

CHAPTER 8

Sample Laboratory Experiments

8.b Identification of Fragrances

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Fragrances/perfumes provide a “Holy Grail” for GC-MS analysis. As noted in many movies or from a trip to a European fragrance shop (perfumery), a near infinite variety of combinations of fragrances can be made. In this laboratory exercise, “name brand” fragrances will be compared to their more inexpensive counterparts in an effort to determine if a difference exists in their “fingerprint” based on GC-MS. A fingerprint, in this context, is a characteristic chromatogram of a complex mixture of compounds.

Perfumes consists of (1) primary scents at the parts per million concentration, (2) modifiers that alter the primary scent to give the perfume a certain desired character, (3) blenders (ingredients that smooth out the transitions of a perfume between different bases; top, middle, and base notes of a fragrance may have separate scents), and (4) fixatives (natural or synthetic substance used to reduce the evaporation rate).

Sources of primary scents include: (1) Plant sources (bark, flowers and blossoms, fruits, leaves and twigs, resins, roots, rhizomes and bulbs, seeds, woods, (2) Animal sources (Ambergris which are lumps of oxidized fatty compounds, Castoreum from the odorous sacs of the North American beaver, Civet Musk obtained from the odorous sacs of the animals related to the Mongoose, Honeycombs, Musk originally derived from the musk sacs from the Asian musk deer), (3) and Other natural sources (extracts of lichens and seaweed). Synthetic sources of the natural compounds mentioned above are used today, as well as calone, linalool and coumarin from terpenes, and salicylates (orchid scents) are also used today.

Experimental Procedures

Chemicals and Supplies:

A variety of perfume samples can be analyzed. In this experiment, Light Blue by Dolce and Gabbana, Shades of Blue by Belcam, Drakkar Noir by Guy Karoche, Classic Match by Belcam, Unforgivable by Sean John, Unjustified by Belcam, and Bring It by Parfums were used.

GC-MS Settings:

Capillary Column:	DB-5 Poly(phenylmethyldimethyl) siloxane (5 % phenyl) 30 m x 0.25 mm; 0.25 μ m phase coating
Injection Volume:	1.00 μ L
Split Mode of Injection	
Split Flow Rate:	131 mL/min.
Column Flow:	1.3 mL/min.
Linear Velocity:	42 cm/s
Injector Temperature:	250°C
MS Transfer Line	
Detector Temperature:	230°C
Quadrupole Temperature:	150 °C
Oven Program:	Initial Temp. at 40.0°C for zero minutes, 2.0°C to 280°C, hold for five minutes.
Total Run Time:	125 min.

Procedures:

Analyze a variety of perfume samples on a GC-MS using the instrumental conditions given above.

Results

(1) The relatively expensive “Light Blue” and a generic blend “Shades of Blue”:

