

Telegram-bot for the furanocoumarin database in Apiaceae

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Motivation and aim: Furanocoumarins are naturally occurring substances with numerous biologically active properties. The most well-known are their phototoxicity and mutagenicity. They are widely used in the treatment of skin diseases (vitiligo and psoriasis), their neuroprotective, anti-inflammatory, antidiabetic, antiviral, insecticidal and other properties are being studied. Knowledge of the biosynthetic pathways of certain substances in plants can be used to develop a theoretical basis for increasing their synthesis or neutralizing their negative effects. The biosynthesis of furanocoumarins in plants has not been fully studied; only a few enzymes in a small number of plant species have been studied. In order to study biochemical pathways, it is necessary to have a comprehensive understanding of which substances are found in certain plant species. Existing databases have insufficient coverage, focusing only on species of pharmaceutical importance. The resulting database is limited to the Apiaceae family, but claims to be comprehensive in covering all species of this family studied to date.

Materials and methods: Using literature data analysis from the base <https://scifinder-n.cas.org/> and manual verification, three types of information were collected:

- 1) taxonomic position of the species specified in the publication, as well as its modern taxonomic position,
 - 2) data on the structure of furanocoumarins isolated from the plant (links to PubChem, Cas number, SMILES code of the structure),
 - 3) literature reference indicating the publication in which a specific substance was isolated from a specific plant species.
- The Telegram bot that allows using the database was created using Python 3.11 tools, the SQLite library, and python-telegram-bot.

Results: The furanocoumarin database in the Apiaceae family contains about 12.5 thousand manually verified records, includes information on 650 species and 400 planar structures (taking into account isomers – 1100 structures). The Telegram bot, available at the link <https://t.me/borshevicBot>, allows you to search by name or by a specified PubChemID of a substance (database <https://pubchem.ncbi.nlm.nih.gov/>), as well as by the genus-species name of the plant or its LSID (database www.ipni.org). The bot provides information on which substances of the furanocoumarin structure are identified in a given plant species and how many publications describe this fact. The bot also allows you to save the search results in xls format, including unique publication identifiers for each fact of determination.

Conclusions: A database of furanocoumarin structures in the Apiaceae family and a telegram bot based on it have been created, allowing one to determine which substances have been identified in which plant species to date.

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