Molecule of the Month: trans-2-Dodecenal

Organoleptic characteristics and F&F applications

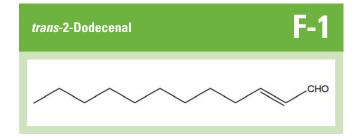
Michael Zviely, CIC

rans-2-Dodecenal, a colorless to slightly yellow liquid, is found in dairy products, chicken, coriander oil (*Coriandrum sativum* L.), peanuts, citrus oils and rice (**see F-1**). Previously known to occur only in plants, this material has been identified in the defensive secretion of the spiroboloid millipede *Rhinocricus insulates*, and shows promising antiviral and antibacterial properties. ¹⁻³

The aroma profile of *trans*-2-dodecenal can be described as intensely fatty, waxy, mandarin orange and somewhat citrusy on dilution. In addition to its application in dairy and meaty flavorings, citrus fruits, coriander, dairy products, mandarin, orange and tangerine flavors, this material can also be used in formulation of tropical blends. In fragrances, *trans*-2-dodecenal can be used to obtain the heavy notes in a citrus complex for cosmetic purposes. Likewise, it finds usage in several applications; however considerable experience and skill is required to fully utilize the character of this aldehyde, without letting its unpleasant notes dominate the composition.⁴

Mandarine aldehyde is commercially offered as 10% solution of *trans*-2-dodecenal in ethyl citrate. It possesses a powerful and complex olfactive note, coupled with distinct mandarin and coriander aspects. In perfumery, this material is used to obtain a uniquely long-lasting citrus mandarin note with superior diffusion—a characteristic that is versatile in a wide range of fragrance types. **Clearly, mandarine aldehyde can be applied to many products, including fine fragrances, shampoos, shower gels, soaps, detergents, softeners and candles.

^{**} Firmenich Compendium



T-1 shows an example of a citrus-related flavor base that can be created using *trans*-2-dodecenal.⁵
T-2 summarizes *trans*-2-alkenals—a family to which *trans*-2-dodecenal belongs, and F-2 shows a preparation route of *trans*-2-dodecenal, directly from decanal, by the addition of two carbon atoms.

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Physical Data

CAS# 20407-84-5

FEMA# 2402

CoE 124

Synonyms: (E)-2-Dodecen-1-al,

cilantro aldehyde,

mandarine aldehyde^a

Appearance Colorless to slightly

yellow liquid

Molecular Weight 182.3

Molecular Formula $C_{12}H_{22}O$

Refractive Index (20°C) 1.450-1.460

Specific Gravity (25°C) 0.840-0.850

Acid Value (mg KOH/g) 10 max.

Boiling Point (760 torr) 269–271°C

Flash Point (cc) 93°C

 $^{\rm a}$ Cilantro aldehyde is a name used by Frutarom; mandarine aldehyde 10% CITR is the name used by Firmenich.

 $[\]ensuremath{^\circ}$ Frutarom and Bedoukian product information

An example of a citrus-related flavor can be created using <i>trans</i> -2-dodec	
<u>Components</u>	Use levels (parts)
Lemon oil Italy	300
Grapefruit oil	100
cis-3-Hexenol (10% in DPG)	5
cis-3-Hexenyl acetate (10% in DPG)	4
trans-2-Dodecenal (10% in DPG)	2
Linalool synt.	10
β-lonone	3
Nerol extra	10
Nerolidol extra	50
Farnesol synt.	50
2,3-Dihydrofarnesal	50
Cedrol crist. extra	10
cis-3-Hexenyl benzoate	2
Methyl jasmonate	30
Citral	20
Dipropylene glycol (DPG)	354
Total	1000

References

- JW Wheeler, J Meinwald, JJ Hurst and T Eisner, trans-2-Dodecenal and 2-methyl-1, 4-quinone produced by a Millipede, Science, 144 (3618), 540–541 (1964)
- 2. K Zafar, S Urdaneta, T Odesanya, J Fraietta, B Neha, F Krebs and MK Howett, A broad-spectrum microbicide from cilantro with antiviral activity, presented at: 3rd International AIDS Society Conference on HIV Pathogenesis and Treatment, Rio de Janeiro (2005)

A family of *trans*-2-alkenals

trans-2-Alkenal	Organoleptic profile [†]
trans-2-butenal	Nauseous, gassy, somewhat fruity on dilution
trans-2-pentenal	Pungent, green, fruity; apple- and orangelike
trans-2-hexenal	Powerful, green, leafy, fruity, fatty, apple character; plumlike, fresh, herbal, citrus
trans-2-heptenal	Intense green, sweet, fresh fruity apple skin nuances
trans-2-octenal	Fruity, cheeselike, earthy with mushroom character
trans-2-nonenal	Green, soapy, cucumber/melonlike with an aldehydic-fatty nuance
trans-2-decenal	Slightly fatty, citrusy on dilution, orangelike
trans-2-undecenal	Fresh, fatty and slightly fruity, citrus note
trans-2-tridecenal	Powerful waxy, mandarin- and tangerinelike; fatty, green and creamy
trans-2-tetradecenal	Waxy, slight green, soapy and fatty with cilantro and chickenlike notes and nuances of cucumber, herbs and citrus lemon ⁶

[†] Some information on organoleptic properties and uses is taken from the FRM 2001 and PMP 96 Databases of Perfumery Materials & Performance, Boelens Aroma Chemicals Information Services, Netherlands.

- 3. I Kubo et al., J Agric Food Chem, 52, 3329 (2004)
- 4. S Arctander, Arctander's Perfume and Flavor Chemicals & Perfume and Flavor Materials of Natural Origin, Allured Publishing Corp., Carol Stream, IL (1961)
- US Pat 20080248177, 3- and 4-methyl dodecenal and their use in fragrance and flavour compositions, R Kaiser, Givaudan SA (June 15, 2006)
- 6. G Mosciano, Organoleptic characteristics of flavor materials, $Perfum\ Flavor,\,34,\,53\,(2009)$

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