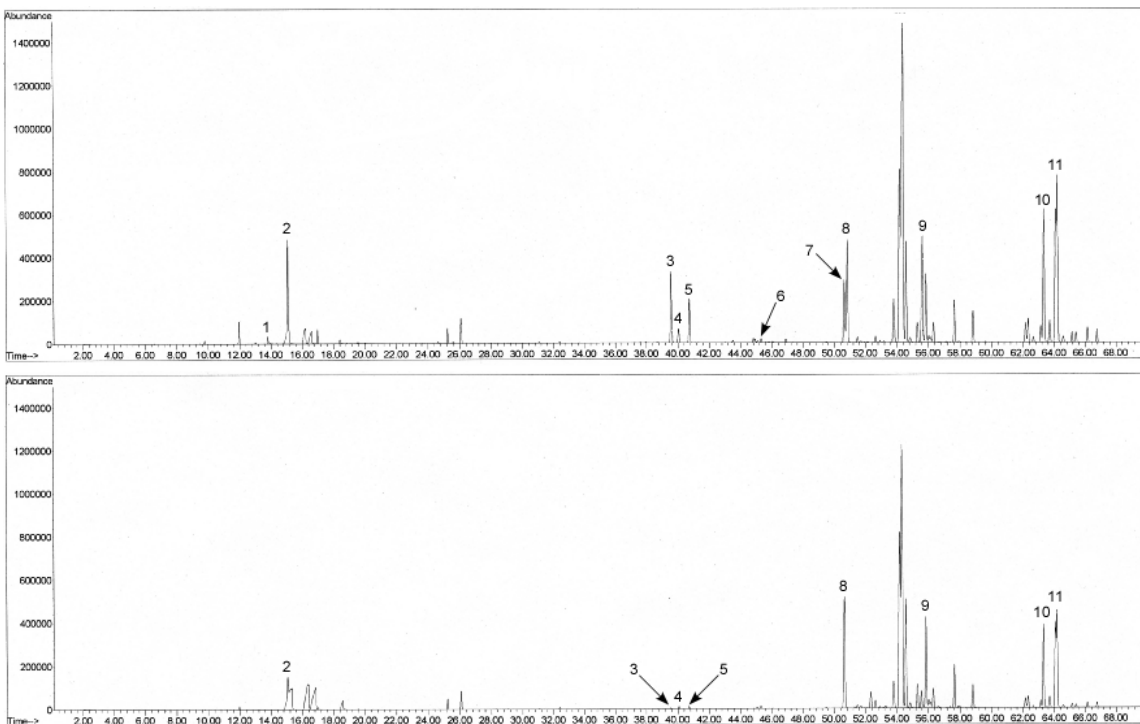


Figure 8b-1. Chromatogram of Light Blue (top figure) and Shades of Blue (bottom figure).

Note the presence, absence, or reduced concentrations of the components between the two perfumes. Names and chemical structures for the numbered components are given in the following table.

Table 8b-1. Labeled Components in Chromatograms of Light Blue by Dolce & Gabbana vs Shades of Blue by Belcam.

	Name	Structure	
1)	diethylene glycol monoethyl ether (preservative)	<input type="text"/>	
2)	limonene (lemon scent)	<input type="text"/>	<input type="text"/>
3)	a-cedrene (wood scent)	<input type="text"/>	<input type="text"/>

4)	b-cedrene (wood scent)			
5)	thujopsene (wood scent)			
6)	cuparene (wood scent)			
7)	cedrol (wood scent)			
8)	diethyl phthalate (preservative)			
9)	methyl dihydrojasmonate (jasmine)			
10)	isopropyl myristate (skin binder)			
11)	1,3,4,6,7,8-hexahydro- 4,6,6,7,8,8- hexamethylcyclopenta-g- 2-benzopyran (musk scent)			

(2) Drakkar Noir and the generic “Classic Match”:

Drakkar Noir is a blend of citrus, lavender, spices and woods. Top notes are citrus, middle notes are woody and herbaceous and base notes are woody warmed and spiced with aromatic coriander and juniper berries, strengthened by sandalwood, patchouli and fir balsam.

