ATOMIS, AN ALMA ARCHIVE TOOL FOR MOLECULAR INVESTIGATIONS IN SPACE

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Abstract. Over the last decade, the amount of data in astrochemistry has exponentially increased. The Atacama Large Millimeter/submillimeter Array (ALMA) has played an important role in this rise. Indeed, about 500 Tb of raw and reduced data are produced per year and stored on the ALMA Science Archive (ASA). Tools are important to promote the use of these data. To facilitate the search for specific species in the ASA, we developed a web application called ATOMIS (ALMA archive TOol for Molecular Investigations in Space). Through this tool, the user can find all the observations covering the transitions of given species in lists of sources. From the list of results, the user can download the corresponding ALMA fits files or go to the ASA to retrieve the raw data. Currently, the fits files can be directly visualized in the ALADIN software through ATOMIS. Future improvements and direct visualization of the datacubes with other softwares are planned.

Keywords: Astrochemistry, Observations: ALMA, Submillimeter/millimeter, Molecules, Archive data

1 Introduction

The Atacama Large Millimeter/submillimeter Array (ALMA) has led to a revolution in astrochemistry thanks to its outstanding sensitivity and angular resolution. The amount of data produced by ALMA is also extremely high (∼500 Tb per year). All the raw and reduced data are stored on the ALMA Science Archive (ASA) and these data usually become public after one year. To make the best use of these archive data, solutions are needed to facilitate their exploitation. In particular, researchers can be interested in searching for a given molecule or a group of molecules in a list of sources. The search through the ASA is currently limited to frequencies, which makes the search more complicated when the molecule has a very high number of observable transitions. We developed a tool called ATOMIS (ALMA archive TOol for Molecular Investigations in Space) to facilitate the search for molecules in lists of sources.

2 ATOMIS design and implementation

The ATOMIS tool is publicly available at the following address: `https://atomis.irap.omp.eu`. It uses Flask framework and is written in Python, JavaScript, and HTML. It consists in four steps summarized in Fig. 1 and described below:

1. **Searching for ALMA observations**
   In the first step, ATOMIS asks the user to specify a source or a list of sources with their known velocities ($v_{\rm LSR}$) or redshift (z) as well as observation parameters such as the angular and spectral resolutions, the sensitivity, the ALMA receiver bands, the property rights of the data (only public data or all data) and the QA2 status. To search for the corresponding ALMA observations, ATOMIS uses the Astropy package (Astropy Collaboration et al. 2022) and features of the ALminer tool (Ahmadi & Hacar 2023). Some ALminer functions were adapted to achieve the desired results. ADQL(Astronomical Data Query Language) TAP query is used and sent to the PyVo TAP service. ATOMIS calculates the corresponding rest frequencies based on the values of $v_{\rm LSR}$ or redshift that are provided. A table of the filtered observations is then produced. It can be downloaded before getting to the next step.

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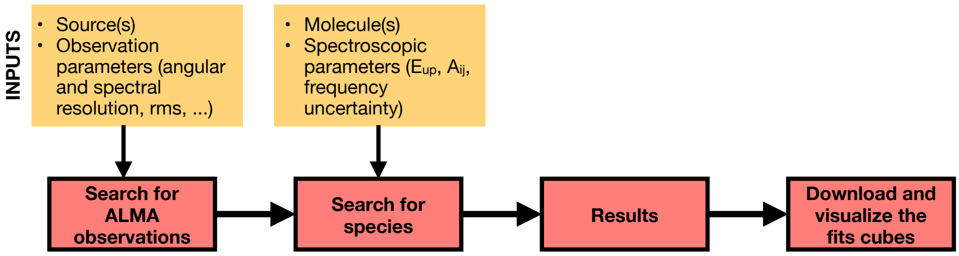

Fig. 1. Schematic view of the ATOMIS tool.

2. **Searching for species**
The second step corresponds to the spectroscopic search. The user can select one or several species from the CASSIS database, which includes the public spectroscopic databases JPL (Pickett et al. 1998), CDMS (Müller et al. 2005), and LSD (Lille Spectroscopic Database) as well as the VASTEL* database. If the desired species is not present in this database, the user can also upload spectroscopic files (.cat file and partition function) or a private database with the CASSIS database format. Different criteria can be applied on the selected species: the minimum and the maximum values of $E_{\rm up}$ and $A_{\rm ij}$ and the maximum frequency uncertainty for the transitions. ATOMIS searches for all the corresponding transitions that are covered in the filtered observations and presents the results under a table format (third step).

3. **Displaying results**
The results are displayed in a table which contains all the ALMA observations (spectral windows) that cover the selected transitions. The table can be adapted with the desired columns (source name, coordinates, project code, covered lines, sensitivity, angular resolution, spectral resolution, ...). The displayed observations can be modified based on the sensitivity and the angular resolution and by deselecting species. Also, ATOMIS provides three additional options to filter the results: only display observations for which all selected species are covered in the same source, in the same project or in the same spectral window. From this table, the user can select an observation and access to the corresponding project in the ALMA archive or click on the link to download the fits files (fourth step).

4. **Downloading and visualizing the datacubes**
The fits files covering the requested transitions available on the ASA are listed on ATOMIS and can be downloaded directly by the user. They can also be directly visualized with Aladin-CASSIS (Glorian et al. 2021), as long as the software Aladin is installed and opened. The interoperability and the communication between ATOMIS and Aladin are ensured by the use of SAMP (Simple Application Messaging Protocol).

3 Conclusion

ATOMIS is a public tool that could present an interest for the astrochemistry community. Future improvements are planned. In particular, interoperabilities with other softwares used to visualize and analyse ALMA data cubes (CARTA, YAFITS, ...) would be useful.

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