

The Importance of New Molecules in Selective Perfumery

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‘Patience dans l’effort’

Maurice Roucel

‘Gravitation is not responsible for people falling in love’

Albert Einstein

Perfumery can only evolve thanks to new ingredients. We highlight herein some key molecules and their use in ‘Selective Perfumery’: the violet odorant undecavertol, the floral nerolione and coumarone, the gourmand cappuccino levistamel, the sandalwood notes *Sandranol[®]* or *Bacdanol[®]*, the fruity top note Magnolia Flower oil, and finally the woody ambery *Ambrocenide[®]*.

Introduction. – Perfumers are always looking for new inspiration, new smells, new ingredients and new molecules to make attractive and glamorous fragrances (for an overview of fragrance chemistry, see [1]). For this, they rely on the ‘molecule creators’ to give them new nuances in their palette of colors. Many important creations have been achieved by using a new chemical substance. First use of ingredients are, for example, salicylates in ‘*Fougère Royale*’ (Houbigant, 1882), coumarin in ‘*Jicky*’ (Guerlain, 1889), aldehydes in ‘*Chanel n°5*’ (Chanel, 1921), hydroxycitronellal in ‘*Muguet des Bois*’ (Coty, 1942), *Calone[®]* in ‘*New West for Her*’ (Aramis, 1990), and ethylmaltol in ‘*Angel*’ (Thierry Mugler, 1992). Usually, when first introduced, new chemicals are used in small amounts until eventually being overdosed. The overdose of a new molecule or ingredient reveals its olfactive character and gives signature to a fragrance.

Undecavertol. – 4-Methyldec-3-en-5-ol (**3**) is obtained from the *Grignard* reaction of pentylmagnesium bromide (**1**) and 2-methylpent-2-enal (**2**; *Scheme 1*) [2] and possesses a powerful, long-lasting, and very diffusive floral violet, fruity green note. When Maurice was working for Donna Karan, New York, he came up with the idea of creating an innovative apple fragrance inspired by the city’s nickname ‘Big Apple’. In this context, undecavertol was used at 8% in ‘*Be Delicious*’ (DKNY, 2004; *Fig. 1*), a very high dosage considering that, before this, it was used at dosages lower than 1% in fine fragrance. ‘*Be Delicious*’ is a floral accord where the principal violet element undecavertol can be interpreted as being a modern methylionone, emphasizing the fruity green-apple facets.

Scheme 1

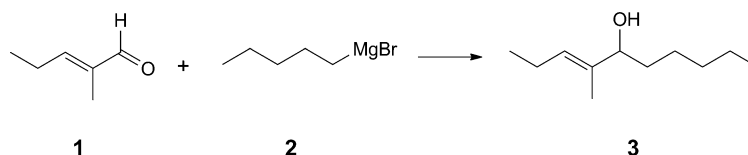
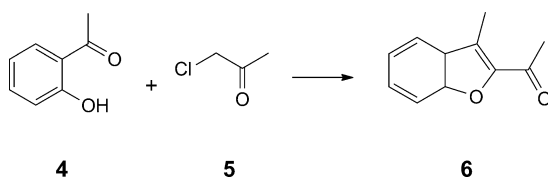


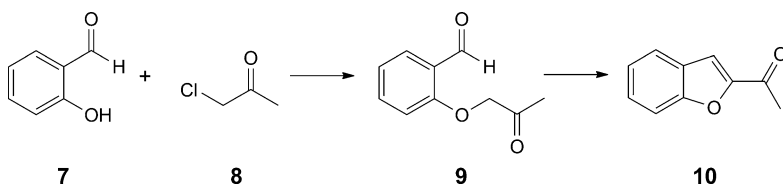
Fig. 1. 'Be Delicious', Donna Karan, 2004

Nerolione and Coumarone. – 1-(3-Methyl-1-benzofuran-2-yl)ethanone (**6**) and 1-(1-benzofuran-2-yl)ethanone (**10**; see *Scheme 3*) are obtained by aldol condensation after the reaction of chloroacetone **5** (**8**) with 2'-hydroxyacetophenone (**4**, see *Scheme 2*) and salicylaldehyde (**7**), respectively [3] (*Scheme 2*). Nerolione is a floral, orange flower, coumarin-like ingredient, and coumarone also has an orange flower, coumarin-like odor but slightly more animalic than nerolione. 'Insolence' (Guerlain, 2006; Fig. 2), has a traditional *Guerlain* structure with an orange-flower note boosted by the explosive mixture of coumarone and nerolione, used in pure in the formula, when it was previously used in dilutions even in technical applications. Nerolione is an extremely powerful, violent ingredient that has the huge advantage over methylantranilate, an ingredient in the same olfactive orange flower direction, that does not cause color-stability issues.

