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Caractérisation et dosage des arômes et antioxydants

Expertises, R&D

ESSAI R&D TWISTAROMA

Sample : Jus de pomme

Analytical method : SBSE

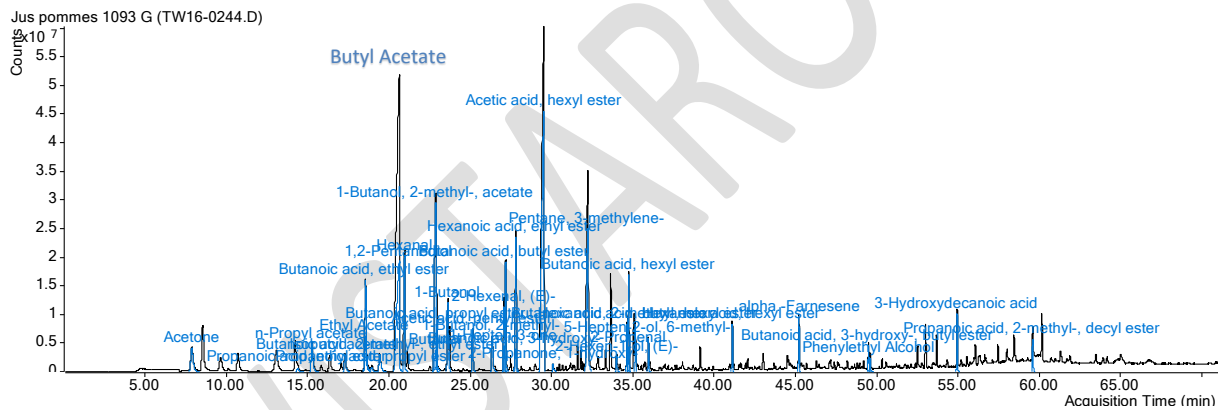
Carrier gas : Helium

GC : Agilent 7890

MS : Agilent 5977B inert MSD

Column : DB-Wax capillary column

Identification : Déconvolution, NIST14 et RI



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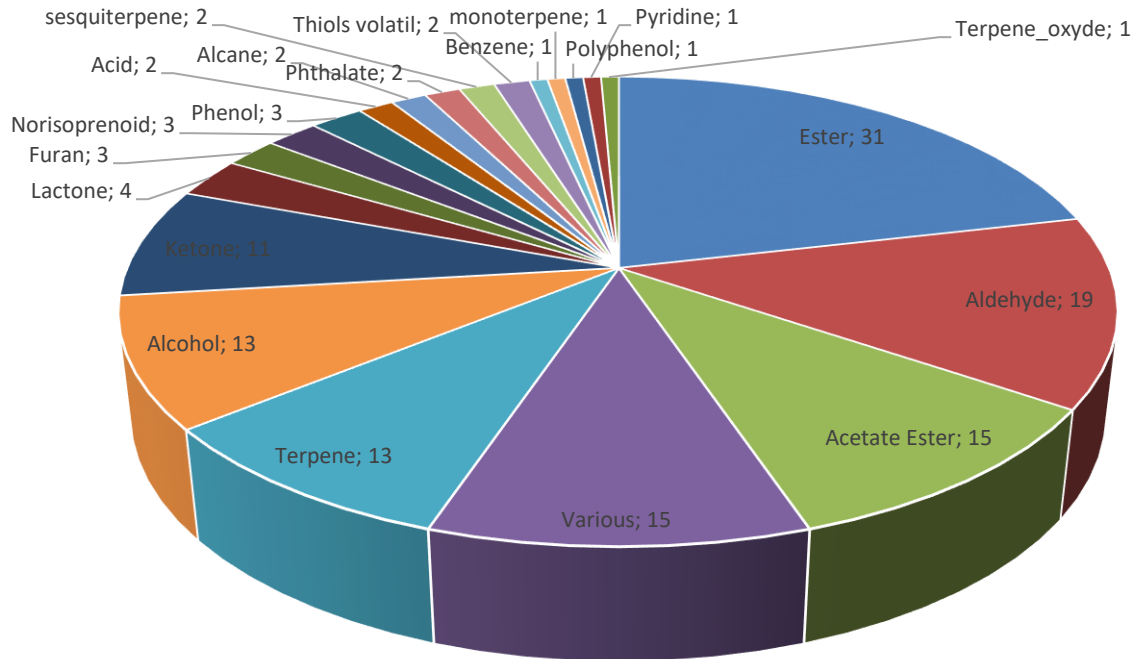
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4 major compounds found :

