Surfing on Scent: The Perfumer's Compendia

What does Peonile, Karanal or Doremox smell like? What are the Cyclemones chemically? Which perfumery raw materials were launched recently? And in general, which compounds are reminiscent of musk? To find some answers to these questions is not easy. When the printed references[1,2] are at their wit's end, the internet can now render some aid.

Quest was the first company to provide an online-compendium separate from their home page.[3] Following obligatory registration, access is granted to their product portfolio, which is presented according to the odor notes in Figure 1. Within these lignes de force the fragrance raw materials are further divided into sub-families and on selection of the names one gets formula, chemical name, molecular weight and odor description in return, besides additional data referring to the use in perfumery. A field for personal comments enables the storage of synonyms of other companies, starting materials or literature references. A search engine allows tracking down compounds outside these restricted categories. However, some practice with the use of odor descriptors is required, since "musky" for instance does not get you very far; while "musk" on the contrary does.

Demo formulae for the application of the materials in perfumery were first introduced on the user-friendly ingredients site of Givaudan, which includes also flavor chemicals.[4] Registration is not necessary, although registering allows users to order samples and access safety data sheets. Products can be listed in order of their commercial or chemical names, CAS and FEMA number, odor families and possible applications. A useful feature is the search function, which allows free navigation around the site. This is shown in Figure 2 with the example of "Geranium". Hits are also returned if the compound is just used in geranium accords without smelling geranium-like. Parts of the output file for Peonile are depicted in Figure 2. Besides the olfactory note and description, physicochemical parameters and stability data are given, and links to demo compositions for different applications are provided as well.

Demo compositions are also incorporated in the site of Firmenich,[5] where one can also open an account for online sample ordering, but one can enter the site without password as well. Searching is possible for names, CAS numbers or fix odor attributes, as is shown for musk in Figure 3. In addition to the perfumistic and physicochemical data, the output data contain a safety data sheet, sample accords and supplementary information concerning the discovery of the respective substances. A short historical outline and a chronology of prominent products are worth reading as well.

Figure 3. Musk search in Firmenich's net with a demo formula for Exaltenon.

IFF has integrated their alphabetic product index in their homepage.[6] Searching for "Cyclemone" and "Isocyclemone" in the ingredients search field will for instance lead you to the Cyclemones. The respective sites of Takasago and Haarmann & Reimer[7] are still in construction.

Since all featured sites address mainly perfumers, the data are quite accurate and reliable—infotainment for all interested in odorants. More on fragrance chemistry can be found in a recent review in *Angewandte Chemie*.[8]

Philip Kraft
Givaudan, Dübendorf (Switzerland)

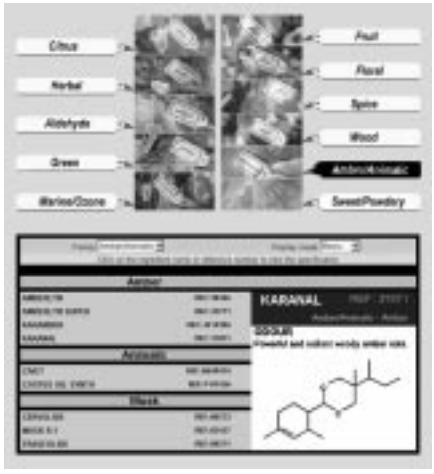

Figure 1. The features of the Quest compendium with Karanal (Karen Rossiter's acetal).

Figure 2. A glimpse into the ingredients site of Givaudan with Peonile (Mario Pesaro's nitrile).

[1] K. Bauer, D. Garbe, H. Surburg, *Common Fragrance and Flavor Materials*, Wiley-VCH, Weinheim, **1997**.
[2] *Allured's Flavor and Fragrance Materials 2001*, Allured Publishing, Carol Stream, Illinois, **2001**.
[3] http://www.questintl.com/compendium/
[4] http://ingredients.givaudan.com/
[5] https://olc-eur.firmenich.com/ oder https://olc-usa.firmenich.com/
[6] http://www.iff.com/Ingredients.nsf/WebDSFrag!OpenView
[7] http://www.haarmann-reimer.de/cgi-bin/hrkat.pl?L=EN&PG=AC&DP=1
[8] P. Kraft, J. A. Bajgrowicz, C. Denis, G. Fráter, *Angew. Chem.* **2000**, *112*, 3106–3138; *Angew. Chem. Int. Ed.* **2000**, *39*, 2980–3010.

  1433-7851/01/4010-1979 $ 17.50+.50/0