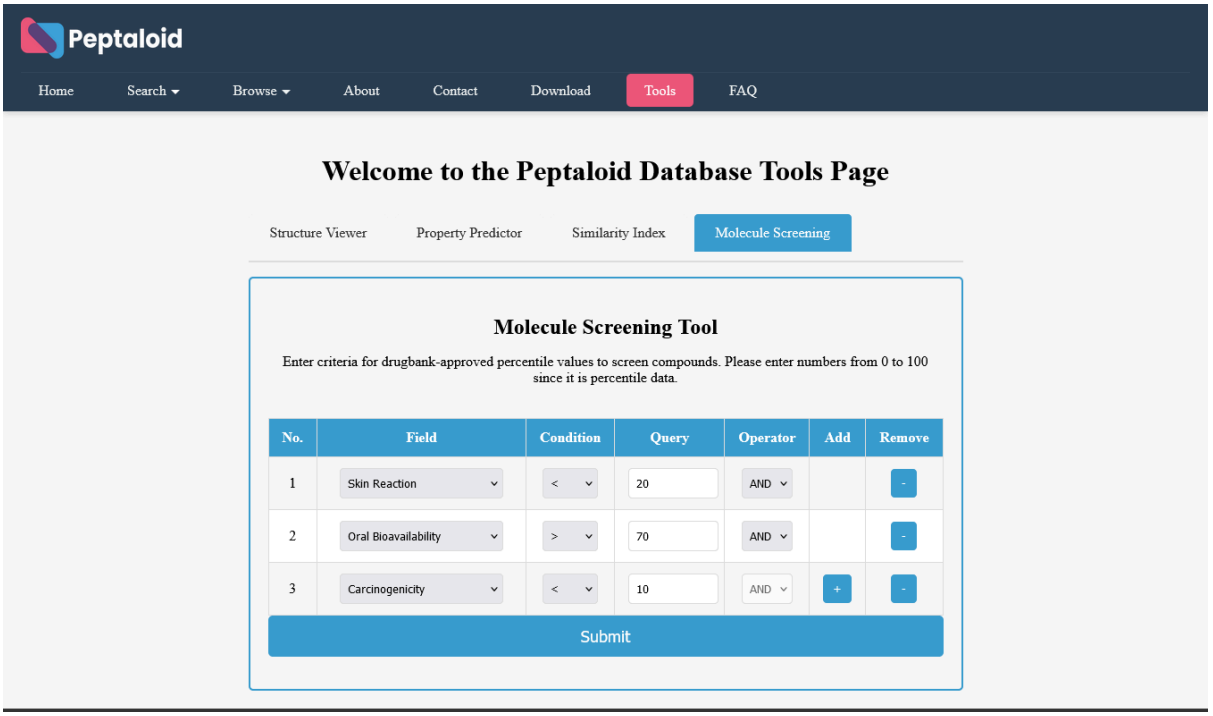
1. Using Similarity Index



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