- butyl acetate (35,3%)
- Hexyl acetate (23,5%)
- 2-methylbutyl acetate (6,4%)
- Ethyl butanoate (2,5%)

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| CAS | Name | RT (min) | Compounds Family | Descriptions (main) | µg/L rel 3-octanol |
|------------|--------------------------|----------|------------------|-----------------------------|--------------------|
| 123-86-4 | butyl acetate | 20,6 | Acetate Ester | fruit, floral, thinner | 1636,3 |
| 142-92-7 | Hexyl acetate | 29,5 | Acetate Ester | fruit, floral, pear | 1089,2 |
| 624-41-9 | 2-methylbutyl acetate | 22,9 | Acetate Ester | fruit, strawberry | 294,8 |
| 105-54-4 | Ethyl butanoate | 18,6 | Ester | fruit, sweet | 117,7 |
| 67-64-1 | 2-Propanone | 7,9 | Ketone | unknown | 115,3 |
| 109-21-7 | butyl butanoate | 27,2 | Ester | unknown | 103,4 |
| 71-36-3 | 1-Butanol | 23,6 | Alcohol | medicinal, alcoholic, fruit | 101,2 |
| 123-66-0 | Ethyl hexanoate | 27,8 | Ester | fruit, green apple, sweet | 90,5 |
| 109-60-4 | propyl acetate | 15,3 | Acetate Ester | sweet, fruit, solvent | 84,4 |
| 141-78-6 | Ethyl acetate | 10,7 | Acetate Ester | fruit, pine apple, sweet | 71,1 |
| 66-25-1 | Hexanal | 21,0 | Aldehyde | green, grassy, fruit | 63,4 |
| 593-75-9 | Methyl isocyanide | 16,4 | Various | | 54,9 |
| 105-66-8 | propyl butanoate | 22,9 | Ester | solvent, pine apple | 49,9 |
| 2639-63-6 | hexyl butanoate | 34,7 | Ester | fruit, floral, pine apple | 48,4 |
| 628-63-7 | Amyl acetate | 25,1 | Acetate Ester | fruit, ripe | 43,1 |
| 110-19-0 | Isobutyl acetate | 17,3 | Acetate Ester | fruit, floral, banana | 40,3 |
| 590-01-2 | butyl propanoate | 23,7 | Ester | | 34,6 |
| 137-32-6 | 2-methylbutanol | 26,3 | Alcohol | vinous | 31,8 |
| 4602-84-0 | Farnesol | 60,2 | Terpene | floral, Fragrant, | 30,1 |
| 6728-26-3 | trans-2-hexenal | 27,1 | Aldehyde | green, fruit, sweet | 29,3 |
| 7452-79-1 | Ethyl 2-methyl butanoate | 19,4 | Ester | fruit, apple, sweet | 27,4 |
| 10032-15-2 | Hexyl 2-methylbutanoate | 35,2 | Ester | pungent, | 24,5 |
| 626-82-4 | butyl hexanoate | 34,6 | Ester | fruit, pine apple, peach | 23,7 |
| 1569-60-4 | 6-methylhept-5-en-2-ol | 36,0 | Alcohol | unknown, sponge | 20,8 |
| 502-61-4 | trans, trans a-Farnesene | 45,2 | Terpene | sweet, wood | 18,8 |
| 6378-65-0 | hexyl hexanoate | 41,1 | Ester | apple, peach, fruit | 18,7 |
| 60-12-8 | 2-Phenylethanol | 49,6 | Alcohol | rose, floral, honey | 18,1 |
| 116-09-6 | Acetol | 30,1 | Ketone | unknown, nutty, | 18,0 |
| 928-95-0 | trans-2-Hexenol | 34,0 | Alcohol | green, fruit, walnut | 15,8 |
| 106-36-5 | Propyl propanoate | 18,9 | Ester | sharp | 11,1 |
| 105-37-3 | Ethyl propanoate | 14,4 | Ester | fruit, sweet | 10,8 |