Scheme 2



Scheme 3



INSOLENCE

GUERLAIN

LVMH GROUP
FEMININE - 2006

FLORAL - FRUITY - POWDERY

top	coeur	drydown
Raspberry	Violet	Musk
	Iris	Tonka bean
	Orange blossom	Sandalwood
	Rose	

Fig. 2. 'Insolence', Guerlain, 2006

Levistamel. – 4,6-Dimethyl-2*H*-pyran-2-one (**14**) is the product of the reaction of ethyl 3-methylbut-2-enoate (**12**) with AcCl (**11**) [4] (*Scheme 4*). Levistamel is a note for gourmands, which can be used either in feminine or masculine fragrances. For '*Rochas Man*' (*Rochas*, 1999, *Fig. 3*), at first, *Maurice* presented an accord of three simple products with the internal name '*Capuccini*', which was a creamy coffee accord for men, quite innovative at that time. Levistamel is an edible note and has a roasted

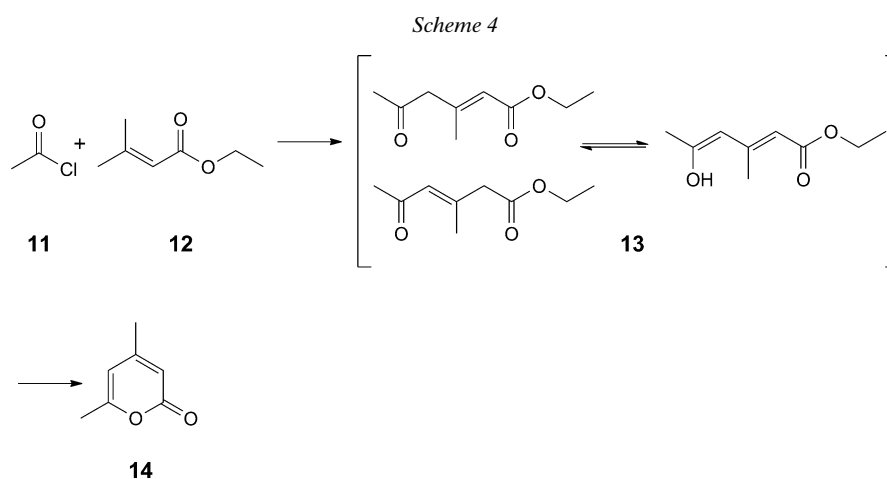


Fig. 3. 'Rochas Man', Rochas, 1999

coffee, malt, cappuccino, fenugrec, and immortelle smell. It is used in pure in the '*Rochas Man*' fragrance, and can be considered as a modern ingredient for immortelle and coffee natural ingredients.

Concerning the creation of 'L' (*Lolita Lempicka*, 2006; *Fig. 4*), Mme. *Lolita Lempicka* wanted a fresh vanilla smelling of the seaside. For *Maurice*, the seaside effect

can be recreated by the salty facets of salicylates and the smell of immortelle, which conjures up images of the Corsican coast. ‘*When the wind carries, you can smell Corsica before seeing it*’. Again, there levistamel is used as an edible, roasted coffee and modern immortelle note.



Fig. 4. ‘L’, Lolita Lempicka, 2006

Sandranol® and Bacdanol®. – Sandranol® (18) or Bacdanol® is obtained from aldol condensation of butanal (16) with campholenaldehyde (15) followed by a partial hydrogenation of the unsaturated aldehyde 17 (Scheme 5) [5]. Maurice used it in ‘K’ (Krizia, 1981; Fig. 5), which was a major success for Krizia, as it stayed in the market for more than 30 years. ‘K’ is a modern sweet oriental with a classical oriental structure with patchouly, spices, musks amber and cassis top notes where the sweet effect is created by an overdose (30%) of sandalwood ingredients. The sandalwood accord is mainly a mixture of Sandranol® and Sandalore®. Sandranol®, apart from its nice sandalwood smell, is an extremely powerful ingredient and brings comfort, softness, long lasting and strength to the creation. It has a wrapping effect and softens the rough aspects of patchouli and coumarin.