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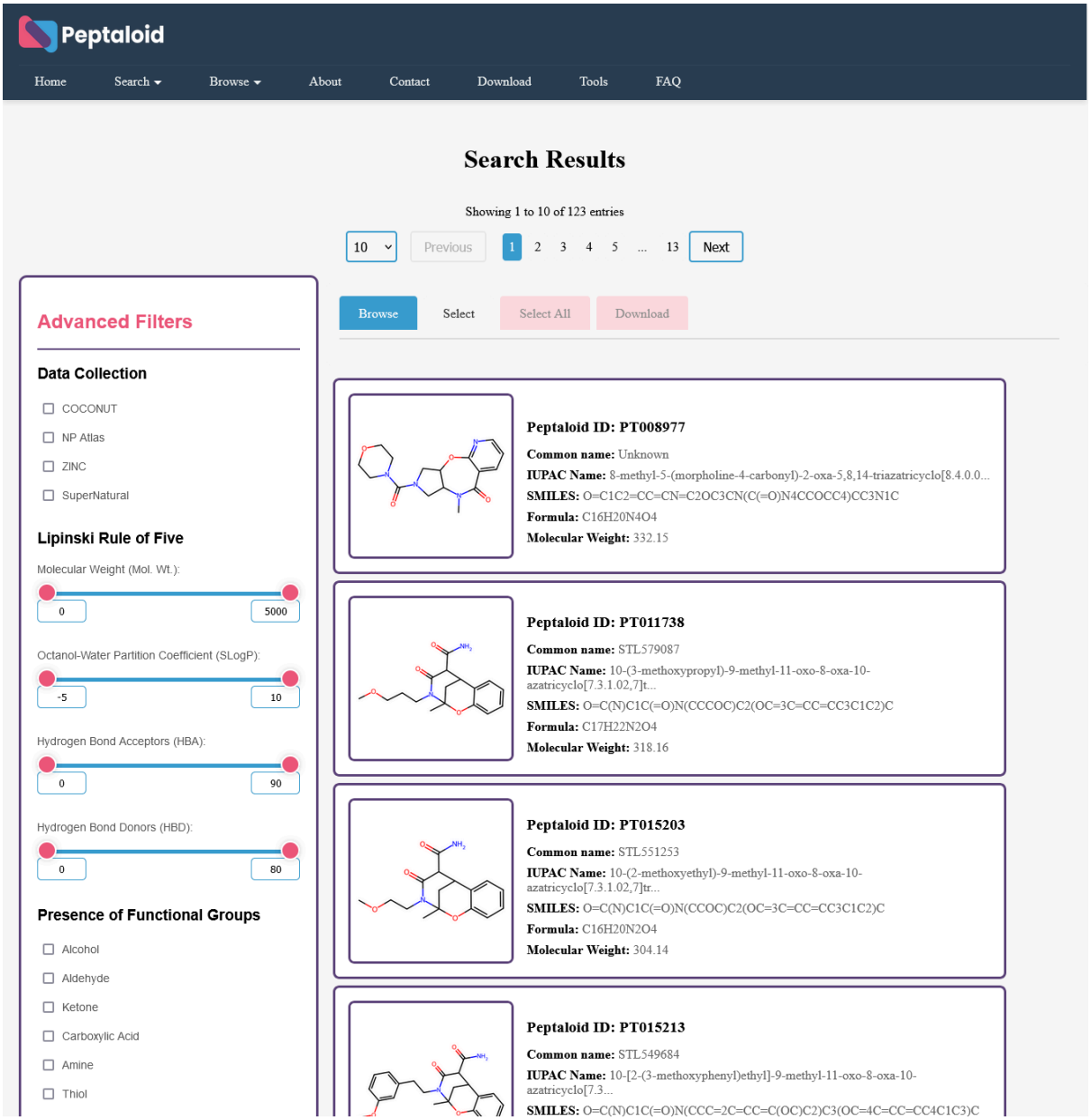
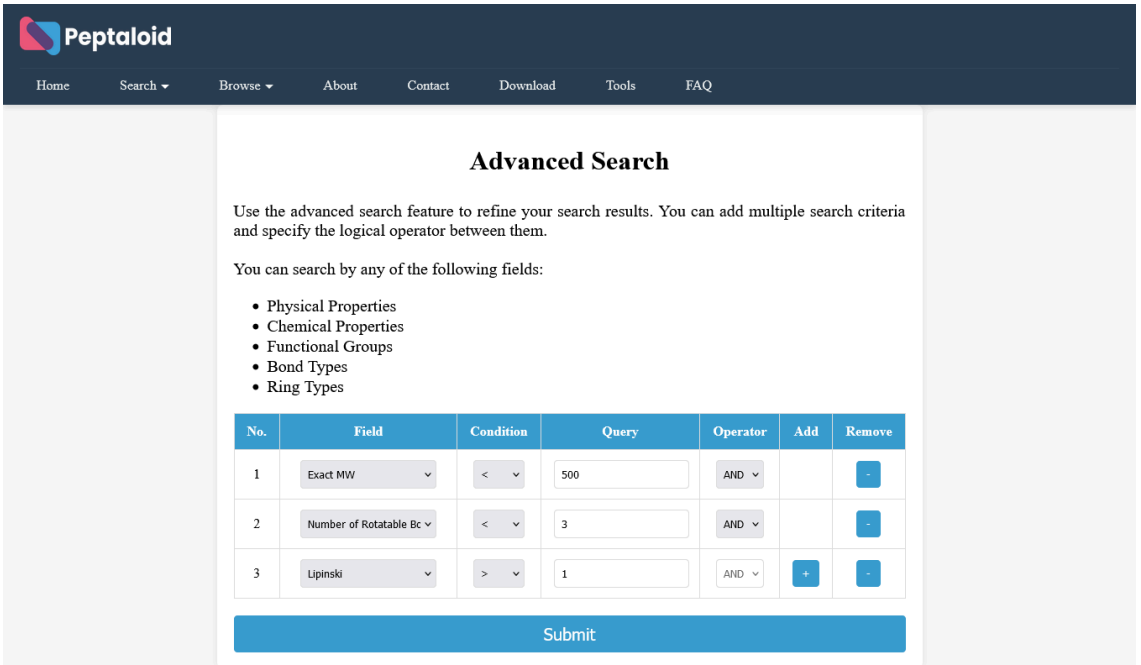