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|------------|-------------------------------|--------------------|----------------|------------------------------|------|
| 103-45-7 | 2-phenylethyl acetate | 47,2 | Acetate Ester | floral, rose, honey | 10,3 |
| 97-99-4 | Tetrahydrofurfuryl alcohol | 34,6 | Various | | 10,2 |
| 110-93-0 | 6-methyl-5-hepten-2-one | 31,8 | Ketone | sweet | 9,9 |
| 111-87-5 | 1-Octanol | 39,1 | Alcohol | green, floral, rose | 8,9 |
| 98-01-1 | Furfural | 36,1 | Aldehyde | alkane, sweet, floral | 7,8 |
| 67-47-0 | 5-hydroxy methylfurfural | 63,5 | Aldehyde | wax | 7,8 |
| 140-67-0 | Estragole | 43,0 | Various | sweet | 7,6 |
| 25152-84-5 | trans, trans 2,4-Decadienal | 46,4 | Various | fatty, fried, wax | 6,9 |
| 623-42-7 | Methyl butanoate | 15,8 | Ester | fruit, sweet | 6,6 |
| 2445-76-3 | hexyl propanoate | 31,9 | Ester | fruit, | 5,7 |
| 37064-20-3 | Propyl 2-methylbutanoate | 23,7 | Ester | sweet, | 5,4 |
| 4312-99-6 | 1-octen-3-one | 30,5 | Ketone | mushroom, metallic, mushroom | 5,3 |
| 142-62-1 | Hexanoic acid | 47,4 | Acid | cheesy, rancid, sweaty | 5,0 |
| 98-00-0 | 2-Furanmethanol | 42,1 | Furan | burnt, sweet | 4,9 |
| 543-49-7 | 2-Heptanol | 30,9 | Alcohol | fruit, earthy, sweet | 4,8 |
| 34995-77-2 | trans-linalool oxide furanoid | 36,3 | Terpene_ oxyde | floral, wood | 4,7 |
| 84-74-2 | di-butyl phtalate | 70,5 1447 71 | Phthalate | plastic, faintodor, | 4,0 |
| 23726-93-4 | trans-b-Damascenone | 46,8 | Norisoprenoid | apple, honey | 3,9 |
| 18679-18-0 | Dodec-6-eno-1,4-lactone | 61,7 | Various | | 3,7 |
| 3879-26-3 | neryl acetone | 48,2 | Various | | 3,7 |
| 706-14-9 | g-Decalactone | 55,8 | Lactone | peach, sweet | 3,3 |
| 626-77-7 | propyl hexanaoate | 31,2 | Ester | fruit, pine apple, sweet | 3,1 |
| 868-57-5 | methyl-2-Methyl butanoate | 17,1 | Ester | fruit, sweet | 3,0 |
| 539-90-2 | isobutyl butanoate | 24,6 | Ester | fruit, | 2,9 |
| 24157-81-1 | 2,6-Diisopropylnaphthalene | 58,1 | Various | sugar | 2,6 |
| 19444-84-9 | 2-Hydroxy-gamma-butyrolactone | 55,9 | Lactone | | 2,5 |
| 123-72-8 | 1-butanal | 10,1 | Aldehyde | pungent | 2,4 |
| 106-32-1 | Ethyl octanoate | 35,3 | Ester | fruit, sweet, floral | 2,4 |
| 110-43-0 | 2-Heptanone | 25,5 | Ketone | fruit, bluecheese, sweet | 2,3 |
| 705-86-2 | d-Decalactone | 57,1 | Lactone | coconut, fruit, lactone | 2,3 |
| 118-71-8 | Maltol | 51,1 | Polyphenol | caramel, burnt sugar, | 2,3 |



