



**National Institute of Immunology
New Delhi 110067 INDIA**

Notification for proprietary purchase

11th Feb 2025

NII is planning the procurement of the following item through proprietary mode.

Name of the item:	CAS SciFinder™
Make:	Chemical Abstract Service (CAS)
Model:	Latest continuously curated version with up-to-date databases

Any other potential competitor firm or vendors meeting the below-mentioned specifications may contact equipment@nii.ac.in by email or send the quotation in two bid system (technical and price bids separately) latest **by 25th Feb 2025.**

Specifications and Features required for the CAS SciFinder™ or equivalent platform:

A robust, user-friendly, state-of-the-art, and browser-based platform for researchers and scientists to conduct comprehensive searches using chemical structures, plan synthetic routes, perform retro-synthetic analysis, design synthons, fragment-based searches, access extensive primary literatures, patent databases, and effective visualization of complex data.

1. Substance and structure search:

- A. Substance Search:** Allow user to search through a database of more than 280 million CAS registry numbers, with comprehensive and accurate information, including the source information.
- B. Structure Search:** Input to either draw or import the structure of interest and perform searches. Output should provide a complete overview of structure property values, spectral data, regulatory information, structure-activity relationships (SAR), absorption, distribution, metabolism, and excretion (ADME), toxicology data, and bioactivity information. Also identify structural variants, scaffold searches, and related structures.

2. Reaction and Retrosynthesis Planner

- A. Reaction Search:** Ability to search for specific compounds as reactants, starting materials, products, reactants, catalysis, solvents, or any other roles. Easy access to locate reactions with experimental methods and supporting primary literature. Provision of filter options to narrow down and pinpoint specific reactions.
- B. Advanced Search Options:** Provision to specify reaction sites, subgroups, moieties, atom mapping, use of protecting groups, locking of atoms and rings, fragment-based searches.
- C. Retrosynthesis Planning:** Ability to plan synthetic routes with possible reaction pathways using retrosynthetic analysis using synthons, both by experimental and

logical predictive routes. Ability to manually select alternate steps at will, explore evidence, and plan synthetic steps with ease. Ability to modify the retrosynthetic route by selection of bonds to break and to protect with selectivity, excluding selected scaffolds and specific reaction steps.

3. Literature and Patent Search

- A. Journal Articles:** Access to a comprehensive collection of scientific literature across multiple disciplines, with user-friendly indexing for locating terms like concepts, reactions, formulations, and analytical methods reported in the primary research articles.
- B. Patents:** Capabilities to search patents comprehensively, covering more than 100 patent offices worldwide.

4. Data Analysis and Visualization

- A. Citation Mapping:** Capability to trace the citation history of important papers and the trail of back-references.
- B. Knowledge Graph:** Capability to locate connections between published primary literature, indexed substances, authors, and companies.
- C. Visualization of structures and reactions:** Featured with enhanced visualization tools for chemical structures, reactions, and inter-conversions.

5. Supplier Information

- A. Commercial availability:** Feature to provide detailed information on suppliers, commercial availability of chemicals and reagents, including purity and country of origin.