

A Graphical Journey of Innovative Organic Architectures That Have Improved Our Lives

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In addition to the need for advancing the frontiers of the field of chemistry, chemists are often faced with the equally important task of finding new and more effective ways to both communicate the results of their research activities and justify why investing in chemistry is important for society. Although classically inspired by the architectures of natural products in many of our chemical development endeavors, we have become equally inspired and intrigued by the diverse pharmaceutical structural space (1). We decided to graphically capture this wealth of information on a single page (poster, Figure 1), which in turn would allow anyone to easily visually mine it for a wealth of interesting information, statistics,

structural patterns, and so forth (2). The fruits of our labor can now be found on the Web (3), where high-resolution PDF files can be downloaded and printed in any size.

We and others (in academia and industry) have learned over the past few years that hanging large printed versions of the posters in public spaces results in a magnetic effect, wherein people tend to be attracted by the visual language of organic chemistry (4). The posters can also serve as useful tools for educating the public, teaching both undergraduate and graduate students, and serving as a spring board of ideas for researchers interested in the development of new synthetic methods and

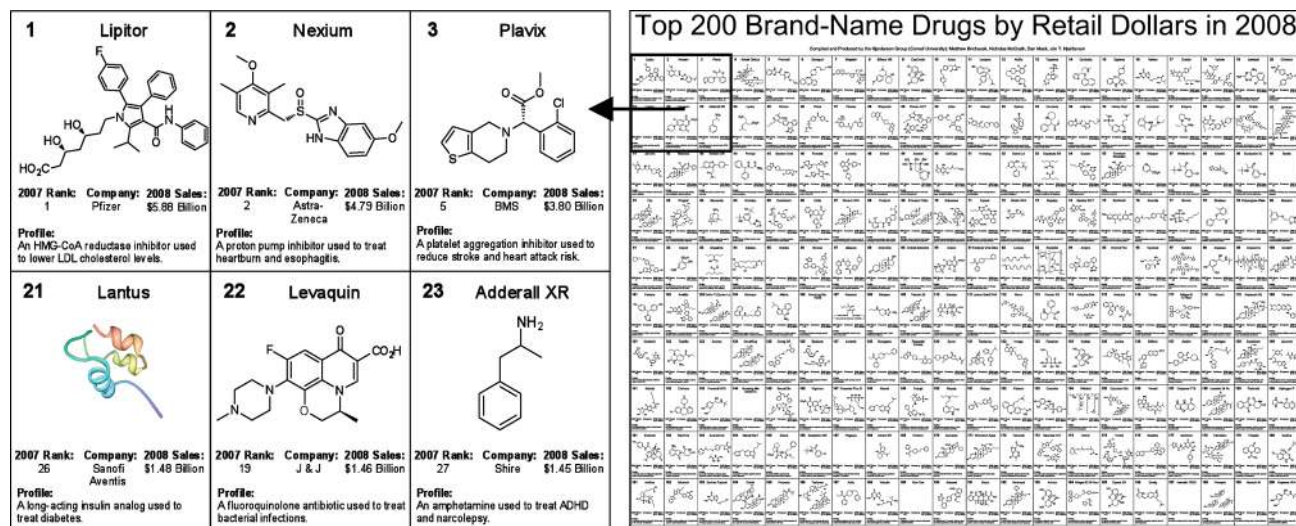


Figure 1. Graphical representation of the 2008 top selling drugs along with an expanded view.

Table 1. Sample Questions

1. How many of the top 20 brand name drugs contain (a) an aromatic ring? (b) a heterocycle? (c) a fused ring system?
2. Which of the top 20 brand name drugs (a) promote cardiovascular health? (b) affect neurotransmitters?
3. In addition to carbon, hydrogen, oxygen, and nitrogen, what are the three most commonly used elements found in brand name drugs?
4. Identify at least one brand name drug that contains (a) an adamantane (b) an alkyne (c) an azide (d) a nitrile (e) a cyclopropane (f) no rings.
5. Locate a brand name drug that is clearly derived from (a) a steroid (b) an alkaloid (c) a nucleoside.
6. Randomly choose 3 generic drugs and assign the hybridization of each carbon atom. Is there a trend in the relative number of sp , sp^2 , and sp^3 hybridized carbons found in generic drugs?
7. Five- and six-membered rings are most frequently used for pharmaceutical structures. In general, are small rings (3–4) or large rings (7+) more common in the generic drugs?
8. Randomly choose three generic drugs and identify all the asymmetric carbon atoms.
9. Are there more macromolecules (biologics or polymers) present in the brand name or generic drug poster?
10. Comparing the brand name and generic drug posters, which has a greater number of drugs with more than one active ingredient (combination therapies)?

strategies. Examples of the wealth of information that can be gathered about the organic architectures used for pharmaceuticals simply by looking at these posters, and without reading a book (5), are listed in Table 1.

Visually exploring the drug posters either on your own or by answering the questions in Table 1 leads to a greater understanding of the organic architectures that affect our everyday life. Displaying this information in the form of an interactive Web site that enables simple mining of the data would serve as a nice supplement to this manuscript and will be explored in the future.

Acknowledgment

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Literature Cited

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Supporting Information Available

PDF files for Top 200 Brand-Name Drugs by Retail Dollars in 2008; Top 200 Generic Drugs by Retail Dollars in 2008; answers to the sample questions. This material is available via the Internet at <http://pubs.acs.org>.