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|-------------|---|--------------------|------------------|-----------------------------------|-----|
| 84-69-5 | Diisobutyl phthalate | 65,1 9662 45 | Phthalate | ether | 2,1 |
| 589-75-3 | Butyl octanoate | 41,2 | Ester | unknown, | 2,1 |
| 108-95-2 | Phenol | 51,7 | Phenol | medicinal, smoky | 2,0 |
| 112-14-1 | octyl acetate | 36,7 | Acetate Ester | fruit, pear | 1,9 |
| 2548-87-0 | trans-2-Octenal | 35,3 | Aldehyde | nutty, fatty, stale | 1,9 |
| 57266-86-1 | cis-2-Heptenal | 31,4 | Aldehyde | green, soapy | 1,9 |
| 101-41-7 | Methyl benzene Acetate | 44,6 | Acetate Ester | sweet, unknown | 1,9 |
| 141-27-5 | Geranial | 44,8 | Terpene | lemon, minty | 1,8 |
| 140-11-4 | Benzyl acetate | 44,6 | Acetate Ester | fresh, jasmin | 1,8 |
| 106-68-3 | 3-Octanone | 28,7 | Ketone | fruit, sweet | 1,8 |
| 5989-27-5 | d-Limonene | 26,5 | Terpene | grassy, | 1,8 |
| 97-62-1 | Ethyl isobutanoate | 14,9 | Ester | fruit, sweet, strawberry | 1,8 |
| 93-15-2 | Methyl eugenol | 52,1 | Phenol | strawberry | 1,8 |
| 505-10-2 | Methionol | 44,1 | Alcohol | potato, vegetable | 1,7 |
| 4440-65-7 | 3-Hexenal | 23,4 | Aldehyde | | 1,7 |
| 80-56-8 | a-Pinene | 17,8 | Terpene | Pine, piney | 1,6 |
| 100-52-7 | Benzaldehyde | 38,4 | Aldehyde | almond, nutty, wood | 1,4 |
| 538-68-1 | Pentylbenzene | 34,9 | Various | | 1,4 |
| 6846-50-0 | [2 4,4-trimethyl-1-(2-methylpropanoyloxy)pentan-3-yl]2-methylpropanoate | 49,0 | Ester | moldy | 1,4 |
| 5405-41-4 | Ethyl 3-hydroxybutanoate | 37,9 | Ester | marshmallow, grape fruit | 1,4 |
| 562-74-3 | 4-Terpineol | 41,0 | Terpene | floral, lilac | 1,3 |
| 18794-84-8 | trans-b-farnesene | 42,8 | Terpene | wood, sweet | 1,2 |
| 106-70-7 | Methyl hexanoate | 25,7 | Ester | fruit, floral, sweet | 1,2 |
| 3681-71-8 | cis-3-hexenyl acetate | 31,0 | Acetate Ester | green, fruit | 1,1 |
| 91-20-3 | Naphthalene | 45,4 | Terpene | pungent, tar | 1,1 |
| 123-35-3 | b-myrcene | 24,8 | Terpene | spicy | 1,1 |
| 102488-09-5 | 3-hydroxy-b-damascone | 64,9 1517 57 | Norisoprenoid | | 1,0 |
| 1604-28-0 | 6-methylhepta-3,5-dien-2-one | 40,6 | Various | cinnamon, coconut, spice, wood | 1,0 |
| 693-54-9 | 2-decanone | 37,4 | Ketone | musty, | 0,9 |
| 2438-20-2 | 2-methylbutyl-2-methyl propanoate | 25,9 | Ester | | 0,9 |
| 620-02-0 | 5-methylfurfural | 39,8 | Aldehyde | caramel, spicy | 0,9 |
| 143-08-8 | 1-Nonanol | 42,3 | Alcohol | roseorange | 0,9 |