Magnolia Flower Oil. – This essential oil is a very good example to show that it is still possible to introduce new natural ingredients in perfumery, which are not just the results of a new extraction technique of a known natural material. At that time, Monique Rémy, director of Laboratoires Monique Rémy, was travelling all around the

Scheme 5

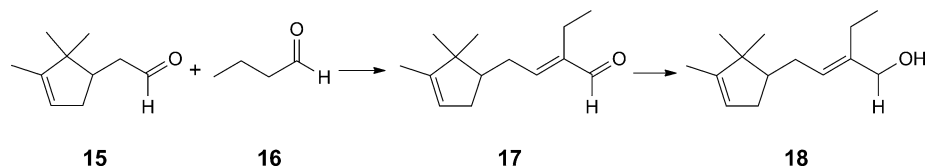


Fig. 5. 'K', Krizia, 1981

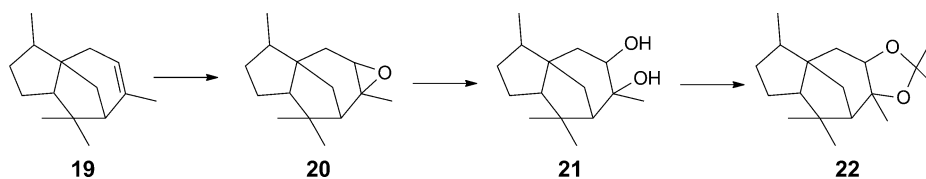
world searching for new natural ingredients for perfumery. She presented to *Maurice* a new essential oil from China: the Magnolia flower oil of *Michelia longifolia* and *M. alba*. The new ingredient began to attract real interest after being used successfully in a fragrance. Unfortunately, only 500 g of the oil were available worldwide, so it could not be used in an overdose. Therefore, *Maurice* used the right dosage for the launch of this product in the feminine fine fragrance 'Tocade' (*Rochas*, 1994; Fig. 6), a bipolar accord of rose and amber. The analysis of the unknown oil revealed that it consisted mainly linalool (ca. 70%), and some of the top-note components were well-known by chemists working in the flavor area, i.e., methyl 2-methylbutanoate and ethyl 2-methylbutanoate, both fruity, very red strawberry with exotic fruits facets. The production of Magnolia flower oil is nowadays reaching ca. 1 t per year, and it is one of *Maurice's* favorite ingredients used in most of his creations, like the above mentioned success 'Be Delicious' (*DKNY*, 2004).



Fig. 6. 'Tocade', Rochas, 1994

Ambrocenide®. – *Ambrocenide®* (**22**) is prepared starting from cedrene (**19**), one of the principal cedarwood oil component, after epoxydation of the C=C bond (\rightarrow **20**), opening of the epoxyde and acetalization of the obtained diol **21** [6]. *Ambrocenide®* is an extremely powerful amber molecule; therefore, it is available as a 10 or 5% solution in DPG (diphosphatidylglycerol), TEC (triethyl citrate), and IPM (isopropyl myristate) and from now on in pure form. For 'Burning Hot' (Avon, 2013; Fig. 7), I had to create a fragrance for South American men who were out seducing in night clubs. Technically, this fragrance had to last the entire hot night, so I immediately thought about *Ambrocenide®*, for its long-lasting character, stability, and strength. 'Burning Hot' is a classical fougere structure with an ambery and woody sensual background, but the whole structure from the top to the base is pushed up by the explosive *Ambrocenide®*. *Ambrocenide®* is the 'Viagra' of the ambery-woody notes of the fragrance.

Scheme 6



BURNING HOT
AVON



AVON
MASCULINE- 2013

FOUGERE - AMBERY - AROMATIC

top	coeur	drydown
Mandarine	Cardamom	Amber gris
Lavandin	Nutmeg	Vanille
Galbanum	Fir balsam abs.	Tonka bean
Marine notes		Patchouli
		Cistus labdanum
		Musk



Fig. 7. 'Burning Hot', Avon, 2013

Conclusions. – A short survey is provided on the use of ingredients for the creation of new perfumes. We tried to highlight that the signature of a perfume depends on a new molecule, essential oil, or an innovative accord with a new ingredient. Finally, we believe that an attractive name for the new material would facilitate its use.

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