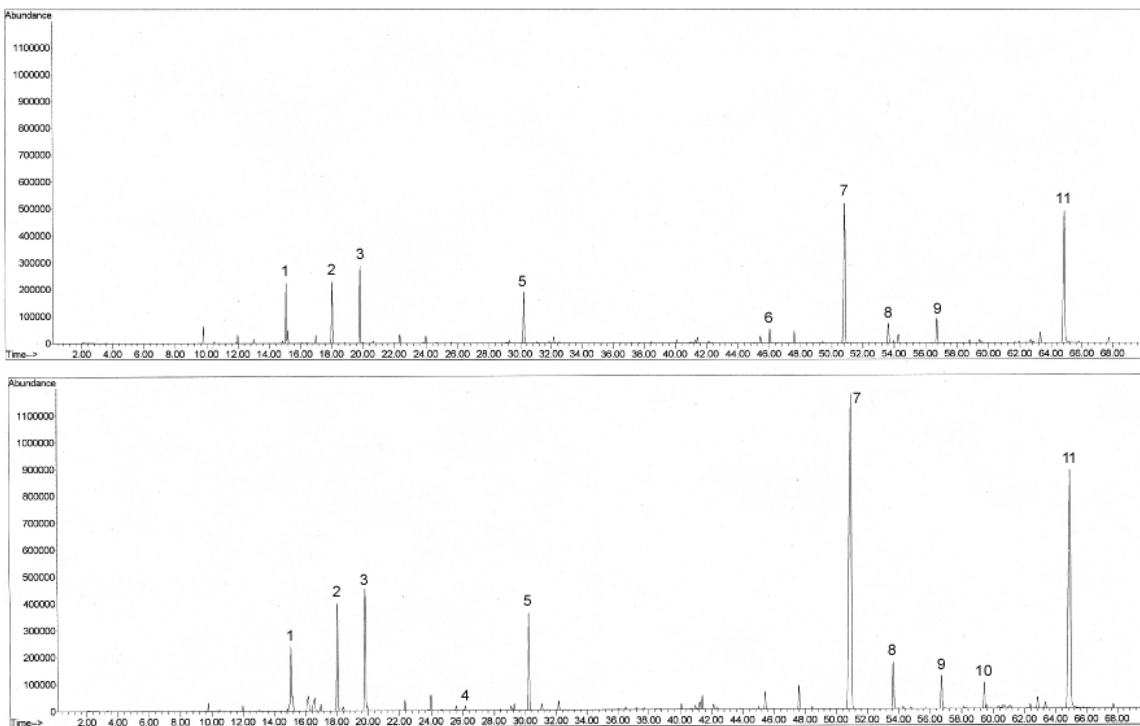


Figure 8b-2. Chromatogram of Drakkar Noir (top figure) and Classic Match (bottom figure).

Table 8b-2. Labeled Components in Chromatograms of Drakkar Noir and Classic Match.

	Name	Structure
1)	limonene (lemon scent)	<input type="text"/>
2)	dihydromyrcenol (lime scent)	<input type="text"/>
3)	linalool (spicy floral scent)	<input type="text"/>
4)	4-Allylanisole (minty sweet scent)	<input type="text"/>
5)	linalyl acetate (sweet scent)	<input type="text"/>
6)	2,6-ditertbutyl-4-methylphenol (antioxidant)	<input type="text"/>

7)	diethyl phthalate (preservative)			
8)	patchouli alcohol (woody scent)			
9)	verymoss (woody scent)			
10)	d-cadinene (woody scent)			
11)	benzyl salicylate (floral scent)			

(3) Unforgivable by Sean John vs Unjustified by Belcam Inc. vs Bring It by Parfums de Coeur