Case Study 4: Advanced Browsing and Filtering Based on Molecular Properties

- **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



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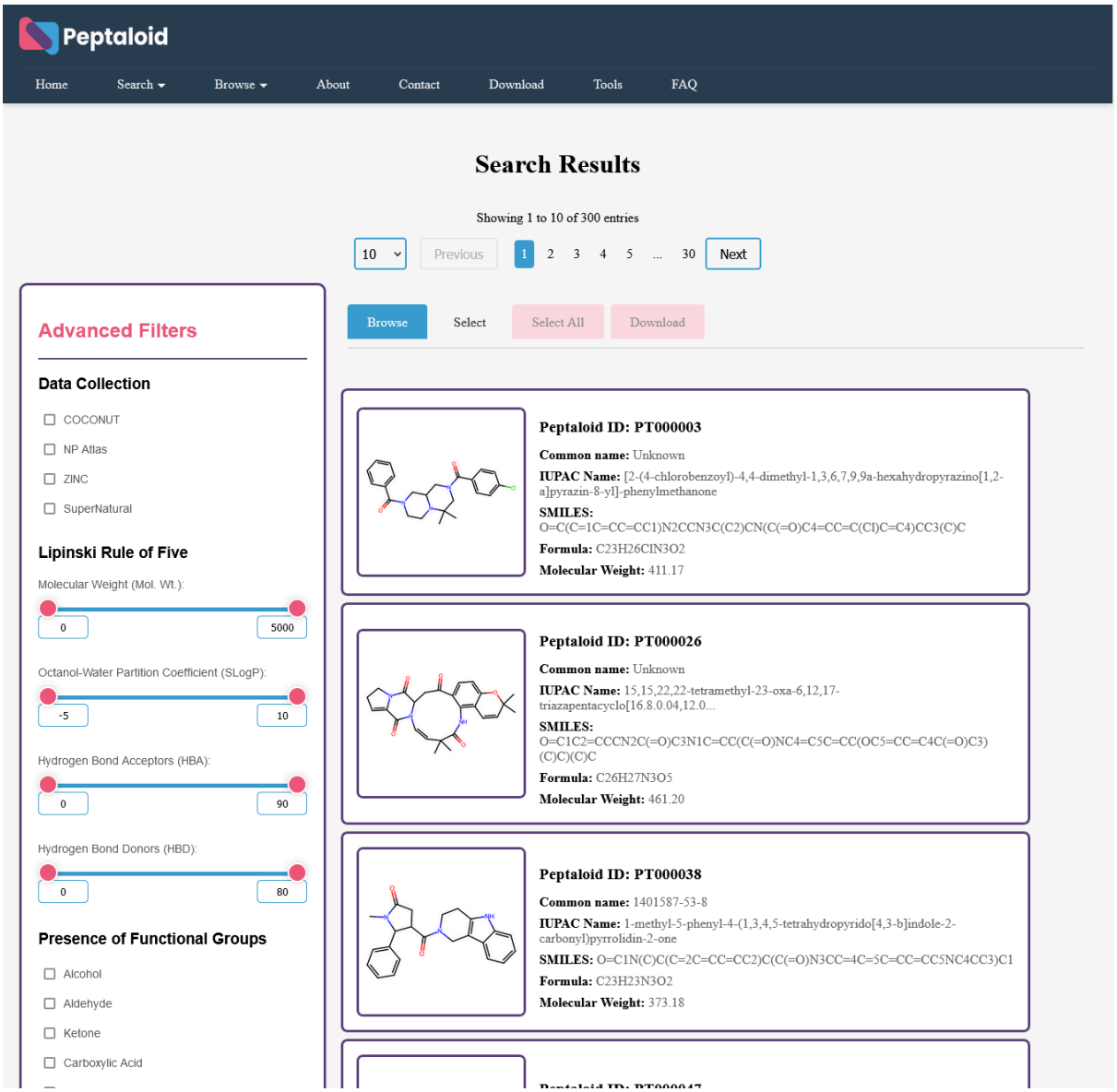

Note: These case studies illustrate just a few of the diverse ways the Peptaloid database can be employed to advance research in peptide alkaloids, from molecular search and property retrieval to drug repurposing and ADMET screening. However, the scope of Peptaloid is not confined to these examples alone. 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.