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|------------|----------------------------------|------|---------------|---|-----|
| 112-06-1 | Heptyl acetate | 33,2 | Acetate Ester | Herbal, wine | 0,9 |
| 881395 | 2,4-Heptadienal, (E,E)- | 37,4 | | | 0,9 |
| 122-99-6 | 2-phenoxyethanol | 55,4 | Alcohol | unknown, | 0,9 |
| 19089-92-0 | hexyltrans-2-butenolate | 39,4 | Ester | | 0,9 |
| 100-41-4 | Ethyl benzene | 23,1 | Various | | 0,8 |
| 108-88-3 | Toluene | 18,6 | Benzene | sweet, synthetic | 0,8 |
| 100-42-5 | Styrene | 28,7 | Phenol | sweet | 0,8 |
| 112-31-2 | Decanal | 37,6 | Aldehyde | green, tallow | 0,8 |
| 80-71-7 | Maple Lactone | 47,2 | Lactone | caramel, maple syrup | 0,8 |
| 5910-87-2 | trans,trans-2,4-nonadienal | 44,0 | Aldehyde | fatty, wax | 0,7 |
| 1195-79-5 | Fenchone | 34,5 | Terpene | | 0,7 |
| 1759-28-0 | 4-methyl-5-vinylthiazol | 38,5 | Alcohol | nutty, | 0,7 |
| 97-87-0 | Butyl isobutanoate | 24,0 | Ester | | 0,6 |
| 14901-07-6 | b-Ionone | 50,8 | Norisoprenoid | floral, wood | 0,6 |
| 101-97-3 | Ethyl-2-phenylacetate | 46,3 | Acetate Ester | sweet, honey, fruit | 0,6 |
| 108-10-1 | Methyl isobutyl ketone | 16,9 | Ketone | grass, fruit, spice | 0,6 |
| 5077-67-8 | 1-hydroxy-2-butanone | 33,0 | Ketone | sweet, coffee, musty, grain, malty, butters cotch | 0,6 |
| 96-17-3 | 2-methyl butanal | 12,0 | Aldehyde | malty, green | 0,6 |
| 124-18-5 | Decane | 16,6 | Alcane | sweet-ethereal | 0,5 |
| 17092-92-1 | Dihydroactinidiolide | 61,0 | Various | musk | 0,5 |
| 1197-01-9 | p-Cymen-8-ol | 47,8 | Terpene | unknown, musty, | 0,5 |
| 538-86-3 | Benzyl methyl ether | 33,9 | Various | | 0,4 |
| 2445-78-5 | 2-methylbutyl-2-methyl butanoate | 29,8 | Ester | | 0,4 |
| 111-71-7 | Heptanal | 25,7 | Aldehyde | grassy, solvent | 0,4 |
| 3387-41-5 | Sabinene | 22,3 | monoterpene | wood, weak | 0,4 |
| 111-65-9 | Octane | 7,5 | Various | alkane, sweet-ethereal | 0,4 |
| 1120-21-4 | Undecane | 21,8 | Alcane | warm | 0,3 |
| 554-12-1 | Methyl propanoate | 11,7 | Ester | rum, strawberry, apple | 0,3 |
| 111-13-7 | 2-Octanone | 29,9 | Ketone | soapy, unripe apple | 0,3 |
| 624-13-5 | Propyl octanoate | 38,2 | Ester | fruit, | 0,3 |
| 3777-69-3 | 2-Pentylfuran | 27,7 | Furan | fruit, sweet | 0,3 |
| 95-47-6 | 1,2 Dimethylbenzene | 23,5 | Various | geranium | 0,3 |
| 106-26-3 | Neral | 43,4 | Aldehyde | lemon, musty | 0,3 |
| 1576-85-8 | 4-pentenyl acetate | 26,0 | Acetate Ester | | 0,2 |
| 106-30-9 | Ethyl heptanoate | 31,7 | Ester | fruit, wine | 0,2 |
| 5986-38-9 | Ocimenol | 43,5 | Terpene | citrus, cologne | 0,2 |

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|------------|------------------------------------|------|----------------|-------------------------------------|------|
| 99-85-4 | g-Terpinene | 28,5 | Terpene | citrus, wood | 0,2 |
| 107-86-8 | 3-methyl-2-butenal | 26,1 | Aldehyde | fruity, pungent, almond, cherry | 0,2 |
| 110-86-1 | Pyridine | 25,4 | Pyridine | burnt, | 0,2 |
| 1192-62-7 | 1-(2-furanyl)-Ethanone | 38,9 | Furan | sweet | 0,2 |
| 483-77-2 | calamenene | 48,1 | sesquiterpene | spicy | 0,2 |
| 1565-81-7 | Decan-3-ol | 40,2 | Alcool | | 0,1 |
| 95-63-6 | 1,2,4-Trimethyl benzene | 29,9 | Various | fruit, | 0,1 |
| 74-93-1 | Methanethiol | 5,7 | Thiols volatil | sulfury | 0,1 |
| 6314-97-2 | phenyl acetaldehyde diethyl acetal | 44,4 | Aldehyde | fruit, | 0,1 |
| 75-18-3 | Dimethyl sulfide | 6,5 | Thiols volatil | sulfury, cabbage, Truffle | 0,1 |
| 590-86-3 | 3-methyl butanal | 12,1 | Aldehyde | malty, chocolate, green | 0,1 |
| 4437-51-8 | Hexan-3,4-dione | 23,4 | Ketone | butter, toasted, almond, caramel | 0,05 |
| 50277-34-4 | b-Calacorene | 50,4 | sesquiterpene | | 0,04 |
| 620-23-5 | Benzaldehyde, 3-methyl- | 41,7 | Aldehyde | | 0,03 |
| 503-74-2 | 3-methyl butanoic acid | 42,4 | Acid | rancid, cheesy, acidic | 0,02 |

RT : Temps de rétention

Illkirch, le 5 mars 2019

Dr. Damien Steyer
Directeur du laboratoire