Chemical-Pharmaceutical Twins *

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Dual names for single entities may be found in the literature and daily speech of all sciences, but they have a special place in medicinal chemistry. There are many instances in which the chemists prefer one name for a chemical compound or product, and the pharmacists another. Several of these are discussed.

Reasons for twinning vary. Perhaps the oldest is the ancient interest of alchemists in finding the elixir of life. They experimented with all manner of weird concoctions, inevitably including some which actually had medicinal properties and are now familiar as chemical entities. Latin names, often fanciful, were translated into European languages, including English and French. The latter was assimilated into English after the Norman conquest. Just as medicine was slower to give up Latin terms and phrases than were most other sciences, so the pharmacists tended to cling longer than did chemists to names derived from alchemy, or descendants of such names.

Another reason for twinning is the persistence of both Greek and Latin derivations as names for drugs. A third reason stems back to the Linnaean botanical nomenclature, when names for the same drug were taken from different parts of a botanical name. Even synthetic drugs are not immune; pharmacists are less scrupulous than chemists about using official chemical nomenclature. Often they prefer an old-fashioned but familiar name for a compound, rather than the correct chemical name.

Not in a strict classification by origins, but grouped in a general way according to the principal reasons for twinning, some examples are presented. They illustrate the trend but are far short of amounting to a glossary of chemical-pharmaceutical twins.

Alchemical-Chemical Pairs. Silver nitrate was lunar caustic. from alchemical association of silver with the moon, and from the use of stick silver nitrate in cauterizing. This name, though obsolescent in modern medical literature, is not yet dead, as are other and still more fanciful alchemical names for the compound.

Two old names still cling to copper sulfate—namely, copperas and blue vitriol. With characteristic alchemical inconsistency, copperas (from Latin cuprosa) was applied just as happily to iron(II) sulfate or green vitriol. The word vitriol (from vitreus, since some vitriols look glassy) had the honor of a Latin acrostic, "visita interiora terrae rectificando invenies occultum lapidem" ("visit the interior of the earth, by rectifying thou shalt find the hidden stone"). A few of the vitriol names still persist: white vitriol is zinc sulfate.

The pharmacists have not yet abandoned all of the many names beginning with Latin sal (salt). Ammonium chloride is still sal ammoniac; potassium bisulfate is sal enixum; potassium bicarbonate is sal aeratus, or more commonly saleratus; and sal has even been dragged over into the jet age in the registered trade name Sal Ethyl, which is ethyl salicylate.

Proper Names. Of course there are old place names and personal names which refuse to play dead. Magnesium sulfate is still Epsom salt (from Epsom, England); potassium sodium tartrate is Rochelle salt or Seignette salt, since Seignette was from La Rochelle. The name Glauber salt persists for sodium sulfate, although J. R. Glauber died in 1670. The French systematic nomenclature of the late 18th century came out against use of proper names in chemical names, and they were given up much earlier in chemistry than in pharmacy. (Mineralogy is still full of them.)

Elements known in early times had various associations with the seven known planets, but two were remarkably constant: gold with the sun and silver with the moon. Planetary names for metals are long obsolete; of the few survivors, lunar caustic is probably the most familiar.

Greek-Latin Pairs. A classic example of anglicized Greek and Latin names for the same drug is found in *epinephrine* (Greek) and *adrenaline* (Latin), both meaning on the kidney. A less familiar instance is the little-used drug *hendecanediamidine* (Greek) or *undecanediamidine* (Latin). Similarity of Greek and Latin is also responsible for the pair chromaphil (Greek) and chromaffin (Latin), not a drug but a cell type.

Plant Origins. Drugs derived from plants acquire names in various ways; thus, hyoscine (hyoscyamos, the pig bean) is scopolamine to chemists (from G. A. Scopoli, the botanist who worked with *Hyoscyamus niger*, henbane). The pharmacists borrowed his name in scopoletin, which chemists call gelsimic (or gelseminic) acid.

The Senses. Taste, smell, color, and appearance gave names to numerous medicinals of early times; some survive. Sugar of lead is lead acetate; butter of antimony is antimony(V) chloride; cream of tartar is potassium bitartrate. One early reformer of nomenclature complained that the kitchen had too much influence. Hydrogen sulfide was once called, for obvious reasons, stinking sulfureous air. Taste entered into naming bitter salt (magnesium

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sulfate), which survived longer as Epsom salt. The element glucinum (now beryllium) was named from glucina (beryl) because the sweet taste of its salts attracted the attention of medical-minded alchemists. Color had much influence; surviving names include white lead, a basic lead carbonate; whiting or refined chalk; blue vitriol or copper sulfate; brunswick green or the green copper carbonate.

Longevity of old names in pharmacy is illustrated by muriatic (hydrochloric), from Latin *muria* (brine), and muriates, still used in pharmacy. Baryta for barium oxide, tartar emetic for potassium antimonyl tartrate, and spirits of hartshorn (an instance of animal origin) for spirit of ammonia are other examples.

Synthetics. Pharmacists commonly prefer old chemical names rather than the official nomenclature for synthetic drugs. They like trimethylene, not cyclopropane; succinodinitrile, not 1,2-dicyanoethane; and they still often call ethyl acetate by its old name, acetic ether. Sulfa drugs and antibiotics have proliferated great numbers of coined names, many under trademark protection. Many of the official chemical names are so long and cumbersome that even the chemists tend to favor short coined names; sometimes their choices agree with those of the pharmacists— $e.\ g..\ sulfapyridine$ for N^1 -2 pyridylsulfanilamide, and tetracycline for 4-dimethylamino-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-2-naphthacenecarboxamide.

Traces of alchemy linger longer in pharmacy than in chemistry; but chemists cannot claim total emancipation.

Aqua regia is still a chemical term for the royal water which dissolves gold. Spirit appears variously—e. g., in proof spirit. To alchemists spiritus was any gas, vapor, or volatile liquid which had notable effects; thus gradually came its principal use for alcohol (wood spirit) and for ethanol, simply spirit. Oleum, stripped of its many companion words designating kinds of oil, survives in chemistry as a name for fuming sulfuric acid.

Habit is strong, and much water will flow under the bridge before pharmacists and chemists join in a standard terminology for medicinals. But some terms, obsolete now in chemistry and obsolescent in pharmacy, will lose their last toehold and the approach to uniformity will be closer.

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Use of the Wiswesser Line Notation for Determining Duplicate Chemical Structures

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A computer (Honeywell 200/400) system has been established for routinely checking, via the Wiswesser chemical line notation, all newly submitted chemical structures against an existing file. A run of 1772 "new" notations against 84,716 file notations required 50 minutes of computer time

Checking a list of "new" compounds against an existing file to avoid duplication is a task which confronts every organization that deals with the acquisition of chemical compounds for its screening programs. (New compounds are those submitted for possible testing and which have been assigned file numbers.) Over 2000 structures per month are submitted for review under the Industry Liaison Program (1). Upon acquiring a list of structures for sample selection the first question is: Which compounds have been screened and are on file? The Wiswesser chemical line notation (2) provides an efficient means of accomplishing this.

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WISWESSER CHEMICAL LINE NOTATION

The Wiswesser chemical line notation has been established to be:

- a unique and unambiguous method of depicting chemical structures.
- 2. a representation which can be processed by unmodified automatic data processing (ADP) equipment.
- concise. (The average notation length for a file of over 90,000 structures has been determined to be 16.5 symbols. The "space" was considered a symbol for this determination.)

These attributes offer a convenient, rapid, unique, and unambiguous automatic file search methodology.