ACD/IUPAC Name Pro 3.6. Advanced Chemistry Developement (www.acdlabs.com). CD-Rom. US$ 1995. (academic discount 50–60%).

The continuous move towards electronic media and electronic searching techniques increases the need for consistent naming of chemical compounds. The wealth of compounds being synthesised demands a systematic approach to naming in order to make them fully searchable electronically. The IUPAC naming system is highly regarded and widely used to identify chemical structures. A system like this lends itself nicely to a computerised naming program.

The ACD/IUPAC Name Pro is straightforward to use, once the user is familiar with any drawing program. The instruction manual smoothly guides the user through different examples and illustrates in simple terms the more elegant features of the program.

The main components of this program are the Chemsketch window, the Name window, the History window and the IUPAC rules window. Movement between these windows is possible at all times.

On opening the program, the user is immediately in the Chemsketch window where a compound can be drawn, either bond by bond or by using ready-made templates or radical tables listing common groups. These tables allow a large selection of compound types to be drawn at the touch of a button and these can be linked together or joined to other groups or modified as required. There is also access to a complete periodic table and any atom can be added directly from this. Atom labels can be edited and groups of atoms added easily. The program will correct valence as you draw and will indicate when incorrect structures are drawn. You can also indicate charge making it possible to name ions or multicomponent charged species. Stereochemical bonds can be drawn and there are various tools available to clean up the structure, perform 3D optimisation and to rotate bonds or indeed the whole molecule as required.

The Names window can then be entered and in most cases the compound will be named within a few seconds. The name will be the correct IUPAC name of the compound and the IUPAC rules leading to this name are retrievable by hyperlinks for a better understanding. Naming preferences can be set which can customise the naming still further, for example using retained replacements such as toluene rather than methylbenzene or naming a compound as 2-propene rather than prop-2-ene. It is also possible to set the preferences to refuse to name certain compound types, such as bridged fused systems, which will not lead to the IUPAC name.

In this window it is possible to highlight any part of the molecule and the corresponding part of the name is highlighted. This allows for simple identification of major parts of the molecule and is something that I personally have found very useful. Atom numbering can be added for clarity, making it easy to understand the naming of an unfamiliar class of compounds quite quickly.

The History window keeps track of every compound named in one session and these can be reviewed as you work. They can be edited and renamed, deleted, used as they are or saved if they will be required again. It is also possible to name several structures at once from the History window.

The IUPAC rules are available to be viewed fully or can be searched for specific information. This gives a very useful background and understanding of how the names are created.

The name or structure can be copied from this program into any other program, for example Microsoft Word, which accepts drawn objects. There exists possibilities to use this program in creating posters as well as for drawing graphs, laboratory apparatus and 3-dimensional molecules. There is also an extensive dictionary where it is possible to look up a drawn structure or search for a common name. This is useful in providing the correct IUPAC name for compounds with common names.

I have used this program over a few months to name a vast variety of compounds in manuscripts from authors in different areas of organic chemistry. It has been easy to use and as far as I could see unfailingly accurate. The naming preferences have been very useful in this instance to allow me to find the name closest to the author's original choice. For consistent naming these preference should be set the same way each time.

Version 3.6 of this program has been considerably updated allowing a much greater range of compounds to be named in a shorter time. Some limitations include difficulty in naming organometallic compounds, bridged fused systems and cyclic systems other than biphenyls. As a minor point, the apparent inability to use delete to go from a double bond to a single bond was somewhat annoying. This program is continuing to be refined, this version being better than the previous and I am certain with time that all classes of compounds will be named within seconds.

I would find this program very useful in many areas of organic chemistry; in industry where accurate names are required in the minimum time and for researchers to ensure that their compounds are named correctly for maximum searchability in electronic media. It would also be a valuable teaching tool. It is easy to use and even drawing a simple compound can yield useful information on atom numbering, finding the principle group and having a look at the compound in 3D. I would unhesitatingly recommend this program for any organic chemist who regularly names compounds. It has certainly provided me with a useful and informative reference source and a reliable bakkup for consistent nomenclature.

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