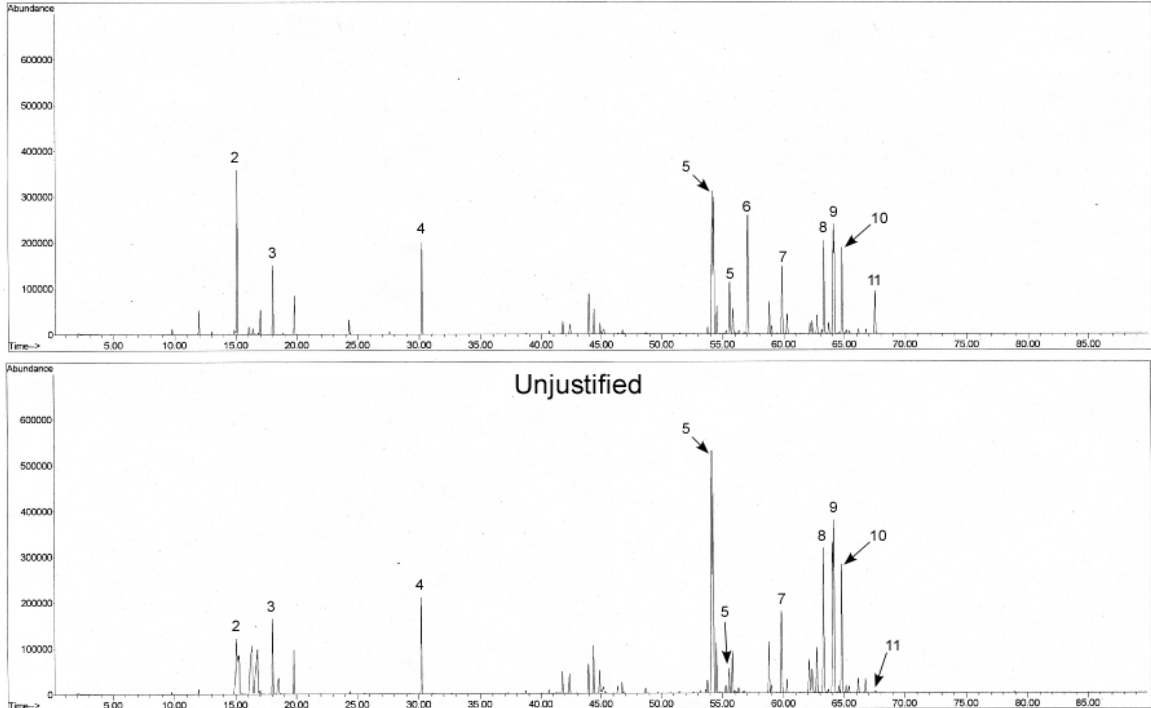


Figure 8b-3. Chromatogram of Unforgivable (top figure) and Unjustified (bottom figure).

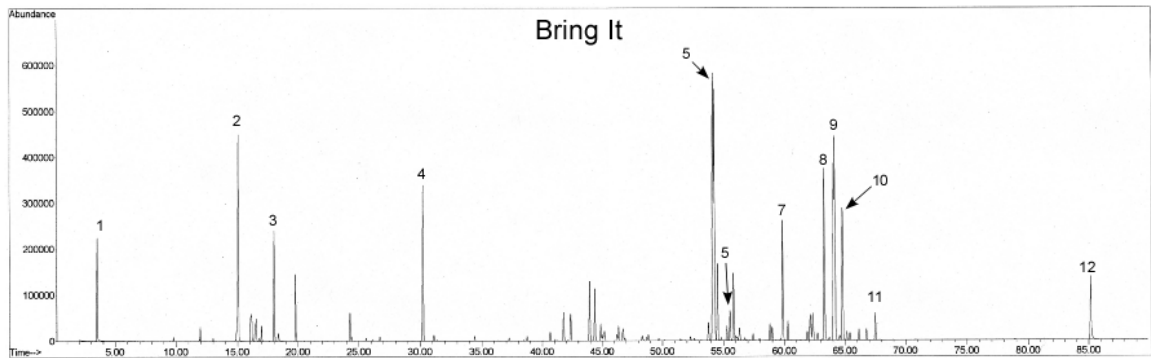


Figure 8b-4. Chromatogram of Bring It.

Table 8b-3. Labeled Components in Chromatograms of Drakkar Noir and Classic Match.

	Name	Structure
1)	propylene glycol	<input type="text"/>
2)	limonene (lemon scent)	<input type="text"/>
3)	dihydromyrcenol (citrus scent)	<input type="text"/>

4)	tricyclene (citrus scent)			
5)	methyl dihydrojasmonate (jasmine)			
6)	1,1,3-trimethyl-3-phenylindan			
7)	acetyl cedrene (musty scent)			
8)	isopropyl myristate (skin binder)			
9)	1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethylcyclopenta-g-2-benzopyran (musk scent)			
10)	Versalide (musky scent)			
11)	6-tert-butyl-3-methyl-2,4-dinitroanisole (musky scent)			
12)	Octyl 4-methoxycinnamate (keratin binder)			

Comparisons of the “real” versus “fake” perfumes show distinct similarities with respect to presence of peaks and their “fingerprint”. However, closer inspection of each peak shows differences. These subtle differences change our olfactory perception of their “smell”.

Note the identification of the components in each table and the type of the compounds present and their purpose.